# **Parsl Documentation**

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Parsl extends parallelism in Python beyond a single computer.

You can use Parsl just like Python's parallel executors but across *multiple cores and nodes*. However, the real power of Parsl is in expressing multi-step workflows of functions. Parsl lets you chain functions together and will launch each function as inputs and computing resources are available.

```
import parsl
from parsl import python_app
# Start Parsl on a single computer
parsl.load()
# Make functions parallel by decorating them
@python_app
def f(x):
   return x + 1
@python_app
def q(x):
   return x * 2
# These functions now return Futures, and can be chained
future = f(1)
assert future.result() == 2
future = g(f(1))
assert future.result() == 4
```

Start with the configuration quickstart to learn how to tell Parsl how to use your computing resource, see if a template configuration for your supercomputer is already available, then explore the parallel computing patterns to determine how to use parallelism best in your application.

Parsl is an open-source code, and available on GitHub: https://github.com/parsl/parsl/

#### CHAPTER

ONE

### WHY USE PARSL?

# 1.1 Parsl is Python

*Everything about a Parsl program is written in Python.* Parsl follows Python's native parallelization approach and functions, how they combine into workflows, and where they run are all described in Python.

# 1.2 Parsl works everywhere

*Parsl can run parallel functions on a laptop and the world's fastest supercomputers.* Scaling from laptop to supercomputer is often as simple as changing the resource configuration. Parsl is tested on many of the top supercomputers.

# 1.3 Parsl is flexible

*Parsl supports many kinds of applications.* Functions can be pure Python or invoke external codes, be single- or multi-threaded or GPUs.

### 1.4 Parsl handles data

Parsl has first-class support for workflows involving files. Data will be automatically moved between workers, even if they reside on different filesystems.

# 1.5 Parsl is fast

Parsl was built for speed. Workflows can manage tens of thousands of parallel tasks and process thousands of tasks per second.

# 1.6 Parsl is a community

#### Parsl is part of a large, experienced community.

The Parsl Project was launched by researchers with decades of experience in workflows as part of a National Science Foundation project to create sustainable research software.

The Parsl team is guided by the community through its GitHub, conversations on Slack, Bi-Weekly developer calls, and engagement with the Workflows Community Initiative.

#### 1.6.1 Table of Contents

#### Quickstart

To try Parsl now (without installing any code locally), experiment with our hosted tutorial notebooks on Binder.

#### Installation

Parsl is available on PyPI and conda-forge.

Parsl requires Python3.8+ and has been tested on Linux and macOS.

#### **Installation using Pip**

While pip can be used to install Parsl, we suggest the following approach for reliable installation when many Python environments are available.

- 1. Install Parsl:
  - \$ python3 -m pip install pars1

To update a previously installed parsl to a newer version, use: python3 -m pip install -U parsl

#### Installation using Conda

1. Create and activate a new conda environment:

```
$ conda create --name parsl_py38 python=3.8
$ source activate parsl_py38
```

2. Install Parsl:

```
$ python3 -m pip install pars1
or
$ conda config --add channels conda-forge
$ conda install pars1
```

The conda documentation provides instructions for installing conda on macOS and Linux.

#### **Getting started**



Parsl has much in common with Python's native concurrency library, but unlocking Parsl's potential requires understanding a few major concepts.

A Parsl program submits tasks to run on Workers distributed across remote computers. The instructions for these tasks are contained within "*apps*" that users define using Python functions. Each remote computer (e.g., a node on a supercomputer) has a single "*Executor*" which manages the workers. Remote resources available to Parsl are acquired by a "*Provider*", which places the executor on a system with a "*Launcher*". Task execution is brokered by a "*Data Flow Kernel*" that runs on your local system.

We describe these components briefly here, and link to more details in the User Guide.

**Note:** Parsl's documentation includes templates for many supercomputers. Even though you may not need to write a configuration from a blank slate, understanding the basic terminology below will be very useful.

#### **Application Types**

Parsl enables concurrent execution of Python functions (python\_app) or external applications (bash\_app). The logic for both are described by Python functions marked with Parsl decorators. When decorated functions are invoked, they run asynchronously on other resources. The result of a call to a Parsl app is an AppFuture, which behaves like a Python Future.

The following example shows how to write a simple Parsl program with hello world Python and Bash apps.

```
import parsl
from parsl import python_app, bash_app

@python_app
def hello_python (message):
    return 'Hello %s' % message

@bash_app
def hello_bash(message, stdout='hello-stdout'):
    return 'echo "Hello %s"' % message

with parsl.load():
    # invoke the Python app and print the result
    print(hello_python('World (Python)').result())
    # invoke the Bash app and read the result from a file
```

```
hello_bash('World (Bash)').result()
with open('hello-stdout', 'r') as f:
    print(f.read())
```

Learn more about the types of Apps and their options here.

#### **Executors**

Executors define how Parsl deploys work on a computer. Many types are available, each with different advantages.

The *HighThroughputExecutor*, like Python's ProcessPoolExecutor, creates workers that are separate Python processes. However, you have much more control over how the work is deployed. You can dynamically set the number of workers based on available memory and pin each worker to specific GPUs or CPU cores among other powerful features.

Learn more about Executors here.

#### **Execution Providers**

Resource providers allow Parsl to gain access to computing power. For supercomputers, gaining resources often requires requesting them from a scheduler (e.g., Slurm). Parsl Providers write the requests to requisition **"Blocks"** (e.g., supercomputer nodes) on your behalf. Parsl comes pre-packaged with Providers compatible with most supercomputers and some cloud computing services.

Another key role of Providers is defining how to start an Executor on a remote computer. Often, this simply involves specifying the correct Python environment and (described below) how to launch the Executor on each acquired computers.

Learn more about Providers here.

#### Launchers

The Launcher defines how to spread workers across all nodes available in a Block. A common example is an MPILauncher, which uses MPI's mechanism for starting a single program on multiple computing nodes. Like Providers, Parsl comes packaged with Launchers for most supercomputers and clouds.

Learn more about Launchers here.

#### **Benefits of a Data-Flow Kernel**

The Data-Flow Kernel (DFK) is the behind-the-scenes engine behind Parsl. The DFK determines when tasks can be started and sends them to open resources, receives results, restarts failed tasks, propagates errors to dependent tasks, and performs the many other functions needed to execute complex workflows. The flexibility and performance of the DFK enables applications with intricate dependencies between tasks to execute on thousands of parallel workers.

Start with the Tutorial or the parallel patterns to see the complex types of workflows you can make with Parsl.

#### **Starting Parsl**

A Parsl script must contain the function definitions, resource configuration, and a call to parsl.load before launching tasks. This script runs on a system that must stay on-line until all of your tasks complete but need not have much computing power, such as the login node for a supercomputer.

The *Config* object holds definitions of Executors and the Providers and Launchers they rely on. An example which launches 512 workers on 128 nodes of the Polaris supercomputer looks like

```
config = Config(
   retires=1, # Restart task if they fail once
    executors=[
       HighThroughputExecutor(
            available_accelerators=4, # Maps one worker per GPU
            address_by_hostname(),
            cpu_affinity="alternating", # Prevents thread contention
            provider=PBSProProvider(
                account="example".
                worker_init="module load conda; conda activate parsl",
                walltime="1:00:00",
               queue="prod",
                scheduler_options="#PBS -1 filesystems=home:eagle", # Change if data on_
→other filesystem
                launcher=MpiExecLauncher(
                   bind_cmd="--cpu-bind", overrides="--depth=64 --ppn 1"
                ), # Ensures 1 manger per node and allows it to divide work to all 64.
⇔cores
                select_options="ngpus=4",
                nodes_per_block=128,
                cpus_per_node=64,
           ),
       ),
   ]
)
```

The documentation has examples for other supercomputers here.

The next step is to load the configuration

parsl.load(config)

You are then ready to use 10 PFLOPS of computing power through Python!

#### **Tutorial**

The best way to learn more about Parsl is by reviewing the Parsl tutorials. There are several options for following the tutorial:

- 1. Use Binder to follow the tutorial online without installing or writing any code locally.
- 2. Clone the Parsl tutorial repository using a local Parsl installation.
- 3. Read through the online tutorial documentation.

#### **Usage Tracking**

To help support the Parsl project, we ask that users opt-in to anonymized usage tracking whenever possible. Usage tracking allows us to measure usage, identify bugs, and improve usability, reliability, and performance. Only aggregate usage statistics will be used for reporting purposes.

As an NSF-funded project, our ability to track usage metrics is important for continued funding.

You can opt-in by setting PARSL\_TRACKING=true in your environment or by setting usage\_tracking=True in the configuration object (*parsl.config*.

To read more about what information is collected and how it is used see Usage statistics collection.

#### **For Developers**

Parsl is an open source community that encourages contributions from users and developers. A guide for contributing to Parsl is available in the Parsl GitHub repository.

The following instructions outline how to set up Parsl from source.

1. Download Parsl:

\$ git clone https://github.com/Parsl/parsl

2. Install:

```
$ cd pars1
$ pip install .
( To install specific extra options from the source :)
$ pip install '.[<optional_package1>...]'
```

3. Use Parsl!

#### **Parsl tutorial**

Parsl is a native Python library that allows you to write functions that execute in parallel and tie them together with dependencies to create workflows. Parsl wraps Python functions as "Apps" using the @python\_app decorator, and Apps that call external applications using the @bash\_app decorator. Decorated functions can run in parallel when all their inputs are ready.

For more comprehensive documentation and examples, please refer our documentation.

```
[]: import parsl
import os
from parsl.app.app import python_app, bash_app
from parsl.configs.local_threads import config
#parsl.set_stream_logger() # <-- log everything to stdout
print(parsl.__version__)
```

#### **Configuring Parsl**

Parsl separates code and execution. To do so, it relies on a configuration model to describe the pool of resources to be used for execution (e.g., clusters, clouds, threads).

We'll come back to configuration later in this tutorial. For now, we configure this example to use a local pool of threads to facilitate local parallel execution.

```
[ ]: parsl.load(config)
```

#### Apps

In Parsl an app is a piece of code that can be asynchronously executed on an execution resource (e.g., cloud, cluster, or local PC). Parsl provides support for pure Python apps (python\_app) and also command-line apps executed via Bash (bash\_app).

#### **Python Apps**

As a first example, let's define a simple Python function that returns the string 'Hello World!'. This function is made into a Parsl App using the **@python\_app** decorator.

```
[]: @python_app
```

```
def hello ():
    return 'Hello World!'
```

print(hello().result())

As can be seen above, Apps wrap standard Python function calls. As such, they can be passed arbitrary arguments and return standard Python objects.

```
[]: @python_app
def multiply(a, b):
    return a * b
print(multiply(5, 9).result())
```

As Parsl apps are potentially executed remotely, they must contain all required dependencies in the function body. For example, if an app requires the time library, it should import that library within the function.

```
[ ]: @python_app
  def slow_hello ():
        import time
        time.sleep(5)
        return 'Hello World!'
```

print(slow\_hello().result())

#### **Bash Apps**

Parsl's Bash app allows you to wrap execution of external applications from the command-line as you would in a Bash shell. It can also be used to execute Bash scripts directly. To define a Bash app, the wrapped Python function must return the command-line string to be executed.

As a first example of a Bash app, let's use the Linux command echo to return the string 'Hello World!'. This function is made into a Bash App using the @bash\_app decorator.

Note that the echo command will print 'Hello World!' to stdout. In order to use this output, we need to tell Parsl to capture stdout. This is done by specifying the stdout keyword argument in the app function. The same approach can be used to capture stderr.

```
[]: @bash_app
```

```
def echo_hello(stdout='echo-hello.stdout', stderr='echo-hello.stderr'):
    return 'echo "Hello World!"'
echo_hello().result()
with open('echo-hello.stdout', 'r') as f:
    print(f.read())
```

#### **Passing data**

Parsl Apps can exchange data as Python objects (as shown above) or in the form of files. In order to enforce dataflow semantics, Parsl must track the data that is passed into and out of an App. To make Parsl aware of these dependencies, the app function includes inputs and outputs keyword arguments.

We first create three test files named hello1.txt, hello2.txt, and hello3.txt containing the text "hello 1", "hello 2", and "hello 3".

```
[]: for i in range(3):
    with open(os.path.join(os.getcwd(), 'hello-{}.txt'.format(i)), 'w') as f:
        f.write('hello {}\n'.format(i))
```

We then write an App that will concentate these files using cat. We pass in the list of hello files (inputs) and concatenate the text into a new file named all\_hellos.txt (outputs). As we describe below we use Parsl File objects to abstract file locations in the event the cat app is executed on a different computer.

#### [ ]: from parsl.data\_provider.files import File

#### **Futures**

When a normal Python function is invoked, the Python interpreter waits for the function to complete execution and returns the results. In case of long running functions, it may not be desirable to wait for completion. Instead, it is preferable that functions are executed asynchronously. Parsl provides such asynchronous behavior by returning a future in lieu of results. A future is essentially an object that allows Parsl to track the status of an asynchronous task so that it may, in the future, be interrogated to find the status, results, exceptions, etc.

Parsl provides two types of futures: AppFutures and DataFutures. While related, these two types of futures enable subtly different workflow patterns, as we will see.

#### **AppFutures**

AppFutures are the basic building block upon which Parsl scripts are built. Every invocation of a Parsl app returns an AppFuture, which may be used to manage execution of the app and control the workflow.

Here we show how AppFutures are used to wait for the result of a Python App.

```
[ ]: @python_app
def hello ():
    import time
    time.sleep(5)
    return 'Hello World!'
app_future = hello()
```

```
# Check if the app_future is resolved, which it won't be
print('Done: {}'.format(app_future.done()))
```

```
# Print the result of the app_future. Note: this
# call will block and wait for the future to resolve
print('Result: {}'.format(app_future.result()))
print('Done: {}'.format(app_future.done()))
```

#### **DataFutures**

While AppFutures represent the execution of an asynchronous app, DataFutures represent the files it produces. Parsl's dataflow model, in which data flows from one app to another via files, requires such a construct to enable apps to validate creation of required files and to subsequently resolve dependencies when input files are created. When invoking an app, Parsl requires that a list of output files be specified (using the outputs keyword argument). A DataFuture for each file is returned by the app when it is executed. Throughout execution of the app, Parsl will monitor these files to 1) ensure they are created, and 2) pass them to any dependent apps.

```
[]: # App that echos an input message to an output file
@bash_app
def slowecho(message, outputs=[]):
    return 'sleep 5; echo %s &> %s' % (message, outputs[0])
# Call slowecho specifying the output file
hello = slowecho('Hello World!', outputs=[File(os.path.join(os.getcwd(), 'hello-world.txt
→'))])
```

```
# The AppFuture's outputs attribute is a list of DataFutures
print(hello.outputs)
# Also check the AppFuture
print('Done: {}'.format(hello.done()))
# Print the contents of the output DataFuture when complete
with open(hello.outputs[0].result(), 'r') as f:
    print(f.read())
# Now that this is complete, check the DataFutures again, and the Appfuture
print(hello.outputs)
print('Done: {}'.format(hello.done()))
```

#### **Data Management**

Parsl is designed to enable implementation of dataflow patterns. These patterns enable workflows, in which the data passed between apps manages the flow of execution, to be defined. Dataflow programming models are popular as they can cleanly express, via implicit parallelism, the concurrency needed by many applications in a simple and intuitive way.

#### Files

Parsl's file abstraction abstracts access to a file irrespective of where the app is executed. When referencing a Parsl file in an app (by calling filepath), Parsl translates the path to the file's location relative to the file system on which the app is executing.

```
[]: from parsl.data_provider.files import File
```

```
# App that copies the contents of a file to another file
@bash_app
def copy(inputs=[], outputs=[]):
    return 'cat %s &> %s' % (inputs[0], outputs[0])
# Create a test file
open(os.path.join(os.getcwd(), 'cat-in.txt'), 'w').write('Hello World!\n')
# Create Parsl file objects
parsl_infile = File(os.path.join(os.getcwd(), 'cat-in.txt'),)
parsl_outfile = File(os.path.join(os.getcwd(), 'cat-out.txt'),)
# Call the copy app with the Parsl file
copy_future = copy(inputs=[parsl_infile], outputs=[parsl_outfile])
# Read what was redirected to the output file
with open(copy_future.outputs[0].result(), 'r') as f:
    print(f.read())
```

#### **Remote Files**

The Parsl file abstraction can also represent remotely accessible files. In this case, you can instantiate a file object using the remote location of the file. Parsl will implicitly stage the file to the execution environment before executing any dependent apps. Parsl will also translate the location of the file into a local file path so that any dependent apps can access the file in the same way as a local file. Parsl supports files that are accessible via Globus, FTP, and HTTP.

Here we create a File object using a publicly accessible file with random numbers. We can pass this file to the sort\_numbers app in the same way we would a local file.

```
[ ]: from parsl.data_provider.files import File
    @python_app
    def sort_numbers(inputs=[]):
        with open(inputs[0].filepath, 'r') as f:
            strs = [n.strip() for n in f.readlines()]
            strs.sort()
            return strs
    unsorted_file = File('https://raw.githubusercontent.com/Parsl/parsl-tutorial/master/
            -_input/unsorted.txt')
    f = sort_numbers(inputs=[unsorted_file])
    print (f.result())
```

#### Composing a workflow

Now that we understand all the building blocks, we can create workflows with Parsl. Unlike other workflow systems, Parsl creates implicit workflows based on the passing of control or data between Apps. The flexibility of this model allows for the creation of a wide range of workflows from sequential through to complex nested, parallel workflows. As we will see below, a range of workflows can be created by passing AppFutures and DataFutures between Apps.

#### Sequential workflow

Simple sequential or procedural workflows can be created by passing an AppFuture from one task to another. The following example shows one such workflow, which first generates a random number and then writes it to a file.

```
[]: # App that generates a random number
@python_app
def generate(limit):
    from random import randint
    return randint(1,limit)
# App that writes a variable to a file
@bash_app
def save(variable, outputs=[]):
    return 'echo %s &> %s' % (variable, outputs[0])
# Generate a random number between 1 and 10
random = generate(10)
print('Random number: %s' % random.result())
```

```
# Save the random number to a file
saved = save(random, outputs=[File(os.path.join(os.getcwd(), 'sequential-output.txt'))])
# Print the output file
with open(saved.outputs[0].result(), 'r') as f:
    print('File contents: %s' % f.read())
```

#### **Parallel workflow**

The most common way that Parsl Apps are executed in parallel is via looping. The following example shows how a simple loop can be used to create many random numbers in parallel. Note that this takes 5 seconds to run (the time needed for the longest delay), not the 15 seconds that would be needed if these generate functions were called and returned in sequence.

```
[]: # App that generates a random number after a delay
@python_app
def generate(limit,delay):
    from random import randint
    import time
    time.sleep(delay)
    return randint(1,limit)
# Generate 5 random numbers between 1 and 10
rand_nums = []
for i in range(5):
    rand_nums.append(generate(10,i))
# Wait for all apps to finish and collect the results
outputs = [i.result() for i in rand_nums]
# Print results
print(outputs)
```

#### **Parallel dataflow**

Parallel dataflows can be developed by passing data between Apps. In this example we create a set of files, each with a random number, we then concatenate these files into a single file and compute the sum of all numbers in that file. The calls to the first App each create a file, and the second App reads these files and creates a new one. The final App returns the sum as a Python integer.

```
[]: # App that generates a semi-random number between 0 and 32,767
@bash_app
def generate(outputs=[]):
    return "echo $(( RANDOM )) &> {}".format(outputs[0])
# App that concatenates input files into a single output file
@bash_app
def concat(inputs=[], outputs=[]):
```

```
(continued from previous page)
```

```
return "cat {0} > {1}".format(" ".join([i.filepath for i in inputs]), outputs[0])
# App that calculates the sum of values in a list of input files
@python_app
def total(inputs=[]):
    total = 0
   with open(inputs[0], 'r') as f:
        for 1 in f:
            total += int(1)
    return total
# Create 5 files with semi-random numbers in parallel
output_files = []
for i in range (5):
     output_files.append(generate(outputs=[File(os.path.join(os.getcwd(), 'random-{}.txt
\rightarrow'.format(i)))]))
# Concatenate the files into a single file
cc = concat(inputs=[i.outputs[0] for i in output_files],
            outputs=[File(os.path.join(os.getcwd(), 'all.txt'))])
# Calculate the sum of the random numbers
total = total(inputs=[cc.outputs[0]])
print (total.result())
```

#### Dynamic workflows with apps that generate other apps

Often there is a need for a workflow to launch apps based on results from prior apps, but it doesn't know what those apps are until some earlier apps are completed. For example, a pre-processing stage might be followed by n middle stages, but the value of n is not known until pre-processing is complete; or the choice of app to run might depend on the output of pre-processing.

Parsl's join\_app is designed to address this situation by allowing you to define sub-workflows. Rather than return a value (like python\_app) a join\_app instead returns a future. When invoked, the join\_app will not complete until the future has completed and the return value will be the return value from the future.

The following example shows how recursive Fibonacci can be implemented using a join\_app. Here the fibonacci app makes calls to a seperate add app for each pair of numbers.

```
[]: from parsl.app.app import join_app, python_app
```

```
@python_app
def add(*args):
    """Add all of the arguments together. If no arguments, then
    zero is returned (the neutral element of +)
    """
    accumulator = 0
    for v in args:
        accumulator += v
    return accumulator
```

```
@join_app
def fibonacci(n):
    if n == 0:
        return add()
    elif n == 1:
        return add(1)
    else:
        return add(fibonacci(n - 1), fibonacci(n - 2))
```

```
print(fibonacci(10).result())
```

#### **Examples**

#### Monte Carlo workflow

Many scientific applications use the Monte Carlo method to compute results.

One example is calculating  $\pi$  by randomly placing points in a box and using the ratio that are placed inside the circle.

Specifically, if a circle with radius r is inscribed inside a square with side length 2r, the area of the circle is  $\pi r^2$  and the area of the square is  $(2r)^2$ .

Thus, if N uniformly-distributed random points are dropped within the square, approximately  $N\pi/4$  will be inside the circle.

Each call to the function pi() is executed independently and in parallel. The avg\_three() app is used to compute the average of the futures that were returned from the pi() calls.

The dependency chain looks like this:

App Calls	pi()	pi()	pi()		
	\		/		
Futures	а	b	с		
	\		/		
App Call	<pre>avg_points()</pre>				
		1			
Future	avg_pi				

```
[]: # App that estimates pi by placing points in a box
@python_app
def pi(num_points):
    from random import random
    inside = 0
    for i in range(num_points):
        x, y = random(), random() # Drop a random point in the box.
        if x**2 + y**2 < 1: # Count points within the circle.
            inside += 1
    return (inside*4 / num_points)
# App that computes the mean of three values
```

```
@python_app
def mean(a, b, c):
    return (a + b + c) / 3
# Estimate three values for pi
a, b, c = pi(10**6), pi(10**6)
# Compute the mean of the three estimates
mean_pi = mean(a, b, c)
# Print the results
print("a: {:.5f} b: {:.5f} c: {:.5f}".format(a.result(), b.result(), c.result()))
print("Average: {:.5f}".format(mean_pi.result()))
```

#### **Execution and configuration**

Parsl is designed to support arbitrary execution providers (e.g., PCs, clusters, supercomputers, clouds) and execution models (e.g., threads, pilot jobs). The configuration used to run the script tells Parsl how to execute apps on the desired environment. Parsl provides a high level abstraction, called a Block, for describing the resource configuration for a particular app or script.

Information about the different execution providers and executors supported is included in the Parsl documentation.

So far in this tutorial, we've used a built-in configuration for running with threads. Below, we will illustrate how to create configs for different environments.

#### Local execution with threads

As we saw above, we can configure Parsl to execute apps on a local thread pool. This is a good way to parallelize execution on a local PC. The configuration object defines the executors that will be used as well as other options such as authentication method (e.g., if using SSH), checkpoint files, and executor specific configuration. In the case of threads we define the maximum number of threads to be used.

```
[]: from parsl.config import Config
from parsl.executors.threads import ThreadPoolExecutor
local_threads = Config(
    executors=[
        ThreadPoolExecutor(
            max_threads=8,
            label='local_threads'
        )
    ]
)
```

#### Local execution with pilot jobs

We can also define a configuration that uses Parsl's HighThroughputExecutor. In this mode, pilot jobs are used to manage the submission. Parsl creates an interchange to manage execution and deploys one or more workers to execute tasks. The following config will instantiate this infrastructure locally, it can be extended to include a remote provider (e.g., the Cori or Theta supercomputers) for execution.

```
[]: from parsl.providers import LocalProvider
    from parsl.channels import LocalChannel
    from parsl.config import Config
    from parsl.executors import HighThroughputExecutor
    local_htex = Config(
         executors=[
            HighThroughputExecutor(
                 label="htex_Local",
                 worker_debug=True,
                 cores_per_worker=1,
                 provider=LocalProvider(
                     channel=LocalChannel(),
                     init_blocks=1,
                     max_blocks=1,
                 ),
             )
        ],
         strategy=None,
    )
[]: parsl.clear()
     #parsl.load(local_threads)
    parsl.load(local_htex)
[]: @bash_app
    def generate(outputs=[]):
        return "echo $(( RANDOM )) &> {}".format(outputs[0])
    @bash_app
    def concat(inputs=[], outputs=[]):
        return "cat {0} > {1}".format(" ".join(i.filepath for i in inputs), outputs[0])
    @python_app
    def total(inputs=[]):
        total = 
        with open(inputs[0], 'r') as f:
             for 1 in f:
                 total += int(1)
        return total
    # Create 5 files with semi-random numbers
    output_files = []
    for i in range (5):
          output_files.append(generate(outputs=[File(os.path.join(os.getcwd(), 'random-%s.txt
                                                                                 (continues on next page)
```

```
→' % i))]))
```

```
print (total.result())
```

#### **User guide**

#### **Overview**

Parsl is designed to enable straightforward parallelism and orchestration of asynchronous tasks into dataflow-based workflows, in Python. Parsl manages the concurrent execution of these tasks across various computation resources, from laptops to supercomputers, scheduling each task only when its dependencies (e.g., input data dependencies) are met.

Developing a Parsl program is a two-step process:

- 1. Define Parsl apps by annotating Python functions to indicate that they can be executed concurrently.
- 2. Use standard Python code to invoke Parsl apps, creating asynchronous tasks and adhering to dependencies defined between apps.

We aim in this section to provide a mental model of how Parsl programs behave. We discuss how Parsl programs create concurrent tasks, how tasks communicate, and the nature of the environment on which Parsl programs can perform operations. In each case, we compare and contrast the behavior of Python programs that use Parsl constructs with those of conventional Python programs.

**Note:** The behavior of a Parsl program can vary in minor respects depending on the Executor used (see *Execution*). We focus here on the behavior seen when using the recommended *parsl.executors.HighThroughputExecutor* (HTEX).

#### **Parsl and Concurrency**

Any call to a Parsl app creates a new task that executes concurrently with the main program and any other task(s) that are currently executing. Different tasks may execute on the same nodes or on different nodes, and on the same or different computers.

The Parsl execution model thus differs from the Python native execution model, which is inherently sequential. A Python program that does not contain Parsl constructs, or make use of other concurrency mechanisms, executes statements one at a time, in the order that they appear in the program. This behavior is illustrated in the following figure, which shows a Python program on the left and, on the right, the statements executed over time when that program is run, from top to bottom. Each time that the program calls a function, control passes from the main program (in black) to the function (in red). Execution of the main program resumes only after the function returns.



In contrast, the Parsl execution model is inherently concurrent. Whenever a program calls an app, a separate thread of execution is created, and the main program continues without pausing. Thus in the example shown in the figure below. There is initially a single task: the main program (black). The first call to double creates a second task (red) and the second call to double creates a third task (orange). The second and third task terminate as the function that they execute returns. (The dashed lines represent the start and finish of the tasks). The calling program will only block (wait) when it is explicitly told to do so (in this case by calling result())



**Note:** Note: We talk here about concurrency rather than parallelism for a reason. Two activities are concurrent if they can execute at the same time. Two activities occur in parallel if they do run at the same time. If a Parsl program creates more tasks that there are available processors, not all concurrent activities may run in parallel.

#### **Parsl and Execution**

We have now seen that Parsl tasks are executed concurrently alongside the main Python program and other Parsl tasks. We now turn to the question of how and where are those tasks executed. Given the range of computers on which parallel programs may be executed, Parsl allows tasks to be executed using different executors (parsl.executors). Executors are responsible for taking a queue of tasks and executing them on local or remote resources.

We briefly describe two of Parsl's most commonly used executors. Other executors are described in *Execution*.

The *pars1.executors.HighThroughputExecutor* (HTEX) implements a *pilot job model* that enables fine-grain task execution using across one or more provisioned nodes. HTEX can be used on a single node (e.g., a laptop) and will make use of multiple processes for concurrent execution. As shown in the following figure, HTEX uses Parsl's provider abstraction (pars1.providers) to communicate with a resource manager (e.g., batch scheduler or cloud

API) to provision a set of nodes (e.g., Parsl will use Slurm's qsub command to request nodes on a Slurm cluster) for the duration of execution. HTEX deploys a lightweight worker agent on the nodes which subsequently connects back to the main Parsl process. Parsl tasks are then sent from the main program to the connected workers for execution and the results are sent back via the same mechanism. This approach has a number of advantages over other methods: it avoids long job scheduler queue delays by acquiring one set of resources for the entire program and it allows for scheduling of many tasks on individual nodes.



The *pars1.executors.ThreadPoolExecutor* allows tasks to be executed on a pool of locally accessible threads. As execution occurs on the same computer, on a pool of threads forked from the main program, the tasks share memory with one another (this is discussed further in the following sections).

#### **Parsl and Communication**

Parsl tasks typically need to communicate in order to perform useful work. Parsl provides for two forms of communication: by parameter passing and by file passing. As described in the next section, Parsl programs may also communicate by interacting with shared filesystems and services its environment.

#### **Parameter Passing**

The figure above illustrates communication via parameter passing. The call double(3) to the app double in the main program creates a new task and passes the parameter value, 3, to that new task. When the task completes execution, its return value, 6, is returned to the main program. Similarly, the second task is passed the value 5 and returns the value 10. In this case, the parameters passed are simple primitive types (i.e., integers); however, complex objects (e.g., Numpy Arrays, Pandas DataFrames, custom objects) can also be passed to/from tasks.

#### **File Passing**

Parsl supports communication via files in both Bash apps and Python apps. Files may be used in place of parameter passing for many reasons, such as for apps are designed to support files, when data to be exchanged are large, or when data cannot be easily serialized into Python objects. As Parsl tasks may be executed on remote nodes, without shared file systems, Parsl offers a Parsl *parsl.data\_provider.files.File* construct for location-independent reference to files. Parsl will translate file objects to worker-accessible paths when executing dependent apps. Parsl is also able to transfer files in, out, and between Parsl apps using one of several methods (e.g., FTP, HTTP(S), Globus and rsync). To accommodate the asynchronous nature of file transfer, Parsl treats data movement like a Parsl app, adding a dependency to the execution graph and waiting for transfers to complete before executing dependent apps. More information is provided in *Passing Python objects*).

#### **Futures**

Communication via parameter and file passing also serves a second purpose, namely synchronization. As we discuss in more detail in *Futures*, a call to an app returns a special object called a future that has a special unassigned state until such time as the app returns, at which time it takes the return value. (In the example program, two futures are thus created, d1 and d2.) The AppFuture function result() blocks until the future to which it is applied takes a value. Thus the print statement in the main program blocks until both child tasks created by the calls to the double app return. The following figure captures this behavior, with time going from left to right rather than top to bottom as in the preceding figure. Task 1 is initially active as it starts Tasks 2 and 3, then blocks as a result of calls to d1.result() and d2.result(), and when those values are available, is active again.



#### **The Parsl Environment**

Regular Python and Parsl-enhanced Python differ in terms of the environment in which code executes. We use the term *environment* here to refer to the variables and modules (the *memory environment*), the file system(s) (the *file system environment*), and the services (the *service environment*) that are accessible to a function.

An important question when it comes to understanding the behavior of Parsl programs is the environment in which this new task executes: does it have the same or different memory, file system, or service environment as its parent task or any other task? The answer, depends on the executor used, and (in the case of the file system environment) where the task executes. Below we describe behavior for the most commonly used *parsl.executors.HighThroughputExecutor* which is representative of all Parsl executors except the *parsl.executors.ThreadPoolExecutor*.

#### **Memory environment**

In Python, the variables and modules that are accessible to a function are defined by Python scoping rules, by which a function has access to both variables defined within the function (*local* variables) and those defined outside the function (*global* variables). Thus in the following code, the print statement in the print\_answer function accesses the global variable "answer", and we see as output "the answer is 42."

```
answer = 42
def print_answer():
    print('the answer is', answer)
print_answer()
```

In Parsl (except when using the *parsl.executors.ThreadPoolExecutor*) a Parsl app is executed in a distinct environment that only has access to local variables associated with the app function. Thus, if the program above is executed with say the *parsl.executors.HighThroughputExecutor*, will print "the answer is 0" rather than "the answer is 42," because the print statement in provide\_answer does not have access to the global variable that has been assigned the value 42. The program will run without errors when using the *parsl.executors.ThreadPoolExecutor*.

Similarly, the same scoping rules apply to import statements, and thus the following program will run without errors with the *parsl.executors.ThreadPoolExecutor*, but raise errors when run with any other executor, because the return statement in ambiguous\_double refers to a variable (factor) and a module (random) that are not known to the function.

```
import random
factor = 5
@python_app
def ambiguous_double(x):
    return x * random.random() * factor
print(ambiguous_double(42))
```

To allow this program to run correctly with all Parsl executors, the random library must be imported within the app, and the factor variable must be passed as an argument, as follows.

```
import random
factor = 5
@python_app
def good_double(factor, x):
    import random
    return x * random.random() * factor
print(good_double(factor, 42))
```

#### File system environment

In a regular Python program the environment that is accessible to a Python program also includes the file system(s) of the computer on which it is executing. Thus in the following code, a value written to a file "answer.txt" in the current directory can be retrieved by reading the same file, and the print statement outputs "the answer is 42."

```
def print_answer_file():
    with open('answer.txt','r') as f:
        print('the answer is', f.read())
with open('answer.txt','w') as f:
    f.write('42')
    f.close()
print_answer_file()
```

The question of which file system environment is accessible to a Parsl app depends on where the app executes. If two tasks run on nodes that share a file system, then those tasks (e.g., tasks A and B in the figure below, but not task C) share a file system environment. Thus the program above will output "the answer is 42" if the parent task and the child task run on nodes 1 and 2, but not if they run on nodes 2 and 3.



#### Service Environment

We use the term service environment to refer to network services that may be accessible to a Parsl program, such as a Redis server or Globus data management service. These services are accessible to any task.

#### **Environment Summary**

As we summarize in the table, if tasks execute with the *parsl.executors.ThreadPoolExecutor*, they share the memory and file system environment of the parent task. If they execute with any other executor, they have a separate memory environment, and may or may not share their file system environment with other tasks, depending on where they are placed. All tasks typically have access to the same network services.

	Share memory en- vironment with par- ent/other tasks	Share file system environment with parent	Share file system environ- ment with other tasks	Share service environment with other tasks
Python without Parsl	Yes	Yes	N/A	N/A
Parsl Thread- PoolEx- ecutor	Yes	Yes	Yes	N/A
Other Parsl executors	No	If executed on the same node with file system access	If tasks are executed on the same node or with access to the same file system	N/A

#### Apps

An **App** defines a computation that will be executed asynchronously by Parsl. Apps are Python functions marked with a decorator which designates that the function will run asynchronously and cause it to return a **Future** instead of the result.

Apps can be one of three types of functions, each with their own type of decorator

- @python\_app: Most Python functions
- @bash\_app: A Python function which returns a command line program to execute
- @join\_app: A function which launches one or more new Apps

The intricacies of Python and Bash apps are documented below. Join apps are documented in a later section (see *Join Apps*).

#### **Python Apps**

```
@python_app
def hello_world(name: str) -> str:
    return f'Hello, {name}!'
print(hello_world('user').result())
```

Python Apps run Python functions. The code inside a function marked by @python\_app is what will be executed either locally or on a remote system.

Most functions can run without modification. Limitations on the content of the functions and their inputs/outputs are described below.

#### **Rules for Function Contents**

Parsl apps have access to less information from the script that defined them than functions run via Python's native multiprocessing libraries. The reason is that functions are executed on workers that lack access to the global variables in the script that defined them. Practically, this means

1. *Functions may need to re-import libraries*. Place the import statements that define functions or classes inside the function. Type annotations should not use libraries defined in the function.

```
import numpy as np
# BAD: Assumes library has been imported
@python_app
def linear_model(x: list[float] | np.ndarray, m: float, b: float):
    return np.multiply(x, m) + b
# GOOD: Function imports libraries on remote worker
@python_app
def linear_model(x: list[float] | 'np.ndarray', m: float, b: float):
    import numpy as np
    return np.multiply(x, m) + b
```

2. *Global variables are inaccessible*. Functions should not use variables defined outside the function. Likewise, do not assume that variables created inside the function are visible elsewhere.

3. *Outputs are only available through return statements*. Parsl does not support generator functions (i.e., those which use yield statements) and any changes to input arguments will not be communicated.

```
# BAD: Assumes changes to inputs will be communicated
@python_app
def append_to_list(input_list: list, new_val):
    input_list.append(new_val)
# GOOD: Changes to inputs are returned
@python_app
def append_to_list(input_list: list, new_val) -> list:
```

input\_list.append(new\_val)
return input\_list

#### **Functions from Modules**

The above rules assume that the user is running the example code from a standalone script or Jupyter Notebook. Functions that are defined in an installed Python module do not need to abide by these guidelines, as they are sent to workers differently than functions defined locally within a script.

Directly convert a function from a library to a Python App by passing it as an argument to python\_app:

```
from module import function
function_app = python_app(function)
```

function\_app will act as Parsl App function of function.

It is also possible to create wrapped versions of functions, such as ones with pinned arguments. Parsl just requires first calling update\_wrapped() with the wrapped function to include attributes from the original function (e.g., its name).

```
from functools import partial, update_wrapped
import numpy as np
my_max = partial(np.max, axis=0, keepdims=True)
my_max = update_wrapper(my_max, max) # Copy over the names
my_max_app = python_app(my_max)
```

The above example is equivalent to creating a new function (as below)

```
@python_app
def my_max_app(*args, **kwargs):
    import numpy as np
    return np.max(*args, keepdims=True, axis=0, **kwargs)
```

#### Inputs and Outputs

Python apps may be passed any Python type as an input and return any Python type, with a few exceptions. There are several classes of allowed types, each with different rules.

- *Python Objects*: Any Python object that can be saved with pickle or dill can be used as an import or output. All primitive types (e.g., floats, strings) are valid as are many complex types (e.g., numpy arrays).
- *Files*: Pass files as inputs as a *File* object. Parsl can transfer them to a remote system and update the File object with a new path. Access the new path with File.filepath attribute.

```
@python_app
def read_first_line(x: File):
    with open(x.filepath, 'r') as fp:
        return fp.readline()
```

Files can also be outputs of a function, but only through the outputs kwargs (described below).

• *Parsl Futures*. Functions can receive results from other Apps as Parsl Future objects. Parsl will establish a dependency on the App(s) which created the Future(s) and start executing as soon as the preceding ones complete.

```
@python_app
def capitalize(x: str):
    return x.upper()

input_file = File('text.txt')
first_line_future = read_first_line(input_file)
capital_future = capitalize(first_line_future)
print(capital_future.result())
```

See the section on Futures for more details.

Learn more about the types of data allowed in the data section.

Note: Any changes to mutable input arguments will be ignored.

#### **Special Keyword Arguments**

Some keyword arguments to the Python function are treated differently by Parsl

1. inputs: (list) This keyword argument defines a list of input *Futures* or files. Parsl will wait for the results of any listed *Futures* to be resolved before executing the app. The inputs argument is useful both for passing files as arguments and when one wishes to pass in an arbitrary number of futures at call time.

```
@python_app()
def map_app(x):
    return x * 2
@python_app()
def reduce_app(inputs = ()):
    return sum(inputs)
map_futures = [map_app(x) for x in range(3)]
reduce_future = reduce_app(inputs=map_futures)
print(reduce_future.result()) # 0 + 1 * 2 + 2 * 2 = 6
```

2. outputs: (list) This keyword argument defines a list of files that will be produced by the app. For each file thus listed, Parsl will create a future, track the file, and ensure that it is correctly created. The future can then be passed to other apps as an input argument.

```
@python_app()
def write_app(message, outputs=()):
    """Write a single message to every file in outputs"""
    for path in outputs:
        with open(path, 'w') as fp:
            print(message, file=fp)

to_write = [
    File(Path(tmpdir) / 'output-0.txt'),
    File(Path(tmpdir) / 'output-1.txt')
]
```

```
write_app('Hello!', outputs=to_write).result()
for path in to_write:
    with open(path) as fp:
        assert fp.read() == 'Hello!\n'
```

3. walltime: (int) This keyword argument places a limit on the app's runtime in seconds. If the walltime is exceed, Parsl will raise an *pars1.app.errors.AppTimeout* exception.

#### **Outputs**

A Python app returns an AppFuture (see *Futures*) as a proxy for the results that will be returned by the app once it is executed. This future can be inspected to obtain task status; and it can be used to wait for the result, and when complete, present the output Python object(s) returned by the app. In case of an error or app failure, the future holds the exception raised by the app.

#### **Options for Python Apps**

The *python\_app()* decorator has a few options which controls how Parsl executes all tasks run with that application. For example, you can ensure that Parsl caches the results of the function and executes tasks on specific sites.

```
@python_app(cache=True, executors=['gpu'])
def expensive_gpu_function():
    # ...
    return
```

See the Parsl documentation for full details.

#### Limitations

To summarize, any Python function can be made a Python App with a few restrictions

- 1. Functions should act only on defined input arguments. That is, they should not use script-level or global variables.
- 2. Functions must explicitly import any required modules if they are defined in script which starts Parsl.
- 3. Parsl uses dill and pickle to serialize Python objects to/from apps. Therefore, Parsl require that all input and output objects can be serialized by dill or pickle. See *Addressing SerializationError*.
- 4. STDOUT and STDERR produced by Python apps remotely are not captured.

#### **Bash Apps**

```
@bash_app
def echo(
    name: str,
    stdout=parsl.AUTO_LOGNAME  # Requests Parsl to return the stdout
):
    return f'echo "Hello, {name}!"'
future = echo('user')
```

```
future.result() # block until task has completed
with open(future.stdout, 'r') as f:
    print(f.read())
```

A Parsl Bash app executes an external application by making a command-line execution. Parsl will execute the string returned by the function as a command-line script on a remote worker.

#### **Rules for Function Contents**

Bash Apps follow the same rules *as Python Apps*. For example, imports may need to be inside functions and global variables will be inaccessible.

#### **Inputs and Outputs**

Bash Apps can use the same kinds of inputs as Python Apps, but only communicate results with Files.

The Bash Apps, unlike Python Apps, can also return the content printed to the Standard Output and Error.

#### **Special Keywords Arguments**

In addition to the inputs, outputs, and walltime keyword arguments described above, a Bash app can accept the following keywords:

- stdout: (string, tuple or parsl.AUTO\_LOGNAME) The path to a file to which standard output should be redirected. If set to parsl.AUTO\_LOGNAME, the log will be automatically named according to task id and saved under task\_logs in the run directory. If set to a tuple (filename, mode), standard output will be redirected to the named file, opened with the specified mode as used by the Python open function.
- 2. stderr: (string or parsl.AUTO\_LOGNAME) Like stdout, but for the standard error stream.
- 3. label: (string) If the app is invoked with stdout=parsl.AUTO\_LOGNAME or stderr=parsl.AUTO\_LOGNAME, this argument will be appended to the log name.

#### **Outputs**

If the Bash app exits with Unix exit code 0, then the AppFuture will complete. If the Bash app exits with any other code, Parsl will treat this as a failure, and the AppFuture will instead contain an *BashExitFailure* exception. The Unix exit code can be accessed through the exitcode attribute of that *BashExitFailure*.

#### **Execution Options**

Bash Apps have the same execution options (e.g., pinning to specific sites) as the Python Apps.

#### **MPI Apps**

Applications which employ MPI to span multiple nodes are a special case of Bash apps, and require special modification of Parsl's execution environment to function. Support for MPI applications is described in a later section.

#### **Futures**

When an ordinary Python function is invoked in a Python program, the Python interpreter waits for the function to complete execution before proceeding to the next statement. But if a function is expected to execute for a long period of time, it may be preferable not to wait for its completion but instead to proceed immediately with executing subsequent statements. The function can then execute concurrently with that other computation.

Concurrency can be used to enhance performance when independent activities can execute on different cores or nodes in parallel. The following code fragment demonstrates this idea, showing that overall execution time may be reduced if the two function calls are executed concurrently.

```
v1 = expensive_function(1)
v2 = expensive_function(2)
result = v1 + v2
```

However, concurrency also introduces a need for **synchronization**. In the example, it is not possible to compute the sum of v1 and v2 until both function calls have completed. Synchronization provides a way of blocking execution of one activity (here, the statement result = v1 + v2) until other activities (here, the two calls to expensive\_function()) have completed.

Parsl supports concurrency and synchronization as follows. Whenever a Parsl program calls a Parsl app (a function annotated with a Parsl app decorator, see *Apps*), Parsl will create a new task and immediately return a future in lieu of that function's result(s). The program will then continue immediately to the next statement in the program. At some point, for example when the task's dependencies are met and there is available computing capacity, Parsl will execute the task. Upon completion, Parsl will set the value of the future to contain the task's output.

A future can be used to track the status of an asynchronous task. For example, after creation, the future may be interrogated to determine the task's status (e.g., running, failed, completed), access results, and capture exceptions. Further, futures may be used for synchronization, enabling the calling Python program to block until the future has completed execution.

Parsl provides two types of futures: *AppFuture* and *DataFuture*. While related, they enable subtly different parallel patterns.

#### **AppFutures**

AppFutures are the basic building block upon which Parsl programs are built. Every invocation of a Parsl app returns an AppFuture that may be used to monitor and manage the task's execution. AppFutures are inherited from Python's concurrent library. They provide three key capabilities:

1. An AppFuture's result() function can be used to wait for an app to complete, and then access any result(s). This function is blocking: it returns only when the app completes or fails. The following code fragment implements an example similar to the expensive\_function() example above. Here, the sleep\_double app simply doubles the input value. The program invokes the sleep\_double app twice, and returns futures in place of results. The example shows how the future's result() function can be used to wait for the results from the two sleep\_double app invocations to be computed.

```
@python_app
def sleep_double(x):
    import time
    time.sleep(2) # Sleep for 2 seconds
    return x*2
# Start two concurrent sleep_double apps. doubled_x1 and doubled_x2 are AppFutures
doubled_x1 = sleep_double(10)
doubled_x2 = sleep_double(5)
# The result() function will block until each of the corresponding app calls have_
    ...completed
print(doubled_x1.result() + doubled_x2.result())
```

2. An AppFuture's done() function can be used to check the status of an app, *without blocking*. The following example shows that calling the future's done() function will not stop execution of the main Python program.

```
@python_app
def double(x):
    return x*2
# doubled_x is an AppFuture
doubled_x = double(10)
# Check status of doubled_x, this will print True if the result is available, else False
print(doubled_x.done())
```

3. An AppFuture provides a safe way to handle exceptions and errors while asynchronously executing apps. The example shows how exceptions can be captured in the same way as a standard Python program when calling the future's result() function.

```
@python_app
def bad_divide(x):
    return 6/x
# Call bad divide with 0, to cause a divide by zero exception
doubled_x = bad_divide(0)
# Catch and handle the exception.
try:
    doubled_x.result()
except ZeroDivisionError as ze:
    print('Oops! You tried to divide by 0')
except Exception as e:
    print('Oops! Something really bad happened')
```

In addition to being able to capture exceptions raised by a specific app, Parsl also raises DependencyErrors when apps are unable to execute due to failures in prior dependent apps. That is, an app that is dependent upon the successful completion of another app will fail with a dependency error if any of the apps on which it depends fail.
### **DataFutures**

While an AppFuture represents the execution of an asynchronous app, a DataFuture represents a file to be produced by that app. Parsl's dataflow model requires such a construct so that it can determine when dependent apps, apps that that are to consume a file produced by another app, can start execution.

When calling an app that produces files as outputs, Parsl requires that a list of output files be specified (as a list of *File* objects passed in via the outputs keyword argument). Parsl will return a DataFuture for each output file as part AppFuture when the app is executed. These DataFutures are accessible in the AppFuture's outputs attribute.

Each DataFuture will complete when the App has finished executing, and the corresponding file has been created (and if specified, staged out).

When a DataFuture is passed as an argument to a subsequent app invocation, that subsequent app will not begin execution until the DataFuture is completed. The input argument will then be replaced with an appropriate File object.

The following code snippet shows how DataFutures are used. In this example, the call to the echo Bash app specifies that the results should be written to an output file ("hello1.txt"). The main program inspects the status of the output file (via the future's outputs attribute) and then blocks waiting for the file to be created (hello.outputs[0].result()).

```
# This app echoes the input string to the first file specified in the
# outputs list
@bash_app
def echo(message, outputs=()):
    return 'echo {} &> {}'.format(message, outputs[0])
# Call echo specifying the output file
hello = echo('Hello World!', outputs=[File('hello1.txt')])
# The AppFuture's outputs attribute is a list of DataFutures
print(hello.outputs)
# Print the contents of the output DataFuture when complete
with open(hello.outputs[0].result().filepath, 'r') as f:
    print(f.read())
```

# **Passing Python objects**

Parsl apps can communicate via standard Python function parameter passing and return statements. The following example shows how a Python string can be passed to, and returned from, a Parsl app.

```
@python_app
def example(name):
    return 'hello {0}'.format(name)
r = example('bob')
print(r.result())
```

Parsl uses the dill and pickle libraries to serialize Python objects into a sequence of bytes that can be passed over a network from the submitting machine to executing workers.

Thus, Parsl apps can receive and return standard Python data types such as booleans, integers, tuples, lists, and dictionaries. However, not all objects can be serialized with these methods (e.g., closures, generators, and system objects), and so those objects cannot be used with all executors. Parsl will raise a *SerializationError* if it encounters an object that it cannot serialize. This applies to objects passed as arguments to an app, as well as objects returned from an app. See *Addressing SerializationError*.

#### **Staging data files**

Parsl apps can take and return data files. A file may be passed as an input argument to an app, or returned from an app after execution. Parsl provides support to automatically transfer (stage) files between the main Parsl program, worker nodes, and external data storage systems.

Input files can be passed as regular arguments, or a list of them may be specified in the special inputs keyword argument to an app invocation.

Inside an app, the filepath attribute of a *File* can be read to determine where on the execution-side file system the input file has been placed.

Output *File* objects must also be passed in at app invocation, through the outputs parameter. In this case, the *File* object specifies where Parsl should place output after execution.

Inside an app, the filepath attribute of an output *File* provides the path at which the corresponding output file should be placed so that Parsl can find it after execution.

If the output from an app is to be used as the input to a subsequent app, then a *DataFuture* that represents whether the output file has been created must be extracted from the first app's AppFuture, and that must be passed to the second app. This causes app executions to be properly ordered, in the same way that passing AppFutures to subsequent apps causes execution ordering based on an app returning.

In a Parsl program, file handling is split into two pieces: files are named in an execution-location independent manner using *File* objects, and executors are configured to stage those files in to and out of execution locations using instances of the *Staging* interface.

### **Parsl files**

Parsl uses a custom *File* to provide a location-independent way of referencing and accessing files. Parsl files are defined by specifying the URL *scheme* and a path to the file. Thus a file may represent an absolute path on the submit-side file system or a URL to an external file.

The scheme defines the protocol via which the file may be accessed. Parsl supports the following schemes: file, ftp, http, https, and globus. If no scheme is specified Parsl will default to the file scheme.

The following example shows creation of two files with different schemes: a locally-accessible data.txt file and an HTTPS-accessible README file.

```
File('file://home/parsl/data.txt')
File('https://github.com/Parsl/parsl/blob/master/README.rst')
```

Parsl automatically translates the file's location relative to the environment in which it is accessed (e.g., the Parsl program or an app). The following example shows how a file can be accessed in the app irrespective of where that app executes.

```
@python_app
def print_file(inputs=()):
    with open(inputs[0].filepath, 'r') as inp:
        content = inp.read()
        return(content)
# create an remote Parsl file
```

```
f = File('https://github.com/Parsl/parsl/blob/master/README.rst')
# call the print_file app with the Parsl file
r = print_file(inputs=[f])
r.result()
```

As described below, the method by which this files are transferred depends on the scheme and the staging providers specified in the Parsl configuration.

### **Staging providers**

Parsl is able to transparently stage files between at-rest locations and execution locations by specifying a list of *Staging* instances for an executor. These staging instances define how to transfer files in and out of an execution location. This list should be supplied as the storage\_access parameter to an executor when it is constructed.

Parsl includes several staging providers for moving files using the schemes defined above. By default, Parsl executors are created with three common staging providers: the NoOpFileStaging provider for local and shared file systems and the HTTP(S) and FTP staging providers for transferring files to and from remote storage locations. The following example shows how to explicitly set the default staging providers.

```
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.data_provider.data_manager import default_staging
config = Config(
    executors=[
    HighThroughputExecutor(
        storage_access=default_staging,
        # equivalent to the following
        # storage_access=[NoOpFileStaging(), FTPSeparateTaskStaging(),
        J
    ]
)
```

Parsl further differentiates when staging occurs relative to the app invocation that requires or produces files. Staging either occurs with the executing task (*in-task staging*) or as a separate task (*separate task staging*) before app execution. In-task staging uses a wrapper that is executed around the Parsl task and thus occurs on the resource on which the task is executed. Separate task staging inserts a new Parsl task in the graph and associates a dependency between the staging task and the task that depends on that file. Separate task staging may occur on either the submit-side (e.g., when using Globus) or on the execution-side (e.g., HTTPS, FTP).

#### NoOpFileStaging for Local/Shared File Systems

The NoOpFileStaging provider assumes that files specified either with a path or with the file URL scheme are available both on the submit and execution side. This occurs, for example, when there is a shared file system. In this case, files will not moved, and the File object simply presents the same file path to the Parsl program and any executing tasks.

Files defined as follows will be handled by the NoOpFileStaging provider.

```
File('file://home/parsl/data.txt')
File('/home/parsl/data.txt')
```

The NoOpFileStaging provider is enabled by default on all executors. It can be explicitly set as the only staging provider as follows.

```
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.data_provider.file_noop import NoOpFileStaging
config = Config(
    executors=[
    HighThroughputExecutor(
        storage_access=[NoOpFileStaging()]
    )
]
)
```

#### FTP, HTTP, HTTPS: separate task staging

Files named with the ftp, http or https URL scheme will be staged in using HTTP GET or anonymous FTP commands. These commands will be executed as a separate Parsl task that will complete before the corresponding app executes. These providers cannot be used to stage out output files.

The following example defines a file accessible on a remote FTP server.

```
File('ftp://www.iana.org/pub/mirror/rirstats/arin/ARIN-STATS-FORMAT-CHANGE.txt')
```

When such a file object is passed as an input to an app, Parsl will download the file to whatever location is selected for the app to execute. The following example illustrates how the remote file is implicitly downloaded from an FTP server and then converted. Note that the app does not need to know the location of the downloaded file on the remote computer, as Parsl abstracts this translation.

```
@python_app
def convert(inputs=(), outputs=()):
    with open(inputs[0].filepath, 'r') as inp:
        content = inp.read()
        with open(outputs[0].filepath, 'w') as out:
        out.write(content.upper())

# create an remote Parsl file
inp = File('ftp://www.iana.org/pub/mirror/rirstats/arin/ARIN-STATS-FORMAT-CHANGE.txt')
# create a local Parsl file
out = File('file:///tmp/ARIN-STATS-FORMAT-CHANGE.txt')
```

```
# call the convert app with the Parsl file
f = convert(inputs=[inp], outputs=[out])
f.result()
```

HTTP and FTP separate task staging providers can be configured as follows.

#### FTP, HTTP, HTTPS: in-task staging

These staging providers are intended for use on executors that do not have a file system shared between each executor node.

These providers will use the same HTTP GET/anonymous FTP as the separate task staging providers described above, but will do so in a wrapper around individual app invocations, which guarantees that they will stage files to a file system visible to the app.

A downside of this staging approach is that the staging tasks are less visible to Parsl, as they are not performed as separate Parsl tasks.

In-task staging providers can be configured as follows.

```
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.data_provider.http import HTTPInTaskStaging
from parsl.data_provider.ftp import FTPInTaskStaging
config = Config(
    executors=[
    HighThroughputExecutor(
        storage_access=[HTTPInTaskStaging(), FTPInTaskStaging()]
    )
]
)
```

#### Globus

The Globus staging provider is used to transfer files that can be accessed using Globus. A guide to using Globus is available here).

A file using the Globus scheme must specify the UUID of the Globus endpoint and a path to the file on the endpoint, for example:

File('globus://037f054a-15cf-11e8-b611-0ac6873fc732/unsorted.txt')

Note: a Globus endpoint's UUID can be found in the Globus Manage Endpoints page.

There must also be a Globus endpoint available with access to a execute-side file system, because Globus file transfers happen between two Globus endpoints.

#### **Globus Configuration**

In order to manage where files are staged, users must configure the default working\_dir on a remote location. This information is specified in the *ParslExecutor* via the working\_dir parameter in the *Config* instance. For example:

```
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
config = Config(
    executors=[
    HighThroughputExecutor(
        working_dir="/home/user/data"
    )
]
)
```

Parsl requires knowledge of the Globus endpoint that is associated with an executor. This is done by specifying the endpoint\_name (the UUID of the Globus endpoint that is associated with the system) in the configuration.

In some cases, for example when using a Globus shared endpoint or when a Globus endpoint is mounted on a supercomputer, the path seen by Globus is not the same as the local path seen by Parsl. In this case the configuration may optionally specify a mapping between the endpoint\_path (the common root path seen in Globus), and the local\_path (the common root path on the local file system), as in the following. In most cases, endpoint\_path and local\_path are the same and do not need to be specified.

```
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.data_provider.globus import GlobusStaging
from parsl.data_provider.data_manager import default_staging
config = Config(
    executors=[
    HighThroughputExecutor(
        working_dir="/home/user/parsl_script",
        storage_access=default_staging + [GlobusStaging(
            endpoint_uuid="7d2dc622-2edb-11e8-b8be-0ac6873fc732",
            endpoint_path="/",
            local_path="/home/user"
        )]
```

) ] )

### **Globus Authorization**

In order to transfer files with Globus, the user must first authenticate. The first time that Globus is used with Parsl on a computer, the program will prompt the user to follow an authentication and authorization procedure involving a web browser. Users can authorize out of band by running the parsl-globus-auth utility. This is useful, for example, when running a Parsl program in a batch system where it will be unattended.

```
$ parsl-globus-auth
Parsl Globus command-line authorizer
If authorization to Globus is necessary, the library will prompt you now.
Otherwise it will do nothing
Authorization complete
```

#### rsync

The rsync utility can be used to transfer files in the file scheme in configurations where workers cannot access the submit-side file system directly, such as when executing on an AWS EC2 instance or on a cluster without a shared file system. However, the submit-side file system must be exposed using rsync.

#### rsync Configuration

rsync must be installed on both the submit and worker side. It can usually be installed by using the operating system package manager: for example, by apt-get install rsync.

An *RSyncStaging* option must then be added to the Parsl configuration file, as in the following. The parameter to RSyncStaging should describe the prefix to be passed to each rsync command to connect from workers to the submitside host. This will often be the username and public IP address of the submitting system.

```
from parsl.data_provider.rsync import RSyncStaging
config = Config(
    executors=[
        HighThroughputExecutor(
        storage_access=[HTTPInTaskStaging(), FTPInTaskStaging(), RSyncStaging("benc@
        ...
        )
        )
```

# rsync Authorization

The rsync staging provider delegates all authentication and authorization to the underlying rsync command. This command must be correctly authorized to connect back to the submit-side system. The form of this authorization will depend on the systems in question.

The following example installs an ssh key from the submit-side file system and turns off host key checking, in the worker\_init initialization of an EC2 instance. The ssh key must have sufficient privileges to run rsync over ssh on the submit-side system.

```
with open("rsync-callback-ssh", "r") as f:
    private_key = f.read()
ssh_init = """
mkdir .ssh
chmod go-rwx .ssh
cat > .ssh/id_rsa <<EOF</pre>
{private_key}
EOF
cat > .ssh/config <<EOF</pre>
Host *
  StrictHostKeyChecking no
EOF
chmod go-rwx .ssh/id_rsa
chmod go-rwx .ssh/config
""".format(private_key=private_key)
config = Config(
    executors=[
        HighThroughputExecutor(
             storage_access=[HTTPInTaskStaging(), FTPInTaskStaging(), RSyncStaging("benc@
\rightarrow" + public_ip)],
            provider=AWSProvider(
            worker_init = ssh_init
             . . .
             )
    )
)
```

#### Execution

Contemporary computing environments may include a wide range of computational platforms or **execution providers**, from laptops and PCs to various clusters, supercomputers, and cloud computing platforms. Different execution providers may require or allow for the use of different **execution models**, such as threads (for efficient parallel execution on a multicore processor), processes, and pilot jobs for running many small tasks on a large parallel system.

Parsl is designed to abstract these low-level details so that an identical Parsl program can run unchanged on different platforms or across multiple platforms. To this end, Parsl uses a configuration file to specify which execution provider(s) and execution model(s) to use. Parsl provides a high level abstraction, called a *block*, for providing a uniform description of a compute resource irrespective of the specific execution provider.

**Note:** Refer to *Configuration* for information on how to configure the various components described below for specific scenarios.

### **Execution providers**

Clouds, supercomputers, and local PCs offer vastly different modes of access. To overcome these differences, and present a single uniform interface, Parsl implements a simple provider abstraction. This abstraction is key to Parsl's ability to enable scripts to be moved between resources. The provider interface exposes three core actions: submit a job for execution (e.g., sbatch for the Slurm resource manager), retrieve the status of an allocation (e.g., squeue), and cancel a running job (e.g., scancel). Parsl implements providers for local execution (fork), for various cloud platforms using cloud-specific APIs, and for clusters and supercomputers that use a Local Resource Manager (LRM) to manage access to resources, such as Slurm, HTCondor, and Cobalt.

Each provider implementation may allow users to specify additional parameters for further configuration. Parameters are generally mapped to LRM submission script or cloud API options. Examples of LRM-specific options are partition, wall clock time, scheduler options (e.g., #SBATCH arguments for Slurm), and worker initialization commands (e.g., loading a conda environment). Cloud parameters include access keys, instance type, and spot bid price

Parsl currently supports the following providers:

- 1. pars1.providers.LocalProvider: The provider allows you to run locally on your laptop or workstation.
- 2. *pars1.providers.CobaltProvider*: This provider allows you to schedule resources via the Cobalt scheduler. This provider is deprecated and will be removed by 2024.04.
- 3. pars1.providers.SlurmProvider: This provider allows you to schedule resources via the Slurm scheduler.
- 4. *pars1.providers.CondorProvider*: This provider allows you to schedule resources via the Condor scheduler.
- 5. *pars1.providers.GridEngineProvider*: This provider allows you to schedule resources via the GridEngine scheduler.
- 6. pars1.providers.TorqueProvider: This provider allows you to schedule resources via the Torque scheduler.
- 7. *pars1.providers.AWSProvider*: This provider allows you to provision and manage cloud nodes from Amazon Web Services.
- 8. *pars1.providers.GoogleCloudProvider*: This provider allows you to provision and manage cloud nodes from Google Cloud.
- 9. *pars1.providers.KubernetesProvider*: This provider allows you to provision and manage containers on a Kubernetes cluster.
- 10. *pars1.providers.AdHocProvider*: This provider allows you manage execution over a collection of nodes to form an ad-hoc cluster.

11. pars1.providers.LSFProvider: This provider allows you to schedule resources via IBM's LSF scheduler.

# Executors

Parsl programs vary widely in terms of their execution requirements. Individual Apps may run for milliseconds or days, and available parallelism can vary between none for sequential programs to millions for "pleasingly parallel" programs. Parsl executors, as the name suggests, execute Apps on one or more target execution resources such as multi-core workstations, clouds, or supercomputers. As it appears infeasible to implement a single execution strategy that will meet so many diverse requirements on such varied platforms, Parsl provides a modular executor interface and a collection of executors that are tuned for common execution patterns.

Parsl executors extend the Executor class offered by Python's concurrent.futures library, which allows Parsl to use existing solutions in the Python Standard Library (e.g., ThreadPoolExecutor) and from other packages such as Work Queue. Parsl extends the concurrent.futures executor interface to support additional capabilities such as automatic scaling of execution resources, monitoring, deferred initialization, and methods to set working directories. All executors share a common execution kernel that is responsible for deserializing the task (i.e., the App and its input arguments) and executing the task in a sandboxed Python environment.

Parsl currently supports the following executors:

- 1. parsl.executors.ThreadPoolExecutor: This executor supports multi-thread execution on local resources.
- 2. *pars1.executors.HighThroughputExecutor*: This executor implements hierarchical scheduling and batching using a pilot job model to deliver high throughput task execution on up to 4000 Nodes.
- 3. pars1.executors.WorkQueueExecutor: This executor integrates Work Queue as an execution backend. Work Queue scales to tens of thousands of cores and implements reliable execution of tasks with dynamic resource sizing.

4. *pars1.executors.taskvine.TaskVineExecutor*: This executor uses TaskVine as the execution backend. TaskVine scales up to tens of thousands of cores and actively uses local storage on compute nodes to offer a diverse array of performance-oriented features, including: smart caching and sharing common large files between tasks and compute nodes, reliable execution of tasks, dynamic resource sizing, automatic Python environment detection and sharing. These executors cover a broad range of execution requirements. As with other Parsl components, there is a standard interface (ParslExecutor) that can be implemented to add support for other executors.

Note: Refer to Configuration for information on how to configure these executors.

# Launchers

Many LRMs offer mechanisms for spawning applications across nodes inside a single job and for specifying the resources and task placement information needed to execute that application at launch time. Common mechanisms include srun (for Slurm), aprun (for Crays), and mpirun (for MPI). Thus, to run Parsl programs on such systems, we typically want first to request a large number of nodes and then to *launch* "pilot job" or **worker** processes using the system launchers. Parsl's Launcher abstraction enables Parsl programs to use these system-specific launcher systems to start workers across cores and nodes.

Parsl currently supports the following set of launchers:

- 1. pars1.launchers.SrunLauncher: Srun based launcher for Slurm based systems.
- 2. pars1.launchers.AprunLauncher: Aprun based launcher for Crays.
- 3. pars1.launchers.SrunMPILauncher: Launcher for launching MPI applications with Srun.

- 4. *pars1.launchers.GnuParallelLauncher*: Launcher using GNU parallel to launch workers across nodes and cores.
- 5. parsl.launchers.MpiExecLauncher: Uses Mpiexec to launch.
- 6. pars1.launchers.SimpleLauncher: The launcher default to a single worker launch.
- 7. parsl.launchers.SingleNodeLauncher: This launcher launches workers\_per\_node count workers on a single node.

Additionally, the launcher interface can be used to implement specialized behaviors in custom environments (for example, to launch node processes inside containers with customized environments). For example, the following launcher uses Srun to launch worker-wrapper, passing the command to be run as parameters to worker-wrapper. It is the responsibility of worker-wrapper to launch the command it is given inside the appropriate environment.

```
class MyShifterSRunLauncher:
    def __init__(self):
        self.srun_launcher = SrunLauncher()
    def __call__(self, command, tasks_per_node, nodes_per_block):
        new_command="worker-wrapper {}".format(command)
        return self.srun_launcher(new_command, tasks_per_node, nodes_per_block)
```

## **Blocks**

One challenge when making use of heterogeneous execution resource types is the need to provide a uniform representation of resources. Consider that single requests on clouds return individual nodes, clusters and supercomputers provide batches of nodes, grids provide cores, and workstations provide a single multicore node

Parsl defines a resource abstraction called a *block* as the most basic unit of resources to be acquired from a provider. A block contains one or more nodes and maps to the different provider abstractions. In a cluster, a block corresponds to a single allocation request to a scheduler. In a cloud, a block corresponds to a single API request for one or more instances. Parsl can then execute *tasks* (instances of apps) within and across (e.g., for MPI jobs) nodes within a block. Blocks are also used as the basis for elasticity on batch scheduling systems (see Elasticity below). Three different examples of block configurations are shown below.

1. A single block comprised of a node executing one task:



2. A single block with one node executing several tasks. This configuration is most suitable for single threaded apps running on multicore target systems. The number of tasks executed concurrently is proportional to the number

of cores available on the system.



3. A block comprised of several nodes and executing several tasks, where a task can span multiple nodes. This configuration is generally used by MPI applications. Starting a task requires using a specific MPI launcher that is supported on the target system (e.g., aprun, srun, mpirun, mpiexec). The MPI Apps documentation page describes how to configure Parsl for this case.



The configuration options for specifying the shape of each block are:

- 1. workers\_per\_node: Number of workers started per node, which corresponds to the number of tasks that can execute concurrently on a node.
- 2. nodes\_per\_block: Number of nodes requested per block.

### Elasticity

Workload resource requirements often vary over time. For example, in the map-reduce paradigm the map phase may require more resources than the reduce phase. In general, reserving sufficient resources for the widest parallelism will result in underutilization during periods of lower load; conversely, reserving minimal resources for the thinnest parallelism will lead to optimal utilization but also extended execution time. Even simple bag-of-task applications may have tasks of different durations, leading to trailing tasks with a thin workload.

To address dynamic workload requirements, Parsl implements a cloud-like elasticity model in which resource blocks are provisioned/deprovisioned in response to workload pressure. Given the general nature of the implementation, Parsl can provide elastic execution on clouds, clusters, and supercomputers. Of course, in an HPC setting, elasticity may be complicated by queue delays.

Parsl's elasticity model includes a flow control system that monitors outstanding tasks and available compute capacity. This flow control monitor determines when to trigger scaling (in or out) events to match workload needs.

The animated diagram below shows how blocks are elastically managed within an executor. The Parsl configuration for an executor defines the minimum, maximum, and initial number of blocks to be used.

The configuration options for specifying elasticity bounds are:

- 1. min\_blocks: Minimum number of blocks to maintain per executor.
- 2. init\_blocks: Initial number of blocks to provision at initialization of workflow.
- 3. max\_blocks: Maximum number of blocks that can be active per executor.

#### Parallelism

Parsl provides a user-managed model for controlling elasticity. In addition to setting the minimum and maximum number of blocks to be provisioned, users can also define the desired level of parallelism by setting a parameter (p). Parallelism is expressed as the ratio of task execution capacity to the sum of running tasks and available tasks (tasks with their dependencies met, but waiting for execution). A parallelism value of 1 represents aggressive scaling where the maximum resources needed are used (i.e., max\_blocks); parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used. By selecting a fraction between 0 and 1, the provisioning aggressiveness can be controlled.

For example:

• When p = 0: Use the fewest resources possible. If there is no workload then no blocks will be provisioned, otherwise the fewest blocks specified (e.g., min\_blocks, or 1 if min\_blocks is set to 0) will be provisioned.

```
if active_tasks == 0:
    blocks = min_blocks
else:
    blocks = max(min_blocks, 1)
```

• When p = 1: Use as many resources as possible. Provision sufficient nodes to execute all running and available tasks concurrently up to the max\_blocks specified.

• When p = 1/2: Queue up to 2 tasks per worker before requesting a new block.

# Configuration

The example below shows how elasticity and parallelism can be configured. Here, a *parsl.executors*. *HighThroughputExecutor* is used with a minimum of 1 block and a maximum of 2 blocks, where each block may host up to 2 workers per node. Thus this setup is capable of servicing 2 tasks concurrently. Parallelism of 0.5 means that when more than 2 \* the total task capacity (i.e., 4 tasks) are queued a new block will be requested. An example *Config* is:

```
from parsl.config import Config
from libsubmit.providers.local.local import Local
from parsl.executors import HighThroughputExecutor
config = Config(
    executors=[
        HighThroughputExecutor(
            label='local_htex',
            workers_per_node=2,
            provider=Local(
                min_blocks=1,
                init_blocks=1,
                max_blocks=2,
                nodes_per_block=1,
                parallelism=0.5
            )
        )
    ]
```

)

The animated diagram below illustrates the behavior of this executor. In the diagram, the tasks are allocated to the first block, until 5 tasks are submitted. At this stage, as more than double the available task capacity is used, Parsl provisions a new block for executing the remaining tasks.

# **Multi-executor**

Parsl supports the use of one or more executors as specified in the configuration. In this situation, individual apps may indicate which executors they are able to use.

The common scenarios for this feature are:

- A workflow has an initial simulation stage that runs on the compute heavy nodes of an HPC system followed by an analysis and visualization stage that is better suited for GPU nodes.
- A workflow follows a repeated fan-out, fan-in model where the long running fan-out tasks are computed on a cluster and the quick fan-in computation is better suited for execution using threads on a login node.
- A workflow includes apps that wait and evaluate the results of a computation to determine whether the app should be relaunched. Only apps running on threads may launch other apps. Often, simulations have stochastic behavior and may terminate before completion. In such cases, having a wrapper app that checks the exit code and determines whether or not the app has completed successfully can be used to automatically re-execute the app (possibly from a checkpoint) until successful completion.

The following code snippet shows how apps can specify suitable executors in the app decorator.

```
#(CPU heavy app) (CPU heavy app) (CPU heavy app) <--- Run on compute queue
#
       1
                       #
     (data)
                      (data)
                                      (data)
#
                      1
                                      /
        #
        (Analysis and visualization phase)
                                                <--- Run on GPU node
# A mock molecular dynamics simulation app
@bash_app(executors=["Theta.Phi"])
def MD_Sim(arg, outputs=()):
   return "MD_simulate {} -o {}".format(arg, outputs[0])
# Visualize results from the mock MD simulation app
@bash_app(executors=["Cooley.GPU"])
def visualize(inputs=(), outputs=()):
   bash_array = " ".join(inputs)
   return "viz {} -o {}".format(bash_array, outputs[0])
```

# Encryption

Users can enable encryption for the HighThroughputExecutor by setting its encrypted initialization argument to True.

For example,

```
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
config = Config(
    executors=[
    HighThroughputExecutor(
        encrypted=True
    )
  ]
)
```

Under the hood, we use CurveZMQ to encrypt all communication channels between the executor and related nodes.

## **Encryption performance**

CurveZMQ depends on libzmq and libsodium, which pyzmq (a Parsl dependency) includes as part of its installation via pip. This installation path should work on most systems, but users have reported significant performance degradation as a result.

If you experience a significant performance hit after enabling encryption, we recommend installing pyzmq with conda:

```
conda install conda-forge::pyzmq
```

Alternatively, you can install libsodium, then install libzmq, then build pyzmq from source:

```
pip3 install parsl --no-binary pyzmq
```

# **MPI Apps**

MPI applications run multiple copies of a program that complete a single task by coordinating using messages passed within or across nodes. Starting MPI application requires invoking a "launcher" code (e.g., mpiexec) from one node with options that define how the copies of a program should be distributed to others. Parsl simplifies this by composing the "launcher" command from the resources specified at the time each app is invoked.

The broad strokes of a complete solution involves the following components:

- 1. Configuring the *HighThroughputExecutor* with: enable\_mpi\_mode=True
- 2. Specify an MPI Launcher from one of the supported launchers ("aprun", "srun", "mpiexec") for the *HighThroughputExecutor* with: mpi\_launcher="srun"
- 3. Specify the provider that matches your cluster, (eg. user SlurmProvider for Slurm clusters)
- 4. Set the non-mpi launcher to SingleNodeLauncher
- 5. Specify resources required by the application via resource\_specification as shown below:

```
# Define HighThroughputExecutor(enable_mpi_mode=True, mpi_launcher="mpiexec", ...)
@bash_app
def lammps_mpi_application(infile: File, parsl_resource_specification: Dict):
    # PARSL_MPI_PREFIX will resolve to `mpiexec -n 4 -ppn 2 -hosts NODE001,NODE002`
    return f"$PARSL_MPI_PREFIX lmp_mpi -in {infile.filepath}"
# Resources in terms of nodes and how ranks are to be distributed are set on a per app
# basis via the resource_spec dictionary.
resource_spec = {
    "num_nodes" = 2,
    "ranks_per_node" = 2,
    "num_ranks" = 4,
}
future = lammps_mpi_application(File('in.file'), resource_specification=resource_spec)
```

# **HTEX and MPI Tasks**

The *HighThroughputExecutor* (HTEX) is the default executor available through Parsl. Parsl Apps which invoke MPI code require MPI specific configuration such that:

- 1. All workers are started on the lead-node (mom-node in case of Crays)
- 2. Resource requirements of Apps are propagated to workers who provision the required number of nodes from within the batch job.

# **Configuring the Provider**

Parsl must be configured to deploy workers on exactly one node per block. This part is simple. Instead of defining a launcher which will place an executor on each node in the block, simply use the *SingleNodeLauncher*. The MPI Launcher that the application will use is to be specified via HighThroughputExecutor(mpi\_launcher="LAUNCHER")

It is also necessary to specify the desired number of blocks for the executor. Parsl cannot determine the number of blocks needed to run a set of MPI Tasks, so they must bet set explicitly (see Issue #1647). The easiest route is to set the max\_blocks and min\_blocks of the provider to the desired number of blocks.

# **Configuring the Executor**

Here are the steps for configuring the executor:

- 1. Set HighThroughputExecutor(enable\_mpi\_mode=True)
- 2. Set HighThroughputExecutor(mpi\_launcher="LAUNCHER") to one from ("srun", "aprun", "mpiexec")
- 3. Set the max\_workers to the number of MPI Apps you expect to run per scheduler job (block).
- 4. Set cores\_per\_worker=1e-6 to prevent HTEx from reducing the number of workers if you request more workers than cores.

### **Example Configuration**

Here's an example configuration which runs MPI tasks on ALCF's Polaris Supercomputer

```
import parsl
from typing import Dict
from parsl.config import Config
# PBSPro is the right provider for Polaris:
from parsl.providers import PBSProProvider
# The high throughput executor is for scaling to HPC systems:
from parsl.executors import HighThroughputExecutor
# address_by_interface is needed for the HighThroughputExecutor:
from parsl.addresses import address_by_interface
# For checkpointing:
from parsl.utils import get_all_checkpoints
# Adjust your user-specific options here:
# run_dir="/lus/grand/projects/yourproject/yourrundir/"
user_opts = {
    "worker_init": "module load conda; conda activate parsl_mpi_py310",
    "scheduler_options":"#PBS -1 filesystems=home:eagle:grand\n#PBS -1 place=scatter" ,
   "account": SET_YOUR_ALCF_ALLOCATION_HERE,
    "queue": "debug-scaling",
    "walltime": "1:00:00",
    "nodes_per_block": 8,
   "available_accelerators": 4, # Each Polaris node has 4 GPUs, setting this ensures_
\rightarrow one worker per GPU
```

```
"cores_per_worker": 8, # this will set the number of cpu hardware threads per worker.
}
config = Config(
        executors=[
            HighThroughputExecutor(
                label="htex",
                enable_mpi_mode=True,
                mpi_launcher="mpiexec",
                cores_per_worker=user_opts["cores_per_worker"],
                address=address_by_interface("bond0"),
                provider=PBSProProvider(
                    account=user_opts["account"],
                    queue=user_opts["queue"],
                    # PBS directives (header lines): for array jobs pass '-J' option
                    scheduler_options=user_opts["scheduler_options"],
                    # Command to be run before starting a worker, such as:
                    worker_init=user_opts["worker_init"],
                    # number of compute nodes allocated for each block
                    nodes_per_block=user_opts["nodes_per_block"],
                    init_blocks=1,
                    min_blocks=0,
                    max_blocks=1, # Can increase more to have more parallel jobs
                    walltime=user_opts["walltime"]
                ),
            ),
        ],
```

### Writing MPI-Compatible Apps

In MPI mode, the *HighThroughputExecutor* can execute both Python or Bash Apps which invokes the MPI application. However, it is important to note that Python Apps that directly use mpi4py is not supported.

For multi-node MPI applications, especially when running multiple applications within a single batch job, it is important to specify the resource requirements for the app so that the Parsl worker can provision the appropriate resources before the application starts. For eg, your Parsl script might contain a molecular dynamics application that requires 8 ranks over 1 node for certain inputs and 32 ranks over 4 nodes for some depending on the size of the molecules being simulated. By specifying resources via resource\_specification, parsl workers will provision the requested resources and then compose MPI launch command prefixes (Eg: mpiexec -n <ranks> -ppn <ranks\_per\_node> -hosts <node1. .nodeN>). These launch command prefixes are shared with the app via environment variables.

```
→specification: Dict):
    total_ranks = os.environ("")
    return f'aprun -N $PARSL_RANKS_PER_NODE -n {total_ranks} /bin/hostname'
```

All valid key-value pairs set in the resource\_specification are exported to the application via env vars, for eg. parsl\_resource\_specification = {'RANKS\_PER\_NODE': 4} `` will set the env var ``PARSL\_RANKS\_PER\_NODE

However, the following options are required for MPI applications :

When the above are supplied, the following launch command prefixes are set:

PARSL\_MPIEXEC\_PREFIX: mpiexec launch command which works for a large number of batch. →systems especially PBS systems PARSL\_SRUN\_PREFIX: srun launch command for Slurm based clusters PARSL\_APRUN\_PREFIX: aprun launch command prefix for some Cray machines PARSL\_MPI\_PREFIX: Parsl sets the MPI prefix to match the mpi\_launcher specified to. →`HighThroughputExecutor` PARSL\_MPI\_NODELIST: List of assigned nodes separated by commas (Eg, NODE1,NODE2) PARSL\_WORKER\_POOL\_ID: Alphanumeric string identifier for the worker pool PARSL\_WORKER\_BLOCK\_ID: Batch job ID that the worker belongs to

### Example Application: CosmicTagger

TODO: Blurb about what CosmicTagger does CosmicTagger implements models and training utilities to train convolutional networks to separate cosmic pixels, background pixels, and neutrino pixels in a neutrinos dataset. There are several variations. A detailed description of the code can be found in:

Cosmic Background Removal with Deep Neural Networks in SBND

Cosmic Background Removal with Deep Neural Networks in SBND This network is implemented in both PyTorch and TensorFlow. To select between the networks, you can use the –framework parameter. It accepts either tensorflow or torch. The model is available in a development version with sparse convolutions in the torch framework.

This example is broken down into three components. First, configure the Executor for Polaris at ALCF. The configuration will use the *PBSProProvider* to connect to the batch scheduler. With the goal of running MPI applications, we set the

```
import parsl
from typing import Dict
from parsl.config import Config
# PBSPro is the right provider for Polaris:
```

```
from parsl.providers import PBSProProvider
# The high throughput executor is for scaling to HPC systems:
from parsl.executors import HighThroughputExecutor
# address_by_interface is needed for the HighThroughputExecutor:
from parsl.addresses import address_by_interface
user_opts = {
    # Make sure to setup a conda environment before using this config
    "worker_init": "module load conda; conda activate parsl_mpi_py310",
    "scheduler_options":"#PBS -1 filesystems=home:eagle:grand\n#PBS -1 place=scatter" ,
    "account": <SET_YOUR_ALLOCATION>,
    "queue": "debug-scaling",
    "walltime": "1:00:00",
    "nodes_per_block": 8,
   "available_accelerators": 4, # Each Polaris node has 4 GPUs, setting this ensures
→one worker per GPU
    "cores_per_worker": 8, # this will set the number of cpu hardware threads per worker.
}
config = Config(
        executors=[
            HighThroughputExecutor(
                label="htex",
                enable_mpi_mode=True,
                mpi_launcher="mpiexec",
                cores_per_worker=user_opts["cores_per_worker"],
                address=address_by_interface("bond0"),
                provider=PBSProProvider(
                    account=user_opts["account"],
                    queue=user_opts["queue"],
                    # PBS directives (header lines): for array jobs pass '-J' option
                    scheduler_options=user_opts["scheduler_options"],
                    # Command to be run before starting a worker, such as:
                    worker_init=user_opts["worker_init"],
                    # number of compute nodes allocated for each block
                    nodes_per_block=user_opts["nodes_per_block"],
                    init_blocks=1,
                    min_blocks=0.
                    max_blocks=1, # Can increase more to have more parallel jobs
                    walltime=user_opts["walltime"]
                ),
           ),
       ],
)
```

Next we define the CosmicTagger MPI application. TODO: Ask Khalid for help.

```
(continued from previous page)
```

```
iterations: int = 500,
                  trial: int = 2,
                  stdout=parsl.AUTO_LOGNAME,
                  stderr=parsl.AUTO_LOGNAME,
                  parsl_resource_specification:Dict={}):
   NRANKS = parsl_resource_specification['num_ranks']
   return f"""
   module purge
   module use /soft/modulefiles/
   module load conda/2023-10-04
   conda activate
   echo "PARSL_MPI_PREFIX : $PARSL_MPI_PREFIX"
   $PARSL_MPI_PREFIX --cpu-bind numa \
       python {workdir}/bin/exec.py --config-name a21 \
            run.id=run_plrs_ParslDemo_g$ {NRANKS }_ {datatype }_b {batchsize }_{ framework }_i
\rightarrow {iterations}_T{trial} \
            run.compute_mode=GPU \
            run.distributed=True \
            framework={framework} \
            run.minibatch_size={batchsize} \
            run.precision={datatype} \
            mode.optimizer.loss_balance_scheme=light \
            run.iterations={iterations}
   .....
```

In this example, we run a simple test that does an exploration over the batchsize parameter while launching the application over 2-4 nodes.

```
def run_cosmic_tagger():
   futures = {}
    for num_nodes in [2, 4]:
        for batchsize in [2, 4, 8]:
            parsl_res_spec = {"num_nodes": num_nodes,
                              "num_tasks": num_nodes * 4,
                              "ranks_per_node": 4}
            future = cosmic_tagger(workdir="/home/yadunand/CosmicTagger",
                                   datatype="float32",
                                   batchsize=str(batchsize),
                                   parsl_resource_specification=parsl_res_spec)
            print(f"Stdout : {future.stdout}")
            print(f"Stderr : {future.stderr}")
            futures[(num_nodes, batchsize)] = future
    for key in futures:
        print(f"Got result for {key}: {futures[key].result()}")
```

run\_cosmic\_tagger()

#### Limitations

Support for MPI tasks in HTEX is limited. It is designed for running many multi-node MPI applications within a single batch job.

- 1. MPI tasks may not span across nodes from more than one block.
- 2. Parsl does not correctly determine the number of execution slots per block (Issue #1647)
- 3. The executor uses a Python process per task, which can use a lot of memory (Issue #2264)

#### **Error handling**

Parsl provides various mechanisms to add resiliency and robustness to programs.

#### Exceptions

Parsl is designed to capture, track, and handle various errors occurring during execution, including those related to the program, apps, execution environment, and Parsl itself. It also provides functionality to appropriately respond to failures during execution.

Failures might occur for various reasons:

- 1. A task failed during execution.
- 2. A task failed to launch, for example, because an input dependency was not met.
- 3. There was a formatting error while formatting the command-line string in Bash apps.
- 4. A task completed execution but failed to produce one or more of its specified outputs.
- 5. Task exceeded the specified walltime.

Since Parsl tasks are executed asynchronously and remotely, it can be difficult to determine when errors have occurred and to appropriately handle them in a Parsl program.

For errors occurring in Python code, Parsl captures Python exceptions and returns them to the main Parsl program. For non-Python errors, for example when a node or worker fails, Parsl imposes a timeout, and considers a task to have failed if it has not heard from the task by that timeout. Parsl also considers a task to have failed if it does not meet the contract stated by the user during invocation, such as failing to produce the stated output files.

Parsl communicates these errors by associating Python exceptions with task futures. These exceptions are raised only when a result is called on the future of a failed task. For example:

```
@python_app
def bad_divide(x):
    return 6 / x
# Call bad divide with 0, to cause a divide by zero exception
doubled_x = bad_divide(0)
```

```
# Catch and handle the exception.
try:
    doubled_x.result()
except ZeroDivisionError as e:
    print('Oops! You tried to divide by 0.')
except Exception as e:
    print('Oops! Something really bad happened.')
```

#### **Retries**

Often errors in distributed/parallel environments are transient. In these cases, retrying failed tasks can be a simple way of overcoming transient (e.g., machine failure, network failure) and intermittent failures. When retries are enabled (and set to an integer > 0), Parsl will automatically re-launch tasks that have failed until the retry limit is reached. By default, retries are disabled and exceptions will be communicated to the Parsl program.

The following example shows how the number of retries can be set to 2:

```
import pars1
from pars1.configs.htex_local import config
config.retries = 2
pars1.load(config)
```

More specific retry handling can be specified using retry handlers, documented below.

### Lazy fail

Parsl implements a lazy failure model through which a workload will continue to execute in the case that some tasks fail. That is, the program will not halt as soon as it encounters a failure, rather it will continue to execute unaffected apps.

The following example shows how lazy failures affect execution. In this case, task C fails and therefore tasks E and F that depend on results from C cannot be executed; however, Parsl will continue to execute tasks B and D as they are unaffected by task C's failure.

```
Here's a workflow graph, where
     (X) is runnable.
     [X] is completed,
     (X*) is failed.
     (!X) is dependency failed
  (A)
                  [A]
                                 (A)
  / 
                 / 
                                 / 
(B) (C)
               [B] (C*)
                               [B] (C*)
    =>
                   =>
 (D) (E)
                               [D] (!E)
               (D) (E)
  \backslash /
                                 \backslash /
                 \setminus /
  (F)
                 (F)
                                 (!F)
  time ---->
```

# **Retry handlers**

The basic parsl retry mechanism keeps a count of the number of times a task has been (re)tried, and will continue retrying that task until the configured retry limit is reached.

Retry handlers generalize this to allow more expressive retry handling: parsl keeps a retry cost for a task, and the task will be retried until the configured retry limit is reached. Instead of the cost being 1 for each failure, user-supplied code can examine the failure and compute a custom cost.

This allows user knowledge about failures to influence the retry mechanism: an exception which is almost definitely a non-recoverable failure (for example, due to bad parameters) can be given a high retry cost (so that it will not be retried many times, or at all), and exceptions which are likely to be transient (for example, where a worker node has died) can be given a low retry cost so they will be retried many times.

A retry handler can be specified in the parsl configuration like this:

```
Config(
    retries=2,
    retry_handler=example_retry_handler
)
```

**example\_retry\_handler** should be a function defined by the user that will compute the retry cost for a particular failure, given some information about the failure.

For example, the following handler will give a cost of 1 to all exceptions, except when a bash app exits with unix exitcode 9, in which case the cost will be 100. This will have the effect that retries will happen as normal for most errors, but the bash app can indicate that there is little point in retrying by exiting with exitcode 9.

```
def example_retry_handler(exception, task_record):
    if isinstance(exception, BashExitFailure) and exception.exitcode == 9:
        return 100
    else
        return 1
```

The retry handler is given two parameters: the exception from execution, and the parsl internal task\_record. The task record contains details such as the app name, parameters and executor.

If a retry handler raises an exception itself, then the task will be aborted and no further tries will be attempted.

# Memoization and checkpointing

When an app is invoked several times with the same parameters, Parsl can reuse the result from the first invocation without executing the app again.

This can save time and computational resources.

This is done in two ways:

- Firstly, *app caching* will allow reuse of results within the same run.
- Building on top of that, *checkpointing* will store results on the filesystem and reuse those results in later runs.

# App caching

There are many situations in which a program may be re-executed over time. Often, large fragments of the program will not have changed and therefore, re-execution of apps will waste valuable time and computation resources. Parsl's app caching solves this problem by storing results from apps that have successfully completed so that they can be re-used.

App caching is enabled by setting the cache argument in the *python\_app()* or *bash\_app()* decorator to True (by default it is False).

```
@bash_app(cache=True)
def hello (msg, stdout=None):
    return 'echo {}'.format(msg)
```

App caching can be globally disabled by setting app\_cache=False in the Config.

App caching can be particularly useful when developing interactive programs such as when using a Jupyter notebook. In this case, cells containing apps are often re-executed during development. Using app caching will ensure that only modified apps are re-executed.

### App equivalence

Parsl determines app equivalence by storing the hash of the app function. Thus, any changes to the app code (e.g., its signature, its body, or even the docstring within the body) will invalidate cached values.

However, Parsl does not traverse the call graph of the app function, so changes inside functions called by an app will not invalidate cached values.

#### Invocation equivalence

Two app invocations are determined to be equivalent if their input arguments are identical.

In simple cases, this follows obvious rules:

```
# these two app invocations are the same and the second invocation will
# reuse any cached input from the first invocation
x = 7
f(x).result()
y = 7
f(y).result()
```

Internally, equivalence is determined by hashing the input arguments, and comparing the hash to hashes from previous app executions.

This approach can only be applied to data types for which a deterministic hash can be computed.

By default Parsl can compute sensible hashes for basic data types: str, int, float, None, as well as more some complex types: functions, and dictionaries and lists containing hashable types.

Attempting to cache apps invoked with other, non-hashable, data types will lead to an exception at invocation.

In that case, mechanisms to hash new types can be registered by a program by implementing the parsl.dataflow. memoization.id\_for\_memo function for the new type.

### Ignoring arguments

On occasion one may wish to ignore particular arguments when determining app invocation equivalence - for example, when generating log file names automatically based on time or run information. Parsl allows developers to list the arguments to be ignored in the ignore\_for\_cache app decorator parameter:

```
@bash_app(cache=True, ignore_for_cache=['stdout'])
def hello (msg, stdout=None):
    return 'echo {}'.format(msg)
```

#### Caveats

It is important to consider several important issues when using app caching:

- Determinism: App caching is generally useful only when the apps are deterministic. If the outputs may be different for identical inputs, app caching will obscure this non-deterministic behavior. For instance, caching an app that returns a random number will result in every invocation returning the same result.
- Timing: If several identical calls to an app are made concurrently having not yet cached a result, many instances of the app will be launched. Once one invocation completes and the result is cached all subsequent calls will return immediately with the cached result.
- Performance: If app caching is enabled, there may be some performance overhead especially if a large number of short duration tasks are launched rapidly. This overhead has not been quantified.

#### Checkpointing

Large-scale Parsl programs are likely to encounter errors due to node failures, application or environment errors, and myriad other issues. Parsl offers an application-level checkpointing model to improve resilience, fault tolerance, and efficiency.

**Note:** Checkpointing builds on top of app caching, and so app caching must be enabled. If app caching is disabled in the config Config.app\_cache, checkpointing will not work.

Parsl follows an incremental checkpointing model, where each checkpoint file contains all results that have been updated since the last checkpoint.

When a Parsl program loads a checkpoint file and is executed, it will use checkpointed results for any apps that have been previously executed. Like app caching, checkpoints use the hash of the app and the invocation input parameters to identify previously computed results. If multiple checkpoints exist for an app (with the same hash) the most recent entry will be used.

Parsl provides four checkpointing modes:

1. task\_exit: a checkpoint is created each time an app completes or fails (after retries if enabled). This mode minimizes the risk of losing information from completed tasks.

```
from parsl.configs.local_threads import config
config.checkpoint_mode = 'task_exit'
```

2. periodic: a checkpoint is created periodically using a user-specified checkpointing interval. Results will be saved to the checkpoint file for all tasks that have completed during this period.

```
from parsl.configs.local_threads import config
config.checkpoint_mode = 'periodic'
config.checkpoint_period = "01:00:00"
```

 dfk\_exit: checkpoints are created when Parsl is about to exit. This reduces the risk of losing results due to premature program termination from exceptions, terminate signals, etc. However it is still possible that information might be lost if the program is terminated abruptly (machine failure, SIGKILL, etc.)

```
from parsl.configs.local_threads import config
config.checkpoint_mode = 'dfk_exit'
```

4. manual: in addition to these automated checkpointing modes, it is also possible to manually initiate a checkpoint by calling DataFlowKernel.checkpoint() in the Parsl program code.

```
import parsl
from parsl.configs.local_threads import config
dfk = parsl.load(config)
....
dfk.checkpoint()
```

In all cases the checkpoint file is written out to the runinfo/RUN\_ID/checkpoint/ directory.

**Note:** Checkpoint modes **periodic**, **dfk\_exit**, and **manual** can interfere with garbage collection. In these modes task information will be retained after completion, until checkpointing events are triggered.

#### Creating a checkpoint

Automated checkpointing must be explicitly enabled in the Parsl configuration. There is no need to modify a Parsl program as checkpointing will occur transparently. In the following example, checkpointing is enabled at task exit. The results of each invocation of the slow\_double app will be stored in the checkpoint file.

```
import pars1
from pars1.app.app import python_app
from pars1.configs.local_threads import config
config.checkpoint_mode = 'task_exit'
pars1.load(config)
@python_app(cache=True)
def slow_double(x):
    import time
    time.sleep(5)
    return x * 2
d = []
for i in range(5):
    d.append(slow_double(i))
print([d[i].result() for i in range(5)])
```

Alternatively, manual checkpointing can be used to explicitly specify when the checkpoint file should be saved. The following example shows how manual checkpointing can be used. Here, the dfk.checkpoint() function will save the results of the prior invocations of the slow\_double app.

```
import parsl
from parsl import python_app
from parsl.configs.local_threads import config
dfk = parsl.load(config)
@python_app(cache=True)
def slow_double(x, sleep_dur=1):
   import time
    time.sleep(sleep_dur)
   return x * 2
N = 5
       # Number of calls to slow double
d = [] # List to store the futures
for i in range(0, N):
   d.append(slow_double(i))
# Wait for the results
[i.result() for i in d]
cpt_dir = dfk.checkpoint()
print(cpt_dir) # Prints the checkpoint dir
```

### **Resuming from a checkpoint**

When resuming a program from a checkpoint Parsl allows the user to select which checkpoint file(s) to use. Checkpoint files are stored in the runinfo/RUNID/checkpoint directory.

The example below shows how to resume using all available checkpoints. Here, the program re-executes the same calls to the slow\_double app as above and instead of waiting for results to be computed, the values from the checkpoint file are are immediately returned.

## Configuration

Parsl separates program logic from execution configuration, enabling programs to be developed entirely independently from their execution environment. Configuration is described by a Python object (*Config*) so that developers can introspect permissible options, validate settings, and retrieve/edit configurations dynamically during execution. A configuration object specifies details of the provider, executors, connection channel, allocation size, queues, durations, and data management options.

The following example shows a basic configuration object (*Config*) for the Frontera supercomputer at TACC. This config uses the *pars1.executors.HighThroughputExecutor* to submit tasks from a login node (*pars1.channels. LocalChannel*). It requests an allocation of 128 nodes, deploying 1 worker for each of the 56 cores per node, from the normal partition. To limit network connections to just the internal network the config specifies the address used by the infiniband interface with address\_by\_interface('ib0')

```
from parsl.config import Config
from parsl.channels import LocalChannel
from parsl.providers import SlurmProvider
from parsl.executors import HighThroughputExecutor
from parsl.launchers import SrunLauncher
from parsl.addresses import address_by_interface
config = Config(
   executors=[
        HighThroughputExecutor(
            label="frontera_htex",
            address=address_by_interface('ib0'),
            max_workers_per_node=56,
            provider=SlurmProvider(
                channel=LocalChannel(),
                nodes_per_block=128,
                init_blocks=1,
                partition='normal'.
                launcher=SrunLauncher(),
            ),
        )
   ],
)
```

#### **Configuration How-To and Examples:**

- Configuration
  - Creating and Using Config Objects
  - How to Configure
  - Heterogeneous Resources
  - Accelerators
  - Multi-Threaded Applications
  - Ad-Hoc Clusters
  - Amazon Web Services
  - ASPIRE 1 (NSCC)

- Illinois Campus Cluster (UIUC)
- Bridges (PSC)
- CC-IN2P3
- CCL (Notre Dame, TaskVine)
- Expanse (SDSC)
- Perlmutter (NERSC)
- Frontera (TACC)
- Kubernetes Clusters
- Midway (RCC, UChicago)
- Open Science Grid
- Polaris (ALCF)
- Stampede2 (TACC)
- Summit (ORNL)
- TOSS3 (LLNL)
- Further help

### **Creating and Using Config Objects**

*Config* objects are loaded to define the "Data Flow Kernel" (DFK) that will manage tasks. All Parsl applications start by creating or importing a configuration then calling the load function.

```
from parsl.configs.htex_local import config
import parsl
with parsl.load(config):
```

The load statement can happen after Apps are defined but must occur before tasks are started. Loading the Config object within context manager like with is recommended for implicit cleaning of DFK on exiting the context manager

The *Config* object may not be used again after loaded. Consider a configuration function if the application will shut down and re-launch the DFK.

```
from parsl.config import Config
import parsl

def make_config() -> Config:
    return Config(...)

with parsl.load(make_config()):
    # Your workflow here
parsl.clear() # Stops Parsl
with parsl.load(make_config()): # Re-launches with a fresh configuration
    # Your workflow here
```

# How to Configure

**Note:** All configuration examples below must be customized for the user's allocation, Python environment, file system, etc.

The configuration specifies what, and how, resources are to be used for executing the Parsl program and its apps. It is important to carefully consider the needs of the Parsl program and its apps, and the characteristics of the compute resources, to determine an ideal configuration. Aspects to consider include: 1) where the Parsl apps will execute; 2) how many nodes will be used to execute the apps, and how long the apps will run; 3) should Parsl request multiple nodes in an individual scheduler job; and 4) where will the main Parsl program run and how will it communicate with the apps.

Stepping through the following question should help formulate a suitable configuration object.

1. Where should apps be executed?

Target	Executor	Provider
Laptop/Workstation	<ul> <li>parsl.executors. HighThroughputExecutor</li> <li>parsl.executors. ThreadPoolExecutor</li> <li>parsl.executors. WorkQueueExecutor</li> <li>parsl.executors. taskvine. TaskVineExecutor</li> </ul>	parsl.providers. LocalProvider
Amazon Web Services	• parsl.executors. HighThroughputExecutor	parsl.providers.AWSProvider
Google Cloud	• parsl.executors. HighThroughputExecutor	parsl.providers. GoogleCloudProvider
Slurm based system	<ul> <li>parsl.executors. HighThroughputExecutor</li> <li>parsl.executors. WorkQueueExecutor</li> <li>parsl.executors. taskvine. TaskVineExecutor</li> </ul>	parsl.providers. SlurmProvider
Torque/PBS based system	<ul> <li>parsl.executors. HighThroughputExecutor</li> <li>parsl.executors. WorkQueueExecutor</li> </ul>	parsl.providers. TorqueProvider
Cobalt based system	<ul> <li>parsl.executors. HighThroughputExecutor</li> <li>parsl.executors. WorkQueueExecutor</li> </ul>	parsl.providers. CobaltProvider
GridEngine based system	<ul> <li>parsl.executors. HighThroughputExecutor</li> <li>parsl.executors. WorkQueueExecutor</li> </ul>	parsl.providers. GridEngineProvider
Condor based cluster or grid	<ul> <li>parsl.executors. HighThroughputExecutor</li> <li>parsl.executors. WorkQueueExecutor</li> <li>parsl.executors. taskvine. TaskVineExecutor</li> </ul>	parsl.providers. CondorProvider
Kubernetes cluster	• parsl.executors. HighThroughputExecutor	parsl.providers. KubernetesProvider
04		Chapter 1. why use Parsi?

2. How many nodes will be used to execute the apps? What task durations are necessary to achieve good performance?

Executor	Number of Nodes <sup>0</sup>	Task duration for good performance
*parsl.executors. ThreadPoolExecutor	1 (Only local)	Any
parsl.executors. HighThroughputExecutor	<=2000	Task duration(s)/#nodes >= 0.01 longer tasks needed at higher scale
parsl.executors. WorkQueueExecutor	<=1000 <sup>+0</sup>	10s+
parsl.executors.taskvine. TaskVineExecutor	<=1000‡ <sup>0</sup>	10s+

3. Should Parsl request multiple nodes in an individual scheduler job? (Here the term block is equivalent to a single scheduler job.)

nodes_per_block = 1 Provider	Executor choice	Suitable Launchers
Systems that don't use Aprun	Any	<ul> <li>parsl.launchers. SingleNodeLauncher</li> <li>parsl.launchers. SimpleLauncher</li> </ul>
Aprun based systems	Any	• parsl.launchers. AprunLauncher

<sup>0</sup> Assuming 32 workers per node. If there are fewer workers launched per node, a larger number of nodes could be supported.

<sup>0</sup> The maximum number of nodes tested for the *pars1.executors.WorkQueueExecutor* is 10,000 GPU cores and 20,000 CPU cores.

<sup>0</sup> The maximum number of nodes tested for the *parsl.executors.taskvine.TaskVineExecutor* is 10,000 GPU cores and 20,000 CPU cores.

nodes_per_block > 1 Provider	Executor choice	Suitable Launchers
parsl.providers. TorqueProvider	Any	<ul> <li>parsl.launchers. AprunLauncher</li> <li>parsl.launchers. MpiExecLauncher</li> </ul>
parsl.providers. CobaltProvider	Any	• parsl.launchers. AprunLauncher
parsl.providers. SlurmProvider	Any	<ul> <li>parsl.launchers. SrunLauncher if native slurm</li> <li>parsl.launchers. AprunLauncher, otherwise</li> </ul>

**Note:** If using a Cray system, you most likely need to use the *pars1.launchers.AprunLauncher* to launch workers unless you are on a **native Slurm** system like *Perlmutter (NERSC)* 

4) Where will the main Parsl program run and how will it communicate with the apps?

Parsl program location	App execution target	Suitable channel
Laptop/Workstation	Laptop/Workstation	parsl.channels.LocalChannel
Laptop/Workstation	Cloud Resources	No channel is needed
Laptop/Workstation	Clusters with no 2FA	parsl.channels.SSHChannel
Laptop/Workstation	Clusters with 2FA	parsl.channels.SSHInteractiveLoginChannel
Login node	Cluster/Supercomputer	parsl.channels.LocalChannel

### Heterogeneous Resources

In some cases, it can be difficult to specify the resource requirements for running a workflow. For example, if the compute nodes a site provides are not uniform, there is no "correct" resource configuration; the amount of parallelism depends on which node (large or small) each job runs on. In addition, the software and filesystem setup can vary from node to node. A Condor cluster may not provide shared filesystem access at all, and may include nodes with a variety of Python versions and available libraries.

The *parsl.executors.WorkQueueExecutor* provides several features to work with heterogeneous resources. By default, Parsl only runs one app at a time on each worker node. However, it is possible to specify the requirements for a particular app, and Work Queue will automatically run as many parallel instances as possible on each node. Work Queue automatically detects the amount of cores, memory, and other resources available on each execution node. To activate this feature, add a resource specification to your apps. A resource specification is a dictionary with the following three keys: cores (an integer corresponding to the number of cores required by the task), memory (an integer corresponding to the task's memory requirement in MB), and disk (an integer corresponding to the task's disk requirement in MB), passed to an app via the special keyword argument parsl\_resource\_specification. The specification can be set for all app invocations via a default, for example:

or updated when the app is invoked:

```
spec = {'cores': 1, 'memory': 500, 'disk': 500}
future = compute(x, parsl_resource_specification=spec)
```

This parsl\_resource\_specification special keyword argument will inform Work Queue about the resources this app requires. When placing instances of compute(x), Work Queue will run as many parallel instances as possible based on each worker node's available resources.

If an app's resource requirements are not known in advance, Work Queue has an auto-labeling feature that measures the actual resource usage of your apps and automatically chooses resource labels for you. With auto-labeling, it is not necessary to provide parsl\_resource\_specification; Work Queue collects stats in the background and updates resource labels as your workflow runs. To activate this feature, add the following flags to your executor config:

```
config = Config(
    executors=[
        WorkQueueExecutor(
            # ...other options go here
            autolabel=True,
            autocategory=True
        )
    ]
)
```

The autolabel flag tells Work Queue to automatically generate resource labels. By default, these labels are shared across all apps in your workflow. The autocategory flag puts each app into a different category, so that Work Queue will choose separate resource requirements for each app. This is important if e.g. some of your apps use a single core and some apps require multiple cores. Unless you know that all apps have uniform resource requirements, you should turn on autocategory when using autolabel.

The Work Queue executor can also help deal with sites that have non-uniform software environments across nodes. Parsl assumes that the Parsl program and the compute nodes all use the same Python version. In addition, any packages your apps import must be available on compute nodes. If no shared filesystem is available or if node configuration varies, this can lead to difficult-to-trace execution problems.

If your Parsl program is running in a Conda environment, the Work Queue executor can automatically scan the imports in your apps, create a self-contained software package, transfer the software package to worker nodes, and run your code inside the packaged and uniform environment. First, make sure that the Conda environment is active and you have the required packages installed (via either pip or conda):

- python
- parsl
- ndcctools
- conda-pack

Then add the following to your config:

```
config = Config(
    executors=[
```

```
WorkQueueExecutor(
    # ...other options go here
    pack=True
)
]
)
```

**Note:** There will be a noticeable delay the first time Work Queue sees an app; it is creating and packaging a complete Python environment. This packaged environment is cached, so subsequent app invocations should be much faster.

Using this approach, it is possible to run Parsl applications on nodes that don't have Python available at all. The packaged environment includes a Python interpreter, and Work Queue does not require Python to run.

**Note:** The automatic packaging feature only supports packages installed via pip or conda. Importing from other locations (e.g. via \$PYTHONPATH) or importing other modules in the same directory is not supported.

### Accelerators

Many modern clusters provide multiple accelerators per compute note, yet many applications are best suited to using a single accelerator per task. Parsl supports pinning each worker to difference accelerators using available\_accelerators option of the *HighThroughputExecutor*. Provide either the number of executors (Parsl will assume they are named in integers starting from zero) or a list of the names of the accelerators available on the node.
#### **Multi-Threaded Applications**

Workflows which launch multiple workers on a single node which perform multi-threaded tasks (e.g., NumPy, Tensorflow operations) may run into thread contention issues. Each worker may try to use the same hardware threads, which leads to performance penalties. Use the cpu\_affinity feature of the *HighThroughputExecutor* to assign workers to specific threads. Users can pin threads to workers either with a strategy method or an explicit list.

The strategy methods will auto assign all detected hardware threads to workers. Allowed strategies that can be assigned to  $cpu_affinity$  are block, block-reverse, and alternating. The block method pins threads to workers in sequential order (ex: 4 threads are grouped (0, 1) and (2, 3) on two workers); block-reverse pins threads in reverse sequential order (ex: (3, 2) and (1, 0)); and alternating alternates threads among workers (ex: (0, 2) and (1, 3)).

Select the best blocking strategy for processor's cache hierarchy (choose alternating if in doubt) to ensure workers to not compete for cores.

```
local_config = Config(
    executors=[
        HighThroughputExecutor(
        label="htex_Local",
        worker_debug=True,
        cpu_affinity='alternating',
        provider=LocalProvider(
            channel=LocalChannel(),
            init_blocks=1,
            max_blocks=1,
            ),
        )
    ],
    strategy='none',
)
```

Users can also use cpu\_affinity to assign explicitly threads to workers with a string that has the format of cpu\_affinity="list:<worker1\_threads>:<worker2\_threads>:<worker3\_threads>".

Each worker's threads can be specified as a comma separated list or a hyphenated range: thread1, thread2, thread3 or thread\_start-thread\_end.

An example for 12 workers on a node with 208 threads is:

```
cpu_affinity="list:0-7,104-111:8-15,112-119:16-23,120-127:24-31,128-135:32-39,136-143:40-

→47,144-151:52-59,156-163:60-67,164-171:68-75,172-179:76-83,180-187:84-91,188-195:92-99,

→196-203"
```

This example assigns 16 threads each to 12 workers. Note that in this example there are threads that are skipped. If a thread is not explicitly assigned to a worker, it will be left idle. The number of thread "ranks" (colon separated thread lists/ranges) must match the total number of workers on the node; otherwise an exception will be raised.

Thread affinity is accomplished in two ways. Each worker first sets the affinity for the Python process using the affinity mask, which may not be available on all operating systems. It then sets environment variables to control OpenMP thread affinity so that any subprocesses launched by a worker which use OpenMP know which processors are valid. These include OMP\_NUM\_THREADS, GOMP\_COMP\_AFFINITY, and KMP\_THREAD\_AFFINITY.

#### **Ad-Hoc Clusters**

Any collection of compute nodes without a scheduler can be considered an ad-hoc cluster. Often these machines have a shared file system such as NFS or Lustre. In order to use these resources with Parsl, they need to set-up for password-less SSH access.

To use these ssh-accessible collection of nodes as an ad-hoc cluster, we use the *parsl.providers.AdHocProvider* with an *parsl.channels.SSHChannel* to each node. An example configuration follows.

```
from parsl.providers import AdHocProvider
from parsl.channels import SSHChannel
from parsl.executors import HighThroughputExecutor
from parsl.config import Config
from typing import Any, Dict
user_opts: Dict[str, Dict[str, Any]]
user_opts = {'adhoc':
             {'username': 'YOUR_USERNAME',
              'script_dir': 'YOUR_SCRIPT_DIR',
              'remote_hostnames': ['REMOTE_HOST_URL_1', 'REMOTE_HOST_URL_2']
              }
             }
config = Config(
    executors=[
        HighThroughputExecutor(
            label='remote_htex',
            max_workers_per_node=2,
            worker_logdir_root=user_opts['adhoc']['script_dir'],
            provider=AdHocProvider(
                # Command to be run before starting a worker, such as:
                # 'module load Anaconda; source activate parsl_env'.
                worker_init='',
                channels=[SSHChannel(hostname=m,
                                     username=user_opts['adhoc']['username'],
                                     script_dir=user_opts['adhoc']['script_dir'],
                                     ) for m in user_opts['adhoc']['remote_hostnames']]
            )
       )
   ],
    # AdHoc Clusters should not be setup with scaling strategy.
    strategy='none',
)
```

**Note:** Multiple blocks should not be assigned to each node when using the *parsl.executors*. *HighThroughputExecutor* 

#### **Amazon Web Services**



Note: To use AWS with Parsl, install Parsl with AWS dependencies via python3 -m pip install 'parsl[aws]'

Amazon Web Services is a commercial cloud service which allows users to rent a range of computers and other computing services. The following snippet shows how Parsl can be configured to provision nodes from the Elastic Compute Cloud (EC2) service. The first time this configuration is used, Parsl will configure a Virtual Private Cloud and other networking and security infrastructure that will be re-used in subsequent executions. The configuration uses the *parsl.providers.AWSProvider* to connect to AWS.

```
from parsl.config import Config
from parsl.providers import AWSProvider
from parsl.executors import HighThroughputExecutor
config = Config(
    executors=[
        HighThroughputExecutor(
            label='ec2_single_node',
            provider=AWSProvider(
                # Specify your EC2 AMI id
                'YOUR_AMI_ID',
                # Specify the AWS region to provision from
                # eg. us-east-1
                region='YOUR_AWS_REGION',
                # Specify the name of the key to allow ssh access to nodes
                key_name='YOUR_KEY_NAME',
                profile="default",
                state_file='awsproviderstate.json',
                nodes_per_block=1,
                init_blocks=1,
                max_blocks=1,
                min_blocks=0,
                walltime='01:00:00',
            ),
```

```
],
```

#### **ASPIRE 1 (NSCC)**

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The following snippet shows an example configuration for accessing NSCC's **ASPIRE 1** supercomputer. This example uses the *parsl.executors.HighThroughputExecutor* executor and connects to ASPIRE1's PBSPro scheduler. It also shows how scheduler\_options parameter could be used for scheduling array jobs in PBSPro.

```
from parsl.providers import PBSProProvider
from parsl.launchers import MpiRunLauncher
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.addresses import address_by_interface
from parsl.monitoring.monitoring import MonitoringHub
config = Config(
        executors=[
            HighThroughputExecutor(
                label="htex",
                heartbeat_period=15,
                heartbeat_threshold=120.
                worker_debug=True,
                max_workers_per_node=4,
                address_by_interface('ib0'),
                provider=PBSProProvider(
                    launcher=MpiRunLauncher(),
                    # PBS directives (header lines): for array jobs pass '-J' option
                    scheduler_options='#PBS -J 1-10',
                    # Command to be run before starting a worker, such as:
                    # 'module load Anaconda; source activate parsl_env'.
                    worker_init='',
                    # number of compute nodes allocated for each block
                    nodes_per_block=3,
                    min_blocks=3.
                    max_blocks=5,
                    cpus_per_node=24,
                    # medium queue has a max walltime of 24 hrs
                    walltime='24:00:00'
                ),
            ),
        ],
        monitoring=MonitoringHub(
            hub_address=address_by_interface('ib0'),
           hub_port=55055,
            resource_monitoring_interval=10,
        ),
        strategy='simple',
        retries=3,
        app_cache=True,
```

checkpoint\_mode='task\_exit'

#### Illinois Campus Cluster (UIUC)

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The following snippet shows an example configuration for executing on the Illinois Campus Cluster. The configuration assumes the user is running on a login node and uses the *parsl.providers.SlurmProvider* to interface with the scheduler, and uses the *parsl.launchers.SrunLauncher* to launch workers.

```
from parsl.config import Config
from parsl.providers import SlurmProvider
from parsl.executors import HighThroughputExecutor
from parsl.launchers import SrunLauncher
""" This config assumes that it is used to launch parsl tasks from the login nodes
of the Campus Cluster at UIUC. Each job submitted to the scheduler will request 2 nodes.
\rightarrow for 10 minutes.
.....
config = Config(
     executors=[
          HighThroughputExecutor(
               label="CC_htex",
               worker_debug=False,
               cores_per_worker=16.0, # each worker uses a full node
               provider=SlurmProvider(
                    partition='secondary-fdr', # partition
                    nodes_per_block=2, # number of nodes
                    init_blocks=1,
                    max_blocks=1,
                    scheduler_options='',
                    cmd_timeout=60,
                    walltime='00:10:00',
                    launcher=SrunLauncher(),
                    worker_init='conda activate envParsl', # requires conda environment_
\rightarrow with parsl
               ),
          )
     ],
)
```

#### **Bridges (PSC)**



The following snippet shows an example configuration for executing on the Bridges supercomputer at the Pittsburgh Supercomputing Center. The configuration assumes the user is running on a login node and uses the *parsl.providers*. *SlurmProvider* to interface with the scheduler, and uses the *parsl.launchers.SrunLauncher* to launch workers.

```
from parsl.config import Config
from parsl.providers import SlurmProvider
from parsl.launchers import SrunLauncher
from parsl.executors import HighThroughputExecutor
from parsl.addresses import address_by_interface
""" This config assumes that it is used to launch parsl tasks from the login nodes
of Bridges at PSC. Each job submitted to the scheduler will request 2 nodes for 10.
⇔minutes.
.....
config = Config(
    executors=[
        HighThroughputExecutor(
            label='Bridges_HTEX_multinode',
            address=address_by_interface('ens3f0'),
            max_workers_per_node=1,
            provider=SlurmProvider(
                'YOUR_PARTITION_NAME', # Specify Partition / QOS, for eg. RM-small
                nodes_per_block=2,
                init_blocks=1,
                # string to prepend to #SBATCH blocks in the submit
                # script to the scheduler eg: '#SBATCH --gres=gpu:type:n'
                scheduler_options='',
                # Command to be run before starting a worker, such as:
                # 'module load Anaconda; source activate parsl_env'.
                worker_init=''.
                # We request all hyperthreads on a node.
                launcher=SrunLauncher(),
                walltime='00:10:00',
```

```
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```

```
# Slurm scheduler on Cori can be slow at times,
# increase the command timeouts
cmd_timeout=120,
),
)
```

#### CC-IN2P3



The snippet below shows an example configuration for executing from a login node on IN2P3's Computing Centre. The configuration uses the *parsl.providers.LocalProvider* to run on a login node primarily to avoid GSISSH, which Parsl does not support yet. This system uses Grid Engine which Parsl interfaces with using the *parsl.providers.GridEngineProvider*.

```
from parsl.config import Config
from parsl.channels import LocalChannel
from parsl.providers import GridEngineProvider
from parsl.executors import HighThroughputExecutor
config = Config(
    executors=[
        HighThroughputExecutor(
            label='cc_in2p3_htex',
            max_workers_per_node=2,
            provider=GridEngineProvider(
                channel=LocalChannel(),
                nodes_per_block=1,
                init_blocks=2,
                max_blocks=2,
                walltime="00:20:00",
                scheduler_options='',
                                          # Input your scheduler_options if needed
                worker_init='',
                                   # Input your worker_init if needed
```

```
),
)
],
)
```

CCL (Notre Dame, TaskVine)



To utilize TaskVine with Parsl, please install the full CCTools software package within an appropriate Anaconda or Miniconda environment (instructions for installing Miniconda can be found in the Conda install guide):

```
$ conda create -y --name <environment> python=<version> conda-pack
$ conda activate <environment>
$ conda install -y -c conda-forge ndcctools parsl
```

This creates a Conda environment on your machine with all the necessary tools and setup needed to utilize TaskVine with the Parsl library.

The following snippet shows an example configuration for using the Parsl/TaskVine executor to run applications on the local machine. This examples uses the *parsl.executors.taskvine.TaskVineExecutor* to schedule tasks, and a local worker will be started automatically. For more information on using TaskVine, including configurations for remote execution, visit the TaskVine/Parsl documentation online.

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TaskVine's predecessor, WorkQueue, may continue to be used with Parsl. For more information on using WorkQueue visit the CCTools documentation online.

#### Expanse (SDSC)



The following snippet shows an example configuration for executing remotely on San Diego Supercomputer Center's **Expanse** supercomputer. The example is designed to be executed on the login nodes, using the *parsl.providers*. *SlurmProvider* to interface with the Slurm scheduler used by Comet and the *parsl.launchers.SrunLauncher* to launch workers.

```
from parsl.config import Config
from parsl.launchers import SrunLauncher
from parsl.providers import SlurmProvider
from parsl.executors import HighThroughputExecutor
config = Config(
   executors=[
       HighThroughputExecutor(
            label='Expanse_CPU_Multinode',
            max_workers_per_node=32,
            provider=SlurmProvider(
                'compute',
                account='YOUR_ALLOCATION_ON_EXPANSE',
                launcher=SrunLauncher(),
                # string to prepend to #SBATCH blocks in the submit
                # script to the scheduler
                scheduler_options='',
                # Command to be run before starting a worker, such as:
```

```
# 'module load Anaconda; source activate parsl_env'.
worker_init='',
walltime='01:00:00',
init_blocks=1,
max_blocks=1,
nodes_per_block=2,
),
]
]
```

#### Perlmutter (NERSC)

NERSC provides documentation on how to use Parsl on Perlmutter.

#### Frontera (TACC)



Deployed in June 2019, Frontera is the 5th most powerful supercomputer in the world. Frontera replaces the NSF Blue Waters system at NCSA and is the first deployment in the National Science Foundation's petascale computing program. The configuration below assumes that the user is running on a login node and uses the *parsl.providers*. *SlurmProvider* to interface with the scheduler, and uses the *parsl.launchers.SrunLauncher* to launch workers.

```
from parsl.config import Config
from parsl.channels import LocalChannel
from parsl.providers import SlurmProvider
from parsl.executors import HighThroughputExecutor
from parsl.launchers import SrunLauncher
""" This config assumes that it is used to launch parsl tasks from the login nodes
of Frontera at TACC. Each job submitted to the scheduler will request 2 nodes for 10.
...minutes.
"""
config = Config(
    executors=[
```

```
HighThroughputExecutor(
            label="frontera_htex",
            max_workers_per_node=1,
                                               # Set number of workers per node
            provider=SlurmProvider(
                                     # Add extra time for slow scheduler responses
                cmd_timeout=60.
                channel=LocalChannel(),
                nodes_per_block=2,
                init_blocks=1,
                min_blocks=1,
                max_blocks=1,
                partition='normal',
                                                                       # Replace with_
→ partition name
                scheduler_options='#SBATCH -A <YOUR_ALLOCATION>',
                                                                       # Enter scheduler_
\rightarrow options if needed
                # Command to be run before starting a worker, such as:
                # 'module load Anaconda; source activate parsl_env'.
                worker_init='',
                # Ideally we set the walltime to the longest supported walltime.
                walltime='00:10:00',
                launcher=SrunLauncher(),
            ),
        )
    ],
)
```

#### **Kubernetes Clusters**



Kubernetes is an open-source system for container management, such as automating deployment and scaling of containers. The snippet below shows an example configuration for deploying pods as workers on a Kubernetes cluster. The KubernetesProvider exploits the Python Kubernetes API, which assumes that you have kube config in ~/.kube/ config.

```
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.providers import KubernetesProvider
from parsl.addresses import address_by_route
```

```
config = Config(
    executors=[
       HighThroughputExecutor(
            label='kube-htex',
            cores_per_worker=1,
            max_workers_per_node=1,
            worker_logdir_root='YOUR_WORK_DIR',
            # Address for the pod worker to connect back
            address_by_route(),
            provider=KubernetesProvider(
                namespace="default",
                # Docker image url to use for pods
                image='YOUR_DOCKER_URL',
                # Command to be run upon pod start, such as:
                # 'module load Anaconda; source activate parsl_env'.
                # or 'pip install parsl'
                worker_init='',
                # The secret key to download the image
                secret="YOUR_KUBE_SECRET",
                # Should follow the Kubernetes naming rules
                pod_name='YOUR-POD-Name',
                nodes_per_block=1,
                init_blocks=1,
                # Maximum number of pods to scale up
                max_blocks=10,
           ),
       ),
    ]
)
```

#### Midway (RCC, UChicago)



This Midway cluster is a campus cluster hosted by the Research Computing Center at the University of Chicago. The snippet below shows an example configuration for executing remotely on Midway. The configuration assumes the user is running on a login node and uses the *parsl.providers.SlurmProvider* to interface with the scheduler, and uses the *parsl.launchers.SrunLauncher* to launch workers.

```
from parsl.config import Config
from parsl.providers import SlurmProvider
from parsl.launchers import SrunLauncher
from parsl.executors import HighThroughputExecutor
from parsl.addresses import address_by_interface
config = Config(
    executors=[
       HighThroughputExecutor(
            label='Midway_HTEX_multinode',
            address_by_interface('bond0'),
            worker_debug=False,
            max_workers_per_node=2.
            provider=SlurmProvider(
                'YOUR_PARTITION', # Partition name, e.g 'broadwl'
                launcher=SrunLauncher(),
                nodes_per_block=2,
                init_blocks=1,
                min_blocks=1,
                max_blocks=1,
                # string to prepend to #SBATCH blocks in the submit
                # script to the scheduler eg: '#SBATCH --constraint=knl,quad,cache'
                scheduler_options='',
                # Command to be run before starting a worker, such as:
                # 'module load Anaconda; source activate parsl_env'.
                worker_init='',
                walltime='00:30:00'
            ),
```

	·	)				
	],					
)						

**Open Science Grid** 



# **Open Science Grid**

The Open Science Grid (OSG) is a national, distributed computing Grid spanning over 100 individual sites to provide tens of thousands of CPU cores. The snippet below shows an example configuration for executing remotely on OSG. You will need to have a valid project name on the OSG. The configuration uses the *parsl.providers*. *CondorProvider* to interface with the scheduler.

```
# will have modules
                scheduler_options="""
                +ProjectName = "MyProject"
                Requirements = HAS_MODULES=?=TRUE
                .....
                # Command to be run before starting a worker, such as:
                # 'module load Anaconda; source activate parsl_env'.
                worker_init='''unset HOME; unset PYTHONPATH; module load python/3.7.0;
python3 -m venv parsl_env; source parsl_env/bin/activate; python3 -m pip install parsl''
⇔',
                walltime="00:20:00",
            ),
            worker_logdir_root='$OSG_WN_TMP',
            worker_ports=(31000, 31001)
        )
   ]
)
```

#### Polaris (ALCF)

ALCF provides documentation on how to use Parsl on Polaris.

#### Stampede2 (TACC)

The following snippet shows an example configuration for accessing TACC's **Stampede2** supercomputer. This example uses the HighThroughput executor and connects to Stampede2's Slurm scheduler.

```
from parsl.config import Config
from parsl.providers import SlurmProvider
from parsl.launchers import SrunLauncher
from parsl.executors import HighThroughputExecutor
from parsl.data_provider.globus import GlobusStaging
from parsl.addresses import address_by_interface
config = Config(
    executors=[
       HighThroughputExecutor(
            label='Stampede2_HTEX',
            address_by_interface('em3'),
            max_workers_per_node=2,
            provider=SlurmProvider(
                nodes_per_block=2,
                init_blocks=1,
                min_blocks=1,
                max_blocks=1,
                partition='YOUR_PARTITION',
                # string to prepend to #SBATCH blocks in the submit
                # script to the scheduler eg: '#SBATCH --constraint=knl,quad,cache'
```

```
scheduler_options='',
    # Command to be run before starting a worker, such as:
    # 'module load Anaconda; source activate parsl_env'.
    worker_init='',
    launcher=SrunLauncher(),
    walltime='00:30:00'
    ),
    storage_access=[GlobusStaging(
        endpoint_uuid='ceea5ca0-89a9-11e7-a97f-22000a92523b',
        endpoint_path='/',
        local_path='/'
    )]
    )
    ],
```

#### Summit (ORNL)

The following snippet shows an example configuration for executing from the login node on Summit, the leadership class supercomputer hosted at the Oak Ridge National Laboratory. The example uses the *parsl. providers.LSFProvider* to provision compute nodes from the LSF cluster scheduler and the *parsl.launchers. JsrunLauncher* to launch workers across the compute nodes.

```
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.launchers import JsrunLauncher
from parsl.providers import LSFProvider
from parsl.addresses import address_by_interface
config = Config(
    executors=[
       HighThroughputExecutor(
            label='Summit_HTEX'.
            # On Summit ensure that the working dir is writeable from the compute nodes,
            # for eg. paths below /gpfs/alpine/world-shared/
            working_dir='YOUR_WORKING_DIR_ON_SHARED_FS',
            address=address_by_interface('ib0'), # This assumes Parsl is running on_
→login node
            worker_port_range=(50000, 55000),
            provider=LSFProvider(
                launcher=JsrunLauncher(),
                walltime="00:10:00",
                nodes_per_block=2,
                init_blocks=1,
                max_blocks=1,
                worker_init='', # Input your worker environment initialization commands
                project='YOUR_PROJECT_ALLOCATION',
                cmd_timeout=60
```

					(continue	ed from previ	ous page)
		),					
	)						
	_						
	],						
)							

#### TOSS3 (LLNL)



The following snippet shows an example configuration for executing on one of LLNL's **TOSS3** machines, such as Quartz, Ruby, Topaz, Jade, or Magma. This example uses the *pars1.executors.FluxExecutor* and connects to Slurm using the *pars1.providers.SlurmProvider*. This configuration assumes that the script is being executed on the login nodes of one of the machines.

```
from parsl.config import Config
from parsl.executors import FluxExecutor
from parsl.providers import SlurmProvider
from parsl.launchers import SrunLauncher

config = Config(
    executors=[
      FluxExecutor(
         provider=SlurmProvider(
            partition="YOUR_PARTITION", # e.g. "pbatch", "pdebug"
            account="YOUR_ACCOUNT",
            launcher=SrunLauncher(overrides="--mpibind=off"),
```

```
nodes_per_block=1,
                init_blocks=1,
                min_blocks=1,
                max_blocks=1,
                walltime="00:30:00",
                # string to prepend to #SBATCH blocks in the submit
                # script to the scheduler, e.g.: '#SBATCH -t 50'
                scheduler_options='',
                # Command to be run before starting a worker, such as:
                # 'module load Anaconda; source activate parsl_env'.
                worker_init='',
                cmd_timeout=120,
            ),
        )
    ]
)
```

#### **Further help**

For help constructing a configuration, you can click on class names such as *Config* or *HighThroughputExecutor* to see the associated class documentation. The same documentation can be accessed interactively at the python command line via, for example:

from parsl.config import Config
help(Config)

#### Monitoring

Parsl includes a monitoring system to capture task state as well as resource usage over time. The Parsl monitoring system aims to provide detailed information and diagnostic capabilities to help track the state of your programs, down to the individual apps that are executed on remote machines.

The monitoring system records information to an SQLite database while a workflow runs. This information can then be visualised in a web dashboard using the parsl-visualize tool, or queried using SQL using regular SQLite tools.

#### **Monitoring configuration**

Parsl monitoring is only supported with the parsl.executors.HighThroughputExecutor.

The following example shows how to enable monitoring in the Parsl configuration. Here the *parsl.monitoring*. *MonitoringHub* is specified to use port 55055 to receive monitoring messages from workers every 10 seconds.

```
import parsl
from parsl.monitoring.monitoring import MonitoringHub
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.addresses import address_by_hostname
```

import logging

```
config = Config(
   executors=[
       HighThroughputExecutor(
           label="local_htex",
           cores_per_worker=1,
           max_workers_per_node=4,
           address=address_by_hostname(),
       )
   ],
  monitoring=MonitoringHub(
       hub_address=address_by_hostname(),
       hub_port=55055,
       monitoring_debug=False,
       resource_monitoring_interval=10,
   ),
   strategy='none'
)
```

#### Visualization

To run the web dashboard utility parsl-visualize you first need to install its dependencies:

\$ pip install 'parsl[monitoring,visualization]'

To view the web dashboard while or after a Parsl program has executed, run the parsl-visualize utility:

\$ parsl-visualize

By default, this command expects that the default monitoring.db database is used in the runinfo directory. Other databases can be loaded by passing the database URI on the command line. For example, if the full path to the database is /tmp/my\_monitoring.db, run:

\$ parsl-visualize sqlite:///tmp/my\_monitoring.db

By default, the visualization web server listens on 127.0.0.1:8080. If the web server is deployed on a machine with a web browser, the dashboard can be accessed in the browser at 127.0.0.1:8080. If the web server is deployed on a remote machine, such as the login node of a cluster, you will need to use an ssh tunnel from your local machine to the cluster:

\$ ssh -L 50000:127.0.0.1:8080 username@cluster\_address

This command will bind your local machine's port 50000 to the remote cluster's port 8080. The dashboard can then be accessed via the local machine's browser at 127.0.0.1:50000.

**Warning:** Alternatively you can deploy the visualization server on a public interface. However, first check that this is allowed by the cluster's security policy. The following example shows how to deploy the web server on a public port (i.e., open to Internet via public\_IP:55555):

\$ parsl-visualize --listen 0.0.0.0 --port 55555

#### **Workflows Page**

The workflows page lists all Parsl workflows that have been executed with monitoring enabled with the selected database. It provides a high level summary of workflow state as shown below:

Parsl Workflows Documentation

### Workflows

Name	Version	Owner	Status	Runtime (s)	Tasks	Actions
test_fan_inout.py	2019-06-13 10:58:14	yadu	Completed	0:00:25	21 0	<u>Lat</u>
test_monitor_on_fail.py	2019-06-13 11:02:02	yadu	Completed	0:00:02	0 1	<u>Lui</u>

Throughout the dashboard, all blue elements are clickable. For example, clicking a specific worklow name from the table takes you to the Workflow Summary page described in the next section.

#### **Workflow Summary**

The workflow summary page captures the run level details of a workflow, including start and end times as well as task summary statistics. The workflow summary section is followed by the *App Summary* that lists the various apps and invocation count for each.



The workflow summary also presents three different views of the workflow:

• Workflow DAG - with apps differentiated by colors: This visualization is useful to visually inspect the dependency structure of the workflow. Hovering over the nodes in the DAG shows a tooltip for the app represented by the node and it's task ID.

## test\_fan\_inout.py

- Started: 2019-06-13 10:58:14
- Completed: 2019-06-13 10:58:39
- Workflow duration: 0:00:25
- Owner: yadu
- host: borgmachine2
- rundir: /home/yadu/src/parsl/parsl/tests/manual\_tests/runinfo/000
- tasks\_failed\_count: 0
- tasks\_completed\_count: 21

#### View workflow DAG -- colors grouped by task states





• Workflow DAG - with task states differentiated by colors: This visualization is useful to identify what tasks have been completed, failed, or are currently pending.

# test\_fan\_inout.py

- Started: 2019-06-13 10:58:14
- Completed: 2019-06-13 10:58:39
- Workflow duration: 0:00:25
- Owner: yadu
- host: borgmachine2
- rundir: /home/yadu/src/parsl/parsl/tests/manual\_tests/runinfo/000
- tasks\_failed\_count: 0
- tasks\_completed\_count: 21

## View workflow DAG -- colors grouped by apps

View workflow task summary



• Workflow resource usage: This visualization provides resource usage information at the workflow level. For example, cumulative CPU/Memory utilization across workers over time.

## test\_fan\_inout.py

- Started: 2019-06-13 10:58:14
- Completed: 2019-06-13 10:58:39
- Workflow duration: 0:00:25
- Owner: yadu
- host: borgmachine2
- rundir: /home/yadu/src/parsl/parsl/tests/manual\_tests/runinfo/000
- tasks\_failed\_count: 0
- tasks\_completed\_count: 21

View workflow DAG -- colors grouped by apps View workflow DAG -- colors grouped by task states View workflow task summary **CPU Usage** 









#### Memory Usage









#### CPU usage







CPU User Time

CPU User Time

Time (seconds)

o 🔍 🕂 🔅 🔗 🖬 🗖 🗶 🚸 👘 🚍 📕

10

#### Memory usage







5

Time (seconds)

#### **Example parallel patterns**

Parsl can be used to implement a wide range of parallel programming patterns, from bag of tasks through to nested workflows. Parsl implicitly assembles a dataflow dependency graph based on the data shared between apps. The flexibility of this model allows for the implementation of a wide range of parallel programming and workflow patterns.

Parsl is also designed to address broad execution requirements, from programs that run many short tasks to those that run a few long tasks.

Below we illustrate a range of parallel programming and workflow patterns. It is important to note that this set of examples is by no means comprehensive.

#### **Bag of Tasks**

Parsl can be used to execute a large bag of tasks. In this case, Parsl assembles the set of tasks (represented as Parsl apps) and manages their concurrent execution on available resources.

```
from parsl import python_app
parsl.load()
# Map function that returns double the input integer
@python_app
def app_random():
    import random
    return random.random()
results = []
for i in range(0, 10):
    x = app_random()
    results.append(x)
for r in results:
    print(r.result())
```

#### Sequential workflows

Sequential workflows can be created by passing an AppFuture from one task to another. For example, in the following program the generate app (a Python app) generates a random number that is consumed by the save app (a Bash app), which writes it to a file. Because save cannot execute until it receives the message produced by generate, the two apps execute in sequence.

```
from parsl import python_app
parsl.load()
# Generate a random number
@python_app
def generate(limit):
    from random import randint
    """Generate a random integer and return it"""
    return randint(1, limit)
```

```
# Write a message to a file
@bash_app
def save(message, outputs=()):
    return 'echo {} &> {}'.format(message, outputs[0])
message = generate(10)
saved = save(message, outputs=['output.txt'])
with open(saved.outputs[0].result(), 'r') as f:
    print(f.read())
```

#### **Parallel workflows**

Parallel execution occurs automatically in Parsl, respecting dependencies among app executions. In the following example, three instances of the wait\_sleep\_double app are created. The first two execute concurrently, as they have no dependencies; the third must wait until the first two complete and thus the doubled\_x and doubled\_y futures have values. Note that this sequencing occurs even though wait\_sleep\_double does not in fact use its second and third arguments.

```
from parsl import python_app
parsl.load()
@python_app
def wait_sleep_double(x, foo_1, foo_2):
     import time
     time.sleep(2) # Sleep for 2 seconds
     return x*2
# Launch two apps, which will execute in parallel, since they do not have to
# wait on any futures
doubled_x = wait_sleep_double(10, None, None)
doubled_y = wait_sleep_double(10, None, None)
# The third app depends on the first two:
#
     doubled_x doubled_y (2 s)
#
           \
                 /
            doublex_z
                               (2 s)
#
doubled_z = wait_sleep_double(10, doubled_x, doubled_y)
# doubled_z will be done in ~4s
print(doubled_z.result())
```

#### Parallel workflows with loops

A common approach to executing Parsl apps in parallel is via loops. The following example uses a loop to create many random numbers in parallel.

```
from parsl import python_app
parsl.load()

Opython_app
def generate(limit):
    """Generate a random integer and return it"""
    from random import randint
    return randint(1, limit)

rand_nums = []
for i in range(1,5):
    rand_nums.append(generate(i))

# Wait for all apps to finish and collect the results
outputs = [r.result() for r in rand_nums]
```

The ParslPoolExecutor simplifies this pattern using the same interface as Python's native Executors.

```
from parsl.concurrent import ParslPoolExecutor
from parsl.configs.htex_local import config

# NOTE: Functions used by the ParslPoolExecutor do _not_ use decorators
def generate(limit):
    """Generate a random integer and return it"""
    from random import randint
    return randint(1, limit)
with ParslPoolExecutor(config) as exec:
```

outputs = pool.map(generate, range(1, 5))

In the preceding example, the execution of different tasks is coordinated by passing Python objects from producers to consumers. In other cases, it can be convenient to pass data in files, as in the following reformulation. Here, a set of files, each with a random number, is created by the generate app. These files are then concatenated into a single file, which is subsequently used to compute the sum of all numbers.

```
from pars1 import python_app, bash_app
pars1.load()
@bash_app
def generate(outputs=()):
    return 'echo $(( RANDOM % (10 - 5 + 1 ) + 5 )) &> {}'.format(outputs[0])
@bash_app
def concat(inputs=(), outputs=(), stdout='stdout.txt', stderr='stderr.txt'):
    return 'cat {0} >> {1}'.format(' '.join(inputs), outputs[0])
```

```
@python_app
def total(inputs=()):
   total = 
   with open(inputs[0].filepath, 'r') as f:
        for 1 in f:
            total += int(1)
   return total
# Create 5 files with random numbers
output_files = []
for i in range (5):
     output_files.append(generate(outputs=['random-%s.txt' % i]))
# Concatenate the files into a single file
cc = concat(inputs=[i.outputs[0] for i in output_files], outputs=['all.txt'])
# Calculate the average of the random numbers
totals = total(inputs=[cc.outputs[0]])
print(totals.result())
```

#### MapReduce

MapReduce is a common pattern used in data analytics. It is composed of a map phase that filters values and a reduce phase that aggregates values. The following example demonstrates how Parsl can be used to specify a MapReduce computation in which the map phase doubles a set of input integers and the reduce phase computes the sum of those results.

```
from parsl import python_app
parsl.load()
# Map function that returns double the input integer
@python_app
def app_double(x):
   return x*2
# Reduce function that returns the sum of a list
@python_app
def app_sum(inputs=()):
   return sum(inputs)
# Create a list of integers
items = range((0, 4))
# Map phase: apply the double *app* function to each item in list
mapped_results = []
for i in items:
   x = app_double(i)
   mapped_results.append(x)
```

```
# Reduce phase: apply the sum *app* function to the set of results
total = app_sum(inputs=mapped_results)
```

print(total.result())

The program first defines two Parsl apps, app\_double and app\_sum. It then makes calls to the app\_double app with a set of input values. It then passes the results from app\_double to the app\_sum app to aggregate values into a single result. These tasks execute concurrently, synchronized by the mapped\_results variable. The following figure shows the resulting task graph.



#### Caching expensive initialisation between tasks

Many tasks in workflows require a expensive "initialization" steps that, once performed, can be used across successive invocations for that task. For example, you may want to reuse a machine learning model for multiple interface tasks and avoid loading it onto GPUs more than once.

This ExaWorks tutorial gives examples of how to do this.

#### **Structuring Parsl programs**

Parsl programs can be developed in many ways. When developing a simple program it is often convenient to include the app definitions and control logic in a single script. However, as a program inevitably grows and changes, like any code, there are significant benefits to be obtained by modularizing the program, including:

- 1. Better readability
- 2. Logical separation of components (e.g., apps, config, and control logic)
- 3. Ease of reuse of components

The following example illustrates how a Parsl project can be organized into modules.

The configuration(s) can be defined in a module or file (e.g., config.py) which can be imported into the control script depending on which execution resources should be used.

```
from parsl.config import Config
from parsl.channels import LocalChannel
from parsl.executors import HighThroughputExecutor
from parsl.providers import LocalProvider
htex_config = Config(
    executors=[
    HighThroughputExecutor(
        label="htex_local",
        cores_per_worker=1,
        provider=LocalProvider(
            channel=LocalChannel(),
        ),
        ),
    ],
)
```

Parsl apps can be defined in separate file(s) or module(s) (e.g., library.py) grouped by functionality.

```
from parsl import python_app
@python_app
def increment(x):
    return x + 1
```

Finally, the control logic for the Parsl program can then be implemented in a separate file (e.g., run\_increment.py). This file must the import the configuration from config.py before calling the increment app from library.py:

```
import pars1
from config import htex_config
from library import increment
pars1.load(htex_config)
for i in range(5):
    print('{} + 1 = {}'.format(i, increment(i).result()))
```

Which produces the following output:

#### Lifted operators

Parsl allows some operators ([] and .) to be used on an AppFuture in a way that makes sense with those operators on the eventually returned result.

#### Lifted [] operator

When an app returns a complex structure such as a dict or a list, it is sometimes useful to pass an element of that structure to a subsequent task, without waiting for that subsequent task to complete.

To help with this, Parsl allows the [] operator to be used on an *AppFuture*. This operator will return another *AppFuture* that will complete after the initial future, with the result of [] on the value of the initial future.

The end result is that this assertion will hold:

```
fut = my_app()
assert fut['x'].result() == fut.result()[x]
```

but more concurrency will be available, as execution of the main workflow code will not stop to wait for result() to complete on the initial future.

*AppFuture* does not implement other methods commonly associated with dicts and lists, such as len, because those methods should return a specific type of result immediately, and that is not possible when the results are not available until the future.

If a key does not exist in the returned result, then the exception will appear in the Future returned by [], rather than at the point that the [] operator is applied. This is because the valid values that can be used are not known until the underlying result is available.

#### Lifted . operator

The . operator works similarly to [] described above:

```
fut = my_app
assert fut.x.result() == fut.result().x
```

Attributes beginning with \_ are not lifted as this usually indicates an attribute that is used for internal purposes, and to try to avoid mixing protocols (such as iteration in for loops) defined on AppFutures vs protocols defined on the underlying result object.

#### Join Apps

Join apps, defined with the @join\_app decorator, are a form of app that can launch other pieces of a workflow: for example a Parsl sub-workflow, or a task that runs in some other system.

#### **Parsl sub-workflows**

One reason for launching Parsl apps from inside a join app, rather than directly in the main workflow code, is because the definitions of those tasks are not known well enough at the start of the workflow.

For example, a workflow might run an expensive step to detect some objects in an image, and then on each object, run a further expensive step. Because the number of objects is not known at the start of the workflow, but instead only after an expensive step has completed, the subsequent tasks cannot be defined until after that step has completed.

In simple cases, the main workflow script can be stopped using Future.result() and join apps are not necessary, but in more complicated cases, that approach can severely limit concurrency.

Join apps allow more naunced dependencies to be expressed that can help with:

- · increased concurrency helping with strong scaling
- · more focused error propagation allowing more of an ultimately failing workflow to complete
- more useful monitoring information

#### Using Futures from other components

Sometimes, a workflow might need to incorporate tasks from other systems that run asynchronously but do not need a Parsl worker allocated for their entire run. An example of this is delegating some work into Globus Compute: work can be given to Globus Compute, but Parsl does not need to keep a worker allocated to that task while it runs. Instead, Parsl can be told to wait for the Future returned by Globus Compute to complete.

#### Usage

A *join\_app* looks quite like a *python\_app*, but should return one or more Future objects, rather than a value. Once the Python code has run, the app will wait for those Futures to complete without occuping a Parsl worker, and when those Futures complete, their contents will be the return value of the *join\_app*.

For example:

```
@python_app
def some_app():
    return 3
@join_app
def example():
    x: Future = some_app()
    return x # note that x is a Future, not a value
assert example.result() == 3
```

#### Example of a Parsl sub-workflow

This example workflow shows a preprocessing step, followed by a middle stage that is chosen by the result of the pre-processing step (either option 1 or option 2) followed by a know post-processing step.

```
@python_app
def pre_process():
  return 3
@python_app
def option_one(x):
  return x*2
@python_app
def option_two(x):
  return (-x) * 2
@join_app
def process(x):
  if x > 0:
    return option_one(x)
  else:
    return option_two(x)
@python_app
def post_process(x):
 return str(x)
assert post_process(process(pre_process()))).result() == "6"
```

• Why can't process be a regular python function?

process needs to inspect the value of x to make a decision about what app to launch. So it needs to defer execution until after the pre-processing stage has completed. In Parsl, the way to defer that is using apps: even though process is invoked at the start of the workflow, it will execute later on, when the Future returned by pre\_process has a value.

• Why can't process be a @python\_app?

A Python app, if run in a *pars1.executors.ThreadPoolExecutor*, can launch more parsl apps; so a python\_app implementation of process() would be able to inspect x and choose and invoke the appropriate option\_{one, two}.

From launching the option\_{one, two} app, the app body python code would get a Future[int] - a Future that will eventually contain int.

But, we want to invoke post\_process at submission time near the start of workflow so that Parsl knows about as many tasks as possible. But we don't want it to execute until the value of the chosen option\_{one, two} app is known.

If we don't have join apps, how can we do this?

We could make process wait for option\_{one, two} to complete, before returning, like this:

```
@python_app
def process(x):
    if x > 0:
        f = option_one(x)
    else:
```

```
f = option_two(x)
return f.result()
```

but this will block the worker running process until option\_{one, two} has completed. If there aren't enough workers to run option\_{one, two} this can even deadlock. (principle: apps should not wait on completion of other apps and should always allow parsl to handle this through dependencies)

We could make process return the Future to the main workflow thread:

```
@python_app
def process(x):
    if x > 0:
        f = option_one(x)
    else:
        f = option_two(x)
    return f # f is a Future[int]
# process(3) is a Future[Future[int]]
```

What comes out of invoking process(x) now is a nested Future[Future[int]] - it's a promise that eventually process will give you a promise (from option\_one, two}) that will eventually give you an int.

We can't pass that future into post\_process... because post\_process wants the final int, and that future will complete before the int is ready, and that (outer) future will have as its value the inner future (which won't be complete yet).

So we could wait for the result in the main workflow thread:

```
f_outer = process(pre_process()) # Future[Future[int]]
f_inner = f_outer.result # Future[int]
result = post_process(f_inner)
# result == "6"
```

But this now blocks the main workflow thread. If we really only need to run these three lines, that's fine, but what about if we are in a for loop that sets up 1000 parametrised iterations:

```
for x in [1..1000]:
    f_outer = process(pre_process(x))  # Future[Future[int]]
    f_inner = f_outer.result()  # Future[int]
    result = post_process(f_inner)
```

The for loop can only iterate after pre\_processing is done for each iteration - it is unnecessarily serialised by the .result() call, so that pre\_processing cannot run in parallel.

So, the rule about not calling .result() applies in the main workflow thread too.

What join apps add is the ability for parsl to unwrap that Future[Future[int]] into a Future[int] in a "sensible" way (eg it doesn't need to block a worker).

#### Example of invoking a Futures-driven task from another system

This example shows launching some activity in another system, without occupying a Parsl worker while that activity happens: in this example, work is delegated to Globus Compute, which performs the work elsewhere. When the work is completed, Globus Compute will put the result into the future that it returns, and then (because the Parsl app is a @join\_app), that result will be used as the result of the Parsl app.

As above, the motivation for doing this inside an app, rather than in the top level is that sufficient information to launch the Globus Compute task might not be available at start of the workflow.

This workflow will run a first stage, const\_five, on a Parsl worker, then using the result of that stage, pass the result as a parameter to a Globus Compute task, getting a Future from that submission. Then, the results of the Globus Compute task will be passed onto a second Parsl local task, times\_two.

```
import parsl
from globus_compute_sdk import Executor
tutorial_endpoint_uuid = '4b116d3c-1703-4f8f-9f6f-39921e5864df'
gce = Executor(endpoint_id=tutorial_endpoint_uuid)
def increment_in_funcx(n):
   return n+1
@parsl.join_app
def increment_in_parsl(n):
    future = gce.submit(increment_in_funcx, n)
   return future
@parsl.python_app
def times_two(n):
   return n*2
@parsl.python_app
def const_five():
   return 5
parsl.load()
workflow = times_two(increment_in_parsl(const_five()))
r = workflow.result()
assert r == (5+1)*2
```

#### Terminology

The term "join" comes from use of monads in functional programming, especially Haskell.

#### Usage statistics collection

Parsl uses an **Opt-in** model to send usage statistics back to the Parsl development team to measure worldwide usage and improve reliability and usability. The usage statistics are used only for improvements and reporting. They are not shared in raw form outside of the Parsl team.

#### Why are we doing this?

The Parsl development team receives support from government funding agencies. For the team to continue to receive such funding, and for the agencies themselves to argue for funding, both the team and the agencies must be able to demonstrate that the scientific community is benefiting from these investments. To this end, it is important that we provide aggregate usage data about such things as the following:

- How many people use Parsl
- Average job length
- · Parsl exit codes

By participating in this project, you help justify continuing support for the software on which you rely. (see *What is sent?* below).

#### Opt-In

We have chosen opt-in collection rather than opt-out with the hope that developers and researchers will choose to send us this information. The reason is that we need this data - it is a requirement for funding.

By opting-in, and allowing these statistics to be reported back, you are explicitly supporting the further development of Parsl.

If you wish to opt in to usage reporting, set PARSL\_TRACKING=true in your environment or set usage\_tracking=True in the configuration object (*parsl.config*).

#### What is sent?

- IP address
- Run UUID
- Start and end times
- Number of executors used
- Number of failures
- Parsl and Python version
- · OS and OS version

#### How is the data sent?

The data is sent via UDP. While this may cause us to lose some data, it drastically reduces the possibility that the usage statistics reporting will adversely affect the operation of the software.

#### When is the data sent?

The data is sent twice per run, once when Parsl starts a script, and once when the script is completed.

#### What will the data be used for?

The data will be used for reporting purposes to answer questions such as:

- How many unique users are using Parsl?
- To determine patterns of usage is activity increasing or decreasing?

We will also use this information to improve Parsl by identifying software faults.

- What percentage of tasks complete successfully?
- Of the tasks that fail, what is the most common fault code returned?

#### Feedback

Please send us your feedback at parsl@googlegroups.com. Feedback from our user communities will be useful in determining our path forward with usage tracking in the future.

#### **Plugins**

Parsl has several places where code can be plugged in. Parsl usually provides several implementations that use each plugin point.

This page gives a brief summary of those places and why you might want to use them, with links to the API guide.

#### Executors

When the parsl dataflow kernel is ready for a task to run, it passes that task to an *ParslExecutor*. The executor is then responsible for running the task's Python code and returning the result. This is the abstraction that allows one executor to run code on the local submitting host, while another executor can run the same code on a large supercomputer.

#### **Providers, Launchers and Channels**

Some executors are based on blocks of workers (for example the *parsl.executors.HighThroughputExecutor*: the submit side requires a batch system (eg slurm, kubernetes) to start worker processes, which then execute tasks.

The particular way in which a system makes those workers start is implemented by providers and launchers.

An *ExecutionProvider* allows a command line to be submitted as a request to the underlying batch system to be run inside an allocation of nodes.
A *Launcher* modifies that command line when run inside the allocation to add on any wrappers that are needed to launch the command (eg srun inside slurm). Providers and launchers are usually paired together for a particular system type.

A *Channel* allows the commands used to interact with an *ExecutionProvider* to be executed on a remote system. The default channel executes commands on the local system, but a few variants of an *parsl.channels.SSHChannel* are provided.

# **File staging**

Parsl can copy input files from an arbitrary URL into a task's working environment, and copy output files from a task's working environment to an arbitrary URL. A small set of data staging providers is installed by default, for file:// http:// and ftp:// URLs. More data staging providers can be added in the workflow configuration, in the storage parameter of the relevant *ParslExecutor*. Each provider should subclass the *Staging* class.

## Default stdout/stderr name generation

Parsl can choose names for your bash apps stdout and stderr streams automatically, with the parsl.AUTO\_LOGNAME parameter. The choice of path is made by a function which can be configured with the std\_autopath parameter of Parsl *Config.* By default, DataFlowKernel.default\_std\_autopath will be used.

# Memoization/checkpointing

When parsl memoizes/checkpoints an app parameter, it does so by computing a hash of that parameter that should be the same if that parameter is the same on subsequent invocations. This isn't straightforward to do for arbitrary objects, so parsl implements a checkpointing hash function for a few common types, and raises an exception on unknown types:

ValueError("unknown type for memoization ...")

You can plug in your own type-specific hash code for additional types that you need and understand using *id\_for\_memo*.

## Invoking other asynchronous components

Parsl code can invoke other asynchronous components which return Futures, and integrate those Futures into the task graph: Parsl apps can be given any concurrent.futures.Future as a dependency, even if those futures do not come from invoking a Parsl app. This includes as the return value of a join\_app.

An specific example of this is integrating Globus Compute tasks into a Parsl task graph. See *Example of invoking a Futures-driven task from another system* 

### Measuring performance with parsl-perf

pars1-perf is tool for making basic performance measurements of Parsl configurations.

It runs increasingly large numbers of no-op apps until a batch takes (by default) 120 seconds, giving a measurement of tasks per second.

This can give a basic measurement of some of the overheads in task execution.

parsl-perf must be invoked with a configuration file, which is a Python file containing a variable config which contains a *Config* object, or a function fresh\_config which returns a *Config* object. The fresh\_config format is the same as used with the pytest test suite.

To specify a parsl\_resource\_specification for tasks, add a --resources argument.

To change the target runtime from the default of 120 seconds, add a --time parameter.

For example:

```
$ python -m parsl.benchmark.perf --config parsl/tests/configs/workqueue_ex.py --
-resources '{"cores":1, "memory":0, "disk":0}'
==== Iteration 1 ====
Will run 10 tasks to target 120 seconds runtime
Submitting tasks / invoking apps
warning: using plain-text when communicating with workers.
warning: use encryption with a key and cert when creating the manager.
All 10 tasks submitted ... waiting for completion
Submission took 0.008 seconds = 1248.676 tasks/second
Runtime: actual 3.668s vs target 120s
Tasks per second: 2.726
[...]
==== Iteration 4 ====
Will run 57640 tasks to target 120 seconds runtime
Submitting tasks / invoking apps
```

All 57640 tasks submitted ... waiting **for** completion Submission took 34.839 seconds = 1654.487 tasks/second Runtime: actual 364.387s vs target 120s Tasks per second: 158.184 Cleaning up DFK The end

# FAQ

#### How can I debug a ParsI script?

Parsl interfaces with the Python logger and automatically logs Parsl-related messages a runinfo directory. The runinfo directory will be created in the folder from which you run the Parsl script and it will contain a series of subfolders for each time you run the code. Your latest run will be the largest number.

Alternatively, you can configure the file logger to write to an output file.

import parsl

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```
# Emit log lines to the screen
parsl.set_stream_logger()
# Write log to file, specify level of detail for logs
parsl.set_file_logger(FILENAME, level=logging.DEBUG)
```

**Note:** Parsl's logging will not capture STDOUT/STDERR from the apps themselves. Follow instructions below for application logs.

### How can I view outputs and errors from apps?

Parsl apps include keyword arguments for capturing stderr and stdout in files.

```
@bash_app
def hello(msg, stdout=None):
    return 'echo {}'.format(msg)
# When hello() runs the STDOUT will be written to 'hello.txt'
hello('Hello world', stdout='hello.txt')
```

#### How can I make an App dependent on multiple inputs?

You can pass any number of futures in to a single App either as positional arguments or as a list of futures via the special keyword inputs=(). The App will wait for all inputs to be satisfied before execution.

### Can I pass any Python object between apps?

This depends on the executor in use. The *parsl.executors.threads.ThreadPoolExecutor* can receive and return any Python object. Other executors will serialize their parameters and return values, so only objects which Parsl knows how to serialize can be passed.

Parsl knows how to serialize objects using the Pickle and Dill libraries.

Pickle provides a list of objects that it knows how to serialize: What can be pickled and unpickled?.

Dill can serialize much more than Pickle, documented in the dill documentation.

For objects that can't be pickled, use object specific methods to write the object into a file and use files to communicate between apps.

### How do I specify where apps should be run?

Parsl's multi-executor support allows you to define the executor (including local threads) on which an App should be executed. For example:

```
@python_app(executors=['SuperComputer1'])
def BigSimulation(...):
    ...
@python_app(executors=['GPUMachine'])
def Visualize (...)
    ...
```

### Workers do not connect back to Parsl

If you are running via ssh to a remote system from your local machine, or from the login node of a cluster/supercomputer, it is necessary to have a public IP to which the workers can connect back. While our remote execution systems can identify the IP address automatically in certain cases, it is safer to specify the address explicitly. Parsl provides a few heuristic based address resolution methods that could be useful, however with complex networks some trial and error might be necessary to find the right address or network interface to use.

For pars1.executors.HighThroughputExecutor the address is specified in the Config as shown below :

**Note:** Another possibility that can cause workers not to connect back to Parsl is an incompatibility between the system and the pre-compiled bindings used for pyzmq. As a last resort, you can try: pip install --upgrade --no-binary pyzmq pyzmq, which forces re-compilation.

For the *parsl.executors.HighThroughputExecutor*, address is a keyword argument taken at initialization. Here is an example for the *parsl.executors.HighThroughputExecutor*:

```
# THIS IS A CONFIG FRAGMENT FOR ILLUSTRATION
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
from parsl.addresses import address_by_route, address_by_query, address_by_hostname
```

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```
config = Config(
    executors=[
    HighThroughputExecutor(
        label='NERSC_Cori',
        address='<AA.BB.CC.DD>'  # specify public ip here
        # address=address_by_route()  # Alternatively you can try this
        # address=address_by_query()  # Alternatively you can try this
        # address=address_by_hostname()  # Alternatively you can try this
        )
    ],
)
```

**Note:** On certain systems such as the Midway RCC cluster at UChicago, some network interfaces have an active intrusion detection system that drops connections that persist beyond a specific duration (~20s). If you get repeated ManagerLost exceptions, it would warrant taking a closer look at networking.

#### parsl.errors.ConfigurationError

The Parsl configuration model underwent a major and non-backward compatible change in the transition to v0.6.0. Prior to v0.6.0 the configuration object was a python dictionary with nested dictionaries and lists. The switch to a class based configuration allowed for well-defined options for each specific component being configured as well as transparency on configuration defaults. The following traceback indicates that the old style configuration was passed to Parsl v0.6.0+ and requires an upgrade to the configuration.

```
File "/home/yadu/src/parsl/parsl/dataflow/dflow.py", line 70, in __init__
    'Expected `Config` class, received dictionary. For help, '
parsl.errors.ConfigurationError: Expected `Config` class, received dictionary. For help,
see http://parsl.readthedocs.io/en/stable/stubs/parsl.config.Config.html
```

For more information on how to update your configuration script, please refer to: Configuration.

#### Remote execution fails with SystemError(unknown opcode)

When running with Ipyparallel workers, it is important to ensure that the Python version on the client side matches that on the side of the workers. If there's a mismatch, the apps sent to the workers will fail with the following error: ipyparallel.error.RemoteError: SystemError(unknown opcode)

**Caution:** It is **required** that both the parsl script and all workers are set to use python with the same Major.Minor version numbers. For example, use Python3.5.X on both local and worker side.

### Parsl complains about missing packages

If parsl is cloned from a Github repository and added to the PYTHONPATH, it is possible to miss the installation of some dependent libraries. In this configuration, parsl will raise errors such as:

ModuleNotFoundError: No module named 'ipyparallel'

You should usually install parsl using a package managment tool such as pip or conda, ideally in a restricted environment such a virtualenv or a conda environment.

For instance, with conda, follow this cheatsheet to create a virtual environment:

```
# Activate an environmentconda install
source activate <my_env>
# Install packages:
conda install <ipyparallel, dill, boto3...>
```

### How do I run code that uses Python2.X?

Modules or code that require Python2.X cannot be run as python apps, however they may be run via bash apps. The primary limitation with python apps is that all the inputs and outputs including the function would be mangled when being transmitted between python interpreters with different version numbers (also see *parsl.errors.ConfigurationError*)

Here is an example of running a python2.7 code as a bash application:

```
@bash_app
def python_27_app (arg1, arg2 ...):
    return '''conda activate py2.7_env # Use conda to ensure right env
    python2.7 my_python_app.py -arg {0} -d {1}
    '''.format(arg1, arg2)
```

### **Parsl hangs**

There are a few common situations in which a Parsl script might hang:

- 1. Circular Dependency in code: If an app takes a list as an input argument and the future returned is added to that list, it creates a circular dependency that cannot be resolved. This situation is described in issue 59 in more detail.
- 2. Workers requested are unable to contact the Parsl client due to one or more issues listed below:
  - Parsl client does not have a public IP (e.g. laptop on wifi). If your network does not provide public IPs, the simple solution is to ssh over to a machine that is public facing. Machines provisioned from cloud-vendors setup with public IPs are another option.
  - Parsl hasn't autodetected the public IP. See Workers do not connect back to Parsl for more details.
  - Firewall restrictions that block certain port ranges. If there is a certain port range that is **not** blocked, you may specify that via configuration:

```
from libsubmit.providers import Cobalt
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
```

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```
config = Config(
    executors=[
        HighThroughputExecutor(
            label='ALCF_theta_local',
            provider=Cobalt(),
            worer_port_range=('50000,55000'),
            interchange_port_range=('50000,55000')
        )
    ],
)
```

### How can I start a Jupyter notebook over SSH?

#### Run

```
jupyter notebook --no-browser --ip=`/sbin/ip route get 8.8.8.8 | awk '{print $NF;exit}'`
```

for a Jupyter notebook, or

jupyter lab --no-browser --ip=`/sbin/ip route get 8.8.8.8 | awk '{print \$NF;exit}'`

for Jupyter lab (recommended). If that doesn't work, see these instructions.

#### How can I sync my conda environment and Jupyter environment?

Run:

conda install nb\_conda

Now all available conda environments (for example, one created by following the instructions *in the quickstart guide*) will automatically be added to the list of kernels.

#### Addressing SerializationError

As of v1.0.0, Parsl will raise a *SerializationError* when it encounters an object that Parsl cannot serialize. This applies to objects passed as arguments to an app, as well as objects returned from the app.

Parsl uses dill and pickle to serialize Python objects to/from functions. Therefore, Python apps can only use input and output objects that can be serialized by dill or pickle. For example the following data types are known to have issues with serializability :

- Closures
- Objects of complex classes with no \_\_dict\_\_ or \_\_getstate\_\_ methods defined
- System objects such as file descriptors, sockets and locks (e.g threading.Lock)

If Parsl raises a SerializationError, first identify what objects are problematic with a quick test:

```
import pickle
# If non-serializable you will get a TypeError
pickle.dumps(YOUR_DATA_OBJECT)
```

If the data object simply is complex, please refer here for more details on adding custom mechanisms for supporting serialization.

# How do I cite Parsl?

To cite Parsl in publications, please use the following:

Babuji, Y., Woodard, A., Li, Z., Katz, D. S., Clifford, B., Kumar, R., Lacinski, L., Chard, R., Wozniak, J., Foster, I., Wilde, M., and Chard, K., Parsl: Pervasive Parallel Programming in Python. 28th ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC). 2019. https://doi.org/10.1145/3307681.3325400

or

@inproceedings	{babuji19parsl,
author	= {Babuji, Yadu and
	Woodard, Anna and
	Li, Zhuozhao and
	Katz, Daniel S. and
	Clifford, Ben and
	Kumar, Rohan and
	Lacinski, Lukasz and
	Chard, Ryan and
	Wozniak, Justin and
	Foster, Ian and
	Wilde, Mike and
	Chard, Kyle},
title	<pre>= {Parsl: Pervasive Parallel Programming in Python},</pre>
booktitle	= {28th ACM International Symposium on High-Performance Parallel and $\Box$
$\rightarrow$ Distributed	Computing (HPDC)},
doi	= {10.1145/3307681.3325400},
year	$= \{2019\},$
url	= {https://doi.org/10.1145/3307681.3325400}
}	

# **API Reference guide**

# Core

parsl.app.app.python_app	Decorator function for making python apps.
parsl.app.app.bash_app	Decorator function for making bash apps.
parsl.app.app.join_app	Decorator function for making join apps
parsl.dataflow.futures.AppFuture	An AppFuture wraps a sequence of Futures which may fail and be retried.
parsl.dataflow.dflow.DataFlowKernelLoader	Manage which DataFlowKernel is active.
parsl.monitoring.MonitoringHub	

### parsl.app.app.python\_app

parsl.app.app.python\_app(function: Callable | None = None, data\_flow\_kernel: DataFlowKernel | None = None, cache: bool = False, executors: List[str] | Literal['all'] = 'all', ignore\_for\_cache: Sequence[str] | None = None)  $\rightarrow$  Callable

Decorator function for making python apps.

### Parameters

- function (function) Do not pass this keyword argument directly. This is needed in order to allow for omitted parenthesis, for example, @python\_app if using all defaults or @python\_app(walltime=120). If the decorator is used alone, function will be the actual function being decorated, whereas if it is called with arguments, function will be None. Default is None.
- data\_flow\_kernel (DataFlowKernel) The DataFlowKernel responsible for managing this app. This can be omitted only after calling parsl.dataflow.dflow. DataFlowKernelLoader.load(). Default is None.
- **executors** (*string or list*) Labels of the executors that this app can execute over. Default is 'all'.
- cache (bool) Enable caching of the app call. Default is False.
- **ignore\_for\_cache** ((*sequence* /*None*)) Names of arguments which will be ignored by the caching mechanism.

#### parsl.app.app.bash\_app

parsl.app.app.bash\_app(function: Callable | None = None, data\_flow\_kernel: DataFlowKernel | None = None, cache: bool = False, executors: List[str] | Literal['all'] = 'all', ignore\_for\_cache: Sequence[str] | None = None)  $\rightarrow$  Callable

Decorator function for making bash apps.

### Parameters

- **function** (*function*) Do not pass this keyword argument directly. This is needed in order to allow for omitted parenthesis, for example, @bash\_app if using all defaults or @bash\_app(walltime=120). If the decorator is used alone, function will be the actual function being decorated, whereas if it is called with arguments, function will be None. Default is None.
- data\_flow\_kernel (DataFlowKernel) The DataFlowKernel responsible for managing this app. This can be omitted only after calling parsl.dataflow.dflow. DataFlowKernelLoader.load(). Default is None.
- walltime (*int*) Walltime for app in seconds. Default is 60.
- **executors** (*string or list*) Labels of the executors that this app can execute over. Default is 'all'.
- cache (bool) Enable caching of the app call. Default is False.
- **ignore\_for\_cache** ((*list*/*None*)) Names of arguments which will be ignored by the caching mechanism.

### parsl.app.app.join\_app

 $parsl.app.app.join_app(function: Callable | None = None, data_flow_kernel: DataFlowKernel | None = None, cache: bool = False, ignore_for_cache: Sequence[str] | None = None) \rightarrow Callable$ 

Decorator function for making join apps

#### Parameters

- **function** (*function*) Do not pass this keyword argument directly. This is needed in order to allow for omitted parenthesis, for example, @python\_app if using all defaults or @python\_app(walltime=120). If the decorator is used alone, function will be the actual function being decorated, whereas if it is called with arguments, function will be None. Default is None.
- data\_flow\_kernel (DataFlowKernel) The DataFlowKernel responsible for managing this app. This can be omitted only after calling parsl.dataflow.dflow. DataFlowKernelLoader.load(). Default is None.
- **cache** (*bool*) Enable caching of the app call. Default is False.
- **ignore\_for\_cache** ((*sequence*/*None*)) Names of arguments which will be ignored by the caching mechanism.

#### parsl.dataflow.futures.AppFuture

#### class parsl.dataflow.futures.AppFuture(task\_record: TaskRecord)

An AppFuture wraps a sequence of Futures which may fail and be retried.

The AppFuture will wait for the DFK to provide a result from an appropriate parent future, through parent\_callback. It will set its result to the result of that parent future, if that parent future completes without an exception. This result setting should cause .result(), .exception() and done callbacks to fire as expected.

The AppFuture will not set its result to the result of the parent future, if that parent future completes with an exception, and if that parent future has retries left. In that case, no result(), exception() or done callbacks should report a result.

The AppFuture will set its result to the result of the parent future, if that parent future completes with an exception and if that parent future has no retries left, or if it has no retry field. .result(), .exception() and done callbacks should give a result as expected when a Future has a result set

The parent future may return a RemoteExceptionWrapper as a result and AppFuture will treat this an an exception for the above retry and result handling behaviour.

**\_\_init\_\_**(*task\_record:* TaskRecord)  $\rightarrow$  None

Initialize the AppFuture.

Args:

#### **KWargs:**

• task\_record : The TaskRecord for the task represented by this future.

init(task_record)	Initialize the AppFuture.
add_done_callback(fn)	Attaches a callable that will be called when the future finishes.
cancel()	Cancel the future if possible.
cancelled()	Return True if the future was cancelled.
done()	Return True if the future was cancelled or finished executing.
<pre>exception([timeout])</pre>	Return the exception raised by the call that the future represents.
result([timeout])	Return the result of the call that the future represents.
<pre>running()</pre>	Return True if the future is currently executing.
<pre>set_exception(exception)</pre>	Sets the result of the future as being the given exception.
<pre>set_result(result)</pre>	Sets the return value of work associated with the fu- ture.
<pre>set_running_or_notify_cancel()</pre>	Mark the future as running or process any cancel no- tifications.
task_status()	Returns the status of the task that will provide the value for this future.

# Attributes

outputs	
stderr	Return app stderr.
stdout	Return app stdout.
tid	

 $cancel() \rightarrow bool$ 

Cancel the future if possible.

Returns True if the future was cancelled, False otherwise. A future cannot be cancelled if it is running or has already completed.

### $cancelled() \rightarrow bool$

Return True if the future was cancelled.

```
property outputs: Sequence[DataFuture]
```

### property stderr: None | str | DataFuture

Return app stderr. If stdout was specified as a string, then this property will return that string. If stdout was specified as a File, then this property will return a DataFuture representing that file stageout. TODO: this can be a tuple too I think?

### property stdout: None | str | DataFuture

Return app stdout. If stdout was specified as a string, then this property will return that string. If stdout was specified as a File, then this property will return a DataFuture representing that file stageout. TODO: this can be a tuple too I think?

#### $task_status() \rightarrow str$

Returns the status of the task that will provide the value for this future. This may not be in-sync with the result state of this future - for example, task\_status might return 'done' but self.done() might not be true (which in turn means self.result() and self.exception() might block).

The actual status description strings returned by this method are likely to change over subsequent versions of parsl, as use-cases and infrastructure are worked out.

It is expected that the status values will be from a limited set of strings (so that it makes sense, for example, to group and count statuses from many futures).

It is expected that might be a non-trivial cost in acquiring the status in future (for example, by communicating with a remote worker).

Returns: str

property tid: int

### parsl.dataflow.dflow.DataFlowKernelLoader

#### class parsl.dataflow.dflow.DataFlowKernelLoader

Manage which DataFlowKernel is active.

This is a singleton class containing only class methods. You should not need to instantiate this class.

\_\_init\_\_()

## Methods

init()	
clear()	Clear the active DataFlowKernel so that a new one can be loaded.
dfk()	Return the currently-loaded DataFlowKernel.
load([config])	Load a DataFlowKernel.
<pre>wait_for_current_tasks()</pre>	Waits for all tasks in the task list to be completed, by waiting for their AppFuture to be completed.

### classmethod clear() $\rightarrow$ None

Clear the active DataFlowKernel so that a new one can be loaded.

#### classmethod dfk() $\rightarrow$ DataFlowKernel

Return the currently-loaded DataFlowKernel.

#### **classmethod load**(*config*: Config | *None* = *None*) → *DataFlowKernel*

Load a DataFlowKernel.

#### **Parameters**

**config** (-) – Configuration to load. This config will be passed to a new DataFlowKernel instantiation which will be set as the active DataFlowKernel.

### Returns

The loaded DataFlowKernel object.

#### **Return type**

### • DataFlowKernel

### <code>classmethod wait\_for\_current\_tasks()</code> $\rightarrow$ None

Waits for all tasks in the task list to be completed, by waiting for their AppFuture to be completed. This method will not necessarily wait for any tasks added after cleanup has started such as data stageout.

## parsl.monitoring.MonitoringHub

\_\_init\_\_(hub\_address: str, hub\_port: int | None = None, hub\_port\_range: Tuple[int, int] = (55050, 56000), workflow\_name: str | None = None, workflow\_version: str | None = None, logging\_endpoint: str | None = None, logdir: str | None = None, monitoring\_debug: bool = False, resource\_monitoring\_enabled: bool = True, resource\_monitoring\_interval: float = 30)

### Parameters

- hub\_address (str) The ip address at which the workers will be able to reach the Hub.
- hub\_port (*int*) The UDP port to which workers will be able to deliver messages to the monitoring router. Note that despite the similar name, this is not related to hub\_port\_range. Default: None
- hub\_port\_range (tuple(int, int)) The port range for a ZMQ channel from an executor process (for example, the interchange in the High Throughput Executor) to deliver monitoring messages to the monitoring router. Note that despite the similar name, this is not related to hub\_port. Default: (55050, 56000)
- **workflow\_name** (*str*) The name for the workflow. Default to the name of the parsl script
- **workflow\_version** (*str*) The version of the workflow. Default to the beginning datetime of the parsl script
- **logging\_endpoint** (*str*) The database connection url for monitoring to log the information. These URLs follow RFC-1738, and can include username, password, hostname, database name. Default: sqlite, in the configured run\_dir.
- logdir (str) Parsl log directory paths. Logs and temp files go here. Default: '.'
- monitoring\_debug (Bool) Enable monitoring debug logging. Default: False
- **resource\_monitoring\_enabled** (*boolean*) Set this field to True to enable logging of information from the worker side. This will include environment information such as start time, hostname and block id, along with periodic resource usage of each task. Default: True
- **resource\_monitoring\_interval** (*float*) The time interval, in seconds, at which the monitoring records the resource usage of each task. If set to 0, only start and end information will be logged, and no periodic monitoring will be made. Default: 30 seconds

init(hub_address[, hub_port,])	<b>param hub_address</b> The ip address at which the workers will be able to reach the Hub.
close()	
send(mtype, message)	
<pre>start(run_id, dfk_run_dir, config_run_dir)</pre>	
$close() \rightarrow None$	

**send**(*mtype: MessageType, message: Any*)  $\rightarrow$  None

**start**(*run\_id: str, dfk\_run\_dir: str, config\_run\_dir: str* | *PathLike*)  $\rightarrow$  int

# Configuration

parsl.config.Config	Specification of Parsl configuration options.
parsl.set_stream_logger	Add a stream log handler.
parsl.set_file_logger	Add a file log handler.
<pre>parsl.addresses.address_by_hostname</pre>	Returns the hostname of the local host.
<pre>parsl.addresses.address_by_interface</pre>	Returns the IP address of the given interface name, e.g.
parsl.addresses.address_by_query	Finds an address for the local host by querying ipify.
<pre>parsl.addresses.address_by_route</pre>	Finds an address for the local host by querying the local
	routing table for the route to Google DNS.
<pre>parsl.utils.get_all_checkpoints</pre>	Finds the checkpoints from all runs in the rundir.
<pre>parsl.utils.get_last_checkpoint</pre>	Finds the checkpoint from the last run, if one exists.

## parsl.config.Config

```
class parsl.config.Config(executors: Iterable[ParslExecutor] | None = None, app_cache: bool = True,
                                 checkpoint_files: Sequence[str] | None = None, checkpoint_mode: None |
                                 Literal['task_exit'] | Literal['periodic'] | Literal['dfk_exit'] | Literal['manual'] =
                                 None, checkpoint_period: str | None = None, garbage_collect: bool = True,
                                 internal_tasks_max_threads: int = 10, retries: int = 0, retry_handler:
                                 Callable[[Exception, TaskRecord], float] | None = None, run_dir: str = 'runinfo',
                                 std_autopath: Callable | None = None, strategy: str | None = 'simple',
                                 strategy_period: float | int = 5, max_idletime: float = 120.0, monitoring:
                                 MonitoringHub | None = None, usage_tracking: bool = False, initialize_logging:
                                 bool = True)
```

Specification of Parsl configuration options.

#### **Parameters**

- **executors** (sequence of ParslExecutor, optional) List (or other iterable) of ParslExecutor instances to use for executing tasks. Default is (*ThreadPoolExecutor()*,).
- app\_cache (bool, optional) Enable app caching. Default is True.
- **checkpoint\_files** (sequence of str, optional) List of paths to checkpoint files. See parsl.utils.get\_all\_checkpoints() and parsl.utils.get\_last\_checkpoint() for helpers. Default is None.
- **checkpoint\_mode** (*str, optional*) Checkpoint mode to use, can be 'dfk\_exit', 'task\_exit', 'periodic' or 'manual'. If set to None, checkpointing will be disabled. Default is None.
- **checkpoint\_period** (*str*, *optional*) Time interval (in "HH:MM:SS") at which to checkpoint completed tasks. Only has an effect if checkpoint\_mode='periodic'.
- **garbage\_collect** (*bool. optional.*) Delete task records from DFK when tasks have completed. Default: True
- **internal\_tasks\_max\_threads** (*int*, *optional*) Maximum number of threads to allocate for submit side internal tasks such as some data transfers or @joinapps Default is 10.
- **monitoring** (MonitoringHub, optional) The config to use for database monitoring. Default is None which does not log to a database.
- **retries** (*int*, *optional*) Set the number of retries (or available retry budget when using retry\_handler) in case of failure. Default is 0.
- **retry\_handler** (*function*, *optional*) A user pluggable handler to decide if/how a task retry should happen. If no handler is specified, then each task failure incurs a retry cost of 1.
- run\_dir (str, optional) Path to run directory. Default is 'runinfo'.
- **std\_autopath** (*function*, *optional*) Sets the function used to generate stdout/stderr specifications when parsl.AUTO\_LOGPATH is used. If no function is specified, generates paths that look like: rundir/NNN/task\_logs/X/task\_{id}\_{name}{label}.{out/err}
- **strategy** (*str*, *optional*) Strategy to use for scaling blocks according to workflow needs. Can be 'simple', 'htex\_auto\_scale', 'none' or None. If 'none' or None, dynamic scaling will be disabled. Default is 'simple'. The literal value None is deprecated.
- **strategy\_period** (*float or int*, *optional*) How often the scaling strategy should be executed. Default is 5 seconds.
- **max\_idletime** (*float*, *optional*) The maximum idle time allowed for an executor before strategy could shut down unused blocks. Default is 120.0 seconds.
- **usage\_tracking** (*bool*, *optional*) Set this field to True to opt-in to Parsl's usage tracking system. Parsl only collects minimal, non personally-identifiable, information used for reporting to our funding agencies. Default is False.
- **initialize\_logging** (*bool*, *optional*) Make DFK optionally not initialize any logging. Log messages will still be passed into the python logging system under the parsl logger name, but the logging system will not by default perform any further log system configuration. Most noticeably, it will not create a parsl.log logfile. The use case for this is when parsl is used as a library in a bigger system which wants to configure logging in a way that makes sense for that bigger system as a whole.

\_\_\_init\_\_\_(executors: Iterable[ParslExecutor] | None = None, app\_cache: bool = True, checkpoint\_files: Sequence[str] | None = None, checkpoint\_mode: None | Literal['task\_exit'] | Literal['periodic'] | Literal['dfk\_exit'] | Literal['manual'] = None, checkpoint\_period: str | None = None, garbage\_collect: bool = True, internal\_tasks\_max\_threads: int = 10, retries: int = 0, retry\_handler: Callable[[Exception, TaskRecord], float] | None = None, run\_dir: str = 'runinfo', std\_autopath: Callable | None = None, strategy: str | None = 'simple', strategy\_period: float | int = 5, max\_idletime: float = 120.0, monitoring: MonitoringHub | None = None, usage\_tracking: bool = False, initialize\_logging: bool = True) → None

## **Methods**

\_\_init\_\_([executors, app\_cache, ...])

get\_usage\_information()

### Attributes

executors

property executors: Sequence[ParslExecutor]

get\_usage\_information()

## parsl.set\_stream\_logger

parsl.set\_stream\_logger(name: str = 'parsl', level: int = 10, format\_string: str | None = None, stream: TextIOWrapper | None = None)  $\rightarrow$  Logger

Add a stream log handler.

### Parameters

- **name** (-) Set the logger name.
- **level** (-) Set to logging.DEBUG by default.
- **format\_string** (-) Set to None by default.
- **stream** (-) Specify sys.stdout or sys.stderr for stream. If not specified, the default stream for logging.StreamHandler is used.

#### Returns

• logger for specified name

# parsl.set\_file\_logger

pars1.set\_file\_logger(filename: str, name: str = 'parsl', level: int = 10, format\_string: str | None = None) →
Logger

Add a file log handler.

#### **Parameters**

- filename (-) Name of the file to write logs to
- name (-) Logger name
- **level** (-) Set the logging level.
- format\_string (-) Set the format string

#### Returns

• logger for specified name

### parsl.addresses.address\_by\_hostname

### parsl.addresses.address\_by\_hostname() $\rightarrow$ str

Returns the hostname of the local host.

This will return an unusable value when the hostname cannot be resolved from workers.

## parsl.addresses.address\_by\_interface

### parsl.addresses.address\_by\_interface(ifname: str) → str

Returns the IP address of the given interface name, e.g. 'eth0'

This is taken from a Stack Overflow answer: https://stackoverflow.com/questions/24196932/ how-can-i-get-the-ip-address-of-eth0-in-python#24196955

### Parameters

ifname (str) – Name of the interface whose address is to be returned. Required.

## parsl.addresses.address\_by\_query

#### pars1.addresses.address\_by\_query(*timeout: float* = 30) $\rightarrow$ str

Finds an address for the local host by querying ipify. This may return an unusable value when the host is behind NAT, or when the internet-facing address is not reachable from workers. Parameters: \_\_\_\_\_

#### timeout

[float] Timeout for the request in seconds. Default: 30s

### parsl.addresses.address\_by\_route

#### parsl.addresses.address\_by\_route() $\rightarrow$ str

Finds an address for the local host by querying the local routing table for the route to Google DNS.

This will return an unusable value when the internet-facing address is not reachable from workers.

### parsl.utils.get\_all\_checkpoints

Finds the checkpoints from all runs in the rundir.

#### **Kwargs:**

• rundir(str) : Path to the runinfo directory

#### Returns

• a list suitable for the checkpoint\_files parameter of Config

### parsl.utils.get\_last\_checkpoint

Finds the checkpoint from the last run, if one exists.

Note that checkpoints are incremental, and this helper will not find previous checkpoints from earlier than the most recent run. If you want that behaviour, see *get\_all\_checkpoints*.

#### **Kwargs:**

• rundir(str) : Path to the runinfo directory

#### Returns

• a list suitable for the checkpoint\_files parameter of *Config*, with 0 or 1 elements

# Channels

parsl.channels.base.Channel	Channels are abstractions that enable Execution- Providers to talk to resource managers of remote compute facilities.
parsl.channels.LocalChannel	This is not even really a channel, since opening a local shell is not heavy and done so infrequently that they do not need a persistent channel
parsl.channels.SSHChannel	SSH persistent channel.
parsl.channels.OAuthSSHChannel	SSH persistent channel.
parsl.channels.SSHInteractiveLoginChannel	SSH persistent channel.

### parsl.channels.base.Channel

#### class parsl.channels.base.Channel

Channels are abstractions that enable ExecutionProviders to talk to resource managers of remote compute facilities.

For certain resources such as campus clusters or supercomputers at research laboratories, resource requirements may require authentication. For instance some resources may allow access to their job schedulers from only their login-nodes which require you to authenticate through SSH, or require two factor authentication.

The simplest Channel, *LocalChannel*, executes commands locally in a shell, while the *SSHChannel* authenticates you to remote systems.

Channels provide the ability to execute commands remotely, using the execute\_wait method, and manipulate the remote file system using methods such as push\_file, pull\_file and makedirs.

Channels should ensure that each launched command runs in a new process group, so that providers (such as AdHocProvider and LocalProvider) which terminate long running commands using process groups can do so.

\_\_init\_\_()

### Methods

init()	
abspath(path)	Return the absolute path.
close()	Closes the channel.
<pre>execute_wait(cmd[, walltime, envs])</pre>	Executes the cmd, with a defined walltime.
<i>isdir</i> (path)	Return true if the path refers to an existing directory.
<i>makedirs</i> (path[, mode, exist_ok])	Create a directory.
<pre>pull_file(remote_source, local_dir)</pre>	Transport file on the remote side to a local directory
<pre>push_file(source, dest_dir)</pre>	Channel will take care of moving the file from source
	to the destination directory

#### Attributes

script\_dir

This is a property.

**abstract abspath**(*path: str*)  $\rightarrow$  str

Return the absolute path.

#### Parameters

**path** (*str*) – Path for which the absolute path will be returned.

abstract close()  $\rightarrow$  bool

Closes the channel. Clean out any auth credentials.

Parameters None –

Returns Bool **abstract execute\_wait**(*cmd: str, walltime: int* = 0, *envs: Dict[str, str]* = {})  $\rightarrow$  Tuple[int, str, str] Executes the cmd, with a defined walltime.

#### Parameters

- cmd (-) Command string to execute over the channel
- walltime (-) Timeout in seconds

#### **KWargs:**

• envs (Dict[str, str]) : Environment variables to push to the remote side

#### Returns

• (exit\_code, stdout, stderr) (int, string, string)

#### **abstract** isdir(*path: str*) $\rightarrow$ bool

Return true if the path refers to an existing directory.

#### Parameters

**path** (*str*) – Path of directory to check.

**abstract makedirs**(*path: str, mode: int = 329, exist\_ok: bool = False*)  $\rightarrow$  None

Create a directory.

If intermediate directories do not exist, they will be created.

#### Parameters

- **path** (*str*) Path of directory to create.
- mode (*int*) Permissions (posix-style) for the newly-created directory.
- exist\_ok (bool) If False, raise an OSError if the target directory already exists.
- **abstract pull\_file**(*remote\_source: str*, *local\_dir: str*)  $\rightarrow$  str

Transport file on the remote side to a local directory

#### Parameters

- remote\_source (string) remote\_source
- **local\_dir** (*string*) Local directory to copy to

#### Returns

destination\_path (string)

**abstract push\_file**(*source: str, dest\_dir: str*) → str

Channel will take care of moving the file from source to the destination directory

### Parameters

- source (string) Full filepath of the file to be moved
- dest\_dir (string) Absolute path of the directory to move to

#### Returns

destination\_path (string)

#### abstract property script\_dir: str

This is a property. Returns the directory assigned for storing all internal scripts such as scheduler submit scripts. This is usually where error logs from the scheduler would reside on the channel destination side.

# Parameters

None (-) –

### Returns

• Channel script dir

# parsl.channels.LocalChannel

### class parsl.channels.LocalChannel(userhome='.', envs={}, script\_dir=None)

This is not even really a channel, since opening a local shell is not heavy and done so infrequently that they do not need a persistent channel

# \_\_init\_\_(userhome='.', envs={}, script\_dir=None)

Initialize the local channel. script\_dir is required by set to a default.

### **KwArgs:**

- userhome (string): (default='.') This is provided as a way to override and set a specific userhome
- envs (dict) : A dictionary of env variables to be set when launching the shell
- script\_dir (string): Directory to place scripts

# Methods

<i>init</i> ([userhome, envs, script_dir])	Initialize the local channel.
abspath(path)	Return the absolute path.
close()	There's nothing to close here, and this really doesn't do anything
<pre>execute_wait(cmd[, walltime, envs])</pre>	Synchronously execute a commandline string on the shell.
<i>isdir</i> (path)	Return true if the path refers to an existing directory.
<i>makedirs</i> (path[, mode, exist_ok])	Create a directory.
<pre>pull_file(remote_source, local_dir)</pre>	Transport file on the remote side to a local directory
<pre>push_file(source, dest_dir)</pre>	If the source files dirpath is the same as dest_dir, a copy is not necessary, and nothing is done.

## Attributes

script_dir	This is a property.
------------	---------------------

### abspath(path)

Return the absolute path.

Parameters

**path** (*str*) – Path for which the absolute path will be returned.

#### close()

There's nothing to close here, and this really doesn't do anything

Returns

• False, because it really did not "close" this channel.

#### execute\_wait(cmd, walltime=None, envs={})

Synchronously execute a commandline string on the shell.

#### **Parameters**

- cmd (-) Commandline string to execute
- walltime (-) walltime in seconds, this is not really used now.

#### **Kwargs:**

• envs (dict) : Dictionary of env variables. This will be used to override the envs set at channel initialization.

#### Returns

Return code from the execution, -1 on fail - stdout : stdout string - stderr : stderr string

#### **Return type**

• retcode

Raises: None.

### isdir(path)

Return true if the path refers to an existing directory.

### Parameters

**path** (*str*) – Path of directory to check.

### makedirs(path, mode=448, exist\_ok=False)

Create a directory.

If intermediate directories do not exist, they will be created.

#### **Parameters**

- **path** (*str*) Path of directory to create.
- mode (*int*) Permissions (posix-style) for the newly-created directory.
- exist\_ok (bool) If False, raise an OSError if the target directory already exists.

#### pull\_file(remote\_source, local\_dir)

Transport file on the remote side to a local directory

### **Parameters**

- **remote\_source** (*string*) remote\_source
- local\_dir (string) Local directory to copy to

#### Returns

destination\_path (string)

### push\_file(source, dest\_dir)

If the source files dirpath is the same as dest\_dir, a copy is not necessary, and nothing is done. Else a copy is made.

#### **Parameters**

- **source** (-) Path to the source file
- **dest\_dir** (-) Path to the directory to which the files is to be copied

#### Returns

Absolute path of the destination file

### **Return type**

• destination\_path (String)

#### Raises

- FileCopyException – If file copy failed.

#### property script\_dir

This is a property. Returns the directory assigned for storing all internal scripts such as scheduler submit scripts. This is usually where error logs from the scheduler would reside on the channel destination side.

#### **Parameters**

None (-) –

### Returns

· Channel script dir

### parsl.channels.SSHChannel

# 

SSH persistent channel. This enables remote execution on sites accessible via ssh. It is assumed that the user has setup host keys so as to ssh to the remote host. Which goes to say that the following test on the commandline should work:

>>> ssh <username>@<hostname>

Initialize a persistent connection to the remote system. We should know at this point whether ssh connectivity is possible

Parameters hostname (-) – Hostname

#### **KWargs:**

- username (string) : Username on remote system
- password (string) : Password for remote system
- port : The port designated for the ssh connection. Default is 22.
- script\_dir (string) : Full path to a script dir where generated scripts could be sent to.
- envs (dict) : A dictionary of environment variables to be set when executing commands
- key\_filename (string or list): the filename, or list of filenames, of optional private key(s)

Raises:

init(hostname[, username, password,])	Initialize a persistent connection to the remote system.
abspath(path)	Return the absolute path on the remote side.
close()	Closes the channel.
<pre>execute_wait(cmd[, walltime, envs])</pre>	Synchronously execute a commandline string on the shell.
<i>isdir</i> (path)	Return true if the path refers to an existing directory.
<i>makedirs</i> (path[, mode, exist_ok])	Create a directory on the remote side.
<pre>prepend_envs(cmd[, env])</pre>	
<pre>pull_file(remote_source, local_dir)</pre>	Transport file on the remote side to a local directory
<pre>push_file(local_source, remote_dir)</pre>	Transport a local file to a directory on a remote ma- chine

## **Attributes**

scrint dir	This is a property
SCI IPC_UII	This is a property.

# abspath(path)

Return the absolute path on the remote side.

Parameters

**path** (*str*) – Path for which the absolute path will be returned.

# close()

Closes the channel. Clean out any auth credentials.

Parameters None –

#### Returns

Bool

### execute\_wait(cmd, walltime=2, envs={})

Synchronously execute a commandline string on the shell.

### **Parameters**

- cmd (-) Commandline string to execute
- walltime (-) walltime in seconds

### **Kwargs:**

• envs (dict) : Dictionary of env variables

#### Returns

Return code from the execution, -1 on fail - stdout : stdout string - stderr : stderr string

### **Return type**

• retcode

Raises: None.

### isdir(path)

Return true if the path refers to an existing directory.

#### Parameters

**path** (*str*) – Path of directory on the remote side to check.

### makedirs(path, mode=448, exist\_ok=False)

Create a directory on the remote side.

If intermediate directories do not exist, they will be created.

### **Parameters**

- **path** (*str*) Path of directory on the remote side to create.
- mode (int) Permissions (posix-style) for the newly-created directory.
- exist\_ok (bool) If False, raise an OSError if the target directory already exists.

#### prepend\_envs(cmd, env={})

### pull\_file(remote\_source, local\_dir)

Transport file on the remote side to a local directory

### Parameters

• **remote\_source** (-) - remote\_source

• local\_dir (-) – Local directory to copy to

#### Returns

Local path to file

#### **Return type**

• str

# Raises

- - FileExists Name collision at local directory.
- - FileCopyException FileCopy failed.

### push\_file(local\_source, remote\_dir)

Transport a local file to a directory on a remote machine

### Parameters

- **local\_source** (-) Path
- remote\_dir (-) Remote path

# Returns

Path to copied file on remote machine

#### **Return type**

• str

# Raises

- - BadScriptPath if script path on the remote side is bad
- - BadPermsScriptPath You do not have perms to make the channel script dir
- - FileCopyException FileCopy failed.

### property script\_dir

This is a property. Returns the directory assigned for storing all internal scripts such as scheduler submit scripts. This is usually where error logs from the scheduler would reside on the channel destination side.

#### **Parameters**

None (-) –

Returns

· Channel script dir

### parsl.channels.OAuthSSHChannel

class pars1.channels.OAuthSSHChannel(hostname, username=None, script\_dir=None, envs=None, port=22)

SSH persistent channel. This enables remote execution on sites accessible via ssh. This channel uses Globus based OAuth tokens for authentication.

\_\_init\_\_(hostname, username=None, script\_dir=None, envs=None, port=22)

Initialize a persistent connection to the remote system. We should know at this point whether ssh connectivity is possible

Parameters hostname (-) – Hostname

### **KWargs:**

- username (string) : Username on remote system
- script\_dir (string) : Full path to a script dir where generated scripts could be sent to.
- envs (dict) : A dictionary of env variables to be set when executing commands
- port (int) : Port at which the SSHService is running

Raises:

# **Methods**

init(hostname[, username, script_dir,])	Initialize a persistent connection to the remote system.
abspath(path)	Return the absolute path on the remote side.
close()	Closes the channel.
<pre>execute_wait(cmd[, walltime, envs])</pre>	Synchronously execute a commandline string on the shell.
isdir(path)	Return true if the path refers to an existing directory.
<pre>makedirs(path[, mode, exist_ok])</pre>	Create a directory on the remote side.
prepend_envs(cmd[, env])	
<pre>pull_file(remote_source, local_dir)</pre>	Transport file on the remote side to a local directory
<pre>push_file(local_source, remote_dir)</pre>	Transport a local file to a directory on a remote ma- chine

### **Attributes**

script\_dir

This is a property.

#### close()

Closes the channel. Clean out any auth credentials.

Parameters None –

Returns Bool

### execute\_wait(cmd, walltime=60, envs={})

Synchronously execute a commandline string on the shell.

This command does NOT honor walltime currently.

#### **Parameters**

**cmd** (-) – Commandline string to execute

#### **Kwargs:**

- walltime (int) : walltime in seconds
- envs (dict) : Dictionary of env variables

#### Returns

Return code from the execution, -1 on fail - stdout : stdout string - stderr : stderr string

#### **Return type**

retcode

Raises: None.

### parsl.channels.SSHInteractiveLoginChannel

### **class** parsl.channels.**SSHInteractiveLoginChannel**(*hostname*, *username=None*, *password=None*,

script\_dir=None, envs=None)

SSH persistent channel. This enables remote execution on sites accessible via ssh. This channel supports interactive login and is appropriate when keys are not set up.

\_\_init\_\_(hostname, username=None, password=None, script\_dir=None, envs=None)

Initialize a persistent connection to the remote system. We should know at this point whether ssh connectivity is possible

Parameters hostname (-) – Hostname

### **KWargs:**

- username (string) : Username on remote system
- password (string) : Password for remote system
- script\_dir (string) : Full path to a script dir where generated scripts could be sent to.

• envs (dict) : A dictionary of env variables to be set when executing commands

Raises:

# Methods

init(hostname[, username, password,])	Initialize a persistent connection to the remote system.
abspath(path)	Return the absolute path on the remote side.
close()	Closes the channel.
<pre>execute_wait(cmd[, walltime, envs])</pre>	Synchronously execute a commandline string on the shell.
isdir(path)	Return true if the path refers to an existing directory.
<pre>makedirs(path[, mode, exist_ok])</pre>	Create a directory on the remote side.
<pre>prepend_envs(cmd[, env])</pre>	
<pre>pull_file(remote_source, local_dir)</pre>	Transport file on the remote side to a local directory
<pre>push_file(local_source, remote_dir)</pre>	Transport a local file to a directory on a remote ma- chine

### Attributes

scrin	t dır
JCTTP	C_GII

This is a property.

# Data management

parsl.app.futures.DataFuture	A datafuture points at an AppFuture.
parsl.data_provider.data_manager.	The DataManager is responsible for transferring input
DataManager	and output data.
parsl.data_provider.staging.Staging	This class defines the interface for file staging providers.
parsl.data_provider.files.File	The Parsl File Class.
parsl.data_provider.ftp. FTPSeparateTaskStaging	Performs FTP staging as a separate parsl level task.
parsl.data_provider.ftp.FTPInTaskStaging	Performs FTP staging as a wrapper around the applica- tion task.
<pre>parsl.data_provider.file_noop.</pre>	
NoOpFileStaging	
parsl.data_provider.globus.GlobusStaging	Specification for accessing data on a remote executor via Globus.
parsl.data_provider.http.	A staging provider that Performs HTTP and HTTPS
HTTPSeparateTaskStaging	staging as a separate parsl-level task.
parsl.data_provider.http.HTTPInTaskStaging	A staging provider that performs HTTP and HTTPS staging as in a wrapper around each task.
<pre>parsl.data_provider.rsync.RSyncStaging</pre>	This staging provider will execute rsync on worker nodes to stage in files from a remote location.

# parsl.app.futures.DataFuture

```
class pars1.app.futures.DataFuture(fut: Future, file_obj: File, tid: int | None = None)
```

A datafuture points at an AppFuture.

We are simply wrapping a AppFuture, and adding the specific case where, if the future is resolved i.e file exists, then the DataFuture is assumed to be resolved.

**\_\_\_init\_\_\_**(*fut: Future, file\_obj: File, tid: int* | *None* = *None*)  $\rightarrow$  None

Construct the DataFuture object.

If the file\_obj is a string convert to a File.

# Parameters

- **fut** (-) AppFuture that this DataFuture will track
- **file\_obj** (-) Something representing file(s)

# **Kwargs:**

• tid (task\_id) : Task id that this DataFuture tracks

# **Methods**

<pre>init(fut, file_obj[, tid])</pre>	Construct the DataFuture object.
<pre>add_done_callback(fn)</pre>	Attaches a callable that will be called when the future
	finishes.
cancel()	Cancel the future if possible.
cancelled()	Return True if the future was cancelled.
done()	Return True if the future was cancelled or finished executing.
<pre>exception([timeout])</pre>	Return the exception raised by the call that the future represents.
<pre>parent_callback(parent_fu)</pre>	Callback from executor future to update the parent.
result([timeout])	Return the result of the call that the future represents.
running()	Return True if the future is currently executing.
<pre>set_exception(exception)</pre>	Sets the result of the future as being the given excep- tion.
<pre>set_result(result)</pre>	Sets the return value of work associated with the fu- ture.
<pre>set_running_or_notify_cancel()</pre>	Mark the future as running or process any cancel no- tifications.

### **Attributes**

filename	Filepath of the File object this datafuture represents.
filepath	Filepath of the File object this datafuture represents.
tid	Returns the task_id of the task that will resolve this
	DataFuture.

### cancel()

Cancel the future if possible.

Returns True if the future was cancelled, False otherwise. A future cannot be cancelled if it is running or has already completed.

## cancelled()

Return True if the future was cancelled.

### property filename

Filepath of the File object this datafuture represents.

### property filepath

Filepath of the File object this datafuture represents.

### parent\_callback(parent\_fu)

Callback from executor future to update the parent.

Updates the future with the result (the File object) or the parent future's exception.

# Parameters

 $\ensuremath{\texttt{parent\_fu}}\xspace(\ensuremath{-}\xspace)$  – Future returned by the executor along with callback

Returns

• None

# running()

Return True if the future is currently executing.

### property tid

Returns the task\_id of the task that will resolve this DataFuture.

## parsl.data\_provider.data\_manager.DataManager

## class parsl.data\_provider.data\_manager.DataManager(dfk: DataFlowKernel)

The DataManager is responsible for transferring input and output data.

# **\_\_\_init\_\_**(*dfk:* DataFlowKernel) $\rightarrow$ None

Initialize the DataManager.

## Parameters

dfk (-) – The DataFlowKernel that this DataManager is managing data for.

init(dfk)	Initialize the DataManager.
<pre>optionally_stage_in(input, func, executor)</pre>	
<pre>replace_task(file, func, executor)</pre>	This will give staging providers the chance to wrap (or replace entirely!) the task function.
<pre>replace_task_stage_out(file, func, executor)</pre>	This will give staging providers the chance to wrap (or replace entirely!) the task function.
<pre>stage_in(file, input, executor)</pre>	Transport the input from the input source to the ex- ecutor, if it is file-like, returning a DataFuture that wraps the stage-in operation.
<pre>stage_out(file, executor, app_fu)</pre>	Transport the file from the local filesystem to the re- mote Globus endpoint.

#### optionally\_stage\_in(input, func, executor)

**replace\_task**(*file:* File, *func:* Callable, executor: str) → Callable

This will give staging providers the chance to wrap (or replace entirely!) the task function.

**replace\_task\_stage\_out**(*file:* File, *func:* Callable, executor: str) → Callable

This will give staging providers the chance to wrap (or replace entirely!) the task function.

#### stage\_in(file: File, input: Any, executor: str) $\rightarrow$ Any

Transport the input from the input source to the executor, if it is file-like, returning a DataFuture that wraps the stage-in operation.

If no staging in is required - because the file parameter is not file-like, then return that parameter unaltered.

#### **Parameters**

- self(-)-
- **input** (-) input to stage in. If this is a File or a DataFuture, stage in tasks will be launched with appropriate dependencies. Otherwise, no stage-in will be performed.
- **executor** (-) an executor the file is going to be staged in to.

#### **stage\_out**(*file:* File, *executor: str*, *app\_fu: Future*) $\rightarrow$ Future | None

Transport the file from the local filesystem to the remote Globus endpoint.

This function returns either a Future which should complete when the stageout is complete, or None, if no staging needs to be waited for.

### Parameters

- **self** (-) -
- file (-) -
- executor (-) -
- **app\_fu** (-) complete before stageout begins.

# parsl.data\_provider.staging.Staging

### class parsl.data\_provider.staging.Staging

This class defines the interface for file staging providers.

For each file to be staged in, the data manager will present the file to each configured Staging provider in turn: first, it will ask if the provider can stage this file by calling can\_stage\_in, and if so, it will call both stage\_in and replace\_task to give the provider the opportunity to perform staging.

For each file to be staged out, the data manager will follow the same pattern using the corresponding stage out methods of this class.

The default implementation of this class rejects all files, and performs no staging actions.

To implement a concrete provider, one or both of the can\_stage\_\* methods should be overridden to match the appropriate files, and then the corresponding stage\_\* and/or replace\_task\* methods should be implemented.

#### \_\_init\_\_()

### Methods

init()	
<pre>can_stage_in(file)</pre>	Given a File object, decide if this staging provider can stage the file.
can_stage_out(file)	Like can_stage_in, but for staging out.
<pre>replace_task(dm, executor, file, func)</pre>	For a file to be staged in, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>replace_task_stage_out(dm, executor, file, func)</pre>	For a file to be staged out, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>stage_in(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.
<pre>stage_out(dm, executor, file, app_fu)</pre>	This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

#### $can_stage_in(file: File) \rightarrow bool$

Given a File object, decide if this staging provider can stage the file. Usually this is be based on the URL scheme, but does not have to be. If this returns True, then other methods of this Staging object will be called to perform the staging.

### $\texttt{can\_stage\_out(\mathit{file:} File)} \rightarrow \texttt{bool}$

Like can\_stage\_in, but for staging out.

### $replace_task(dm: DataManager, executor: str, file: File, func: Callable) \rightarrow Callable | None$

For a file to be staged in, optionally return a replacement app function, which usually should be the original app function wrapped in staging code.

replace\_task\_stage\_out(dm: DataManager, executor: str, file: File, func: Callable)  $\rightarrow$  Callable | None

For a file to be staged out, optionally return a replacement app function, which usually should be the original app function wrapped in staging code.

 $stage_in(dm: DataManager, executor: str, file: File, parent_fut: Future | None) \rightarrow DataFuture | None$ 

This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.

This call will be made with a fresh copy of the File that may be modified for the purposes of this particular staging operation, rather than the original application-provided File. This allows staging specific information (primarily localpath) to be set on the File without interfering with other stagings of the same File.

### The call can return a:

- DataFuture: the corresponding task input parameter will be replaced by the DataFuture, and the main task will not run until that DataFuture is complete. The DataFuture result should be the file object as passed in.
- None: the corresponding task input parameter will be replaced by a suitable automatically generated replacement that container the File fresh copy, or is the fresh copy.

#### **stage\_out**(*dm*: DataManager, *executor*: *str*, *file*: File, *app\_fu*: *Future*) $\rightarrow$ Future | None

This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

Even though it should set up stageout, it will be invoked before the task executes. Any work which needs to happen after the main task should depend on app\_fu.

For a given file, either return a Future which completes when stageout is complete, or return None to indicate that no stageout action need be waited for. When that Future completes, parsl will mark the relevant output DataFuture complete.

Note the asymmetry here between stage\_in and stage\_out: this can return any Future, while stage\_in must return a DataFuture.

## parsl.data\_provider.files.File

## class parsl.data\_provider.files.File(url: PathLike | str)

The Parsl File Class.

This represents the global, and sometimes local, URI/path to a file.

Staging-in mechanisms may annotate a file with a local path recording the path at the far end of a staging action. It is up to the user of the File object to track which local scope that local path actually refers to.

\_\_init\_\_(url: PathLike | str)

Construct a File object from a url string.

#### Parameters

```
url (-) – url of the file e.g. - 'input.txt' - pathlib.Path('input.txt') - 'file:///scratch/
proj101/input.txt' - 'globus://go#ep1/~/data/input.txt' - 'globus://ddb59aef-6d04-11e5-ba46-
22000b92c6ec/home/johndoe/data/input.txt'
```

init(url)	Construct a File object from a url string.
cleancopy()	Returns a copy of the file containing only the global
	immutable state, without any mutable site-local lo-
	cal_path information.

# **Attributes**

filepath	Return the resolved filepath on the side where it is
	called from.

## $cleancopy() \rightarrow File$

Returns a copy of the file containing only the global immutable state, without any mutable site-local local\_path information. The returned File object will be as the original object was when it was constructed.

# property filepath: str

Return the resolved filepath on the side where it is called from.

The appropriate filepath will be returned when called from within an app running remotely as well as regular python on the submit side.

Only file: scheme URLs make sense to have a submit-side path, as other URLs are not accessible through POSIX file access.

#### Returns

• filepath

## parsl.data\_provider.ftp.FTPSeparateTaskStaging

## class parsl.data\_provider.ftp.FTPSeparateTaskStaging

Performs FTP staging as a separate parsl level task.

\_\_init\_\_()

init()	
<pre>can_stage_in(file)</pre>	Given a File object, decide if this staging provider can stage the file.
can_stage_out(file)	Like can_stage_in, but for staging out.
<pre>replace_task(dm, executor, file, func)</pre>	For a file to be staged in, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>replace_task_stage_out(dm, executor, file, func)</pre>	For a file to be staged out, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>stage_in(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.
<pre>stage_out(dm, executor, file, app_fu)</pre>	This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

### can\_stage\_in(file)

Given a File object, decide if this staging provider can stage the file. Usually this is be based on the URL scheme, but does not have to be. If this returns True, then other methods of this Staging object will be called to perform the staging.

### stage\_in(dm, executor, file, parent\_fut)

This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.

This call will be made with a fresh copy of the File that may be modified for the purposes of this particular staging operation, rather than the original application-provided File. This allows staging specific information (primarily localpath) to be set on the File without interfering with other stagings of the same File.

### The call can return a:

- DataFuture: the corresponding task input parameter will be replaced by the DataFuture, and the main task will not run until that DataFuture is complete. The DataFuture result should be the file object as passed in.
- None: the corresponding task input parameter will be replaced by a suitable automatically generated replacement that container the File fresh copy, or is the fresh copy.

## parsl.data\_provider.ftp.FTPInTaskStaging

## class parsl.data\_provider.ftp.FTPInTaskStaging

Performs FTP staging as a wrapper around the application task.

\_\_init\_\_()

init()	
<pre>can_stage_in(file)</pre>	Given a File object, decide if this staging provider can stage the file.
can_stage_out(file)	Like can_stage_in, but for staging out.
<i>replace_task</i> (dm, executor, file, f)	For a file to be staged in, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>replace_task_stage_out(dm, executor, file, func)</pre>	For a file to be staged out, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>stage_in(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.
<pre>stage_out(dm, executor, file, app_fu)</pre>	This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

### can\_stage\_in(file)

Given a File object, decide if this staging provider can stage the file. Usually this is be based on the URL scheme, but does not have to be. If this returns True, then other methods of this Staging object will be called to perform the staging.

#### **replace\_task**(*dm*, *executor*, *file*, *f*)

For a file to be staged in, optionally return a replacement app function, which usually should be the original app function wrapped in staging code.

#### stage\_in(dm, executor, file, parent\_fut)

This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.

This call will be made with a fresh copy of the File that may be modified for the purposes of this particular staging operation, rather than the original application-provided File. This allows staging specific information (primarily localpath) to be set on the File without interfering with other stagings of the same File.

#### The call can return a:

- DataFuture: the corresponding task input parameter will be replaced by the DataFuture, and the main task will not run until that DataFuture is complete. The DataFuture result should be the file object as passed in.
- None: the corresponding task input parameter will be replaced by a suitable automatically generated replacement that container the File fresh copy, or is the fresh copy.
# parsl.data\_provider.file\_noop.NoOpFileStaging

class parsl.data\_provider.file\_noop.NoOpFileStaging

**\_\_\_init\_\_**()

# Methods

init()	
<pre>can_stage_in(file)</pre>	Given a File object, decide if this staging provider can stage the file.
can_stage_out(file)	Like can_stage_in, but for staging out.
<pre>replace_task(dm, executor, file, func)</pre>	For a file to be staged in, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>replace_task_stage_out(dm, executor, file, func)</pre>	For a file to be staged out, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>stage_in(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.
<pre>stage_out(dm, executor, file, app_fu)</pre>	This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

# can\_stage\_in(file)

Given a File object, decide if this staging provider can stage the file. Usually this is be based on the URL scheme, but does not have to be. If this returns True, then other methods of this Staging object will be called to perform the staging.

#### can\_stage\_out(file)

Like can\_stage\_in, but for staging out.

# parsl.data\_provider.globus.GlobusStaging

Specification for accessing data on a remote executor via Globus.

# Parameters

- **endpoint\_uuid** (*str*) Universally unique identifier of the Globus endpoint at which the data can be accessed. This can be found in the Manage Endpoints page.
- **endpoint\_path** (*str*, *optional*) FIXME
- **local\_path** (*str*, *optional*) FIXME

\_\_init\_\_(endpoint\_uuid: str, endpoint\_path: str | None = None, local\_path: str | None = None)

# **Methods**

init(endpoint_uuid[, endpoint_path,])	
<pre>can_stage_in(file)</pre>	Given a File object, decide if this staging provider can stage the file.
<pre>can_stage_out(file)</pre>	Like can_stage_in, but for staging out.
<pre>initialize_globus()</pre>	
<pre>replace_task(dm, executor, file, func)</pre>	For a file to be staged in, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>replace_task_stage_out(dm, executor, file, func)</pre>	For a file to be staged out, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>stage_in(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.
<pre>stage_out(dm, executor, file, app_fu)</pre>	This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

#### can\_stage\_in(file)

Given a File object, decide if this staging provider can stage the file. Usually this is be based on the URL scheme, but does not have to be. If this returns True, then other methods of this Staging object will be called to perform the staging.

# can\_stage\_out(file)

Like can\_stage\_in, but for staging out.

#### initialize\_globus()

#### stage\_in(dm, executor, file, parent\_fut)

This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.

This call will be made with a fresh copy of the File that may be modified for the purposes of this particular staging operation, rather than the original application-provided File. This allows staging specific information (primarily localpath) to be set on the File without interfering with other stagings of the same File.

#### The call can return a:

- DataFuture: the corresponding task input parameter will be replaced by the DataFuture, and the main task will not run until that DataFuture is complete. The DataFuture result should be the file object as passed in.
- None: the corresponding task input parameter will be replaced by a suitable automatically generated replacement that container the File fresh copy, or is the fresh copy.

# stage\_out(dm, executor, file, app\_fu)

This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

Even though it should set up stageout, it will be invoked before the task executes. Any work which needs to happen after the main task should depend on app\_fu.

For a given file, either return a Future which completes when stageout is complete, or return None to indicate that no stageout action need be waited for. When that Future completes, parsl will mark the relevant output DataFuture complete.

Note the asymmetry here between stage\_in and stage\_out: this can return any Future, while stage\_in must return a DataFuture.

# parsl.data\_provider.http.HTTPSeparateTaskStaging

#### class parsl.data\_provider.http.HTTPSeparateTaskStaging

A staging provider that Performs HTTP and HTTPS staging as a separate parsl-level task. This requires a shared file system on the executor.

**\_\_\_init\_\_**()

#### **Methods**

init()	
<pre>can_stage_in(file)</pre>	Given a File object, decide if this staging provider can stage the file.
<pre>can_stage_out(file)</pre>	Like can_stage_in, but for staging out.
<pre>replace_task(dm, executor, file, func)</pre>	For a file to be staged in, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>replace_task_stage_out(dm, executor, file, func)</pre>	For a file to be staged out, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>stage_in(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.
<pre>stage_out(dm, executor, file, app_fu)</pre>	This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

#### can\_stage\_in(file)

Given a File object, decide if this staging provider can stage the file. Usually this is be based on the URL scheme, but does not have to be. If this returns True, then other methods of this Staging object will be called to perform the staging.

#### stage\_in(dm, executor, file, parent\_fut)

This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.

This call will be made with a fresh copy of the File that may be modified for the purposes of this particular staging operation, rather than the original application-provided File. This allows staging specific information (primarily localpath) to be set on the File without interfering with other stagings of the same File.

#### The call can return a:

- DataFuture: the corresponding task input parameter will be replaced by the DataFuture, and the main task will not run until that DataFuture is complete. The DataFuture result should be the file object as passed in.
- None: the corresponding task input parameter will be replaced by a suitable automatically generated replacement that container the File fresh copy, or is the fresh copy.

# parsl.data\_provider.http.HTTPInTaskStaging

#### class parsl.data\_provider.http.HTTPInTaskStaging

A staging provider that performs HTTP and HTTPS staging as in a wrapper around each task. In contrast to HTTPSeparateTaskStaging, this provider does not require a shared file system.

**\_\_\_init\_\_**()

#### **Methods**

init()	
<pre>can_stage_in(file)</pre>	Given a File object, decide if this staging provider can stage the file.
<pre>can_stage_out(file)</pre>	Like can_stage_in, but for staging out.
<i>replace_task</i> (dm, executor, file, f)	For a file to be staged in, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>replace_task_stage_out(dm, executor, file, func)</pre>	For a file to be staged out, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>stage_in(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.
<pre>stage_out(dm, executor, file, app_fu)</pre>	This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

#### can\_stage\_in(file)

Given a File object, decide if this staging provider can stage the file. Usually this is be based on the URL scheme, but does not have to be. If this returns True, then other methods of this Staging object will be called to perform the staging.

#### **replace\_task**(*dm*, *executor*, *file*, *f*)

For a file to be staged in, optionally return a replacement app function, which usually should be the original app function wrapped in staging code.

## stage\_in(dm, executor, file, parent\_fut)

This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.

This call will be made with a fresh copy of the File that may be modified for the purposes of this particular staging operation, rather than the original application-provided File. This allows staging specific information (primarily localpath) to be set on the File without interfering with other stagings of the same File.

# The call can return a:

- DataFuture: the corresponding task input parameter will be replaced by the DataFuture, and the main task will not run until that DataFuture is complete. The DataFuture result should be the file object as passed in.
- None: the corresponding task input parameter will be replaced by a suitable automatically generated replacement that container the File fresh copy, or is the fresh copy.

# parsl.data\_provider.rsync.RSyncStaging

# class parsl.data\_provider.rsync.RSyncStaging(hostname)

This staging provider will execute rsync on worker nodes to stage in files from a remote location.

Worker nodes must be able to authenticate to the rsync server without interactive authentication - for example, worker initialization could include an appropriate SSH key configuration.

The submit side will need to run an rsync-compatible server (for example, an ssh server with the rsync binary installed)

\_\_init\_\_(hostname)

# **Methods**

init(hostname)	
<pre>can_stage_in(file)</pre>	Given a File object, decide if this staging provider can stage the file.
can_stage_out(file)	Like can_stage_in, but for staging out.
<i>replace_task</i> (dm, executor, file, f)	For a file to be staged in, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>replace_task_stage_out(dm, executor, file, f)</pre>	For a file to be staged out, optionally return a replace- ment app function, which usually should be the orig- inal app function wrapped in staging code.
<pre>stage_in(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.
<pre>stage_out(dm, executor, file, parent_fut)</pre>	This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

#### can\_stage\_in(file)

Given a File object, decide if this staging provider can stage the file. Usually this is be based on the URL scheme, but does not have to be. If this returns True, then other methods of this Staging object will be called to perform the staging.

# can\_stage\_out(file)

Like can\_stage\_in, but for staging out.

## **replace\_task**(*dm*, *executor*, *file*, *f*)

For a file to be staged in, optionally return a replacement app function, which usually should be the original app function wrapped in staging code.

#### replace\_task\_stage\_out(dm, executor, file, f)

For a file to be staged out, optionally return a replacement app function, which usually should be the original app function wrapped in staging code.

## stage\_in(dm, executor, file, parent\_fut)

This call gives the staging provider an opportunity to prepare for stage-in and to launch arbitrary tasks which must complete as part of stage-in.

This call will be made with a fresh copy of the File that may be modified for the purposes of this particular staging operation, rather than the original application-provided File. This allows staging specific information (primarily localpath) to be set on the File without interfering with other stagings of the same File.

# The call can return a:

- DataFuture: the corresponding task input parameter will be replaced by the DataFuture, and the main task will not run until that DataFuture is complete. The DataFuture result should be the file object as passed in.
- None: the corresponding task input parameter will be replaced by a suitable automatically generated replacement that container the File fresh copy, or is the fresh copy.

# stage\_out(dm, executor, file, parent\_fut)

This call gives the staging provider an opportunity to prepare for stage-out and to launch arbitrary tasks which must complete as part of stage-out.

Even though it should set up stageout, it will be invoked before the task executes. Any work which needs to happen after the main task should depend on app\_fu.

For a given file, either return a Future which completes when stageout is complete, or return None to indicate that no stageout action need be waited for. When that Future completes, parsl will mark the relevant output DataFuture complete.

Note the asymmetry here between stage\_in and stage\_out: this can return any Future, while stage\_in must return a DataFuture.

# Executors

parsl.executors.base.ParslExecutor	Executors are abstractions that represent available com- pute resources to which you could submit arbitrary App tasks.
<pre>parsl.executors.status_handling.</pre>	A base class for executors which scale using blocks.
BlockProviderExecutor	
parsl.executors.ThreadPoolExecutor	A thread-based executor.
parsl.executors.HighThroughputExecutor	Executor designed for cluster-scale
parsl.executors.WorkQueueExecutor	Executor to use Work Queue batch system
parsl.executors.taskvine.TaskVineExecutor	Executor to use TaskVine dynamic workflow system
parsl.executors.FluxExecutor	Executor that uses Flux to schedule and run jobs.
parsl.executors.radical.	Executor is designed for executing heterogeneous tasks
RadicalPilotExecutor	

# parsl.executors.base.ParslExecutor

Executors are abstractions that represent available compute resources to which you could submit arbitrary App tasks.

This is an abstract base class that only enforces concrete implementations of functionality by the child classes.

Can be used as a context manager. On exit, calls self.shutdown() with no arguments and re-raises any thrown exception.

In addition to the listed methods, a ParslExecutor instance must always have a member field:

#### label: str - a human readable label for the executor, unique

with respect to other executors.

Per-executor monitoring behaviour can be influenced by exposing:

**radio\_mode: str - a string describing which radio mode should be used to** send task resource data back to the submit side.

An executor may optionally expose:

#### storage\_access: List[parsl.data\_provider.staging.Staging] - a list of staging

providers that will be used for file staging. In the absence of this attribute, or if this attribute is None, then a default value of parsl.data\_provider.staging.default\_staging will be used by the staging code.

Typechecker note: Ideally storage\_access would be declared on executor \_\_init\_\_ methods as List[Staging] - however, lists are by default invariant, not co-variant, and it looks like @typeguard cannot be persuaded otherwise. So if you're implementing an executor and want to @typeguard the constructor, you'll have to use List[Any] here.

# Methods

<pre>init(*[, hub_address, hub_port,])</pre>	
<pre>monitor_resources()</pre>	Should resource monitoring happen for tasks on run- ning on this executor?
<pre>shutdown()</pre>	Shutdown the executor.
start()	Start the executor.
<pre>submit(func, resource_specification, *args,)</pre>	Submit.

# Attributes

hub_address	Address to the Hub for monitoring.
hub_port	Port to the Hub for monitoring.
label	
<pre>monitoring_radio</pre>	Local radio for sending monitoring messages
radio_mode	
run_dir	Path to the run directory.
run_id	UUID for the enclosing DFK.

#### property hub\_address: str | None

Address to the Hub for monitoring.

#### property hub\_port: int | None

Port to the Hub for monitoring.

```
label: str = 'undefined'
```

#### $\texttt{monitor\_resources()} \rightarrow \texttt{bool}$

Should resource monitoring happen for tasks on running on this executor?

Parsl resource monitoring conflicts with execution styles which use threads, and can deadlock while running.

This function allows resource monitoring to be disabled per executor implementation.

## property monitoring\_radio: MonitoringRadio | None

Local radio for sending monitoring messages

```
radio_mode: str = 'udp'
```

#### property run\_dir: str

Path to the run directory.

#### property run\_id: str | None

UUID for the enclosing DFK.

#### abstract shutdown() $\rightarrow$ None

Shutdown the executor.

This includes all attached resources such as workers and controllers.

#### abstract start() $\rightarrow$ None

Start the executor.

Any spin-up operations (for example: starting thread pools) should be performed here.

# **abstract submit**(func: Callable, resource\_specification: Dict[str, Any], \*args: Any, \*\*kwargs: Any) $\rightarrow$ Future

Submit.

The executor can optionally set a parsl\_executor\_task\_id attribute on the Future that it returns, and in that case, parsl will log a relationship between the executor's task ID and parsl level try/task IDs.

# parsl.executors.status\_handling.BlockProviderExecutor

A base class for executors which scale using blocks.

This base class is intended to help with executors which:

- use blocks of workers to execute tasks
- blocks of workers are launched on a batch system through an *ExecutionProvider*

An implementing class should implement the abstract methods required by *ParslExecutor* to submit tasks, as well as BlockProviderExecutor abstract methods to provide the executor-specific command to start a block of workers (the \_get\_launch\_command method), and some basic scaling information (outstanding and workers\_per\_node properties).

This base class provides a scale\_out method which will launch new blocks. It does not provide a scale\_in method, because scale-in behaviour is not well defined in the Parsl scaling model and so behaviour is left to individual executors.

Parsl scaling will provide scaling between min\_blocks and max\_blocks by invoking scale\_out, but it will not initialize the blocks requested by any init\_blocks parameter. Subclasses must implement that behaviour themselves.

BENC: TODO: block error handling: maybe I want this more user pluggable? I'm not sure of use cases for switchability at the moment beyond "yes or no"

\_\_init\_\_(\*, provider: ExecutionProvider | None, block\_error\_handler: bool | Callable[[BlockProviderExecutor, Dict[str, JobStatus]], None])

# Methods

<pre>init(*, provider, block_error_handler)</pre>	
<pre>create_monitoring_info(status)</pre>	Create a monitoring message for each block based on the poll status.
handle_errors(status)	This method is called by the error management in- frastructure after a status poll.
<pre>monitor_resources()</pre>	Should resource monitoring happen for tasks on run- ning on this executor?
<pre>poll_facade()</pre>	
<pre>scale_in(blocks)</pre>	Scale in method.
<pre>scale_in_facade(n[, max_idletime])</pre>	
<pre>scale_out([blocks])</pre>	Scales out the number of blocks by "blocks"
<pre>scale_out_facade(n)</pre>	
<pre>send_monitoring_info(status)</pre>	
<pre>set_bad_state_and_fail_all(exception)</pre>	Allows external error handlers to mark this executor as irrecoverably bad and cause all tasks submitted to it now and in the future to fail.
<pre>shutdown()</pre>	Shutdown the executor.
start()	Start the executor.
status()	Return the status of all jobs/blocks currently known to this executor.
<pre>submit(func, resource_specification, *args,)</pre>	Submit.

# **Attributes**

bad_state_is_set	Returns true if this executor is in an irrecoverable error state.
executor_exception	Returns an exception that indicates why this executor is in an irrecoverable state.
hub_address	Address to the Hub for monitoring.
hub_port	Port to the Hub for monitoring.
label	
<pre>monitoring_radio</pre>	Local radio for sending monitoring messages
outstanding	This should return the number of tasks that the execu- tor has been given to run (waiting to run, and running now)
provider	
radio_mode	
run_dir	Path to the run directory.
run_id	UUID for the enclosing DFK.
status_facade	Return the status of all jobs/blocks of the executor of this poller.
status_polling_interval	Returns the interval, in seconds, at which the status method should be called.
tasks	
workers_per_node	

### property bad\_state\_is\_set

Returns true if this executor is in an irrecoverable error state. If this method returns true, :property:executor\_exception should contain an exception indicating the cause.

#### **create\_monitoring\_info**(*status: Dict[str*, JobStatus]) → Sequence[object]

Create a monitoring message for each block based on the poll status.

#### property executor\_exception

Returns an exception that indicates why this executor is in an irrecoverable state.

#### handle\_errors(*status: Dict[str*, JobStatus]) → None

This method is called by the error management infrastructure after a status poll. The executor implementing this method is then responsible for detecting abnormal conditions based on the status of submitted jobs. If the executor does not implement any special error handling, this method should return False, in which case a generic error handling scheme will be used. :param status: status of all jobs launched by this executor

#### abstract property outstanding: int

This should return the number of tasks that the executor has been given to run (waiting to run, and running now)

 $poll_facade() \rightarrow None$ 

#### property provider

abstract scale\_in(*blocks: int*)  $\rightarrow$  List[str]

Scale in method.

Cause the executor to reduce the number of blocks by count.

Returns

A list of block ids corresponding to the blocks that were removed.

**scale\_in\_facade**(*n*: *int*, *max\_idletime*: *float* | *None* = *None*) → List[str]

scale\_out(*blocks: int* = l)  $\rightarrow$  List[str]

Scales out the number of blocks by "blocks"

**scale\_out\_facade**(*n*: *int*) → List[str]

send\_monitoring\_info(status: Dict)  $\rightarrow$  None

#### set\_bad\_state\_and\_fail\_all(exception: Exception)

Allows external error handlers to mark this executor as irrecoverably bad and cause all tasks submitted to it now and in the future to fail. The executor is responsible for checking :method:bad\_state\_is\_set() in the :method:submit() method and raising the appropriate exception, which is available through :method:executor\_exception().

**status()**  $\rightarrow$  Dict[str, *JobStatus*]

Return the status of all jobs/blocks currently known to this executor.

Returns

a dictionary mapping block ids (in string) to job status

# property status\_facade: Dict[str, JobStatus]

Return the status of all jobs/blocks of the executor of this poller.

#### Returns

a dictionary mapping block ids (in string) to job status

#### property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called. The assumption here is that, once initialized, an executor's polling interval is fixed. In practice, at least given the current situation, the executor uses a single task provider and this method is a delegate to the corresponding method in the provider.

#### Returns

the number of seconds to wait between calls to status() or zero if no polling should be done

property tasks: Dict[object, Future]

abstract property workers\_per\_node: int | float

#### parsl.executors.ThreadPoolExecutor

A thread-based executor.

#### Parameters

• max\_threads (Optional[int]) – Number of threads. Default is 2.

- thread\_name\_prefix (string) Thread name prefix
- storage\_access (list of Staging) Specifications for accessing data this executor remotely.

\_\_init\_\_(label: str = 'threads', max\_threads: int | None = 2, thread\_name\_prefix: str = ", storage\_access: List[Staging] | None = None, working\_dir: str | None = None)

# Methods

init([label, max_threads,])	
<pre>monitor_resources()</pre>	Resource monitoring sometimes deadlocks when us-
	ing threads, so this function returns false to disable it.
<pre>shutdown([block])</pre>	Shutdown the ThreadPool.
start()	Start the executor.
<pre>submit(func, resource_specification, *args,)</pre>	Submits work to the thread pool.

#### **Attributes**

hub_address	Address to the Hub for monitoring.
hub_port	Port to the Hub for monitoring.
label	
monitoring_radio	Local radio for sending monitoring messages
radio_mode	
run_dir	Path to the run directory.
run_id	UUID for the enclosing DFK.

#### monitor\_resources()

Resource monitoring sometimes deadlocks when using threads, so this function returns false to disable it.

#### shutdown(block=True)

Shutdown the ThreadPool. The underlying concurrent.futures thread pool implementation will not terminate tasks that are being executed, because it does not provide a mechanism to do that. With block set to false, this will return immediately and it will appear as if the DFK is shut down, but the python process will not be able to exit until the thread pool has emptied out by task completions. In either case, this can be a very long wait.

# **Kwargs:**

• block (Bool): To block for confirmations or not

## start()

Start the executor.

Any spin-up operations (for example: starting thread pools) should be performed here.

submit(func, resource\_specification, \*args, \*\*kwargs)

Submits work to the thread pool.

This method is simply pass through and behaves like a submit call as described here Python docs:

# parsl.executors.HighThroughputExecutor

class	parsl.executors.	.HighThroughputExecu	tor(label: str	= 'H	HighThroughputExecutor', provider:	

ExecutionProvider = LocalProvider(channel=LocalChannel(envs={}, script\_dir=None, userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/l cmd timeout=30, init blocks=1, launcher=SingleNodeLauncher(debug=True, fail on any=False), max blocks=1, min blocks=0, move\_files=None, nodes\_per\_block=1, parallelism=1, worker\_init="), launch\_cmd: str | None = None, address: *str* | *None* = *None*, *worker\_ports: Tuple[int, int]* | *None* = None, worker\_port\_range: Tuple[int, int] | None = (54000, 55000), interchange port range: Tuple[int, int] *None* = (55000, 56000), *storage\_access: List*[Staging] | *None* = *None*, *working\_dir: str* | *None* = *None*, worker\_debug: bool = False, cores\_per\_worker: float = 1.0, mem\_per\_worker: float | None = None, max\_workers: *int* | *float* | *None* = *None*, *max\_workers\_per\_node: int* | float | None = None, cpu\_affinity: str = 'none',  $available\_accelerators: int | Sequence[str] = (),$ prefetch\_capacity: int = 0, heartbeat\_threshold: int = *120, heartbeat\_period: int = 30, drain\_period: int | None* = None, poll period: int = 10, address probe timeout: int | None = None, worker logdir root: str | None = None, enable mpi mode: bool = False, mpi launcher: str = 'mpiexec', block\_error\_handler: bool | Callable[[BlockProviderExecutor, Dict[str, JobStatus]], *None*] = *True*, *encrypted*: *bool* = *False*)

Executor designed for cluster-scale

#### The HighThroughputExecutor system has the following components:

- 1. The HighThroughputExecutor instance which is run as part of the Parsl script.
- 2. The Interchange which acts as a load-balancing proxy between workers and Parsl
- 3. The multiprocessing based worker pool which coordinates task execution over several cores on a node.
- 4. ZeroMQ pipes connect the HighThroughputExecutor, Interchange and the process\_worker\_pool

Here is a diagram

Data	Executor   Inte	erchange   External	Process(es)
Flow			
Task   Kernel			
+>	> ->outg	joing_q -> process	s_worker_pool
	batch	ing	
Parsl <fut- < th=""><th>  load-</th><th>balancing  result</th><th>exception</th></fut- <>	load-	balancing  result	exception
^	watch	idogs	
	Q_mngmnt	V	V
	Thread< -incom	ing_q<  +	+
+update_f	t+		

Each of the workers in each process\_worker\_pool has access to its local rank through an environmental variable, PARSL\_WORKER\_RANK. The local rank is unique for each process and is an integer in the range from 0 to the number of workers per in the pool minus 1. The workers also have access to the ID of the worker pool as PARSL\_WORKER\_POOL\_ID and the size of the worker pool as PARSL\_WORKER\_COUNT.

#### **Parameters**

• provider (ExecutionProvider) -

Provider to access computation resources. Can be one of EC2Provider,

Cobalt, Condor, GoogleCloud, GridEngine, Local, GridEngine, Slurm, or Torque.

- **label** (*str*) Label for this executor instance.
- **launch\_cmd** (*str*) Command line string to launch the process\_worker\_pool from the provider. The command line string will be formatted with appropriate values for the following values (debug, task\_url, result\_url, cores\_per\_worker, nodes\_per\_block, heartbeat\_period ,heartbeat\_threshold, logdir). For example: launch\_cmd="process\_worker\_pool.py {debug} -c {cores\_per\_worker} -task\_url={task\_url} -result\_url={result\_url}"
- **address** (*string*) An address to connect to the main Parsl process which is reachable from the network in which workers will be running. This field expects an IPv4 address (xxx.xxx.xxx). Most login nodes on clusters have several network interfaces available, only some of which can be reached from the compute nodes. This field can be used to limit the executor to listen only on a specific interface, and limiting connections to the internal network. By default, the executor will attempt to enumerate and connect through all possible addresses. Setting an address here overrides the default behavior. default=None
- worker\_ports ((*int*, *int*)) Specify the ports to be used by workers to connect to Parsl. If this option is specified, worker\_port\_range will not be honored.
- worker\_port\_range ((int, int)) Worker ports will be chosen between the two integers provided.
- **interchange\_port\_range** ((*int*, *int*)) Port range used by Parsl to communicate with the Interchange.
- working\_dir (str) Working dir to be used by the executor.
- worker\_debug (Bool) Enables worker debug logging.
- **cores\_per\_worker** (*float*) cores to be assigned to each worker. Oversubscription is possible by setting cores\_per\_worker < 1.0. Default=1
- **mem\_per\_worker** (*float*) GB of memory required per worker. If this option is specified, the node manager will check the available memory at startup and limit the number of workers such that the there's sufficient memory for each worker. Default: None
- max\_workers (int) Deprecated. Please use max\_workers\_per\_node instead.
- **max\_workers\_per\_node** (*int*) Caps the number of workers launched per node. Default: None
- **cpu\_affinity** (*string*) Whether or how each worker process sets thread affinity. Options include "none" to forgo any CPU affinity configuration, "block" to assign adjacent cores to workers (ex: assign 0-1 to worker 0, 2-3 to worker 1), and "alternating" to assign cores to workers in round-robin (ex: assign 0,2 to worker 0, 1,3 to worker 1). The "block-reverse" option assigns adjacent cores to workers, but assigns the CPUs with large indices to low index workers (ex: assign 2-3 to worker 1, 0,1 to worker 2)

• **available\_accelerators** (*int | list*) – Accelerators available for workers to use. Each worker will be pinned to exactly one of the provided accelerators, and no more workers will be launched than the number of accelerators.

Either provide the list of accelerator names or the number available. If a number is provided, Parsl will create names as integers starting with 0.

default: empty list

- **prefetch\_capacity** (*int*) Number of tasks that could be prefetched over available worker capacity. When there are a few tasks (<100) or when tasks are long running, this option should be set to 0 for better load balancing. Default is 0.
- address\_probe\_timeout (*int | None*) Managers attempt connecting over many different addresses to determine a viable address. This option sets a time limit in seconds on the connection attempt. Default of None implies 30s timeout set on worker.
- **heartbeat\_threshold** (*int*) Seconds since the last message from the counterpart in the communication pair: (interchange, manager) after which the counterpart is assumed to be un-available. Default: 120s
- **heartbeat\_period** (*int*) Number of seconds after which a heartbeat message indicating liveness is sent to the counterpart (interchange, manager). Default: 30s
- **poll\_period** (*int*) Timeout period to be used by the executor components in milliseconds. Increasing poll\_periods trades performance for cpu efficiency. Default: 10ms
- **drain\_period** (*int*) The number of seconds after start when workers will begin to drain and then exit. Set this to a time that is slightly less than the maximum walltime of batch jobs to avoid killing tasks while they execute. For example, you could set this to the walltime minus a grace period for the batch job to start the workers, minus the expected maximum length of an individual task.
- **worker\_logdir\_root** (*string*) In case of a remote file system, specify the path to where logs will be kept.
- **enable\_mpi\_mode** (*boo1*) If enabled, MPI launch prefixes will be composed for the batch scheduler based on the nodes available in each batch job and the resource\_specification dict passed from the app. This is an experimental feature, please refer to the following doc section before use: https://parsl.readthedocs.io/en/stable/userguide/mpi\_apps.html
- **mpi\_launcher** (*str*) This field is only used if enable\_mpi\_mode is set. Select one from the list of supported MPI launchers = ("srun", "aprun", "mpiexec"). default: "mpiexec"
- encrypted (bool) Flag to enable/disable encryption (CurveZMQ). Default is False.

\_\_init\_\_(label: str = 'HighThroughputExecutor', provider: ExecutionProvider = LocalProvider(channel=LocalChannel(envs={}, script\_dir=None, userhome='/home/docs/checkouts/readthedocs.org/user builds/parsl/checkouts/latest/docs'), cmd\_timeout=30, init\_blocks=1, launcher=SingleNodeLauncher(debug=True, fail\_on\_any=False), max\_blocks=1, min\_blocks=0, move\_files=None, nodes\_per\_block=1, parallelism=1, worker\_init="), launch\_cmd: str | None = None, address: str | None = None, worker ports: Tuple[int, int] | None = None, worker port range: Tuple[int, int] | None = (54000, 55000), interchange\_port\_range: Tuple[int, int] | None = (55000, 56000), storage\_access: *List*[Staging] | *None* = *None*, *working\_dir: str* | *None* = *None*, *worker\_debug: bool* = *False*, cores\_per\_worker: float = 1.0, mem\_per\_worker: float | None = None, max\_workers: int | float | *None* = *None*, *max\_workers\_per\_node: int* | *float* | *None* = *None*, *cpu\_affinity: str* = '*none*', available\_accelerators: int | Sequence[str] = (), prefetch\_capacity: int = 0, heartbeat\_threshold: int = 120, heartbeat\_period: int = 30, drain\_period: int | None = None, poll\_period: int = 10, address\_probe\_timeout: int | None = None, worker\_logdir\_root: str | None = None, enable\_mpi\_mode: bool = False, mpi\_launcher: str = 'mpiexec', block\_error\_handler: bool | *Callable*[[BlockProviderExecutor, *Dict[str*, JobStatus]], *None*] = *True*, *encrypted: bool* = *False*)

# Methods

<i>init</i> ([label, provider, launch_cmd,])	
<pre>connected_blocks()</pre>	List of connected block ids
<pre>connected_managers()</pre>	Returns a list of dicts one for each connected managers.
<pre>create_monitoring_info(status)</pre>	Create a monitoring message for each block based on the poll status.
<pre>get_usage_information()</pre>	
handle_errors(status)	This method is called by the error management in- frastructure after a status poll.
<pre>hold_worker(worker_id)</pre>	Puts a worker on hold, preventing scheduling of ad- ditional tasks to it.
<pre>initialize_scaling()</pre>	Compose the launch command and scale out the initial blocks.
<pre>monitor_resources()</pre>	Should resource monitoring happen for tasks on run- ning on this executor?
<pre>poll_facade()</pre>	
<pre>scale_in(blocks[, max_idletime])</pre>	Scale in the number of active blocks by specified amount.
<pre>scale_in_facade(n[, max_idletime])</pre>	
<pre>scale_out([blocks])</pre>	Scales out the number of blocks by "blocks"
<pre>scale_out_facade(n)</pre>	
<pre>send_monitoring_info(status)</pre>	
<pre>set_bad_state_and_fail_all(exception)</pre>	Allows external error handlers to mark this executor as irrecoverably bad and cause all tasks submitted to it now and in the future to fail.
<pre>shutdown([timeout])</pre>	Shutdown the executor, including the interchange.
start()	Create the Interchange process and connect to it.
status()	Return the status of all jobs/blocks currently known to this executor.
<pre>submit(func, resource_specification, *args,)</pre>	Submits work to the outgoing_q.

# **Attributes**

<pre>bad_state_is_set</pre>	Returns true if this executor is in an irrecoverable error state.
connected_workers	Returns the count of workers across all connected managers
executor_exception	Returns an exception that indicates why this executor is in an irrecoverable state.
hub_address	Address to the Hub for monitoring.
hub_port	Port to the Hub for monitoring.
label	
logdir	
max_workers	
monitoring_radio	Local radio for sending monitoring messages
outstanding	Returns the count of tasks outstanding across the in- terchange and managers
provider	
radio_mode	
run_dir	Path to the run directory.
run_id	UUID for the enclosing DFK.
status_facade	Return the status of all jobs/blocks of the executor of this poller.
status_polling_interval	Returns the interval, in seconds, at which the status method should be called.
tasks	
worker_logdir	
workers_per_node	

#### $connected_blocks() \rightarrow List[str]$

List of connected block ids

# $\texttt{connected\_managers()} \rightarrow \texttt{List[Dict[str, Any]]}$

Returns a list of dicts one for each connected managers. The dict contains info on manager(str:manager\_id), block\_id, worker\_count, tasks(int), idle\_durations(float), active(bool)

# property connected\_workers: int

Returns the count of workers across all connected managers

#### get\_usage\_information()

# **hold\_worker**(*worker\_id: str*) $\rightarrow$ None

Puts a worker on hold, preventing scheduling of additional tasks to it.

This is called "hold" mostly because this only stops scheduling of tasks, and does not actually kill the worker.

Parameters worker\_id (str) – Worker id to be put on hold

#### initialize\_scaling()

Compose the launch command and scale out the initial blocks.

#### property logdir

#### property max\_workers

#### property outstanding: int

Returns the count of tasks outstanding across the interchange and managers

#### radio\_mode: str = 'htex'

```
scale_in(blocks: int, max_idletime: float | None = None) → List[str]
```

Scale in the number of active blocks by specified amount.

The scale in method here is very rude. It doesn't give the workers the opportunity to finish current tasks or cleanup. This is tracked in issue #530

#### **Parameters**

- **blocks** (*int*) Number of blocks to terminate and scale\_in by
- **max\_idletime** (*float*) A time to indicate how long a block should be idle to be a candidate for scaling in.

If None then blocks will be force scaled in even if they are busy.

If a float, then only idle blocks will be terminated, which may be less than the requested number.

# **Return type**

List of block IDs scaled in

#### **shutdown**(*timeout: float* = 10.0)

Shutdown the executor, including the interchange. This does not shut down any workers directly - workers should be terminated by the scaling mechanism or by heartbeat timeout.

#### **Parameters**

**timeout** (*float*) – Amount of time to wait for the Interchange process to terminate before we forcefully kill it.

#### start()

Create the Interchange process and connect to it.

#### **status()** $\rightarrow$ Dict[str, *JobStatus*]

Return the status of all jobs/blocks currently known to this executor.

#### Returns

a dictionary mapping block ids (in string) to job status

submit(func, resource\_specification, \*args, \*\*kwargs)

Submits work to the outgoing\_q.

The outgoing\_q is an external process listens on this queue for new work. This method behaves like a submit call as described here Python docs:

#### **Parameters**

• **func** (-) – Callable function

- **resource\_specification** (-) Dictionary containing relevant info about task that is needed by underlying executors.
- **args** (-) List of arbitrary positional arguments.

# Kwargs:

• kwargs (dict) : A dictionary of arbitrary keyword args for func.

# Returns

Future

# property worker\_logdir

property workers\_per\_node: int | float

# parsl.executors.WorkQueueExecutor

<pre>class parsl.executors.WorkQueueExecuto</pre>	<b>r</b> ( <i>label: str</i> = 'WorkQueueExecutor', provider: ExecutionProvider
	= LocalProvider(channel=LocalChannel(envs={},
	script_dir=None, user-
	home='/home/docs/checkouts/readthedocs.org/user_builds/parsl/checkouts/latest/a
	cmd_timeout=30, init_blocks=1,
	launcher=SingleNodeLauncher(debug=True,
	fail_on_any=False), max_blocks=1, min_blocks=0,
	move_files=None, nodes_per_block=1, parallelism=1,
	worker_init="), working_dir: str = '.', project_name: str   None
	= None, project_password_file: str   None = None, address: str
	<i>None</i> = <i>None</i> , <i>port</i> : <i>int</i> = 0, <i>env</i> : <i>Dict</i>   <i>None</i> = <i>None</i> , <i>shared_fs</i> :
	bool = False, storage_access: List[Staging]   None = None,
	use_cache: bool = False, source: bool = False, pack: bool =
	False, extra_pkgs: List[str]   None = None, autolabel: bool =
	<i>False</i> , <i>autolabel_window: int</i> = 1, <i>autocategory: bool</i> = <i>True</i> ,
	<i>max_retries: int</i> = 1, <i>init_command: str</i> = ", <i>worker_options:</i>
	<i>str</i> = ", <i>full_debug: bool</i> = <i>True, worker_executable: str</i> =
	'work_queue_worker', function_dir: str   None = None,
	coprocess: bool = False)

Executor to use Work Queue batch system

The WorkQueueExecutor system utilizes the Work Queue framework to efficiently delegate Parsl apps to remote machines in clusters and grids using a fault-tolerant system. Users can run the work\_queue\_worker program on remote machines to connect to the WorkQueueExecutor, and Parsl apps will then be sent out to these machines for execution and retrieval.

# Parameters

- **label** (*str*) A human readable label for the executor, unique with respect to other Work Queue master programs. Default is "WorkQueueExecutor".
- **working\_dir** (*str*) Location for Parsl to perform app delegation to the Work Queue system. Defaults to current directory.
- **project\_name** (*str*) If a project\_name is given, then Work Queue will periodically report its status and performance back to the global WQ catalog, which can be viewed here: http://ccl.cse.nd.edu/software/workqueue/status Default is None. Overrides address.

- **project\_password\_file** (*str*) Optional password file for the work queue project. Default is None.
- **address** (*str*) The ip to contact this work queue master process. If not given, uses the address of the current machine as returned by socket.gethostname(). Ignored if project\_name is specified.
- **port** (*int*) TCP port on Parsl submission machine for Work Queue workers to connect to. Workers will connect to Parsl using this port.

If 0, Work Queue will allocate a port number automatically. In this case, environment variables can be used to influence the choice of port, documented here: https://ccl.cse.nd.edu/software/manuals/api/html/work\_queue\_8h.html#a21714a10bcdfcf5c3bd44a96f5dcbda6 Default: WORK\_QUEUE\_DEFAULT\_PORT.

- **env** (*dict{str}*) Dictionary that contains the environmental variables that need to be set on the Work Queue worker machine.
- **shared\_fs** (*bool*) Define if working in a shared file system or not. If Parsl and the Work Queue workers are on a shared file system, Work Queue does not need to transfer and rename files for execution. Default is False.
- **use\_cache** (*bool*) Whether workers should cache files that are common to tasks. Warning: Two files are considered the same if they have the same filepath name. Use with care when reusing the executor instance across multiple parsl workflows. Default is False.
- **source** (*bool*) Choose whether to transfer parsl app information as source code. (Note: this increases throughput for @python\_apps, but the implementation does not include functionality for @bash\_apps, and thus source=False must be used for programs utilizing @bash\_apps.) Default is False. Set to True if pack is True
- **pack** (*bool*) Use conda-pack to prepare a self-contained Python evironment for each task. This greatly increases task latency, but does not require a common environment or shared FS on execution nodes. Implies source=True.
- **extra\_pkgs** (*list*) List of extra pip/conda package names to include when packing the environment. This may be useful if the app executes other (possibly non-Python) programs provided via pip or conda. Scanning the app source for imports would not detect these dependencies, so they need to be manually specified.
- **autolabel** (*bool*) Use the Resource Monitor to automatically determine resource labels based on observed task behavior.
- **autolabel\_window** (*int*) Set the number of tasks considered for autolabeling. Work Queue will wait for a series of N tasks with steady resource requirements before making a decision on labels. Increasing this parameter will reduce the number of failed tasks due to resource exhaustion when autolabeling, at the cost of increased resources spent collecting stats.
- **autocategory** (*bool*) Place each app in its own category by default. If all invocations of an app have similar performance characteristics, this will provide a reasonable set of categories automatically.
- **max\_retries** (*int*) Set the number of retries that Work Queue will make when a task fails. This is distinct from Parsl level retries configured in parsl.config.Config. Set to None to allow Work Queue to retry tasks forever. By default, this is set to 1, so that all retries will be managed by Parsl.
- **init\_command** (*str*) Command line to run before executing a task in a worker. Default is ".

- worker\_options (str) Extra options passed to work\_queue\_worker. Default is ''.
- worker\_executable (*str*) The command used to invoke work\_queue\_worker. This can be used when the worker needs to be wrapped inside some other command (for example, to run the worker inside a container). Default is 'work\_queue\_worker'.
- **function\_dir** (*str*) The directory where serialized function invocations are placed to be sent to workers. If undefined, this defaults to a directory under runinfo/. If shared\_filesystem=True, then this directory must be visible from both the submitting side and workers.
- **coprocess** (*boo1*) Use Work Queue's coprocess facility to avoid launching a new Python process for each task. Experimental. This requires a version of Work Queue / cctools after commit 874df524516441da531b694afc9d591e8b134b73 (release 7.5.0 is too early). Default is False.

\_\_init\_\_(label: str = 'WorkQueueExecutor', provider: ExecutionProvider =

LocalProvider(channel=LocalChannel(envs={}, script\_dir=None, userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), cmd\_timeout=30, init\_blocks=1, launcher=SingleNodeLauncher(debug=True, fail\_on\_any=False), max\_blocks=1, min\_blocks=0, move\_files=None, nodes\_per\_block=1, parallelism=1, worker\_init=''), working\_dir: str = '.', project\_name: str | None = None, project\_password\_file: str | None = None, address: str | None = None, port: int = 0, env: Dict | None = None, shared\_fs: bool = False, storage\_access: List[Staging] | None = None, use\_cache: bool = False, source: bool = False, pack: bool = False, extra\_pkgs: List[str] | None = None, autolabel: bool = False, autolabel\_window: int = 1, autocategory: bool = True, max\_retries: int = 1, init\_command: str = '', worker\_options: str = '', full\_debug: bool = True, worker\_executable: str = 'work\_queue\_worker', function\_dir: str | None = None, coprocess: bool = False)

# Methods

<pre>init([label, provider, working_dir,])</pre>	
<pre>atexit_cleanup()</pre>	
<pre>create_monitoring_info(status)</pre>	Create a monitoring message for each block based on the poll status.
handle_errors(status)	This method is called by the error management in- frastructure after a status poll.
<pre>initialize_scaling()</pre>	Compose the launch command and call scale out
<pre>monitor_resources()</pre>	Should resource monitoring happen for tasks on run- ning on this executor?
<pre>poll_facade()</pre>	
<pre>scale_in(count)</pre>	Scale in method.
<pre>scale_in_facade(n[, max_idletime])</pre>	
<pre>scale_out([blocks])</pre>	Scales out the number of blocks by "blocks"
<pre>scale_out_facade(n)</pre>	
<pre>send_monitoring_info(status)</pre>	
<pre>set_bad_state_and_fail_all(exception)</pre>	Allows external error handlers to mark this executor as irrecoverably bad and cause all tasks submitted to it now and in the future to fail.
<pre>shutdown(*args, **kwargs)</pre>	Shutdown the executor.
start()	Create submit process and collector thread to create, send, and retrieve Parsl tasks within the Work Queue system.
status()	Return the status of all jobs/blocks currently known to this executor.
<pre>submit(func, resource_specification, *args,)</pre>	Processes the Parsl app by its arguments and submits the function information to the task queue, to be exe- cuted using the Work Queue system.

# **Attributes**

<pre>bad_state_is_set</pre>	Returns true if this executor is in an irrecoverable error state.
executor_exception	Returns an exception that indicates why this executor is in an irrecoverable state.
hub_address	Address to the Hub for monitoring.
hub_port	Port to the Hub for monitoring.
label	
monitoring_radio	Local radio for sending monitoring messages
outstanding	Count the number of outstanding tasks.
provider	
radio_mode	
run_dir	Path to the run directory.
run_id	UUID for the enclosing DFK.
status_facade	Return the status of all jobs/blocks of the executor of this poller.
status_polling_interval	Returns the interval, in seconds, at which the status method should be called.
tasks	
workers_per_node	

## atexit\_cleanup()

# initialize\_scaling()

Compose the launch command and call scale out

Scales the workers to the appropriate nodes with provider

#### property outstanding: int

Count the number of outstanding tasks. This is inefficiently implemented and probably could be replaced with a counter.

#### radio\_mode: str = 'filesystem'

scale\_in(*count: int*)  $\rightarrow$  List[str]

Scale in method.

# shutdown(\*args, \*\*kwargs)

Shutdown the executor. Sets flag to cancel the submit process and collector thread, which shuts down the Work Queue system submission.

#### start()

Create submit process and collector thread to create, send, and retrieve Parsl tasks within the Work Queue system.

#### submit(func, resource\_specification, \*args, \*\*kwargs)

Processes the Parsl app by its arguments and submits the function information to the task queue, to be executed using the Work Queue system. The args and kwargs are processed for input and output files to the Parsl app, so that the files are appropriately specified for the Work Queue task.

## **Parameters**

- func (function) Parsl app to be submitted to the Work Queue system
- **args** (*list*) Arguments to the Parsl app
- kwargs (dict) Keyword arguments to the Parsl app

property workers\_per\_node: int | float

# parsl.executors.taskvine.TaskVineExecutor

**class** parsl.executors.taskvine.**TaskVineExecutor**(*label: str = 'TaskVineExecutor'*,

worker\_launch\_method: Literal['provider'] | *Literal['factory']* | *Literal['manual']* = 'factory', function\_exec\_mode: Literal['regular'] *Literal*['serverless'] = 'regular', manager\_config: TaskVineManagerConfig = TaskVineManagerConfig(port=0, address=None, project\_name=None, project\_password\_file=None, env\_vars=None, init\_command=", env\_pack=None, app pack=False, extra pkgs=None, max retries=1, library config=None, shared fs=False, autolabel=False, autolabel\_algorithm='max-xput', autolabel\_window=None, autocategory=True, enable\_peer\_transfers=True, wait for workers=None, vine log dir=None), factory\_config: TaskVineFactoryConfig = TaskVineFactoryConfig(factory\_timeout=300, scratch\_dir=None, min\_workers=1, max\_workers=1, workers\_per\_cycle=1, worker\_options=None, worker\_executable='vine\_worker', worker\_timeout=300, cores=None, gpus=None, memory=None, disk=None, python\_env=None, *batch\_type='local', condor\_requirements=None,* batch\_options=None, \_project\_port=0, \_project\_address=None, \_project\_name=None, \_project\_password\_file=None), provider: ExecutionProvider | None = LocalProvider(channel=LocalChannel(envs={}, script dir=None, userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/ cmd\_timeout=30, init\_blocks=1, launcher=SingleNodeLauncher(debug=True, fail\_on\_any=False), max\_blocks=1, min\_blocks=0, move\_files=None, nodes\_per\_block=1, parallelism=1, worker\_init="), storage\_access: *List*[Staging] | *None* = *None*)

Executor to use TaskVine dynamic workflow system

The TaskVineExecutor system utilizes the TaskVine framework to efficiently delegate Parsl apps to remote machines in clusters and grids using a fault-tolerant system. Users can run the vine\_worker program on remote machines to connect to the TaskVineExecutor, and Parsl apps will then be sent out to these machines for execution and retrieval.

This Executor sets up configurations for the TaskVine manager, TaskVine factory, and run both in separate processes. Sending tasks and receiving results are done through multiprocessing module native to Python.

## Parameters

- **label** (*str*) A human readable label for the executor, unique with respect to other executors. Default is "TaskVineExecutor".
- worker\_launch\_method (Union[Literal['provider'], Literal['factory'], Literal['manual']]) – Choose to use Parsl provider, TaskVine factory, or manual userprovided workers to scale workers. Options are among {'provider', 'factory', 'manual'}. Default is 'factory'.
- **function\_exec\_mode** (Union[Literal['regular'], Literal['serverless']]) Choose to execute functions with a regular fresh python process or a pre-warmed forked python process. Default is 'regular'.
- **manager\_config** (*TaskVineManagerConfig*) Configuration for the TaskVine manager. Default
- **factory\_config** (*TaskVineFactoryConfig*) Configuration for the TaskVine factory. Use of factory is disabled by default.
- **provider** (ExecutionProvider) The Parsl provider that will spawn worker processes. Default to spawning one local vine worker process.
- **storage\_access** (*List*[Staging]) Define Parsl file staging providers for this executor. Default is None.

**\_\_\_init\_\_**(*label: str = 'TaskVineExecutor', worker launch method: Literal['provider']* | *Literal['factory']* | *Literal['manual'] = 'factory', function\_exec\_mode: Literal['regular'] | Literal['serverless'] =* 'regular', manager\_config: TaskVineManagerConfig = TaskVineManagerConfig(port=0, address=None, project\_name=None, project\_password\_file=None, env\_vars=None, init command=", env pack=None, app pack=False, extra pkgs=None, max retries=1, *library\_config=None, shared\_fs=False, autolabel=False, autolabel\_algorithm='max-xput',* autolabel\_window=None, autocategory=True, enable\_peer\_transfers=True, wait\_for\_workers=None, vine\_log\_dir=None), factory\_config: TaskVineFactoryConfig = TaskVineFactoryConfig(factory\_timeout=300, scratch\_dir=None, min\_workers=1, max\_workers=1, workers\_per\_cycle=1, worker\_options=None, worker\_executable='vine\_worker', worker timeout=300, cores=None, gpus=None, memory=None, disk=None, python env=None, batch\_type='local', condor\_requirements=None, batch\_options=None, \_project\_port=0, \_project\_address=None, \_project\_name=None, \_project\_password\_file=None), provider: ExecutionProvider | None = LocalProvider(channel=LocalChannel(envs={}, script\_dir=None, userhome='/home/docs/checkouts/readthedocs.org/user builds/parsl/checkouts/latest/docs'), cmd timeout=30, init blocks=1, launcher=SingleNodeLauncher(debug=True, fail on any=False), max blocks=1, min blocks=0, move files=None, nodes per block=1, parallelism=1, worker init="), storage access: List[Staging] | None = None)

# Methods

init([label, worker_launch_method,])			
<pre>atexit_cleanup()</pre>			
<pre>create_monitoring_info(status)</pre>	Create a monitoring message for each block based on the poll status.		
handle_errors(status)	This method is called by the error management in- frastructure after a status poll.		
<pre>initialize_scaling()</pre>	Compose the launch command and call scale out		
<pre>monitor_resources()</pre>	Should resource monitoring happen for tasks on run- ning on this executor?		
<pre>poll_facade()</pre>			
<pre>scale_in(count)</pre>	Scale in method.		
<pre>scale_in_facade(n[, max_idletime])</pre>			
<pre>scale_out([blocks])</pre>	Scales out the number of blocks by "blocks"		
<pre>scale_out_facade(n)</pre>			
<pre>send_monitoring_info(status)</pre>			
<pre>set_bad_state_and_fail_all(exception)</pre>	Allows external error handlers to mark this executor as irrecoverably bad and cause all tasks submitted to it now and in the future to fail.		
<pre>shutdown(*args, **kwargs)</pre>	Shutdown the executor.		
start()	Create submit process and collector thread to create, send, and retrieve Parsl tasks within the TaskVine sys- tem.		
status()	Return the status of all jobs/blocks currently known to this executor.		
<pre>submit(func, resource_specification, *args,)</pre>	Processes the Parsl app by its arguments and submits the function information to the task queue, to be exe- cuted using the TaskVine system.		

# **Attributes**

<pre>bad_state_is_set</pre>	Returns true if this executor is in an irrecoverable error state.
executor_exception	Returns an exception that indicates why this executor is in an irrecoverable state.
hub_address	Address to the Hub for monitoring.
hub_port	Port to the Hub for monitoring.
label	
monitoring_radio	Local radio for sending monitoring messages
outstanding	Count the number of outstanding tasks.
provider	
radio_mode	
run_dir	Path to the run directory.
run_id	UUID for the enclosing DFK.
status_facade	Return the status of all jobs/blocks of the executor of this poller.
status_polling_interval	Returns the interval, in seconds, at which the status method should be called.
tasks	
workers_per_node	

# atexit\_cleanup()

#### initialize\_scaling()

Compose the launch command and call scale out

Scales the workers to the appropriate nodes with provider

#### property outstanding: int

Count the number of outstanding tasks.

#### radio\_mode: str = 'filesystem'

```
scale_in(count: int) \rightarrow List[str]
```

Scale in method. Cancel a given number of blocks

# shutdown(\*args, \*\*kwargs)

Shutdown the executor. Sets flag to cancel the submit process and collector thread, which shuts down the TaskVine system submission.

# start()

Create submit process and collector thread to create, send, and retrieve Parsl tasks within the TaskVine system.

#### submit(func, resource\_specification, \*args, \*\*kwargs)

Processes the Parsl app by its arguments and submits the function information to the task queue, to be executed using the TaskVine system. The args and kwargs are processed for input and output files to the Parsl app, so that the files are appropriately specified for the TaskVine task.

**Parameters** 

- **func** (*function*) Parsl app to be submitted to the TaskVine system
- **resource\_specification** (*dict*) Dictionary containing relevant info about task. Include information about resources of task, execution mode of task (out of {regular, server-less}).
- **args** (*list*) Arguments to the Parsl app
- **kwargs** (*dict*) Keyword arguments to the Parsl app

property workers\_per\_node: int | float

# parsl.executors.FluxExecutor

Executor that uses Flux to schedule and run jobs.

Every callable submitted to the executor is wrapped into a Flux job.

This executor requires that there be a Flux installation available locally, and that it can be located either in PATH or through the flux\_path argument.

Flux jobs are fairly heavyweight. As of Flux v0.25, a single Flux instance is (on many systems) capped at 50 jobs per second. As such, this executor is not a good fit for use-cases consisting of large numbers of small, fast jobs.

However, Flux is great at handling jobs with large resource requirements, and collections of jobs with varying resource requirements.

Note that due to vendor-specific extensions, on certain Cray machines like ALCF's Theta or LANL's Trinitite/Trinity, Flux cannot run applications that use the default MPI library. Generally the only workaround is to recompile with another MPI library like OpenMPI.

This executor acts as a sort of wrapper around a flux.job.FluxExecutor, which can be confusing since both wrapped and wrapper classes share the same name. Whenever possible, the underlying executor is referred by its fully qualified name, flux.job.FluxExecutor.

#### Parameters

- working\_dir (*str*) Directory in which the executor should place its files, possibly overwriting existing files. If None, generate a unique directory.
- **label** (*str*) Label for this executor instance.
- **flux\_handle\_args** (*collections.abc.Sequence*) Positional arguments to flux. Flux() instance, if any. The first positional argument, **url**, is provided by this executor.
- **flux\_executor\_kwargs** (*collections.abc.Mapping*) Keyword arguments to pass to the underlying flux.job.FluxExecutor() instance, if any. Note that the handle\_args keyword argument is provided by this executor, in order to supply the URL of a remote Flux instance.
- **flux\_path** (*str*) Path to flux installation to use, or None to search PATH for flux.
- **launch\_cmd** (*str*) The command to use when launching the executor's backend. The default command is available as the DEFAULT\_LAUNCH\_COMMAND attribute. The default command starts a new Flux instance, which may not be desirable if a Flux instance will already be provisioned (this is not likely).

\_\_init\_\_(provider: ExecutionProvider | None = None, working\_dir: str | None = None, label: str =
'FluxExecutor', flux\_executor\_kwargs: Mapping = {}, flux\_path: str | None = None, launch\_cmd:
str | None = None)

# **Methods**

init([provider, working_dir, label,])	
<pre>monitor_resources()</pre>	Should resource monitoring happen for tasks on run- ning on this executor?
<pre>shutdown([wait])</pre>	Shut down the executor, causing further calls to submit to fail.
start()	Called when DFK starts the executor when the config is loaded.
<pre>submit(func, resource_specification, *args,)</pre>	Wrap a callable in a Flux job and submit it to Flux.

# **Attributes**

DEFAULT_LAUNCH_CMD	
hub_address	Address to the Hub for monitoring.
hub_port	Port to the Hub for monitoring.
label	
monitoring_radio	Local radio for sending monitoring messages
radio_mode	
run_dir	Path to the run directory.
run_id	UUID for the enclosing DFK.

# DEFAULT\_LAUNCH\_CMD = '{flux} start {python} {manager} {protocol} {hostname} {port}'

#### shutdown(wait=True)

Shut down the executor, causing further calls to submit to fail.

# Parameters

wait – If True, do not return until all submitted Futures are done.

#### start()

Called when DFK starts the executor when the config is loaded.

submit(func: Callable, resource\_specification: Dict[str, Any], \*args: Any, \*\*kwargs: Any)

Wrap a callable in a Flux job and submit it to Flux.

## Parameters

- **func** The callable to submit as a job to Flux
- **resource\_specification** A mapping defining the resources to allocate to the Flux job.

Only the following keys are checked for:

- num\_tasks: the number of tasks to launch (MPI ranks for an MPI job), default 1
- cores\_per\_task: cores per task, default 1
- gpus\_per\_task: gpus per task, default 1
- num\_nodes: if > 0, evenly distribute the allocated cores/gpus across the given number of nodes. Does *not* give the job exclusive access to those nodes; this option only affects distribution.
- args positional arguments for the callable
- kwargs keyword arguments for the callable

#### parsl.executors.radical.RadicalPilotExecutor

# Executor is designed for executing heterogeneous tasks

in terms of type/resource.

The RadicalPilotExecutor system has the following main components:

- 1. "start": Create and start the RADICAL-Pilot runtime components rp.Session, rp.PilotManager and rp.TaskManager.
- 2. "translate": Unwrap, identify, and parse Parsl apps into rp.TaskDescription.
- 3. "submit": Submit Parsl apps to rp.TaskManager.
- 4. "shut\_down": Shut down the RADICAL-Pilot runtime and all associated components.

Here is a diagram

The RadicalPilotExecutor creates a rp.Session, rp.TaskManager, and rp.PilotManager. The executor receives the Parsl apps from the DFK and translates these apps (in-memory) into rp.TaskDescription object to be passed to the rp.TaskManager. This executor has two submission mechanisms:

- 1. Default\_mode: where the executor submits the tasks directly to RADICAL-Pilot.
- 2. Bulk\_mode: where the executor accumulates N tasks (functions and executables) and submit them.

#### Parameters

- **rpex\_cfg** a dataclass specifying resource configuration. Default is ResourceConfig instance.
- label (*str*) Label for this executor instance. Default is "RPEX".

- **bulk\_mode** (*bool*) Enable bulk mode submission and execution. Default is False (stream).
- **resource** (*Optional[str]*) The resource name of the targeted HPC machine or cluster. Default is local.localhost (user local machine).
- runtime (*int*) The maximum runtime for the entire job in minutes. Default is 30.
- **working\_dir** (*str*) The working dir to be used by the executor.
- **rpex\_pilot\_kwargs** (Dict of kwargs that are passed directly to the rp.PilotDescription object.) –
- information (For more) -

# **Methods**

init(resource[, label, bulk_mode,])	
<pre>monitor_resources()</pre>	Should resource monitoring happen for tasks on run- ning on this executor?
<pre>shutdown([hub, targets, block])</pre>	Shutdown the executor, including all RADICAL- Pilot components.
start()	Create the Pilot component and pass it.
<pre>submit(func, resource_specification, *args,)</pre>	Submits tasks in stream mode or bulks (bulk mode) to RADICAL-Pilot rp.TaskManager.
<pre>task_state_cb(task, state)</pre>	Update the state of Parsl Future apps Based on RP task state callbacks.
<pre>task_translate(tid, func,)</pre>	Convert Parsl function to RADICAL-Pilot rp.TaskDescription
unwrap(func, args)	Unwrap a Parsl app and its args for further processing.

### Attributes

hub_address	Address to the Hub for monitoring.
hub_port	Port to the Hub for monitoring.
label	
monitoring_radio	Local radio for sending monitoring messages
radio_mode	
run_dir	Path to the run directory.
run_id	UUID for the enclosing DFK.

shutdown(hub=True, targets='all', block=False)

Shutdown the executor, including all RADICAL-Pilot components.

#### start()

Create the Pilot component and pass it.

submit(func, resource\_specification, \*args, \*\*kwargs)

Submits tasks in stream mode or bulks (bulk mode) to RADICAL-Pilot rp.TaskManager.

task\_state\_cb(task, state)

Update the state of Parsl Future apps Based on RP task state callbacks.

task\_translate(tid, func, parsl\_resource\_specification, args, kwargs)

Convert Parsl function to RADICAL-Pilot rp.TaskDescription

# unwrap(func, args)

Unwrap a Parsl app and its args for further processing.

# Parameters

- **func** (*callable*) The function to be unwrapped.
- **args** (*tuple*) The arguments associated with the function.

# Returns

A tuple containing the unwrapped function, adjusted arguments, and task type information.

# Return type

tuple

# Launchers

parsl.launchers.base.Launcher	Launchers are basically wrappers for user submitted scripts as they are submitted to a specific execution re- source.
parsl.launchers.SimpleLauncher	Does no wrapping.
parsl.launchers.SingleNodeLauncher	Worker launcher that wraps the user's command with the framework to launch multiple command invocations in parallel.
parsl.launchers.SrunLauncher	Worker launcher that wraps the user's command with the SRUN launch framework to launch multiple cmd invo- cations in parallel on a single job allocation.
parsl.launchers.AprunLauncher	Worker launcher that wraps the user's command with the Aprun launch framework to launch multiple cmd invoca- tions in parallel on a single job allocation
parsl.launchers.SrunMPILauncher	Launches as many workers as MPI tasks to be executed concurrently within a block.
parsl.launchers.GnuParallelLauncher	Worker launcher that wraps the user's command with the framework to launch multiple command invocations via GNU parallel sshlogin.
parsl.launchers.MpiExecLauncher	Worker launcher that wraps the user's command with the framework to launch multiple command invocations via mpiexec.
parsl.launchers.JsrunLauncher	Worker launcher that wraps the user's command with the Jsrun launch framework to launch multiple cmd invoca- tions in parallel on a single job allocation
parsl.launchers.WrappedLauncher	Wraps the command by prepending commands before a user's command

# parsl.launchers.base.Launcher

class parsl.launchers.base.Launcher(debug: bool = True)

Launchers are basically wrappers for user submitted scripts as they are submitted to a specific execution resource.

\_\_init\_\_(debug: bool = True)

# **Methods**

\_\_init\_\_([debug])

# parsl.launchers.SimpleLauncher

```
class parsl.launchers.SimpleLauncher(debug: bool = True)
```

Does no wrapping. Just returns the command as-is

**\_\_init\_\_**(*debug: bool* = *True*)  $\rightarrow$  None

# Methods

\_\_init\_\_([debug])

# parsl.launchers.SingleNodeLauncher

```
class pars1.launchers.SingleNodeLauncher(debug: bool = True, fail_on_any: bool = False)
```

Worker launcher that wraps the user's command with the framework to launch multiple command invocations in parallel. This wrapper sets the bash env variable CORES to the number of cores on the machine. By setting task\_blocks to an integer or to a bash expression the number of invocations of the command to be launched can be controlled.

\_\_init\_\_(debug: bool = True, fail\_on\_any: bool = False)

# **Methods**

\_\_\_init\_\_([debug, fail\_on\_any])

# parsl.launchers.SrunLauncher

**class** parsl.launchers.**SrunLauncher**(*debug: bool = True, overrides: str = "*)

Worker launcher that wraps the user's command with the SRUN launch framework to launch multiple cmd invocations in parallel on a single job allocation.

\_\_init\_\_(debug: bool = True, overrides: str = ")

#### **Parameters**

overrides (str) – This string will be passed to the srun launcher. Default: "

### **Methods**

\_\_init\_\_([debug, overrides])

param overrides This string will be passed to the srun launcher. Default: "

# parsl.launchers.AprunLauncher

```
class parsl.launchers.AprunLauncher(debug: bool = True, overrides: str = ")
```

Worker launcher that wraps the user's command with the Aprun launch framework to launch multiple cmd invocations in parallel on a single job allocation

\_\_init\_\_(debug: bool = True, overrides: str = ")

Parameters

overrides (str) – This string will be passed to the aprun launcher. Default: "

#### **Methods**

\_\_init\_\_([debug, overrides])

param overrides This string will be passed to the aprun launcher. Default: "

#### parsl.launchers.SrunMPILauncher

**class** parsl.launchers.**SrunMPILauncher**(*debug: bool = True, overrides: str = "*)

Launches as many workers as MPI tasks to be executed concurrently within a block.

Use this launcher instead of SrunLauncher if each block will execute multiple MPI applications at the same time. Workers should be launched with independent Srun calls so as to setup the environment for MPI application launch.
\_\_init\_\_(debug: bool = True, overrides: str = ")

```
Parameters
overrides (str) – This string will be passed to the launcher. Default: "
```

# **Methods**

\_\_\_init\_\_([debug, overrides])

param overrides

This string will be passed to the launcher. Default: "

### parsl.launchers.GnuParallelLauncher

### class parsl.launchers.GnuParallelLauncher(debug: bool = True)

Worker launcher that wraps the user's command with the framework to launch multiple command invocations via GNU parallel sshlogin.

This wrapper sets the bash env variable CORES to the number of cores on the machine.

This launcher makes the following assumptions:

- GNU parallel is installed and can be located in \$PATH
- Paswordless SSH login is configured between the controller node and the target nodes.
- The provider makes available the \$PBS\_NODEFILE environment variable

\_\_init\_\_(debug: bool = True)

# Methods

\_\_init\_\_([debug])

# parsl.launchers.MpiExecLauncher

**class** parsl.launchers.**MpiExecLauncher**(*debug: bool = True, bind\_cmd: str = '--bind-to', overrides: str =* 

Worker launcher that wraps the user's command with the framework to launch multiple command invocations via mpiexec.

This wrapper sets the bash env variable CORES to the number of cores on the machine.

")

This launcher makes the following assumptions: - mpiexec is installed and can be located in \$PATH - The provider makes available the \$PBS\_NODEFILE environment variable

\_\_init\_\_(debug: bool = True, bind\_cmd: str = '--bind-to', overrides: str = '')

### Parameters

- **bind\_cmd** (*str*) Name of the argument for binding ranks to CPUs
- overrides (str) Additional arguments to add to the invocation

# Methods

\_\_init\_\_([debug, bind\_cmd, overrides])

param bind\_cmd Name of the argument for binding ranks to CPUs

### parsl.launchers.JsrunLauncher

```
class parsl.launchers.JsrunLauncher(debug: bool = True, overrides: str = ")
```

Worker launcher that wraps the user's command with the Jsrun launch framework to launch multiple cmd invocations in parallel on a single job allocation

\_\_init\_\_(debug: bool = True, overrides: str = ")

Parameters

overrides (str) – This string will be passed to the JSrun launcher. Default: "

# **Methods**

\_\_init\_\_([debug, overrides])

param overrides This string will be passed to the JSrun launcher. Default: "

### parsl.launchers.WrappedLauncher

**class** parsl.launchers.**WrappedLauncher**(*prepend: str, debug: bool = True*)

Wraps the command by prepending commands before a user's command

As an example, the wrapped launcher can be used to launch a command inside a docker container by prepending the proper docker invocation

\_\_init\_\_(prepend: str, debug: bool = True)

**Parameters prepend** (*str*) – Command to use before the launcher (e.g., time)

# Methods

\_\_\_*init\_\_\_*(prepend[, debug])

### param prepend

Command to use before the launcher (e.g., time)

# **Providers**

parsl.providers.AdHocProvider	Ad-hoc execution provider
parsl.providers.AWSProvider	A provider for using Amazon Elastic Compute Cloud (EC2) resources.
parsl.providers.CobaltProvider	Cobalt Execution Provider
parsl.providers.CondorProvider	HTCondor Execution Provider.
parsl.providers.GoogleCloudProvider	A provider for using resources from the Google Compute Engine.
parsl.providers.GridEngineProvider	A provider for the Grid Engine scheduler.
parsl.providers.LocalProvider	Local Execution Provider
parsl.providers.LSFProvider	LSF Execution Provider
parsl.providers.SlurmProvider	Slurm Execution Provider
parsl.providers.TorqueProvider	Torque Execution Provider
parsl.providers.KubernetesProvider	Kubernetes execution provider
parsl.providers.PBSProProvider	PBS Pro Execution Provider
parsl.providers.base.ExecutionProvider	Execution providers are responsible for managing exe- cution resources that have a Local Resource Manager (LRM).
<pre>parsl.providers.cluster_provider.</pre>	This class defines behavior common to all
ClusterProvider	cluster/supercompute-style scheduler systems.

# parsl.providers.AdHocProvider

Ad-hoc execution provider

This provider is used to provision execution resources over one or more ad hoc nodes that are each accessible over a Channel (say, ssh) but otherwise lack a cluster scheduler.

- **channels** (*list of Channel ojects*) Each channel represents a connection to a remote node
- **worker\_init** (*str*) Command to be run before starting a worker, such as 'module load Anaconda; source activate env'. Since this provider calls the same worker\_init across all nodes in the ad-hoc cluster, it is recommended that a single script is made available across nodes such as ~/setup.sh that can be invoked.
- **cmd\_timeout** (*int*) Duration for which the provider will wait for a command to be invoked on a remote system. Defaults to 30s

• **parallelism** (*float*) – Determines the ratio of workers to tasks as managed by the strategy component

\_\_init\_\_(channels=[], worker\_init=", cmd\_timeout=30, parallelism=1, move\_files=None)

# **Methods**

init([channels, worker_init,])	
<pre>cancel(job_ids)</pre>	Cancel a list of jobs with job_ids
<pre>status(job_ids)</pre>	Get status of the list of jobs with job_ids
<pre>submit(command, tasks_per_node[, job_name])</pre>	Submits the command onto a channel from the list of
	channels

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancel a list of jobs with job\_ids

# **Parameters**

job\_ids (list of strings) - List of job id strings

### Returns

list of confirmation bools

# Return type

[True, False...]

# property label

Provides the label for this provider

# status(job\_ids)

Get status of the list of jobs with job\_ids

# Parameters

job\_ids (list of strings) – List of job id strings

# **Return type**

list of JobStatus objects

# property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

submit(command, tasks\_per\_node, job\_name='parsl.adhoc')

Submits the command onto a channel from the list of channels

Submit returns an ID that corresponds to the task that was just submitted.

### **Parameters**

- command ((String)) Commandline invocation to be made on the remote side.
- tasks\_per\_node ((int)) command invocations to be launched per node
- job\_name ((String)) Name of the job. Default : parsl.adhoc

### Returns

- None At capacity, cannot provision more
- **job\_id** ((*string*)) Identifier for the job

# parsl.providers.AWSProvider

A provider for using Amazon Elastic Compute Cloud (EC2) resources.

One of 3 methods are required to authenticate: keyfile, profile or environment variables. If neither keyfile or profile are set, the following environment variables must be set: AWS\_ACCESS\_KEY\_ID (the access key for your AWS account), AWS\_SECRET\_ACCESS\_KEY (the secret key for your AWS account), and (optionaly) the AWS\_SESSION\_TOKEN (the session key for your AWS account).

- image\_id (str) Identification of the Amazon Machine Image (AMI).
- **worker\_init** (*str*) String to append to the Userdata script executed in the cloudinit phase of instance initialization.
- walltime (str) Walltime requested per block in HH:MM:SS.
- key\_file (str) Path to json file that contains 'AWSAccessKeyId' and 'AWSSecretKey'.
- nodes\_per\_block (*int*) This is always 1 for ec2. Nodes to provision per block.
- **profile** (*str*) Profile to be used from the standard aws config file ~/.aws/config.
- nodes\_per\_block Nodes to provision per block. Default is 1.
- **init\_blocks** (*int*) Number of blocks to provision at the start of the run. Default is 1.
- min\_blocks (int) Minimum number of blocks to maintain. Default is 0.
- max\_blocks (int) Maximum number of blocks to maintain. Default is 10.
- **instance\_type** (*str*) EC2 instance type. Instance types comprise varying combinations of CPU, memory, storage, and networking capacity For more information on possible instance types, see here. Default is 't2.small'.
- **region** (*str*) Amazon Web Service (AWS) region to launch machines. Default is 'useast-2'.

- **key\_name** (*str*) Name of the AWS private key (.pem file) that is usually generated on the console to allow SSH access to the EC2 instances. This is mostly used for debugging.
- **spot\_max\_bid** (*float*) Maximum bid price (if requesting spot market machines).
- iam\_instance\_profile\_arn (str) Launch instance with a specific role.
- **state\_file** (*str*) Path to the state file from a previous run to re-use.
- walltime Walltime requested per block in HH:MM:SS. This option is not currently honored by this provider.
- **launcher** (Launcher) Launcher for this provider. With AWS, usually the default *SingleNodeLauncher* will be appropriate.
- **linger** (*Bool*) When set to True, the workers will not halt. The user is responsible for shutting down the node.

# Methods

init(image_id, key_name[, init_blocks,])	
cancel(job_ids)	Cancel the jobs specified by a list of job ids.
<pre>config_route_table(vpc, internet_gateway)</pre>	Configure route table for Virtual Private Cloud (VPC).
<pre>create_name_tag_spec(resource_type, name)</pre>	Create a new tag specification for a resource name.
create_session()	Create a session.
<pre>create_vpc()</pre>	Create and configure VPC
<pre>generate_aws_id()</pre>	Generate a new ID for AWS resources.
<pre>get_instance_state([instances])</pre>	Get states of all instances on EC2 which were started by this file.
goodbye()	
<pre>initialize_boto_client()</pre>	Initialize the boto client.
<pre>read_state_file(state_file)</pre>	Read the state file, if it exists.
<pre>security_group(vpc, name)</pre>	Create and configure a new security group.
show_summary()	Print human readable summary of current AWS state to log and to console.
<pre>shut_down_instance([instances])</pre>	Shut down a list of instances, if provided.
<pre>spin_up_instance(command, job_name)</pre>	Start an instance in the VPC in the first available subnet.
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by their ids.
<pre>submit([command, tasks_per_node, job_name])</pre>	Submit the command onto a freshly instantiated AWS EC2 instance.
teardown()	Teardown the EC2 infastructure.
<pre>write_state_file()</pre>	Save information that must persist to a file.
xstr(s)	

# **Attributes**

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancel the jobs specified by a list of job ids.

Parameters

job\_ids (list of str) - List of of job identifiers

#### Returns

Each entry in the list will contain False if the operation fails. Otherwise, the entry will be True.

Return type list of bool

config\_route\_table(vpc, internet\_gateway)

Configure route table for Virtual Private Cloud (VPC).

#### Parameters

- **vpc** (*dict*) Representation of the VPC (created by create\_vpc()).
- **internet\_gateway** (*dict*) Representation of the internet gateway (created by create\_vpc()).

### create\_name\_tag\_spec(resource\_type, name)

Create a new tag specification for a resource name.

### Parameters

- **resource\_type** (*str*) The AWS resource type
- **name** (*str*) The name to assign to the resource

# Returns

A TagSpecifications record to be passed into the creation of a new AWS resource.

Return type record

#### create\_session()

Create a session.

First we look in self.key\_file for a path to a json file with the credentials. The key file should have 'AWSAccessKeyId' and 'AWSSecretKey'.

Next we look at self.profile for a profile name and try to use the Session call to automatically pick up the keys for the profile from the user default keys file ~/.aws/config.

Finally, boto3 will look for the keys in environment variables: AWS\_ACCESS\_KEY\_ID: The access key for your AWS account. AWS\_SECRET\_ACCESS\_KEY: The secret key for your AWS account. AWS\_SESSION\_TOKEN: The session key for your AWS account. This is only needed when you are using temporary credentials. The AWS\_SECURITY\_TOKEN environment variable can also be used, but is only

supported for backwards compatibility purposes. AWS\_SESSION\_TOKEN is supported by multiple AWS SDKs besides python.

# create\_vpc()

Create and configure VPC

We create a VPC with CIDR 10.0.0/16, which provides up to 64,000 instances.

We attach a subnet for each availability zone within the region specified in the config. We give each subnet an ip range like 10.0.X.0/20, which is large enough for approx. 4000 instances.

Security groups are configured in function security\_group.

# generate\_aws\_id()

Generate a new ID for AWS resources.

### Returns

An ID of the form 'parsl.aws.123456.789' for giving resources unique identifiers.

### **Return type**

str

### get\_instance\_state(instances=None)

Get states of all instances on EC2 which were started by this file.

### goodbye()

### initialize\_boto\_client()

Initialize the boto client.

# property label

Provides the label for this provider

# read\_state\_file(state\_file)

Read the state file, if it exists.

If this script has been run previously, resource IDs will have been written to a state file. On starting a run, a state file will be looked for before creating new infrastructure. Information on VPCs, security groups, and subnets are saved, as well as running instances and their states.

AWS has a maximum number of VPCs per region per account, so we do not want to clutter users' AWS accounts with security groups and VPCs that will be used only once.

### security\_group(vpc, name)

Create and configure a new security group.

Allows all ICMP in, all TCP and UDP in within VPC.

This security group is very open. It allows all incoming ping requests on all ports. It also allows all outgoing traffic on all ports. This can be limited by changing the allowed port ranges.

### **Parameters**

- **vpc** (*VPC instance*) VPC in which to set up security group.
- **name** (*str*) Name tag for the newly created security group.

# show\_summary()

Print human readable summary of current AWS state to log and to console.

# shut\_down\_instance(instances=None)

Shut down a list of instances, if provided.

If no instance is provided, the last instance started up will be shut down.

### spin\_up\_instance(command, job\_name)

Start an instance in the VPC in the first available subnet.

N instances will be started if nodes\_per\_block > 1. Not supported. We only do 1 node per block.

### Parameters

- **command** (*str*) Command string to execute on the node.
- **job\_name** (*str*) Name associated with the instances.

### status(job\_ids)

Get the status of a list of jobs identified by their ids.

### Parameters

job\_ids (list of str) – Identifiers for the jobs.

#### Returns

The status codes of the requsted jobs.

# Return type

list of int

### property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

submit(command='sleep 1', tasks\_per\_node=1, job\_name='parsl.aws')

Submit the command onto a freshly instantiated AWS EC2 instance.

Submit returns an ID that corresponds to the task that was just submitted.

### Parameters

- command (str) Command to be invoked on the remote side.
- **tasks\_per\_node** (*int* (*default=1*)) Number of command invocations to be launched per node
- job\_name (str) Prefix for the job name.

### Returns

If at capacity, None will be returned. Otherwise, the job identifier will be returned.

#### **Return type**

None or str

# teardown()

Teardown the EC2 infastructure.

Terminate all EC2 instances, delete all subnets, delete security group, delete VPC, and reset all instance variables.

### write\_state\_file()

Save information that must persist to a file.

We do not want to create a new VPC and new identical security groups, so we save information about them in a file between runs.

# xstr(s)

# parsl.providers.CobaltProvider

```
class parsl.providers.CobaltProvider(channel=LocalChannel(envs={}, script_dir=None, user-
```

home='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs' nodes\_per\_block=1, init\_blocks=0, min\_blocks=0, max\_blocks=1, parallelism=1, walltime='00:10:00', account=None, queue=None, scheduler\_options=", worker\_init=", launcher=AprunLauncher(debug=True, overrides="), cmd\_timeout=10)

Cobalt Execution Provider

WARNING: CobaltProvider is deprecated and will be removed by 2024.04

This provider uses cobalt to submit (qsub), obtain the status of (qstat), and cancel (qdel) jobs. Theo script to be used is created from a template file in this same module.

# Parameters

- **channel** (Channel) Channel for accessing this provider. Possible channels include *LocalChannel* (the default), *SSHChannel*, or *SSHInteractiveLoginChannel*.
- **nodes\_per\_block** (*int*) Nodes to provision per block.
- **min\_blocks** (*int*) Minimum number of blocks to maintain.
- max\_blocks (int) Maximum number of blocks to maintain.
- walltime (str) Walltime requested per block in HH:MM:SS.
- **account** (*str*) Account that the job will be charged against.
- queue (*str*) Torque queue to request blocks from.
- scheduler\_options (str) String to prepend to the submit script to the scheduler.
- **worker\_init** (*str*) Command to be run before starting a worker, such as 'module load Anaconda; source activate env'.
- **launcher** (Launcher) Launcher for this provider. Possible launchers include *AprunLauncher* (the default) or, *SingleNodeLauncher*

# \_\_init\_\_(channel=LocalChannel(envs={}, script\_dir=None,

userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), nodes\_per\_block=1, init\_blocks=0, min\_blocks=0, max\_blocks=1, parallelism=1, walltime='00:10:00', account=None, queue=None, scheduler\_options='', worker\_init='', launcher=AprunLauncher(debug=True, overrides=''), cmd\_timeout=10)

# Methods

init([channel, nodes_per_block,])	
<pre>cancel(job_ids)</pre>	Cancels the jobs specified by a list of job ids
<pre>execute_wait(cmd[, timeout])</pre>	
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	Submits the command onto an Local Resource Manager job of parallel elements.

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancels the jobs specified by a list of job ids

Args: job\_ids : [<job\_id> ...]

Returns : [True/False...] : If the cancel operation fails the entire list will be False.

# property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

#### Returns

the number of seconds to wait between calls to status()

submit(command, tasks\_per\_node, job\_name='parsl.cobalt')

Submits the command onto an Local Resource Manager job of parallel elements. Submit returns an ID that corresponds to the task that was just submitted.

If tasks\_per\_node < 1 : ! This is illegal. tasks\_per\_node should be integer

```
If tasks_per_node == 1:
```

A single node is provisioned

```
If tasks_per_node > 1 :
```

tasks\_per\_node number of nodes are provisioned.

### **Parameters**

- command (-) (String) Commandline invocation to be made on the remote side.
- tasks\_per\_node (-) command invocations to be launched per node

# **Kwargs:**

• job\_name (String): Name for job, must be unique

### Returns

At capacity, cannot provision more - job\_id: (string) Identifier for the job

# **Return type**

• None

# parsl.providers.CondorProvider

```
class pars1.providers.CondorProvider(channel: Channel = LocalChannel(envs={}, script_dir=None, user-
home='/home/docs/checkouts/readthedocs.org/user_builds/parsl/checkouts/latest/docs'
nodes_per_block: int = 1, cores_per_slot: int | None = None,
mem_per_slot: float | None = None, init_blocks: int = 1,
min_blocks: int = 0, max_blocks: int = 1, parallelism: float = 1,
environment: Dict[str, str] | None = None, project: str = '',
scheduler_options: str = '', transfer_input_files: List[str] = [],
walltime: str = '00:10:00', worker_init: str = '', launcher: Launcher
= SingleNodeLauncher(debug=True, fail_on_any=False),
requirements: str = '', cmd_timeout: int = 60, cmd_chunk_size: int
= 100)
```

HTCondor Execution Provider.

- **channel** (Channel) Channel for accessing this provider. Possible channels include *LocalChannel* (the default), *SSHChannel*, or *SSHInteractiveLoginChannel*.
- **nodes\_per\_block** (*int*) Nodes to provision per block.
- **cores\_per\_slot** (*int*) Specify the number of cores to provision per slot. If set to None, executors will assume all cores on the node are available for computation. Default is None.
- **mem\_per\_slot** (*float*) Specify the real memory to provision per slot in GB. If set to None, no explicit request to the scheduler will be made. Default is None.
- init\_blocks (int) Number of blocks to provision at time of initialization
- min\_blocks (int) Minimum number of blocks to maintain
- max\_blocks (int) Maximum number of blocks to maintain.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.
- **environment** (*dict of str*) A dictionary of environmant variable name and value pairs which will be set before running a task.
- project (str) Project which the job will be charged against
- **scheduler\_options** (*str*) String to add specific condor attributes to the HTCondor submit script.
- **transfer\_input\_files** (*list(str)*) List of strings of paths to additional files or directories to transfer to the job
- worker\_init (*str*) Command to be run before starting a worker.
- **requirements** (*str*) Condor requirements.

- **launcher** (Launcher) Launcher for this provider. Possible launchers include *SingleNodeLauncher* (the default),
- cmd\_timeout (int) Timeout for commands made to the scheduler in seconds.
- **cmd\_chunk\_size** (*int*) Calls to the scheduler will be made for chunks of blocks with this size.

\_\_init\_\_(channel: Channel = LocalChannel(envs={}, script\_dir=None,

userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), nodes\_per\_block: int = 1, cores\_per\_slot: int | None = None, mem\_per\_slot: float | None = None, init\_blocks: int = 1, min\_blocks: int = 0, max\_blocks: int = 1, parallelism: float = 1, environment: Dict[str, str] | None = None, project: str = '', scheduler\_options: str = '', transfer\_input\_files: List[str] = [], walltime: str = '00:10:00', worker\_init: str = '', launcher: Launcher = SingleNodeLauncher(debug=True, fail\_on\_any=False), requirements: str = '', cmd\_timeout: int = 60, cmd\_chunk\_size: int = 100)  $\rightarrow$  None

# **Methods**

Cancels the jobs specified by a list of job IDs.
Get the status of a list of jobs identified by their ids.
Submits the command onto an Local Resource Manager job.

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
status_polling_interval	Returns the interval, in seconds, at which the status
	method should be called.

### cancel(job\_ids)

Cancels the jobs specified by a list of job IDs.

### Parameters

job\_ids (list of str) – The job IDs to cancel.

### Returns

Each entry in the list will be True if the job is cancelled succesfully, otherwise False.

# **Return type**

list of bool

# status(job\_ids)

Get the status of a list of jobs identified by their ids.

### **Parameters**

job\_ids (list of int) – Identifiers of jobs for which the status will be returned.

# Returns

Status codes for the requested jobs.

# **Return type**

List of int

# property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

submit(command, tasks\_per\_node, job\_name='parsl.condor')

Submits the command onto an Local Resource Manager job.

# example file with the complex case of multiple submits per job:

Universe =vanilla output = out.(Cluster).(Process) error = err.(Cluster).(Process) log = log.(Cluster) leave\_in\_queue = true executable = test.sh queue 5 executable = foo queue 1

\$ condor\_submit test.sub Submitting job(s)..... 5 job(s) submitted to cluster 118907. 1 job(s) submitted to cluster 118908.

### **Parameters**

- command (*str*) Command to execute
- job\_name (str) Job name prefix.
- tasks\_per\_node (int) command invocations to be launched per node

### Returns

None if at capacity and cannot provision more; otherwise the identifier for the job.

### **Return type**

None or str

# parsl.providers.GoogleCloudProvider

A provider for using resources from the Google Compute Engine.

- **project\_id** (*str*) Project ID from Google compute engine.
- **key\_file** (*str*) Path to authorization private key json file. This is required for auth. A new one can be generated here: https://console.cloud.google.com/apis/credentials
- region (str) Region in which to start instances
- **os\_project** (*str*) OS project code for Google compute engine.
- **os\_family** (*str*) OS family to request.
- **google\_version** (*str*) Google compute engine version to use. Possibilies include 'v1' (default) or 'beta'.
- instance\_type (str) 'n1-standard-1',

- **init\_blocks** (*int*) Number of blocks to provision immediately. Default is 1.
- min\_blocks (*int*) Minimum number of blocks to maintain. Default is 0.
- max\_blocks (int) Maximum number of blocks to maintain. Default is 10.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.

# Methods

init(project_id, key_file, region,)	
bye()	
<pre>cancel(job_ids)</pre>	Cancels the resources identified by the job_ids pro- vided by the user.
<pre>create_instance([command])</pre>	
<pre>delete_instance(name)</pre>	
get_zone(region)	
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	The submit method takes the command string to be executed upon instantiation of a resource most often to start a pilot.

# Attributes

status\_polling\_interval

# bye()

```
cancel(job_ids)
```

Cancels the resources identified by the job\_ids provided by the user.

Parameters

**job\_ids** (-) – A list of job identifiers

# Returns

• A list of status from cancelling the job which can be True, False

### Raises

# - ExecutionProviderException or its subclasses -

create\_instance(command=")

### delete\_instance(name)

### get\_zone(region)

# status(job\_ids)

Get the status of a list of jobs identified by the job identifiers returned from the submit request.

# **Parameters**

job\_ids (-) - A list of job identifiers

### Returns

• A list of JobStatus objects corresponding to each job\_id in the job\_ids list.

### Raises

- ExecutionProviderException or its subclasses -

# property status\_polling\_interval

# submit(command, tasks\_per\_node, job\_name='parsl.gcs')

The submit method takes the command string to be executed upon instantiation of a resource most often to start a pilot.

### Args :

- command (str) : The bash command string to be executed.
- tasks\_per\_node (int) : command invocations to be launched per node

### **KWargs:**

• job\_name (str) : Human friendly name to be assigned to the job request

### Returns

• A job identifier, this could be an integer, string etc

### Raises

- ExecutionProviderException or its subclasses -

# parsl.providers.GridEngineProvider

class parsl.providers.GridEngineProvider(channel=LocalChannel(envs={}, script\_dir=None, user-

home='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/ nodes\_per\_block=1, init\_blocks=1, min\_blocks=0, max\_blocks=1, parallelism=1, walltime='00:10:00', scheduler\_options='', worker\_init='',

launcher=SingleNodeLauncher(debug=True,

```
fail_on_any=False), cmd_timeout: int = 60, queue=None)
```

A provider for the Grid Engine scheduler.

# Parameters

• **channel** (Channel) – Channel for accessing this provider. Possible channels include *LocalChannel* (the default), *SSHChannel*, or *SSHInteractiveLoginChannel*.

- nodes\_per\_block (int) Nodes to provision per block.
- min\_blocks (int) Minimum number of blocks to maintain.
- max\_blocks (int) Maximum number of blocks to maintain.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.
- walltime (str) Walltime requested per block in HH:MM:SS.
- **scheduler\_options** (*str*) String to prepend to the #\$\$ blocks in the submit script to the scheduler.
- **worker\_init** (*str*) Command to be run before starting a worker, such as 'module load Anaconda; source activate env'.
- **launcher** (Launcher) Launcher for this provider. Possible launchers include *SingleNodeLauncher* (the default),
- cmd\_timeout (int) Timeout for commands made to the scheduler in seconds

# \_\_init\_\_(channel=LocalChannel(envs={}, script\_dir=None,

userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), nodes\_per\_block=1, init\_blocks=1, min\_blocks=0, max\_blocks=1, parallelism=1, walltime='00:10:00', scheduler\_options='', worker\_init='', launcher=SingleNodeLauncher(debug=True, fail\_on\_any=False), cmd\_timeout: int = 60, queue=None)

# **Methods**

init([channel, nodes_per_block,])	
<pre>cancel(job_ids)</pre>	Cancels the resources identified by the job_ids pro- vided by the user.
<pre>execute_wait(cmd[, timeout])</pre>	
<pre>get_configs(command, tasks_per_node)</pre>	Compose a dictionary with information for writing the submit script.
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	The submit method takes the command string to be executed upon instantiation of a resource most often to start a pilot.

# **Attributes**

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
status_polling_interval	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancels the resources identified by the job\_ids provided by the user.

# Parameters

job\_ids (-) - A list of job identifiers

### Returns

• A list of status from cancelling the job which can be True, False

### Raises

# - ExecutionProviderException or its subclasses -

# get\_configs(command, tasks\_per\_node)

Compose a dictionary with information for writing the submit script.

# property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

# submit(command, tasks\_per\_node, job\_name='parsl.sge')

The submit method takes the command string to be executed upon instantiation of a resource most often to start a pilot.

# Args :

- command (str) : The bash command string to be executed.
- tasks\_per\_node (int) : command invocations to be launched per node

# **KWargs:**

• job\_name (str) : Human friendly name to be assigned to the job request

### Returns

• A job identifier, this could be an integer, string etc

#### Raises

- ExecutionProviderException or its subclasses -

# parsl.providers.LocalProvider

```
class pars1.providers.LocalProvider(channel=LocalChannel(envs={), script_dir=None, user-
```

home='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'),
nodes\_per\_block=1, launcher=SingleNodeLauncher(debug=True,
fail\_on\_any=False), init\_blocks=1, min\_blocks=0, max\_blocks=1,
worker\_init='', cmd\_timeout=30, parallelism=1, move\_files=None)

Local Execution Provider

This provider is used to provide execution resources from the localhost.

### Parameters

- min\_blocks (int) Minimum number of blocks to maintain.
- max\_blocks (int) Maximum number of blocks to maintain.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.
- move\_files (*Optional[Bool]*) Should files be moved? By default, Parsl will try to figure this out itself (= None). If True, then will always move. If False, will never move.
- **worker\_init** (*str*) Command to be run before starting a worker, such as 'module load Anaconda; source activate env'.

\_\_init\_\_(channel=LocalChannel(envs={}, script\_dir=None,

userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), nodes\_per\_block=1, launcher=SingleNodeLauncher(debug=True, fail\_on\_any=False), init\_blocks=1, min\_blocks=0, max\_blocks=1, worker\_init='', cmd\_timeout=30, parallelism=1, move\_files=None)

# Methods

init([channel, nodes_per_block,])	
<pre>cancel(job_ids)</pre>	Cancels the jobs specified by a list of job ids
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by their ids.
<pre>submit(command, tasks_per_node[, job_name])</pre>	Submits the command onto an Local Resource Man-
	ager job.

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancels the jobs specified by a list of job ids

Args: job\_ids : [<job\_id> ...]

# Returns: [True] Always returns true for every job\_id, regardless of

whether an individual cancel failed (unless an exception is raised)

# property label

Provides the label for this provider

# status(job\_ids)

Get the status of a list of jobs identified by their ids.

# Parameters

 $job_ids$  (-) – List of identifiers for the jobs

# Returns

• List of status codes.

# property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

# Returns

the number of seconds to wait between calls to status()

# submit(command, tasks\_per\_node, job\_name='parsl.localprovider')

Submits the command onto an Local Resource Manager job. Submit returns an ID that corresponds to the task that was just submitted.

# If tasks\_per\_node < 1: 1/tasks\_per\_node is provisioned

If tasks\_per\_node == 1: A single node is provisioned

# If tasks\_per\_node > 1 : tasks\_per\_node nodes are provisioned.

### **Parameters**

- command (-) (String) Commandline invocation to be made on the remote side.
- tasks\_per\_node (-) command invocations to be launched per node

### **Kwargs:**

• job\_name (String): Name for job, must be unique

# Returns

At capacity, cannot provision more - job\_id: (string) Identifier for the job

# **Return type**

• None

# parsl.providers.LSFProvider

```
class pars1.providers.LSFProvider(channel=LocalChannel(envs={), script_dir=None, user-
```

home='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'),
nodes\_per\_block=1, cores\_per\_block=None, cores\_per\_node=None,
init\_blocks=1, min\_blocks=0, max\_blocks=1, parallelism=1,
walltime='00:10:00', scheduler\_options='', worker\_init='',
project=None, queue=None, cmd\_timeout=120, move\_files=True,
bsub\_redirection=False, request\_by\_nodes=True,
launcher=SingleNodeLauncher(debug=True, fail on any=False))

# LSF Execution Provider

This provider uses by to submit, bjobs for status and bkill to cancel jobs. The by script to be used is created from a template file in this same module.

- **channel** (Channel) Channel for accessing this provider. Possible channels include *LocalChannel* (the default), *SSHChannel*, or *SSHInteractiveLoginChannel*.
- **nodes\_per\_block** (*int*) Nodes to provision per block. When request\_by\_nodes is False, it is computed by cores\_per\_block / cores\_per\_node.
- **cores\_per\_block** (*int*) Cores to provision per block. Enabled only when request\_by\_nodes is False.
- **cores\_per\_node** (*int*) Cores to provision per node. Enabled only when request\_by\_nodes is False.
- **init\_blocks** (*int*) Number of blocks to request at the start of the run.
- min\_blocks (int) Minimum number of blocks to maintain.
- **max\_blocks** (*int*) Maximum number of blocks to maintain.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.
- walltime (*str*) Walltime requested per block in HH:MM:SS.
- **project** (*str*) Project to which the resources must be charged
- **queue** (*str*) Queue to which to submit the job request
- **scheduler\_options** (*str*) String to prepend to the #BSUB blocks in the submit script to the scheduler.
- **worker\_init** (*str*) Command to be run before starting a worker, such as 'module load Anaconda; source activate env'.
- **cmd\_timeout** (*int*) Seconds after which requests to the scheduler will timeout. Default: 120s
- **launcher** (Launcher) Launcher for this provider. Possible launchers include *SingleNodeLauncher* (the default), *SrunLauncher*, or *AprunLauncher*
- move\_files (Optional[Bool]: should files be moved? by default, Parsl will try to move files.)-
- **bsub\_redirection** (*Boo1*) Should a redirection symbol "<" be included when submitting jobs, i.e., Bsub < job\_script.

- **request\_by\_nodes** (*Boo1*) Request by nodes or request by cores per block. When this is set to false, nodes\_per\_block is computed by cores\_per\_block / cores\_per\_node. Default is True.
- \_\_init\_\_(channel=LocalChannel(envs={}, script\_dir=None,

userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), nodes\_per\_block=1, cores\_per\_block=None, cores\_per\_node=None, init\_blocks=1, min\_blocks=0, max\_blocks=1, parallelism=1, walltime='00:10:00', scheduler\_options='', worker\_init='', project=None, queue=None, cmd\_timeout=120, move\_files=True, bsub\_redirection=False, request\_by\_nodes=True, launcher=SingleNodeLauncher(debug=True, fail\_on\_any=False))

# Methods

init([channel, nodes_per_block,])	
<pre>cancel(job_ids)</pre>	Cancels the jobs specified by a list of job ids
<pre>execute_wait(cmd[, timeout])</pre>	
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	Submit the command as an LSF job.

# **Attributes**

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancels the jobs specified by a list of job ids

Args: job\_ids : [<job\_id> ...]

Returns : [True/False...] : If the cancel operation fails the entire list will be False.

# property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

submit(command, tasks\_per\_node, job\_name='parsl.lsf')

Submit the command as an LSF job.

- command (str) Command to be made on the remote side.
- tasks\_per\_node (int) Command invocations to be launched per node
- job\_name (*str*) Name for the job (must be unique).

### Returns

If at capacity, returns None; otherwise, a string identifier for the job

### Return type

None or str

# parsl.providers.SlurmProvider

### Slurm Execution Provider

This provider uses sbatch to submit, squeue for status and scancel to cancel jobs. The sbatch script to be used is created from a template file in this same module.

- **partition** (*str*) Slurm partition to request blocks from. If unspecified or None, no partition slurm directive will be specified.
- **account** (*str*) Slurm account to which to charge resources used by the job. If unspecified or None, the job will use the user's default account.
- **qos** (*str*) Slurm queue to place job in. If unspecified or None, no queue slurm directive will be specified.
- **constraint** (*str*) Slurm job constraint, often used to choose cpu or gpu type. If unspecified or None, no constraint slurm directive will be added.
- **channel** (Channel) Channel for accessing this provider. Possible channels include *LocalChannel* (the default), *SSHChannel*, or *SSHInteractiveLoginChannel*.
- nodes\_per\_block (int) Nodes to provision per block.
- **cores\_per\_node** (*int*) Specify the number of cores to provision per node. If set to None, executors will assume all cores on the node are available for computation. Default is None.
- **mem\_per\_node** (*int*) Specify the real memory to provision per node in GB. If set to None, no explicit request to the scheduler will be made. Default is None.
- **init\_blocks** (*int*) Number of blocks to provision at the start of the run. Default is 1.
- min\_blocks (*int*) Minimum number of blocks to maintain.
- max\_blocks (int) Maximum number of blocks to maintain.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.
- walltime (*str*) Walltime requested per block in HH:MM:SS.

- **scheduler\_options** (*str*) String to prepend to the #SBATCH blocks in the submit script to the scheduler.
- **regex\_job\_id** (*str*) The regular expression used to extract the job ID from the sbatch standard output. The default is r"Submitted batch job (?P<id>\S\*)", where id is the regular expression symbolic group for the job ID.
- **worker\_init** (*str*) Command to be run before starting a worker, such as 'module load Anaconda; source activate env'.
- **exclusive** (*bool* (*Default* = *True*)) Requests nodes which are not shared with other running jobs.
- **launcher** (Launcher) Launcher for this provider. Possible launchers include *SingleNodeLauncher* (the default), *SrunLauncher*, or *AprunLauncher*
- move\_files (Optional[Bool]: should files be moved? by default, Parsl will try to move files.)-

\_\_init\_\_\_(partition: str | None = None, account: str | None = None, qos: str | None = None, constraint: str | None = None, channel: Channel = LocalChannel(envs={}, script\_dir=None, userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), nodes\_per\_block: int = 1, cores\_per\_node: int | None = None, mem\_per\_node: int | None = None, init\_blocks: int = 1, min\_blocks: int = 0, max\_blocks: int = 1, parallelism: float = 1, walltime: str = '00:10:00', scheduler\_options: str = '', regex\_job\_id: str = 'Submitted batch job (?P<id>\\S\*)', worker\_init: str = '', cmd\_timeout: int = 10, exclusive: bool = True, move\_files: bool = True, launcher: Launcher = SingleNodeLauncher(debug=True, fail\_on\_any=False))

# Methods

init([partition, account, qos,])	
<pre>cancel(job_ids)</pre>	Cancels the jobs specified by a list of job ids
<pre>execute_wait(cmd[, timeout])</pre>	
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	Submit the command as a slurm job.

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
<pre>mem_per_node</pre>	Real memory to provision per node in GB.
status_polling_interval	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancels the jobs specified by a list of job ids

Args: job\_ids : [<job\_id> ... ]

Returns : [True/False...] : If the cancel operation fails the entire list will be False.

### property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

Submit the command as a slurm job.

### Parameters

- command (str) Command to be made on the remote side.
- tasks\_per\_node (int) Command invocations to be launched per node
- job\_name (str) Name for the job

### Returns

job id – A string identifier for the job

**Return type** 

str

# parsl.providers.TorqueProvider

**class** pars1.providers.**TorqueProvider**(*channel=LocalChannel(envs={*), script\_dir=None, user-

home='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs', account=None, queue=None, scheduler\_options='', worker\_init='', nodes\_per\_block=1, init\_blocks=1, min\_blocks=0, max\_blocks=1, parallelism=1, launcher=AprunLauncher(debug=True, overrides=''), walltime='00:20:00', cmd\_timeout=120)

# Torque Execution Provider

This provider uses qsub to submit, qstat for status, and qdel to cancel jobs. The qsub script to be used is created from a template file in this same module.

- **channel** (Channel) Channel for accessing this provider. Possible channels include *LocalChannel* (the default), *SSHChannel*, or *SSHInteractiveLoginChannel*.
- **account** (*str*) Account the job will be charged against.
- **queue** (*str*) Torque queue to request blocks from.
- **nodes\_per\_block** (*int*) Nodes to provision per block.
- init\_blocks (int) Number of blocks to provision at the start of the run. Default is 1.
- min\_blocks (int) Minimum number of blocks to maintain. Default is 0.
- max\_blocks (int) Maximum number of blocks to maintain.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.
- walltime (*str*) Walltime requested per block in HH:MM:SS.

- **scheduler\_options** (*str*) String to prepend to the #PBS blocks in the submit script to the scheduler. WARNING: scheduler\_options should only be given #PBS strings, and should not have trailing newlines.
- **worker\_init** (*str*) Command to be run before starting a worker, such as 'module load Anaconda; source activate env'.
- **launcher** (Launcher) Launcher for this provider. Possible launchers include *AprunLauncher* (the default), or *SingleNodeLauncher*,

# \_\_init\_\_(channel=LocalChannel(envs={}, script\_dir=None, userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), account=None, queue=None, scheduler\_options='', worker\_init='', nodes\_per\_block=1, init\_blocks=1, min\_blocks=0, max\_blocks=1, parallelism=1, launcher=AprunLauncher(debug=True, overrides=''), walltime='00:20:00', cmd\_timeout=120)

# Methods

init([channel, account, queue,])	
<pre>cancel(job_ids)</pre>	Cancels the jobs specified by a list of job ids
<pre>execute_wait(cmd[, timeout])</pre>	
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	Submits the command onto an Local Resource Manager job.

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
status_polling_interval	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancels the jobs specified by a list of job ids

Args: job\_ids : [<job\_id> ...]

Returns : [True/False...] : If the cancel operation fails the entire list will be False.

# property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

### submit(command, tasks\_per\_node, job\_name='parsl.torque')

Submits the command onto an Local Resource Manager job. Submit returns an ID that corresponds to the task that was just submitted.

If tasks\_per\_node < 1 : ! This is illegal. tasks\_per\_node should be integer

### If tasks\_per\_node == 1:

A single node is provisioned

### If tasks\_per\_node > 1 :

tasks\_per\_node number of nodes are provisioned.

### Parameters

- **command** (-) (String) Commandline invocation to be made on the remote side.
- tasks\_per\_node (-) command invocations to be launched per node

# **Kwargs:**

• job\_name (String): Name for job, must be unique

# Returns

At capacity, cannot provision more - job\_id: (string) Identifier for the job

# Return type

• None

# parsl.providers.KubernetesProvider

class parsl.providers.KubernetesProvider(*image: str*, *namespace: str* = 'default', *nodes\_per\_block: int* = 1, *init\_blocks: int* = 4, *min\_blocks: int* = 0, *max\_blocks: int* = 10, *max\_cpu: float* = 2, *max\_mem: str* = '500Mi', *init\_cpu: float* = 1, *init\_mem: str* = '250Mi', *parallelism: float* = 1, *worker\_init: str* = '', *pod\_name: str* | *None* = None, *user\_id: str* | *None* = None, *group\_id: str* | *None* = None, *run\_as\_non\_root: bool* = False, *secret: str* | *None* = None, *persistent\_volumes: List[Tuple[str, str]]* = [])

Kubernetes execution provider

- namespace (str) Kubernetes namespace to create deployments.
- **image** (*str*) Docker image to use in the deployment.
- **nodes\_per\_block** (*int*) Nodes to provision per block.
- **init\_blocks** (*int*) Number of blocks to provision at the start of the run. Default is 1.
- min\_blocks (int) Minimum number of blocks to maintain.
- **max\_blocks** (*int*) Maximum number of blocks to maintain.
- **max\_cpu** (*float*) CPU limits of the blocks (pods), in cpu units. This is the cpu "limits" option for resource specification. Check kubernetes docs for more details. Default is 2.
- **max\_mem** (*str*) Memory limits of the blocks (pods), in Mi or Gi. This is the memory "limits" option for resource specification on kubernetes. Check kubernetes docs for more details. Default is 500Mi.
- **init\_cpu**(*float*) CPU limits of the blocks (pods), in cpu units. This is the cpu "requests" option for resource specification. Check kubernetes docs for more details. Default is 1.

- **init\_mem** (*str*) Memory limits of the blocks (pods), in Mi or Gi. This is the memory "requests" option for resource specification on kubernetes. Check kubernetes docs for more details. Default is 250Mi.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.
- worker\_init (str) Command to be run first for the workers, such as python start.py.
- secret (str) The Kubernetes ImagePullSecret secret to use to pull images
- **pod\_name** (*str*) The name for the pod, will be appended with a timestamp. Default is None, meaning parsl automatically names the pod.
- user\_id (str) Unix user id to run the container as.
- group\_id (str) Unix group id to run the container as.
- run\_as\_non\_root (bool) Run as non-root (True) or run as root (False).
- **persistent\_volumes** (*list[(str, str)]*) List of tuples describing persistent volumes to be mounted in the pod. The tuples consist of (PVC Name, Mount Directory).
- \_\_init\_\_\_(image: str, namespace: str = 'default', nodes\_per\_block: int = 1, init\_blocks: int = 4, min\_blocks: int = 0, max\_blocks: int = 10, max\_cpu: float = 2, max\_mem: str = '500Mi', init\_cpu: float = 1, init\_mem: str = '250Mi', parallelism: float = 1, worker\_init: str = '', pod\_name: str | None = None, user\_id: str | None = None, group\_id: str | None = None, run\_as\_non\_root: bool = False, secret: str | None = None, persistent\_volumes: List[Tuple[str, str]] = []) → None

# **Methods**

init(image[, namespace,])	
<pre>cancel(job_ids)</pre>	Cancels the jobs specified by a list of job ids Args: job_ids : [ <job_id>] Returns : [True/False] : If the cancel operation fails the entire list will be False.</job_id>
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(cmd_string, tasks_per_node[, job_name])</pre>	Submit a job :param - cmd_string: (String) - Name of the container to initiate :param - tasks_per_node: command invocations to be launched per node :type - tasks_per_node: int

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

# cancel(job\_ids)

Cancels the jobs specified by a list of job ids Args: job\_ids : [<job\_id> ...] Returns : [True/False...] : If the cancel operation fails the entire list will be False.

# property label

Provides the label for this provider

# status(job\_ids)

Get the status of a list of jobs identified by the job identifiers returned from the submit request. :param - job\_ids: A list of job identifiers :type - job\_ids: list

# Returns

• A list of JobStatus objects corresponding to each job\_id in the job\_ids list.

### Raises

# - ExecutionProviderExceptions or its subclasses -

### property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

# submit(cmd\_string, tasks\_per\_node, job\_name='parsl')

Submit a job :param - cmd\_string: (String) - Name of the container to initiate :param - tasks\_per\_node: command invocations to be launched per node :type - tasks\_per\_node: int

### **Kwargs:**

• job\_name (String): Name for job, must be unique

# Returns

At capacity, cannot provision more - job\_id: (string) Identifier for the job

# **Return type**

• None

# parsl.providers.PBSProProvider

class parsl.providers.PBSProProvider(channel=LocalChannel(envs={}, script\_dir=None, user-

home='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs' account=None, queue=None, scheduler\_options=", select\_options=", worker\_init=", nodes\_per\_block=1, cpus\_per\_node=1, init\_blocks=1, min\_blocks=0, max\_blocks=1, parallelism=1, launcher=SingleNodeLauncher(debug=True, fail\_on\_any=False), walltime='00:20:00', cmd\_timeout=120)

PBS Pro Execution Provider

- **channel** (Channel) Channel for accessing this provider. Possible channels include *LocalChannel* (the default), *SSHChannel*, or *SSHInteractiveLoginChannel*.
- account (str) Account the job will be charged against.
- queue (*str*) Queue to request blocks from.
- **nodes\_per\_block** (*int*) Nodes to provision per block.

- cpus\_per\_node (int) CPUs to provision per node.
- **init\_blocks** (*int*) Number of blocks to provision at the start of the run. Default is 1.
- min\_blocks (int) Minimum number of blocks to maintain. Default is 0.
- max\_blocks (int) Maximum number of blocks to maintain.
- **parallelism** (*float*) Ratio of provisioned task slots to active tasks. A parallelism value of 1 represents aggressive scaling where as many resources as possible are used; parallelism close to 0 represents the opposite situation in which as few resources as possible (i.e., min\_blocks) are used.
- walltime (str) Walltime requested per block in HH:MM:SS.
- **scheduler\_options** (*str*) String to prepend to the #PBS blocks in the submit script to the scheduler.
- **select\_options** (*str*) String to append to the #PBS -l select block in the submit script to the scheduler. This can be used to specify ngpus.
- **worker\_init** (*str*) Command to be run before starting a worker, such as 'module load Anaconda; source activate env'.
- launcher (Launcher) Launcher for this provider. The default is SingleNodeLauncher.

\_\_init\_\_(channel=LocalChannel(envs={}, script\_dir=None,

userhome='/home/docs/checkouts/readthedocs.org/user\_builds/parsl/checkouts/latest/docs'), account=None, queue=None, scheduler\_options=", select\_options=", worker\_init=", nodes\_per\_block=1, cpus\_per\_node=1, init\_blocks=1, min\_blocks=0, max\_blocks=1, parallelism=1, launcher=SingleNodeLauncher(debug=True, fail\_on\_any=False), walltime='00:20:00', cmd\_timeout=120)

# Methods

init([channel, account, queue,])	
cancel(job_ids)	Cancels the jobs specified by a list of job ids
<pre>execute_wait(cmd[, timeout])</pre>	
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	Submits the command job.

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

# property status\_polling\_interval

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

submit(command, tasks\_per\_node, job\_name='parsl')

Submits the command job.

### **Parameters**

- command (str) Command to be executed on the remote side.
- **tasks\_per\_node** (*int*) Command invocations to be launched per node.
- job\_name (str) Identifier for job.

# Returns

- None If at capacity and cannot provision more
- **job\_id** (*str*) Identifier for the job

# parsl.providers.base.ExecutionProvider

### class parsl.providers.base.ExecutionProvider

Execution providers are responsible for managing execution resources that have a Local Resource Manager (LRM). For instance, campus clusters and supercomputers generally have LRMs (schedulers) such as Slurm, Torque/PBS, Condor and Cobalt. Clouds, on the other hand, have API interfaces that allow much more finegrained composition of an execution environment. An execution provider abstracts these types of resources and provides a single uniform interface to them.

The providers abstract away the interfaces provided by various systems to request, monitor, and cancel compute resources.

script\_string ----->| submit id <------+ [ ids ] ----->| status [statuses] <------+ [ ids ] ----->| cancel [cancel] <-----+ |



# **Methods**

init()	
<pre>cancel(job_ids)</pre>	Cancels the resources identified by the job_ids pro- vided by the user.
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	The submit method takes the command string to be executed upon instantiation of a resource most often to start a pilot (such as for HighThroughputExecutor or WorkQueueExecutor).

# **Attributes**

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

# **abstract cancel**(*job\_ids: List[object]*) → List[bool]

Cancels the resources identified by the job\_ids provided by the user.

# Parameters

 $job_ids(-) - A$  list of job identifiers

# Returns

• A list of status from cancelling the job which can be True, False

# Raises

# - ExecutionProviderException or its subclasses -

# property cores\_per\_node: int | None

Number of cores to provision per node.

Providers which set this property should ask for cores\_per\_node cores when provisioning resources, and set the corresponding environment variable PARSL\_CORES before executing submitted commands.

If this property is set, executors may use it to calculate how many tasks can run concurrently per node.

# abstract property label: str

Provides the label for this provider

### property mem\_per\_node: float | None

Real memory to provision per node in GB.

Providers which set this property should ask for mem\_per\_node of memory when provisioning resources, and set the corresponding environment variable PARSL\_MEMORY\_GB before executing submitted commands.

If this property is set, executors may use it to calculate how many tasks can run concurrently per node.

# **abstract** status(*job\_ids: List[object]*) $\rightarrow$ List[*JobStatus*]

Get the status of a list of jobs identified by the job identifiers returned from the submit request.

### Parameters

**job\_ids** (-) – A list of job identifiers

Returns

• A list of JobStatus objects corresponding to each job\_id in the job\_ids list.

Raises

### - ExecutionProviderException or its subclasses -

### abstract property status\_polling\_interval: int

Returns the interval, in seconds, at which the status method should be called.

### Returns

the number of seconds to wait between calls to status()

**abstract submit**(*command: str, tasks\_per\_node: int, job\_name: str = 'parsl.auto'*)  $\rightarrow$  object

The submit method takes the command string to be executed upon instantiation of a resource most often to start a pilot (such as for HighThroughputExecutor or WorkQueueExecutor).

### Args :

- command (str) : The bash command string to be executed
- tasks\_per\_node (int) : command invocations to be launched per node

# **KWargs:**

• job\_name (str) : Human friendly name to be assigned to the job request

# Returns

• A job identifier, this could be an integer, string etc or None or any other object that evaluates to boolean false if submission failed but an exception isn't thrown.

### Raises

- ExecutionProviderException or its subclasses -

# parsl.providers.cluster\_provider.ClusterProvider

This class defines behavior common to all cluster/supercompute-style scheduler systems.

- **label** (*str*) Label for this provider.
- **channel** (Channel) Channel for accessing this provider. Possible channels include *LocalChannel* (the default), *SSHChannel*, or *SSHInteractiveLoginChannel*.
- walltime (str) Walltime requested per block in HH:MM:SS.
- launcher (Launcher) Launcher for this provider.
- cmd\_timeout (int) Timeout for commands made to the scheduler in seconds

+----script\_string ----->| submit id <-----+ [ ids ] ----->| status [statuses] <-----+ | [ ids ] ----->| cancel [cancel] <-----+

# **Methods**

init(label, channel, nodes_per_block,)	
<pre>cancel(job_ids)</pre>	Cancels the resources identified by the job_ids pro- vided by the user.
<pre>execute_wait(cmd[, timeout])</pre>	
<pre>status(job_ids)</pre>	Get the status of a list of jobs identified by the job identifiers returned from the submit request.
<pre>submit(command, tasks_per_node[, job_name])</pre>	The submit method takes the command string to be executed upon instantiation of a resource most often to start a pilot (such as for HighThroughputExecutor or WorkQueueExecutor).

# Attributes

cores_per_node	Number of cores to provision per node.
label	Provides the label for this provider
mem_per_node	Real memory to provision per node in GB.
<pre>status_polling_interval</pre>	Returns the interval, in seconds, at which the status
	method should be called.

### execute\_wait(cmd, timeout=None)

# property label

Provides the label for this provider

# status(job\_ids)

Get the status of a list of jobs identified by the job identifiers returned from the submit request.

Parameters

job\_ids (-) - A list of job identifiers

# Returns

• A list of JobStatus objects corresponding to each job\_id in the job\_ids list.

Raises

- ExecutionProviderException or its subclasses -

# **Batch jobs**

parsl.jobs.states.JobState
parsl.jobs.states.JobStatus
parsl.jobs.error\_handlers.
noop\_error\_handler
parsl.jobs.error\_handler
parsl.jobs.error\_handlers.
windowed\_error\_handler

Defines a set of states that a job can be in Encapsulates a job state together with other details:

# parsl.jobs.states.JobState

Defines a set of states that a job can be in

\_\_init\_\_(\*args, \*\*kwds)

# Methods

<pre>init(*args, **kwds)</pre>	
<pre>as_integer_ratio()</pre>	Return integer ratio.
<pre>bit_count()</pre>	Number of ones in the binary representation of the absolute value of self.
<pre>bit_length()</pre>	Number of bits necessary to represent self in binary.
conjugate	Returns self, the complex conjugate of any int.
<pre>from_bytes([byteorder, signed])</pre>	Return the integer represented by the given array of bytes.
<pre>to_bytes([length, byteorder, signed])</pre>	Return an array of bytes representing an integer.

# Attributes

UNKNOWN	The batch provider is unable to determinate a state for this job
PENDING	"This job is in the batch queue but has not started run- ning
RUNNING	This job is running in the batch system
CANCELLED	This job has been cancelled
COMPLETED	This job has completed
FAILED	This job has failed
TIMEOUT	This job has ended due to walltime expiry.
HELD	This job is held/suspended in the batch system
MISSING	This job has reached a terminal state without the re- sources(managers/workers) launched in the job con- necting back to the Executor.
denominator	the denominator of a rational number in lowest terms
imag	the imaginary part of a complex number
numerator	the numerator of a rational number in lowest terms
real	the real part of a complex number

# CANCELLED = 3

This job has been cancelled

# COMPLETED = 4

This job has completed

# FAILED = 5

This job has failed

# HELD = 7

This job is held/suspended in the batch system

# MISSING = 8

This job has reached a terminal state without the resources(managers/workers) launched in the job connecting back to the Executor. This state is set by HTEX when it is able to infer that the block failed to start workers for eg due to bad worker environment or network connectivity issues.

# PENDING = 1

"This job is in the batch queue but has not started running

# RUNNING = 2

This job is running in the batch system

# TIMEOUT = 6

This job has ended due to walltime expiry. This is different from other error states, because in the pilot job model, a timeout is usually expected and not a failure. Timeouts should not be reported with FAILED state: if they are reported as FAILED, Parsl's error handling code in *simple\_error\_handler* will eventually regard the batch system as broken and shut down.

# UNKNOWN = 0

The batch provider is unable to determinate a state for this job
#### parsl.jobs.states.JobStatus

Encapsulates a job state together with other details:

**Parameters** 

- state The machine-readable state of the job this status refers to
- message Optional human readable message
- exit\_code Optional exit code
- **stdout\_path** Optional path to a file containing the job's stdout
- stderr\_path Optional path to a file containing the job's stderr

\_\_init\_\_(state: JobState, message: str | None = None, exit\_code: int | None = None, stdout\_path: str | None = None, stderr\_path: str | None = None)

## **Methods**

\_\_init\_\_(state[, message, exit\_code, ...])

#### **Attributes**

SUMMARY\_TRUNCATION\_THRESHOLD

status\_name

stderr

stderr\_summary

stdout

stdout\_summary

terminal

SUMMARY\_TRUNCATION\_THRESHOLD = 2048

property status\_name: str

property stderr: str | None

property stderr\_summary: str | None

property stdout: str | None

property stdout\_summary: str | None

property terminal: bool

## parsl.jobs.error\_handlers.noop\_error\_handler

parsl.jobs.error\_handlers.noop\_error\_handler(*executor*: BlockProviderExecutor, *status*: *Dict[str*, JobStatus], *threshold*: *int* = 3)  $\rightarrow$  None

## parsl.jobs.error\_handlers.simple\_error\_handler

parsl.jobs.error\_handlers.simple\_error\_handler(*executor*: BlockProviderExecutor, *status*: *Dict[str*, JobStatus], *threshold*: *int* = 3)  $\rightarrow$  None

## parsl.jobs.error\_handlers.windowed\_error\_handler

parsl.jobs.error\_handlers.windowed\_error\_handler(*executor*: BlockProviderExecutor, *status*: Dict[str, JobStatus], *threshold*: int = 3)  $\rightarrow$  None

## **Exceptions**

parsl.app.errors.AppBadFormatting	An error raised during formatting of a bash function.
parsl.app.errors.AppException	An error raised during execution of an app.
<pre>parsl.app.errors.AppTimeout</pre>	An error raised during execution of an app when it exceeds its allotted walltime.
<pre>parsl.app.errors.BadStdStreamFile</pre>	Error raised due to bad filepaths specified for STDOUT/ STDERR.
parsl.app.errors.BashAppNoReturn	Bash app returned no string.
parsl.app.errors.BashExitFailure	A non-zero exit code returned from a @bash_app
parsl.app.errors.MissingOutputs	Error raised at the end of app execution due to missing output files.
parsl.app.errors.ParslError	Base class for all exceptions.
parsl.errors.ConfigurationError	Raised when a component receives an invalid configura-
	tion.
parsl.errors.OptionalModuleMissing	Error raised when a required module is missing for a op- tional/extra component
parsl.executors.errors.ExecutorError	Base class for executor related exceptions.
parsl.executors.errors.ScalingFailed	Scaling failed due to error in Execution provider.
<pre>parsl.executors.errors.BadMessage</pre>	Mangled/Poorly formatted/Unsupported message re- ceived
parsl.dataflow.errors.DataFlowException	Base class for all exceptions.
parsl.dataflow.errors.BadCheckpoint	Error raised at the end of app execution due to missing output files.
<pre>parsl.dataflow.errors.DependencyError</pre>	Error raised if an app cannot run because there was an error
parsl.dataflow.errors.JoinError	Error raised if apps joining into a join_app raise exceptions.

continues on next page

parsl.launchers.errors.BadLauncher	Error raised when an object of inappropriate type is supplied as a Launcher
parsl.providers.errors. ExecutionProviderException	Base class for all exceptions Only to be invoked when only a more specific error is not available.
parsl.providers.errors.ScaleOutFailed	Scale out failed in the submit phase on the provider side
parsl.providers.errors.	Error raised when the template used to compose the sub-
SchedulerMissingArgs	mit script to the local resource manager is missing re- quired arguments
parsl.providers.errors.ScriptPathError	Error raised when the template used to compose the sub- mit script to the local resource manager is missing re- quired arguments
parsl.channels.errors.ChannelError	Base class for all exceptions
<pre>parsl.channels.errors.BadHostKeyException</pre>	SSH channel could not be created since server's host keys could not be verified
parsl.channels.errors.BadScriptPath	An error raised during execution of an app.
<pre>parsl.channels.errors.BadPermsScriptPath</pre>	User does not have permissions to access the script_dir on the remote site
parsl.channels.errors.FileExists	Push or pull of file over channel fails since a file of the name already exists on the destination.
parsl.channels.errors.AuthException	An error raised during execution of an app.
parsl.channels.errors.SSHException	if there was any other error connecting or establishing an SSH session
parsl.channels.errors.FileCopyException	File copy operation failed
parsl.executors.high_throughput.errors. WorkerLost	Exception raised when a worker is lost
<pre>parsl.executors.high_throughput. interchange.ManagerLost</pre>	Task lost due to manager loss.
parsl.serialize.errors. DeserializationError	Failure at the deserialization of results/exceptions from remote workers.
<pre>parsl.serialize.errors.SerializationError</pre>	Failure to serialize task objects.

Table 1	- continued	from	previous	page

# parsl.app.errors.AppBadFormatting

# exception parsl.app.errors.AppBadFormatting

An error raised during formatting of a bash function.

# parsl.app.errors.AppException

## exception parsl.app.errors.AppException

An error raised during execution of an app.

What this exception contains depends entirely on context

# parsl.app.errors.AppTimeout

## exception parsl.app.errors.AppTimeout

An error raised during execution of an app when it exceeds its allotted walltime.

# parsl.app.errors.BadStdStreamFile

## exception parsl.app.errors.BadStdStreamFile(reason: str)

Error raised due to bad filepaths specified for STDOUT/ STDERR.

## **Contains:**

reason(string)

# parsl.app.errors.BashAppNoReturn

## exception parsl.app.errors.BashAppNoReturn(reason: str)

Bash app returned no string.

Contains: reason(string)

## parsl.app.errors.BashExitFailure

**exception** parsl.app.errors.**BashExitFailure**(*app\_name: str, exitcode: int*) A non-zero exit code returned from a @bash\_app

Contains: app name (str) exitcode (int)

# parsl.app.errors.MissingOutputs

# **exception** parsl.app.errors.**MissingOutputs**(*reason: str, outputs: List*[File]) Error raised at the end of app execution due to missing output files.

Contains: reason(string) outputs(List of files)

## parsl.app.errors.ParslError

#### exception parsl.app.errors.ParslError

Base class for all exceptions.

Only to be invoked when a more specific error is not available.

## parsl.errors.ConfigurationError

## exception parsl.errors.ConfigurationError

Raised when a component receives an invalid configuration.

## parsl.errors.OptionalModuleMissing

**exception** parsl.errors.**OptionalModuleMissing**(*module\_names: List[str], reason: str*) Error raised when a required module is missing for a optional/extra component

## parsl.executors.errors.ExecutorError

**exception** parsl.executors.errors.**ExecutorError**(*executor*: ParslExecutor, *reason: str*) Base class for executor related exceptions.

Only to be invoked when only a more specific error is not available.

#### parsl.executors.errors.ScalingFailed

**exception** parsl.executors.errors.**ScalingFailed**(*executor*: ParslExecutor, *reason: str*) Scaling failed due to error in Execution provider.

#### parsl.executors.errors.BadMessage

**exception** parsl.executors.errors.**BadMessage**(*reason*) Mangled/Poorly formatted/Unsupported message received

## parsl.dataflow.errors.DataFlowException

**exception** parsl.dataflow.errors.**DataFlowException** Base class for all exceptions.

Only to be invoked when only a more specific error is not available.

# parsl.dataflow.errors.BadCheckpoint

## exception parsl.dataflow.errors.BadCheckpoint(reason: str)

Error raised at the end of app execution due to missing output files.

Parameters

reason (-) –

Contains: reason (string) dependent\_exceptions

# parsl.dataflow.errors.DependencyError

## exception parsl.dataflow.errors.DependencyError(dependent\_exceptions\_tids:

Sequence[Tuple[Exception, str]], task\_id: int)

Error raised if an app cannot run because there was an error in a dependency.

## in a dependence

# Parameters

- **dependent\_exceptions\_tids** (-) List of exceptions and identifiers for dependencies which failed. The identifier might be a task ID or the repr of a non-DFK Future.
- task\_id (-) Task ID of the task that failed because of the dependency error

# parsl.dataflow.errors.JoinError

# 

Error raised if apps joining into a join\_app raise exceptions. There can be several exceptions (one from each joining app), and JoinError collects them all together.

## parsl.launchers.errors.BadLauncher

# exception parsl.launchers.errors.BadLauncher(launcher: Launcher)

Error raised when an object of inappropriate type is supplied as a Launcher

## parsl.providers.errors.ExecutionProviderException

## exception parsl.providers.errors.ExecutionProviderException

Base class for all exceptions Only to be invoked when only a more specific error is not available.

## parsl.providers.errors.ScaleOutFailed

**exception** parsl.providers.errors.**ScaleOutFailed**(*provider*, *reason*) Scale out failed in the submit phase on the provider side

## parsl.providers.errors.SchedulerMissingArgs

exception parsl.providers.errors.SchedulerMissingArgs(missing\_keywords, sitename)

Error raised when the template used to compose the submit script to the local resource manager is missing required arguments

#### parsl.providers.errors.ScriptPathError

exception parsl.providers.errors.ScriptPathError(script\_path, reason)

Error raised when the template used to compose the submit script to the local resource manager is missing required arguments

#### parsl.channels.errors.ChannelError

exception parsl.channels.errors.ChannelError(reason: str, e: Exception, hostname: str)

Base class for all exceptions

Only to be invoked when only a more specific error is not available.

#### parsl.channels.errors.BadHostKeyException

exception parsl.channels.errors.BadHostKeyException(e: Exception, hostname: str)
 SSH channel could not be created since server's host keys could not be verified
 Contains: reason(string) e (paramiko exception object) hostname (string)

## parsl.channels.errors.BadScriptPath

exception parsl.channels.errors.BadScriptPath(e: Exception, hostname: str)

An error raised during execution of an app. What this exception contains depends entirely on context Contains: reason(string) e (paramiko exception object) hostname (string)

#### parsl.channels.errors.BadPermsScriptPath

**exception** parsl.channels.errors.**BadPermsScriptPath**(*e: Exception, hostname: str*) User does not have permissions to access the script\_dir on the remote site

## parsl.channels.errors.FileExists

**exception** parsl.channels.errors.**FileExists**(*e: Exception, hostname: str, filename: str* | *None* = *None*) Push or pull of file over channel fails since a file of the name already exists on the destination.

Contains: reason(string) e (paramiko exception object) hostname (string)

#### parsl.channels.errors.AuthException

exception parsl.channels.errors.AuthException(e: Exception, hostname: str)
An error raised during execution of an app. What this exception contains depends entirely on context Contains:
reason(string) e (paramiko exception object) hostname (string)

#### parsl.channels.errors.SSHException

exception parsl.channels.errors.SSHException(e: Exception, hostname: str)
if there was any other error connecting or establishing an SSH session
Contains: reason(string) e (paramiko exception object) hostname (string)

#### parsl.channels.errors.FileCopyException

exception parsl.channels.errors.FileCopyException(e: Exception, hostname: str)
File copy operation failed

Contains: reason(string) e (paramiko exception object) hostname (string)

#### parsl.executors.high\_throughput.errors.WorkerLost

**exception** parsl.executors.high\_throughput.errors.**WorkerLost**(*worker\_id*, *hostname*) Exception raised when a worker is lost

## parsl.executors.high\_throughput.interchange.ManagerLost

## exception parsl.executors.high\_throughput.interchange.ManagerLost(manager\_id: bytes, hostname:

Task lost due to manager loss. Manager is considered lost when multiple heartbeats have been missed.

#### parsl.serialize.errors.DeserializationError

# **exception** parsl.serialize.errors.**DeserializationError**(*reason: str*) Failure at the deserialization of results/exceptions from remote workers.

str)

## parsl.serialize.errors.SerializationError

## exception parsl.serialize.errors.SerializationError(fname: str)

Failure to serialize task objects.

## Internal

parsl.app.app.AppBase	This is the base class that defines the two external facing functions that an App must define.
parsl.app.bash.BashApp	
parsl.app.python.PythonApp	Extends AppBase to cover the Python App.
parsl.dataflow.dflow.DataFlowKernel	The DataFlowKernel adds dependency awareness to an existing executor.
<pre>parsl.dataflow.memoization.id_for_memo</pre>	This should return a byte sequence which identifies the supplied value for memoization purposes: for any two calls of id_for_memo, the byte sequence should be the same when the "same" value is supplied, and different otherwise.
parsl.dataflow.memoization.Memoizer	Memoizer is responsible for ensuring that identical work is not repeated.
parsl.dataflow.states.FINAL_STATES	States from which we will never move to another state, because the job has either definitively completed or failed.
parsl.dataflow.states.States	Enumerates the states a parsl task may be in.
parsl.dataflow.taskrecord.TaskRecord	This stores most information about a Parsl task
parsl.jobs.job_status_poller. JobStatusPoller	
parsl.jobs.strategy.Strategy	Scaling strategy.
parsl.utils.Timer	This class will make a callback periodically, with a period specified by the interval parameter.

## parsl.app.app.AppBase

class pars1.app.app.AppBase(func: Callable, data\_flow\_kernel: DataFlowKernel | None = None, executors: List[str] | Literal['all'] = 'all', cache: bool = False, ignore\_for\_cache: Sequence[str] | None = None)

This is the base class that defines the two external facing functions that an App must define.

The \_\_init\_\_() which is called when the interpreter sees the definition of the decorated function, and the \_\_call\_\_() which is invoked when a decorated function is called by the user.

**\_\_init\_\_**(func: Callable, data\_flow\_kernel: DataFlowKernel | None = None, executors: List[str] | Literal['all'] = 'all', cache: bool = False, ignore\_for\_cache: Sequence[str] | None = None)  $\rightarrow$  None

Construct the App object.

Parameters

func (-) – Takes the function to be made into an App

**Kwargs:** 

- data\_flow\_kernel (DataFlowKernel): The DataFlowKernel responsible for managing this app. This can be omitted only after calling parsl.dataflow.dflow.DataFlowKernelLoader. load().
- executors (str|list) : Labels of the executors that this app can execute over. Default is 'all'.
- cache (Bool) : Enable caching of this app ?
- ignore\_for\_cache (sequence|None): Names of arguments which will be ignored by the caching mechanism.

#### Returns

• App object.

# Methods

\_\_init\_\_(func[, data\_flow\_kernel, ...]) Construct the App object.

## parsl.app.bash.BashApp

\_\_init\_\_(func, data\_flow\_kernel=None, cache=False, executors='all', ignore\_for\_cache=None) Construct the App object.

**Parameters func** (-) – Takes the function to be made into an App

## **Kwargs:**

- data\_flow\_kernel (DataFlowKernel): The DataFlowKernel responsible for managing this app. This can be omitted only after calling parsl.dataflow.dflow.DataFlowKernelLoader. load().
- executors (str|list) : Labels of the executors that this app can execute over. Default is 'all'.
- cache (Bool) : Enable caching of this app ?
- ignore\_for\_cache (sequence|None): Names of arguments which will be ignored by the caching mechanism.

## Returns

• App object.

## **Methods**

\_\_\_*init\_\_*(func[, data\_flow\_kernel, cache, ...])

Construct the App object.

## parsl.app.python.PythonApp

Extends AppBase to cover the Python App.

\_\_init\_\_(func, data\_flow\_kernel=None, cache=False, executors='all', ignore\_for\_cache=None, join=False) Construct the App object.

#### **Parameters**

**func** (-) – Takes the function to be made into an App

## Kwargs:

- data\_flow\_kernel (DataFlowKernel): The DataFlowKernel responsible for managing this app. This can be omitted only after calling parsl.dataflow.dflow.DataFlowKernelLoader. load().
- executors (str|list) : Labels of the executors that this app can execute over. Default is 'all'.
- cache (Bool) : Enable caching of this app ?
- ignore\_for\_cache (sequence|None): Names of arguments which will be ignored by the caching mechanism.

#### Returns

• App object.

## Methods

\_\_init\_\_(func[, data\_flow\_kernel, cache, ...]) Construct the App object.

#### parsl.dataflow.dflow.DataFlowKernel

#### class parsl.dataflow.dflow.DataFlowKernel(config: Config)

The DataFlowKernel adds dependency awareness to an existing executor.

It is responsible for managing futures, such that when dependencies are resolved, pending tasks move to the runnable state.

Here is a simplified diagram of what happens internally:

User		DFK	I	Executor	
Task	> +5	Submit			
					(continues on next page)

(continued from previous page)

App_Fu<+-	-
	Dependencies met
	<pre>task&gt; +Submit</pre>
1	Ex_Fu<

**\_\_init\_\_**(*config:* Config)  $\rightarrow$  None

Initialize the DataFlowKernel.

## Parameters

**config** (Config) – A specification of all configuration options. For more details see the :class:~`parsl.config.Config` documentation.

# Methods

init(config)		Initialize the DataFlowKernel.
add_executors(executors)		
atexit_cleanup()		
<pre>check_staging_inhibited(kwargs)</pre>		
<pre>checkpoint([tasks])</pre>		Checkpoint the dfk incrementally to a checkpoint file.
cleanup()		DataFlowKernel cleanup.
<pre>default_std_autopath(taskrecord, kw)</pre>		
<pre>handle_app_update(task_record, future)</pre>		This function is called as a callback when an AppFu- ture is in its final state.
<pre>handle_exec_update(task_record, future)</pre>		This function is called only as a callback from an ex- ecution attempt reaching a final state (either success- fully or failing).
<pre>handle_join_update(task_record, ner_app_future)</pre>	in-	
<pre>launch_if_ready(task_record)</pre>		launch_if_ready will launch the specified task, if it is ready to run (for example, without dependencies, and in pending state).
<pre>launch_task(task_record)</pre>		Handle the actual submission of the task to the executor layer.
<pre>load_checkpoints(checkpointDirs)</pre>		Load checkpoints from the checkpoint files into a dic- tionary.
<pre>log_task_states()</pre>		
<pre>submit(func, app_args, executors, cache,)</pre>		Add task to the dataflow system.
<pre>update_task_state(task_record, new_state)</pre>		Updates a task record state, and recording an appropriate change to task state counters.
<pre>wait_for_current_tasks()</pre>		Waits for all tasks in the task list to be completed, by waiting for their AppFuture to be completed.
<pre>wipe_task(task_id)</pre>		Remove task with task_id from the internal tasks table

## Attributes

config	Returns the fully initialized config that the DFK is
	actively using.

**add\_executors**(*executors*: *Sequence*[ParslExecutor]) → None

```
atexit_cleanup() \rightarrow None
```

**checkpoint**(*tasks: Sequence*[TaskRecord] | *None* = *None*)  $\rightarrow$  str

Checkpoint the dfk incrementally to a checkpoint file.

When called, every task that has been completed yet not checkpointed is checkpointed to a file.

#### **Kwargs:**

#### • tasks (List of task records)

[List of task ids to checkpoint. Default=None] if set to None, we iterate over all tasks held by the DFK.

Note: Checkpointing only works if memoization is enabled

#### Returns

Checkpoint dir if checkpoints were written successfully. By default the checkpoints are written to the RUNDIR of the current run under RUNDIR/checkpoints/{tasks.pkl, dfk.pkl}

## $\texttt{cleanup()} \rightarrow None$

DataFlowKernel cleanup.

This involves releasing all resources explicitly.

We call scale\_in on each of the executors and call executor.shutdown.

# property config: Config

Returns the fully initialized config that the DFK is actively using.

Returns

· Config object

default\_std\_autopath(taskrecord, kw)

#### **handle\_app\_update**(*task\_record:* TaskRecord, *future:* AppFuture) $\rightarrow$ None

This function is called as a callback when an AppFuture is in its final state.

It will trigger post-app processing such as checkpointing.

#### **Parameters**

- task\_record Task record
- **future** (*Future*) The relevant app future (which should be consistent with the task structure 'app\_fu' entry

#### handle\_exec\_update(*task\_record:* TaskRecord, *future: Future*) → None

This function is called only as a callback from an execution attempt reaching a final state (either successfully or failing).

It will launch retries if necessary, and update the task structure.

#### Parameters

- task\_record (dict) Task record
- future (Future) The future object corresponding to the task which
- callback (makes this) -

handle\_join\_update(task\_record: TaskRecord, inner\_app\_future: AppFuture | None)  $\rightarrow$  None

#### **launch\_if\_ready**(*task\_record:* TaskRecord) $\rightarrow$ None

launch\_if\_ready will launch the specified task, if it is ready to run (for example, without dependencies, and in pending state).

This should be called by any piece of the DataFlowKernel that thinks a task may have become ready to run.

It is not an error to call launch\_if\_ready on a task that is not ready to run - launch\_if\_ready will not incorrectly launch that task.

It is also not an error to call launch\_if\_ready on a task that has already been launched - launch\_if\_ready will not re-launch that task.

launch\_if\_ready is thread safe, so may be called from any thread or callback.

#### **launch\_task**(*task\_record:* TaskRecord) $\rightarrow$ Future

Handle the actual submission of the task to the executor layer.

## Parameters

task\_record – The task record

#### Returns

Future that tracks the execution of the submitted function

**load\_checkpoints**(*checkpointDirs: Sequence[str]* | *None*)  $\rightarrow$  Dict[str, Future]

Load checkpoints from the checkpoint files into a dictionary.

The results are used to pre-populate the memoizer's lookup\_table

## **Kwargs:**

• checkpointDirs (list) : List of run folder to use as checkpoints Eg. ['runinfo/001', 'runinfo/002']

# Returns

• dict containing, hashed -> future mappings

#### $log_task_states() \rightarrow None$

**submit**(func: Callable, app\_args: Sequence[Any], executors: str | Sequence[str], cache: bool, ignore\_for\_cache: Sequence[str] | None, app\_kwargs: Dict[str, Any], join: bool = False)  $\rightarrow$ AppFuture

Add task to the dataflow system.

If the app task has the executors attributes not set (default=='all') the task will be launched on a randomly selected executor from the list of executors. If the app task specifies a particular set of executors, it will be targeted at the specified executors.

#### Parameters

**func** (-) - A function object

## **KWargs**:

- app\_args : Args to the function
- executors (list or string) [List of executors this call could go to.] Default='all'
- cache (Bool) : To enable memoization or not
- ignore\_for\_cache (sequence) : List of kwargs to be ignored for memoization/checkpointing
- app\_kwargs (dict) : Rest of the kwargs to the fn passed as dict.

#### Returns

(AppFuture) [DataFutures,]

#### **update\_task\_state**(*task\_record:* TaskRecord, *new\_state:* States) → None

Updates a task record state, and recording an appropriate change to task state counters.

#### $\texttt{wait\_for\_current\_tasks()} \rightarrow None$

Waits for all tasks in the task list to be completed, by waiting for their AppFuture to be completed. This method will not necessarily wait for any tasks added after cleanup has started (such as data stageout?)

#### wipe\_task(*task\_id: int*) $\rightarrow$ None

Remove task with task\_id from the internal tasks table

## parsl.dataflow.memoization.id\_for\_memo

```
parsl.dataflow.memoization.id_for_memo(obj: object, output_ref: bool = False) \rightarrow bytes
parsl.dataflow.memoization.id_for_memo(denormalized_list: list, output_ref: bool = False) \rightarrow bytes
parsl.dataflow.memoization.id_for_memo(denormalized_tuple: tuple, output_ref: bool = False) \rightarrow bytes
parsl.dataflow.memoization.id_for_memo(denormalized_tuple: tuple, output_ref: bool = False) \rightarrow bytes
parsl.dataflow.memoization.id_for_memo(denormalized_dict: dict, output_ref: bool = False) \rightarrow bytes
parsl.dataflow.memoization.id_for_memo(denormalized_dict: dict, output_ref: bool = False) \rightarrow bytes
```

This should return a byte sequence which identifies the supplied value for memoization purposes: for any two calls of id\_for\_memo, the byte sequence should be the same when the "same" value is supplied, and different otherwise.

"same" is in quotes about because sameness is not as straightforward as serialising out the content.

For example, for two dicts x, y:

 $x = {$ "a":3, "b":4 $} y = {$ "b":4, "a":3 $}$ 

then: x == y, but their serialization is not equal, and some other functions on x and y are not equal: list(x.keys()) != list(y.keys())

id\_for\_memo is invoked with output\_ref=True when the parameter is an output reference (a value in the outputs=[] parameter of an app invocation).

Memo hashing might be different for such parameters: for example, a user might choose to hash input File content so that changing the content of an input file invalidates memoization. This does not make sense to do for output files: there is no meaningful content stored where an output filename points at memoization time.

## parsl.dataflow.memoization.Memoizer

Memoizer is responsible for ensuring that identical work is not repeated.

When a task is repeated, i.e., the same function is called with the same exact arguments, the result from a previous execution is reused. wiki

The memoizer implementation here does not collapse duplicate calls at call time, but works **only** when the result of a previous call is available at the time the duplicate call is made.

For instance:

```
No advantage from Memoization helps
memoization here: here:
TaskA TaskB
| TaskA |
| | TaskA |
| | TaskA done (TaskB)
| | | (TaskB)
done |
done |
done
```

The memoizer creates a lookup table by hashing the function name and its inputs, and storing the results of the function.

When a task is ready for launch, i.e., all of its arguments have resolved, we add its hash to the task datastructure.

\_\_init\_\_(dfk: DataFlowKernel, memoize: bool = True, checkpoint: Dict[str, Future[Any]] = {})

Initialize the memoizer.

Parameters dfk (-) – The DFK object

**KWargs:** 

- memoize (Bool): enable memoization or not.
- checkpoint (Dict): A checkpoint loaded as a dict.

# Methods

<pre>init(dfk[, memoize, checkpoint])</pre>	Initialize the memoizer.
check_memo(task)	Create a hash of the task and its inputs and check the
	lookup table for this hash.
hash_lookup(hashsum)	Lookup a hash in the memoization table.
<pre>make_hash(task)</pre>	Create a hash of the task inputs.
update_memo(task, r)	Updates the memoization lookup table with the result
	from a task.

## **check\_memo**(*task:* TaskRecord) $\rightarrow$ Future[Any] | None

Create a hash of the task and its inputs and check the lookup table for this hash.

If present, the results are returned.

**Parameters task** (-) – task from the dfk.tasks table

cask (-) = task from the drk.tasks

# Returns

• Result of the function if present in table, wrapped in a Future

This call will also set task['hashsum'] to the unique hashsum for the func+inputs.

#### **hash\_lookup**(*hashsum: str*) $\rightarrow$ Future[Any]

Lookup a hash in the memoization table.

#### **Parameters**

hashsum (-) - The same hashes used to uniquely identify apps+inputs

#### Returns

· Lookup result

#### Raises

- KeyError – if hash not in table

## **make\_hash**(*task:* TaskRecord) $\rightarrow$ str

Create a hash of the task inputs.

## Parameters

task (-) – Task dictionary from dfk.tasks

#### Returns

A unique hash string

## **Return type**

• hash (str)

#### **update\_memo**(*task:* TaskRecord, *r: Future*[*Any*]) $\rightarrow$ None

Updates the memoization lookup table with the result from a task.

#### **Parameters**

- task (-) A task dict from dfk.tasks
- **r** (-) Result future

# parsl.dataflow.states.FINAL\_STATES

# parsl.dataflow.states.FINAL\_STATES = [<States.exec\_done: 3>, <States.memo\_done: 9>, <States.failed: 4>, <States.dep\_fail: 5>]

States from which we will never move to another state, because the job has either definitively completed or failed.

## parsl.dataflow.states.States

Enumerates the states a parsl task may be in.

These states occur inside the task record for a task inside a DataFlowKernel and in the monitoring database.

In a single successful task execution, tasks will progress in this sequence:

pending -> launched -> running -> running\_ended -> exec\_done

Other states represent deviations from this path, either due to failures, or to deliberate changes to how tasks are executed (for example due to join\_app, or memoization).

All tasks should end up in one of the states listed in *FINAL\_STATES*.

\_\_init\_\_(\*args, \*\*kwds)

## Methods

init(*args, **kwds)	
<pre>as_integer_ratio()</pre>	Return integer ratio.
<pre>bit_count()</pre>	Number of ones in the binary representation of the absolute value of self.
<pre>bit_length()</pre>	Number of bits necessary to represent self in binary.
conjugate	Returns self, the complex conjugate of any int.
<pre>from_bytes([byteorder, signed])</pre>	Return the integer represented by the given array of bytes.
<pre>to_bytes([length, byteorder, signed])</pre>	Return an array of bytes representing an integer.

## **Attributes**

unsched	
pending	Task is known to parsl but cannot run yet.
running	Task is running on a resource.
exec_done	Task has been executed successfully.
failed	Task has failed and no more attempts will be made to run it.
dep_fail	Dependencies of this task failed, so it is marked as failed without even an attempt to launch it.
launched	Task has been passed to a <i>ParslExecutor</i> for execution.
fail_retryable	Task has failed, but can be retried
memo_done	Task was found in the memoization table, so it is marked as done without even an attempt to launch it.
joining	Task is a join_app, joining on internal tasks.
running_ended	Like States.running, this state is also not observed by the DFK, but instead only by monitoring.
denominator	the denominator of a rational number in lowest terms
imag	the imaginary part of a complex number
numerator	the numerator of a rational number in lowest terms
real	the real part of a complex number

#### dep\_fail = 5

Dependencies of this task failed, so it is marked as failed without even an attempt to launch it.

## $exec_done = 3$

Task has been executed successfully.

#### fail\_retryable = 8

Task has failed, but can be retried

# failed = 4

Task has failed and no more attempts will be made to run it.

#### joining = 10

Task is a join\_app, joining on internal tasks. The task has run its own Python code, and is now waiting on other tasks before it can make further progress (to a done/failed state).

## launched = 7

Task has been passed to a *ParslExecutor* for execution.

#### $memo\_done = 9$

Task was found in the memoization table, so it is marked as done without even an attempt to launch it.

## pending = 0

Task is known to parsl but cannot run yet. Usually, a task cannot run because it is waiting for dependency tasks to complete.

#### running = 2

Task is running on a resource. This state is special - a DFK task record never goes to States.running state; but the monitoring database may represent a task in this state based on non-DFK information received from monitor\_wrapper.

## running\_ended = 11

Like States.running, this state is also not observed by the DFK, but instead only by monitoring. This state does not record anything about task success or failure, merely that the wrapper ran long enough to record it as finished.

unsched = -1

## parsl.dataflow.taskrecord.TaskRecord

# class parsl.dataflow.taskrecord.TaskRecord

This stores most information about a Parsl task

\_\_init\_\_(\*args, \*\*kwargs)

# Methods

<pre>init(*args, **kwargs)</pre>	
clear()	
copy()	
<pre>fromkeys([value])</pre>	Create a new dictionary with keys from iterable and values set to value.
<pre>get(key[, default])</pre>	Return the value for key if key is in the dictionary, else default.
<pre>items()</pre>	
keys()	
pop(k[,d])	If the key is not found, return the default if given; oth- erwise, raise a KeyError.
<pre>popitem()</pre>	Remove and return a (key, value) pair as a 2-tuple.
<pre>setdefault(key[, default])</pre>	Insert key with a value of default if key is not in the dictionary.
update([E,]**F)	If E is present and has a .keys() method, then does: for k in E: $D[k] = E[k]$ If E is present and lacks a .keys() method, then does: for k, v in E: $D[k] = v$ In either case, this is followed by: for k in F: $D[k] = F[k]$
values()	

# Attributes

dfk	The DataFlowKernel which is managing this task.
func_name	
status	
depends	
app_fu	The Future which was returned to the user when an app was invoked.
exec_fu	When a task has been launched on an executor, stores the Future returned by that executor.
executor	The name of the executor which this task will be/is
retries_left	being/was executed on.
fail_count	
fail_cost	
fail_history	
checkpoint	Should this task be checkpointed?
hashsum	The hash used for checkpointing and memoisation.
task_launch_lock	This lock is used to ensure that task launch only hap-
	pens once.
func	
fn_hash	
args	
kwargs	
time_invoked	
time returned	
cime_i etainea	
try_time_launched	
try_time_returned	
memoize	Should this task be memoized?
ignore_for_cache	
from_memo	
id	
14	
try_id	
	continues on next page

resource_specification	Dictionary containing relevant info for a task execu-
	uon.
join	Is this a join_app?
joins	If this is a join app and the python body has executed,
	then this contains the Future or list of Futures that the
	join app will join.
join_lock	Restricts access to end-of-join behavior to ensure that
	joins only complete once, even if several joining Fu-
	tures complete close together in time.

Table 2 – continued from previous page

## app\_fu: AppFuture

The Future which was returned to the user when an app was invoked.

#### args: Sequence[Any]

#### checkpoint: bool

Should this task be checkpointed?

# depends: List[Future]

#### dfk: dflow.DataFlowKernel

The DataFlowKernel which is managing this task.

#### exec\_fu: Future | None

When a task has been launched on an executor, stores the Future returned by that executor.

#### executor: str

The name of the executor which this task will be/is being/was executed on.

## fail\_cost: float

fail\_count: int

fail\_history: List[str]

fn\_hash: str

from\_memo: bool | None

#### func: Callable

func\_name: str

#### hashsum: str | None

The hash used for checkpointing and memoisation. This is not known until at least all relevant dependencies have completed, and will be None before that.

# id: int

## ignore\_for\_cache: Sequence[str]

#### join: bool

Is this a join\_app?

## join\_lock: threading.Lock

Restricts access to end-of-join behavior to ensure that joins only complete once, even if several joining Futures complete close together in time.

## joins: None | Future | List[Future]

If this is a join app and the python body has executed, then this contains the Future or list of Futures that the join app will join.

## kwargs: Dict[str, Any]

#### memoize: bool

Should this task be memoized?

## resource\_specification: Dict[str, Any]

Dictionary containing relevant info for a task execution. Includes resources to allocate and execution mode as a given executor permits.

## retries\_left: int

## status: States

#### task\_launch\_lock: threading.Lock

This lock is used to ensure that task launch only happens once. A task can be launched by dependencies completing from arbitrary threads, and a race condition would exist when dependencies complete in multiple threads very close together in time, which this lock prevents.

```
time_invoked: datetime.datetime | None
```

time\_returned: datetime.datetime | None

try\_id: int

try\_time\_launched: datetime.datetime | None

try\_time\_returned: datetime.datetime | None

#### parsl.jobs.job\_status\_poller.JobStatusPoller

**\_\_init\_\_**(\*, strategy: str | None, max\_idletime: float, strategy\_period: float | int, monitoring: MonitoringRadio | None = None)  $\rightarrow$  None

Initialize the Timer object. We start the timer thread here

#### KWargs:

- interval (int or float) : number of seconds between callback events
- name (str) : a base name to use when naming the started thread

## **Methods**

<pre>init(*, strategy, max_idletime,[,])</pre>	Initialize the Timer object.
add_executors(executors)	
close([timeout])	Merge the threads and terminate.
<pre>make_callback()</pre>	Makes the callback and resets the timer.
poll()	

add\_executors(executors: Sequence[BlockProviderExecutor])  $\rightarrow$  None

**close**(*timeout: float* | *None* = *None*)  $\rightarrow$  None Merge the threads and terminate.

 $poll() \rightarrow None$ 

## parsl.jobs.strategy.Strategy

class pars1.jobs.strategy.Strategy(\*, strategy: str | None, max\_idletime: float)

Scaling strategy.

As a workflow dag is processed by Parsl, new tasks are added and completed asynchronously. Parsl interfaces executors with execution providers to construct scalable executors to handle the variable work-load generated by the workflow. This component is responsible for periodically checking outstanding tasks and available compute capacity and trigger scaling events to match workflow needs.

Here's a diagram of an executor. An executor consists of blocks, which are usually created by single requests to a Local Resource Manager (LRM) such as slurm, condor, torque, or even AWS API. The blocks could contain several task blocks which are separate instances on workers.

```
executor = | | task task | ... | task task | |
```

## The relevant specification options are:

- 1. min\_blocks: Minimum number of blocks to maintain
- 2. init\_blocks: number of blocks to provision at initialization of workflow
- 3. max\_blocks: Maximum number of blocks that can be active due to one workflow

```
active_tasks = pending_tasks + running_tasks
```

```
Parallelism = slots / tasks
= [0, 1] (i.e, 0 \le p \le 1)
```

For example:

#### When p = 0,

=> compute with the least resources possible. infinite tasks are stacked per slot.

```
blocks = min_blocks { if active_tasks = 0
    max(min_blocks, 1) { else
```

## When p = 1,

=> compute with the most resources. one task is stacked per slot.

#### When p = 1/2,

=> We stack upto 2 tasks per slot before we overflow and request a new block

let's say min:init:max = 0:0:4 and task\_blocks=2 Consider the following example: min\_blocks = 0 init\_blocks = 0 max\_blocks = 4 tasks\_per\_node = 2 nodes\_per\_block = 1

In the diagram, X <- task

at 2 tasks:

+---Block---| | | | | | | X X | |slot slot| +-----+

at 5 tasks, we overflow as the capacity of a single block is fully used.

+B1	ock		+Blo	ock
X	X	>		
X	X		X	
slot	slot		slot	slot
+	+		+	+

**\_\_init\_\_**(\*, *strategy: str* | *None*, *max\_idletime: float*)  $\rightarrow$  None Initialize strategy.

## **Methods**

init(*, strategy, max_idletime)	Initialize strategy.
add_executors(executors)	

add\_executors(*executors: Sequence*[ParslExecutor]) → None

## parsl.utils.Timer

**class** parsl.utils.**Timer**(*callback: Callable*, \**args: Any, interval: float* | *int* = 5, *name: str* | *None* = *None*) This class will make a callback periodically, with a period specified by the interval parameter.

This is based on the following logic :

```
BEGIN (INTERVAL, THRESHOLD, callback) :
   start = current_time()
   while (current_time()-start < INTERVAL) :
        wait()
        break
   callback()</pre>
```

**\_\_init\_\_**(*callback: Callable*, \**args: Any, interval: float* | *int* = 5, *name: str* | *None* = *None*)  $\rightarrow$  None Initialize the Timer object. We start the timer thread here

#### **KWargs:**

- interval (int or float) : number of seconds between callback events
- name (str) : a base name to use when naming the started thread

## Methods

<pre>init(callback, *args[, interval, name])</pre>	Initialize the Timer object.
close([timeout])	Merge the threads and terminate.
<pre>make_callback()</pre>	Makes the callback and resets the timer.

**close**(*timeout: float* | *None* = *None*)  $\rightarrow$  None Merge the threads and terminate.

 $make_callback() \rightarrow None$ 

Makes the callback and resets the timer.

## **Developer documentation**

## Contributing

Parsl is an open source project that welcomes contributions from the community.

If you're interested in contributing, please review our contributing guide.

## Roadmap

## **OVERVIEW**

While we follow best practices in software development processes (e.g., CI, flake8, code review), there are opportunities to make our code more maintainable and accessible. This roadmap, written in the fall of 2023, covers our major activities planned through 2025 to increase efficiency, productivity, user experience, and community building.

Features and improvements are documented via GitHub issues and pull requests.

## **Code Maintenance**

- **Type Annotations and Static Type Checking**: Add static type annotations throughout the codebase and add typeguard checks.
- **Release Process**: Improve the overall release process to synchronize docs and code releases, automatically produce changelog documentation.
- **Components Maturity Model**: Defines the component maturity model and tags components with their appropriate maturity level.
- **Define and Document Interfaces**: Identify and document interfaces via which external components can augment the Parsl ecosystem.
- **Distributed Testing Process**: All tests should be run against all possible schedulers, using different executors, on a variety of remote systems. Explore the use of containerized schedulers and remote testing on real systems.

## **New Features and Integrations**

- Enhanced MPI Support: Extend Parsl's MPI model with MPI apps and runtime support capable of running MPI apps in different environments (MPI flavor and launcher).
- Serialization Configuration: Enable users to select what serialization methods are used and enable users to supply their own serializer.
- **PSI/J integration**: Integrate PSI/J as a common interface for schedulers.
- **Internal Concurrency Model**: Revisit and rearchitect the concurrency model to reduce areas that are not well understood and reduce the likelihood of errors.
- Common Model for Errors: Make Parsl errors self-describing and understandable by users.
- Plug-in Model for External Components: Extend Parsl to implement interfaces defined above.
- User Configuration Validation Tool: Provide tooling to help users configure Parsl and diagnose and resolve errors.
- Anonymized Usage Tracking: Usage tracking is crucial for our data-oriented approach to understand the adoption of Parsl, which components are used, and where errors occur. This allows us to prioritize investment in components, progress components through the maturity levels, and identify bugs. Revisit prior usage tracking and develop a service that enables users to control tracking information.
- Support for Globus Compute: Enable execution of Parsl tasks using Globus Compute as an executor.
- Update Globus Data Management: Update Globus integration to use the new Globus Connect v5 model (i.e., needing specific scopes for individual endpoints).
- Performance Measurement: Improve ability to measure performance metrics and report to users.
- Enhanced Debugging: Application-level logging to understand app execution.

## Tutorials, Training, and User Support

- **Configuration and Debugging**: Tutorials showing how to configure Parsl for different resources and debug execution.
- Functional Serialization 101: Tutorial describing how serialization works and how you can integrate custom serializers.
- **ProxyStore Data Management**: Tutorial showing how you can use ProxyStore to manage data for both inter and intra-site scenarios.
- **Open Dev Calls on Zoom**: The internal core team holds an open dev call/office hours every other Thursday to help users troubleshoot issues, present and share their work, connect with each other, and provide community updates.
- Project Documentation: is maintained and updated in Read the Docs.

#### **Longer-term Objectives**

- **Globus Compute Integration**: Once Globus Compute supports multi-tenancy, Parsl will be able to use it to run remote tasks on initially one and then later multiple resources.
- **Multi-System Optimization**: Once Globus Compute integration is complete, it is best to use multiple systems for multiple tasks as part of a single workflow.
- HPC Checkpointing and Job Migration: As new resources become available, HPC tasks will be able to be checkpointed and moved to the system with more resources.

#### Packaging

Currently packaging is managed by @annawoodard and @yadudoc.

Steps to release

- 1. Update the version number in parsl/parsl/version.py
- 2. Check the following files to confirm new release information \* parsl/setup.py \* requirements.txt \* parsl/docs/devguide/changelog.rst \* parsl/README.rst
- 3. Commit and push the changes to github
- 4. Run the tag\_and\_release.sh script. This script will verify that version number matches the version specified.

./tag\_and\_release.sh <VERSION\_FOR\_TAG>

Here are the steps that is taken by the tag\_and\_release.sh script:

```
# Create a new git tag :
git tag <MAJOR>.<MINOR>.<BUG_REV>
# Push tag to github :
git push origin <TAG_NAME>
# Depending on permission all of the following might have to be run as root.
sudo su
# Make sure to have twine installed
pip3 install twine
```

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```
# Create a source distribution
python3 setup.py sdist
# Create a wheel package, which is a prebuilt package
python3 setup.py bdist_wheel
# Upload the package with twine
twine upload dist/*
```

## **Doc Docs**

## **Documentation location**

Documentation is maintained in Python docstrings throughout the code. These are imported via the autodoc Sphinx extension in docs/reference.rst. Individual stubs for user-facing classes (located in stubs) are generated automatically via sphinx-autogen. Parsl modules, classes, and methods can be cross-referenced from a docstring by enclosing it in backticks (`).

#### **Remote builds**

Builds are automatically performed by readthedocs.io and published to parsl.readthedocs.io upon git commits.

## Local builds

To build the documentation locally, use:

```
$ make clean html
```

To view the freshly rebuilt docs, use:

```
$ cd _build/html
$ python3 -m http.server 8080
```

Once the python http server is launched, point your browser to http://localhost:8080

#### **Regenerate module stubs**

If necessary, docstring stubs can be regenerated using:

\$ sphinx-autogen reference.rst

# **Historical Documents**

# **Historical: Changelog**

**Note:** After Parsl 1.2.0, releases moved to a lighter weight automated model. This manual changelog is no longer updated and is now marked as historical.

Change information is delivered as commit messages on individual pull requests, which can be see using any relevant git history browser - for example, on the web at https://github.com/Parsl/parsl/commits/master/ or on the commandline using using git log.

# Parsl 1.2.0

Release date: January 13th, 2022.

Parsl v1.2.0 includes 99 pull requests with contributions from:

Ben Clifford @benclifford, Daniel S. Katz @danielskatz, Douglas Thain @dthain, James Corbett @jameshcorbett, Jonas Rübenach @jrueb, Logan Ward @WardLT, Matthew R. Becker @beckermr, Vladimir @vkhodygo, Yadu Nand Babuji @yadudoc, Yo Yehudi @yochannah, Zhuozhao Li @ZhuozhaoLi, yongyanrao @yongyanrao, Tim Jenness @timj, Darko Marinov @darko-marinov, Quentin Le Boulc'h

# **High Throughput Executor**

- Remove htex self.tasks race condition that shows under high load (#2034)
- Fix htex scale down breakage due to overly aggressive result heartbeat (#2119) [TODO: this fixes a bug introduced since 1.1.0 so note that? #2104 ]
- Send heartbeats via results connection (#2104)

# **Work Queue Executor**

- Allow use of WorkQueue running\_time\_min resource constraint (#2113) WQ recently introduced an additional resource constraint: workers can be aware of their remaining wall time, and tasks can be constrained to only go to workers with sufficient remaining time.
- Implement priority as a Work Queue resource specification (#2067) The allows a workflow script to influence the order in which queued tasks are executed using Work Queue's existing priority mechanism.
- Disable WQ-level retries with an option to re-enable (#2059) Previously by default, Work Queue will retry tasks that fail at the WQ level (for example, because of worker failure) an infinite number of times, inside the same parsl-level execution try. That hides the repeated tries from parsl (so monitoring does not report start/end times as might naively be expected for a try, and parsl retry counting does not count).
- Document WorkqueueExecutor project\_name remote reporting better (#2089)
- wq executor should show itself using representation mixin (#2064)
- Make WorkQueue worker command configurable (#2036)

## **Flux Executor**

The new FluxExecutor class uses the Flux resource manager (github: flux-framework/flux-core) to launch tasks. Each task is a Flux job.

## **Condor Provider**

• Fix bug in condor provider for unknown jobs (#2161)

## **LSF Provider**

• Update LSF provider to make it more friendly for different LSF-based computers (#2149)

## **SLURM Provider**

• Improve docs and defaults for slurm partition and account parameters. (#2126)

## **Grid Engine Provider**

• missing queue from self - causes config serialisation failure (#2042)

## Monitoring

- Index task\_hashsum to give cross-run query speedup (#2085)
- Fix monitoring "db locked" errors occuring at scale (#1917)
- Fix worker efficiency plot when tasks are still in progress (#2048)
- Fix use of previously removed reg\_time monitoring field (#2020)
- Reorder debug message so it happens when the message is received, without necessarily blocking on the resource\_msgs queue put (#2093)

#### **General new features**

• Workflow-pluggable retry scoring (#2068) - When a task fails, instead of causing a retry "cost" of 1 (the previous behaviour), this PR allows that cost to be determined by a user specified function which is given some context about the failure.

# **General bug fixes**

- Fix type error when job status output is large. (#2129)
- Fix a race condition in the local channel (#2115)
- Fix incorrect order of manager and interchange versions in error text (#2108)
- Fix to macos multiprocessing spawn and context issues (#2076)
- Tidy tasks\_per\_node in strategy (#2030)
- Fix and test wrong type handling for joinapp returns (#2063)
- FIX: os independent path (#2043)

# Platform and packaging

- Improve support for Windows (#2107)
- Reflect python 3.9 support in setup.py metadata (#2023)
- Remove python <3.6 handling from threadpoolexecutor (#2083)
- Remove breaking .[all] install target (#2069)

# Internal tidying

- Remove ipp logging hack in PR #204 (#2170)
- Remove BadRegistration exception definition which has been unused since PR #1671 (#2142)
- Remove AppFuture.\_\_repr\_\_, because superclass Future repr is sufficient (#2143)
- Make monitoring hub exit condition more explicit (#2131)
- Replace parsl's logging NullHandler with python's own NullHandler (#2114)
- Remove a commented out line of dead code in htex (#2116)
- Abstract more block handling from HighThroughputExecutor and share with WorkQueue (#2071)
- Regularise monitoring RESOURCE\_INFO messages (#2117)
- Pull os x multiprocessing code into a single module (#2099)
- Describe monitoring protocols better (#2029)
- Remove task\_id param from memo functions, as whole task record is available (#2080)
- remove irrelevant \_\_\_\_\_\_ stub of local provider (#2026)
- remove unused weakref\_cb (#2022)
- Remove unneeded task\_id param from sanitize\_and\_wrap (#2081)
- Remove outdated IPP related comment in memoization (#2058)
- Remove unused AppBase status field (#2053)
- Do not unwrap joinapp future exceptions unnecessarily (#2084)
- Eliminate self.tasks[id] calls from joinapp callback (#2015)
- Looking at eliminating passing of task IDs and passing task records instead (#2016)

- Eliminate self.tasks[id] from launch\_if\_ready
- Eliminate self.tasks[id] calls from launch\_task (#2061)
- Eliminate self.tasks[id] from app done callback (#2017)
- Make process\_worker\_pool pass mypy (#2052)
- Remove unused walltime from LocalProvider (#2057)
- Tidy human readable text/variable names around DependencyError (#2037)
- Replace old string formatting with f-strings in utils.py (#2055)

#### Documentation, error messages and human-readable text

- Add a documentation chapter summarizing plugin points (#2066)
- Correct docstring for set\_file\_logger (#2156)
- Fix typo in two db error messages and make consistent with each other (#2152)
- Update slack join links to currently unexpired link (#2146)
- small typo fix in doc (#2134)
- Update CONTRIBUTING.rst (#2144)
- trying to fix broken link in GitHub (#2133)
- Add CITATION.cff file (#2100)
- Refresh the sanitize\_and\_wrap docstring (#2086)
- Rephrase ad-hoc config doc now that AdHocProvider (PR #1297) is implemented (#2096)
- Add research notice to readme (#2097)
- Remove untrue claim that parsl\_resource\_specification keys are case insensitive (#2095)
- Use zsh compatible install syntax (#2009)
- Remove documentation that interchange is walltime aware (#2082)
- Configure sphinx to put in full documentation for each method (#2094)
- autogenerate sphinx stubs rather than requiring manual update each PR (#2087)
- Update docstring for handle\_app\_update (#2079)
- fix a typo (#2024)
- Switch doc verb from invocated to invoked (#2088)
- Add documentation on meanings of states (#2075)
- Fix summary sentence of ScaleOutException (#2021)
- clarify that max workers is per node (#2056)
- Tidy up slurm state comment (#2035)
- Add nscc singapore example config (#2003)
- better formatting (#2039)
- Add missing f for an f-string (#2062)
- Rework \_\_repr\_\_ and \_\_str\_\_ for OptionalModuleMissing (#2025)

• Make executor bad state exception log use the exception (#2155)

# **CI/testing**

- Make changes for CI reliability (#2118)
- Make missing worker test cleanup DFK at end (#2153)
- Tidy bash error codes tests. (#2130)
- Upgrade CI to use recent ubuntu, as old version was deprecated (#2111)
- Remove travis config, replaced by GitHub Actions in PR #2078 (#2112)
- Fix CI broken by dependency package changes (#2105)
- Adding github actions for CI (#2078)
- Test combine() pattern in joinapps (#2054)
- Assert that there should be no doc stubs in version control (#2092)
- Add monitoring dependency to local tests (#2074)
- Put viz test in a script (#2019)
- Reduce the size of recursive fibonacci joinapp testing (#2110)
- Remove disabled midway test (#2028)

# Parsl 1.1.0

Released on April 26th, 2021.

Parsl v1.1.0 includes 59 closed issues and 243 pull requests with contributions (code, tests, reviews and reports) from:

Akila Ravihansa Perera @ravihansa3000, Anna Woodard @annawoodard, @bakerjl, Ben Clifford @benclifford, Daniel S. Katz @danielskatz, Douglas Thain @dthain, @gerrick, @JG-Quarknet, Joseph Moon @jmoon1506, Kelly L. Rowland @kellyrowland, Lars Bilke @bilke, Logan Ward @WardLT, Kirill Nagaitsev @Loonride, Marcus Schwarting @meschw04, Matt Baughman @mattebaughman, Mihael Hategan @hategan, @radiantone, Rohan Kumar @rohankumar42, Sohit Miglani @sohitmiglani, Tim Shaffer @trshaffer, Tyler J. Skluzacek @tskluzac, Yadu Nand Babuji @yadudoc, and Zhuozhao Li @ZhuozhaoLi

# **Deprecated and Removed features**

- Python 3.5 is no longer supported.
- Almost definitely broken Jetstream provider removed (#1821)

## **New Functionality**

- Allow HTEX to set CPU affinity (#1853)
- New serialization system to replace IPP serialization (#1806)
- Support for Python 3.9
- @join\_apps are a variation of @python\_apps where an app can launch more apps and then complete only after the launched apps are also completed.

These are described more fully in docs/userguide/joins.rst

- Monitoring:
  - hub.log is now named monitoring\_router.log
  - Remove denormalised workflow duration from monitoring db (#1774)
  - Remove hostname from status table (#1847)
  - Clarify distinction between tasks and tries to run tasks (#1808)
  - Replace 'done' state with 'exec\_done' and 'memo\_done' (#1848)
  - Use repr instead of str for monitoring fail history (#1966)
- Monitoring visualization:
  - Make task list appear under .../task/ not under .../app/ (#1762)
  - Test that parsl-visualize does not return HTTP errors (#1700)
  - Generate Gantt chart from status table rather than task table timestamps (#1767)
  - Hyperlinks for app page to task pages should be on the task ID, not the app name (#1776)
  - Use real final state to color DAG visualization (#1812)
- Make task record garbage collection optional. (#1909)
- Make checkpoint\_files = get\_all\_checkpoints() by default (#1918)

# Parsl 1.0.0

Released on June 11th, 2020

Parsl v1.0.0 includes 59 closed issues and 243 pull requests with contributions (code, tests, reviews and reports) from:

Akila Ravihansa Perera @ravihansa3000, Aymen Alsaadi @AymenFJA, Anna Woodard @annawoodard, Ben Clifford @benclifford, Ben Glick @benhg, Benjamin Tovar @btovar, Daniel S. Katz @danielskatz, Daniel Smith @dgasmith, Douglas Thain @dthain, Eric Jonas @ericmjonas, Geoffrey Lentner @glentner, Ian Foster @ianfoster, Kalpani Ranasinghe @kalpanibhagya, Kyle Chard @kylechard, Lindsey Gray @lgray, Logan Ward @WardLT, Lyle Hayhurst @lhayhurst, Mihael Hategan @hategan, Rajini Wijayawardana @rajiniw95, @saktar-unr, Tim Shaffer @trshaffer, Tom Glanzman @TomGlanzman, Yadu Nand Babuji @yadudoc and, Zhuozhao Li @ZhuozhaoLi

## **Deprecated and Removed features**

- **Python3.5** is now marked for deprecation, and will not be supported after this release. Python3.6 will be the earliest Python3 version supported in the next release.
- **App** decorator deprecated in 0.8 is now removed issue#1539 bash\_app and python\_app are the only supported App decorators in this release.
- IPyParallelExecutor is no longer a supported executor issue#1565

## **New Functionality**

- parsl.executors.WorkQueueExecutor introduced in v0.9.0 is now in beta. parsl. executors.WorkQueueExecutor is designed as a drop-in replacement for parsl.executors. HighThroughputExecutor. Here are some key features:
  - Support for packaging the python environment and shipping it to the worker side. This mechanism addresses propagating python environments in grid-like systems that lack shared-filesystems or cloud environments.
  - pars1.executors.WorkQueueExecutor supports resource function tagging and resource specification
  - Support for resource specification kwarg issue#1675
- Limited type-checking in Parsl internal components (as part of an ongoing effort)
- Improvements to caching mechanism including ability to mark certain arguments to be not counted for memoization.
  - Normalize known types for memoization, and reject unknown types (#1291). This means that previous unreliable behaviour for some complex types such as dicts will become more reliable; and that other previous unreliable behaviour for other unknown complex types will now cause an error. Handling can be added for those types using parsl.memoization.id\_for\_memo.
  - Add ability to label some arguments in an app invocation as not memoized using the ignore\_for\_cache app keyword (PR 1568)
- Special keyword args: 'inputs', 'outputs' that are used to specify files no longer support strings and now require *File* objects. For example, the following snippet is no longer supported in v1.0.0:

```
@bash_app
def cat(inputs=(), outputs=()):
    return 'cat {} > {}'.format(inputs[0], outputs[0])
concat = cat(inputs=['hello-0.txt'],
    outputs=['hello-1.txt'])
```

This is the new syntax:
Since filenames are no longer passed to apps as strings, and the string filepath is required, it can be accessed from the File object using the filepath attribute.

```
from pars1 import File
@bash_app
def cat(inputs=(), outputs=()):
    return 'cat {} > {}'.format(inputs[0].filepath, outputs[0].filepath)
```

- New launcher: pars1.launchers.WrappedLauncher for launching tasks inside containers.
- parsl.channels.SSHChannel now supports a key\_filename kwarg issue#1639
- Newly added Makefile wraps several frequent developer operations such as:
  - Run the test-suite: make test
  - Install parsl: make install
  - Create a virtualenv: make virtualenv
  - Tag release and push to release channels: make deploy
- Several updates to the parsl.executors.HighThroughputExecutor:
  - By default, the pars1.executors.HighThroughputExecutor will now use heuristics to detect and try
    all addresses when the workers connect back to the parsl master. An address can be configured manually
    using the HighThroughputExecutor(address=<address\_string>) kwarg option.
  - Support for Mac OS. (pull#1469, pull#1738)
  - Cleaner reporting of version mismatches and automatic suppression of non-critical errors.
  - Separate worker log directories by block id issue#1508
- Support for garbage collection to limit memory consumption in long-lived scripts.
- All cluster providers now use max\_blocks=1 by default issue#1730 to avoid over-provisioning.
- New JobStatus class for better monitoring of Jobs submitted to batch schedulers.

#### **Bug Fixes**

- Ignore AUTO\_LOGNAME for caching issue#1642
- Add batch jobs to PBS/torque job status table issue#1650
- Use higher default buffer threshold for serialization issue#1654
- Do not pass mutable default to ignore\_for\_cache issue#1656
- · Several improvements and fixes to Monitoring
- Fix sites/test\_ec2 failure when aws user opts specified issue#1375
- Fix LocalProvider to kill the right processes, rather than all processes owned by user issue#1447
- Exit htex probe loop with first working address issue#1479
- Allow slurm partition to be optional issue#1501
- Fix race condition with wait\_for\_tasks vs task completion issue#1607
- Fix Torque job\_id truncation issue#1583
- Cleaner reporting for Serialization Errors issue#1355

- Results from zombie managers do not crash the system, but will be ignored issue#1665
- Guarantee monitoring will send out at least one message issue#1446
- Fix monitoring ctrlc hang issue#1670

#### Parsl 0.9.0

Released on October 25th, 2019

Parsl v0.9.0 includes 199 closed issues and pull requests with contributions (code, tests, reviews and reports) from:

Andrew Litteken @AndrewLitteken, Anna Woodard @annawoodard, Ben Clifford @benclifford, Ben Glick @benhg, Daniel S. Katz @danielskatz, Daniel Smith @dgasmith, Engin Arslan @earslan58, Geoffrey Lentner @glentner, John Hover @jhover Kyle Chard @kylechard, TJ Dasso @tjdasso, Ted Summer @macintoshpie, Tom Glanzman @TomGlanzman, Levi Naden @LNaden, Logan Ward @WardLT, Matthew Welborn @mattwelborn, @MatthewBM, Raphael Fialho @rapguit, Yadu Nand Babuji @yadudoc, and Zhuozhao Li @ZhuozhaoLi

#### **New Functionality**

 Parsl will no longer do automatic keyword substitution in @bash\_app in favor of deferring to Python's format method and newer f-strings. For example,

```
# The following example worked until v0.8.0
@bash_app
def cat(inputs=(), outputs=()):
    return 'cat {inputs[0]} > {outputs[0]}' # <-- Relies on Parsl auto_
    formatting the string
# Following are two mechanisms that will work going forward from v0.9.0
@bash_app
def cat(inputs=(), outputs=()):
    return 'cat {} > {}'.format(inputs[0], outputs[0]) # <-- Use str.format_
    method
@bash_app
def cat(inputs=(), outputs=()):
    return f'cat {inputs[0]} > {outputs[0]}' # <-- OR use f-strings_
    -introduced in Python3.6
```

- @python\_app now takes a walltime kwarg to limit the task execution time.
- New file staging API *pars1.data\_provider.staging.Staging* to support pluggable file staging methods. The methods implemented in 0.8.0 (HTTP(S), FTP and Globus) are still present, along with two new methods which perform HTTP(S) and FTP staging on worker nodes to support non-shared-filesystem executors such as clouds.
- Behaviour change for storage\_access parameter. In 0.8.0, this was used to specify Globus staging configuration. In 0.9.0, if this parameter is specified it must specify all desired staging providers. To keep the same staging providers as in 0.8.0, specify:

```
from parsl.data_provider.data_manager import default_staging
storage_access = default_staging + [GlobusStaging(...)]
```

GlobusScheme in 0.8.0 has been renamed *GlobusStaging* and moved to a new module, parsl.data\_provider.globus

- *parsl.executors.WorkQueueExecutor*: a new executor that integrates functionality from Work Queue is now available.
- New provider to support for Ad-Hoc clusters parsl.providers.AdHocProvider
- New provider added to support LSF on Summit pars1.providers.LSFProvider
- Support for CPU and Memory resource hints to providers (github).
- The logging\_level=logging.INFO in *parsl.monitoring.MonitoringHub* is replaced with monitoring\_debug=False:

```
monitoring=MonitoringHub(
    hub_address=address_by_hostname(),
    hub_port=55055,
    monitoring_debug=False,
    resource_monitoring_interval=10,
),
```

- Managers now have a worker watchdog thread to report task failures that crash a worker.
- Maximum idletime after which idle blocks can be relinquished can now be configured as follows:

```
config=Config(
    max_idletime=120.0 , # float, unit=seconds
    strategy='simple'
)
```

- Several test-suite improvements that have dramatically reduced test duration.
- Several improvements to the Monitoring interface.
- Configurable port on *parsl.channels.SSHChannel*.
- suppress\_failure now defaults to True.
- *parsl.executors.HighThroughputExecutor* is the recommended executor, and IPyParallelExecutor is deprecated.
- *parsl.executors.HighThroughputExecutor* will expose worker information via environment variables: PARSL\_WORKER\_RANK and PARSL\_WORKER\_COUNT

#### **Bug Fixes**

- ZMQError: Operation cannot be accomplished in current state bug issue#1146
- Fix event loop error with monitoring enabled issue#532
- Tasks per app graph appears as a sawtooth, not as rectangles issue#1032.
- Globus status processing failure issue#1317.
- Sporadic globus staging error issue#1170.
- RepresentationMixin breaks on classes with no default parameters issue#1124.
- File localpath staging conflict issue#1197.
- Fix IndexError when using CondorProvider with strategy enabled issue#1298.

- Improper dependency error handling causes hang issue#1285.
- Memoization/checkpointing fixes for bash apps issue#1269.
- CPU User Time plot is strangely cumulative issue#1033.
- Issue requesting resources on non-exclusive nodes issue#1246.
- parsl + htex + slurm hangs if slurm command times out, without making further progress issue#1241.
- Fix strategy overallocations issue#704.
- max\_blocks not respected in SlurmProvider issue#868.
- globus staging does not work with a non-default workdir issue#784.
- Cumulative CPU time loses time when subprocesses end issue#1108.
- Interchange KeyError due to too many heartbeat missed issue#1128.

#### Parsl 0.8.0

Released on June 13th, 2019

Parsl v0.8.0 includes 58 closed issues and pull requests with contributions (code, tests, reviews and reports)

from: Andrew Litteken @AndrewLitteken, Anna Woodard @annawoodard, Antonio Villarreal @villarrealas, Ben Clifford @benc, Daniel S. Katz @danielskatz, Eric Tatara @etatara, Juan David Garrido @garri1105, Kyle Chard @@kylechard, Lindsey Gray @lgray, Tim Armstrong @timarmstrong, Tom Glanzman @TomGlanzman, Yadu Nand Babuji @yadudoc, and Zhuozhao Li @ZhuozhaoLi

#### **New Functionality**

- Monitoring is now integrated into parsl as default functionality.
- parsl.AUTO\_LOGNAME: Support for a special AUTO\_LOGNAME option to auto generate stdout and stderr file paths.
- *File* no longer behaves as a string. This means that operations in apps that treated a *File* as a string will break. For example the following snippet will have to be updated:

- Cleaner user app file log management.
- Updated configurations using *parsl.executors.HighThroughputExecutor* in the configuration section of the userguide.
- Support for OAuth based SSH with pars1. channels. OAuthSSHChannel.

#### **Bug Fixes**

- Monitoring resource usage bug issue#975
- Bash apps fail due to missing dir paths issue#1001
- Viz server explicit binding fix issue#1023
- Fix sqlalchemy version warning issue#997
- All workflows are called typeguard issue#973
- Fix ModuleNotFoundError: No module named 'monitoring' issue#971
- Fix sqlite3 integrity error issue#920
- HTEX interchange check python version mismatch to the micro level issue#857
- Clarify warning message when a manager goes missing issue#698
- Apps without a specified DFK should use the global DFK in scope at call time, not at other times. issue#697

### Parsl 0.7.2

Released on Mar 14th, 2019

#### **New Functionality**

- Monitoring: Support for reporting monitoring data to a local sqlite database is now available.
- Parsl is switching to an opt-in model for anonymous usage tracking. Read more here: Usage statistics collection.
- *bash\_app* now supports specification of write modes for stdout and stderr.
- Persistent volume support added to pars1.providers.KubernetesProvider.
- Scaling recommendations from study on Bluewaters is now available in the userguide.

### Parsl 0.7.1

Released on Jan 18th, 2019

#### **New Functionality**

- parsl.executors.LowLatencyExecutor: a new executor designed to address use-cases with tight latency requirements such as model serving (Machine Learning), function serving and interactive analyses is now available.
- New options in parsl.executors.HighThroughputExecutor:
  - suppress\_failure: Enable suppression of worker rejoin errors.
  - max\_workers: Limit workers spawned by manager
- Late binding of DFK, allows apps to pick DFK dynamically at call time. This functionality adds safety to cases where a new config is loaded and a new DFK is created.

#### **Bug fixes**

• A critical bug in *pars1.executors.HighThroughputExecutor* that led to debug logs overflowing channels and terminating blocks of resource is fixed issue#738

#### Parsl 0.7.0

Released on Dec 20st, 2018

Parsl v0.7.0 includes 110 closed issues with contributions (code, tests, reviews and reports) from: Alex Hays @ahayschi, Anna Woodard @annawoodard, Ben Clifford @benc, Connor Pigg @ConnorPigg, David Heise @daheise, Daniel S. Katz @danielskatz, Dominic Fitzgerald @djf604, Francois Lanusse @EiffL, Juan David Garrido @garri1105, Gordon Watts @gordonwatts, Justin Wozniak @jmjwozniak, Joseph Moon @jmoon1506, Kenyi Hurtado @khurtado, Kyle Chard @kylechard, Lukasz Lacinski @lukaszlacinski, Ravi Madduri @madduri, Marco Govoni @mgovoni-devel, Reid McIlroy-Young @reidmcy, Ryan Chard @ryanchard, @sdustrud, Yadu Nand Babuji @yadudoc, and Zhuozhao Li @ZhuozhaoLi

#### **New functionality**

- *parsl.executors.HighThroughputExecutor*: a new executor intended to replace the IPyParallelExecutor is now available. This new executor addresses several limitations of IPyParallelExecutor such as:
  - Scale beyond the ~300 worker limitation of IPP.
  - Multi-processing manager supports execution on all cores of a single node.
  - Improved worker side reporting of version, system and status info.
  - Supports failure detection and cleaner manager shutdown.

Here's a sample configuration for using this executor locally:

```
from parsl.providers import LocalProvider
from parsl.channels import LocalChannel
from parsl.config import Config
from parsl.executors import HighThroughputExecutor
config = Config(
    executors=[
        HighThroughputExecutor(
            label="htex_local",
            cores_per_worker=1,
            provider=LocalProvider(
                channel=LocalChannel(),
                init_blocks=1,
                max_blocks=1,
            ),
        )
    ],
)
```

More information on configuring is available in the Configuration section.

• ExtremeScaleExecutor - a new executor targeting supercomputer scale (>1000 nodes) workflows is now available.

Here's a sample configuration for using this executor locally:

```
from parsl.providers import LocalProvider
from parsl.channels import LocalChannel
from parsl.launchers import SimpleLauncher
from parsl.config import Config
from parsl.executors import ExtremeScaleExecutor
config = Config(
    executors=[
        ExtremeScaleExecutor(
            label="extreme_local",
            ranks_per_node=4,
            provider=LocalProvider(
                channel=LocalChannel(),
                init_blocks=0,
                max_blocks=1,
                launcher=SimpleLauncher(),
            )
        )
    ],
    strategy=None,
)
```

More information on configuring is available in the Configuration section.

- The libsubmit repository has been merged with Parsl to reduce overheads on maintenance with respect to documentation, testing, and release synchronization. Since the merge, the API has undergone several updates to support the growing collection of executors, and as a result Parsl 0.7.0+ will not be backwards compatible with the standalone libsubmit repos. The major components of libsubmit are now available through Parsl, and require the following changes to import lines to migrate scripts to 0.7.0:
  - from libsubmit.providers import <ProviderName> is now from parsl.providers import <ProviderName>
  - from libsubmit.channels import <ChannelName> is now from parsl.channels import <ChannelName>
  - from libsubmit.launchers import <LauncherName> is now from parsl.launchers import <LauncherName>

Warning: This is a breaking change from Parsl v0.6.0

- To support resource-based requests for workers and to maintain uniformity across interfaces, tasks\_per\_node is no longer a **provider** option. Instead, the notion of tasks\_per\_node is defined via executor specific options, for eg:
  - IPyParallelExecutor provides workers\_per\_node
  - pars1.executors.HighThroughputExecutor provides cores\_per\_worker to allow for worker launches to be determined based on the number of cores on the compute node.
  - ExtremeScaleExecutor uses ranks\_per\_node to specify the ranks to launch per node.

**Warning:** This is a breaking change from Parsl v0.6.0

- Major upgrades to the monitoring infrastructure.
  - Monitoring information can now be written to a SQLite database, created on the fly by Parsl
  - Web-based monitoring to track workflow progress
- Determining the correct IP address/interface given network firewall rules is often a nuisance. To simplify this, three new methods are now supported:
  - parsl.addresses.address\_by\_route
  - parsl.addresses.address\_by\_query
  - parsl.addresses.address\_by\_hostname
- *pars1.launchers.AprunLauncher* now supports overrides option that allows arbitrary strings to be added to the aprun launcher call.
- DataFlowKernel has a new method wait\_for\_current\_tasks()
- *DataFlowKernel* now uses per-task locks and an improved mechanism to handle task completions improving performance for workflows with large number of tasks.

#### **Bug fixes (highlights)**

- Ctlr+C should cause fast DFK cleanup issue#641
- Fix to avoid padding in wtime\_to\_minutes() issue#522
- Updates to block semantics issue#557
- Updates public\_ip to address for clarity issue#557
- Improvements to launcher docs issue#424
- Fixes for inconsistencies between stream\_logger and file\_logger issue#629
- Fixes to DFK discarding some un-executed tasks at end of workflow issue#222
- Implement per-task locks to avoid deadlocks issue#591
- Fixes to internal consistency errors issue#604
- Removed unnecessary provider labels issue#440
- Fixes to pars1.providers.TorqueProvider to work on NSCC issue#489
- Several fixes and updates to monitoring subsystem issue#471
- DataManager calls wrong DFK issue#412
- Config isn't reloading properly in notebooks issue#549
- Cobalt provider partition should be queue issue#353
- bash AppFailure exceptions contain useful but un-displayed information issue#384
- Do not CD to engine\_dir issue#543
- Parsl install fails without kubernetes config file issue#527
- Fix import error issue#533
- Change Local Database Strategy from Many Writers to a Single Writer issue#472

- All run-related working files should go in the rundir unless otherwise configured issue#457
- Fix concurrency issue with many engines accessing the same IPP config issue#469
- Ensure we are not caching failed tasks issue#368
- File staging of unknown schemes fails silently issue#382
- Inform user checkpointed results are being used issue#494
- Fix IPP + python 3.5 failure issue#490
- File creation fails if no executor has been loaded issue#482
- Make sure tasks in dep\_fail state are retried issue#473
- Hard requirement for CMRESHandler issue#422
- Log error Globus events to stderr issue#436
- Take 'slots' out of logging issue#411
- Remove redundant logging issue#267
- Zombie ipcontroller processes Process cleanup in case of interruption issue#460
- IPyparallel failure when submitting several apps in parallel threads issue#451
- pars1.providers.SlurmProvider + pars1.launchers.SingleNodeLauncher starts all engines on a single core issue#454
- IPP engine\_dir has no effect if indicated dir does not exist issue#446
- Clarify AppBadFormatting error issue#433
- confusing error message with simple configs issue#379
- Error due to missing kubernetes config file issue#432
- parsl.configs and parsl.tests.configs missing init files issue#409
- Error when Python versions differ issue#62
- Fixing ManagerLost error in HTEX/EXEX issue#577
- Write all debug logs to rundir by default in HTEX/EXEX issue#574
- Write one log per HTEX worker issue#572
- Fixing ManagerLost error in HTEX/EXEX issue#577

#### Parsl 0.6.1

Released on July 23rd, 2018.

This point release contains fixes for issue#409

#### Parsl 0.6.0

Released July 23rd, 2018.

#### **New functionality**

• Switch to class based configuration issue#133

Here's a the config for using threads for local execution

```
from parsl.config import Config
from parsl.executors.threads import ThreadPoolExecutor
config = Config(executors=[ThreadPoolExecutor()])
```

Here's a more complex config that uses SSH to run on a Slurm based cluster

```
from libsubmit.channels import SSHChannel
from libsubmit.providers import SlurmProvider
from parsl.config import Config
from parsl.executors.ipp import IPyParallelExecutor
from parsl.executors.ipp_controller import Controller
config = Config(
    executors=[
        IPyParallelExecutor(
            provider=SlurmProvider(
                'westmere',
                channel=SSHChannel(
                    hostname='swift.rcc.uchicago.edu',
                    username=<USERNAME>,
                    script_dir=<SCRIPTDIR>
                ),
                init_blocks=1,
                min_blocks=1,
                max_blocks=2,
                nodes_per_block=1,
                tasks_per_node=4,
                parallelism=0.5,
                overrides=<SPECIFY_INSTRUCTIONS_TO_LOAD_PYTHON3>
            ),
            label='midway_ipp',
            controller=Controller(public_ip=<PUBLIC_IP>),
        )
    ]
)
```

• Implicit Data Staging issue#281

```
# create an remote Parsl file
inp = File('ftp://www.iana.org/pub/mirror/rirstats/arin/ARIN-STATS-FORMAT-CHANGE.txt
___')
```

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```
# create a local Parsl file
out = File('file:///tmp/ARIN-STATS-FORMAT-CHANGE.txt')
# call the convert app with the Parsl file
f = convert(inputs=[inp], outputs=[out])
f.result()
```

- Support for application profiling issue#5
- Real-time usage tracking via external systems issue#248, issue#251
- Several fixes and upgrades to tests and testing infrastructure issue#157, issue#159, issue#128, issue#192, issue#196
- Better state reporting in logs issue#242
- Hide DFK issue#50
  - Instead of passing a config dictionary to the DataFlowKernel, now you can call parsl.load(Config)
  - Instead of having to specify the dfk at the time of App declaration, the DFK is a singleton loaded at call time :

```
import parsl
from parsl.tests.configs.local_ipp import config
parsl.load(config)

@App('python')
def double(x):
    return x * 2

fut = double(5)
fut.result()
```

• Support for better reporting of remote side exceptions issue#110

#### **Bug Fixes**

- Making naming conventions consistent issue#109
- Globus staging returns unclear error bug issue#178
- Duplicate log-lines when using IPP issue#204
- Usage tracking with certain missing network causes 20s startup delay. issue#220
- task\_exit checkpointing repeatedly truncates checkpoint file during run bug issue#230
- Checkpoints will not reload from a run that was Ctrl-C'ed issue#232
- Race condition in task checkpointing issue#234
- Failures not to be checkpointed issue#239
- Naming inconsitencies with maxThreads, max\_threads, max\_workers are now resolved issue#303
- Fatal not a git repository alerts issue#326
- Default kwargs in bash apps unavailable at command-line string format time issue#349

- Fix launcher class inconsistencies issue#360
- Several fixes to AWS provider issue#362
  - Fixes faulty status updates
  - Faulty termination of instance at cleanup, leaving zombie nodes.

#### Parsl 0.5.1

Released. May 15th, 2018.

#### **New functionality**

- Better code state description in logging issue#242
- String like behavior for Files issue#174
- Globus path mapping in config issue#165

### **Bug Fixes**

- Usage tracking with certain missing network causes 20s startup delay. issue#220
- Checkpoints will not reload from a run that was Ctrl-C'ed issue#232
- Race condition in task checkpointing issue#234
- task\_exit checkpointing repeatedly truncates checkpoint file during run issue#230
- Make dfk.cleanup() not cause kernel to restart with Jupyter on Mac issue#212
- Fix automatic IPP controller creation on OS X issue#206
- Passing Files breaks over IPP issue#200
- repr call after AppException instantiation raises AttributeError issue#197
- Allow DataFuture to be initialized with a str file object issue#185
- Error for globus transfer failure issue#162

#### Parsl 0.5.2

Released. June 21st, 2018. This is an emergency release addressing issue#347

#### **Bug Fixes**

• Parsl version conflict with libsubmit 0.4.1 issue#347

### Parsl 0.5.0

Released. Apr 16th, 2018.

#### **New functionality**

• Support for Globus file transfers issue#71

**Caution:** This feature is available from Parsl v0.5.0 in an experimental state.

#### • PathLike behavior for Files issue#174

- Files behave like strings here :

```
myfile = File("hello.txt")
f = open(myfile, 'r')
```

• Automatic checkpointing modes issue#106

```
config = {
    "globals": {
        "lazyErrors": True,
        "memoize": True,
        "checkpointMode": "dfk_exit"
    }
}
```

• Support for containers with docker issue#45

```
localDockerIPP = {
     "sites": [
         {"site": "Local_IPP",
          "auth": {"channel": None},
          "execution": {
              "executor": "ipp",
              "container": {
                  "type": "docker",
                                       # <---- Specify Docker
                  "image": "app1_v0.1", # <-----Specify docker image</pre>
              },
              "provider": "local",
              "block": {
                  "initBlocks": 2, # Start with 4 workers
              },
          }
          }],
     "globals": {"lazyErrors": True}
                                             }
```

**Caution:** This feature is available from Parsl v0.5.0 in an experimental state.

• Cleaner logging issue#85

- Logs are now written by default to runinfo/RUN\_ID/parsl.log.
- INFO log lines are more readable and compact
- Local configs are now packaged issue#96

```
from parsl.configs.local import localThreads
from parsl.configs.local import localIPP
```

#### **Bug Fixes**

- Passing Files over IPP broken issue#200
- Fix DataFuture.\_\_repr\_\_ for default instantiation issue#164
- Results added to appCache before retries exhausted issue#130
- Missing documentation added for Multisite and Error handling issue#116
- TypeError raised when a bad stdout/stderr path is provided. issue#104
- Race condition in DFK issue#102
- Cobalt provider broken on Cooley.alfc issue#101
- No blocks provisioned if parallelism/blocks = 0 issue#97
- Checkpoint restart assumes rundir issue#95
- Logger continues after cleanup is called issue#93

#### Parsl 0.4.1

Released. Feb 23rd, 2018.

#### **New functionality**

- GoogleCloud provider support via libsubmit
- · GridEngine provider support via libsubmit

#### **Bug Fixes**

- Cobalt provider issues with job state issue#101
- · Parsl updates config inadvertently issue#98
- No blocks provisioned if parallelism/blocks = 0 issue#97
- Checkpoint restart assumes rundir bug issue#95
- Logger continues after cleanup called enhancement issue#93
- Error checkpointing when no cache enabled issue#92
- Several fixes to libsubmit.

#### Parsl 0.4.0

Here are the major changes included in the Parsl 0.4.0 release.

#### **New functionality**

• Elastic scaling in response to workflow pressure. issue#46 Options minBlocks, maxBlocks, and parallelism now work and controls workflow execution.

Documented in: Elasticity

• Multisite support, enables targetting apps within a single workflow to different sites issue#48

```
@App('python', dfk, sites=['SITE1', 'SITE2'])
def my_app(...):
    ...
```

• Anonymized usage tracking added. issue#34

Documented in: Usage statistics collection

• AppCaching and Checkpointing issue#43

Documented in: Checkpointing, App caching

- · Parsl now creates a new directory under ./runinfo/ with an incrementing number per workflow invocation
- Troubleshooting guide and more documentation
- PEP8 conformance tests added to travis testing issue#72

#### **Bug Fixes**

- Missing documentation from libsubmit was added back issue#41
- Fixes for script\_dir | scriptDir inconsistencies issue#64
  - We now use scriptDir exclusively.
- Fix for caching not working on jupyter notebooks issue#90
- Config defaults module failure when part of the option set is provided issue#74
- Fixes for network errors with usage\_tracking issue#70
- PEP8 conformance of code and tests with limited exclusions issue#72
- Doc bug in recommending max\_workers instead of maxThreads issue#73

#### Parsl 0.3.1

This is a point release with mostly minor features and several bug fixes

- · Fixes for remote side handling
- Support for specifying IPythonDir for IPP controllers
- · Several tests added that test provider launcher functionality from libsubmit
- This upgrade will also push the libsubmit requirement from  $0.2.4 \rightarrow 0.2.5$ .

Several critical fixes from libsubmit are brought in:

- Several fixes and improvements to Condor from @annawoodard.
- Support for Torque scheduler
- Provider script output paths are fixed
- Increased walltimes to deal with slow scheduler system
- Srun launcher for slurm systems
- SSH channels now support file\_pull() method While files are not automatically staged, the channels provide support for bi-directional file transport.

#### Parsl 0.3.0

Here are the major changes that are included in the Parsl 0.3.0 release.

#### **New functionality**

• Arguments to DFK has changed:

# Old dfk(executor\_obj)

# New, pass a list of executors dfk(executors=[list\_of\_executors])

# Alternatively, pass the config from which the DFK will #instantiate resources dfk(config=config\_dict)

- · Execution providers have been restructured to a separate repo: libsubmit
- Bash app styles have changes to return the commandline string rather than be assigned to the special keyword cmd\_line. Please refer to RFC #37 for more details. This is a **non-backward** compatible change.
- Output files from apps are now made available as an attribute of the AppFuture. Please refer #26 for more details. This is a **non-backward** compatible change

```
# This is the pre 0.3.0 style
app_fu, [file1, file2] = make_files(x, y, outputs=['f1.txt', 'f2.txt'])
#This is the style that will be followed going forward.
app_fu = make_files(x, y, outputs=['f1.txt', 'f2.txt'])
[file1, file2] = app_fu.outputs
```

- DFK init now supports auto-start of IPP controllers
- Support for channels via libsubmit. Channels enable execution of commands from execution providers either locally, or remotely via ssh.

- Bash apps now support timeouts.
- Support for cobalt execution provider.

#### **Bug fixes**

- Futures have inconsistent behavior in bash app fn body #35
- Parsl dflow structure missing dependency information #30

#### Parsl 0.2.0

Here are the major changes that are included in the Parsl 0.2.0 release.

#### **New functionality**

- Support for execution via IPythonParallel executor enabling distributed execution.
- · Generic executors

#### Parsl 0.1.0

Here are the major changes that are included in the Parsl 0.1.0 release.

#### **New functionality**

- Support for Bash and Python apps
- Support for chaining of apps via futures handled by the DataFlowKernel.
- Support for execution over threads.
- Arbitrary DAGs can be constructed and executed asynchronously.

#### **Bug Fixes**

• Initial release, no listed bugs.

### Historical: Libsubmit Changelog

**Note:** As of Parsl 0.7.0 the libsubmit repository has been merged into Parsl and nothing more will appear in this changelog.

#### Libsubmit 0.4.1

Released. June 18th, 2018. This release folds in massive contributions from @annawoodard.

#### **New functionality**

- · Several code cleanups, doc improvements, and consistent naming
- All providers have the initialization and actual start of resources decoupled.

#### Libsubmit 0.4.0

Released. May 15th, 2018. This release folds in contributions from @ahayschi, @annawoodard, @yadudoc

#### **New functionality**

- Several enhancements and fixes to the AWS cloud provider (#44, #45, #50)
- Added support for python3.4

#### **Bug Fixes**

- Condor jobs left in queue with X state at end of completion issue#26
- Worker launches on Cori seem to fail from broken ENV issue#27
- EC2 provider throwing an exception at initial run issue#46

#### Historical: Swift vs Parsl

**Note:** This section describes comparisons between Parsl and an earlier workflow system, Swift, as part of a justification for the early prototyping stages of Parsl development. It is no longer relevant for modern Parsl users, but remains of historical interest.

The following text is not well structured, and is mostly a brain dump that needs to be organized. Moving from Swift to an established language (python) came with its own tradeoffs. We get the backing of a rich and very well known language to handle the language aspects as well as the libraries. However, we lose the parallel evaluation of every statement in a script. The thesis is that what we lose is minimal and will not affect 95% of our workflows. This is not yet substantiated.

Please note that there are two Swift languages: Swift/K and Swift/T. These have diverged in syntax and behavior. Swift/K is designed for grids and clusters runs the java based Karajan (hence, /K) execution framework. Swift/T is a completely new implementation of Swift/K for high-performance computing. Swift/T uses Turbine(hence, /T) and and ADLB runtime libraries for highly scalable dataflow processing over MPI, without single-node bottlenecks.

#### **Parallel Evaluation**

In Swift (K&T), every statement is evaluated in parallel.

```
y = f(x);
z = g(x);
```

We see that y and z are assigned values in different order when we run Swift multiple times. Swift evaluates both statements in parallel and the order in which they complete is mostly random.

We will not have this behavior in Python. Each statement is evaluated in order.

```
int[] array;
foreach v,i in [1:5] {
    array[i] = 2*v;
}
foreach v in array {
    trace(v)
}
```

Another consequence is that in Swift, a foreach loop that consumes results in an array need not wait for the foreach loop that fill the array. In the above example, the second foreach loop makes progress along with the first foreach loop as it fills the array.

In parsl, a for loop that **launches** tasks has to complete launches before the control may proceed to the next statement. The first for loop has to simply finish iterating, and launching jobs, which should take ~length\_of\_iterable/1000 (items/task\_launch\_rate).

```
futures = {};
for i in range(0,10):
    futures[i] = app_double(i);
for i in fut_array:
    print(i, futures[i])
```

The first for loop first fills the futures dict before control can proceed to the second for loop that consumes the contents.

The main conclusion here is that, if the iteration space is sufficiently large (or the app launches are throttled), then it is possible that tasks that are further down the control flow have to wait regardless of their dependencies being resolved.

#### Mappers

In Swift/K, a mapper is a mechanism to map files to variables. Swift need's to know files on disk so that it could move them to remote sites for execution or as inputs to applications. Mapped file variables also indicate to swift that, when files are created on remote sites, they need to be staged back. Swift/K provides several mappers which makes it convenient to map files on disk to file variables.

There are two choices here :

- 1. Have the user define the mappers and data objects
- 2. Have the data objects be created only by Apps.

In Swift, the user defines file mappings like this :

```
# Mapping a single file
file f <"f.txt">;
# Array of files
file texts[] <filesys_mapper; prefix="foo", suffix=".txt">;
```

The files mapped to an array could be either inputs or outputs to be created. Which is the case is inferred from whether they are on the left-hand side or right-hand side of an assignment. Variables on the left-hand side are inferred to be outputs that have future-like behavior. To avoid conflicting values being assigned to the same variable, Swift variables are all immutable.

For instance, the following would be a major concern *if* variables were not immutable:

x = 0; x = 1; trace(x);

The results that trace would print would be non-deterministic, if x were mutable. In Swift, the above code would raise an error. However this is perfectly legal in python, and the x would take the last value it was assigned.

#### **Remote-Execution**

In Swift/K, remote execution is handled by coasters. This is a pilot mechanism that supports dynamic resource provisioning from cluster managers such as PBS, Slurm, Condor and handles data transport from the client to the workers. Swift/T on the other hand is designed to run as an MPI job on a single HPC resource. Swift/T utilized shared-filesystems that almost every HPC resource has.

To be useful, Parsl will need to support remote execution and file transfers. Here we will discuss just the remoteexecution aspect.

Here is a set of features that should be implemented or borrowed :

- [Done] New remote execution system must have the executor interface.
- [Done] Executors must be memory efficient wrt to holding jobs in memory.
- [Done] Continue to support both BashApps and PythonApps.
- [Done] Capable of using templates to submit jobs to Cluster resource managers.
- [Done] Dynamically launch and shutdown workers.

**Note:** Since the current roadmap to remote execution is through ipython-parallel, we will limit support to Python3.5+ to avoid library naming issues.

### Design

Under construction.

### Historical: Performance and Scalability

**Note:** This scalability review summarises results in a paper, Parsl: Pervasive Parallel Programming in Python, which was published in 2019. The results have not been updated since then. For that reason, this section is marked as historical.

Parsl is designed to scale from small to large systems .

#### Scalability

We studied strong and weak scaling on the Blue Waters supercomputer. In strong scaling, the total problem size is fixed; in weak scaling, the problem size per CPU core is fixed. In both cases, we measure completion time as a function of number of CPU cores. An ideal framework should scale linearly, which for strong scaling means that speedup scales with the number of cores, and for weak scaling means that completion time remains constant as the number of cores increases.

To measure the strong and weak scaling of Parsl executors, we created Parsl programs to run tasks with different durations, ranging from a "no-op"–a Python function that exits immediately—to tasks that sleep for 10, 100, and 1,000 ms. For each executor we deployed a worker per core on each node.

While we compare here with IPP, Fireworks, and Dask Distributed, we note that these systems are not necessarily designed for Parsl-like workloads or scale.

Further results are presented in our HPDC paper.

### Strong scaling

The figures below show the strong scaling results for 5,000 1-second sleep tasks. HTEX provides good performance in all cases, slightly exceeding what is possible with EXEX, while EXEX scales to significantly more workers than the other executors and frameworks. Both HTEX and EXEX remain nearly constant, indicating that they likely will continue to perform well at larger scales.



#### Weak scaling

Here, we launched 10 tasks per worker, while increasing the number of workers. (We limited experiments to 10 tasks per worker, as on 3,125 nodes, that represents 3,125 nodes × 32 workers/node × 10 tasks/worker, or 1M tasks.) The figure below shows our results. We observe that HTEX and EXEX outperform other executors and frameworks with more than 4,096 workers (128 nodes). All frameworks exhibit similar trends, with completion time remaining close to constant initially and increasing rapidly as the number of workers increases.



### Throughput

We measured the maximum throughput of all the Parsl executors, on the UChicago Research Computing Center's Midway Cluster. To do so, we ran 50,000 "no-op" tasks on a varying number of workers and recorded the completion times. The throughout is computed as the number of tasks divided by the completion time. HTEX, and EXEX achieved maximum throughputs of 1,181 and 1,176 tasks/s, respectively.

### Summary

The table below summarizes the scale at which we have tested Parsl executors. The maximum number of nodes and workers for HTEX and EXEX is limited by the size of allocation available during testing on Blue Waters. The throughput results are collected on Midway.

Executor	Max # workers	Max # nodes	Max tasks/second
IPP	2,048	64	330
HTEX	65,536	2,048	1,181
EXEX	262,144	8,192	1,176

# CHAPTER

TWO

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