QCEngine Documentation

Release v0.12.0+0.g2d1cc42.dirty

The QCArchive Development Team

Nov 20, 2019
## CONTENTS:

1 Program Execution ................................................. 3
2 Backends ............................................................... 5
3 Configuration Determination ...................................... 7
4 Program and Procedure Information ............................. 9
5 Index ................................................................. 11
   5.1 Install QCEngine ................................................. 11
   5.2 Single Compute .................................................. 12
   5.3 Environment Detection ......................................... 14
   5.4 Command Line Interface ....................................... 15
   5.5 Program Overview ............................................... 17
   5.6 QCEngine API ..................................................... 18
   5.7 Changelog ......................................................... 28

Python Module Index ................................................. 35

Index ........................................................................ 37
Quantum chemistry program executor and IO standardizer (QCSchema) for quantum chemistry.
A simple example of QC Engine’s capabilities is as follows:

```python
>>> import qcengine as qcng
>>> import qcelemental as qcel

>>> mol = qcel.models.Molecule.from_data('"
O  0.0   0.000  -0.129
H  0.0  -1.494   1.027
H  0.0   1.494   1.027
""

>>> input = qcel.models.AtomicInput(
     molecule=mol,
     driver="energy",
     model={"method": "SCF", "basis": "sto-3g"},
     keywords={"scf_type": "df"}
)

These input specifications can be executed with the compute syntax along with a program specifier:

```python
>>> ret = qcng.compute(input, "psi4")
```

The results contain a complete record of the computation:

```python
>>> ret.return_result
-74.45994963230625

>>> ret.properties.scf_dipole_moment
[0.0, 0.0, 0.6635967188869244]

>>> ret.provenance.cpu
Intel(R) Core(TM) i7-7820HQ CPU @ 2.90GHz
Currently available compute backends for single results are as follow:

- **Quantum Chemistry:**
  - Entos
  - Molpro
  - Psi4
  - Terachem
- **Semi-Emperical:**
  - MOPAC
- **AI Potential:**
  - TorchANI
- **Molecular Mechanics:**
  - RDKit
- **Analytical Corrections:**
  - DFTD3

In addition, several procedures are available:

- **Geometry Optimization:**
  - geomeTRIC
In addition, QCengine can automatically determine the following quantities:

- The number of physical cores on the system and to use.
- The amount of physical memory on the system and the amount to use.
- The provenance of a computation (hardware, software versions, and compute resources).
- Location of scratch disk space.
- Location of quantum chemistry programs binaries or Python modules.

Each of these options can be specified by the user as well.

```python
>>> qcng.get_config()
<JobConfig ncores=2 memory=2.506 scratch_directory=None>

>>> qcng.get_config(local_options={"scratch_directory": "/tmp"})
<JobConfig ncores=2 memory=2.506 scratch_directory='/tmp'>

>>> os.environ["SCRATCH"] = "/my_scratch"
>>> qcng.get_config(local_options={"scratch_directory": "$SCRATCH"})
<JobConfig ncores=2 memory=2.506 scratch_directory='/my_scratch'>
```
Available programs and procedures may be printed using the *CLI*:

```bash
>>> qcengine info
>> Version information
QCEngine version: v0.11.0
QCEElemental version: v0.11.0

>> Program information
Available programs:
mopac v2016
psi4 v1.3.2
rdkit v2019.03.4

Other supported programs:
cfour dftd3 entos gamess molpro mp2d nwchem terachem torchani
```
Getting Started

- Install QCEngine

5.1 Install QCEngine

You can install qcengine with conda or with pip.

5.1.1 Conda

You can install qcengine using conda:

```bash
>>> conda install qcengine -c conda-forge
```

This installs QCEngine and its dependencies. The qcengine package is maintained on the conda-forge channel.

5.1.2 Pip

You can also install QCEngine using pip:

```bash
>>> pip install qcengine
```

5.1.3 Test the Installation

**Note:** QCEngine is a wrapper for other quantum chemistry codes. The tests for QCEngine will only test the wrapper for a given code if its detected in the $PATH or current Python Environment, otherwise the tests for that package are skipped. Keep this in mind if you see many `skip` or `s` codes output from PyTest.

You can test to make sure that Engine is installed correctly by first installing pytest.

From conda:

```bash
>>> conda install pytest -c conda-forge
```

From pip:
>>> pip install pytest

Then, run the following command:

>>> pytest --pyargs qcengine

5.1.4 Developing from Source

If you are a developer and want to make contributions to Engine, you can access the source code from GitHub.

User Interface

- Single Compute
- Environment Detection
- Command Line Interface

5.2 Single Compute

QCEngine’s primary purpose is to consume the MolSSI QCSchema and produce QCSchema results for a variety of quantum chemistry, semiempirical, and molecular mechanics programs. Single QCSchema representation comprises a single energy, gradient, hessian, or properties evaluation.

5.2.1 Input Description

An input description has the following fields:

- **molecule** - A QCSchema compliant dictionary or Molecule model.
- **driver** - The energy, gradient, hessian, or properties option.
- **model** - A description of the evaluation model. For quantum chemistry this is typically method and basis. However, non-quantum chemistry models are often a simple method as in method = 'UFF' for forcefield evaluation.
- **keywords** - a dictionary of keywords to pass to the underlying program. These are program-specific keywords.

An example input is as follows:

```python
>>> import qcengine as qcng
>>> import qcelemental as qcel

>>> mol = qcel.models.Molecule.from_data(''
>>> O 0.0 0.000 -0.129
>>> H 0.0 -1.494 1.027
>>> H 0.0 1.494 1.027
>>> '')

>>> inp = qcel.models.AtomicInput(
>>> molecule=mol,
>>> driver="energy",
>>> model=("method": "SCF", "basis": "sto-3g"),
>>> keywords=("scf_type": "df")
>>> )
```
5.2.2 Computation

A single computation can be evaluated with the `compute` function as follows:

```python
>>> ret = qcng.compute(inp, "psi4")
```

By default the job is given resources relating to the compute environment it is in; however, these variables can be overridden:

```python
>>> ret = qcng.compute(inp, "psi4", local_options={"memory": 2, "ncores": 3})
```

5.2.3 Results

The results contain a complete record of the computation:

```python
>>> ret.return_result
-74.45994963230625

>>> ret.properties.scf_dipole_moment
[0.0, 0.0, 0.6635967188869244]

>>> ret.provenance.cpu
Intel(R) Core(TM) i7-7820HQ CPU @ 2.90GHz
```

5.2.4 Input Fields

class qcelemental.models.AtomicInput

The MolSSI Quantum Chemistry Schema

Parameters

- `id` (str, Optional) – An optional ID of the ResultInput object.
- `schema_name` (ConstrainedStrValue, Default: qcschema_input)
- `schema_version` (int, Default: 1)
- `molecule` (Molecule) – The molecule to use in the computation.
- `driver` ({energy, gradient, hessian, properties}) – Allowed quantum chemistry driver values.
- `model` (Model) – The quantum chemistry model specification for a given operation to compute against.
- `keywords` (Dict[str, Any], Default: {}) – The program specific keywords to be used.
- `protocols` (AtomicResultProtocols, Optional) – Protocols regarding the manipulation of a Result output data.
- `extras` (Dict[str, Any], Default: {}) – Extra fields that are not part of the schema.
- `provenance` (Provenance, Optional) – Provenance information.

5.2.5 Returned Fields

class qcelemental.models.AtomicResult

Parameters
- **id** (*str, Optional*) – An optional ID of the ResultInput object.
- **schema_name** (*ConstrainedStrValue, Default: qcschema_output*)
- **schema_version** (*int, Default: 1*)
- **molecule** (*Molecule*) – The molecule to use in the computation.
- **driver** (**energy, gradient, hessian, properties**) – Allowed quantum chemistry driver values.
- **model** (*Model*) – The quantum chemistry model specification for a given operation to compute against
- **keywords** (*Dict[str, Any], Default: {}*) – The program specific keywords to be used.
- **protocols** (*AtomicResultProtocols, Optional*) – Protocols regarding the manipulation of a Result output data.
- **extras** (*Dict[str, Any], Default: {}*) – Extra fields that are not part of the schema.
- **provenance** (*Provenance*) – Provenance information.
- **properties** (*AtomicResultProperties*) – Named properties of quantum chemistry computations following the MolSSI QCSchema.
- **wavefunction** (*WavefunctionProperties, Optional*) – None
- **return_result** (*Union[float, Array, Dict[str, Any]]*) – The value requested by the ‘driver’ attribute.
- **stdout** (*str, Optional*) – The standard output of the program.
- **stderr** (*str, Optional*) – The standard error of the program.
- **success** (*bool*) – The success of a given programs execution. If False, other fields may be blank.
- **error** (*ComputeError, Optional*) – A complete description of the error.

## 5.3 Environment Detection

QCEngine can inspect the current compute environment to determine the resources available to it.

### 5.3.1 Node Description

QCEngine can detect node descriptions to obtain general information about the current node.

```python
>>> qcng.config.get_node_descriptor()
<NodeDescriptor hostname_pattern='*' name='default' scratch_directory=None
  memory=5.568 memory_safety_factor=10 ncores=4 jobs_per_node=2>
```

### 5.3.2 Config

The configuration file operated based on the current node descriptor and can be overridden:
>>> qcng.get_config()
<JobConfig ncores=2 memory=2.506 scratch_directory=None>

>>> qcng.get_config(local_options={"scratch_directory": "/tmp"})
<JobConfig ncores=2 memory=2.506 scratch_directory="/tmp"/>

>>> os.environ["SCRATCH"] = "/my_scratch"
>>> qcng.get_config(local_options={"scratch_directory": "$SCRATCH"})
<JobConfig ncores=2 memory=2.506 scratch_directory="/my_scratch"/>

5.3.3 Global Environment

The global environment can also be inspected directly.

>>> qcng.config.get_global()
{
    'hostname': 'qcarchive.molssi.org',
    'memory': 5.568,
    'username': 'user',
    'ncores': 4,
    'cpuinfo': {
        'python_version': '3.6.7.final.0 (64 bit)',
        'brand': 'Intel(R) Core(TM) i7-7820HQ CPU @ 2.90GHz',
        'hz_advertised': '2.9000 GHz',
        ...
    },
    'cpu_brand': 'Intel(R) Core(TM) i7-7820HQ CPU @ 2.90GHz'
}

5.4 Command Line Interface

QCEngine provides a command line interface with three commands:

- **qcengine info** displays information about the environment detected by QCEngine.
- **qcengine run** runs a program.
- **qcengine run-procedure** runs a procedure.

5.4.1 Info Command

**Command Invocation**

qcengine info <options>

**Command Description**

This command prints information about the QCEngine environment.
Arguments

category  The information categories to show. Choices include:

- version: Print version of QC Engine and QC Elemental.
- programs: Print detected and supported programs.
- procedures: Print detected and supported procedures.
- config: Print host, compute, and job configuration.
- all: Print all available information.

By default, all available information is printed.

5.4.2 Run Command

Command Invocation

```
qcengine run <program> <data>
```

Command Description

This command runs a program on a given task and outputs the result as a JSON blob.

Arguments

program  The program to run.

data  Data describing the task. One of:

- A JSON blob.
- A file name.
- `-` indicating data will be read from STDIN.

5.4.3 Run-Procedure Command

Command Invocation

```
qcengine run-procedure <program> <data>
```

Command Description

This command runs a procedure on a given task and outputs the result as a JSON blob.
Arguments

**procedure** The procedure to run.

**data** Data describing the task. One of:
  - A JSON blob.
  - A file name.
  - `-', indicating data will be read from STDIN.

Programs

- *Program Overview*

## 5.5 Program Overview

The general capabilities available through QCEngine for each program can be found below:

### 5.5.1 Quantum Chemistry

<table>
<thead>
<tr>
<th>Program</th>
<th>Production</th>
<th>E</th>
<th>G</th>
<th>H</th>
<th>Properties</th>
<th>Wavefunction</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFOUR</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Entos</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GAMESS</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Molpro</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NWChem</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Psi4</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>Q-Chem</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Terachem</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Turbomole</td>
<td>✓</td>
<td>✓</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 5.5.2 Semi-Emperical

<table>
<thead>
<tr>
<th>Program</th>
<th>Production</th>
<th>E</th>
<th>G</th>
<th>H</th>
<th>Properties</th>
<th>Wavefunction</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOPAC</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td></td>
</tr>
</tbody>
</table>

### 5.5.3 AI Potential

<table>
<thead>
<tr>
<th>Program</th>
<th>Production</th>
<th>E</th>
<th>G</th>
<th>H</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>TorchANI</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>
5.5.4 Molecular Mechanics

<table>
<thead>
<tr>
<th>Program</th>
<th>Production</th>
<th>E</th>
<th>G</th>
<th>H</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>RDKit</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

5.5.5 Analytical Corrections

<table>
<thead>
<tr>
<th>Program</th>
<th>Production</th>
<th>E</th>
<th>G</th>
<th>H</th>
<th>Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>DFTD3</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>

Developer Documentation

- QC Engine API
- Changelog

5.6 QC Engine API

5.6.1 qcengine Package

Base file for the dqm_compute module.

Functions

```python
compute(input_data: Union[Dict[str, Any], AtomicInput], program: str, raise_error: bool = False, local_options: Optional[Dict[str, Any]] = None, return_dict: bool = False) → AtomicResult
```

Executes a single quantum chemistry program given a QC Schema input.
The full specification can be found at: http://molssi-qc-schema.readthedocs.io/en/latest/index.html#

**Parameters**

- **input_data** *(Union[Dict[str, Any], ‘AtomicInput’])* – A QCSchema input specification in dictionary or model from QCElemental.models
- **program** *(str)* – The program to execute the input with.
- **raise_error** *(bool, optional)* – Determines if compute should raise an error or not.
- **retries** *(int, optional)* – The number of random tries to retry for.
- **local_options** *(Optional[Dict[str, Any]], optional)* – A dictionary of local configuration options
- **return_dict** *(bool, optional)* – Returns a dict instead of qcelemental.models.AtomicInput

**Returns** A computed AtomicResult object.

**Return type** result

```
compute_procedure
```

```
qcengine.compute_procedure(input_data: Union[Dict[str, Any], BaseModel], procedure: str, raise_error: bool = False, local_options: Optional[Dict[str, str]] = None, return_dict: bool = False) → BaseModel
```

Runs a procedure (a collection of the quantum chemistry executions)

**Parameters**

- **input_data** *(dict or qcelemental.models.OptimizationInput)* – A JSON input specific to the procedure executed in dictionary or model from QCElemental.models
- **procedure** *(f“geometric”)* – The name of the procedure to run
- **raise_error** *(bool, option)* – Determines if compute should raise an error or not.
- **local_options** *(dict, optional)* – A dictionary of local configuration options
- **return_dict** *(bool, optional, default True)* – Returns a dict instead of qcelemental.models.AtomicInput

**Returns** A QC Schema representation of the requested output, type depends on return_dict key.

**Return type** dict, OptimizationResult, FailedOperation

```
get_config
```

```
qcengine.get_config(*, hostname: Optional[str] = None, local_options: Dict[str, Any] = None) →
qcengine.config.JobConfig
```

Returns the configuration key for qcengine.

```
get_molecule
```

```
qcengine.get_molecule(name)
```

Returns a QC JSON representation of a test molecule.
get_procedure

qcengine.get_procedure(name: str) → ProcedureHarness
Returns a procedures executor class

get_program

qcengine.get_program(name: str, check: bool = True) → ProgramHarness
Returns a program’s executor class

Parameters check – True Do raise error if program not found. False is handy for the specialized
case of calling non-execution methods (like parsing for testing) on the returned Harness.

list_all_procedures

qcengine.list_all_procedures() → Set[str]
List all procedures registered by QC Engine.

list_all_programs

qcengine.list_all_programs() → Set[str]
List all programs registered by QC Engine.

list_available_procedures

qcengine.list_available_procedures() → Set[str]
List all procedures that can be executed (found) by QC Engine.

list_available_programs

qcengine.list_available_programs() → Set[str]
List all programs that can be executed (found) by QC Engine.

register_program

qcengine.register_program(entry_point: ProgramHarness) → None
Register a new ProgramHarness with QC Engine.

unregister_program

qcengine.unregister_program(name: str) → None
Unregisters a given program.

Classes
**MDIServer**

```python
MDIServer(mdi_options, program, molecule,...)
```

**class** `qcengine.MDIServer` *(mdi_options: str, program: str, molecule, model, keywords, raise_error: bool = False, local_options: Optional[Dict[str, Any]] = None)*

*Bases:* `object`

**Methods Summary**

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>recv_coords(coords)</code></td>
<td>Receive a set of nuclear coordinates through MDI and assign them to the atoms in the current molecule</td>
</tr>
<tr>
<td><code>recv_elements(elements)</code></td>
<td>Receive a set of atomic numbers through MDI and assign them to the atoms in the current molecule</td>
</tr>
<tr>
<td><code>recv_masses(masses)</code></td>
<td>Receive a set of nuclear masses through MDI and assign them to the atoms in the current molecule</td>
</tr>
<tr>
<td><code>recv_multiplicity(multiplicity)</code></td>
<td>Receive the electronic multiplicity through MDI</td>
</tr>
<tr>
<td><code>recv_total_charge(charge)</code></td>
<td>Receive the total system charge through MDI</td>
</tr>
<tr>
<td><code>run_energy()</code></td>
<td>Run an energy calculation</td>
</tr>
<tr>
<td><code>send_commands()</code></td>
<td>Send the supported MDI commands through MDI</td>
</tr>
<tr>
<td><code>send_coords()</code></td>
<td>Send the nuclear coordinates through MDI</td>
</tr>
<tr>
<td><code>send_elements()</code></td>
<td>Send the atomic number of each nucleus through MDI</td>
</tr>
<tr>
<td><code>send_energy()</code></td>
<td>Send the total energy through MDI</td>
</tr>
<tr>
<td><code>send_forces()</code></td>
<td>Send the nuclear forces through MDI</td>
</tr>
<tr>
<td><code>send_masses()</code></td>
<td>Send the nuclear masses through MDI</td>
</tr>
<tr>
<td><code>send_multiplicity()</code></td>
<td>Send the electronic multiplicity through MDI</td>
</tr>
<tr>
<td><code>send_natoms()</code></td>
<td>Send the number of atoms through MDI</td>
</tr>
<tr>
<td><code>send_ncommands()</code></td>
<td>Send the number of supported MDI commands through MDI</td>
</tr>
<tr>
<td><code>send_total_charge()</code></td>
<td>Send the total system charge through MDI</td>
</tr>
<tr>
<td><code>start()</code></td>
<td>Receive commands through MDI and respond to them as defined by the MDI Standard</td>
</tr>
<tr>
<td><code>stop()</code></td>
<td>Stop listening for MDI commands</td>
</tr>
<tr>
<td><code>update_molecule(key, value)</code></td>
<td>Update the molecule</td>
</tr>
</tbody>
</table>

**Methods Documentation**

- **recv_coords**(coords: Optional[np.ndarray] = None) → None
  
  Receive a set of nuclear coordinates through MDI and assign them to the atoms in the current molecule

  **Parameters**
  - coords (np.ndarray, optional) – New nuclear coordinates. If None, receive through MDI.

- **recv_elements**(elements: Optional[List[int]] = None)
  
  Receive a set of atomic numbers through MDI and assign them to the atoms in the current molecule

  **Parameters**
  - elements (list of int, optional) – New element numbers. If None, receive through MDI.

- **recv_masses**(masses: Optional[List[float]] = None) → None
  
  Receive a set of nuclear masses through MDI and assign them to the atoms in the current molecule
Parameters masses (list of float, optional) – New nuclear masses. If None, receive through MDI.

recv_multiplicity (multiplicity: Optional[int] = None) → None
Receive the electronic multiplicity through MDI
Parameters multiplicity (int, optional) – New multiplicity of the system. If None, receive through MDI.

recv_total_charge (charge: Optional[float] = None) → None
Receive the total system charge through MDI
Parameters charge (float, optional) – New charge of the system. If None, receive through MDI.

run_energy () → None
Run an energy calculation

send_commands () → str
Send the supported MDI commands through MDI
Returns command_string – String containing the name of each supported command
Return type str

send_coords () → numpy.ndarray
Send the nuclear coordinates through MDI
Returns coords – Nuclear coordinates
Return type np.ndarray

send_elements ()
Send the atomic number of each nucleus through MDI
Returns elements – Element of each atom
Return type list of int

send_energy () → float
Send the total energy through MDI
Returns energy – Energy of the system
Return type float

send_forces () → numpy.ndarray
Send the nuclear forces through MDI
Returns forces – Forces on the nuclei
Return type np.ndarray

send_masses () → numpy.ndarray
Send the nuclear masses through MDI
Returns masses – Atomic masses
Return type np.ndarray

send_multiplicity () → int
Send the electronic multiplicity through MDI
Returns multiplicity – Multiplicity of the system
Return type int
send_natoms() → int
Send the number of atoms through MDI
  Returns natom – Number of atoms
  Return type int

send_ncommands() → int
Send the number of supported MDI commands through MDI
  Returns ncommands – Number of supported commands
  Return type int

send_total_charge() → float
Send the total system charge through MDI
  Returns charge – Total charge of the system
  Return type float

start() → None
Receive commands through MDI and respond to them as defined by the MDI Standard

stop() → None
Stop listening for MDI commands

update_molecule(key: str, value)
Update the molecule
  Parameters
  • key (str) – Key of the molecular element to update
  • value – Update value

Class Inheritance Diagram

5.6.2 qcengine.compute Module
Integrates the computes together

Functions

compute(input_data, program[, raise_error, ...])
  Executes a single quantum chemistry program given a QC Schema input.

Continued on next page
Table 4 – continued from previous page

compute_procedure(input_data, procedure[, ...]) Runs a procedure (a collection of the quantum chemistry executions)

compute

qcengine.compute.compute(input_data: Union[Dict[str, Any], AtomicInput], program: str, raise_error: bool = False, local_options: Optional[Dict[str, Any]] = None, return_dict: bool = False) → AtomicResult
Executes a single quantum chemistry program given a QC Schema input.

The full specification can be found at: http://molssi-qc-schema.readthedocs.io/en/latest/index.html#

Parameters

- **input_data** (Union[Dict[str, Any], ‘AtomicInput’]) – A QCSchema input specification in dictionary or model from QCElemental.models
- **program** (str) – The program to execute the input with.
- **raise_error** (bool, optional) – Determines if compute should raise an error or not.
- **retries** (int, optional) – The number of random tries to retry for.
- **local_options** (Optional[Dict[str, Any]], optional) – A dictionary of local configuration options
- **return_dict** (bool, optional) – Returns a dict instead of qcelemental.models.AtomicInput

Returns A computed AtomicResult object.

Return type result

compute_procedure

qcengine.compute.compute_procedure(input_data: Union[Dict[str, Any], BaseModel], procedure: str, raise_error: bool = False, local_options: Optional[Dict[str, str]] = None, return_dict: bool = False) → BaseModel
Runs a procedure (a collection of the quantum chemistry executions)

Parameters

- **input_data** (dict or qcelemental.models.OptimizationInput) – A JSON input specific to the procedure executed in dictionary or model from QCElemental.models
- **procedure** (f’“geometric”’) – The name of the procedure to run
- **raise_error** (bool, option) – Determines if compute should raise an error or not.
- **local_options** (dict, optional) – A dictionary of local configuration options
- **return_dict** (bool, optional, default True) – Returns a dict instead of qcelemental.models.AtomicInput

Returns A QC Schema representation of the requested output, type depends on return_dict key.

Return type dict, OptimizationResult, FailedOperation
5.6.3 qcengine.config Module

Creates globals for the qcengine module

**Functions**

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>get_config(*[, hostname, local_options])</code></td>
<td>Returns the configuration key for qcengine.</td>
</tr>
<tr>
<td><code>get_provenance_augments()</code></td>
<td>A representation of the current global configuration.</td>
</tr>
<tr>
<td><code>global_repr()</code></td>
<td>A representation of the current global configuration.</td>
</tr>
</tbody>
</table>

**get_config**

qcengine.config.get_config (*, hostname: Optional[str] = None, local_options: Dict[str, Any] = None) \rightarrow qcengine.config.JobConfig

Returns the configuration key for qcengine.

**get_provenance_augments**

qcengine.config.get_provenance_augments () \rightarrow Dict[str, str]

**global_repr**

qcengine.config.global_repr () \rightarrow str

A representation of the current global configuration.

**Classes**

**NodeDescriptor(**data)**

Description of an individual node

**NodeDescriptor**

```python
class qcengine.config.NodeDescriptor(**data: Dict[str, Any]):
   _bases: pydantic.main.BaseModel
    Description of an individual node
```

**Class Inheritance Diagram**

```
BaseModel ───> NodeDescriptor
```
5.6.4 qcengine.util Module

Several import utilities

Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>compute_wrapper([capture_output, raise_error])</code></td>
<td>Wraps compute for timing, output capturing, and raise protection</td>
</tr>
<tr>
<td><code>model_wrapper(input_data, model)</code></td>
<td>Wrap input data in the given model, or return a controlled error</td>
</tr>
<tr>
<td><code>handle_output_metadata(output_data, metadata)</code></td>
<td>Fuses general metadata and output together.</td>
</tr>
</tbody>
</table>

**compute_wrapper**

cqengine.util.compute_wrapper(capture_output: bool = True, raise_error: bool = False) → Dict[str, Any]

Wraps compute for timing, output capturing, and raise protection

**model_wrapper**

cqengine.util.model_wrapper(input_data: Dict[str, Any], model: BaseModel) → BaseModel

Wrap input data in the given model, or return a controlled error

**handle_output_metadata**

cqengine.util.handle_output_metadata(output_data: Union[Dict[str, Any], BaseModel], metadata: Dict[str, Any], raise_error: bool = False, return_dict: bool = True) → Union[Dict[str, Any], BaseModel]

Fuses general metadata and output together.

**Returns result** – Output type depends on return_dict or a dict if an error was generated in model construction

**Return type** dict or pydantic.models.AtomicResult

5.6.5 qcengine.programs Package

Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>get_program(name[, check])</code></td>
<td>Returns a program’s executor class</td>
</tr>
<tr>
<td><code>list_all_programs()</code></td>
<td>List all programs registered by QC Engine.</td>
</tr>
<tr>
<td><code>list_available_programs()</code></td>
<td>List all programs that can be executed (found) by QC Engine.</td>
</tr>
<tr>
<td><code>register_program(entry_point)</code></td>
<td>Register a new ProgramHarness with QC Engine.</td>
</tr>
<tr>
<td><code>unregister_program(name)</code></td>
<td>Unregisters a given program.</td>
</tr>
</tbody>
</table>
get_program

qcengine.programs.get_program(name: str, check: bool = True) → ProgramHarness
Returns a program’s executor class

    Parameters check – True Do raise error if program not found. False is handy for the specialized
case of calling non-execution methods (like parsing for testing) on the returned Harness.

list_all_programs

qcengine.programs.list_all_programs() → Set[str]
List all programs registered by QCEngine.

list_available_programs

qcengine.programs.list_available_programs() → Set[str]
List all programs that can be executed (found) by QCEngine.

register_program

qcengine.programs.register_program(entry_point: ProgramHarness) → None
Register a new ProgramHarness with QCEngine.

unregister_program

qcengine.programs.unregister_program(name: str) → None
Unregisters a given program.

Classes

ProgramHarness(**kwargs)

ProgramHarness

class qcengine.programs.ProgramHarness(**kwargs)
    Bases: pydantic.main.BaseModel, abc.ABC
5.7 Changelog

5.7.1 v0.12.0 / 2019-11-13

New Features

- (GH#159) Adds MolSSI Driver Interface support. - (GH#160) Adds Turbomole support. - (GH#164) Adds Q-Chem support.

Enhancements

- (GH#155) Support for Psi4 Wavefunctions using v1.4a2 or greater. - (GH#162) Adds test for geometry optimization with trajectory protocol truncation. - (GH#167) CFOUR and NWChem parsing improvements for CCSD(T) properties. - (GH#168) Standardizes on `dispatch.out` for the common output files. - (GH#170) Increases coverage and begins a common documentation page. - (GH#171) Add Molpro to the standard suite. - (GH#172) Models renamed according to https://github.com/MolSSI/QCEElemental/issues/155, particularly

\[ \text{ResultInput} \rightarrow \text{AtomicInput}, \text{Result} \rightarrow \text{AtomicResult}, \text{Optimization} \rightarrow \text{OptimizationResult}. \]

Bug Fixes

5.7.2 v0.11.0 / 2019-10-01

New Features

- (GH#162) Adds a test to take advantage of Elemental’s Protocols. Although this PR does not technically change anything in Engine, bumping the minor version here allows upstream programs to note when this feature was available because the minimum version dependency on Elemental has been bumped as well.

Enhancements

- (GH#143) Updates to Entos and Molpro to allow Entos to execute functions from the Molpro Harness. Also helps the two drivers to conform to GH#86.
- (GH#145, GH#148) Initial CLI tests have been added to help further ensure Engine is running proper.
• (GH#149) The GAMESS Harness has been improved by adding testing.

• (GH#150, GH#153) TorchANI has been improved by adding a Hessian driver to it and additional information is returned in the extra field when energy is the driver. This also bumped the minimum version of TorchANI Engine supports from 0.5 to 0.9.

• (GH#154) Molpro’s harness has been improved to support callinfo_X properties, unrestricted HF and DFT calculations, and the initial support for parsing local correlation calculations.

• (GH#158) Entos’ output parsing has been improved to read the json dictionary produced by the program directly. Also updates the input file generation.

• (GH#161) Updates MOPAC to have more sensible quantum-chemistry like keywords by default.

Bug Fixes

• (GH#156) Fixed a compatibility bug in specific version of Intel-OpenMP by skipping version 2019.5-281.

• (GH#161) Improved error handling in MOPAC if the execution was incorrect.

5.7.3 v0.10.0 / 2019-08-25

New Features

• (GH#132) Expands CLI for info, run, and run-procedure options.

• (GH#137) A new CI pipeline through Azure has been developed which uses custom, private Docker images to house non-public code which will enable us to test Engine through integrated CI on these codes securely.

• (GH#140) GAMESS, CFOUR, NWChem preliminary implementations.

Enhancements

• (GH#138) Documentation on Azure triggers.

• (GH#139) Overhauls install documentation and clearly defines dev install vs production installs.

5.7.4 v0.9.0 / 2019-08-14

New Features

• (GH#120) Engine now takes advantage of Elemental’s new Msgpack serialization option for Models. Serialization defaults to msgpack when available (conda install msgpack-python [-c conda-forge]), falling back to JSON otherwise. This results in substantial speedups for both serialization and deserialization actions and should be a transparent replacement for users within Engine and Elemental themselves.

Enhancements

• (GH#112) The MolproHarness has been updated to handle DFT and CCSD(T) energies and gradients.

• (GH#116) An environment context manager has been added to catch NumPy style parallelization with Python functions.

• (GH#117) MOPAC and DFTD3 can now accept an extras field which can pass around additional data, conforming to the rest of the Harnesses.
• (GH#119) Small visual improvements to the docs have been made.
• (GH#120) Lists inside models are now generally converted to numpy arrays for internal storage to maximize the benefit of the new Msgpack feature from Elemental.
• (GH#133) The GAMESS Harness now collects the CCSD as part of its output.

Bug Fixes

• (GH#127) Removed unused imports from the NWChem Harvester module.
• (GH#129) Missing type hints from the MolproHarness have been added.
• (GH#131) A code formatting redundancy in the GAMESS input file parser has been removed.

5.7.5 v0.8.2 / 2019-07-25

Bug Fixes

• (GH#114) Make compute and compute_procedure not have required kwargs while debugging a Fractal serialization issue. This is intended to be a temporary change and likely reverted in a later release.

5.7.6 v0.8.1 / 2019-07-22

Enhancements

• (GH#110) Psi4’s auto-retry exception handlers now catch more classes of random errors

Bug Fixes

• (GH#109) Geometric auto-retry settings now correctly propagate through the base code.

5.7.7 v0.8.0 / 2019-07-19

New Features

• (GH#95, GH#96, GH#97, and GH#98) The NWChem interface from QCDB has been added. Thanks to @vivacebelles and @jygrace for this addition!
• (GH#100) The MOPAC interface has now been added to QCEngine thanks help to from @godotalgorithm.

Enhancements

• (GH#94) The gradient and molecule parsed from a GAMESS calculation output file are now returned in parse_output
• (GH#101) Enabled extra files in TeraChem scratch folder to be requested by users, collected after program execution, and recorded in the Result object as extras.
• (GH#103) Random errors can now be retried a finite, controllable number of times (current default is zero retries). Geometry optimizations automatically set retries to 2. This only impacts errors which are categorized as RandomError by QCEngine and all other errors are raised as normal.
Bug Fixes

- **(GH#99)** QCEngine now manages an explicit folder for each Psi4 job to write into and passes the scratch directory via `−s` command line. This resolves a key mismatch which could cause an error.
- **(GH#102)** DFTD3 errors are now correctly returned as a `FailedOperation` instead of a raw dict.

5.7.8 v0.7.1 / 2019-06-18

Bug Fixes

- **(GH#92)** Added an `__init__.py` file to the `programs/tests` directory so they are correctly bundled with the package.

5.7.9 v0.7.0 / 2019-06-17

Breaking Changes

- **(GH#85)** The resource file `programs.dftd3.dashparam.py` has relocated and renamed to `programs.empirical_dispersion_resources.py`.
- **(GH#89)** Function `util.execute` forgot `str` argument `scratch_location` and learned `scratch_directory` in the same role of existing directory within which temporary directories are created and cleaned up. Non-user-facing function `util.scratch_directory` renamed to `util.temporary_directory`.

New Features

- **(GH#60)** WIP: QCEngine interface to GAMESS can run the program (after light editing of rungms) and parse selected output (HF, CC, FCI) into QCSchema.
- **(GH#73)** WIP: QCEngine interface to CFOUR can run the program and parse a variety of output into QCSchema.
- **(GH#59, GH#71, GH#75, GH#76, GH#78, GH#88)** Molpro improvements: Molpro can be run by QCEngine; and the input generator and output parser now supports CCSD energy and gradient calculations. Large thanks to @sjrl for many of the improvements
- **(GH#69)** Custom Exceptions have been added to QCEngine’s returns which will make parsing and diagnosing them easier and more programmatic for codes which invoke QCEngine. Thanks to @dgasmith for implementation.
- **(GH#82)** QCEngine interface to entos can create input files (dft energy and gradients), run the program, and parse the output.
- **(GH#85)** MP2D interface switched to upstream repo (https://github.com/Chandemonium/MP2D v1.1) and now produces correct analytic gradients.

Enhancements

- **(GH#62, GH#67, GH#83)** A large block of TeraChem improvements thanks to @ffangliu contributions. Changed the input parser to call qcelemental `to_string` method with bohr unit, improved output of parser to turn stdout into Result, and modified how version is parsed.

5.7. Changelog
• (GH#63) QCEngine functions `util.which`, `util.which_version`, `util.parse_version`, and `util.safe_version` removed after migrating to QCElemental.

• (GH#65) Torchani can now handle the ANI1-x and ANI1-ccx models. Credit to @dgasmith for implementation

• (GH#74) Removes caching and reduces pytorch overhead from Travis CI. Credit to @dgasmith for implementation

• (GH#77) Rename `ProgramExecutor` to `ProgramHarness` and `BaseProcedure` to `ProcedureHarness`.

• (GH#77) Function `util.execute(..., outfiles=[])` learned to collect output files matching a globed filename.

• (GH#81) Function `util.execute` learned list argument `as_binary` to handle input or output files as binary rather than string.

• (GH#81) Function `util.execute` learned bool argument `scratch_exist_ok` to run in a preexisting directory. This is handy for stringing together execute calls.

• (GH#84) Function `util.execute` learned str argument `scratch_suffix` to identify temp dictionaries for debugging.

• (GH#90) DFTD3 now supports preliminary parameters for zero and Becke-Johnson damping to use with SAPT0-D

**Bug Fixes**

• (GH#80) Fix “psi4:qcvars” handling for older Psi4 versions.

**5.7.10 v0.6.4 / 2019-03-21**

**Bug Fixes**

• (GH#54) Psi4’s Engine implementation now checks its key words in a case insensitive way to give the same value whether you called Psi4 or Engine to do the compute.

• (GH#55) Fixed an error handling routine in Engine to match Psi4.

• (GH#56) Complex inputs are now handled better through Psi4’s wrapper which caused Engine to hang while trying to write to stdout.

**5.7.11 v0.6.3 / 2019-03-15**

**New Features**

• (GH#28) TeraChem is now a registered executor in Engine! Thanks to @ffangliu for implementing.

• (GH#46) MP2D is now a registered executor in Engine! Thanks to @loriab for implementing.

**Enhancements**

• (GH#46) dftd3’s workings received an overhaul. The mol keyword has been replaced with dtype=2, full Psi4 support is now provided, and an MP2D interface has been added.
Bug Fixes

- (GH#50 and GH#51) Executing Psi4 on a single node with multiprocessing is more stable because Psi4 temps are moved to scratch directories. This behavior is now better documented with an example as well.

- (GH#52) Psi4 calls are now executed through the subprocess module to prevent possible multiprocessing issues and memory leak after thousands of runs. A trade off is this adds about 0.5 seconds to task start-up, but its safe. A future Psi4 release will correct this issue and the change can be reverted.

5.7.12 v0.6.2 / 2019-03-07

Enhancements

- (GH#38 and GH#39) Documentation now pulls from the custom QC Archive Sphinx Theme, but can fall back to the standard RTD theme. This allows all docs across QCA to appear consistent with each other.

- (GH#43) Added a base model for all Procedure objects to derive from. This allows procedures’ interactions with compute programs to be more unified. This PR also ensured GeomeTRIC provides Provenance information.

Bug Fixes

- (GH#40) This PR improved numerous back-end and testing quality of life aspects. Fixed setup.py to call pytest instead of unittest when running tests on install. Some conda packages for Travis-CI are cached to reduce the download time of the larger computation codes. Psi4 is now pinned to the 1.3 version to fix build-level pin of libint. Conda-build recipe removed to avoid possible confusion for everyone who isn’t a Conda-Forge recipe maintainer. Tests now rely exclusively on the conda env setups.

5.7.13 v0.6.1 / 2019-02-20

Bug Fixes

- (GH#37) Fixed an issue where RDKit methods were not case agnostic.

5.7.14 v0.6.0 / 2019-02-28

Breaking Changes

- (GH#36) breaking change Model objects are returned by default rather than a dictionary.

New Features

- (GH#18) Add the dftd3 program to available computers.

- (GH#29) Adds preliminary support for the Molpro compute engine.

- (GH#31) Moves all computation to ProgramExecutor to allow for a more flexible input generation, execution, output parsing interface.

- (GH#32) Adds a general execute process which safely runs subprocess jobs.
Enhancements

- (GH#33) Moves the dftd3 executor to the new ProgramExecutor interface.
- (GH#34) Updates models to the more strict QCElemental v0.3.0 model classes.
- (GH#35) Updates CI to avoid pulling CUDA libraries for torchani.
- (GH#36) First pass at documentation.

5.7.15 v0.5.2 / 2019-02-13

Enhancements

- (GH#24) Improves load times dramatically by delaying imports and cpuutils.
- (GH#30) Ensures Psi4 output is already returned and Pydantic v0.20+ changes.

5.7.16 v0.5.1 / 2019-01-29

Enhancements

- (GH#22) Compute results are now returned as a dict of Python Primals which have been serialized-deserialized through Pydantic instead of returning un-processed Python objects or json-compatible string.

5.7.17 v0.5.0 / 2019-01-28

New Features

- (GH#8) Adds the TorchANI program for ANI-1 like energies and potentials.
- (GH#16) Adds QCElemental models based off QCSchema to QCEngine for both validation and object-based manipulation of input and output data.

Enhancements

- (GH#14) Migrates option to Pydantic objects for validation and creation.
- (GH#14) Introduces NodeDescriptor (for individual node description) and JobConfig (individual job configuration) objects.
- (GH#17) NodeDescriptor overhauled to work better with Parsl/Balsam/Dask/etc.
q
qcengine, 18
qcengine.compute, 23
qcengine.config, 25
qcengine.programs, 26
qcengine.util, 26
INDEX

A
AtomicInput (class in qcelemental.models), 13
AtomicResult (class in qcelemental.models), 13

C
compute () (in module qcengine), 18
compute() (in module qcengine.compute), 24
compute_procedure() (in module qcengine), 19
compute_procedure() (in module qcengine.compute), 24
compute_wrapper() (in module qcengine.util), 26

G
get_config() (in module qcengine), 19
get_config() (in module qcengine.config), 25
get_molecule() (in module qcengine), 19
get_procedure() (in module qcengine), 20
get_program() (in module qcengine), 20
get_program() (in module qcengine.programs), 27
global_repr() (in module qcengine.config), 25

H
handle_output_metadata() (in module qcengine.util), 26

L
list_all_procedures() (in module qcengine), 20
list_all_programs() (in module qcengine), 20
list_all_programs() (in module qcengine.programs), 27
list_all_available_procedures() (in module qcengine), 20
list_all_available_programs() (in module qcengine), 20
list_all_available_programs() (in module qcengine.programs), 27

M
MDIServer (class in qcengine), 21
model_wrapper() (in module qcengine.util), 26

N
NodeDescriptor (class in qcengine.config), 25

P
ProgramHarness (class in qcengine.programs), 27

Q
qcengine (module), 18
qcengine.compute (module), 23
qcengine.config (module), 25
qcengine.programs (module), 26
qcengine.util (module), 26

R
recv_coords() (qcengine.MDIServer method), 21
recv_elements() (qcengine.MDIServer method), 21
recv_masses() (qcengine.MDIServer method), 21
recv_multiplicity() (qcengine.MDIServer method), 22
recv_total_charge() (qcengine.MDIServer method), 22
register_program() (in module qcengine), 20
register_program() (in module qcengine.programs), 27
run_energy() (qcengine.MDIServer method), 22

S
send_commands() (qcengine.MDIServer method), 22
send_coords() (qcengine.MDIServer method), 22
send_elements() (qcengine.MDIServer method), 22
send_energy() (qcengine.MDIServer method), 22
send_forces() (qcengine.MDIServer method), 22
send_masses() (qcengine.MDIServer method), 22
send_multiplicity() (qcengine.MDIServer method), 22
send_natoms() (qcengine.MDIServer method), 22
send_ncommands() (qcengine.MDIServer method), 23
send_total_charge() (qcengine.MDIServer method), 23
start() (qcengine.MDIServer method), 23
stop() (qcengine.MDIServer method), 23

U
unregister_program() (in module qcengine), 20
unregister_program() (in module qcengine.programs), 27
update_molecule() (qcengine.MDIServer method), 23