SOLVCON Architecture

Release 0.1.2

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August 07, 2013

Contents

SOLVCON is built upon two keystones: (i) unstructured meshes for spatial discretization and (ii) two-level loop structure of partial differential equation (PDE) solvers.

1 Unstructured Meshes

We usually discretize the spatial domain of interest before solving PDEs with digital computers. The discretized space is called a *mesh* [Mavriplis97]. When discretization is done by exploiting regularity in space, like cutting along each of the Cartesian coordinate axes, the discretized space is called a *structured mesh*. If the discretization does not follow any spatial order, we call the spatial domain an *unstructured mesh*. Both meshing strategies have their strength and weakness. Sometimes a structured mesh is also call a *grid*. Numerical methods that rely on spatial discretization are called *mesh-based* or *grid-based*. Most PDE-solving methods in production uses are mesh-based, but meshless methods have their advantages.

To accommodate complex geometry, SOLVCON chose to use unstructured meshes of mixed elements. Because no structure is assumed for the geometry to be modeled, the mesh can be automatically generated by using computer programs. For example, the following image shows a triangular mesh of a two-dimensional irregular domain:

which is generated by using the Gmsh commands listed in ustmesh_2d_sample.geo. On the other hand, creation of structured meshes often needs a large amount of manual operations and will not be discussed in this document.

In SOLVCON, we assume a mesh is fully covered by a finite number of non-overlapping sub-regions, and only composed by these sub-regions. The sub-regions are called *mesh elements*. In one-dimensional space, SOLVCON also defines one type of mesh elements, *line*, as shown in Figure *One-dimensional mesh element*.

SOLVCON allows two types of two-dimensional mesh elements, *quadrilaterals* and *triangles*, as shown in Figure *Two-dimensional mesh elements*, and four types of three-dimensional mesh elements, *hexahedra*, *tetrahedra*, *prisms*, and *pyramids*, as shown in Figure *Three-dimensional mesh elements*.

The numbers annotated in the figures are the order of the vertices of the elements. A SOLVCON mesh can be a mixture of elements of the same dimension, although it is often composed of one type of element. Two modules provide the support of the meshes: (i) `solvcon.block` defines and manages various look-up tables that form the data structure of the mesh in Python, and (ii) `solvcon.mesh` serves as the interface of the mesh data in C.

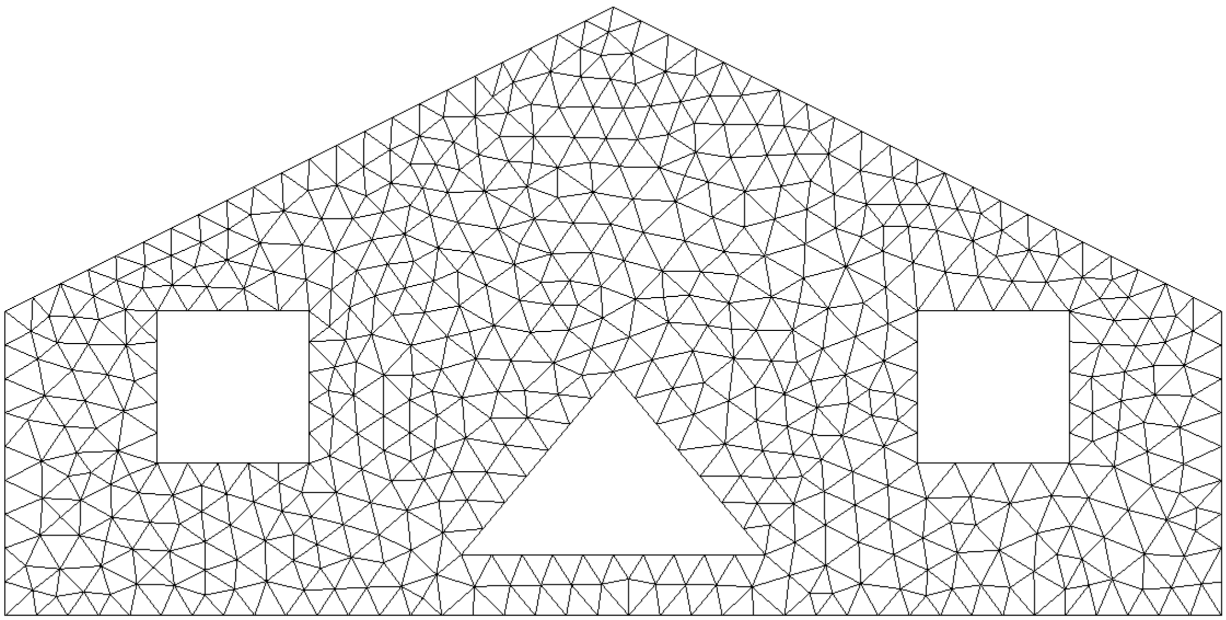

Figure 1: Two-dimensional sample mesh

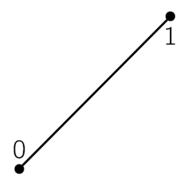

Figure 2: One-dimensional mesh element

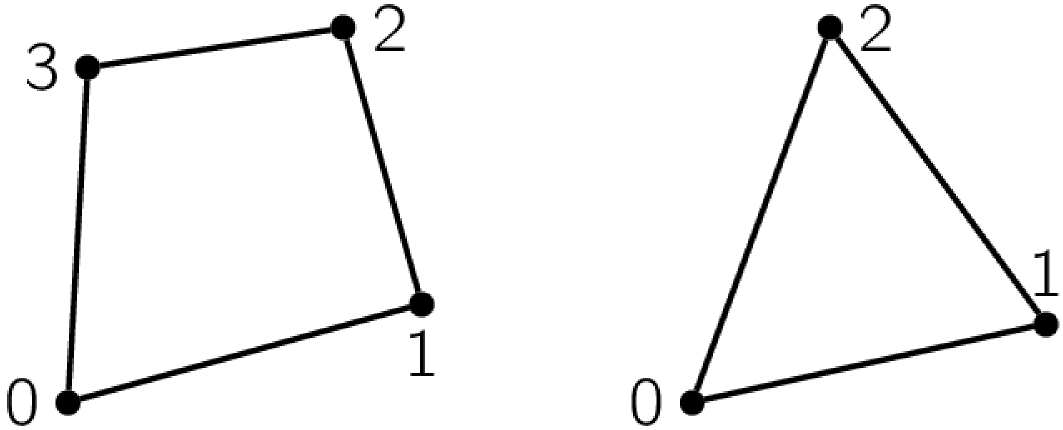

Figure 3: Two-dimensional mesh elements

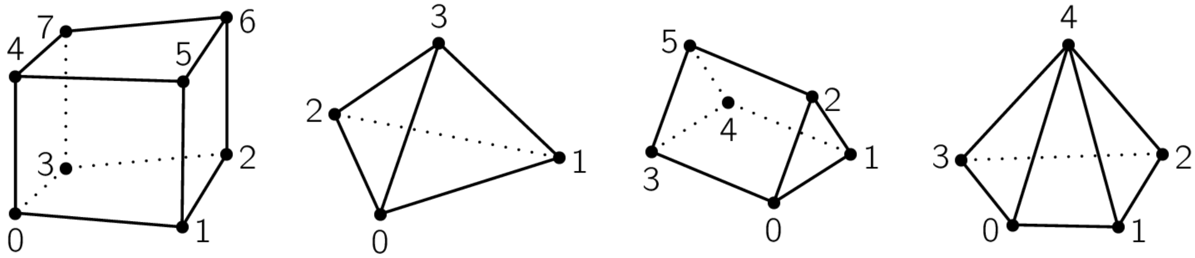

Figure 4: Three-dimensional mesh elements

1.1 Entities

Before explaining the data structure of the meshes, we need to introduce some basic terminologies and definitions. In SOLVCON, a *cell* means a mesh element. The dimensionality of a cell equals to that of the mesh it belongs to, e.g., a two-dimensional mesh is composed by two-dimensional cells. A cell is assumed to be concave, and enclosed by a set of *faces*. The dimensionality of a face is one less than that of a cell. A face is also assumed to be concave, and formed by connecting a sequence of *nodes*. The dimensionality of a node is at least one less than that of a face. Cells, faces, and nodes are the basic constructs, which we call *entities*, of a SOLVCON mesh.

Defining the term "entity" for SOLVCON facilitates a unified treatment of two- and three-dimensional meshes and the corresponding solvers [1]. A cell can be either two- or three-dimensional, and the associated faces become one- or two-dimensional, respectively. Because a face is either one- or two-dimensional, it can always be formed by a sequence of points, which is zero-dimensional. In this treatment, a point is equivalent to a node defined in the previous passage.

Take the two-dimensional mesh shown above as an example, triangular elements are used as the cells. The triangles are formed by three lines (one-dimensional shapes), which are the faces. Each line has two points (zero-dimensional). If we have a three-dimensional mesh composed by hexahedral cells, then the faces should be quadrilaterals (two-dimensional shapes).

All the mesh elements supported by SOLVCON are listed in the following table. The first column is the name of the element, and the second column is the type ID used in SOLVCON. The third column lists the dimensionality. The fourth, fifth, and sixth columns show the number of zero-, one-, and two-dimensional *sub*-entities belong to the element type, respectively. Note that the terms "point" and "line" appear in both the first row and first column, for they are the only element type in the space of the corresponding dimensionality.

Name	Type	Dim	Point#	Line#	Surface#
Point	0	0	0	0	0
Line	1	1	2	0	0
Quadrilateral	2	2	4	4	0
Triangle	3	2	3	3	0
Hexahedron	4	3	8	12	6
Tetrahedron	5	3	4	4	4
Prism	6	3	6	9	5
Pyramid	7	3	5	8	5

Although SOLVCON doesn't support one-dimensional solvers, for completeness, we define the relation between one-dimensional cells (lines) and their sub-entities as:

Shape (type)	Face	= Point
Line (0) 1	0 · 1	· 0

[1] SOLVCON focuses on two- and three-dimensional meshes. But if we put an additional constraint on the mesh elements: Requiring them to be simplices, it wouldn't be difficult to extend the data structure of SOLVCON meshes into higher-dimensional space.

That is, as shown in Figure *One-dimensional mesh element*, a one-dimensional “cell” (line) has two “faces”, which are essentially point 0 and point 1. Symbol · indicates a point.

It will be more practical to illustrate the relation between two-dimensional cells and their sub-entities in a table (see Figure *Two-dimensional mesh elements* for point locations):

Shape (type)	Face	= Line formed by points
Quadrilateral (2)	0	╱ 0 1
	1	╱ 1 2
	2	╱ 2 3
	3	╱ 3 0
Triangle (3)	0	╱ 0 1
	1	╱ 1 2
	2	╱ 2 0

Symbol ╱ indicates a line. The orientation of lines of each two-dimensional shape is defined to follow the right-hand rule. The shape enclosed by the lines has an area normal vector points to the direction of $+z$ (outward paper/screen).

The relation between three-dimensional cells and their sub-entities is defined in the table (see Figure *Three-dimensional mesh elements* for point locations):

Shape (type)	Face	= Surface formed by points
Hexahedron (4)	0	□ 0 3 2 1
	1	□ 1 2 6 5
	2	□ 4 5 6 7
	3	□ 0 4 7 3
	4	□ 0 1 5 4
	5	□ 2 3 7 6
Tetrahedron (5)	0	△ 0 2 1
	1	△ 0 1 3
	2	△ 0 3 2
	3	△ 1 2 3
Prism (6)	0	△ 0 1 2
	1	△ 3 5 4
	2	□ 0 3 4 1
	3	□ 0 2 5 3
	4	□ 1 4 5 2
Pyramid (7)	0	△ 0 4 3
	1	△ 1 4 0
	2	△ 2 4 1
	3	△ 3 4 2
	4	□ 0 3 2 1

Symbol □ indicates a quadrilateral, while symbol △ indicates a triangle.

Because a face is associated to two adjacent cells unless it’s a boundary face, it needs to identify to which cell it belongs, and to which cell it is neighbor. The area normal vector of a face is always point from the belonging cell to neighboring cell. The same rule applies to faces of two-dimensional meshes (lines) too.

1.2 Data Structure Defined in `solvcon.block`

Real data of unstructured meshes are stored in module `solvcon.block`. A simple table for all element types is defined as `elemtype`:

`solvcon.block.`**`elemtype`**

A `numpy.ndarray` object of shape (8, 5) and type `int32`. This array is a reference table for element types in SOLVCON. The content is shown in the first table in Section Entities. Each row represents an element type. The first column is the index of the element type, the second the dimensionality, the third column the number of points, the fourth the number lines, and the fifth the number of surfaces.

Class Block contains descriptive information, look-up tables, and other miscellaneous information for a SOLVCON mesh. There are three steps required to fully construct a Block object: (i) instantiation, (ii) definition, and (iii) build-up. In the first step, when instantiating an object, shape information must be provided to the constructor to allocate arrays for look-up tables:

```
from solvcon.block import Block
blk = Block(ndim=2, nnode=4, ncell=3)
```

Second, we fill the definition of the look-up tables into the object. We at least need to provide the node coordinates and the node lists of cells:

```
blk.ndcrd[:,:] = (0,0), (-1,-1), (1,-1), (0,1)
blk.cltpn[:] = 3
blk.clnds[:,:4] = (3, 0,1,2), (3, 0,2,3), (3, 0,3,1)
```

Third and finally, we build up the rest of the object by calling:

```
blk.build_interior()
blk.build_boundary()
blk.build_ghost()
```

By running the additional code, the block can be saved as a VTK file for viewing:

```
from solvcon.io.vtkxml import VtkXmlUstGridWriter
iodev = VtkXmlUstGridWriter(blk)
iodev.write('block_2d_sample.vtu')
```

class `solvcon.block.`**`Block`**(*ndim=0*, *nnode=0*, *nface=0*, *ncell=0*, *nbound=0*, *use_incenter=False*)

This class represents the unstructured meshes used in SOLVCON. As such, in SOLVCON, an unstructured mesh is also called a *block*. The following six attributes can be passed into the constructor. `ndim`, `nnode`, and `ncell` need to be non-zero to instantiate a valid block. `nface` and `nbound` might be different to the given value after building up the object. `use_incenter` is an optional flag.

`ndim`

Type `int`

Number of dimensionalities of this mesh. Read only after instantiation.

`nnode`

Type `int`

Total number of (non-ghost) nodes of this mesh. Read only after instantiation.

`nface`

Type `int`

Total number of (non-ghost) faces of this mesh. Read only after instantiation.

`ncell`

Type `int`

Total number of (non-ghost) cells of this mesh. Read only after instantiation.

`nbound`

Type `int`

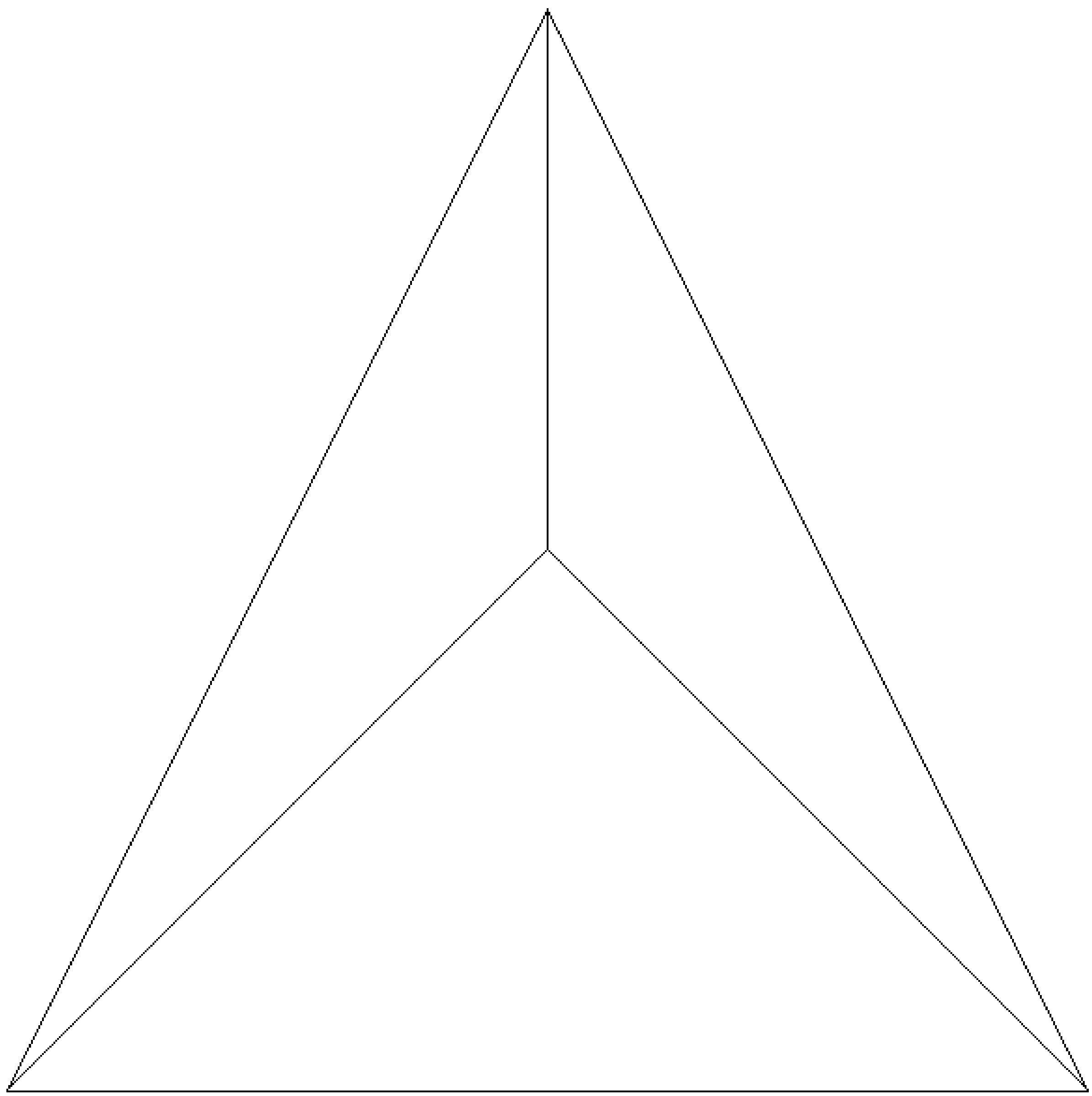

Figure 5: A simple `Block` object

Total number of boundary faces or ghost cells of this mesh. Read only after instantiation.

use_incenter

Type `bool`

Indicates calculating incenters instead of centroids for cells. Default is `False` (using centroids of cells).

To construct a block object, SOLVCON needs to know the dimensionalities (`ndim`), the number of nodes (`nnode`), faces (`nface`), and cells (`ncell`), and the number of boundary faces (`nbound`) of the mesh. These keyword parameters are taken to initialize the following properties:

The meshes are mainly defined by three sets of look-up tables (arrays). The first set is the geometry arrays, which store the coordinate values of mesh elements:

ndcrd
Coordinates of nodes. It's a two-dimensional `numpy.ndarray` array of shape (`nnode`, `ndim`) of type `float64`.

fccnd
Centroids of faces. It's a two-dimension `numpy.ndarray` of shape (`nface`, `ndim`) of type `float64`.

fcnml
Unit normal vectors of faces. It's a two-dimension `numpy.ndarray` of shape (`nface`, `ndim`) of type `float64`.

fcara
Areas of faces. The value should always be non-negative. It's a one-dimension `numpy.ndarray` of shape (`nface`,) of type `float64`.

clcnd
Centroids of cells. It's a two-dimension `numpy.ndarray` of shape (`ncell`, `ndim`) of type `float64`.

clvol
Volumes of cells. It's a one-dimension `numpy.ndarray` of shape (`ncell`,) of type `float64`.

The second set is the meta-data or type data arrays:

fctpn
Type ID of faces. It's a one-dimensional `numpy.ndarray` of shape (`nface`,) of type `int32`.

cltpn
Type ID of cells. It's a one-dimensional `numpy.ndarray` of shape (`ncell`,) of type `int32`.

clgrp
Group ID of cells. It's a one-dimensional `numpy.ndarray` of shape (`ncell`,) of type `int32`. For a new `Block` object, it should be initialized with `-1`.

The third and last set is the connectivity arrays:

fcnds
Lists of the nodes of each face. It's a two-dimensional `numpy.ndarray` of shape (`nface`, `FCMND`+1) and type `int32`.

fccls
Lists of the cells connected by each face. It's a two-dimensional `numpy.ndarray` of shape (`nface`, 4) and type `int32`.

clnds
Lists of the nodes of each cell. It's a two-dimensional `numpy.ndarray` of shape (`ncell`, `CLMND`+1) and type `int32`.

clfcs

Lists of the faces of each cell. It's a two-dimensional `numpy.ndarray` of shape (`ncell`, `CLMFC`+1) and type `int32`.

Every look-up array has two associated arrays distinguished by different prefixes: (i) `gst` (denoting for "ghost") and (ii) `sh` (denoting for "shared"). SOLVCON uses the technique of ghost cells to treat boundary conditions [Mavriplis97], and the `gst` arrays store the information for ghost cells. However, to facilitate efficient indexing in solvers, each of the ghost arrays should be put in a continuous block of memory adjacent to its interior counterpart. In SOLVCON, the `sh` arrays are the continuous memory blocks for both ghost and interior look-up tables, and a pair of `gst` and normal arrays is simply the views of two consecutive, non-overlapping sub-regions of a memory block. More details of the technique of ghost cells will be given in module `solvcon.mesh`.

There are some attributes associated with ghost cells:

ngstnode

Type `int`

Number of nodes only associated with ghost cells. Only valid after build-up. Read only.

ngstface

Type `int`

Number of faces only associated with ghost cells. Only valid after build-up. Read only.

ngstcell

Type `int`

Number of ghost cells. Only valid after build-up. Read only.

Three arrays need to be defined before we can build up a `Block` object: (i) `ndcrd`, (ii) `cltpn`, and (iii) `clnds`. With these information, `build_interior()` builds up the interior arrays for a `Block` object. `build_boundary()` then organizes the information for boundary conditions. Finally, `build_ghost()` builds up the shared and ghost arrays for the `Block` object. Only after the build-up process, the `Block` object can be used by solvers.

build_interior()

Returns Nothing.

Building up a `Block` object includes two steps. First, the method extracts arrays `clfcs`, `fctpn`, `fcnds`, and `fccls` from the defined arrays `cltpn` and `clnds`. If the number of extracted faces is not the same as that passed into the constructor, arrays related to faces are recreated.

Second, the method calculates the geometry information and fills the corresponding arrays.

build_boundary(*unspec_type=None*, *unspec_name='unspecified'*)

Parameters

- **unspec_type** (`type`) – BC type for the unspecified boundary faces. Set to `None` indicates the default to `solvcon.boundcond.unspecified`.
- **unspec_name** (`str`) – Name for the unspecified BC.

Returns Nothing.

This method iterates over each of the `solvcon.boundcond.BC` objects listed in `bclist` to collect boundary-condition information and build boundary faces. If a face belongs to only one cell (i.e., has no neighboring cell), it is regarded as a boundary face.

Unspecified boundary faces will be collected to form an additional `solvcon.boundcond.BC` object. It sets `bndfcs` for later use by `build_ghost()`.

build_ghost()

Returns Nothing.

This method creates the shared arrays, calculates the information for ghost cells, and reassigns interior arrays as the right portions of the shared arrays.

A Block object also contains three instance variables for boundary-condition treatments:

bclist

Type list

The list of associated solvcon.boundcond.BC objects.

nbound

Type int

Number of boundary faces. Only valid after build-up. It should equals to ngstcell.

bndfcs

Type numpy.ndarray

The array is of shape (nbound, 2) and type int32. Each row contains the data for a boundary face. The first column is the 0-based index of the face, while the second column is the serial number of the associated solvcon.boundcond.BC object.

create_msh()

Returns An object contains the sc_mesh_t variable for C code to use data in the Block object.

Return type solvcon.mesh.Mesh

The following code shows how and when to use this method:

```
>>> blk = Block(ndim=2, nnode=4, nface=6, ncell=3, nbound=3)
>>> blk.ndcrd[:,:] = (0,0), (-1,-1), (1,-1), (0,1)
>>> blk.cltpn[:] = 3
>>> blk.clnds[:,:4] = (3, 0,1,2), (3, 0,2,3), (3, 0,3,1)
>>> blk.build_interior()
>>> # it's OK to get a msh when its content is still invalid.
>>> msh = blk.create_msh()
>>> blk.build_boundary()
>>> blk.build_ghost()
>>> # now the msh is valid for the blk is fully built-up.
>>> msh = blk.create_msh()
```

In class Block there are also useful constants defined:

Block.**FCMND**

Type int

The maximum number of nodes that a face can have. From the first table in Section Entities, its value should be 4.

Block.**CLMND**

Type int

The maximum number of nodes that a cell can have. From the first table in Section Entities, its value should be 8.

Block.**CLMFC**

Type `int`

The maximum number of faces that a cell can have. From the first table in Section Entities, its value should be 6.

1.3 Low-Level Interface to C Defined in `solvcon.mesh`

Although it is convenient to have data structure defined in the Python module `solvcon.block`, kernel of numerical methods are usually implemented in C. To bridge Python and C, we use Cython to write an interfacing module `solvcon.mesh`. This module enables C code to use the mesh data held by a `solvcon.block.Block` object, and allows Python to use those C functions.

A header file `mesh.h` contains the essential declarations to use the mesh data:

sc_mesh_t

This `struct` is the counterpart of the Python class `solvcon.block.Block` in C. It contains four sections of fields in order.

The first field section is for shape. These fields correspond to the instance properties (attributes) in `solvcon.block.Block` of the same names:

int **ndim**

int **nnode**

int **nface**

int **ncell**

int **nbound**

int **ngstnode**

int **ngstface**

int **ngstcell**

The second field section is for geometry arrays. These fields correspond to the instance variables (attributes) in `solvcon.block.Block` of the same names:

Note: All arrays in `sc_mesh_t` are shared arrays but the pointers point to the start of their interior portion. In this way, access to ghost information can be efficiently done by using negative indices of nodes, faces, and cells in the first dimension of these arrays. But negative indices in higher dimensions of the arrays is meaningless.

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double* **ndcrd**

double* **fccnd**

double* **fcnml**

double* **fcara**

double* **clcnd**

double* **clvol**

The third field section is for type/meta arrays. These fields correspond to the instance variables (attributes) in `solvcon.block.Block` of the same names:

int* **fctpn**

int* **cltpn**

int* **clgrp**

The fourth and final field section is for connectivity arrays. These fields correspond to the instance variables (attributes) in `solvcon.block.Block` of the same names:

int* **fcnds**

int* **fccls**

int* **clnds**

int* **clfcs**

The SOLVCON C library (`libsolvcon.a`) contains five mesh-related functions that are used internally in `Mesh`. These functions are not meant to be part of the interface, but can be a reference about the usage of `sc_mesh_t`:

int **sc_mesh_extract_faces_from_cells** (sc_mesh_t **msd*, int *mface*, int **pnface*, int **clfcs*, int **fctpn*, int **fcnds*, int **fccls*)

This function extracts interior faces from the node lists of the cells given in the first argument `msd`. The second argument `mface` is also an input, which sets the maximum value of possible number of faces to be extracted.

The rest of the arguments is outputs. The arrays pointed by the last four arguments need to be pre-allocated with appropriate size or the memory will be corrupted.

int **sc_mesh_calc_metric** (sc_mesh_t **msd*, int *use_incenter*)

This function calculates the geometry information and stores the calculated values into the arrays specified in `msd`. The second argument `use_incenter` is a flag. When it is set to `1`, the function calculates and stores the incenter of the cells. Otherwise, the function calculates and stores the centroids of the cells.

void **sc_mesh_build_ghost** (sc_mesh_t **msd*, int **bndfcs*)

Build all information for ghost cells by mirroring information from interior cells. The arrays in the first argument `msd` will be altered, but data in the second argument `bndfcs` will remain intact. The action includes:

1. Define indices and build connectivities for ghost nodes, faces, and cells. In the same loop, mirror the coordinates of interior nodes to ghost nodes.
2. Compute center coordinates for faces for ghost cells.
3. Compute normal vectors and areas for faces for ghost cells.
4. Compute center coordinates for ghost cells.
5. Compute volume for ghost cells.

It should be noted that all the geometry, type/meta and connectivity data used in this function are SHARED arrays rather than interior arrays. The indices for ghost information should be carefully treated. All the ghost indices are negative in shared arrays.

int **sc_mesh_build_rcells** (sc_mesh_t **msd*, int **rcells*, int **rcellno*)

This is a utility function used by `Mesh.create_csr()`. The first argument `msd` is input and will not be changed, and the output will be write to the second and third arguments, `rcells` and `rcellno`. Sufficient memory must be pre-allocated for the output arrays before calling or memory can be corrupted.

int **sc_mesh_build_csr** (sc_mesh_t **msd*, int **rcells*, int **adjncy*)

This is a utility function used by `Mesh.create_csr()`. The first argument `msd` and the second argument `rcells` are input and will not be changed, while the third argument `adjncy` is output. Sufficient memory must be pre-allocated for the output array before calling or memory can be corrupted.

A Python class `Mesh` is written by using Cython to convert a Python-space `solvcon.block.Block` object into a `sc_mesh_t` `struct` variable for use in C. This class is meant to be subclassed to implement the core number-crunching algorithm of a numerical method. In addition, this class also provides functionalities that need the C utility functions listed above.

class `solvcon.mesh.`**`Mesh`**

This class associates the C functions for mesh operations to the mesh data and exposes the functions to Python.

`_msd`

This attribute holds a C `struct` `sc_mesh_t` for internal use.

`setup_mesh`(*blk*)

Parameters **blk** (`solvcon.block.Block`) – The block object to be copied from.

`extract_faces_from_cells`(*max_nfc*)

Parameters **max_nfc** (C `int`) – Maximum value of possible number of faces to be extracted.

Returns Four interior `numpy.ndarray` for `solvcon.block.Block.clfcs`, `solvcon.block.Block.fctpn`, `solvcon.block.Block.fcnds`, and `solvcon.block.Block.fccls`.

Internally calls `sc_mesh_extract_face_from_cells()`.

`calc_metric`()

Returns Nothing.

Calculates geometry information including normal vector and area of faces, and centroid/incenter coordinates and volume of cells. Internally calls `sc_mesh_calc_metric()`.

`build_ghost`()

Returns Nothing.

Builds data for ghost cells. Internally calls `sc_mesh_build_ghost()`.

`create_csr`()

Returns xadj, adjncy

Return type tuple of `numpy.ndarray`

Builds the connectivity graph in the CSR (compressed storage format) used by SCOTCH/METIS. Internally calls `sc_mesh_build_rcells()` and `sc_mesh_build_csr()`.

`partition`(*npart*, *vwgtarr=None*)

Parameters

- **npart** (C `int`) – Number of parts to be partitioned to.
- **vwgtarr** (`numpy.ndarray`) – vwgt weighting settings. Default is `None`.

Returns A 2-tuple of (i) number of cut edges for the partitioning and (ii) a `numpy.ndarray` of shape (`solvcon.block.Block.ncell`,) and type `int32` that indicates the partition number of each cell in the mesh.

Return type `int`, `numpy.ndarray`

Internally calls `METIS_PartGraphKway()` of the SCOTCH library for mesh partitioning.

2 Numerical Code

The numerical calculations in SOLVCON rely on exploiting a two-level loop structure, i.e., the temporal loop and the spatial loops. For time-accurate solvers, there is always an outer loop that coordinates the time-marching. The outer loop is called the *temporal loop*, and it should be implemented in subclasses of `MeshCase`. Inside the temporal loop, there can be one or many inner loops that calculate the new values of the fields. The inner loops are called the *spatial loops*, and they should be implemented in subclasses of `MeshSolver`.

The outer temporal loop is more responsible for coordinating, while the inner spatial loops is closer to numerical algorithms. These two levels allow us to segregate code. An object of `MeshCase` can be seen as the realization of a simulation case in SOLVCON (as a convention the object's name should contain or just be `cse`). Code in `MeshCase` is mainly about obtaining settings, input and output, and provision of the execution environment. On the other hand, we implement the numerical algorithm in `MeshSolver` to manipulate the field data (as a convention the object's name should contain or just be `svr`). Its code shouldn't involve input nor output (excepting that for debugging) but needs to take parallelism into account.

Code for data processing should go to `MeshHook` (as a convention the objects should be named with `hok`), which is the companion of `MeshCase`. Code that processes data close to numerical methods should go to `MeshAnchor` (as a convention the objects should be named with `ank`), which is the companion of `MeshSolver`.

In this section, for conciseness, the terms solver, anchor, case, and hook are used to denote the classes `MeshSolver`, `MeshAnchor`, `MeshCase`, and `MehsHook` or their instances, respectively. In the issue tracking system, solver, anchor, case, and hook form a component "sach".

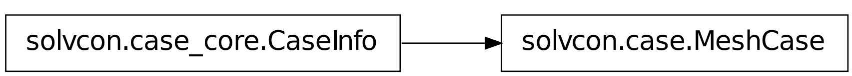
2.1 `solvcon.case`

Module `solvcon.case` contains code for making a simulation case (subclasses of `solvcon.case.MeshCase`). Because a case coordinates the whole process of a simulation run, for parallel execution, there can be only one `MeshCase` object residing in the controller (head) node.

By the design, `MeshCase` itself cannot be directly used. It must be subclassed to implement control logic for a specific application. The application can be a concrete model for a certain physical process, or an abstraction of a group of related physical processes, which can be further subclassed.

class `solvcon.case.`**`MeshCase`**`(`***kw*`)`

Base class for simulation cases based on `solvcon.mesh.Mesh`.



`init()` and `run()` are the two primary methods responsible for the execution of the simulation case object. Both methods accept a keyword parameter "level":

- run level 0: fresh run (default),
- run level 1: restart run,
- run level 2: initialization only.

`cleanup``(`*signum=None*, *frame=None*`)`

Parameters

- **signum** – Signal number.
- **frame** – Current stack frame.

A signal handler for cleaning up the simulation case on termination or when errors occur. This method can be overridden in subclasses. The base implementation is trivial, but usually doesn't need to be overridden.

An example to connect this method to a signal:

```
>>> from .testing import create_trivial_2d_blk
>>> from .solver import MeshSolver
>>> blk = create_trivial_2d_blk()
>>> cse = MeshCase(basefn='meshcase', mesher=lambda *arg: blk,
...                domaintype=domain.Domain, solvertype=MeshSolver)
>>> cse.info.muted = True
>>> signal.signal(signal.SIGTERM, cse.cleanup)
0
```

An example to call this method explicitly:

```
>>> cse.init()
>>> cse.run()
>>> cse.cleanup()
```

Initialize

`MeshCase.init(level=0)`

Parameters **level** (`int`) – Run level; higher level does less work.

Returns Nothing

Load a block and initialize the solver from the geometry information in the block and conditions in the self case. If parallel run is specified (through domaintype), split the domain and perform corresponding tasks.

For a `MeshCase` to be initialized, some information needs to be supplied to the constructor:

```
>>> cse = MeshCase()
>>> cse.info.muted = True
>>> cse.init()
Traceback (most recent call last):
    ...
TypeError: coercing to Unicode: need string or buffer, NoneType found
```

1. Mesh information. We can provide *meshfn* that specifying the path of a valid mesh file, or provide *mesher*, which is a function that generates the mesh and returns the `solvcon.block.Block` object, like the following code:

```
>>> from solvcon.testing import create_trivial_2d_blk
>>> blk = create_trivial_2d_blk()
>>> cse = MeshCase(mesher=lambda *arg: blk)
>>> cse.info.muted = True
>>> cse.init()
Traceback (most recent call last):
    ...
TypeError: isinstance() arg 2 must be a class, type, or tuple of classes and types
```

2. Type of the spatial domain. This information is used for detemining sequential or parallel execution, and performing related operations:

```
>>> cse = MeshCase(mesher=lambda *arg: blk, domaintype=domain.Domain)
>>> cse.info.muted = True
>>> cse.init()
Traceback (most recent call last):
    ...
TypeError: 'NoneType' object is not callable
```

3.The type of solver. It is used to specify the underlying numerical method:

```
>>> from solvcon.solver import MeshSolver
>>> cse = MeshCase(mesher=lambda *arg: blk, domaintype=domain.Domain,
...                solvertype=MeshSolver)
>>> cse.info.muted = True
>>> cse.init()
Traceback (most recent call last):
    ...
TypeError: cannot concatenate 'str' and 'NoneType' objects
```

4.The base name. It is used to name its output files:

```
>>> cse = MeshCase(
...     mesher=lambda *arg: blk, domaintype=domain.Domain,
...     solvertype=MeshSolver, basefn='meshcase')
>>> cse.info.muted = True
>>> cse.init()
```

Time-March

`MeshCase.`**`run`**(*level=0*)

Parameters **level** (`int`) – Run level; higher level does less work.

Returns Nothing

Temporal loop for the incorporated solver. A simple example:

```
>>> from .testing import create_trivial_2d_blk
>>> from .solver import MeshSolver
>>> blk = create_trivial_2d_blk()
>>> cse = MeshCase(basefn='meshcase', mesher=lambda *arg: blk,
...                domaintype=domain.Domain, solvertype=MeshSolver)
>>> cse.info.muted = True
>>> cse.init()
>>> cse.run()
```

Arrangement

`solvcon.case.`**`arrangements`**

The module-level registry for arrangements.

`MeshCase.`**`arrangements`**

The class-level registry for arrangements.

classmethod `MeshCase.`**`register_arrangement`**(*func*, *casename=None*)

Returns Simulation function.

Return type callable

This class method is a decorator that creates a closure (internal function) that turns the decorated function to an arrangement, and registers the arrangement into the module-level registry and the class-level registry. The decorator function should return a `MeshCase` object `cse`, and the closure performs a simulation run by the following code:

```
try:
    signal.signal(signal.SIGTERM, cse.cleanup)
    signal.signal(signal.SIGINT, cse.cleanup)
    cse.init(level=runlevel)
    cse.run(level=runlevel)
    cse.cleanup()
except:
    cse.cleanup()
    raise
```

The usage of this decorator can be exemplified by the following code, which creates four arrangements (although the first three are erroneous):

```
>>> @MeshCase.register_arrangement
... def arg1():
...     return None
>>> @MeshCase.register_arrangement
... def arg2(wrongname):
...     return None
>>> @MeshCase.register_arrangement
... def arg3(casename):
...     return None
>>> @MeshCase.register_arrangement
... def arg4(casename):
...     from .testing import create_trivial_2d_blk
...     from .solver import MeshSolver
...     blk = create_trivial_2d_blk()
...     cse = MeshCase(basefn='meshcase', mesher=lambda *arg: blk,
...                    domaintype=domain.Domain, solvertype=MeshSolver)
...     cse.info.muted = True
...     return cse
```

The created arrangements are collected to a class attribute `arrangements`, i.e., the class-level registry:

```
>>> sorted(MeshCase.arrangements.keys())
['arg1', 'arg2', 'arg3', 'arg4']
```

The arrangements in the class attribute `arrangements` are also put into a module-level attribute `solvcon.case.arrangements`:

```
>>> arrangements == MeshCase.arrangements
True
```

The first example arrangement is a bad one, because it allows no argument:

```
>>> arrangements.arg1()
Traceback (most recent call last):
  ...
TypeError: arg1() takes no arguments (1 given)
```

The second example arrangement is still a bad one, because although it has an argument, the name of the argument is incorrect:

```
>>> arrangements.arg2()
Traceback (most recent call last):
  ...
TypeError: arg2() got an unexpected keyword argument 'casename'
```

The third example arrangement is a bad one for another reason. It doesn't return a `MeshCase`:

```
>>> arrangements.arg3()
Traceback (most recent call last):
  ...
AttributeError: 'NoneType' object has no attribute 'cleanup'
```

The fourth example arrangement is finally good:

```
>>> arrangements.arg4()
```

2.2 solvcon.solver

Module `solvcon.solver` provides the basic facilities for implementing numerical methods by subclassing `MeshSolver`. The base class is defined as:

class `solvcon.solver.`**`MeshSolver`**(*blk*, *time=0.0*, *time_increment=0.0*, *enable_mesg=False*, ***kw*)

Base class for all solving code that take `Mesh`, which is usually needed to write efficient C/C++ code for implementing numerical methods.

Here're some examples about using `MeshSolver`. The first example shows that we can't directly use it. A vanilla `MeshSolver` can't march:

```
>>> from .testing import create_trivial_2d_blk
>>> svr = MeshSolver(create_trivial_2d_blk())
>>> svr.march(0.0, 0.1, 1)
Traceback (most recent call last):
    ...
TypeError: 'NoneType' object has no attribute '__getitem__'
```

At minimal we need to override the `_MMNAMES` class attribute:

```
>>> class DerivedSolver(MeshSolver):
...     _MMNAMES = MeshSolver.new_method_list()
>>> svr = DerivedSolver(create_trivial_2d_blk())
>>> svr.march(0.0, 0.1, 1)
{}
```

Of course the above derived solver did nothing. Let's see another example solver that does non-trivial things:

```
>>> class ExampleSolver(MeshSolver):
...     _MMNAMES = MeshSolver.new_method_list()
...     @_MMNAMES.register
...     def calcsomething(self, worker=None):
...         self.marchret['key'] = 'value'
>>> svr = ExampleSolver(create_trivial_2d_blk())
>>> svr.march(0.0, 0.1, 1)
{'key': 'value'}
```

Two instance attributes are used to record the temporal information:

`time` = **None**

The current time of the solver. By default, `time` is initialized to `0.0`, which is usually desired value. The default value can be overridden from the constructor.

`time_increment` = **None**

The temporal interval between the current and the next time steps. It is usually referred to as Δt in the numerical literature. By default, `time_increment` is initialized to `0.0`, but the default should be overridden from the constructor.

Four instance attributes are used to track the status of time-marching:

step_current = None
It is an int that records the current step of the solver. It is initialized to 0.

step_global = None
It is similar to step_current, but persists over restart. Without restarts, step_global should be identical to step_current.

substep_run = None
The number of sub-steps that a single time step should be split into. It is initialized to 1 and should be overidden in subclasses if needed.

substep_current = None
The current sub-step of the solver. It is initialized to 0.

Derived classes of MeshSolver should use the following method new_method_list() to make a new class variable _MMNAMES to define numerical methods:

static new_method_list()

Returns An object to be set to _MMNAMES.

Return type _MethodList

In subclasses of MeshSolver, implementors can use this utility method to creates an instance of _MethodList, which should be set to _MMNAMES.

_MMNAMES = None
This class attribute holds the names of the methods to be called in march(). It is of type _MethodList. The default value is None and must be reset in subclasses by calling new_method_list().

Time-Marching

MeshSolver.**march**(*time_current*, *time_increment*, *steps_run*, *worker=None*)

Parameters

- **time_current** (*float*) – Starting time of this set of marching steps.
- **time_increment** (*float*) – Temporal interval Δt of the time step.
- **steps_run** (*int*) – The count of time steps to run.

Returns marchret

This method performs time-marching. The parameters *time_current* and *time_increment* are used to reset the instance attributes time and time_increment, respectively.

There is a nested two-level loop in this method for time-marching. The outer loop iterates for time steps, and the inner loop iterates for sub time steps. The outer loop runs steps_run times, while the inner loop runs substep_run times. In total, the inner loop runs *steps_run* * substep_run times. In each sub time step (in the inner loop), the increment of the attribute time is time_increment/substep_run. The temporal increment per time step is effectively time_increment, with a slight error because of round-off.

Before entering and after leaving the outer loop, premarch and postmarch anchors will be run (through the attribute runanchors). Similarly, before entering and after leaving the inner loop, prefull and postfull anchors will be run. Inside the inner loop of sub steps, before and after executing all the marching methods, presub and postsub anchors will be run. Lastly, before and after invoking every marching method, a pair of anchors will be run. The anchors for a marching method are related to the name of the marching method itself. For example, if a marching method is named “calcsome”, anchor precalcsome will be run before the invocation, and anchor postcalcsome will be run afterward.

Derived classes can set `marchret` dictionary, and `march()` will return the dictionary at the end of execution. The dictionary is reset to empty at the begninning of the execution.

`MeshSolver.`**`marchret`** **= None**

Values to be returned by this solver. It will be set to a `dict` in `march()`.

`MeshSolver.`**`runanchors`** **= None**

This instance attribute is of type `AnchorList`, and the foundation of the anchor mechanism of SOLVCON. An `AnchorList` object like this collects a set of `Anchor` #: objects, and is callable. When being called, `runanchors` iterates the contained `Anchor` objects and invokes the corresponding methods of the individual `Anchor`.

`MeshSolver.`**`der`** **= None**

Derived data container as a `dict`.

class `solvcon.solver.`**`_MethodList`**

A custom `list` that provides a decorator for keeping names of functions.

```
>>> mmnames = _MethodList()
>>> @mmnames.register
... def func_of_a_name():
...     pass
>>> mmnames
['func_of_a_name']
```

This class is a private helper and should only be used in `solvcon.solver`.

Parallel Computing

For distributed-memory parallel computing (i.e., MPI runs), the member `svrn` indicates the serial number (0-based) the object is. The value of `svrn` comes from `blk`. Another member, `nsvr`, is the total number of collaborative solvers in the parallel run, and is initialized to `None`.

2.3 `solvcon.hook`

`MeshHook` performs custom operations at certain pre-defined stages.

class `solvcon.hook.`**`Hook`**(*cse*, ***kw*)

Organizer class for hooking subroutines for BaseCase.

@ivar cse: Case object. @itype cse: BaseCase @ivar info: information output function. @itype info: callable @ivar psteps: the interval number of steps between printing. @itype psteps: int @ivar kws: excessive keywords. @itype kws: dict

2.4 `solvcon.anchor`

class `solvcon.anchor.`**`Anchor`**(*svr*, ***kw*)

Anchor that called by solver objects at various stages.

@ivar svr: the solver object to be attached to. @itype svr: solvcon.solver.Solver @ivar kws: excessive keywords. @itype kws: dict

3 References

3.1 ustmesh_2d_sample.geo

```
/*
 * A Gmsh template file for a rectangle domain.
 */
lc = 0.1;
// vertices.
Point(1) = {4,1,0,lc};
Point(2) = {2,2,0,lc};
Point(3) = {0,1,0,lc};
Point(4) = {0,0,0,lc};
Point(5) = {4,0,0,lc};
Point(6) = {3.5,  1,0,lc};
Point(7) = {  3,  1,0,lc};
Point(8) = {  3,0.5,0,lc};
Point(9) = {3.5,0.5,0,lc};
Point(10) = {  1,  1,0,lc};
Point(11) = {0.5,  1,0,lc};
Point(12) = {0.5,0.5,0,lc};
Point(13) = {  1,0.5,0,lc};
Point(14) = {  2,0.8,0,lc};
Point(15) = {1.5,0.2,0,lc};
Point(16) = {2.5,0.2,0,lc};
// lines.
Line(1) = {1,2};
Line(2) = {2,3};
Line(3) = {3,4};
Line(4) = {4,5};
Line(5) = {5,1};
Line(6) = {6,7};
Line(7) = {7,8};
Line(8) = {8,9};
Line(9) = {9,6};
Line(10) = {10,11};
Line(11) = {11,12};
Line(12) = {12,13};
Line(13) = {13,10};
Line(14) = {14,15};
Line(15) = {15,16};
Line(16) = {16,14};
// surface.
Line Loop(1) = {1,2,3,4,5};
Line Loop(2) = {6,7,8,9};
Line Loop(3) = {10,11,12,13};
Line Loop(4) = {14,15,16};
Plane Surface(1) = {1,2,3,4};
// physics.
Physical Line("upper") = {1,2};
Physical Line("left") = {3};
Physical Line("lower") = {4};
Physical Line("right") = {5};
Physical Line("rwin") = {6,7,8,9};
Physical Line("lwin") = {10,11,12,13};
Physical Line("cwin") = {14,15,16};
Physical Surface("domain") = {1};
```

```
// vim: set ai et nu ff=unix ft=c:
```

The following command generate the mesh:

```
gmsh ustmesh_2d_sample.geo -3
```

The following command converts the mesh to a VTK file for ParaView:

```
scg mesh ustmesh_2d_sample.msh ustmesh_2d_sample.vtk
```

References

[Mavriplis97] D. J. Mavriplis, Unstructured grid techniques, Annual Review of Fluid Mechanics 29. (1997)

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