SimPhoNy-Mayavi Documentation

Release 0.2.0

SimPhoNy FP7 Collaboration

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Contents

A plugin-library for the Simphony framework (http://www.simphony-project.eu/) to provide visualization support of the CUDS highlevel components.

CHAPTER 1

Repository

Simphony-mayavi is hosted on github: https://github.com/simphony/simphony-mayavi

CHAPTER 2

Requirements

- mayavi >= 4.4.0
- simphony >= 0.1.3, < 0.2.0

2.1 Optional requirements

To support the documentation built you need the following packages:

- sphinx >= 1.2.3
- sectiondoc commit 8a0c2be, https://github.com/enthought/sectiondoc
- trait-documenter, https://github.com/enthought/trait-documenter
- mock

Alternative running **`pip install -r doc_requirements`** should install the minimum necessary components for the documentation built.

CHAPTER 3

Installation

The package requires python 2.7.x, installation is based on setuptools:

```
# build and install
python setup.py install
```

or:

```
# build for in-place development
python setup.py develop
```

CHAPTER 4

Testing

To run the full test-suite run:

```
python -m unittest discover
```

CHAPTER 5

Documentation

To build the documentation in the doc/build directory run:

```
python setup.py build_sphinx
```

Note:

- One can use the –help option with a setup.py command to see all available options.
- The documentation will be saved in the `./build` directory.

CHAPTER 6

Usage

After installation the user should be able to import the `mayavi` visualization plugin module by:

```
from simphony.visualisation import mayavi_tools
mayavi_tools.show(cuds)
```

CHAPTER 7

Directory structure

- simphony-mayavi – Main package folder.
  - sources – Wrap CUDS objects to provide Mayavi Sources.
  - cuds – Wrap VTK Dataset objects to provide the CUDS container api.
  - core – Utility classes and tools to manipulate vtk and cuds objects.
- examples – Holds examples of loading and visualising SimPhoNy objects with simphony-mayavi.
- doc – Documentation related files: - The rst source files for the documentation

CHAPTER 8

User Manual

8.1 SimPhoNy

Mayavi tools are available in the simphony library through the visualisation plug-in named `mayavi_tools`.

e.g:

```
from simphony.visualisation import mayavi_tools
```

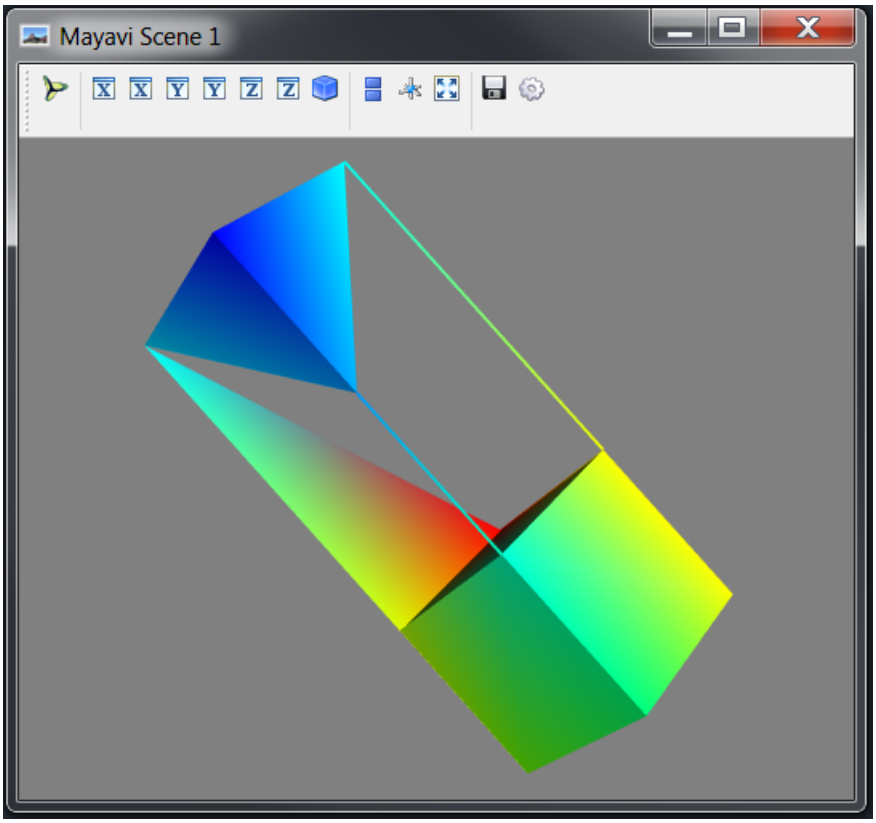
8.1.1 Visualizing CUDS

The *show()* function is available to visualise any top level CUDS container. The function will open a window containing a 3D view and a mayavi toolbar. Interaction allows the common mayavi operations.

Mesh example

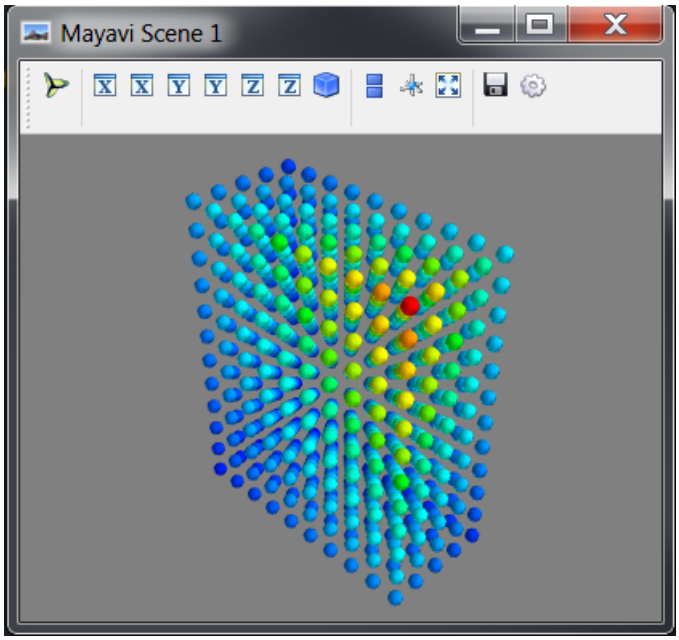
```
from numpy import array

from simphony.cuds.mesh import Mesh, Point, Cell, Edge, Face
from simphony.core.data_container import DataContainer


points = array([
    [0, 0, 0], [1, 0, 0], [0, 1, 0], [0, 0, 1],
    [2, 0, 0], [3, 0, 0], [3, 1, 0], [2, 1, 0],
    [2, 0, 1], [3, 0, 1], [3, 1, 1], [2, 1, 1]],
    'f')

cells = [
    [0, 1, 2, 3],  # tetra
    [4, 5, 6, 7, 8, 9, 10, 11]]  # hex

faces = [[2, 7, 11]]
edges = [[1, 4], [3, 8]]

mesh = Mesh('example')

# add points
uids = [
    mesh.add_point(
```

```
        Point(coordinates=point, data=DataContainer(TEMPERATURE=index)))
    for index, point in enumerate(points)]

# add edges
edge_uids = [
    mesh.add_edge(
        Edge(points=[uids[index] for index in element]))
    for index, element in enumerate(edges)]

# add faces
face_uids = [
    mesh.add_face(
        Face(points=[uids[index] for index in element]))
    for index, element in enumerate(faces)]

# add cells
cell_uids = [
    mesh.add_cell(
        Cell(points=[uids[index] for index in element]))
    for index, element in enumerate(cells)]


if __name__ == '__main__':
    from simphony.visualisation import mayavi_tools

    # Visualise the Mesh object
    mayavi_tools.show(mesh)
```



Lattice example

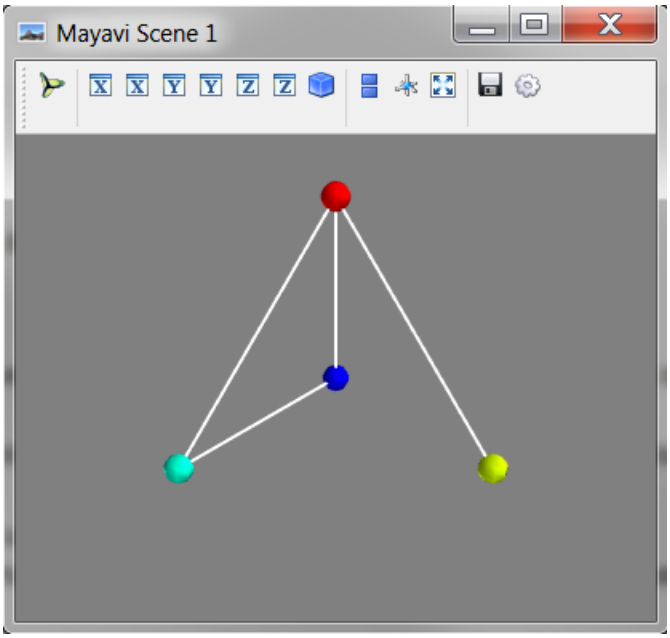
```
import numpy

from simphony.cuds.lattice import make_cubic_lattice
from simphony.core.cuba import CUBA

lattice = make_cubic_lattice('test', 0.1, (5, 10, 12))

for node in lattice.iter_nodes():
    index = numpy.array(node.index) + 1.0
    node.data[CUBA.TEMPERATURE] = numpy.prod(index)
    lattice.update_node(node)


if __name__ == '__main__':
    from simphony.visualisation import mayavi_tools

    # Visualise the Lattice object
    mayavi_tools.show(lattice)
```



Particles example

```
from numpy import array

from simphony.cuds.particles import Particles, Particle, Bond
from simphony.core.data_container import DataContainer

points = array([[0, 0, 0], [1, 0, 0], [0, 1, 0], [0, 0, 1]], 'f')
bonds = array([[0, 1], [0, 3], [1, 3, 2]])
temperature = array([10., 20., 30., 40.])

particles = Particles('test')
```

```
uids = []
for index, point in enumerate(points):
    uid = particles.add_particle(
        Particle(
            coordinates=point,
            data=DataContainer(TEMPERATURE=temperature[index])))
    uids.append(uid)

for indices in bonds:
    particles.add_bond(Bond(particles=[uids[index] for index in indices]))


if __name__ == '__main__':
    from simphony.visualisation import mayavi_tools

    # Visualise the Particles object
    mayavi_tools.show(particles)
```



8.1.2 Create VTK backed CUDS

Three objects (i.e class:~. *VTKMesh*, class:~.*VTKLattice*, ~.*VTKParticles*) that wrap a VTK dataset and provide the CUDS top level container API are also available. The vtk backed objects are expected to provide memory and some speed advantages when Mayavi aided visualisation and processing is a major part of the working session. The provided examples are equivalent to the ones in section *Visualizing CUDS*.

Note: Note all CUBA keys are supported for the *data* attribute of the contained items. Please see documentation for more details.

VTK Mesh example

```
from numpy import array

from simphony.cuds.mesh import Point, Cell, Edge, Face
from simphony.core.data_container import DataContainer
from simphony.visualisation import mayavi_tools


points = array([
    [0, 0, 0], [1, 0, 0], [0, 1, 0], [0, 0, 1],
    [2, 0, 0], [3, 0, 0], [3, 1, 0], [2, 1, 0],
    [2, 0, 1], [3, 0, 1], [3, 1, 1], [2, 1, 1]],
    'f')

cells = [
    [0, 1, 2, 3],  # tetra
    [4, 5, 6, 7, 8, 9, 10, 11]]  # hex

faces = [[2, 7, 11]]
edges = [[1, 4], [3, 8]]

mesh = mayavi_tools.VTKMesh('example')

# add points
uids = [
    mesh.add_point(
        Point(coordinates=point, data=DataContainer(TEMPERATURE=index)))
    for index, point in enumerate(points)]

# add edges
edge_uids = [
    mesh.add_edge(
        Edge(points=[uids[index] for index in element]))
    for index, element in enumerate(edges)]

# add faces
face_uids = [
    mesh.add_face(
        Face(points=[uids[index] for index in element]))
    for index, element in enumerate(faces)]

# add cells
cell_uids = [
    mesh.add_cell(
        Cell(points=[uids[index] for index in element]))
    for index, element in enumerate(cells)]


if __name__ == '__main__':

    # Visualise the Mesh object
    mayavi_tools.show(mesh)
```

VTK Lattice example

```
import numpy

from simphony.core.cuba import CUBA
from simphony.visualisation import mayavi_tools

lattice = mayavi_tools.VTKLattice.empty(
    'test', 'Cubic', (0.1, 0.1, 0.1), (5, 10, 12), (0, 0, 0))

for node in lattice.iter_nodes():
    index = numpy.array(node.index) + 1.0
    node.data[CUBA.TEMPERATURE] = numpy.prod(index)
    lattice.update_node(node)


if __name__ == '__main__':

    # Visualise the Lattice object
    mayavi_tools.show(lattice)
```

VTK Particles example

```
from numpy import array

from simphony.core.data_container import DataContainer
from simphony.cuds.particles import Particle, Bond
from simphony.visualisation import mayavi_tools

points = array([[0, 0, 0], [1, 0, 0], [0, 1, 0], [0, 0, 1]], 'f')
bonds = array([[0, 1], [0, 3], [1, 3, 2]])
temperature = array([10., 20., 30., 40.])

particles = mayavi_tools.VTKParticles('test')
uids = []
for index, point in enumerate(points):
    uid = particles.add_particle(
        Particle(
            coordinates=point,
            data=DataContainer(TEMPERATURE=temperature[index])))
    uids.append(uid)

for indices in bonds:
    particles.add_bond(Bond(particles=[uids[index] for index in indices]))


if __name__ == '__main__':

    # Visualise the Particles object
    mayavi_tools.show(particles)
```

8.1.3 Adapting VTK datasets

The *adapt2cuds()* function is available to wrap common VTK datsets into top level CUDS containers. The function will attempt to automatically adapt the (t)vtk Dataset into a CUDS container. When automatic conversion

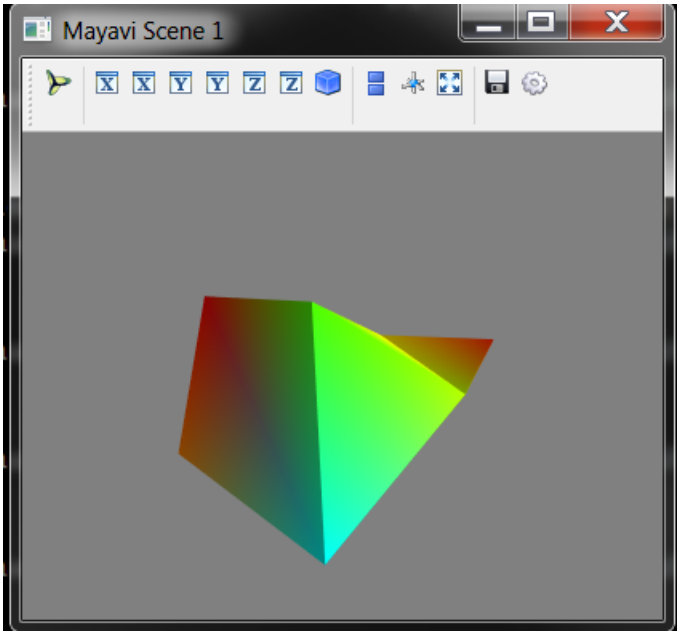
fails the user can always force the kind of the container to adapt into. Furthermore, the user can define the mapping of the included attribute data into corresponding CUBA keys (a common case for vtk datasets that come from vtk reader objects).

Example

```
from numpy import array, random
from tvtk.api import tvtk
from simphony.core.cuba import CUBA
from simphony.visualisation import mayavi_tools


def create_unstructured_grid(array_name='scalars'):
    points = array(
        [[0, 1.2, 0.6], [1, 0, 0], [0, 1, 0], [1, 1, 1],  # tetra
         [1, 0, -0.5], [2, 0, 0], [2, 1.5, 0], [0, 1, 0],
         [1, 0, 0], [1.5, -0.2, 1], [1.6, 1, 1.5], [1, 1, 1]], 'f')  # Hex
    cells = array(
        [4, 0, 1, 2, 3,  # tetra
         8, 4, 5, 6, 7, 8, 9, 10, 11])  # hex
    offset = array([0, 5])
    tetra_type = tvtk.Tetra().cell_type  # VTK_TETRA == 10
    hex_type = tvtk.Hexahedron().cell_type  # VTK_HEXAHEDRON == 12
    cell_types = array([tetra_type, hex_type])
    cell_array = tvtk.CellArray()
    cell_array.set_cells(2, cells)
    ug = tvtk.UnstructuredGrid(points=points)
    ug.set_cells(cell_types, offset, cell_array)
    scalars = random.random(points.shape[0])
    ug.point_data.scalars = scalars
    ug.point_data.scalars.name = array_name
    scalars = random.random((2, 1))
    ug.cell_data.scalars = scalars
    ug.cell_data.scalars.name = array_name
    return ug

# Create an example
vtk_dataset = create_unstructured_grid()

# Adapt to a mesh by converting the scalars attribute to TEMPERATURE
container = mayavi_tools.adapt2cuds(
    vtk_dataset, 'test',
    rename_arrays={'scalars': CUBA.TEMPERATURE})

if __name__ == '__main__':

    # Visualise the Lattice object
    mayavi_tools.show(container)
```

8.1.4 Loading into CUDS

The *load()* function is available to load mayavi readable files (e.g. VTK xml format) into top level CUDS containers. Using `load` the user can import inside their simulation scripts files that have been created by other simulation application and export data into one of the Mayavi supported formats.



8.2 Mayavi2

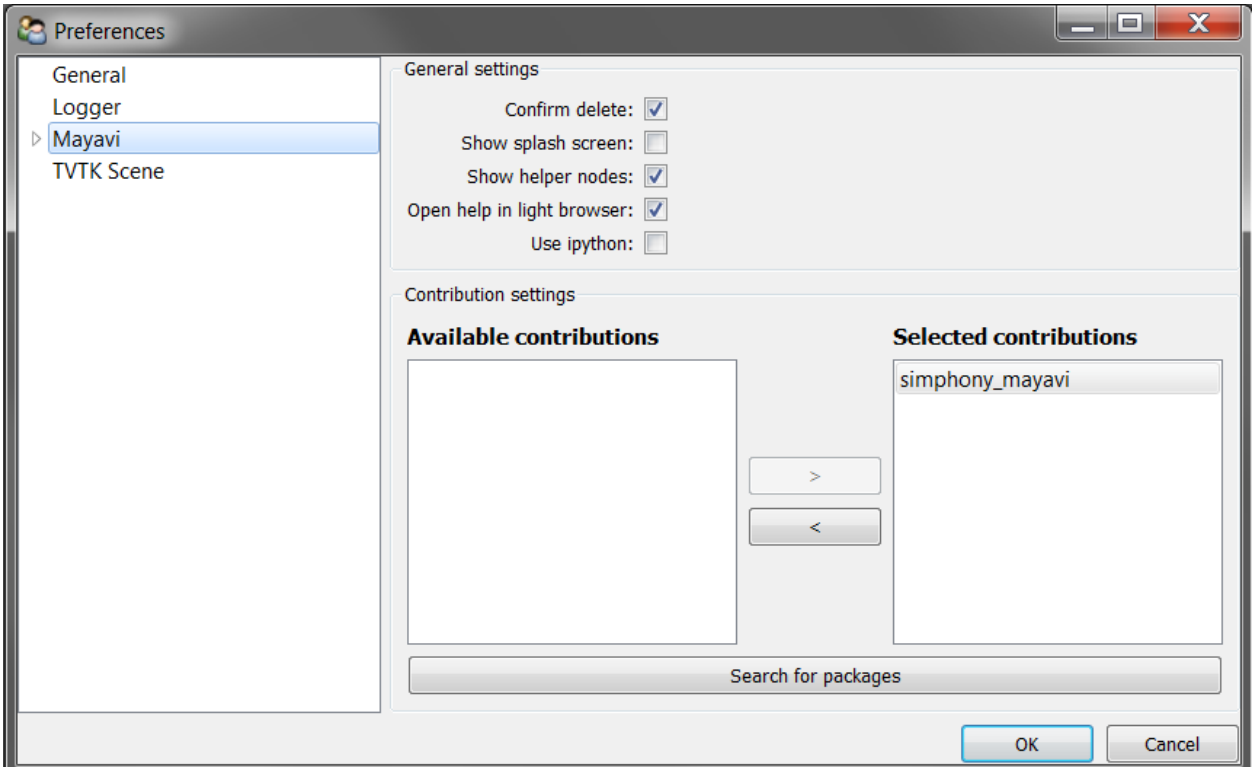
The Simphony-Mayavi library provides a plugin for Mayavi2 to easily create mayavi `Source` instances from SimPhoNy CUDS containers and files. With the provided tools one can use the SimPhoNy libraries to work inside the Mayavi2 application, as it is demonstrated in the examples.

Setup plugin

To setup the mayavi2 plugin one needs to make sure that the simpony_mayavi plugin has been selected and activated in the Mayavi2 preferences dialog.

Source from a CUDS Mesh

```
from numpy import array
from mayavi.scripts import mayavi2

from simphony.cuds.mesh import Mesh, Point, Cell, Edge, Face
from simphony.core.data_container import DataContainer


points = array([
    [0, 0, 0], [1, 0, 0], [0, 1, 0], [0, 0, 1],
    [2, 0, 0], [3, 0, 0], [3, 1, 0], [2, 1, 0],
    [2, 0, 1], [3, 0, 1], [3, 1, 1], [2, 1, 1]],
    'f')

cells = [
    [0, 1, 2, 3],  # tetra
    [4, 5, 6, 7, 8, 9, 10, 11]]  # hex

faces = [[2, 7, 11]]
```




```
edges = [[1, 4], [3, 8]]

container = Mesh('test')

# add points
uids = [
    container.add_point(
        Point(coordinates=point, data=DataContainer(TEMPERATURE=index)))
    for index, point in enumerate(points)]

# add edges
edge_uids = [
    container.add_edge(
        Edge(
            points=[uids[index] for index in element],
            data=DataContainer(TEMPERATURE=index + 20)))
    for index, element in enumerate(edges)]

# add faces
face_uids = [
    container.add_face(
        Face(
            points=[uids[index] for index in element],
            data=DataContainer(TEMPERATURE=index + 30)))
    for index, element in enumerate(faces)]

# add cells
cell_uids = [
    container.add_cell(
        Cell(
```

```
            points=[uids[index] for index in element],
            data=DataContainer(TEMPERATURE=index + 40)))
    for index, element in enumerate(cells)]


# Now view the data.
@mayavi2.standalone
def view():
    from mayavi.modules.surface import Surface
    from simphony_mayavi.sources.api import CUDSSource

    mayavi.new_scene()  # noqa
    src = CUDSSource(cuds=container)
    mayavi.add_source(src)  # noqa
    s = Surface()
    mayavi.add_module(s)  # noqa

if __name__ == '__main__':
    view()
```

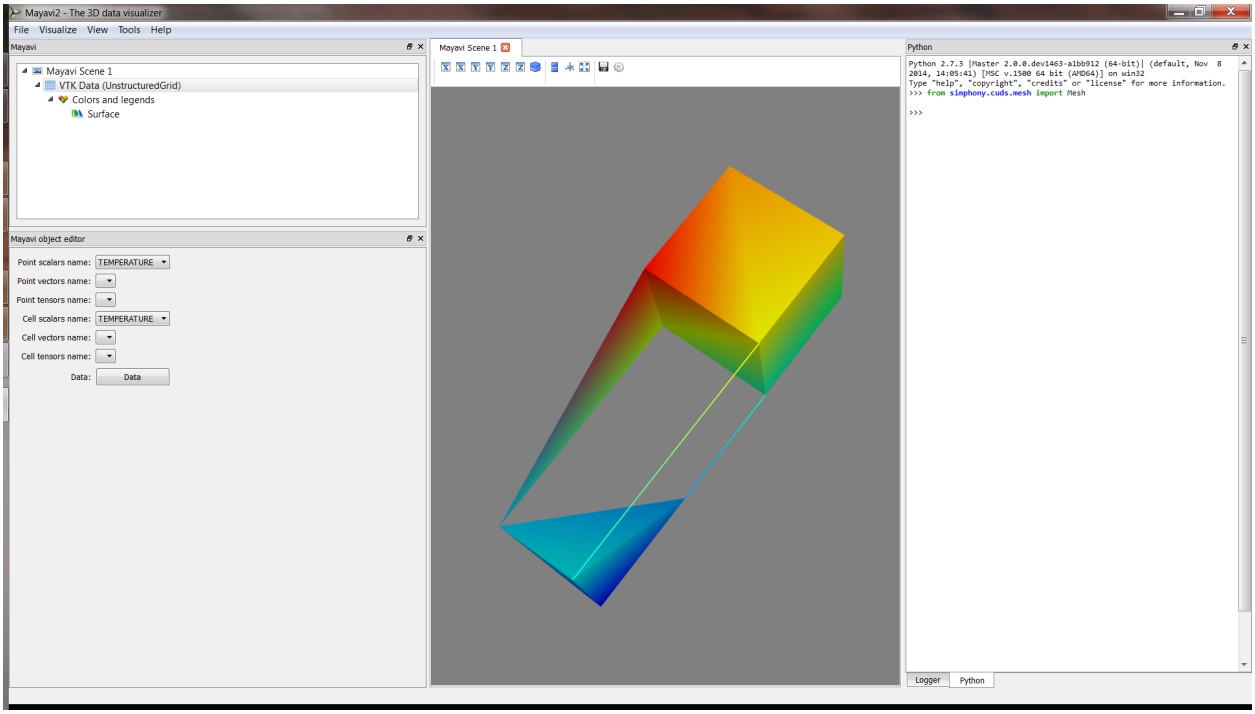


Fig. 8.1: Use the provided example to create a CUDS Mesh and visualise directly in Mayavi2.

Source from a CUDS Lattice

```
import numpy

from mayavi.scripts import mayavi2
from simphony.cuds.lattice import (
    make_hexagonal_lattice, make_cubic_lattice, make_square_lattice)
from simphony.core.cuba import CUBA
```

```
hexagonal = make_hexagonal_lattice('test', 0.1, (5, 4))
square = make_square_lattice('test', 0.1, (5, 4))
cubic = make_cubic_lattice('test', 0.1, (5, 10, 12))


def add_temperature(lattice):
    for node in lattice.iter_nodes():
        index = numpy.array(node.index) + 1.0
        node.data[CUBA.TEMPERATURE] = numpy.prod(index)
        lattice.update_node(node)

add_temperature(hexagonal)
add_temperature(cubic)
add_temperature(square)


# Now view the data.
@mayavi2.standalone
def view(lattice):
    from mayavi.modules.glyph import Glyph
    from simphony_mayavi.sources.api import CUDSSource
    mayavi.new_scene()  # noqa
    src = CUDSSource(cuds=lattice)
    mayavi.add_source(src)  # noqa
    g = Glyph()
    gs = g.glyph.glyph_source
    gs.glyph_source = gs.glyph_dict['sphere_source']
    g.glyph.glyph.scale_factor = 0.02
    g.glyph.scale_mode = 'data_scaling_off'
    mayavi.add_module(g)  # noqa

if __name__ == '__main__':
    view(cubic)
```

Source for a CUDS Particles

```
from numpy import array
from mayavi.scripts import mayavi2

from simphony.cuds.particles import Particles, Particle, Bond
from simphony.core.data_container import DataContainer

points = array([[0, 0, 0], [1, 0, 0], [0, 1, 0], [0, 0, 1]], 'f')
bonds = array([[0, 1], [0, 3], [1, 3, 2]])
temperature = array([10., 20., 30., 40.])

container = Particles('test')
uids = []
for index, point in enumerate(points):
    uid = container.add_particle(
        Particle(
            coordinates=point,
            data=DataContainer(TEMPERATURE=temperature[index])))
    uids.append(uid)

for indices in bonds:
```

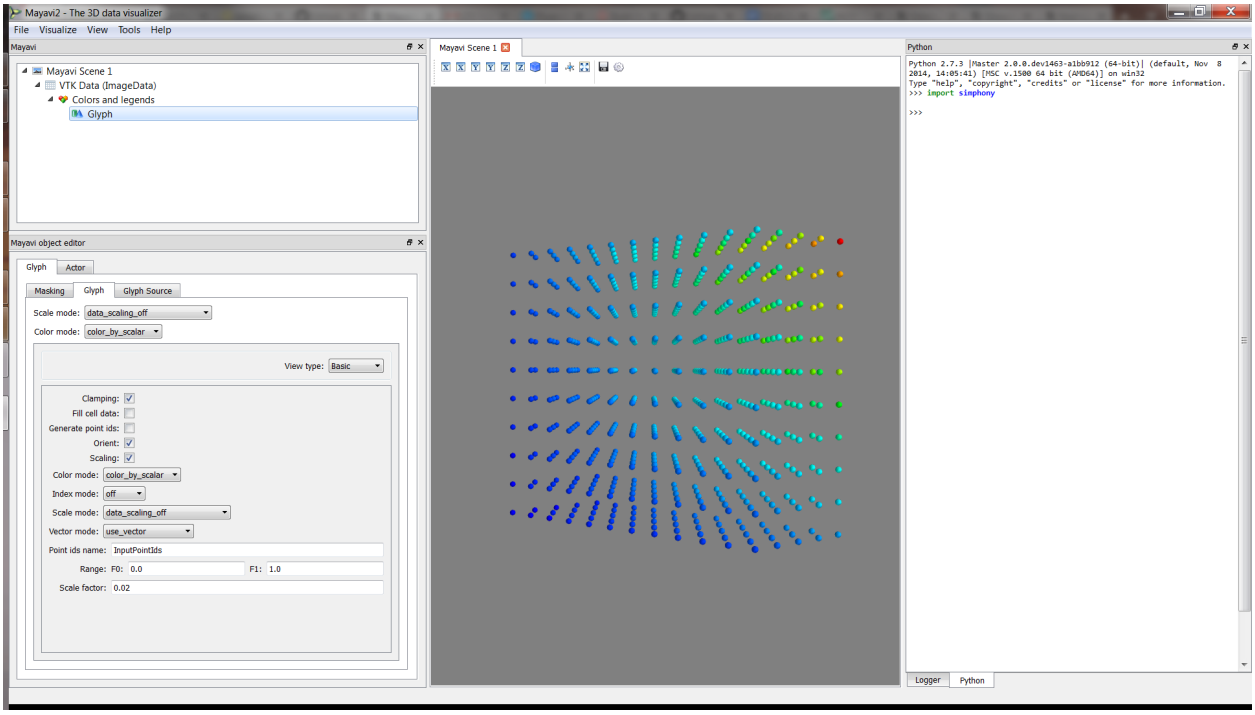


Fig. 8.2: Use the provided example to create a CUDS Lattice and visualise directly in Mayavi2.

```
    container.add_bond(Bond(particles=[uids[index] for index in indices]))


# Now view the data.
@mayavi2.standalone
def view():
    from mayavi.modules.surface import Surface
    from mayavi.modules.glyph import Glyph
    from simphony_mayavi.sources.api import CUDSSource

    mayavi.new_scene()  # noqa
    src = CUDSSource(cuds=container)
    mayavi.add_source(src)  # noqa
    g = Glyph()
    gs = g.glyph.glyph_source
    gs.glyph_source = gs.glyph_dict['sphere_source']
    g.glyph.glyph.scale_factor = 0.05
    g.glyph.scale_mode = 'data_scaling_off'
    s = Surface()
    s.actor.mapper.scalar_visibility = False

    mayavi.add_module(g)  # noqa
    mayavi.add_module(s)  # noqa

if __name__ == '__main__':
    view()
```

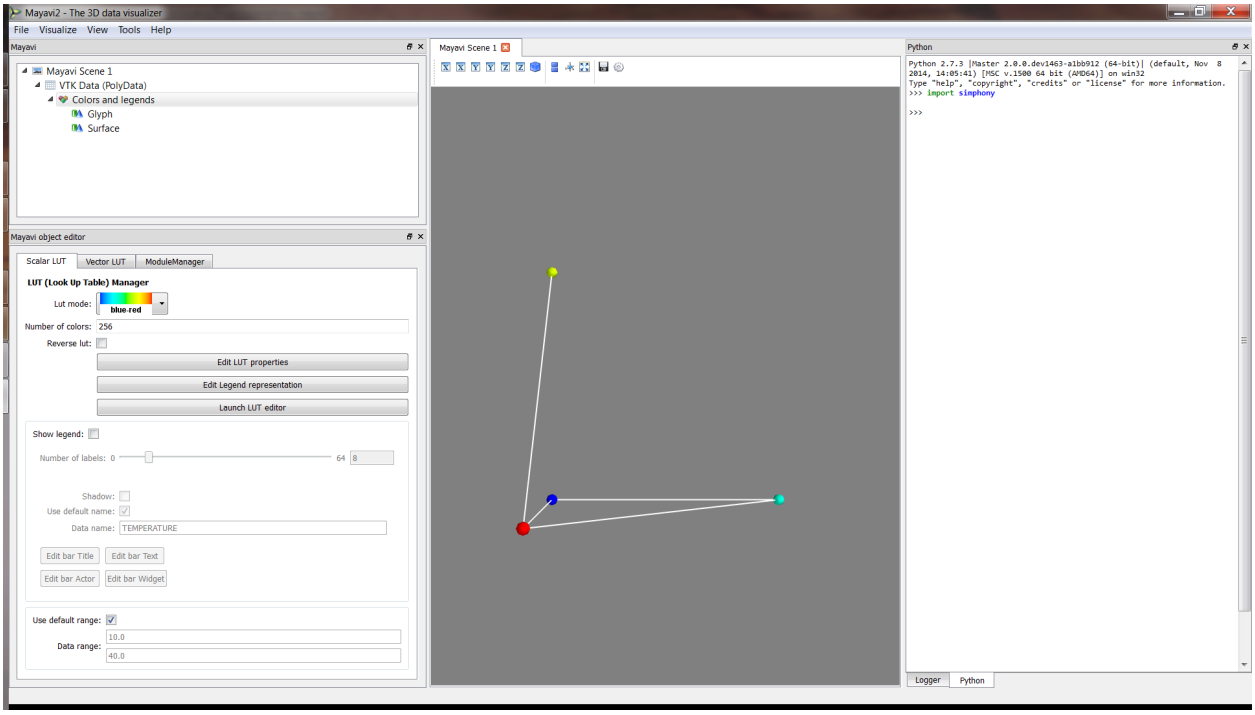


Fig. 8.3: Use the provided example to create a CUDS Particles and visualise directly in Mayavi2.

Source from a CUDS File

```
from contextlib import closing

from mayavi.scripts import mayavi2
import numpy
from numpy import array
from simphony.core.data_container import DataContainer
from simphony.core.cuba import CUBA
from simphony.cuds.particles import Particles, Particle, Bond
from simphony.cuds.lattice import (
    make_hexagonal_lattice, make_cubic_lattice, make_square_lattice)
from simphony.cuds.mesh import Mesh, Point, Cell, Edge, Face
from simphony.io.h5_cuds import H5CUDS

points = array([[0, 0, 0], [1, 0, 0], [0, 1, 0], [0, 0, 1]], 'f')
bonds = array([[0, 1], [0, 3], [1, 3, 2]])
temperature = array([10., 20., 30., 40.])

particles = Particles('particles_example')
uids = []
for index, point in enumerate(points):
    uid = particles.add_particle(
        Particle(
            coordinates=point,
            data=DataContainer(TEMPERATURE=temperature[index])))
    uids.append(uid)
for indices in bonds:
    particles.add_bond(Bond(particles=[uids[index] for index in indices]))
```

```
hexagonal = make_hexagonal_lattice('hexagonal', 0.1, (5, 4))
square = make_square_lattice('square', 0.1, (5, 4))
cubic = make_cubic_lattice('cubic', 0.1, (5, 10, 12))


def add_temperature(lattice):
    for node in lattice.iter_nodes():
        index = numpy.array(node.index) + 1.0
        node.data[CUBA.TEMPERATURE] = numpy.prod(index)
        lattice.update_node(node)


def add_velocity(lattice):
    for node in lattice.iter_nodes():
        node.data[CUBA.VELOCITY] = node.index
        lattice.update_node(node)

add_temperature(hexagonal)
add_temperature(cubic)
add_temperature(square)
add_velocity(hexagonal)
add_velocity(cubic)
add_velocity(square)

points = array([
    [0, 0, 0], [1, 0, 0], [0, 1, 0], [0, 0, 1],
    [2, 0, 0], [3, 0, 0], [3, 1, 0], [2, 1, 0],
    [2, 0, 1], [3, 0, 1], [3, 1, 1], [2, 1, 1]],
    'f')

cells = [
    [0, 1, 2, 3],  # tetra
    [4, 5, 6, 7, 8, 9, 10, 11]]  # hex

faces = [[2, 7, 11]]
edges = [[1, 4], [3, 8]]

mesh = Mesh('mesh_example')

# add points
uids = [
    mesh.add_point(
        Point(coordinates=point, data=DataContainer(TEMPERATURE=index)))
    for index, point in enumerate(points)]

# add edges
edge_uids = [
    mesh.add_edge(
        Edge(
            points=[uids[index] for index in element],
            data=DataContainer(TEMPERATURE=index + 20)))
    for index, element in enumerate(edges)]

# add faces
face_uids = [
    mesh.add_face(
        Face(
            points=[uids[index] for index in element],
```

```
            data=DataContainer(TEMPERATURE=index + 30)))
    for index, element in enumerate(faces)]

# add cells
cell_uids = [
    mesh.add_cell(
        Cell(
            points=[uids[index] for index in element],
            data=DataContainer(TEMPERATURE=index + 40)))
    for index, element in enumerate(cells)]


# save the data into cuds.
with closing(H5CUDS.open('example.cuds', 'w')) as handle:
    handle.add_mesh(mesh)
    handle.add_particles(particles)
    handle.add_lattice(hexagonal)
    handle.add_lattice(cubic)
    handle.add_lattice(square)


# Now view the data.
@mayavi2.standalone
def view():
    mayavi.new_scene()  # noqa

if __name__ == '__main__':
    view()
```

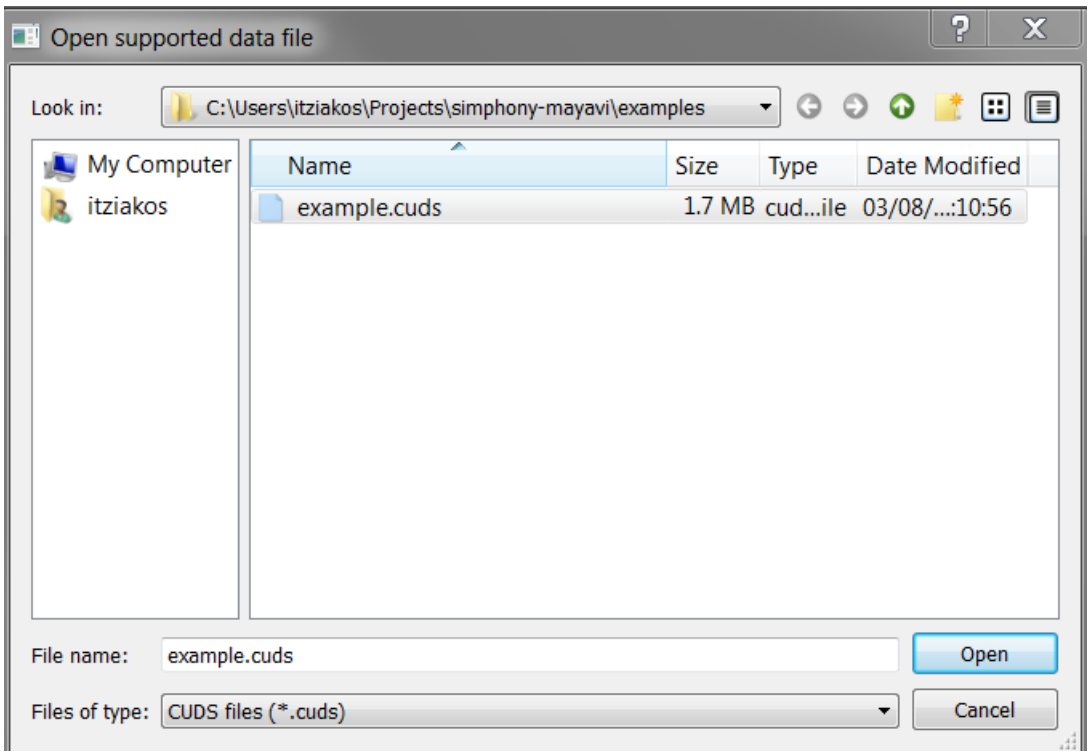


Fig. 8.4: Cuds files are supported in the `Open File..` dialog. After running the provided example load the `example.cuds` file into Mayavi2.

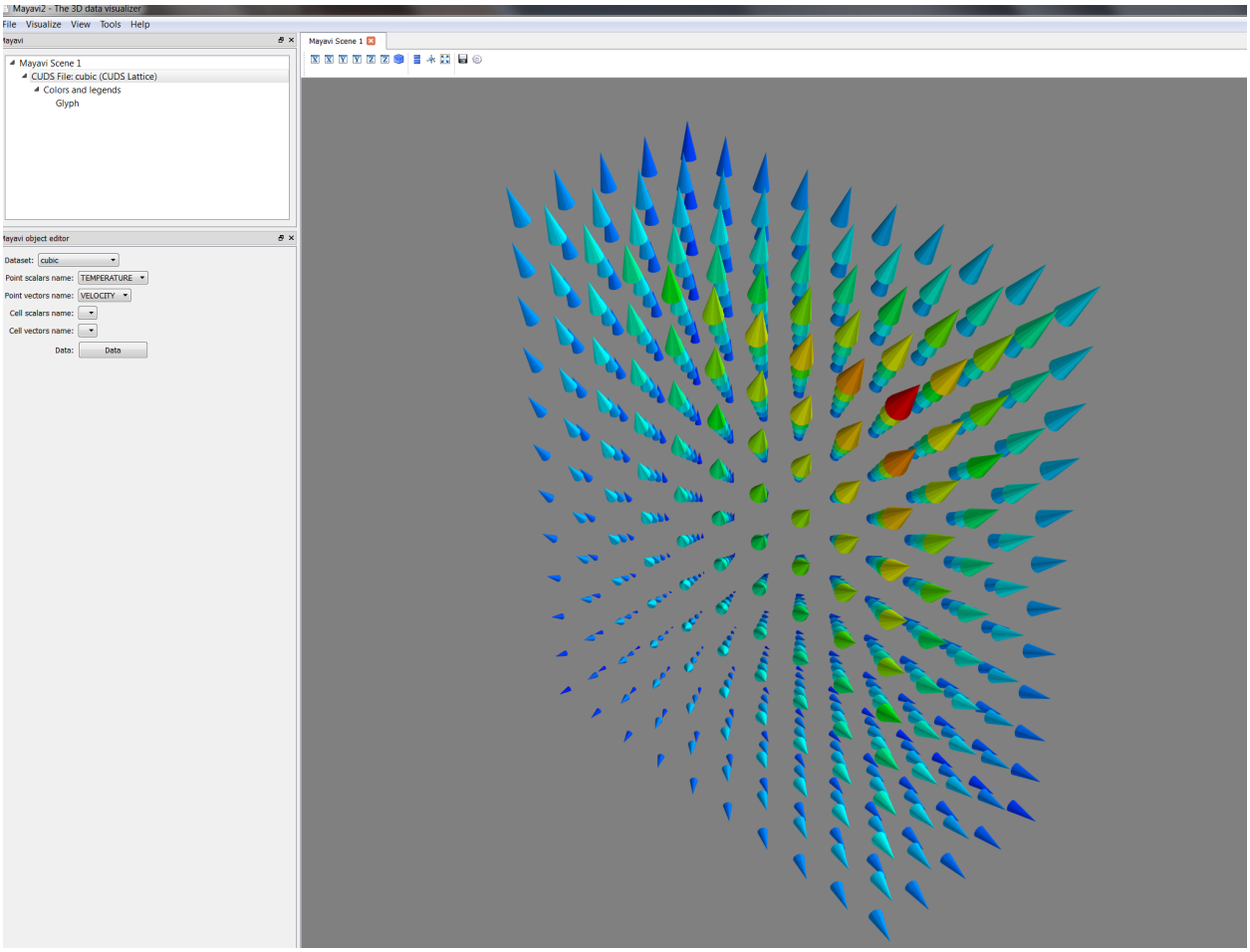


Fig. 8.5: When loaded a CUDSFile is converted into a Mayavi Source and the user can add normal Mayavi modules to visualise the currently selected CUDS container from the available containers in the file.

In the example we load the container named `cubic` and attach the Glyph module to draw a cone at each point to visualise `TEMPERATURE` and `VELOCITY` in the Mayavi Scene.

CHAPTER 9

API Reference

9.1 Plugin module

This module `simphony_mayavi.plugin` provides a set of tools to visualize CUDS objects. The tools are also available as a visualisation plug-in to the simphony library.

`simphony_mayavi.show.`**`show`**(*cuds*)
Show the cuds objects using the default visualisation.

Parameters **`cuds`** – A top level cuds object (e.g. a mesh). The method will detect the type of object and create the appropriate visualisation.

`simphony_mayavi.snapshot.`**`snapshot`**(*cuds*, *filename*)
Shave a snapshot of the cuds object using the default visualisation.

Parameters

- **`cuds`** – A top level cuds object (e.g. a mesh). The method will detect the type of object and create the appropriate visualisation.
- **`filename`** (*string*) – The filename to use for the output file.

`simphony_mayavi.adapt2cuds.`**`adapt2cuds`**(*data_set*, *name='CUDS container'*, *kind=None*, *rename_arrays=None*)
Adapt a TVTK dataset to a CUDS container.

Parameters

- **`data_set`** (*tvtk.Dataset*) – The dataset to import and wrap into CUDS container.
- **`name`** (*string*) – The name of the CUDS container. Default is 'CUDS container'.

kind [{'mesh', 'lattice', 'particles'}] The kind of the container to return. Default is None, where the function will use some heuristics to infer the most appropriate type of CUDS container to return

rename_array [dict] Dictionary mapping the array names used in the dataset object to their related CUBA keywords that will be used in the returned CUDS container.

Note: When set a shallow copy of the input data_set is created and used by the related vtk -> cuds wrapper.

Raises

ValueError: When `kind` is not a valid CUDS container type.

TypeError: When it is not possible to wrap the provided data_set.

simphony_mayavi.load.**load**(*filename*, *name=None*, *kind=None*, *rename_arrays=None*)
Load the file data into a CUDS container.

Parameters

- **filename** (*string*) – The file name of the file to load.
- **name** (*string*) – The name of the returned CUDS container. Default is 'CUDS container'.

kind [{'mesh', 'lattice', 'particles'}] The kind of the container to return. Default is None, where the function will use some heuristics to infer the most appropriate type of CUDS container to return (using adapt2cuds).

rename_array [dict] Dictionary mapping the array names used in the dataset object to their related CUBA keywords that will be used in the returned CUDS container.

Note: Only CUBA keywords are supported for array names so use this option to provide a translation mapping to the CUBA keys.

9.2 Sources module

A module containing objects that wrap CUDS objects and files to Mayavi compatible sources. Please use the simphony_mayavi.sources.api module to access the provided tools.

Classes

CUDSSource	A mayavi source of a SimPhoNy CUDS container.
CUDSFileSource	A mayavi source of a SimPhoNy CUDS File.

9.2.1 Description

class simphony_mayavi.sources.cuds_source.**CUDSSource**
Bases: mayavi.sources.vtk_data_source.VTKDataSource

A mayavi source of a SimPhoNy CUDS container.

cuds = Property(depends_on='_cuds')
The CUDS container

output_info = PipelineInfo(datasets=['image_data', 'poly_data', 'unstructured_grid'], attribute_types=['any'], attribu
Output information for the processing pipeline.

class simphony_mayavi.sources.cuds_file_source.**CUDSFileSource**
Bases: *simphony_mayavi.sources.cuds_source.CUDSSource*

A mayavi source of a SimPhoNy CUDS File.

dataset = DEnum(values_name='datasets')
The name of the CUDS container that is currently loaded.

datasets = ListStr
The names of the contained datasets.

file_path = Instance(FilePath, '', desc='the current file name')
The file path of the cuds file to read.

initialize(*filename*)
Initialise the CUDS file source.

start()

update()

9.3 Cuds module

A module containing tvtk dataset wrappers to simphony CUDS containers.

Classes

VTKParticles(name[, data, data_set, mappings])	Constructor.
VTKMesh(name[, data, data_set, mappings])	Constructor.
VTKLattice(name, type_, data_set[, data])	Constructor.

9.3.1 Description

class simphony_mayavi.cuds.vtk_particles.**VTKParticles**(*name*, *data=None*, *data_set=None*, *mappings=None*)
Bases: simphony.cuds.abstractparticles.ABCParticles

Constructor.

Parameters

- **name** (*string*) – The name of the container.
- **data** (*DataContainer*) – The data attribute to attach to the container. Default is None.
- **data_set** (*tvtk.DataSet*) – The dataset to wrap in the CUDS api. Default is None which will create a tvtk.PolyData
- **mappings** (*dict*) – A dictionary of mappings for the particle2index, index2particle, bond2index and bond2element. Should be provided if the particles and bonds described in data_set are already assigned uids. Default is None and will result in the uid <-> index mappings being generated at construction.

add_bond(*bond*)
Adds the bond to the container.

Also like with particles, if the bond has a defined uid, it won't add the bond if a bond with the same uid already exists, and if the bond has no uid the particle container will generate an uid. If the user wants to replace an existing bond in the container there is an 'update_bond' method for that purpose.

Parameters **bond** (*Bond*) – the new bond that will be included in the container.

Returns **uid** (*uuid.UID*) – The uid of the added bond.

Raises **ValueError** – When the new particle already exists in the container.

Examples

Add a bond to a Particles container.

```
>>> bond = Bond()
>>> particles = Particles(name="foo")
>>> particles.add_bond(bond)
```

add_particle(*particle*)
Adds the particle to the container.

If the new particle has no uid, the particle container will generate a new uid for it. If the particle has already an uid, it won't add the particle if a particle with the same uid already exists. If the user wants to replace an existing particle in the container there is an 'update_particle' method for that purpose.

Parameters **particle** (*Particle*) – the new particle that will be included in the container.

Returns **uid** (*uuid.UUID*) – The uid of the added particle.

Raises **ValueError** – when the new particle already exists in the container.

Examples

Add a particle to a Particles container.

```
>>> particle = Particle()
>>> particles = Particles(name="foo")
>>> particles.add_particle(part)
```

bond2index = None
The mapping from uid to bond index

data
Easy access to the vtk CellData structure

data_set = None
The vtk.PolyData dataset

classmethod from_dataset(*name*, *data_set*, *data=None*)
Wrap a plain dataset into a new VTKParticles.

The constructor makes some sanity checks to make sure that the tvtk.DataSet is compatible and all the information can be properly used.

Raises **TypeError** – When the sanity checks fail.

classmethod from_particles(*particles*)
Create a new VTKParticles copy from a CUDS particles instance.

get_bond(*uid*)
Returns a copy of the bond with the 'bond_id' id.

Parameters **uid** (*uuid.UUID*) – the uid of the bond

Raises **KeyError** – when the bond is not in the container.

Returns **bond** (*Bond*) – A copy of the internally stored bond info.

get_particle(*uid*)
Returns a copy of the particle with the 'particle_id' id.

Parameters **uid** (*uuid.UUID*) – the uid of the particle

Raises **KeyError** – when the particle is not in the container.

Returns **particle** (*Particle*) – A copy of the internally stored particle info.

has_bond(*uid*)
Checks if a bond with the given uid already exists in the container.

has_particle(*uid*)
Checks if a particle with the given uid already exists in the container.

index2bond = None
The reverse mapping from index to bond uid

index2particle = None
The reverse mapping from index to point uid

iter_bonds(*uids=None*)
Generator method for iterating over the bonds of the container.

It can receive any kind of sequence of bond ids to iterate over those concrete bond. If nothing is passed as parameter, it will iterate over all the bonds.

uids [iterable of uuid.UUID, optional] sequence containing the id's of the bond that will be iterated. When the uids are provided, then the bonds are returned in the same order the uids are returned by the iterable. If uids is None, then all bonds are returned by the interable and there is no restriction on the order that they are returned.

Yields **bond** (*Bond*) – The next Bond item

Raises **KeyError** – if any of the ids passed as parameters are not in the container.

Examples

It can be used with a sequence as parameter or without it:

```
>>> particles = Particles(name="foo")
>>> ...
>>> for bond in particles.iter_bonds([id1, id2, id3]):
        ...  #do stuff
        #take the bond back to the container so it will be updated
        #in case we need it
        particles.update_bond(bond)
```

```
>>> for bond in particles.iter_bond():
        ...  #do stuff; it will iterate over all the bond
        #take the bond back to the container so it will be updated
        #in case we need it
        particles.update_bond(bond)
```

iter_particles(*uids=None*)
Generator method for iterating over the particles of the container.

It can receive any kind of sequence of particle uids to iterate over those concrete particles. If nothing is passed as parameter, it will iterate over all the particles.

uids [iterable of uuid.UUID, optional] sequence containing the uids of the particles that will be iterated. When the uids are provided, then the particles are returned in the same order the uids are returned by the iterable. If uids is None, then all particles are returned by the interable and there is no restriction on the order that they are returned.

Yields **particle** (*Particle*) – The Particle item.

Raises **KeyError** – if any of the ids passed as parameters are not in the container.

Examples

It can be used with a sequence as parameter or without it:

```
>>> particles = Particles(name="foo")
>>> ...
>>> for particle in particles.iter_particles([uid1, uid2, uid3]):
        ...  #do stuff
        #take the particle back to the container so it will be updated
        #in case we need it
        part_container.update_particle(particle)
```

```
>>> for particle in particles.iter_particles():
        ...  #do stuff; it will iterate over all the particles
        #take the particle back to the container so it will be updated
        #in case we need it
        particles.update_particle(particle)
```

particle2index = None
The mapping from uid to point index

remove_bond(*uid*)
Removes the bond with the uid from the container.

The uid passed as parameter should exists in the container. If it doesn't exists, nothing will happen.

Parameters **uid** (*uuid.UUID*) – the uid of the bond to be removed.

Examples

Having an uid of an existing bond, pass it to the function.

```
>>> particles = Particles(name="foo")
>>> ...
>>> bond = particles.get_bond(uid)
>>> ...
>>> particles.remove_bond(bond.uid)
or
>>> particles.remove_bond(uid)
```

remove_particle(*uid*)
Removes the particle with uid from the container.

The uid passed as parameter should exists in the container. Otherwise an exception will be raised.

Parameters **uid** (*uuid.UUID*) – the uid of the particle to be removed.

Raises **KeyError** – If the particle doesn't exist.

Examples

Having an uid of an existing particle, pass it to the function.

```
>>> particles = Particles(name="foo")
>>> ...
>>> particle = particles.get_particle(uid)
>>> ...
>>> particles.remove_particle(part.uid)
or directly
>>> particles.remove_particle(uid)
```

supported_cuba = None
The currently supported and stored CUBA keywords.

update_bond(*bond*)
Replaces an existing bond.

Takes the uid of 'bond' and searches inside the container for that bond. If the bond exists, it is replaced with the new bond passed as parameter. If the bond doesn't exist, it will raise an exception.

Parameters **bond** (*Bond*) – the bond that will be replaced.

Raises **ValueError** – If the bond doesn't exist.

Examples

Given a Bond that already exists in the Particles container (taken with the 'get_bond' method for example) just call the function passing the Bond as parameter.

```
>>> particles = Particles(name="foo")
>>> ...
>>> bond = particles.get_bond(uid)
>>> ... #do whatever you want with the bond
>>> particles.update_bond(bond)
```

update_particle(*particle*)
Replaces an existing particle.

Takes the uid of 'particle' and searches inside the container for that particle. If the particle exists, it is replaced with the new particle passed as parameter. If the particle doesn't exist, it will raise an exception.

Parameters **particle** (*Particle*) – the particle that will be replaced.

Raises **ValueError** – If the particle does not exist.

Examples

Given a Particle that already exists in the Particles container (taken with the 'get_particle' method for example), just call the function passing the Particle as parameter.

```
>>> part_container = Particles(name="foo")
>>> ...
>>> part = part_container.get_particle(uid)
>>> ... #do whatever you want with the particle
>>> part_container.update_particle(part)
```

class simphony_mayavi.cuds.vtk_mesh.**VTKMesh**(*name*, *data=None*, *data_set=None*, *mappings=None*)
Bases: simphony.cuds.abstractmesh.ABCMesh

Constructor.

Parameters

- **name** (*string*) – The name of the container
- **data** (*DataContainer*) – The data attribute to attach to the container. Default is None.
- **data_set** (*tvtk.DataSet*) – The dataset to wrap in the CUDS api. Default is None which will create a tvtk.UnstructuredGrid.
- **mappings** (*dict*) – A dictionary of mappings for the point2index, index2point, element2index and index2element. Should be provided if the points and elements described in `data_set` are already assigned uids. Default is None and will result in the uid <-> index mappings being generated at construction.

add_cell(*cell*)

add_edge(*edge*)

add_face(*face*)

add_point(*point*)

data
Easy access to the vtk PointData structure

data_set = None
The vtk.PolyData dataset

element2index = None
The mapping from uid to bond index

element_data = None
Easy access to the vtk CellData structure

classmethod from_dataset(*name*, *data_set*, *data=None*)
Wrap a plain dataset into a new VTKMesh.

The constructor makes some sanity checks to make sure that the tvtk.DataSet is compatible and all the information can be properly used.

Raises **TypeError** – When the sanity checks fail.

classmethod from_mesh(*mesh*)
Create a new VTKMesh copy from a CUDS mesh instance.

get_cell(*uid*)

get_edge(*uid*)

get_face(*uid*)

get_point(*uid*)

has_cells()

has_edges()

has_faces()

index2element = None
The reverse mapping from index to bond uid

index2point = None
The reverse mapping from index to point uid

iter_cells(*uids=None*)

iter_edges(*uids=None*)

iter_faces(*uids=None*)

iter_points(*uids=None*)

point2index = None
The mapping from uid to point index

supported_cuba = None
The currently supported and stored CUBA keywords.

update_cell(*element*)

update_edge(*element*)

update_face(*element*)

update_point(*point*)

class simphony_mayavi.cuds.vtk_lattice.**VTKLattice**(*name*, *type_*, *data_set*, *data=None*)
Bases: simphony.cuds.abstractlattice.ABCLattice

Constructor.

Parameters

- **name** (*string*) – The name of the container.
- **type_** (*string*) – The type of the container.
- **data_set** (*tvtk.DataSet*) – The dataset to wrap in the CUDS api
- **data** (*DataContainer*) – The data attribute to attach to the container. Default is None.

base_vect

data
The container data

classmethod empty(*name*, *type_*, *base_vector*, *size*, *origin*, *data=None*)
Create a new empty Lattice.

classmethod from_dataset(*name*, *data_set*, *data=None*)
Create a new Lattice and try to guess the type.

classmethod from_lattice(*lattice*)
Create a new Lattice from the provided one.

get_coordinate(*index*)
Get coordinate of the given index coordinate.

index [int[3]] node index coordinate

Returns

coordinates : float[3]

get_node(*index*)
Get the lattice node corresponding to the given index.

index [int[3]] node index coordinate

Returns **node** (*LatticeNode*)

iter_nodes (*indices=None*)
Get an iterator over the LatticeNodes described by the indices.

indices [iterable set of int[3], optional] When indices (i.e. node index coordinates) are provided, then nodes are returned in the same order of the provided indices. If indices is None, there is no restriction on the order the nodes that are returned.

Returns

iterator: An iterator over LatticeNode objects

origin

point_data = None
Easy access to the vtk PointData structure

size

supported_cuba = None
The currently supported and stored CUBA keywords.

type

update_node (*node*)
Update the corresponding lattice node.

Parameters **node** (*LatticeNode*) –

9.4 Core module

A module containing core tools and wrappers for vtk data containers used in simphony_mayavi.

Classes

CubaData(attribute_data[, stored_cuba, ...])	Map a vtkCellData or vtkPointData object to a sequence of DataContainers.
CellCollection([cell_array])	A mutable sequence of cells wrapping a tvtk.CellArray.
mergedocs(other)	Merge the docstrings of other class to the decorated.
CUBADataAccumulator([keys])	Accumulate data information per CUBA key.
CUBADataExtractor(**traits)	Extract cuba data from cuds items iterable.

Functions

supported_cuba()	Return the list of CUBA keys that can be supported by vtk.
default_cuba_value(cuba)	Return the default value of the CUBA key as a scalar or numpy array.
cell_array_slicer(data)	Iterate over cell components on a vtk cell array
mergedoc(function, other)	Merge the docstring from the other function to the decorated function.

9.4.1 Description

class simphony_mayavi.core.cuba_data.**CubaData** (*attribute_data*, *stored_cuba=None*, *size=None*, *masks=None*)

Bases: _abcoll.MutableSequence

Map a vtkCellData or vtkPointData object to a sequence of DataContainers.

The class implements the `MutableSequence` api to wrap a `tvtk.CellData` or `tvtk.PointData` array where each CUBA key is a `tvtk.DataArray`. The aim is to help the conversion between column based structure of the `vtkCellData` or `vtkPointData` and the row based access provided by a list of `~.DataContainer`.

While the wrapped tvkt container is empty the following behaviour is active:

- Using `len` will return the `initial_size`, if defined, or 0.
- Using element access will return an empty *class:~.DataContainer*.
- No field arrays have been allocated.

When values are first added/updated with non-empty `DataContainers` then the necessary arrays are created and the `initial_size` info is not used anymore.

Note: Missing values for the attribute arrays are stored in separate attribute arrays named "<CUBA.name>-mask" as `0` while present values are designated with a `1`.

Constructor

attribute_data: tvtk.DataSetAttributes The vtk attribute container.

stored_cuba [set] The CUBA keys that are going to be stored default is the result of running `supported_cuba()`

size [int] The initial size of the container. Default is None. Setting a value will activate the virtual size behaviour of the container.

mask [tvtk.FieldData] A data arrays containing the mask of some of the CUBA data in `attribute_data`.

Raises

ValueError : When a non-empty `attribute_data` container is provided while size != None.

`cubas`
The set of currently stored CUBA keys.

For each cuba key there is an associated `DataArray` connected to the `PointData` or `CellData`

classmethod `empty` (*type_=<AttributeSetType.POINTS: 1>*, *size=0*)
Return an empty sequence based wrapping a vtkAttributeDataSet.

Parameters

- **`size`** (*int*) – The virtual size of the container.
- **`type_`** (*AttributeSetType*) – The type of the vtkAttributeSet to create.

`insert` (*index*, *value*)
Insert the values of the DataContainer in the arrays at row=''index''.

If the provided DataContainer contains new, but supported, cuba keys then a new empty array is created for them and updated with the associated values of `value`. Unsupported CUBA keys are ignored.

Note: The underline data structure is better suited for append operations. Inserting values in the middle or at the front will be less efficient.

---

class simphony_mayavi.core.cell_collection.**CellCollection**(*cell_array=None*)
Bases: _abcoll.MutableSequence

A mutable sequence of cells wrapping a tvtk.CellArray.

Constructor

Parameters **cell_array** (*tvtk.CellArray*) – The tvtk object to wrap. Default value is an empty tvtk.CellArray.

__delitem__(*index*)
Remove cell at index.

Note: This operation will need to create temporary arrays in order to keep the data info consistent.

__getitem__(*index*)
Return the connectivity list for the cell at index.

__len__()
The number of contained cells.

__setitem__(*index*, *value*)
Update the connectivity list for cell at index.

Note: If the size of the connectivity list changes a slower path creating temporary arrays is used.

insert(*index*, *value*)
Insert cell at index.

Note: This operation needs to use a slower path based on temporary array when index < sequence length.

class simphony_mayavi.core.cuba_data_accumulator.**CUBADataAccumulator**(*keys=()*)
Bases: object

Accumulate data information per CUBA key.

A collector object that stores :class:DataContainer data into a list of values per CUBA key. By appending DataContainer instanced the user can effectively convert the per item mapping of data values in a CUDS container to a per CUBA key mapping of the data values (useful for coping data to vtk array containers).

The Accumulator has two modes of operation fixed and expand. fixed means that data will be stored for a predefined set of keys on every append call and missing values will be saved as None. Where expand will extend the internal table of values whenever a new key is introduced.

expand operation

```
>>> accumulator = CUBADataAccumulator():
>>> accumulator.append(DataContainer(TEMPERATURE=34))
>>> accumulator.keys()
{CUBA.TEMPERATURE}
>>> accumulator.append(DataContainer(VELOCITY=(0.1, 0.1, 0.1))
>>> accumulator.append(DataContainer(TEMPERATURE=56))
>>> accumulator.keys()
{CUBA.TEMPERATURE, CUBA.VELOCITY}
>>> accumulator[CUBA.TEMPERATURE]
[34, None, 56]
>>> accumulator[CUBA.VELOCITY]
[None, (0.1, 0.1, 0.1), None]
```

fixed operation

```
>>> accumulator = CUBADataAccumulator([CUBA.TEMPERATURE, CUBA.PRESSURE]):
>>> accumulator.keys()
{CUBA.TEMPERATURE, CUBA.PRESSURE}
>>> accumulator.append(DataContainer(TEMPERATURE=34))
>>> accumulator.append(DataContainer(VELOCITY=(0.1, 0.1, 0.1))
>>> accumulator.append(DataContainer(TEMPERATURE=56))
>>> accumulator.keys()
{CUBA.TEMPERATURE, CUBA.PRESSURE}
>>> accumulator[CUBA.TEMPERATURE]
[34, None, 56]
>>> accumulator[CUBA.PRESSURE]
[None, None, None]
>>> accumulator[CUBA.VELOCITY]
KeyError(...)
```

Constructor

Parameters **keys** (*list*) – The list of keys that the accumulator should care about. Providing this value at initialisation sets up the accumulator to operate in `fixed` mode. If no keys are provided then accumulator operates in `expand` mode.

__getitem__(*key*)
Get the list of accumulated values for the CUBA key.

Parameters **key** (*CUBA*) – A CUBA Enum value

Returns **result** (*list*) – A list of data values collected for `key`. Missing values are designated with `None`.

__len__()
The number of values that are stored per key

Note: Behaviour is temporary and will probably change soon.

---

append(*data*)
Append info from a `DataContainer`.

Parameters **data** (*DataContainer*) – The data information to append.

If the accumulator operates in `fixed` mode:

- Any keys in `self.keys()` that have values in `data` will be stored (appended to the related key lits).
- Missing keys will be stored as `None`

If the accumulator operates in `expand` mode:

- Any new keys in *Data* will be added to the `self.keys()` list and the related list of values with length equal to the current record size will be initialised with values of `None`.
- Any keys in the modified `self.keys()` that have values in `data` will be stored (appended to the list of the related key).
- Missing keys will be store as `None`.

keys
The set of CUBA keys that this accumulator contains.

load_onto_vtk(*vtk_data*)
Load the stored information onto a vtk data container.

Parameters **vtk_data** (*vtkPointData or vtkCellData*) – The vtk container to load the value onto.

Data are loaded onto the vtk container based on their data type. The name of the added array is the name of the CUBA key (i.e. *CUBA*.name). Currently only scalars and three dimensional vectors are supported.

class simphony_mayavi.core.cuba_data_extractor.**CUBADataExtractor**(***traits*)
Bases: traits.has_traits.HasStrictTraits

Extract cuba data from cuds items iterable.

The class that supports extracting data values of a specific CUBA key from an iterable that returns low level CUDS objects (e.g. Point).

available = Property(Set(CUBATrait), depends_on='_available')
The list of cuba keys that are available (read only). The value is recalculated at initialisation and when the reset method is called.

data = Property(Dict(UUID, Any), depends_on='_data')
The dictionary mapping of item uid to the extracted data value. A change Event is fired for data when selected or keys change or the reset method is called.

function = ReadOnly
The function to call that returns a generator over the desired items (e.g. Mesh.iter_points). This value cannot be changed after initialisation.

keys = Either(None, Set(UUID))
The list of uuid keys to restrict the data extraction. This attribute is passed to the function generator method to restrict iteration over the provided keys (e.g Mesh.iter_points(uids=keys))

reset()
Reset the available and data attributes.

selected = CUBATrait
Currently selected CUBA key. Changing the selected key will fire events that will result in executing the generator function and extracting the related values from the CUDS items that the iterator yields. The resulting mapping of uid -> value will be stored in data.

class simphony_mayavi.core.doc_utils.**mergedocs**(*other*)
Bases: object

Merge the docstrings of other class to the decorated.

simphony_mayavi.core.cuba_utils.**supported_cuba**()
Return the list of CUBA keys that can be supported by vtk.

simphony_mayavi.core.cuba_utils.**default_cuba_value**(*cuba*)
Return the default value of the CUBA key as a scalar or numpy array.

Int type values have -1 as default, while float type values have numpy.nan.

Note: Only vector and scalar values are currently supported.

---

simphony_mayavi.core.cell_array_tools.**cell_array_slicer**(*data*)
Iterate over cell components on a vtk cell array

VTK stores the associated point index for each cell in a one dimensional array based on the following template:

```
    [n, id0, id1, id2, ..., idn, m, id0, ...]
```

The iterator takes a cell array and returns the point indices for each cell.

simphony_mayavi.core.doc_utils.**mergedoc**(*function*, *other*)
Merge the docstring from the other function to the decorated function.

CHAPTER 10

Simphony-Mayavi

A plugin-library for the Simphony framework (http://www.simphony-project.eu/) to provide visualization support of the CUDS highlevel components.

10.1 Repository

Simphony-mayavi is hosted on github: https://github.com/simphony/simphony-mayavi

10.2 Requirements

- mayavi >= 4.4.0
- simphony >= 0.1.3, < 0.2.0

10.2.1 Optional requirements

To support the documentation built you need the following packages:

- sphinx >= 1.2.3
- sectiondoc commit 8a0c2be, https://github.com/enthought/sectiondoc
- trait-documenter, https://github.com/enthought/trait-documenter
- mock

Alternative running **`pip install -r doc_requirements`** should install the minimum necessary components for the documentation built.

10.3 Installation

The package requires python 2.7.x, installation is based on setuptools:

```
# build and install
python setup.py install
```

or:

```
# build for in-place development
python setup.py develop
```

10.4 Testing

To run the full test-suite run:

```
python -m unittest discover
```

10.5 Documentation

To build the documentation in the doc/build directory run:

```
python setup.py build_sphinx
```

Note:

- One can use the –help option with a setup.py command to see all available options.
- The documentation will be saved in the `./build` directory.

10.6 Usage

After installation the user should be able to import the `mayavi` visualization plugin module by:

```
from simphony.visualisation import mayavi_tools
mayavi_tools.show(cuds)
```

10.7 Directory structure

- simphony-mayavi – Main package folder.
  - sources – Wrap CUDS objects to provide Mayavi Sources.
  - cuds – Wrap VTK Dataset objects to provide the CUDS container api.
  - core – Utility classes and tools to manipulate vtk and cuds objects.
- examples – Holds examples of loading and visualising SimPhoNy objects with simphony-mayavi.
- doc – Documentation related files: - The rst source files for the documentation

Symbols

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