

SimPhoNy-Mayavi Documentation

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SimPhoNy FP7 Collaboration

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

Repository

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

Requirements

- `mayavi[app] >= 4.4.0`
- `simphony[H5IO] >= 0.3.0`

2.1 Optional requirements

To support testing, you will need the following packages:

- `PIL`
- `mock`

Alternatively unning `pip install -r dev-requirements.txt` should install the packages needed for development purposes.

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>

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

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
```

Testing

To run the full test-suite run:

```
python -m unittest discover
```

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.
-

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)
```

Note:

- It is also recommended that the user uses `qt4` as the user interface backends by setting the environment variable `ETS_TOOLKIT`. In Bash, that is:

```
export ETS_TOOLKIT=qt4
```

Known Issues

- *Segmentation fault during loading or running test suites*

This may be caused by installing BOTH `simphony-paraview` and `simphony-mayavi` in the same environment. Since `paraview` and `mayavi` use different versions of VTK, work-around is limited. Here are two possible solutions.

- If you don't need both `simphony-mayavi` and `simphony-paraview`, uninstall one of them, e.g.:

```
pip uninstall simphony-paraview
```

- If you must retain both plugins, choose to remove one of them from the `simphony.visualisation` entry points. The plugin removed from `simphony.visualisation` is still accessible via `import simphony_paraview.plugin` or `import simphony_mayavi.plugin`. Notice that this change would cause plugin loading tests to fail.

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.
 - `plugins` – GUI for Mayavi2
 - `modules` – default modules for visualising SimPhoNy objects
 - `examples` – Holds examples of loading and visualising SimPhoNy objects with `simphony-mayavi`.
- `doc` – Documentation related files: - The rst source files for the documentation

9.1 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
```

9.1.1 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
point_iter = (Point(coordinates=point, data=DataContainer(TEMPERATURE=index))
               for index, point in enumerate(points))
```

```
uids = mesh.add_points(point_iter)

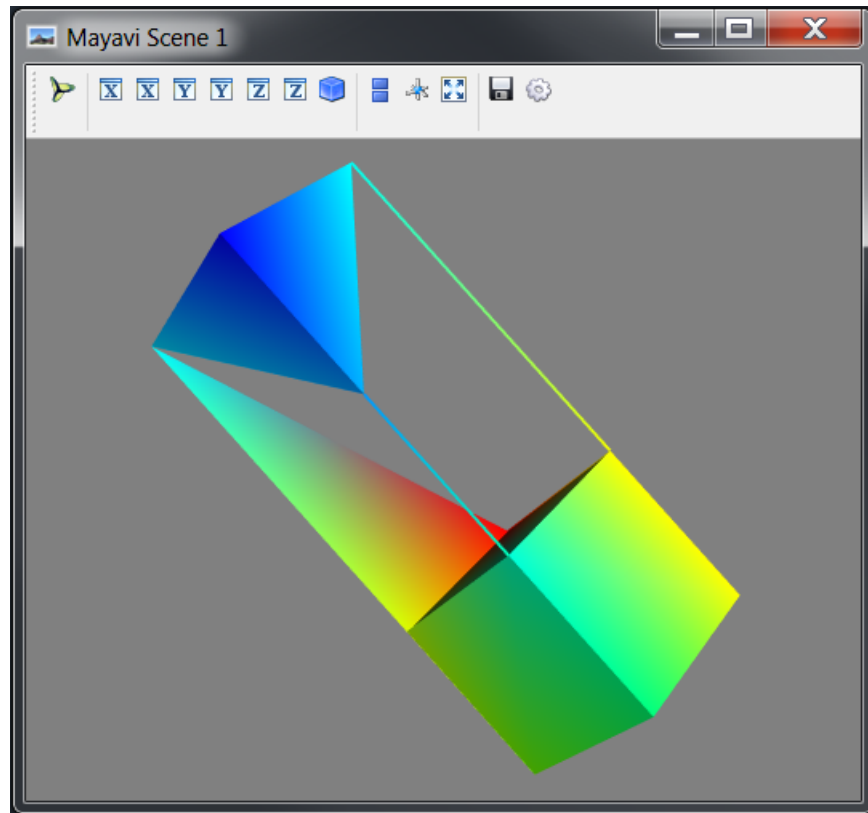
# add edges
edge_iter = (Edge(points=[uids[index] for index in element])
             for index, element in enumerate(edges))
edge_uids = mesh.add_edges(edge_iter)

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

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

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

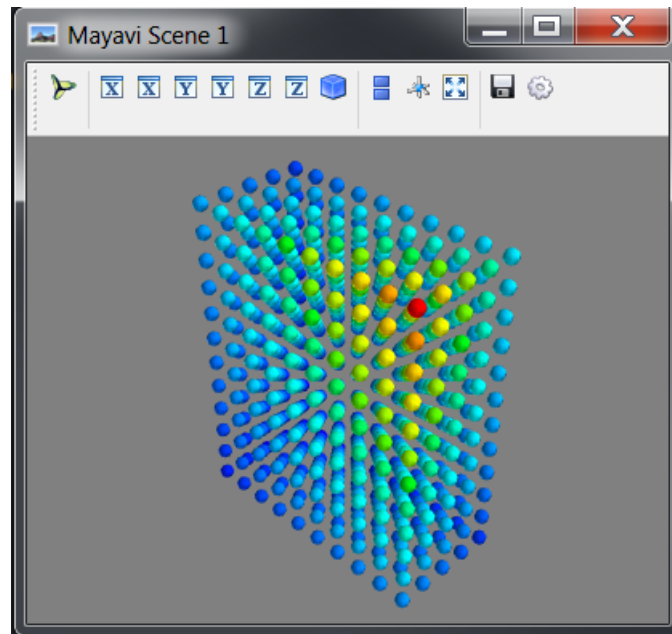
lattice = make_cubic_lattice('test', 0.1, (5, 10, 12))

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

lattice.update_nodes(new_nodes)

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.])

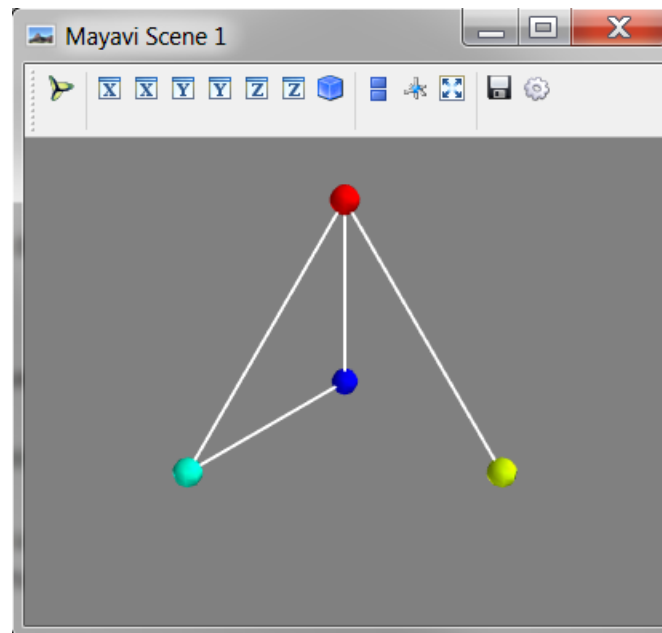
particles = Particles('test')

# add particles
particle_iter = (Particle(coordinates=point,
                           data=DataContainer(TEMPERATURE=temperature[index]))
                 for index, point in enumerate(points))
uids = particles.add_particles(particle_iter)

# add bonds
bond_iter = (Bond(particles=[uids[index] for index in indices]
                  for indices in bonds)
             for indices in bonds)
particles.add_bonds(bond_iter)

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

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



9.1.2 Create VTK backed CUDS

Three objects (i.e. *VTKMesh*, *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
point_iter = (Point(coordinates=point, data=DataContainer(TEMPERATURE=index))
               for index, point in enumerate(points))
uids = mesh.add_points(point_iter)

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

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

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

if __name__ == '__main__':
    # Visualise the Mesh object
    mayavi_tools.show(mesh)

```

VTK Lattice example

```

import numpy

from simphony.core.cuba import CUBA
from simphony.cuds.primitive_cell import PrimitiveCell

```

```
from simphony.visualisation import mayavi_tools

cubic = mayavi_tools.VTKLattice.empty(
    "test", PrimitiveCell.for_cubic_lattice(0.1),
    (5, 10, 12), (0, 0, 0))

lattice = cubic

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

lattice.update_nodes(new_nodes)

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')

# add particles
particle_iter = (Particle(coordinates=point,
                          data=DataContainer(TEMPERATURE=temperature[index]))
                 for index, point in enumerate(points))
uids = particles.add_particles(particle_iter)

# add bonds
bond_iter = (Bond(particles=[uids[index] for index in indices])
              for indices in bonds)
particles.add_bonds(bond_iter)

if __name__ == '__main__':
    # Visualise the Particles object
    mayavi_tools.show(particles)
```

9.1.3 Adapting VTK datasets

The `adapt2cuds()` function is available to wrap common VTK datasets 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

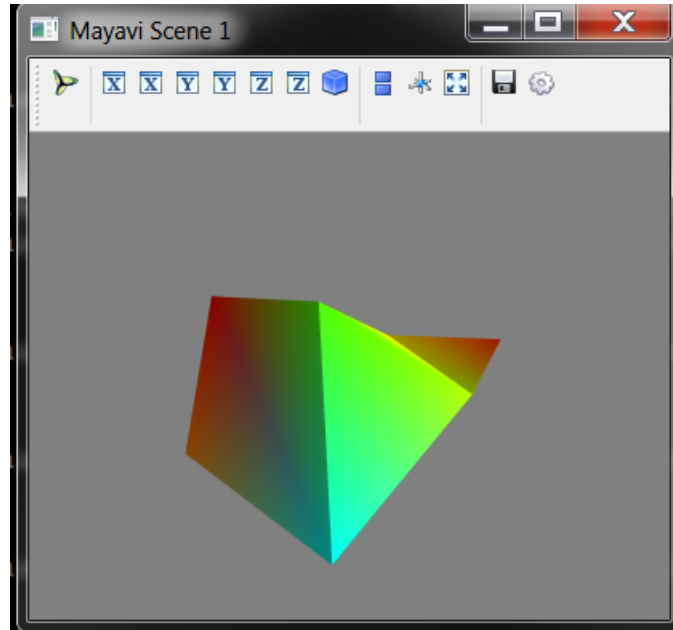
def create_unstructured_grid(array_name='scalars'):
    points = array(
        [[0, 1.2, 0.6], [1, 0, 0], [0, 1, 0], [1, 1, 1], # tetra
         [1, 0, -0.5], [2, 0, 0], [2, 1.5, 0], [0, 1, 0],
         [1, 0, 0], [1.5, -0.2, 1], [1.6, 1, 1.5], [1, 1, 1]], 'f') # Hex
    cells = array(
        [4, 0, 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)
```



9.1.4 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.

9.2 Mayavi2

The Simphony-Mayavi library provides a plugin for Mayavi2 to easily create mayavi `Source` instances from SimPhoNy CUDS datasets and files.

Any CUDS dataset can be adapted as a mayavi `Source` using `CUDSSource`. If CUDS datasets are to be loaded from a CUDS native file, it may be easier to use `CUDSFileSource` which does the loading for you. Similarly, if the CUDS datasets are from a SimPhoNy engine wrapper, `EngineSource` may be used. All of these `Source` objects provide an `update` function that allows the user to refresh visualisation once the CUDS dataset is modified.

With the provided tools one can use the SimPhoNy libraries to work inside the Mayavi2 application, as it is demonstrated in the examples.

9.2.1 Open CUDS Files in Mayavi2

In order for mayavi2 to understand `*.cuds` files one needs to make sure that the `simphony_mayavi` plugin has been selected and activated in the Mayavi2 preferences dialog.

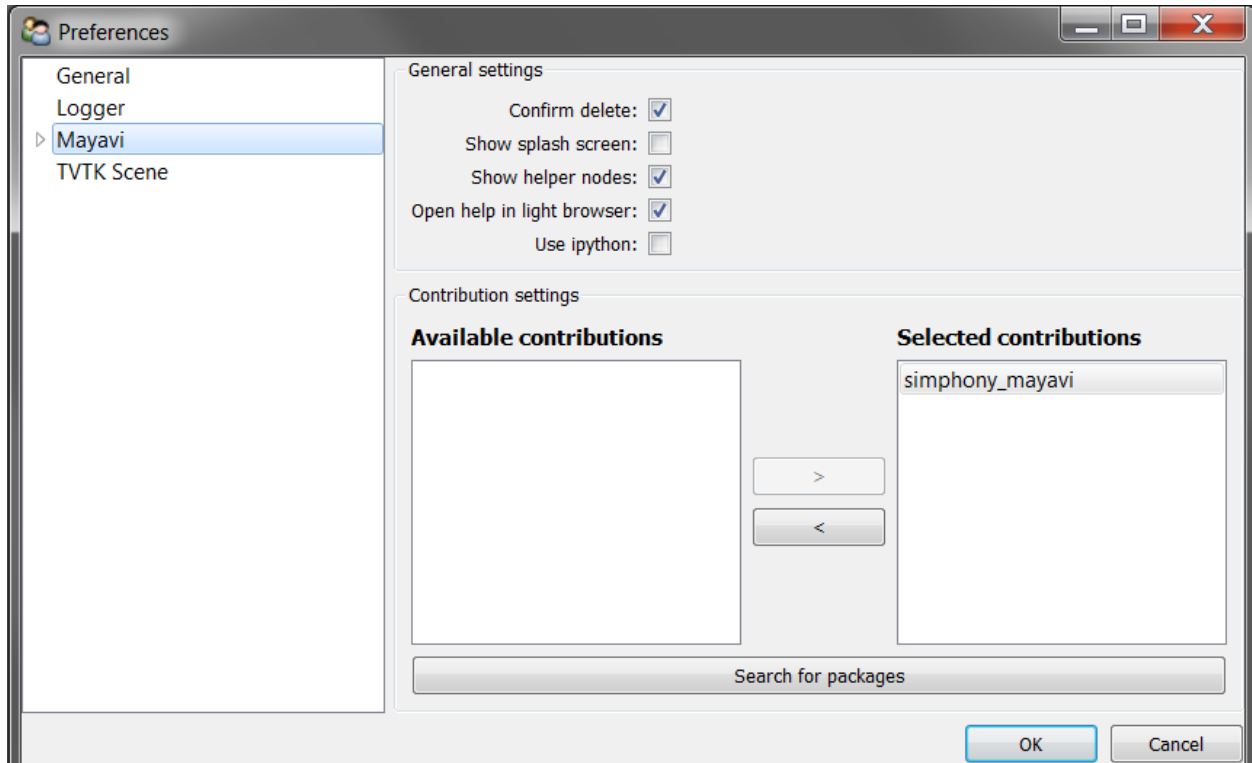
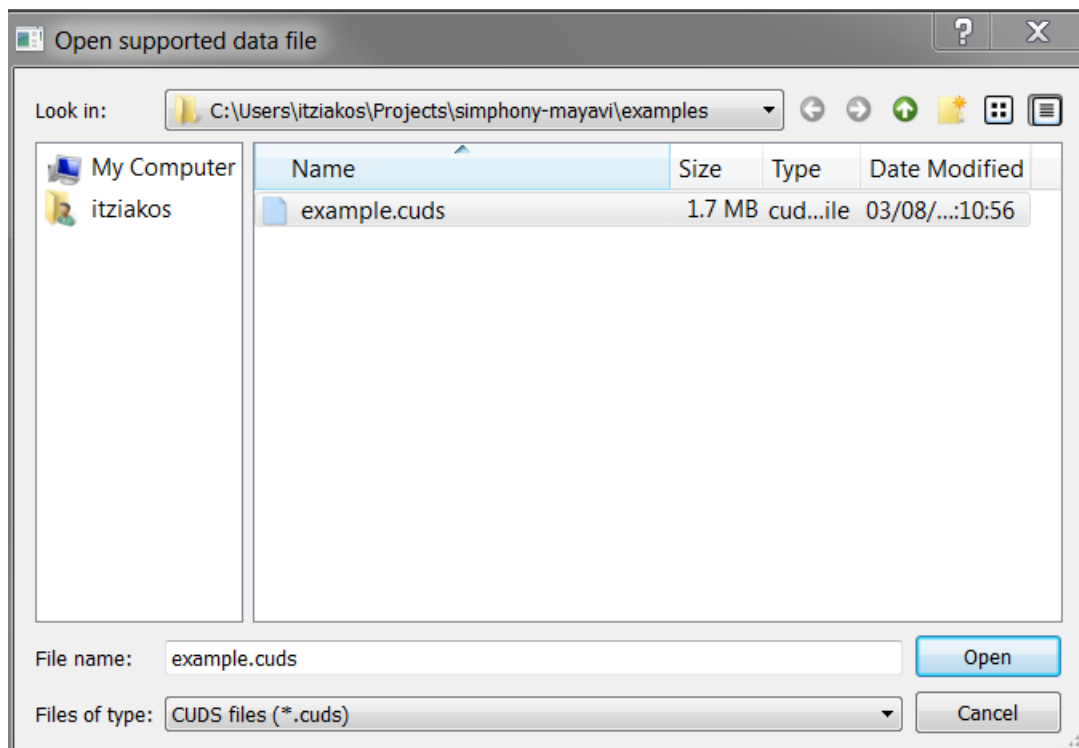


Fig. 9.1: Cuds files are supported in the Open File... dialog. After running the provided example, load the example.cuds file into Mayavi2.



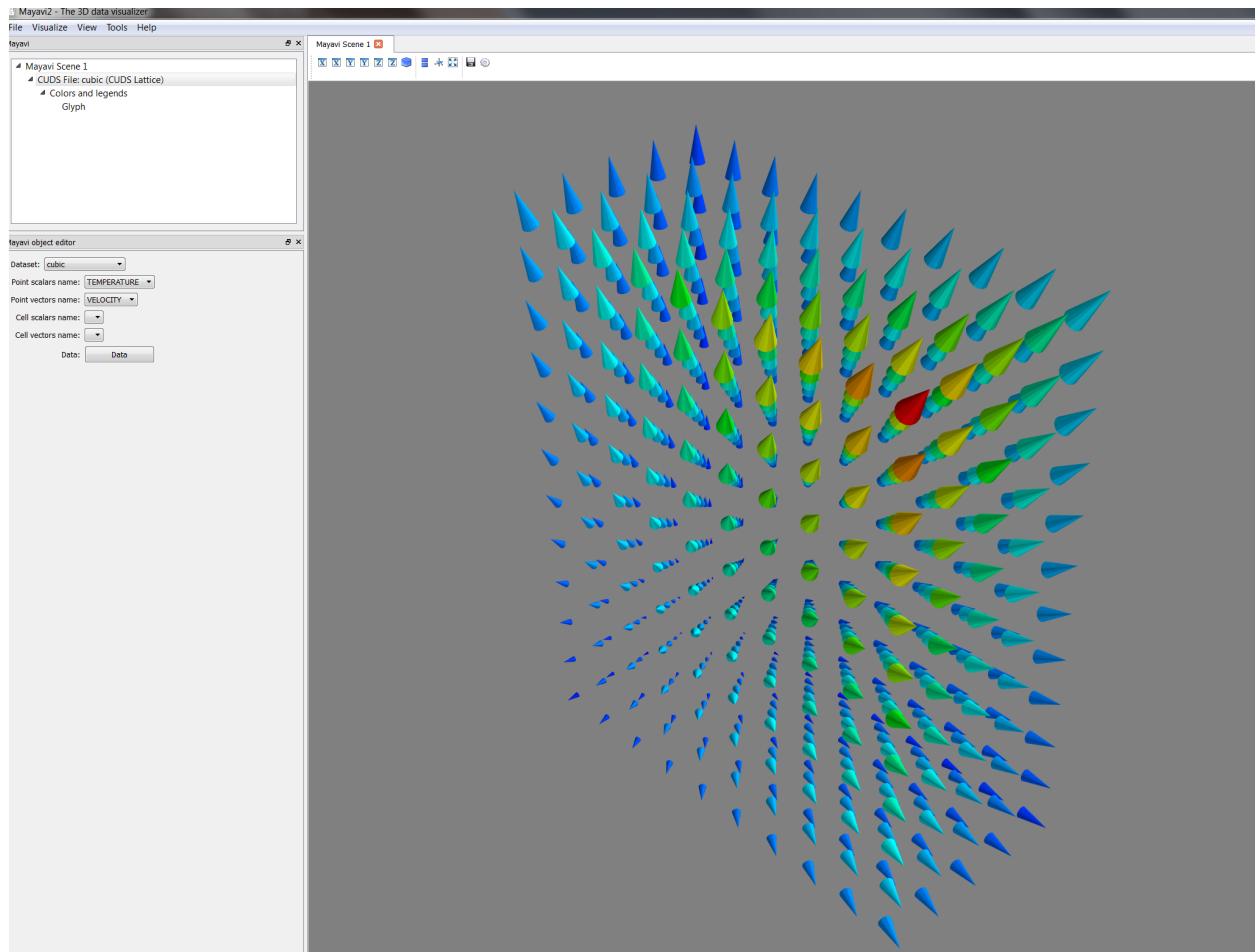


Fig. 9.2: When loaded a CUDSFile is converted into a Mayavi Source and the user can add normal Mayavi modules to visualise the currently selected CUDS container from the available containers in the file.

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.

9.2.2 View CUDS in Mayavi2

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
point_iter = (Point(coordinates=point, data=DataContainer(TEMPERATURE=index))
               for index, point in enumerate(points))
uids = container.add_points(point_iter)

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

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

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

# 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()

```

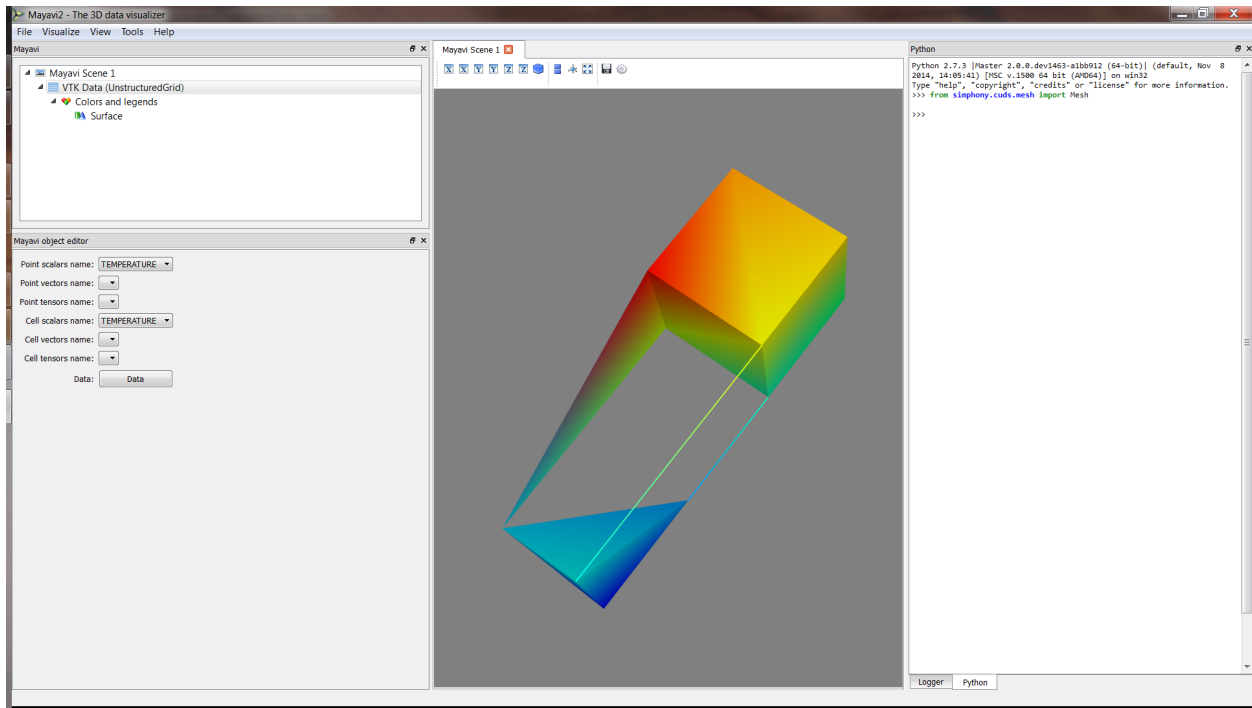


Fig. 9.3: Use the provided example to create a CUDS Mesh and visualise directly in Mayavi2.

Source from a CUDS Lattice

```

import numpy

from mayavi.scripts import mayavi2
from simphony.cuds.lattice import make_cubic_lattice
from simphony.core.cuba import CUBA

cubic = make_cubic_lattice("cubic", 0.1, (5, 10, 12))

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

add_temperature(cubic)

```

```
# 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)
```

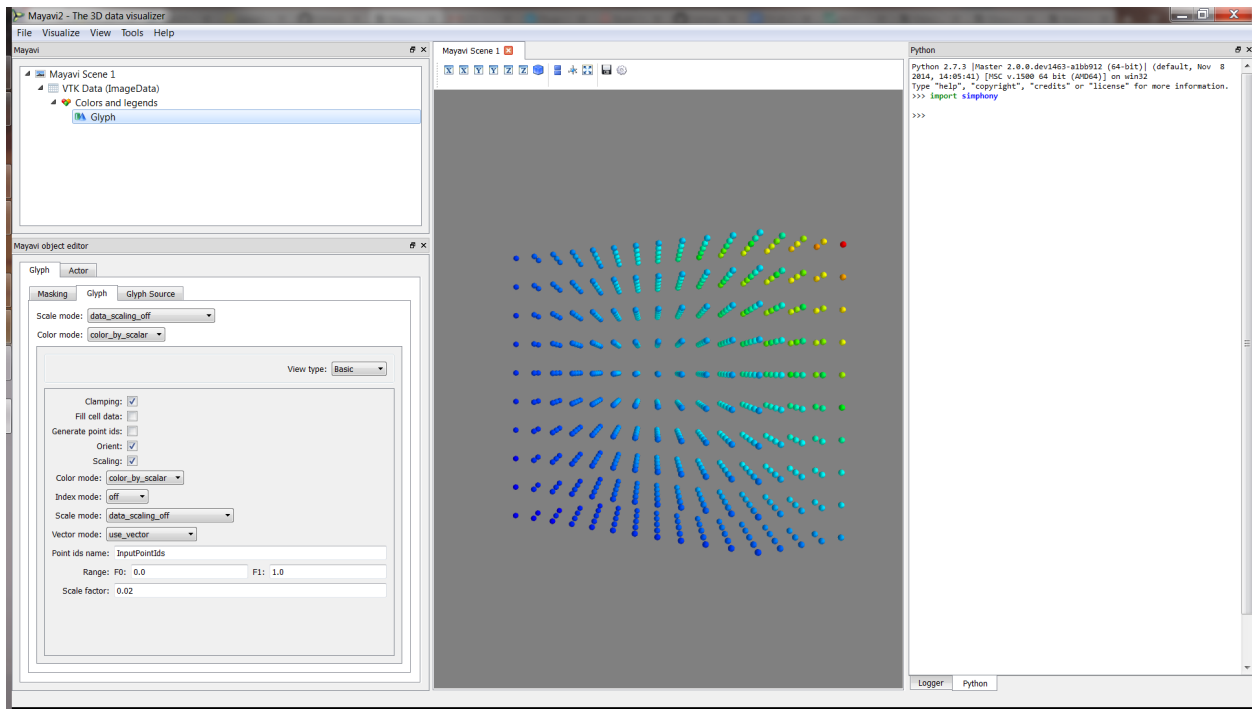


Fig. 9.4: Use the provided example to create a CUDS Lattice and visualise directly in Mayavi2.

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')

# add particles
particle_iter = (Particle(coordinates=point,
                           data=DataContainer(TEMPERATURE=temperature[index]))
                 for index, point in enumerate(points))
uids = container.add_particles(particle_iter)

# add bonds
bond_iter = (Bond(particles=[uids[index] for index in indices]
                  for indices in bonds)
             container.add_bonds(bond_iter)

# 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()
```

Source from a CUDS native file

```
from contextlib import closing

import numpy
from mayavi.scripts import mayavi2

from simphony.core.cuba import CUBA
from simphony.cuds.lattice import (make_hexagonal_lattice,
                                   make_orthorhombic_lattice)
from simphony.io.h5_cuds import H5CUDS

# create some datasets to be saved in a file
hexagonal = make_hexagonal_lattice(
    'hexagonal', 0.1, 0.1, (5, 5, 5), (5, 4, 0))

orthorhombic = make_orthorhombic_lattice(
    'orthorhombic', (0.1, 0.2, 0.3), (5, 5, 5), (5, 4, 0))
```

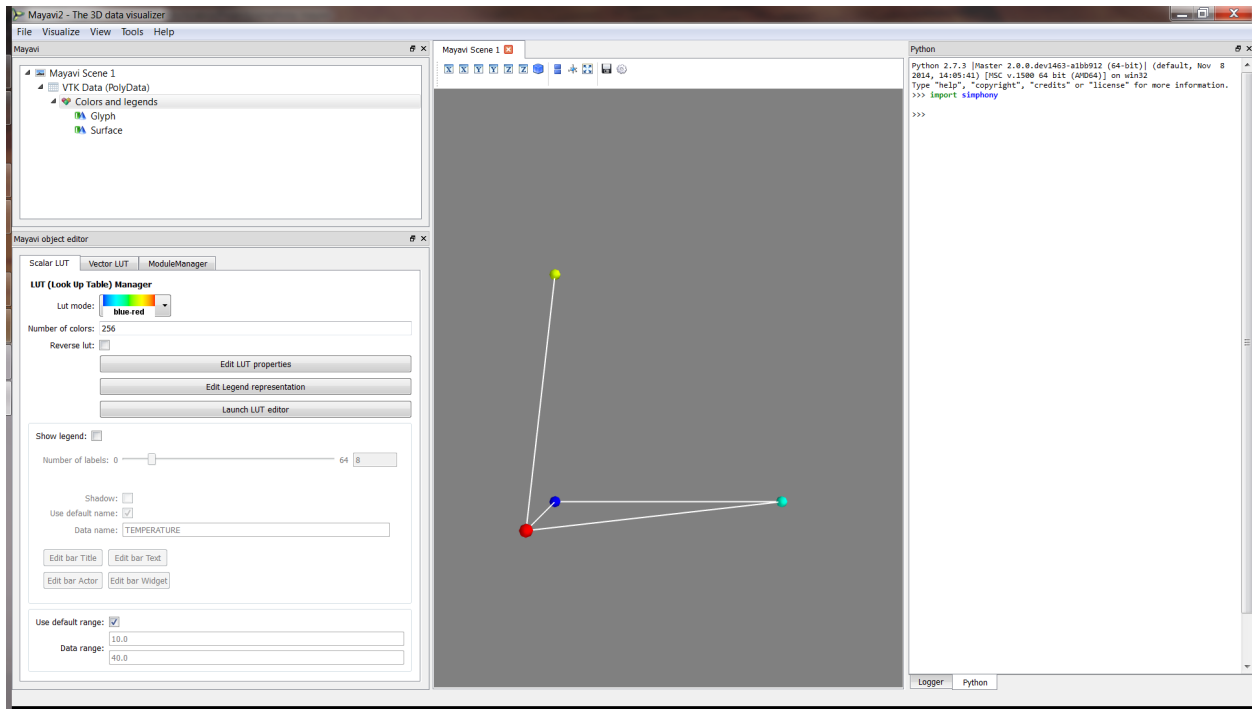


Fig. 9.5: Use the provided example to create a CUDS Particles and visualise directly in Mayavi2.

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

# add some scalar data (i.e. temperature)
add_temperature(hexagonal)
add_temperature(orthorhombic)

# save the data into cuds.
with closing(H5CUDS.open('lattices.cuds', 'w')) as handle:
    handle.add_dataset(hexagonal)
    handle.add_dataset(orthorhombic)

@mayavi2.standalone
def view():
    from mayavi import mlab
    from mayavi.modules.glyph import Glyph
    from simphony_mayavi.sources.api import CUDSFileSource

    mayavi.new_scene()

    # Mayavi Source
    src = CUDSFileSource()
    src.initialize('lattices.cuds')
```

```
# choose a dataset for display
src.dataset = 'orthorhombic'

mayavi.add_source(src)

# customise the visualisation
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'
mayavi.add_module(g)

# add legend
module_manager = src.children[0]
module_manager.scalar_lut_manager.show_scalar_bar = True
module_manager.scalar_lut_manager.show_legend = True

# customise the camera
mlab.view(63., 38., 3., [5., 4., 0.])

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

Source from a SimPhoNy engine wrapper

```
from mayavi.scripts import mayavi2
from simphony_mayavi.tests.testing_utils import DummyEngine

# Comply to SimPhoNy modeling engine API
engine_wrapper = DummyEngine()

@mayavi2.standalone
def view():
    from mayavi.modules.glyph import Glyph
    from simphony_mayavi.sources.api import EngineSource
    from mayavi import mlab

    # Define EngineSource, choose dataset
    src = EngineSource(engine=engine_wrapper,
                       dataset="particles")

    # choose the CUBA attribute for display
    src.point_scalars_name = "TEMPERATURE"

    mayavi.add_source(src)

    # customise the visualisation
    g = Glyph()
    gs = g.glyph.glyph_source
    gs.glyph_source = gs.glyph_dict['sphere_source']
    g.glyph.glyph.scale_factor = 0.2
    g.glyph.scale_mode = 'data_scaling_off'
    mayavi.add_module(g)
```

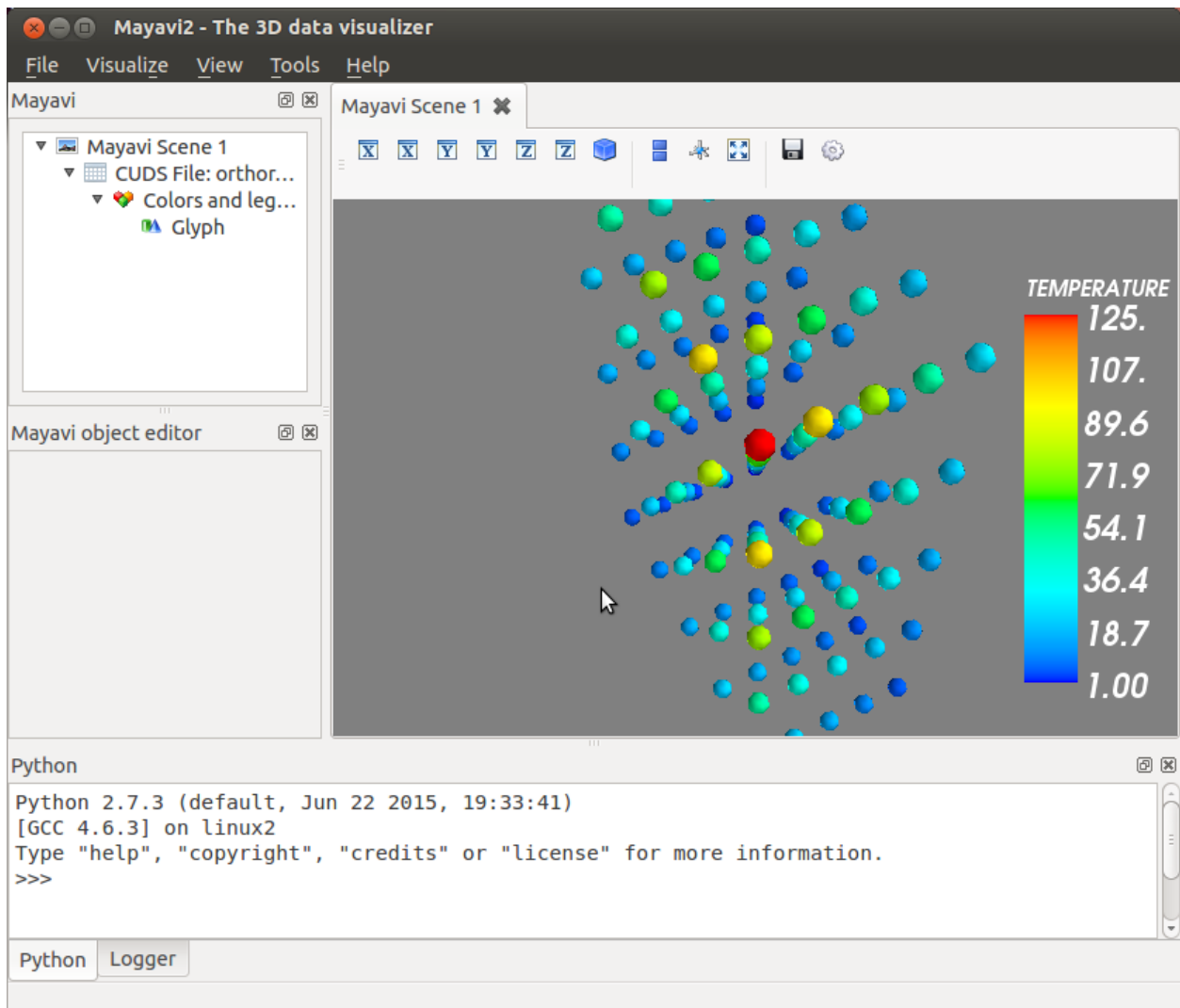


Fig. 9.6: Use the provided example to load data from a CUDS file and visualise directly in Mayavi2.

```
# add legend
module_manager = src.children[0]
module_manager.scalar_lut_manager.show_scalar_bar = True
module_manager.scalar_lut_manager.show_legend = True

# set camera
mlab.view(-65., 60., 14., [1.5, 2., 2.5])

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

9.3 Interacting with Symphony Engine

9.3.1 Batch scripting

Mayavi *mlab* library provides an easy way to visualise data in a script in ways similar to the matplotlib's *pylab* module. As illustrated with examples in *View CUDS in Mayavi2*, the user can easily adapt SimPhoNy CUDS datasets, files, or engines into a native Mayavi *Source* object, and then make use of the *mlab* library to set up the visualisation. More details on how to use *mlab* can be found on its [documentation](#).

Here is an example for visualising a dataset from a SimPhoNy engine, updating the visualisation and saving the image while the engine is being run.

```
from mayavi import mlab

from simphony_mayavi.tests.testing_utils import DummyEngine
from simphony_mayavi.sources.api import EngineSource

# Comply to SimPhoNy modeling engine API
engine_wrapper = DummyEngine()

# Define EngineSource, choose dataset
src = EngineSource(engine=engine_wrapper,
                   dataset="particles")

# choose the CUBA attribute for display
src.point_scalars_name = "TEMPERATURE"

# use glyph to show the particles
mlab.pipeline.glyph(src, scale_factor=0.2, scale_mode='none')

# add legend
module_manager = src.children[0]
module_manager.scalar_lut_manager.show_scalar_bar = True
module_manager.scalar_lut_manager.show_legend = True

# set camera
mlab.view(-65., 60., 14., [1.5, 2., 2.5])

# save the figure
mlab.savefig("figures/particles_001.png")

# run the engine and update the visualisatioin
```

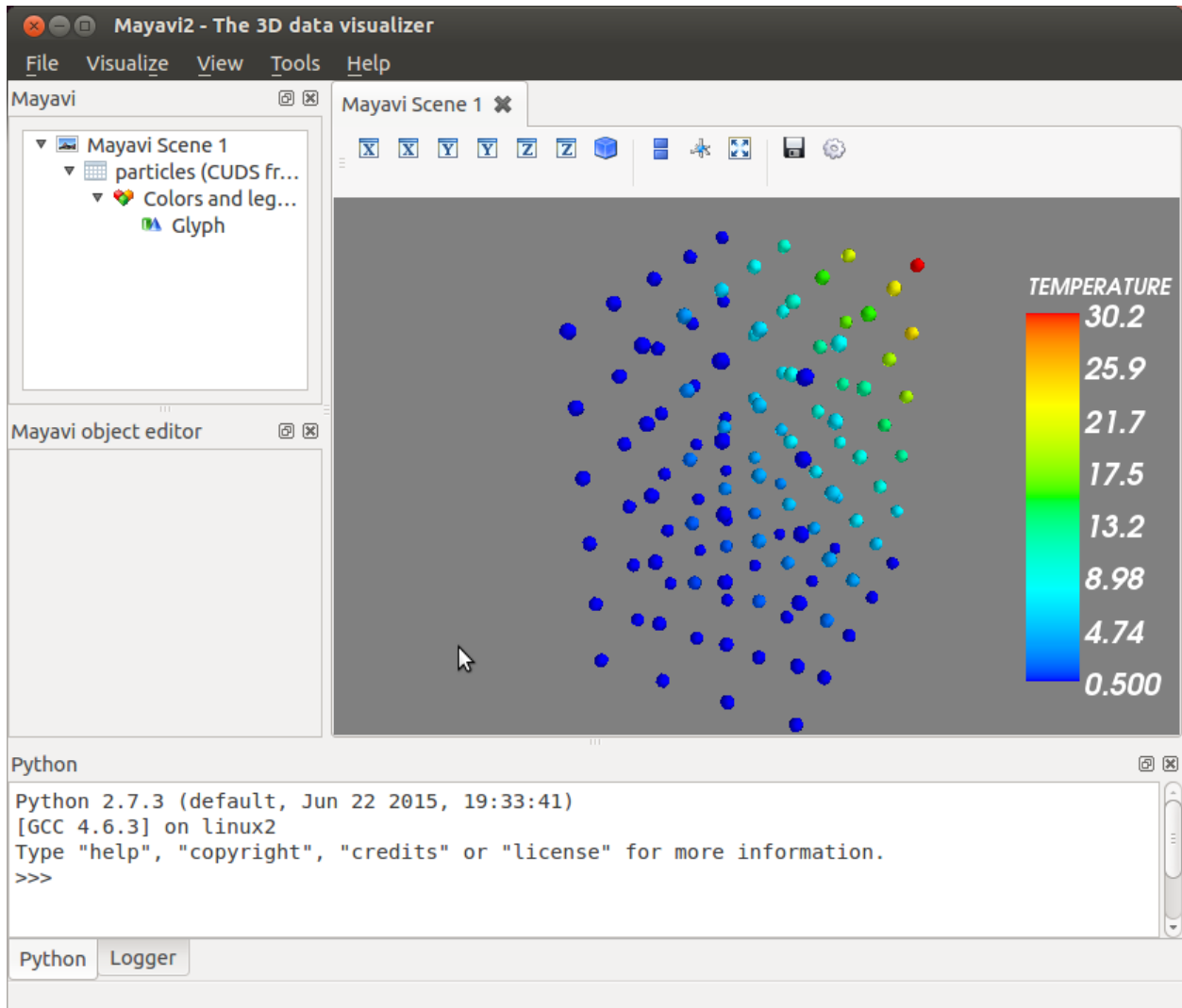



Fig. 9.7: Use the provided example to load data from a SimPhoNy engine and visualise directly in Mayavi2.

In the Mayavi2 embedded python interpreter, the user can access the SimPhoNy engine wrapper associated with the *EngineSource* via its *engine* attribute:

```
# Retrieve the EngineSource
source = engine.scenes[0].children[0]

# The SimPhoNy engine wrapper originally defined
source.engine

# Run the engine
source.engine.run()

# update the visualisation
source.update()
```

```
for i in range(2, 20):
    engine_wrapper.run()
    src.update()
    mlab.savefig("figures/particles_{:03d}.png".format(i))
```

Making a video is just a step away!

9.3.2 Interactive scripting

Non-GUI approach

The `EngineManagerStandalone` is available for the user to select and visualise datasets from a Simphony Modeling Engine via the Python shell. It also allows the user to run the engine (locally) and animate the visualisation after each run.

Example (`EngineManagerStandalone`)

```
from simphony.visualisation import mayavi_tools
from simphony_mayavi.tests.testing_utils import DummyEngine

# Dummy Modeling Engine for demonstration
# The dummy engine has datasets "particles", "lattice", "mesh"
modeling_engine = DummyEngine()

manager = mayavi_tools.EngineManagerStandalone(modeling_engine)

# visualise "particles"
manager.add_dataset_to_scene("particles")

# run the engine for 100 times and animate the
# visualised "particles" after each run
# show a GUI for control the speed of animation
manager.animate(100, delay=100, ui=True)
```

One can visualise multiple datasets in different scenes and animate all of them as the engine runs.

```
from simphony_mayavi.tests.testing_utils import DummyEngine
from simphony.visualisation import mayavi_tools

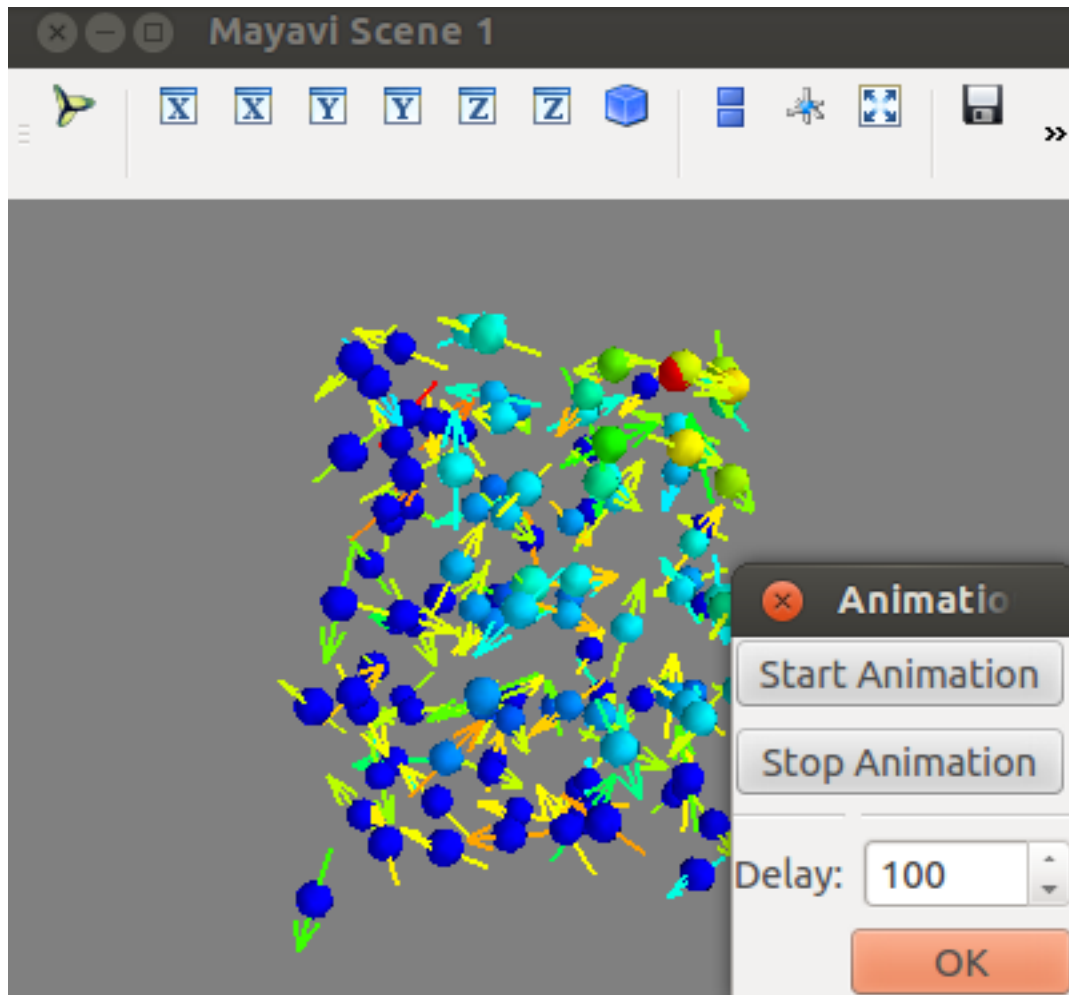
# Dummy Modeling Engine
# The dummy engine has datasets "particles", "lattice", "mesh"
modeling_engine = DummyEngine()

manager = mayavi_tools.EngineManagerStandalone(modeling_engine)

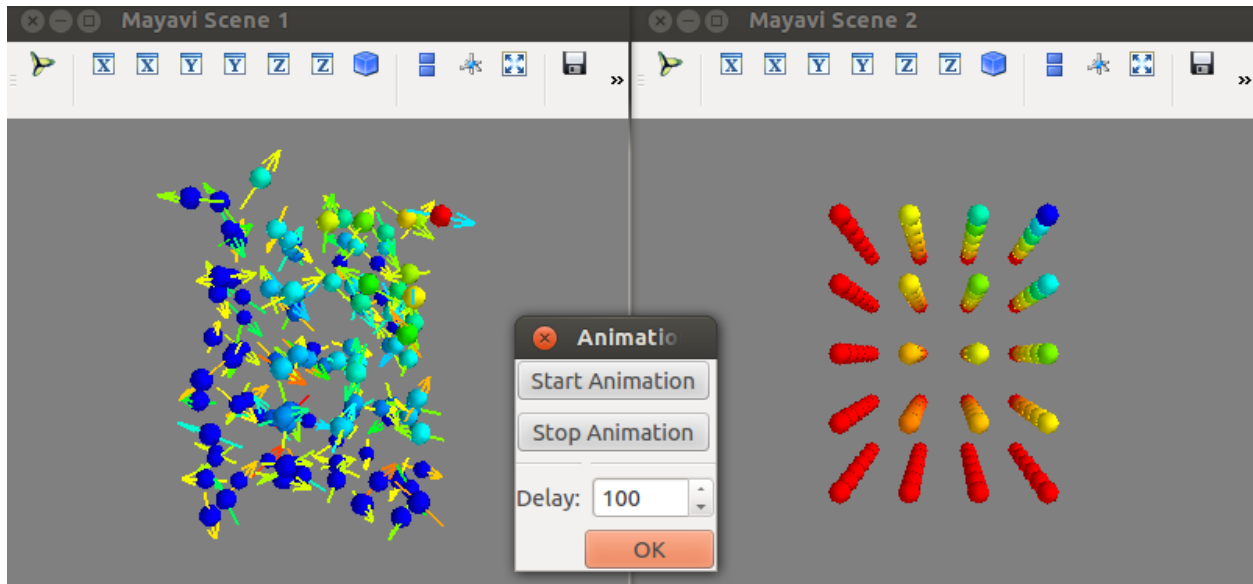
# visualise "particles" to scene 1
manager.add_dataset_to_scene("particles")

# add a new scene
manager.mayavi_engine.new_scene()

# visualise "lattice" in the new scene
# choose to visualise "temperature" as the point scalar data
manager.add_dataset_to_scene("lattice", "TEMPERATURE")
```



```
# run the engine for 100 times and animate the
# datasets in all scenes
manager.animate(100, delay=100, ui=True, update_all_scenes=True)
```



GUI approach

`EngineManagerStandaloneUI` provides a user-friendly and interactive approach to manage multiple engines, visualise datasets from a particular engine, locally run an engine and animate the results.

Multiple engines can be added to or removed from the manager using `add_engine` and `remove_engine`.

Example (Interactive: `EngineManagerStandaloneUI`)

```
from simphony_mayavi.tests.testing_utils import DummyEngine
from simphony.visualisation import mayavi_tools

# GUI for Interacting with the engine and mayavi
gui = mayavi_tools.EngineManagerStandaloneUI()

gui.show_config()

# you can add an engine from the python shell
engine_wrapper = DummyEngine()

# "test" is used as a label for representing the engine in the GUI
gui.add_engine("test", engine_wrapper)

# you can remove the engine from the GUI
# Notice that this may not destroy the instance if the instance
# is referenced elsewhere (i.e. ``engine_wrapper``)
gui.remove_engine("test")
```



Fig. 9.8: Panel for adding more engine wrappers.

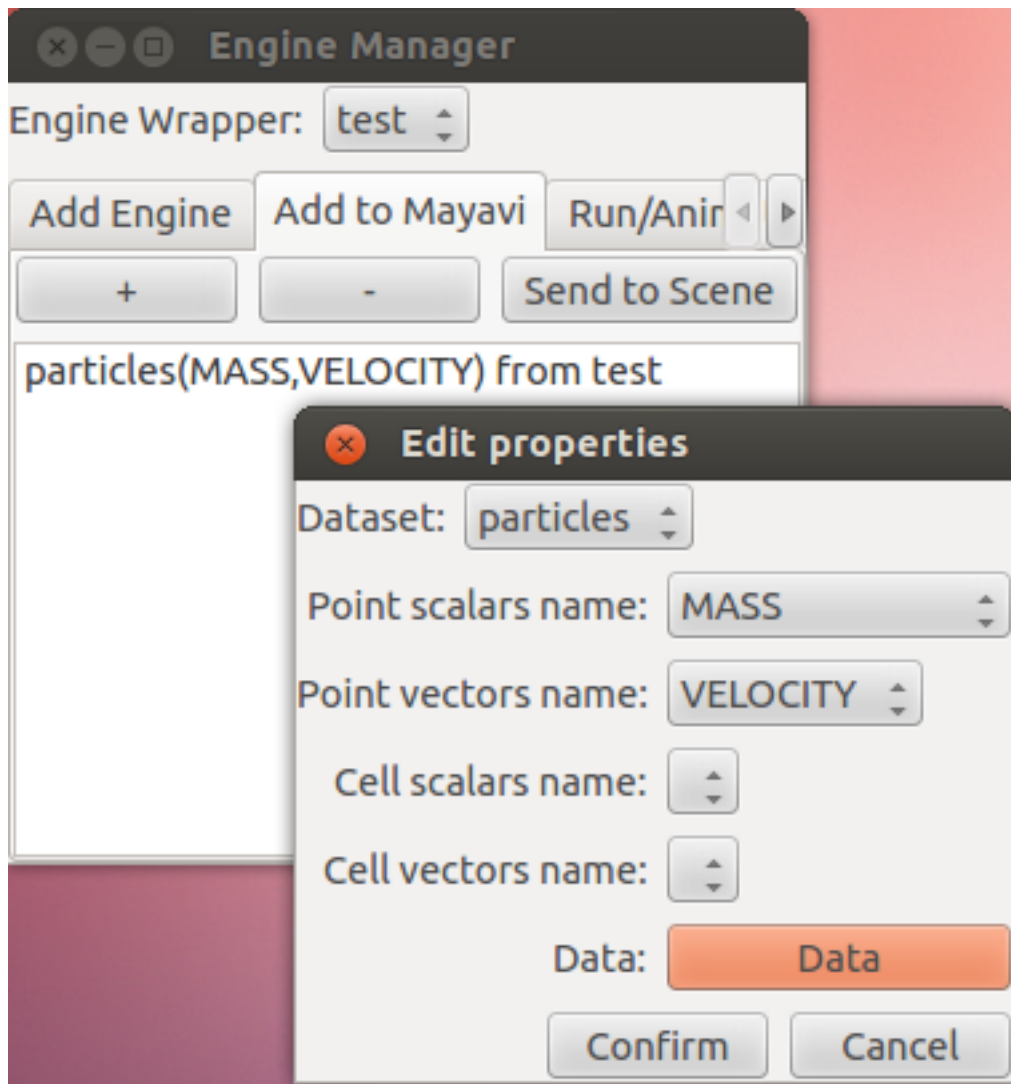


Fig. 9.9: Use *EngineManagerStandaloneUI* to add datasets to Mayavi.

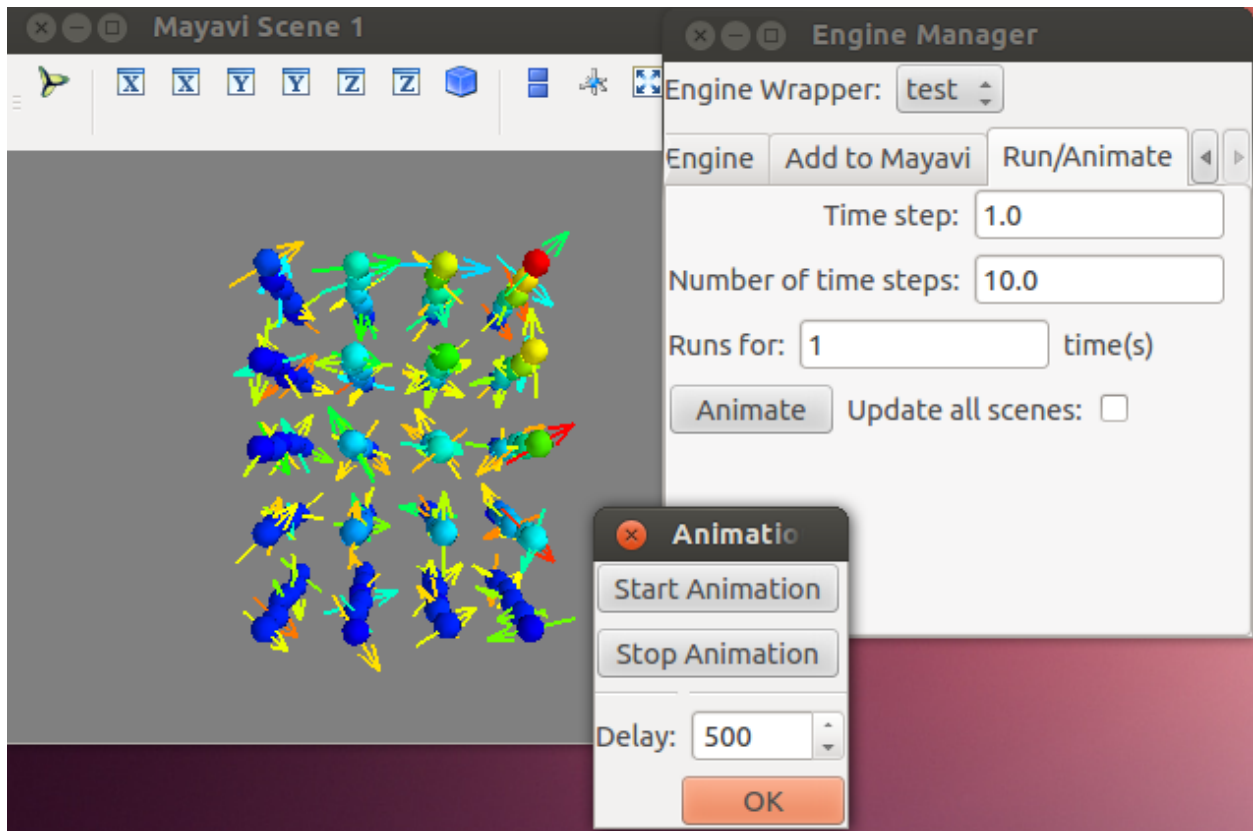


Fig. 9.10: Use *EngineManagerStandaloneUI* to run the engine and animate the results.

9.3.3 Symphony GUI within Mayavi2

A GUI essentially identical to the `EngineManagerStandaloneUI` is provided for the Mayavi2 application. In order to use it, one needs to first activate the plugin in Preferences, following the instructions in *Open CUDS Files in Mayavi2*. After that, **restart** Mayavi2. Then the EngineManager panel can be added by selecting View -> Other... -> Symphony.

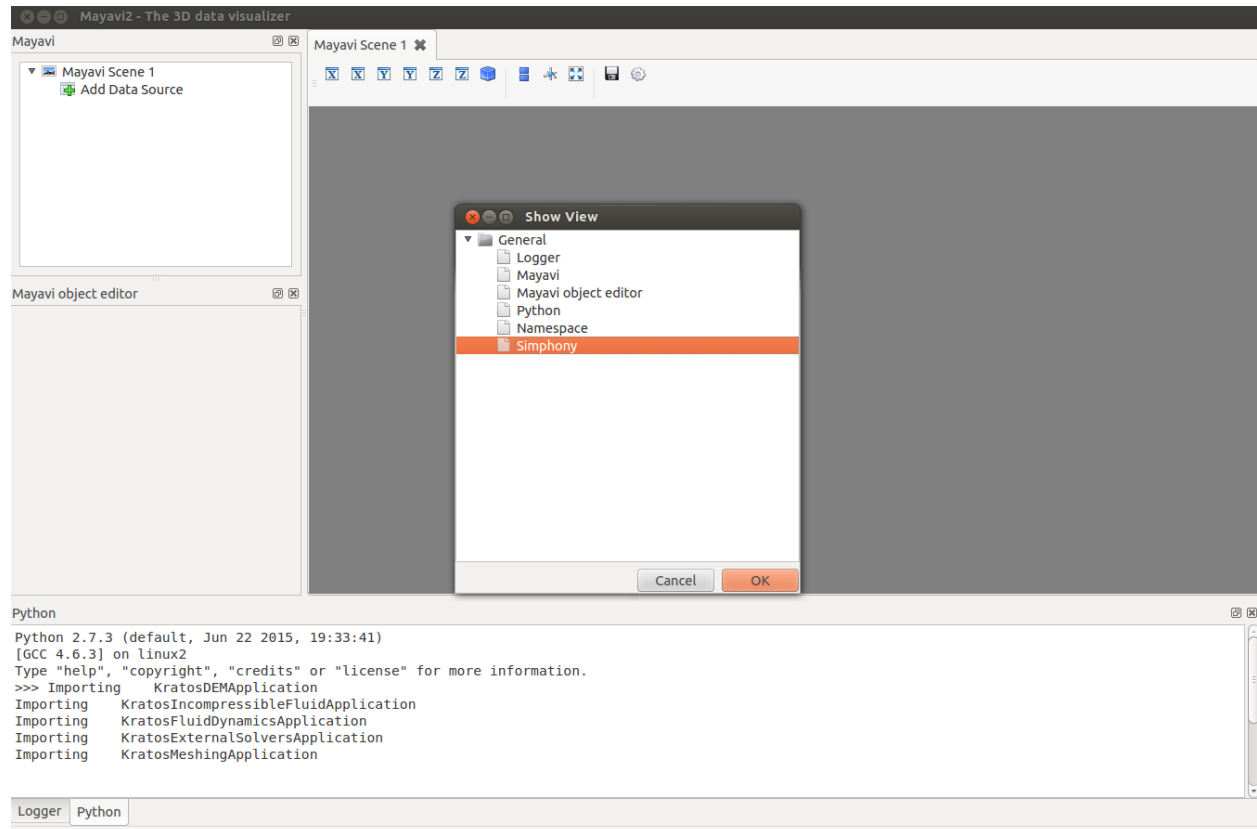


Fig. 9.11: Add the Symphony panel to Mayavi2

The Symphony panel is binded to the embedded Python shell within Mayavi2 as `simphony_panel`. Alternatively the user can access the panel from `simphony.visualisation.mayavi_tools.get_simphony_panel`. With that the user can use the same methods as described in *GUI approach*, such as `add_engine` and `remove_engine`.

Alternatively, the user can setup and load a SimPhoNy engine to Mayavi2 by running a python script from a shell or via Mayavi2 (File->Run Python Script).

The `add_engine_to_mayavi2` method in the `simphony.visualisation.mayavi_tools` namespace is provided for this purpose as illustrated in the following example.

```
""" Modified from simphony-lammps-md/examples/dem_billiards/dem_billiards.py
Requires file:
github.com/simphony/simphony-lammps-md/examples/dem_billiards/billiards_init.data
"""
import os

from mayavi.scripts import mayavi2
```

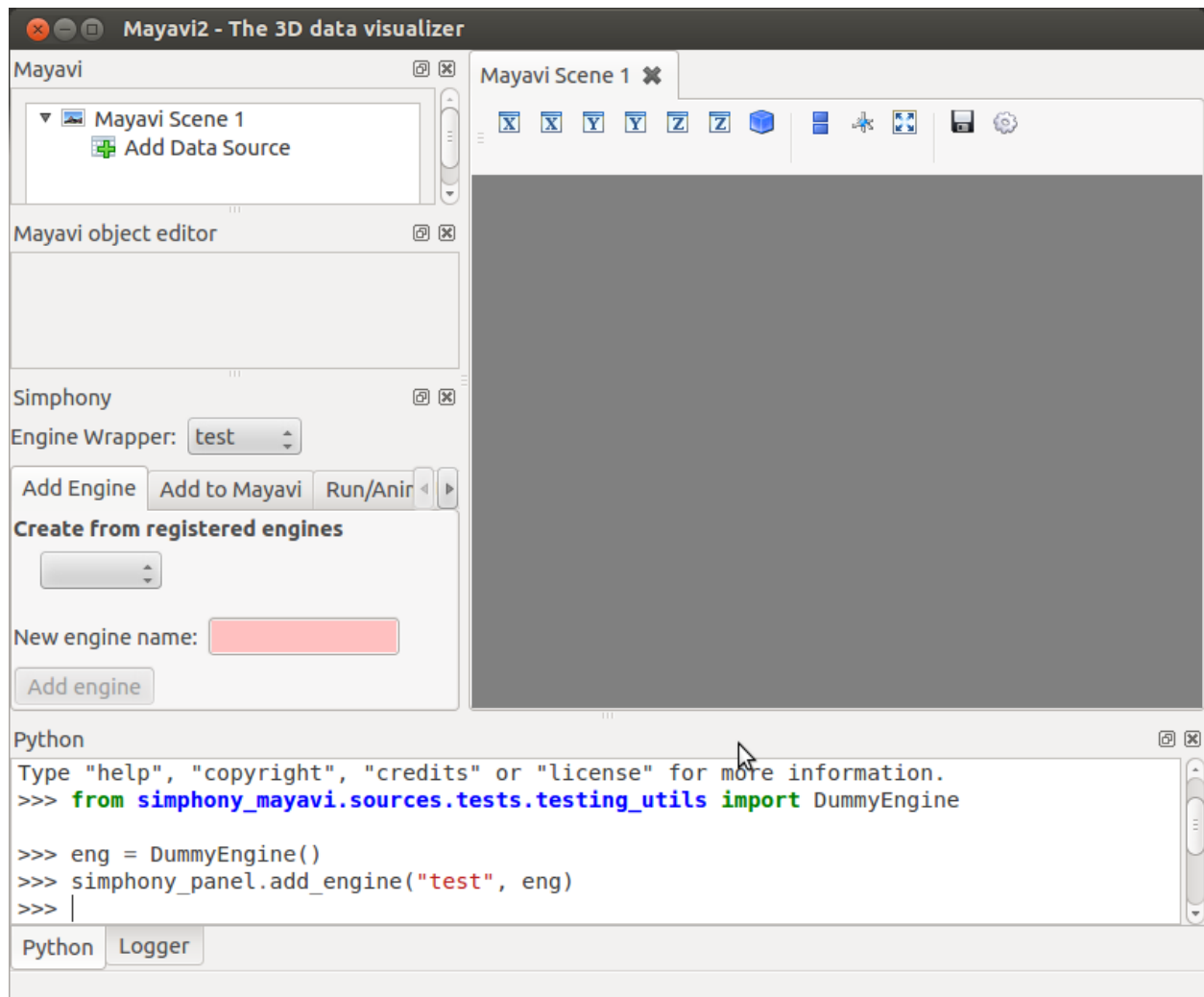



Fig. 9.12: The panel is identical to the *EngineManagerStandaloneUI*

```
from simphony.engine import lammps
from simlammps import EngineType
from simphony.core.cuba import CUBA
from simphony.visualisation import mayavi_tools

# read data
particles = lammps.read_data_file(
    os.path.join(os.path.dirname(__file__),
                 "billiards_init.data"))[0]

# configure dem-wrapper
dem = lammps.LammpsWrapper(engine_type=EngineType.DEM)

dem.CM_extension[lammps.CUBAExtension.THERMODYNAMIC_ENSEMBLE] = "NVE"
dem.CM[CUBA.NUMBER_OF_TIME_STEPS] = 1000
dem.CM[CUBA.TIME_STEP] = 0.001

# Define the BC component of the SimPhoNy application model:
dem.BC_extension[lammps.CUBAExtension.BOX_FACES] = ["fixed",
                                                    "fixed",
                                                    "fixed"]
dem.BC_extension[lammps.CUBAExtension.BOX_VECTORS] = None

# add particles to engine
dem.add_dataset(particles)

# Run the engine
dem.run()

@mayavi2.standalone
def view():
    mayavi_tools.add_engine_to_mayavi2("lammps", dem)

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

This example sets up a Simphony LAMMPS engine and starts Mayavi2 with the engine loaded in the GUI.

API Reference

10.1 Core module

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

Classes

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

Functions

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

10.1.1 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 tvtk 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=None*)
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. An empty list is acceptable, and returns a trivial accumulator providing no data. If *None* is passed, then the 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 lists).
- 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 initialialisation 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.

10.2 Cuds module

A module containing tvtk dataset wrappers to simphony CUDS containers.

Classes

| | |
|-----------------------------------------------------------------------|--------------|
| <u><code>VTKParticles</code>(name[, data, data_set, mappings])</u> | Constructor. |
| <u><code>VTKMesh</code>(name[, data, data_set, mappings])</u> | Constructor. |
| <u><code>VTKLattice</code>(name, primitive_cell, data_set[, ...])</u> | Constructor. |

10.2.1 Description

class `simphony_mayavi.cuds.vtk_particles.VTKParticles` (*name*, *data*, *data_set*, *mappings*)
data=None, *data_set*=None, *mappings*=None)

Bases: `simphony.cuds.abc_particles.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_bonds (*iterable*)

Adds a set of bonds to the container.

Also like with particles, if any 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_bonds' method for that purpose.

iterable [iterable of `Bond` objects] the new bond that will be included in the container.

Returns

uuid [list of `uuid.UUID`] The uuids of the added bonds.

Raises **ValueError** – when there is a bond with an uid that already exists in the container.

Examples

Add a set of bonds to a Particles container.

```
>>> bonds_list = [Bond(), Bond()]
>>> particles = Particles(name="foo")
>>> particles.add_bonds(bonds_list)
```

add_particles (*iterable*)

Adds a set of particles from the provided iterable to the container.

If any particle have no uids, the container will generate a new uids for it. If the particle has already an uids, 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_particles' method for that purpose.

iterable [iterable of Particle objects] the new set of particles that will be included in the container.

Returns

uids [list of uuid.UUID] The uids of the added particles.

Raises ValueError – when there is a particle with an uids that already exists in the container.

Examples

Add a set of particles to a Particles container.

```
>>> particle_list = [Particle(), Particle()]
>>> particles = Particles(name="foo")
>>> uids = particles.add_particles(particle_list)
```

bond2index = None

The mapping from uid to bond index

count_of (*item_type*)

Return the count of item_type in the container.

Parameters **item_type** (*CUDSItem*) – The CUDSItem enum of the type of the items to return the count of.

Returns **count** (*int*) – The number of items of item_type in the container.

Raises ValueError – If the type of the item is not supported in the current container.

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.

Parameters

- **name** (*str*) – The name of the container.

- **data_set** (*tvtk.DataSet*) – The dataset to wrap in the CUDS api. Default is None which will create a tvtk.PolyData
- **data** (*DataContainer*) – The data attribute to attach to the container. Default is None.

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

classmethod **from_particles** (*particles, particle_keys=None, bond_keys=None*)

Create a new VTKParticles copy from a CUDS particles instance.

Parameters

- **particles** (*ABCParticles*) – CUDS Particles dataset
- **particle_keys** (*list*) – A list of point CUBA keys that we want to copy, and only those. If None, all available and compatible keys will be copied.
- **bond_keys** (*list*) – A list of cell CUBA keys that we want to copy, and only those. If None, all available and compatible keys will be copied.

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

is_connected (*bond*)

Test if the connectivity described in bonds is valid i.e. the particles are part of the container

Parameters **bond** (*Bond*) –

Returns **valid** (*bool*)

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 iterable 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
```

```
>>> for bond in particles.iter_bond():
...     #do stuff; it will iterate over all the 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 iterable 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
>>> for particle in particles.iter_particles():
...     #do stuff
```

particle2index = None

The mapping from uid to point index

remove_bonds (*uids*)

Remove the bonds with the provided uids.

The uids passed as parameter should exist in the container. If any uid doesn't exist, an exception will be raised.

uids [iterable of uuid.UUID] the uids of the bond to be removed.

Raises **KeyError** – If any bond doesn't exist.

Examples

Having a set of uids of existing bonds, pass it to the method.

```
>>> particles = Particles(name="foo")
>>> ...
>>> particles.remove_bonds([uid1, uid2])
```

remove_particles (*uids*)

Remove the particles with the provided uids from the container.

The uids inside the iterable should exists in the container. Otherwise an exception will be raised.

uids [iterable of uuid.UUID] the uids of the particles to be removed.

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

Examples

Having a set of uids of existing particles, pass it to the method.

```
>>> particles = Particles(name="foo")
>>> ...
>>> particles.remove_particles([uid1, uid2])
```

supported_cuba = None

The currently supported and stored CUBA keywords.

update_bonds (*iterable*)

Updates a set of bonds from the provided iterable.

Takes the uids of the bonds and searches inside the container for those bond. If the bonds exists, they are replaced in the container. If any bond doesn't exist, it will raise an exception.

iterable [iterable of Bond objects] the bonds that will be replaced.

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

Examples

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

```
>>> particles = Particles(name="foo")
>>> ...
>>> bond1 = particles.get_bond(uid1)
>>> bond2 = particles.get_bond(uid2)
>>> ... #do whatever you want with the bonds
>>> particles.update_bonds([bond1, bond2])
```

update_particles (*iterable*)

Updates a set of particles from the provided iterable.

Takes the uids of the particles and searches inside the container for those particles. If the particles exists, they are replaced in the container. If any particle doesn't exist, it will raise an exception.

iterable [iterable of Particle objects] the particles that will be replaced.

Raises ValueError – If any particle inside the iterable does not exist.

Examples

Given a set of Particle objects that already exists in the container (taken with the ‘get_particle’ method for example), just call the function passing the Particle items as parameter.

```
>>> part_container = Particles(name="foo")
>>> ... #do whatever you want with the particles
>>> part_container.update_particles([part1, part2])
```

```
class simphony_mayavi.cuds.vtk_mesh.VTKMesh(name, data=None, data_set=None, mappings=None)
```

Bases: `simphony.cuds.abc_mesh.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_cells (*cells*)

Adds a set of new cells to the mesh.

cells [iterable of Cell] Cell to be added to the mesh

Raises ValueError – If other cell with a duplicated uid was already in the mesh

add_edges (*edges*)

Adds a set of new edges to the mesh.

edges [iterable of Edge] Edge to be added to the mesh

Raises ValueError – If other edge with a duplicated uid was already in the mesh

add_faces (*faces*)

Adds a set of new faces to the mesh.

faces [iterable of Face] Face to be added to the mesh

Raises ValueError – If other face with a duplicated uid was already in the mesh

add_points (*points*)

Adds a set of new points to the mesh.

points [iterable of Point] Points to be added to the mesh

Raises ValueError – If other point with a duplicated uid was already in the mesh.

count_of (*item_type*)

Return the count of *item_type* in the container.

Parameters *item_type* (*CUDSItem*) – The CUDSItem enum of the type of the items to return the count of.

Returns *count* (*int*) – The number of items of *item_type* in the container.

Raises *ValueError* – If the type of the item is not supported in the current container.

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.

Parameters

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

Raises *TypeError* – When the sanity checks fail.

classmethod from_mesh (*mesh*, *point_keys*=None, *cell_keys*=None)

Create a new VTKMesh copy from a CUDS mesh instance.

Parameters

- **mesh** (*ABCMesh*) – The original mesh to create the new one.
- **point_keys** (*list*) – A list of point CUBA keys that we want to copy, and only those. If None, all available and compatible keys will be copied.
- **cell_keys** (*list*) – A list of cell CUBA keys that we want to copy, and only those. If None, all available and compatible keys will be copied.

get_cell (*uid*)

Returns a cell with a given uid.

Returns the cell stored in the mesh identified by uid. If such a cell does not exists an exception is raised.

Parameters *uid* (*uuid.UUID*) – uid of the desired cell.

Returns *cell* (*Cell*) – Cell identified by uid

Raises

- **KeyError** – If the cell identified by uuid was not found
- **TypeError** – When *uid* is not *uuid.UUID*

get_edge (*uid*)

Returns an edge with a given uid.

Returns the edge stored in the mesh identified by uid. If such edge do not exists an exception is raised.

Parameters **uid** (*uuid.UUID*) – uid of the desired edge.

Returns **edge** (*Edge*) – Edge identified by uid

Raises

- **KeyError** – If the edge identified by uid was not found
- **TypeError** – When uid is not uuid.UUID

get_face (*uid*)

Returns a face with a given uid.

Returns the face stored in the mesh identified by uid. If such a face does not exists an exception is raised.

Parameters **uid** (*uuid.UUID*) – uid of the desired face.

Returns **face** (*Face*) – Face identified by uid

Raises

- **KeyError** – If the face identified by uid was not found
- **TypeError** – When uid is not uuid.UUID

get_point (*uid*)

Returns a point with a given uid.

Returns the point stored in the mesh identified by uid. If such point do not exists an exception is raised.

Parameters **uid** (*uuid.UUID*) – uid of the desired point.

Returns **point** (*Point*) – Mesh point identified by uuid

Raises

- **KeyError** – If the point identified by uid was not found
- **TypeError** – When uid is not uuid.UUID

has_cells ()

Check if the mesh has cells

Returns **result** (*bool*) – True of there are cells inside the mesh, False otherwise

has_edges ()

Check if the mesh has edges

Returns **result** (*bool*) – True of there are edges inside the mesh, False otherwise

has_faces ()

Check if the mesh has faces

Returns **result** (*bool*) – True of there are faces inside the mesh, False otherwise

index2element = None

The reverse mapping from index to bond uid

index2point = None

The reverse mapping from index to point uid

iter_cells (*uids=None*)

Returns an iterator over cells.

uids [iterable of uuid.UUID or None] When the uids are provided, then the cells are returned in the same order the uids are returned by the iterable. If uids is None, then all cells are returned by the iterable and there is no restriction on the order that they are returned.

Yields cell (*Cell*)

iter_edges (*uids=None*)

Returns an iterator over edges.

uids [iterable of uuid.UUID or None] When the uids are provided, then the edges are returned in the same order the uids are returned by the iterable. If uids is None, then all edges are returned by the iterable and there is no restriction on the order that they are returned.

Yields edge (*Edge*)

iter_faces (*uids=None*)

Returns an iterator over faces.

uids [iterable of uuid.UUID or None] When the uids are provided, then the faces are returned in the same order the uids are returned by the iterable. If uids is None, then all faces are returned by the iterable and there is no restriction on the order that they are returned.

Yields face (*Face*)

iter_points (*uids=None*)

Returns an iterator over points.

uids [iterable of uuid.UUID or None] When the uids are provided, then the points are returned in the same order the uids are returned by the iterable. If uids is None, then all points are returned by the iterable and there is no restriction on the order that they are returned.

Yields point (*Point*)

point2index = None

The mapping from uid to point index

supported_cuba = None

The currently supported and stored CUBA keywords.

update_cells (*cells*)

Updates the information of a set of cells.

Gets the mesh cell identified by the same uid as the provided cell and updates its information with the one provided with the new cell.

cells [iterable of Cell] Cell to be updated

Raises ValueError – If the any cell was not found in the mesh

update_edges (*edges*)

Updates the information of a set of edges.

Gets the mesh edge identified by the same uid as the provided edge and updates its information with the one provided with the new edge.

edges [iterable of Edge] Edge to be updated

Raises ValueError – If the any edge was not found in the mesh

update_faces (*faces*)

Updates the information of a set of faces.

Gets the mesh face identified by the same uid as the provided face and updates its information with the one provided with the new face.

faces [iterable of Face] Face to be updated

Raises ValueError – If the any face was not found in the mesh

update_points (*points*)

Updates the information of a set of points.

Gets the mesh point identified by the same uid as the provided point and updates its information with the one provided with the new point.

points [iterable of Point] Point to be updated

Raises ValueError – If the any point was not found in the mesh

```
class simphony_mayavi.cuds.vtk_lattice.VTKLattice(name, primitive_cell, data_set,
                                                  data=None)
```

Bases: `simphony.cuds.abc_lattice.ABCLattice`

Constructor.

Parameters

- **name** (*string*) – The name of the container.
- **primitive_cell** (*PrimitiveCell*) – primitive cell specifying the 3D Bravais lattice
- **data_set** (*tvtk.DataSet*) – The dataset to wrap in the CUDS api. If it is a `tvtk.PolyData`, the points are assumed to be arranged in C-contiguous order so that the first point is the origin and the last point is furthest away from the origin
- **data** (*DataContainer*) – The data attribute to attach to the container. Default is None.

count_of (*item_type*)

Return the count of *item_type* in the container.

Parameters *item_type* (*CUDSItem*) – The CUDSItem enum of the type of the items to return the count of.

Returns *count* (*int*) – The number of items of *item_type* in the container.

Raises ValueError – If the type of the item is not supported in the current container.

data

The container data

```
classmethod empty(name, primitive_cell, size, origin, data=None)
```

Create a new empty Lattice.

Parameters

- **name** (*string*) – The name of the container.
- **primitive_cell** (*PrimitiveCell*) – Primitive cell specifying the 3D Bravais lattice
- **size** (*tuple*) – lattice dimensions (nx, ny, nz)
- **origin** (*tuple*) – lattice origin (x, y, z)

- **data** (*DataContainer*) – The data attribute to attach to the container. Default is None.

Returns *lattice* (*VTKLattice*)

classmethod **from_dataset** (*name, data_set, data=None*)

Create a new Lattice and try to guess the *primitive_cell*

Parameters

- **name** (*str*) –
- **data_set** (*tvtk.ImageData* or *tvtk.PolyData*) – The dataset to wrap in the CUDS api. If it is a PolyData, the points are assumed to be arranged in C-contiguous order
- **data** (*DataContainer*) – The data attribute to attach to the container. Default is None.

Returns *lattice* (*VTKLattice*)

Raises **TypeError** – If *data_set* is not either *tvtk.ImageData* or *tvtk.PolyData*

IndexError: If the lattice nodes are not arranged in C-contiguous order

classmethod **from_lattice** (*lattice, node_keys=None*)

Create a new Lattice from the provided one.

Parameters

- **lattice** (*simphony.cuds.lattice.Lattice*) –
- **node_keys** (*list*) – A list of point CUBA keys that we want to copy, and only those. If None, all available and compatible keys will be copied.

Returns *lattice* (*VTKLattice*)

Raises

ValueError

- if *bravais_lattice* attribute of the primitive cell indicates a cubic/tetragonal/orthorhombic lattice but the primitive vectors are inconsistent with this attribute
- if *bravais_lattice* is not a member of *BravaisLattice*

get_coordinate (*ind*)

Get coordinate of the given index coordinate.

ind [*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 of the returned nodes.

Returns

iterator: An iterator over LatticeNode objects

origin

lattice origin (x, y, z)

point_data = None

Easy access to the vtk PointData structure

primitive_cell

Primitive cell specifying the 3D Bravais lattice

size

lattice dimensions (nx, ny, nz)

supported_cuba = None

The currently supported and stored CUBA keywords.

update_nodes (*nodes*)

Update the corresponding lattice nodes.

nodes : iterator of LatticeNodes

10.3 Modules module

`simphony_mayavi.modules.default_module.default_module` (*source*)

Mapping for module appropriate for the selected data

Parameters *source* (CUDSSource) –

Returns *modules* (*list*) – mayavi modules to be added to the pipeline

`simphony_mayavi.modules.default_module.default_scalar_module` (*scale_factor=1.0*)

Returns a Glyph with a sphere glyph source and scale_mode turned off. Suitable for points/nodes with scalar data

`simphony_mayavi.modules.default_module.default_vector_module` (*scale_factor=1.0*)

Returns a Glyph in its original mayavi defaults plus the scale_mode turned off

10.4 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.

Classes

`EngineManagerStandalone`

`EngineManagerStandaloneUI`

Functions

| |
|-----------------------------------------------------------|
| <code>simphony_mayavi.plugin.show</code> |
| <code>simphony_mayavi.plugin.snapshot</code> |
| <code>simphony_mayavi.plugin.adapt2cuds</code> |
| <code>simphony_mayavi.plugin.load</code> |
| <code>simphony_mayavi.plugin.add_engine_to_mayavi2</code> |
| <code>simphony_mayavi.plugin.get_simphony_panel</code> |
| <code>simphony_mayavi.plugin.restore_scene</code> |

10.4.1 Description

10.5 Plugins module

This module contains classes the Symphony plugins for the Mayavi2 application.

Classes

| | |
|---------------------------------------------------------------------------------------------|------------------|
| <code>simphony_mayavi.plugins.add_source_panel.AddSourcePanel</code> | |
| <code>AddEnginePanel</code> | A panel to add |
| <code>simphony_mayavi.plugins.add_engine_source_to_mayavi.AddEngineSourceToMayavi</code> | |
| <code>EngineManager</code> | A basic contain |
| <code>EngineManagerMayavi2</code> | The Symphony |
| <code>simphony_mayavi.plugins.engine_manager_standalone.EngineManagerStandalone</code> | |
| <code>simphony_mayavi.plugins.engine_manager_standalone_ui.EngineManagerStandaloneUI</code> | |
| <code>RunAndAnimate</code> | Standalone no |
| <code>RunAndAnimatePanel</code> | GUI for runni |
| <code>TabbedPanelCollection</code> | Collect a list o |

Functions

| |
|--------------------------------------------------------------------------------------------------|
| <code>simphony_mayavi.plugins.add_engine_source_to_mayavi.add_source_and_modules_to_scene</code> |
|--------------------------------------------------------------------------------------------------|

10.5.1 Descriptions

class `simphony_mayavi.plugins.add_engine_panel.AddEnginePanel`

Bases: `traits.has_traits.HasTraits`

A panel to add a new modeling engine by creating one from a factory function. Then send it to the EngineManager instance `engine_manager`

class `simphony_mayavi.plugins.engine_manager.EngineManager`

Bases: `traits.has_traits.HasTraits`

A basic container of Symphony Engine that comes with a GUI.

Additional panel can be added to support more operations related to the modeling engines

engines = dict
 Mappings of Symphony Modeling Engines in this manager

engine_name = str
 Name of the Symphony Modeling Engine

engine = ABCModelingEngine
 Symphony Modeling Engine

add_engine (*name, modeling_engine*)
 Add a Symphony Engine to the manager

Parameters

- **name** (*str*) – Name to be associated with the modeling engine
- **modeling_engine** (*ABCModelingEngine*) – Symphony Engine Wrapper

remove_engine (*name*)
 Remove a modeling engine from the manager. If modeling engine to be removed is currently selected, select the one of the remaining engines

Parameters **name** (*str*) – Name associated with the engine to be removed

class `simphony_mayavi.plugins.engine_manager_mayavi2.EngineManagerMayavi2`
 Bases: `simphony_mayavi.plugins.engine_manager.EngineManager`

The Symphony panel in the Mayavi2 application

get_mayavi ()
 Get the mayavi engine in Mayavi2

class `simphony_mayavi.plugins.run_and_animate.RunAndAnimate` (*engine, mayavi_engine*)
 Bases: `object`

Standalone non-GUI based controller for running a Symphony Modeling Engine and animating the CUDS dataset in Mayavi.

Precondition: The required CUDS datasets are already visible in the Mayavi scene(s)

Parameters

- **engine** (*ABCModelingEngine*) – Symphony Modeling Engine
- **mayavi_engine** (*mayavi.api.Engine*) – for retrieving scenes and visible datasets

animate (*number_of_runs, delay=None, ui=False, update_all_scenes=False*)
 Run the modeling engine, and animate the scene. If there is no source in the scene or none of the sources belongs to the selected Engine *engine*, a `RuntimeError` is raised.

Parameters

- **number_of_runs** (*int*) – the number of times the `engine.run()` is called
- **delay** (*int*) – delay between each run. If `None`, use previous setting or the Mayavi's default (500)
- **ui** (*bool*) – whether an UI is shown, default is `False`
- **update_all_scenes** (*bool*) – whether all scenes are updated, default is `False`: i.e. only the current scene is updated

Raises

RuntimeError if nothing in scene(s) belongs to *engine*

```
class simphony_mayavi.plugins.run_and_animate_panel.RunAndAnimatePanel
    Bases: traits.has_traits.HasTraits

    GUI for running a Symphony Modeling Engine and animating the result in an existing scene

    engine = ABCModelingEngine
        Symphony Engine

    mayavi_engine = mayavi.api.Engine
        The mayavi engine that manages the scenes

    time_step = float
        CUBA.TIME_STEP of the Symphony Engine

    number_of_time_steps = float
        CUBA.NUMBER_OF_TIME_STEPS of the Symphony Engine

    show_config()
        Show the GUI

class simphony_mayavi.plugins.tabbed_panel_collection.TabbedPanelCollection
    Bases: traits.has_traits.HasTraits

    Collect a list of HasTraits instances and display each of them as a tab in a tabbed notebook using ListEditor

    panels = list
        Instances of HasTraits to be displayed in tabs

    selected_panel = HasTraits
        Currently selected (visible) instance

    classmethod create(**kwargs)
        Create a TabbedPanelCollection containing the given HasTraits instances.

        **kwargs The values are the HasTraits instances to be collected. The keys in the keyword arguments are
            used to define attributes of the TabbedPanelCollection so that the HasTraits instances can be retrieved
            easily. As with any keyword arguments, the order of the keys is lost.

    Raises

    AttributeError If the given key is a pre-defined attribute/method
```

Examples

```
>>> all_panels = TabbedPanelCollection(panel_a=PanelA(),
                                         panel_b=PanelB())

>>> all_panels.panel_a
<PanelA at 0x7fdc974febd0>
```

```
>>> all_panels.configure_traits() # should display a notebook
```

10.5.2 Engine_wrapper module

```
class simphony_mayavi.plugins.engine_wrappers.abc_engine_factory.ABCEngineFactory
    Bases: traits.has_traits.ABCHasStrictTraits

    create()
        Return a new engine wrapper instance
```

```

class simphony_mayavi.plugins.engine_wrappers.jyulb.JyulbFileIOEngineFactory
    Bases: simphony_mayavi.plugins.engine_wrappers.abc_engine_factory.ABCEngineFactory

class simphony_mayavi.plugins.engine_wrappers.jyulb.JyulbInternalEngineFactory
    Bases: simphony_mayavi.plugins.engine_wrappers.abc_engine_factory.ABCEngineFactory

class simphony_mayavi.plugins.engine_wrappers.kratos.KratosEngineFactory
    Bases: simphony_mayavi.plugins.engine_wrappers.abc_engine_factory.ABCEngineFactory

class simphony_mayavi.plugins.engine_wrappers.lammps_md.LammpsEngineFactory
    Bases: simphony_mayavi.plugins.engine_wrappers.abc_engine_factory.ABCEngineFactory

class simphony_mayavi.plugins.engine_wrappers.openfoam.OpenFoamFileIOEngineFactory
    Bases: simphony_mayavi.plugins.engine_wrappers.abc_engine_factory.ABCEngineFactory

class simphony_mayavi.plugins.engine_wrappers.openfoam.OpenFoamInternalEngineFactory
    Bases: simphony_mayavi.plugins.engine_wrappers.abc_engine_factory.ABCEngineFactory

```

10.6 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

| | |
|-----------------------------------------------------|---------------------------------------------------------|
| <code>CUDSSource([cuds, point_scalars, ...])</code> | A mayavi source of a SimPhoNy CUDS container. |
| <code>CUDSFileSource(**traits)</code> | A mayavi source of a SimPhoNy CUDS File. |
| <code>EngineSource([engine, dataset, ...])</code> | A mayavi source for reading data from a SimPhoNy Engine |

10.6.1 Description

```

class simphony_mayavi.sources.cuds_source.CUDSSource (cuds=None, point_scalars=None,
                                                         point_vectors=None,
                                                         cell_scalars=None,
                                                         cell_vectors=None, **traits)
    Bases: mayavi.sources.vtk_data_source.VTKDataSource

```

A mayavi source of a SimPhoNy CUDS container.

cuds [instance of ABCParticle/ABCMesh/ABCLattice/H5Mesh] The CUDS container to be wrapped as VTK data source

The `cuds` attribute holds a reference to the CUDS instance it is assigned to, as oppose to making a copy. Therefore in any given time after setting `cuds`, the CUDS container could be modified internally and divert from the VTK data source. The `update` function can be called to update the visualisation.

Constructor

Parameters

- **cuds** (*Instance*) – The CUDS dataset to be wrapped as VTK data source (i.e. *ABCParticles*, *ABCLattice*, *ABCMesh* or *H5Mesh*)
- **point_scalars** (*str*) – CUBA name of the data to be selected as point scalars. Default is the first available point scalars.

- **point_vectors** (*str*) – CUBA name of the data to be selected as point vectors. Default is the first available point vectors.
- **cell_scalars** (*str*) – CUBA name of the data to be selected as cell scalars. Default is the first available cell scalars.
- **cell_vectors** (*str*) – CUBA name of the data to be selected as cell vectors. Default is the first available cell vectors.

Note: To turn off visualisation for a point/cell scalar/vector data, assign the attribute to an empty string (i.e. `point_scalars=""`)

Other optional keyword parameters are parsed to `VTKDataSource`.

Examples

```
>>> cuds = Particles("test")
```

```
>>> # Say each particle has scalars "TEMPERATURE" and "MASS"
>>> # and vector data: "VELOCITY"
>>> cuds.add_particles([...])
```

```
>>> # Initialise the source and specify scalar data to visualise
>>> # but turn off the visualisation for point vectors
>>> source = CUDSSource(cuds=cuds, point_scalars="MASS",
                        point_vectors="")
```

```
>>> # Show it in Mayavi!
>>> from mayavi import mlab
>>> mlab.pipeline.glyph(source)
```

cuds = Property(depends_on='_cuds')

The CUDS container

output_info = PipelineInfo(datasets=['image_data', 'poly_data', 'unstructured_grid'], attribute_types=['any'], attribut

Output information for the processing pipeline.

update ()

Recalculate the VTK data from the CUDS dataset. Useful when `cuds` is modified after assignment.

Examples

```
>>> # Add content to cuds after visualisation is set up
>>> source.cuds.add_particles([...])
```

```
>>> # update the scene!
>>> source.update()
```

class `simphony_mayavi.sources.cuds_file_source.CUDSFileSource` (****traits**)

Bases: `simphony_mayavi.sources.cuds_source.CUDSSource`

A mayavi source of a SimPhoNy CUDS File.

Create a `CUDSFileSource` instance

Example

```
>>> source = CUDSFileSource()
>>> source.initialize("path/to/cuds_file.cuds")
```

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.

initialized = Bool(False)

whether the source is initialized

start ()

update ()

```
class simphony_mayavi.sources.engine_source.EngineSource (engine=None,
                                                           dataset=None,
                                                           point_scalars=None,
                                                           point_vectors=None,
                                                           cell_scalars=None,
                                                           cell_vectors=None,
                                                           **traits)
```

Bases: `simphony_mayavi.sources.cuds_source.CUDSSource`

A mayavi source for reading data from a SimPhoNy Engine

Constructor

Parameters

- **engine** (*ABCModelingEngine*) – The SimPhoNy Modeling Engine where dataset is loaded from. Default is None.
- **dataset** (*str*) – Name of the dataset to be extracted from engine. Default is the first available dataset if engine is defined, otherwise it is an empty string
- **point_scalars** (*str*) – CUBA name of the data to be selected as point scalars. Default is the first available point scalars.
- **point_vectors** (*str*) – CUBA name of the data to be selected as point vectors. Default is the first available point vectors.
- **cell_scalars** (*str*) – CUBA name of the data to be selected as cell scalars. Default is the first available cell scalars.
- **cell_vectors** (*str*) – CUBA name of the data to be selected as cell vectors. Default is the first available cell vectors.

Note: To turn off visualisation for a point/cell scalar/vector data, assign the attribute to an empty string (i.e. `point_scalars=""`)

Other optional keyword parameters are parsed to CUDSSource

Examples

```
>>> source = EngineSource(engine=some_engine)
>>> source.datasets
["particles", "lattice"]
>>> source.dataset = "particles"
```

```
>>> # Alternatively
>>> source = EngineSource(engine=some_engine, dataset="particles")
```

```
>>> from mayavi import mlab
>>> mlab.pipeline.glyphy(source)
```

update()

Recalculate the VTK data from the CUDS dataset. Useful when `cuds` is modified after assignment.

Examples

```
>>> # Add content to cuds after visualisation is set up
>>> source.cuds.add_particles([...])
```

```
>>> # update the scene!
>>> source.update()
```

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