SimPhoNy UI

Release 0.2.0.dev0

Jul 05, 2017

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Simphony-ui

A GUI which allows one to run a computation using Liggghts and OpenFOAM and visualize the result with Mayavi

Repository

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

Requirements

- futures
- simphony-framework == 0.3.1

Optional requirements

To support the documentation built you need the following packages:

- sphinx >= 1.3.1

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
```

Quick start:

Once installed, you can run SimPhoNy-UI with:

```
# run simphony-ui
openfoam_liggghts_ui
```

Testing

To run the full test-suite run:

```
python -m unittest discover
```

Directory structure

The module is structured as following:

- simphony_ui – Core of the simphony_ui module
    - liggghts_model – The Liggghts trait model and wrapper creation
    - openfoam_model – The OpenFOAM trait model and wrapper creation
    - couple_openfoam_liggghts – Main routine which run the calculation
    - ui – Main trait model which contains the whole UI with the Mayavi view
- doc – Documentation related files
    - source – Sphinx rst source files
    - build – Documentation build directory, if documentation has been generated using the `make` script in the `doc` directory.

EDM packages

The repository supports generation of EDM packages with the command:

```
python edmsetup.py egg
```

Check the simphony/buildrecipes-common documentation for more information.

User Manual

SimPhoNy-UI

You can use SimPhoNy-UI to run a calculation using OpenFOAM and Liggghts at the same time and visualize the result with Mayavi.

Input parameters

Using the UI, you will be able to set the following parameters:

- General parameters
- LIGGGHTS specific parameters
- OpenFoam specific parameters

You must specify input files for OpenFOAM and Liggghts. You can find examples of input files in the simphony_ui/tests/fixtures directory.

General parameters

The following parameters are available in the general configuration tab:

- Number of iterations: It is the total number of full steps the evaluation will perform.
- Update frequency: Allows to specify the number of iterations at which the data will be snapshot. For example, 10000 iterations with an update frequency of 1000 will produce image frames at iterations 1000, 2000, 3000 etc.
- Force type: the force type to use, common between liggghts and openfoam.

LIGGGHTS parameters

This dialog contains parameters specific to LIGGGHTS. Their documentation can be found on the appropriate sources for LIGGGHTS.

OpenFoam parameters

This dialog contains parameters specific to OpenFoam. Their documentation can be found on the appropriate sources for OpenFoam.

Run the calculation

Once input parameters are correctly set, you'll be able to run the calculation with the "Run" button at the bottom of the dialog. A progress bar dialog should appear. It can take a few minutes for large number of iterations.

Visualize result

Once the calculation terminated, the result should automatically appears in the 3D Mayavi scene. You could then see the Mayavi pipeline and change some parameters of the visualization, and play the movie or change frames using the buttons on the bottom part of the visualization.

The "Save..." button allows to save the rendered frames as png files. Once pressed, a dialog will request a directory. Files in the format "frame-N.png" with N the frame number will be created.

If you run the calculation again, Mayavi input datasets will be overwritten.

CHAPTER 3

Indices and tables

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