FDEM Post-Processing

Release 0.0

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Dec 28, 2022

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CHAPTER

ONE

PYFDEMPP - AN FDEM VISUALISER POST-PROCESSING PACKAGE

python 3.5|3.6|3.7|3.8|3.9|3.10 pip3 install pyfdempp

1.1 About

This Python package performs transformations on hybrid finite-discrete element method (FDEM) models with an unstructured grid in vtk/vtu/vtp format. It currently supports arrays of simulation files from the FDEM solvers:

- Geomechanica's Irazu software,
- Y-Geo (and its common derivatives), as well as
- OpenFDEM.

The package is heavily dependent on `pyvista` and is limited to `Python >=3.5`. The package is maintained by the Grasselli's Geomechanics Group at the University of Toronto, Canada, and is part of a collaborative effort by the open-source pacakge OpenFDEM.

1.2 Functionality

The functionality of this script was developed with the objective of extracting common information needed when running simulations. Highlights of the script are:

- Get model information.

```
import pyfdempp as fd
model = fd.Model("abs_model_path_on_machine")
# Getting number of points in your model.
model.n_points
```

Output:

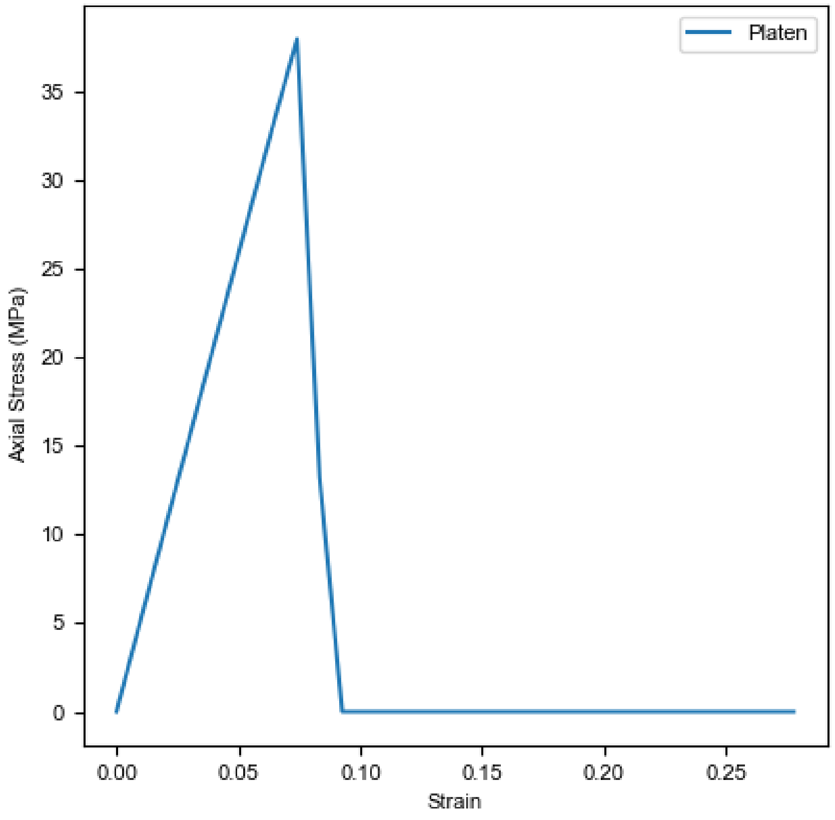
```
11904
```

- Extract information within the FDEM Model based on the name of the array (e.g., Stress, Strain, Temperature, etc…) Works in 2D and 3D.
- Extract stress-strain information for UCS and BD Simulations (Works in 2D and 3D). Optional addition of virtual strain gauges (Limited to 2D).

```
import pyfdempp as fd
model = fd.Model("abs_model_path_on_machine")
model.complete_stress_strain(progress_bar=True)
```

Output:

```
Script Identifying Platen
   Platen Material ID found as [1]
   Progress: |//////////////////////////////////////////////////| 100.0% Complete
   1.51 seconds
     Platen Stress  Platen Strain
 0    0.000000e+00       0.000000
 1    4.825237e+00       0.009259
 2    9.628823e+00       0.018519
 3    1.441437e+01       0.027778
 4    1.919164e+01       0.037037
 ..            ...            ...
 57   2.036137e-30       0.240741
 58   2.036137e-30       0.250000
 59   2.036137e-30       0.259259
 60   2.036137e-30       0.268519
 61   2.036137e-30       0.277778

 [62 rows x 2 columns]
```



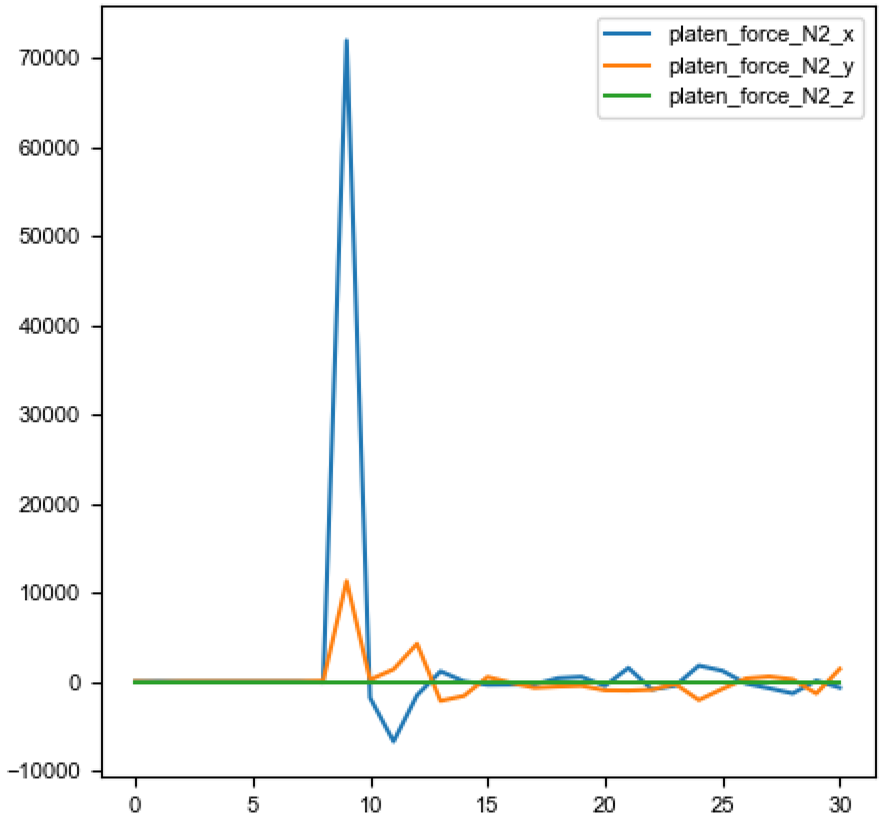
- Plotting stress vs strain curve.
- Calculate the Elastic Modulus of the dataset. Eavg, Esec and Etan can be evaluated. Works in 2D and 3D.

```
import pyfdempp as fd
model = fd.Model("abs_model_path_on_machine")
df_1 = model.complete_UCS_stress_strain(st_status=True)

# Variants of E tangent
print('Etan at 50%%: %.2fMPa' % model.Etan50_mod(df_1)[0])
print('Etan at 50%% with linear best fit disabled: %.2fMPa' % model.Etan50_mod(df_1,␣
↪linear_bestfit=False)[0])
print('Etan at 50%% using strain gauge data: %.2fMPa' % model.Etan50_mod(df_1, loc_
↪strain='Gauge Displacement Y', plusminus_range=1)[0])
# Variants of E secant
print('Esec at 70%%: %.2fMPa' % model.Esec_mod(df_1, 70))
print('Esec at 50%%: %.2fMPa' % model.Esec_mod(df_1, 0.5))
# Variants of E average
print('Eavg between 50-60%%: %.2fMPa' % model.Eavg_mod(df_1, 0.5, 0.6)[0])
print('Eavg between 20-70%% with linear best fit disabled: %.2fMPa' % model.Eavg_mod(df_
↪1, 0.2, 0.7, linear_bestfit=False)[0])
```

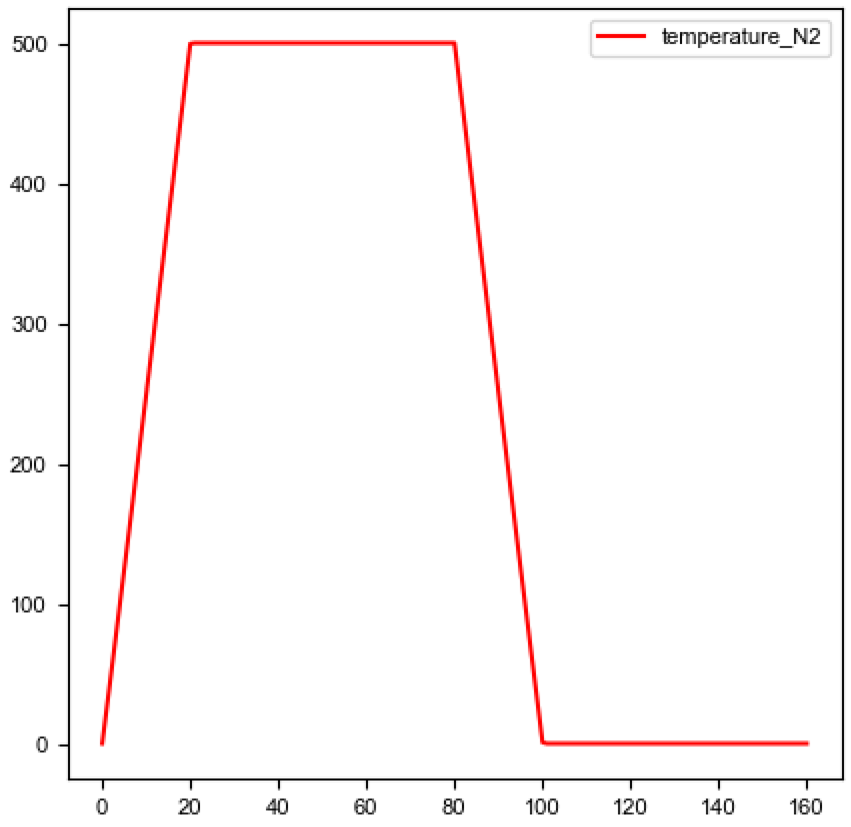
Output:

```
    Etan at 50%: 51683.94MPa
    Etan at 50% with linear best fit disabled: 51639.22MPa
    Etan at 50% using strain gauge data: 50275.03MPa

    Esec at 70%: 51681.01MPa
    Esec at 50%: 51817.43MPa

    Eavg between 50-60%: 51594.49MPa
    Eavg between 20-70% with linear best fit disabled: 51660.62MPa
```

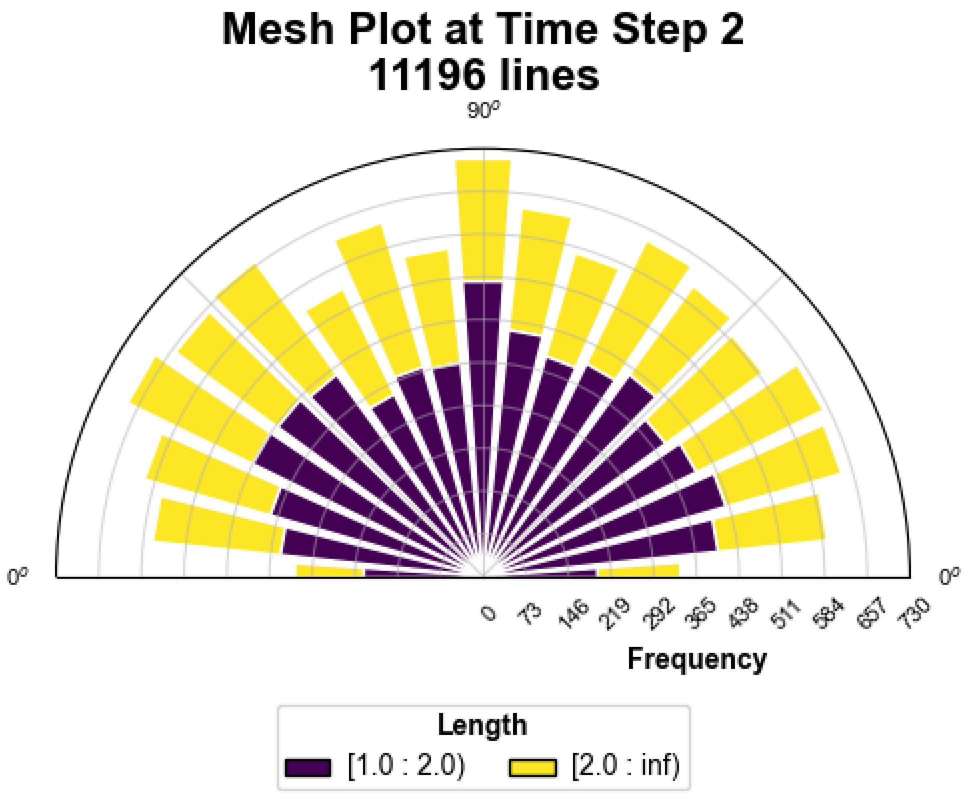
- Extract information of a particular cell based on a sequence of array names. This can be extended to extracting information along a line. Works in 2D and 3D.



- Extract information of a threshold dataset criteria based on a sequence of array names. Works in 2D and 3D.



- Extract mesh information and plot rosette/polar plots. Limited to 2D.



- Automatic detection/ User-defined assigment of loading direction when analysing mechanical simulations, namely UCS, BD, and PLT, in both 2D and 3D simulations.

```
Script Identifying Platen
        Platen Material ID found as [1]
        3D Loading direction detected as [1] is Y-direction
Values used in calculations are
        Area        3721.00
        Length        122.00
Progress: |//////////////////////////////////////////////////| 100.0% Complete
```

1.3 Additional Support

Please refer to the user manual for detailed information pertaining to the various functions and their usage/arguments. For specific script requests and bug, please report them on our github page.

CHAPTER

TWO

PYFDEMPP

2.1 pyfdempp package

2.1.1 Submodules

pyfdempp.pyfdempp

class `pyfdempp.pyfdempp.`**`Model`**(*dir_path=None*, *runfile=None*, *fdem_engine=None*)

Bases: `object`

Collects datafiles into one Class. Returns the data array ordered by simulation timestep.

Example

```
>>> import pyfdempp as fdem
>>> model = fdem.Model("../example_outputs/Irazu_UCS")
```

`Eavg_mod`(*ucs_data*, *upperrange*, *lowerrange*, *linear_bestfit=True*, *loc_stress='Platen Stress'*, *loc_strain='Platen Strain'*)

Average Elastic modulus between two ranges

Parameters

- **`ucs_data`** (*`pandas.DataFrame`*) – DataFrame containing the stress-strain data
- **`upperrange`** (*`float`*) – Upper range to calculate the average
- **`lowerrange`** (*`float`*) – Lower range to calculate the average
- **`linear_bestfit`** (*`bool`*) – Calculate data based on range extents or linear best fit line.
- **`loc_stress`** (*`str`*) – Column to obtain stress from. Defaults to Platen Stress
- **`loc_strain`** (*`str`*) – Column to obtain strain from. Defaults to Platen Strain

Returns

Average Elastic modulus

Return type

list[float]

Raises

`ZeroDivisionError` – The range over which to calculate the Eavg is too small. Consider a larger range.

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> df_1 = data.complete_UCS_stress_strain(st_status=True)
>>> data.Eavg_mod(df_1, 0.5, 0.6)[0]
51594.490217007056
>>> data.Eavg_mod(df_1, 0.5, 0.6, loc_strain='Gauge Displacement Y
↪')[0]
51110.06292512191
```

Esec_mod(*ucs_data*, *upperrange*, *loc_stress='Platen Stress'*, *loc_strain='Platen Strain'*)

Secant Modulus between 0 and upperrange. The upperrange can be a % or a fraction.

Parameters

- **ucs_data** (*pandas.DataFrame*) – DataFrame containing the stress-strain data
- **upperrange** (*float*) – Range over which to calculate the Secant Modulus
- **loc_stress** (*str*) – Column to obtain stress from. Defaults to Platen Stress
- **loc_strain** (*str*) – Column to obtain strain from. Defaults to Platen Strain

Returns

Secant Elastic modulus between 0 and upperrange

Return type

float

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> df_1 = data.complete_UCS_stress_strain(st_status=True)
>>> data.Esec_mod(df_1, 0.5)
51817.43019752671
>>> data.Esec_mod(df_1, 0.5, loc_strain='Gauge Displacement Y')
51355.860814069754
```

Etan50_mod(*ucs_data*, *linear_bestfit=True*, *loc_stress='Platen Stress'*, *loc_strain='Platen Strain'*, *plusminus_range=1*)

Tangent Elastic modulus at 50%. Calculates +/- number of datapoint from the 50% Stress. Defaults to +/- 1 datapoint.

Parameters

- **ucs_data** (*pandas.DataFrame*) – DataFrame containing the stress-strain data
- **linear_bestfit** (*bool*) – Calculate data based on range extents or linear best fit line.
- **loc_stress** (*str*) – Column to obtain stress from. Defaults to Platen Stress
- **loc_strain** (*str*) – Column to obtain strain from. Defaults to Platen Strain
- **plusminus_range** (*int*) – Range over which to calculate the Elastic modulus

Returns

Tangent Elastic modulus at 50% as a slope and Y-Intercept. Y-Intercept = 0 if linear_bestfit is False

Return type

list[float]

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> df_1 = data.complete_UCS_stress_strain()
>>> data.Etan50_mod(df_1)[0]
51683.94337878284
>>> data.Etan50_mod(df_1, linear_bestfit=False)[0]
51639.21679789497
>>> df_1 = data.complete_UCS_stress_strain(st_status=True)
>>> data.Etan50_mod(df_1, loc_strain='Gauge Displacement Y',␣
↪plusminus_range=1)[0]
51216.33411269702
```

complete_BD_stress_strain(*st_status=False*, *gauge_width=0*, *gauge_length=0*, *c_center=None*, *progress_bar=True*)

Calculate the full stress-strain curve for an indirect tensile simulation.

Parameters

- **st_status** (*bool*) – Enable/Disable SG
- **gauge_width** (*float*) – width of the virtual strain gauge
- **gauge_length** (*float*) – length of the virtual strain gauge
- **c_center** (*None or list[float, float, float]*) – User-defined center of the SG
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns

full stress-strain information

Return type

pandas.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("/external/Speed_Cal_Using_Flowstone/BD/BD_c_17_
↪5_ts_2_55_GII_90000_v_0_6")
# full stress-strain without SG
>>> df_wo_SG = data.complete_BD_stress_strain(False)
Columns:
    Name: Platen Stress, dtype=float64, nullable: False
    Name: Platen Strain, dtype=float64, nullable: False
Script Identifying Platen
    Platen Material ID found as [1]
Progress: |//////////////////////////////////////////////////| 100.0%␣
↪Complete
# full stress-strain with SG and default dimensions
>>> df_Def_SG = data.complete_BD_stress_strain(True)
Columns:
    Name: Platen Stress, dtype=float64, nullable: False
    Name: Platen Strain, dtype=float64, nullable: False
    Name: Gauge Displacement X, dtype=float64, nullable: False
    Name: Gauge Displacement Y, dtype=float64, nullable: False
    Script Identifying Platen
```

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```
Platen Material ID found as [1]
Dimensions of SG are 12.0 x 12.0
Vertical Gauges
    extends between [[6.0, -6.0, 0.0], [-6.0, -6.0, 0.0], [6.0, 6.0,␣
↪0.0], [-6.0, 6.0, 0.0]]
    cover cells ID [3644, 7481, 4635, 2872]
Horizontal Gauges
    extends between [[6.0, 6.0, 0.0], [6.0, -6.0, 0.0], [-6.0, 6.0, 0.
↪0], [-6.0, -6.0, 0.0]]
    cover cells ID [4635, 3644, 2872, 7481]
Progress: |//////////////////////////////////////////////////| 100.0%␣
↪Complete
# full stress-strain with SG and user-defined dimensions
>>> df_userdf_SG = data.complete_BD_stress_strain(True, 10, 10)
Columns:
    Name: Platen Stress, dtype=float64, nullable: False
    Name: Platen Strain, dtype=float64, nullable: False
    Name: Gauge Displacement X, dtype=float64, nullable: False
    Name: Gauge Displacement Y, dtype=float64, nullable: False
Script Identifying Platen
    Platen Material ID found as [1]
    Dimensions of SG are 10 x 10
    Vertical Gauges
        extends between [[5.0, -5.0, 0.0], [-5.0, -5.0, 0.0], [5.0, 5.
↪0, 0.0], [-5.0, 5.0, 0.0]]
        cover cells ID [1898, 5999, 5249, 6806]
    Horizontal Gauges
        extends between [[5.0, 5.0, 0.0], [5.0, -5.0, 0.0], [-5.0, 5.
↪0, 0.0], [-5.0, -5.0, 0.0]]
        cover cells ID [5249, 1898, 6806, 5999]
Progress: |//////////////////////////////////////////////////| 100.0%␣
↪Complete
```

complete_PLT_stress_strain(*load_config*, *platen_id=None*, *axis_of_loading=None*, *De_squared=None*, *progress_bar=True*)

Calculate the full stress-strain curve for a point load simulation.

Parameters

- **load_config** (*str*) – type of PLT Test. “A” “D” “B”
- **platen_id** (*None or int*) – Manual override of Platen ID
- **axis_of_loading** (*None or int*) – Loading Direction
- **De_squared** (*None or float*) – equivalent core diameter (i.e., the value of De_squared)
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns
full stress-strain information

Return type
pandas.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("/external/Yusuf_PLT/Axial")
# Minimal Arguments
>>> df = data.complete_PLT_stress_strain(load_config="A", platen_id=1)
Columns:
    Name: Platen Stress, dtype=float64, nullable: False
```

complete_UCS_stress_strain(*platen_id=None*, *st_status=False*, *axis_of_loading=None*, *gauge_width=0*, *gauge_length=0*, *c_center=None*, *samp_A=None*, *samp_L=None*, *progress_bar=True*)

Calculate the full stress-strain curve for a uniaxial compressive strength simulation

Parameters

- **platen_id** (*None or int*) – Manual override of Platen ID
- **st_status** (*bool*) – Enable/Disable SG
- **axis_of_loading** (*None or int*) – Loading Direction
- **gauge_width** (*float*) – width of the virtual strain gauge
- **gauge_length** (*float*) – length of the virtual strain gauge
- **c_center** (*None or list[float, float, float]*) – User-defined center of the SG
- **samp_A** (*None or float*) – Sample Area
- **samp_L** (*None or float*) – Sample Length
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns

full stress-strain information

Return type

pandas.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
# Minimal Arguments
>>> df_wo_SG = data.complete_UCS_stress_strain()
Columns:
    Name: Platen Stress, dtype=float64, nullable: False
    Name: Platen Strain, dtype=float64, nullable: False
Script Identifying Platen
    Platen Material ID found as [1]
    Predefined loading Axis [1] is Y-direction
Values used in calculations are
    Area    52.00
    Length  108.00
Progress: |//////////////////////////////////////////////////| 100.0%␣
↪Complete
# full stress-strain without SG
>>> df_Def_SG = data.complete_UCS_stress_strain(None, True)
Columns:
    Name: Platen Stress, dtype=float64, nullable: False
```

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```
    Name: Platen Strain, dtype=float64, nullable: False
    Name: Gauge Displacement X, dtype=float64, nullable: False
    Name: Gauge Displacement Y, dtype=float64, nullable: False
Script Identifying Platen
    Platen Material ID found as [1]
        Predefined loading Axis [1] is Y-direction
    Values used in calculations are
        Area        52.00
        Length      108.00
        Dimensions of SG are 27.0 x 13.0
        Vertical Gauges
            extends between [[6.5, -13.5, 0.0], [-6.5, -13.5, 0.0],␣
↪[6.5, 13.5, 0.0], [-6.5, 13.5, 0.0]]
            cover cells ID [2744, 1377, 3466, 3789]
        Horizontal Gauges
            extends between [[13.5, 6.5, 0.0], [13.5, -6.5, 0.0], [-
↪13.5, 6.5, 0.0], [-13.5, -6.5, 0.0]]
            cover cells ID [2089, 1582, 2210, 1504]
    Progress: |///////////////////////////////////////////////////|␣
↪100.0% Complete
# full stress-strain with SG and user-defined dimensions
>>> df_userdf_SG = data.complete_UCS_stress_strain(None, True, gauge_
↪width=10, gauge_length=10)
Columns:
    Name: Platen Stress, dtype=float64, nullable: False
    Name: Platen Strain, dtype=float64, nullable: False
    Name: Gauge Displacement X, dtype=float64, nullable: False
    Name: Gauge Displacement Y, dtype=float64, nullable: False
Script Identifying Platen
    Platen Material ID found as [1]
    Predefined loading Axis [1] is Y-direction
Values used in calculations are
    Area    52.00
    Length  108.00
    Dimensions of SG are 10 x 10
    Vertical Gauges
        extends between [[5.0, -5.0, 0.0], [-5.0, -5.0, 0.0], [5.0, 5.
↪0, 0.0], [-5.0, 5.0, 0.0]]
        cover cells ID [1186, 1397, 1669, 1148]
    Horizontal Gauges
        extends between [[5.0, 5.0, 0.0], [5.0, -5.0, 0.0], [-5.0, 5.
↪0, 0.0], [-5.0, -5.0, 0.0]]
        cover cells ID [1669, 1186, 1148, 1397]
Progress: |///////////////////////////////////////////////////| 100.0%␣
↪Complete
```

`convert_to_xyz_array`(*node_df*)

Convert extracted node information into summation based on X, Y and Z

Parameters

node_df (*pandas.DataFrame*) – Extracted node information

Returns

A DataFrame with summations along X, Y, Z axis. Column names are [“sum_X”, “sum_Y”, “sum_Z”]

Return type
pandas.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_3D_UCS")
>>> # # Extract all cells that meet the criteria and split to␣
↪nodewise data for each time step.
>>> # In this case "BOUNDARY CONDITION" is set to "1" for the␣
↪threshold with the "FORCE" being extracted at each node.
>>> df = data.extract_threshold_info(thres_id=1, thres_array='boundary
↪', arrays_needed=['platen_force'])
>>> # Sum the X,Y,Z of all nodes for each time step.
>>> df_sum = data.convert_to_xyz_array(df)
>>> print(df_sum)
              sum_X          sum_Y          sum_Z
    0   0.000000e+00  0.000000e+00  0.000000e+00
    1  -1.224291e+05 -2.348118e+09  4.645789e+04
    2  -8.768720e+04 -4.663436e+09  7.953211e+03
    3  -5.580583e+04 -6.948494e+09 -1.039933e+04
    4  -1.602602e+05 -9.240063e+09  1.065935e+04
    5  -1.588623e+05 -1.152608e+10  4.616695e+04
    ...
```

crack_failure_mode(*remove_boundary=True*, *progress_bar=True*)

Get all failure modes in every timestep. Boundaries Optional. This will create a dataframe that has the failure mode for every crack. The time the crack first appears would be the time it inititated.

Parameters

- **remove_boundary** (*bool*) – Optional. Keep or remove boundaries in DataFrame
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns
A DataFrame containing the failure mode for each crack at every time step.

Return type
pd.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> df_cracks = data.crack_failure_mode()
```

crack_failure_mode_clustering(*crack_LUT=None*, *crack_LUT_name=None*, *remove_boundary=True*, *progress_bar=True*)

Cluster the crack modes based on their failure moed values. By default, it uses the Irazu convention which is 1=pure tensile; 1-1.5= tensile dominant; 1.5-2= shear dominant, 2= pure shear; 3= mixed mode. The crack LUT can also be user defined to get a specific range within the dataset.

Parameters

- **crack_LUT** (*list[float]*) – LUT range for the crack failure (float)

- **crack_LUT_name** (*list[str]*) – LUT range for the crack failure (name)
- **remove_boundary** (*bool*) – Optional. Keep or remove boundaries in DataFrame
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns
A DataFrame containing the total number of cracks in every time step.

Return type
pd.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> df_crack_default_clustering = data.crack_failure_mode_clustering()
>>> df_crack_userdefined_clustering = data.crack_failure_mode_clustering(crack_
↪LUT=[1,2], crack_LUT_name=['tensile_and_shear'])
```

crack_number(*progress_bar=True*)

Get the total number of cracks at every timestep. Excluding boundaries.

Parameters
progress_bar (*bool*) – Show/Hide progress bar

Returns
A DataFrame containing the total number of cracks at every time step.

Return type
pd.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> crack_number_total = data.crack_number()
>>> max(crack_number_total['crack number'])
222.0
>>> crack_number_total
            crack number
0             0.0
1             0.0
2             0.0
3             0.0
4             0.0
5             0.0
6             0.0
7             0.0
8             0.0
9           117.0
10          212.0
11          219.0
12          221.0
13          221.0
14          221.0
15          221.0
16          221.0
```

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```
17          221.0
18          222.0
19          222.0
20          222.0
21          222.0
22          222.0
23          222.0
24          222.0
25          222.0
26          222.0
27          222.0
28          222.0
29          222.0
30          222.0
```

direct_shear_calculation(*platen_id*, *array*, *progress_bar=True*)

Analyse direcr shear simulation built with a rigid platen on the outside.

Parameters

- **platen_id** (*int*) – Material id of the platen
- **array** (*str*) – the name of the array to be extracted
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns

DataFrame containing the absolute value of the array for each identified corner. Absolute sum of the extracted array split in Top/Bottom ane Left/Rigth sub-set into Top/Bottom.

Return type

pandas.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("/external/2D_shear_4mm_profile_normal_load_test")
>>> df = data.direct_shear_calculation(platen_id=1, array='platen_force',␣
↪progress_bar=True)
User Defined Platen ID
    Platen Material ID found as 1
No. of points
    Left        158
    Left_Top    78
    Left_Bottom 80
    Right       158
    Right_Top   76
    Right_Bottom        82
    Top 35
    Bottom      38
>>> import matplotlib.pyplot as plt
>>> plt.plot(df['Left_Top'], label='Left Top')
[<matplotlib.lines.Line2D object at 0x7fe71f187320>]
>>> plt.plot(df['Left_Bottom'], label='Left Bottom')
[<matplotlib.lines.Line2D object at 0x7f65cf8975f8>]
```

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```
>>> plt.plot(df['Left'], label='Left')
[<matplotlib.lines.Line2D object at 0x7fe71f187390>]
>>> plt.legend()
<matplotlib.legend.Legend object at 0x7fe71f187668>
>>> plt.show()
```

draw_rose_diagram(*t_step*, *rose_data=None*, *thres_id=None*, *thres_array='mineral_type'*, *rose_range='Length'*)

Draw a wind rose diagram based on the information passed.

Parameters

- **t_step** (*int*) – Time step in model. Default 0
- **rose_data** (*DataFrame*) – User can bypass requirement and pass a DataFrame with the data. Should be 2 columns with the Angle being the 2nd. Default None
- **thres_id** (*int*) – ID of item to threshold. Default None.
- **thres_array** (*str*) – Array name of item to threshold. Default "mineral_type".
- **rose_range** (*str*) – Range to calculate the windrose bins. Default "length"

Returns
windrose figure

Return type
matplotlib.pyplot

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> data.draw_rose_diagram(t_step=0)
<module 'matplotlib.pyplot' from '/usr/local/lib/python3.8/dist-packages/
↪matplotlib/pyplot.py'>
>>> data.draw_rose_diagram(t_step=0, rose_range='Length', thres_id=0, thres_
↪array='boundary')
<module 'matplotlib.pyplot' from '/usr/local/lib/python3.8/dist-packages/
↪matplotlib/pyplot.py'>
>>> # If you want to save the figure to a pyplot format.
>>> figure_name = data.draw_rose_diagram(t_step=0, rose_range='Length', thres_
↪id=0, thres_array='boundary')
```

extract_based_coord(*thres_model*, *coord_xyz*, *location*, *include_cells=False*, *adjacent_cells=False*)

Extract the vtkdata set based on the defined coord location in the x=0 y=1 z=2 location.

Parameters

- **thres_model** (*pyvista.core.pointset.UnstructuredGrid*) – threshold dataset of the material id of the rock
- **coord_xyz** (*int*) – x=0 y=1 z=2
- **location** (*float*) – Xmin/Xmax/Ymin/Ymax/Zmin/Zmax
- **include_cells** (*bool*) – If True, extract the cells that contain at least one of the extracted points. If False, extract the cells that contain exclusively points from the extracted points list.

- **adjacent_cells** (*bool*) – Specifies if the cells shall be returned or not

Returns
Pointset of the data being filtered

Return type
pyvista.core.pointset.UnstructuredGrid

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("/external/2D_shear_4mm_profile_normal_load_test
↪")
>>> data.rock_sample_dimensions()
Script Identifying Platen
    Platen Material ID found as [1]
(31.713071, 30.111493, 0.0, [-0.2, 31.513071, -14.92642, 15.185073, 0.
↪0, 0.0])
>>> extracted_left = data.extract_based_coord(data.rock_model, 0,␣
↪data.rock_model.bounds[0])
```

extract_cell_info(*cell_id*, *arrays_needed*, *progress_bar=True*)

Returns the information of the cell based on the array requested. If the array is a point data, the array is suffixed with _Nx where x is the node on that cell. Also shows a quick example on how to plot the information extracted.

Parameters

- **cell_id** (*int*) – Cell ID to extract
- **arrays_needed** (*list[str]*) – list of array names to extract
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns
unpacked DataFrame

Return type
pandas.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> import matplotlib.pyplot as plt
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> # Extract data platen_force', 'mineral_type' from Cell ID 1683
>>> extraction_of_cellinfo = data.extract_cell_info(1683, ['platen_
↪force', 'mineral_type'])
Columns:
    Name: platen_force_N1, dtype=object, nullable: False
    Name: platen_force_N2, dtype=object, nullable: False
    Name: platen_force_N3, dtype=object, nullable: False
    Name: mineral_type, dtype=object, nullable: False
>>> # For noded information => PLOTTING METHOD ONE
>>> x, y = [], []
>>> for i, row in extraction_of_cellinfo.iterrows():
>>>     x.append(i)
>>>     y.append(row['platen_force_N2'][0])
```

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```
>>> plt.plot(x, y, c='red', label='platen_force_N2_x')
[<matplotlib.lines.Line2D object at 0x7f08fe98a310>]
>>> plt.legend()
 <matplotlib.legend.Legend object at 0x7f08fe9854c0>
>>> plt.show()
# For noded information => PLOTTING METHOD TWO
>>> lx = extraction_of_cellinfo['platen_force_N2'].to_list()
>>> lx1 = list(zip(*lx))
>>> plt.plot(lx1[0], label='platen_force_N2_x')
[<matplotlib.lines.Line2D object at 0x7f08fe859b20>]
>>> plt.plot(lx1[1], label='platen_force_N2_y')
[<matplotlib.lines.Line2D object at 0x7f08fe859e50>]
>>> plt.plot(lx1[2], label='platen_force_N2_z')
[<matplotlib.lines.Line2D object at 0x7f08fe86a160>]
>>> plt.legend()
<matplotlib.legend.Legend object at 0x7f08fe86a340>
>>> plt.show()
# For non-nonded information
>>> plt.plot(lx1[0], label='mineral_type')
[<matplotlib.lines.Line2D object at 0x7f08fe7e39a0>]
>>> plt.legend()
<matplotlib.legend.Legend object at 0x7f08fe7e39d0>
>>> plt.show()
```

extract_crack_info(*arrays_needed*, *progress_bar=True*)

Returns the information based on the array requested.

Parameters

- **arrays_needed** (*list[str]*) – list of array names to extract
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns

unpacked DataFrame

Return type

pandas.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> extraction_of_cracks = data.extract_crack_info(arrays_needed=[
↪'area', 'length'])
Progress: |//////////////////////////////////////////////////| 100.0%␣
↪Complete
```

extract_threshold_info(*thres_id*, *thres_array*, *arrays_needed*, *dataset_to_load='basic'*, *progress_bar=True*)

Returns the information of the cell based on the array requested. If the array is a point data, the array is suffixed with _Nx where x is cell ID. Also shows a quick example on how to plot the information extracted.

Parameters

- **thres_id** (*int*) – Threshold ID to extract

- **thres_array** (*str*) – Array name of item to threshold.
- **arrays_needed** (*list[str]*) – list of array names to extract
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns
A DataFrame or a series of DataFrames nested in a dictionary with the key being the name of the array needed

Return type
pandas.DataFrame or dict[pandas.DataFrame]

Example

```
>>> import pyfdempp as fdem
>>> import matplotlib.pyplot as plt
>>> data = fdem.Model("../example_outputs/Irazu_3D_UCS")
>>> # Extract all cells that meet the criteria and split to nodewise␣
↪data for each time step.
>>> # In this case "BOUNDARY CONDITION" is set to "1" for the␣
↪threshold with the "FORCE" being extracted at each node.
>>> df = data.extract_threshold_info(thres_id=1, thres_array='boundary
↪', arrays_needed=['platen_force'])
Progress: |//////////////////////////////////////////////////| 100.0%␣
↪Complete
54.74 seconds.
>>> # Sum the X,Y,Z of all nodes for each time step.
>>> df_sum = data.convert_to_xyz_array(df)
```

find_cell(*model_point*)

Identify the containing cell in the model to the defined point. Will return an error if the point is not within a cell.

Parameters
model_point (*list[float, float, float]*) – x,y,z of a point in the model which

Returns
The cell that contains the point.

Return type
int

Raises
IndexError – Point outside model domain.

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> data.find_cell([0, 0, 0])
2167
>>> data.find_cell([2000, 2000, 0])
IndexError: Point outside model domain.
X=56.0, Y=116.0, Z=0.0
```

mesh_geometry(*vertices*)

Returns a unique set of vertices and calculates their length and orientation.

Parameters
: **vertices** (*list[tuples]*) – list of vertices in the model at a given time step

Returns
: DataFrame of the vertices length and orientation

Return type
: pandas.DataFrame

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> vert = data.model_vertices(t_step=0, thres_id=1, thres_array='mineral_type')
>>> data.mesh_geometry(vert)
       Length       Angle
0    2.236068   63.434949
1    2.000000    0.000000
2    2.363608   59.436301
3    2.000000    0.000000
4    2.244731  117.123188
..        ...         ...
409  2.116948    0.287685
410  2.000000    0.000000
411  2.000000    0.000000
412  1.802781   45.829911
413  2.227619  116.002627

[414 rows x 2 columns]
```

model_dimensions(*mat_id=None*)

Function to get the "INITIAL" model bounds and returns the width, height, thickness

Parameters
: **mat_id** (*int*) – Optional, if a threshold is specific to a material type

Returns
: model width, model height, model thickness

Type
: tuple[float, float, float]

Example

```
>>> import pyfdempp as fdem
>>> model = fdem.Model("../example_outputs/Irazu_UCS")
>>> # Returns the overall model dimensions
>>> model.model_dimensions()
(56.0, 116.0, 0.0)
>>> # Returns the model dimensions based on material id 1
>>> model.model_dimensions(1)
(56.0, 116.0, 0.0)
>>> # Error when material is not found
>>> model.model_dimensions(3)
IndexError: Material ID for platen out of range.
Material Range 0-1
```

model_domain()

Identifies the model domain by confirming the simulation cell vertex.
2D (3 Points - Triangle) 3D (4 Points - Tetrahedral)

Returns
number of nodes to skip in analysis

Return type
int

Raises
Warning – Simulation partially supported.

Example

```
>>> import pyfdempp as fdem
>>> model = fdem.Model("../example_outputs/Irazu_UCS")
>>> model.model_domain()
2D Simulation
4
```

model_vertices(*t_step=0*, *thres_id=None*, *thres_array='mineral_type'*)

Returns a list of the vertices in the form of Point1, Point 2

Parameters

- **t_step** (*int*) – Time step in model. Default 0
- **thres_id** (*int*) – ID of item to threshold. Default None.
- **thres_array** (*str*) – Array name of item to threshold. Default "mineral_type".

Returns
list of the verticies in the model and/or the threshold of it.

Return type
list[tuples]

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> len(data.model_vertices(t_step=0, thres_id=0, thres_array='mineral_type'))
11196
>>> len(data.model_vertices(t_step=0, thres_id=1, thres_array='boundary'))
354
```

openfdem_att_check(*att*, *dict_to_check=None*)

Checks that the attribute is a valid choice.

Param
Attribute

Type
str

Returns
Attribute

Return type
str

Raises
KeyError – Attribute does not exist.

Example

```
>>> import pyfdempp as fdem
>>> model = fdem.Model("../example_outputs/Irazu_UCS")
>>> model.openfdem_att_check('mineral_type')
'mineral_type'
>>> model.openfdem_att_check('material_property')
KeyError: Attribute does not exist.
Available options are mineral_type, boundary, platen_force, platen_
↪displacement, gauge_displacement'
```

platen_info(*pv_cells*, *platen_boundary_id*, *var_property*)

This function thresholds cells based on boundary condition and sums them based on the defined parameter var_property

Parameters

- **pv_cells** (*pyvista.core.pointset.UnstructuredGrid or DataSet*) –
- **platen_boundary_id** (*float*) – boundary id that the threshold should be based on
- **var_property** (*str*) – name of the property (array to b returned)

Returns
array of the property based on the threshold

Return type
ndarray

plot_stress_strain(*strain*, *stress*, *ax=None*, ***plt_kwargs*)

Simple plot of the stress-strain curve of a given dataframe

Parameters

- **strain** (*pandas.DataFrame*) – X-axis data [Strain]
- **stress** (*pandas.DataFrame*) – Y-axis data [Stress]
- **ax** (*matplotlib*) – Matplotlib Axis
- **plt_kwargs** – *~matplotlib.Modules* submodules

Returns
Matplotlib AxesSubplots

Return type
Matplotlib Axis

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
# Minimal Arguments
>>> df_wo_SG = data.complete_UCS_stress_strain()
Columns:
    Name: Platen Stress, dtype=float64, nullable: False
```

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```
    Name: Platen Strain, dtype=float64, nullable: False.
    Script Identifying Platen
Platen Material ID found as [1]
    UCS Simulation
        Predefined loading Axis [1] is Y-direction
    Values used in calculations are
        Area        52.00
        Length      108.00
Progress: |//////////////////////////////////////////////////| 100.0%␣
↪Complete
>>> data.plot_stress_strain(df_wo_SG['Platen Strain'], df_wo_SG[
↪'Platen Stress'], label='stress-strain', color='green')
<AxesSubplot:xlabel='Strain (-)', ylabel='Axial Stress (MPa)'>
```

rock_sample_dimensions(*platen_id=None*)

Lookup cell element ID on the top center and then trace points Using this information, we obtain the platen prop ID. Alternatively the user can define the ID of thresholding

Parameters

platen_id (*None or int*) – Manual override of Platen ID

Returns

sample width, sample height, sample thickness

Return type

tuple[float, float, float]

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> # Let the script try to identify the platen material ID
>>> data.rock_sample_dimensions()
Script Identifying Platen
    Platen Material ID found as [1]
(52.0, 108.0, 0.0, [-26.0, 26.0, -54.0, 54.0, 0.0, 0.0])
>>> # Explicitly defined the platen material ID
>>> data.rock_sample_dimensions(0)
User Defined Platen ID
    Platen Material ID found as 0
(56.0, 116.0, 0.0, [-28.0, 28.0, -58.0, 58.0, 0.0, 0.0])
>>> # Explicitly defined the platen material ID is out of range
>>> data.rock_sample_dimensions(3)
IndexError: Threshold ID out of range.
boundary Range -1-1
```

simulation_type()

Identifies the type of simulation running. BD or UCS. Checks the top left corner of the model. If it contains material it is assumed as a rectangle.

Returns

Type of simulation. BD/UCS

Return type

str

Example

```
>>> import pyfdempp as fdem
>>> data = fdem.Model("../example_outputs/Irazu_UCS")
>>> data.rock_sample_dimensions()
Script Identifying Platen
    Platen Material ID found as [1]
(52.0, 108.0, 0.0, [-26.0, 26.0, -54.0, 54.0, 0.0, 0.0])
>>> data.simulation_type()
'UCS Simulation'
>>> data_bd = fdem.Model("../example_outputs/openfdem_BD", runfile='.y
↪')
>>> data_bd.rock_sample_dimensions()
Script Identifying Platen
    Platen Material ID found as [1]
(100.0, 99.94999694824219, 0.0, [-50.0, 50.0, -49.974998474121094, 49.
↪974998474121094, 0.0, 0.0])
>>> data_bd.simulation_type()
'BD Simulation'
```

threshold_bound_check(*thres_id*, *thres_array='boundary'*)

Checks the material ID is a valid choice.

Parameters

- **thres_id** (*int*) – ID of the item ot be threshold
- **thres_array** (*str*) – Array name of the item ot be threshold

Returns
ID of the material

Return type
int

Raises
IndexError – ID out of range.

Example

```
>>> import pyfdempp as fdem
>>> model = fdem.Model("../example_outputs/Irazu_UCS")
>>> model.threshold_bound_check(0)
0
>>> model.threshold_bound_check(5)
IndexError: Material ID for platen out of range.
Material Range 0-1
```

unpack_DataFrame(*packed_cell_info*)

Unpacking of the original array produced by pyvista If the array is a point data, the array is suffixed with _Nx where x is the node on that cell.

Parameters
packed_cell_info (*pandas.DataFrame*) –

Returns
Unpacked DataFrame

Return type
pandas.DataFrame

class `pyfdempp.pyfdempp.`**`Timestep`**(*file*, *runfile=None*)

Bases: `object`

A class handling the data of each timestep.

Each data array returns for only the timestep handles spatial manipulations

2.1.2 Supporting Modules

pyfdempp.aggregate_storage module

class `pyfdempp.aggregate_storage.`**`aggregate_storage`**(*file_directory*, *h5filename=None*, *overwrite=False*, *compression=None*, *verbose=True*)

Bases: `object`

Aggregator class to store VTK files in a single h5 file for faster access to data.

`file_group_key`(*vtkfilename*)

Produces a standard group/key based on VTK file name

Parameters
vtkfilename (*`str path`*) – VTK file name to be stored/read

Returns
Key described using timestep and filename

Return type
str

`read_file`(*filename*, *verbose=False*)

Extract VTK file from HDF5 file given original filename

The VTK file is reconstructed from the data arrays stored in the HDF5 file. It will be similar but different from the original.

Parameters

- **filename** (*`str path`*) – File name to be extracted (unaltered since HDF5 file creation)
- **verbose** (*`bool, optional`*) – Print progress statements, defaults to False

Returns
VTK Unstructured Grid as if read from a *.vtp or *.vtu file

Return type
VTK Unstructured Grid

`store_file`(*vtkfilename*)

Stores VTK file into HDF5 file

Parameters
vtkfilename (*`str path`*) – VTK file name

pyfdempp.complete_BD_thread_pool_generators module

`pyfdempp.complete_BD_thread_pool_generators.`**`history_strain_func`**`(`*f_name*, *model*, *cv*, *ch*`)`

Calculate the axial stress from platens, axial strain from platens and SG as well as lateral strain from SG

Parameters

- **`f_name`** (*`str`*) – name of vtu file being processed
- **`model`** (*`openfdem.pyfdempp.Model`*) – FDEM Model Class
- **`cv`** (*`list`*) – list of cells at the corner of the vertical strain gauge
- **`ch`** (*`list`*) – list of cells at the corner of the horizontal strain gauge

Returns

Stress, Platen Strain, SG Strain, SG Lateral Strain

Return type

Generator[Tuple[list, list, list, list], Any, None]

`pyfdempp.complete_BD_thread_pool_generators.`**`main`**`(`*model*, *st_status*, *gauge_width*, *gauge_length*, *c_center*, *progress_bar=False*`)`

Main concurrent Thread Pool to calculate the full stress-strain

Parameters

- **`model`** (*`openfdem.pyfdempp.Model`*) – FDEM Model Class
- **`st_status`** (*`bool`*) – Enable/Disable SG Calculations
- **`gauge_width`** (*`float`*) – SG width
- **`gauge_length`** (*`float`*) – SG length
- **`c_center`** (*`None or list[float, float, float]`*) – User-defined center of the SG
- **`progress_bar`** (*`bool`*) – Show/Hide progress bar

Returns

full stress-strain information

Return type

pd.DataFrame

`pyfdempp.complete_BD_thread_pool_generators.`**`set_strain_gauge`**`(`*model*, *gauge_length=None*, *gauge_width=None*, *c_center=None*`)`

Calculate local strain based on the dimensions of a virtual strain gauge placed at the center of teh model with x/y dimensions. By default set to 0.25 of the length/width.

Parameters

- **`model`** (*`openfdem.pyfdempp.Model`*) – FDEM Model Class
- **`gauge_length`** (*`float`*) – length of the virtual strain gauge
- **`gauge_width`** (*`float`*) – width of the virtual strain gauge
- **`c_center`** (*`None or list[float, float, float]`*) – User-defined center of the SG

Returns

Cells that cover the horizontal and vertical gauges as well as the gauge width and length

Return type

[list, list, float, float]

pyfdempp.complete_UCS_thread_pool_generators module

pyfdempp.complete_UCS_thread_pool_generators.**check_loading_direction**(*model*, *f1*, *f2*)

pyfdempp.complete_UCS_thread_pool_generators.**history_strain_func**(*f_name*, *model*, *cv*, *ch*, *axis*)

Calculate the axial stress from platens, axial strain from platens and SG as well as lateral strain from SG

Parameters

- **f_name** (*str*) – name of vtu file being processed
- **model** (*openfdem.pyfdempp.Model*) – FDEM Model Class
- **cv** (*list[int]*) – list of cells at the corner of the vertical strain gauge
- **ch** (*list[int]*) – list of cells at the corner of the horizontal strain gauge

Returns

Stress, Platen Strain, SG Strain, SG Lateral Strain

Return type

Generator[Tuple[list, list, list, list], Any, None]

pyfdempp.complete_UCS_thread_pool_generators.**main**(*model*, *platen_id*, *st_status*, *axis_of_loading*, *gauge_width*, *gauge_length*, *c_center*, *user_samp_A=None*, *user_samp_L=None*, *progress_bar=False*)

Main concurrent Thread Pool to calculate the full stress-strain

Parameters

- **model** (*openfdem.pyfdempp.Model*) – FDEM Model Class
- **platen_id** (*None or int*) – Manual override of Platen ID
- **st_status** (*bool*) – Enable/Disable SG Calculations
- **axis_of_loading** (*None or int*) – Enable/Disable SG
- **gauge_width** (*float*) – SG width
- **gauge_length** (*float*) – SG length
- **c_center** (*None or list[float, float, float]*) – User-defined center of the SG
- **user_samp_A** (*None or float*) – Sample Area
- **user_samp_L** (*None or float*) – Sample Length
- **progress_bar** (*bool*) – Show/Hide progress bar

Returns

full stress-strain information

Return type

pd.DataFrame

pyfdempp.complete_UCS_thread_pool_generators.**set_strain_gauge**(*model*, *gauge_length=None*, *gauge_width=None*, *c_center=None*)

Calculate local strain based on the dimensions of a virtual strain gauge placed at the center of teh model with x/y dimensions. By default, set to 0.25 of the length/width.

Parameters

- **model** (*openfdem.pyfdempp.Model*) – FDEM Model Class
- **gauge_length** (*float*) – length of the virtual strain gauge
- **gauge_width** (*float*) – width of the virtual strain gauge
- **c_center** (*None or list[float, float, float]*) – User-defined center of the SG

Returns
Cells that cover the horizontal and vertical gauges as well as the gauge width and length

Return type
[list, list, float, float]

pyfdempp.extract_cell_thread_pool_generators module

pyfdempp.extract_cell_thread_pool_generators.**history_cellinfo_func**(*f_name*, *model*, *cell_id*, *array_needed*, *thres_array=None*)

Generate a dictionary of the various array being interrogated for the said cell ID

Parameters

- **f_name** (*str*) – name of vtu file being processed
- **model** (*openfdem.pyfdempp.Model*) – FDEM Model Class
- **cell_id** (*int*) – ID of the cell from which the data needs to be extracted
- **array_needed** (*list[str]*) – Name of the property to extract

Returns
The value of the property from the cell being extracted

Return type
Generator[Tuple()]

pyfdempp.extract_cell_thread_pool_generators.**main**(*model*, *cellid*, *arrayname*, *progress_bar=False*)

Main concurrent Thread Pool to get value of the property from the cell being extracted

Parameters

- **model** (*openfdem.pyfdempp.Model*) – FDEM Model Class
- **cellid** (*int*) – ID of the cell from which the data needs to be extracted
- **arrayname** (*list[str]*) – Name of the property to extract
- **progress_bar** – Show/Hide progress bar

Returns
DataFrame of the values of the property from the cell being extracted

Return type
pandas.DataFrame

pyfdempp.formatting_codes module

`pyfdempp.formatting_codes.`**`bold_text`**`(`*val*`)`

Returns text as bold

Parameters
`val` (*`str`*) – Text

Returns
Text as bold

Return type
str

`pyfdempp.formatting_codes.`**`calc_timer_values`**`(`*end_time*`)`

Function to calculate the time

Parameters
`end_time` (*`float`*) – Time (Difference in time in seconds)

Returns
Time in minutes and seconds

Return type
float

`pyfdempp.formatting_codes.`**`docstring_creator`**`(`*df*`)`

Write the example output for a docstring DataFrame

Parameters
`df` (*`pandas.DataFrame`*) – DataFrame to be read

Returns
prints the docstring and type for each element in the DataFrame

Return type
str

`pyfdempp.formatting_codes.`**`green_text`**`(`*val*`)`

Returns text as bold in green font color

Parameters
`val` (*`str`*) – Text

Returns
Text as bold in green font color

Return type
str

`pyfdempp.formatting_codes.`**`print_progress`**`(`*iteration*, *total*, *prefix=''*, *suffix=''*, *decimals=1*, *bar_length=50*`)`

Call in a loop to create terminal progress bar Adjusted bar length to 50, to display on small screen

Parameters

- **`iteration`** (*`int`*) – current iteration
- **`total`** (*`int`*) – total iteration
- **`prefix`** (*`str`*) – prefix string
- **`suffix`** (*`str`*) – suffix string

- **decimals** (*int*) – positive number of decimals in percent complete
- **bar_length** (*int*) – character length of bar

Returns
system output showing progress

Return type

pyfdempp.formatting_codes.**red_text**(*val*)

Returns text as bold in red font color

Parameters
val (*str*) – Text

Returns
Text as bold in red font color

Return type
str

pyfdempp.model_reader module

pyfdempp.model_reader.**mp_read**(**args*, ***kwargs*)

pyfdempp.model_reader.**multiprocess_async**(**args*, ***kwargs*)

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pyfdempp.model_reader.**normal_read**(**args*, ***kwargs*)

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