pyCFS

A COMPANION LIBRARY FOR openCFS

PART 2: DATA MANIPULATION

FOCUS

- Test case generation
  - Create `.cfs` files from scratch
- Pre-Processing
  - Mesh preparation
  - Data processing
- Post-Processing
  - Compare to analytic computations
  - Plot time series (faster than ParaView)
- Small to medium size problems!
  - Many parts are parallelized
  - Some Python operations are still slow for large problems

GETTING STARTED

INSTALLATION

- Install in `pip` environment

```
pip install pyCFS
```

INSTALLATION

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```
pip install pyCFS
```

Update from current main branch ```pip pip install git+https://gitlab.com/openCFS/pycfs@main --upgrade --force-reinstall ```

ADDITIONAL DEPENDENCIES

- Large dependencies excluded from standard install
- Install dependencies for all functionality

```
pip install pyCFS[data]
```

DOCUMENTATION

- Documentation page
  - Installation Guide
  - Basic usage Guide
    - Contains only some features
  - API-Documenation

FUNCTIONALITY

OVERVIEW

Structured into submodules

```python
from pyCFS.data import io, operators, util, extras
```

- `io`
  - I/O operations for CFS type HDF5 format
- `operators`
  - Basic mesh/data operations
- `util`
  - Various useful functions when working with *pyCFS*
- `extras`
  - I/O compatibilty methods to other file formats
  - Additional functionality not directly related to *openCFS*

I/O (`CFSReader`)

```python
from pyCFS.data.io import CFSReader
```

- Reading CFS-type HDF5 files
  - Mesh
  - Data (on Nodes/Elements, History data)

```xml
<surfRegionResult type="acouPower">
  <surfRegionList>
    <surfRegion name="S_body" outputIds="hdf5" writeAsHistResult="ye
  </surfRegionList>
</surfRegionResult>
```

I/O (CFSReader)

Usage

```
with CFSReader(filename="file.cfs") as reader:
    # Print file information
    print(reader)

    # Read the whole mesh
    mesh = reader.MeshData

    # Read coordinates, connectivity
    coordinates = reader.Coordinates
    connectivity = reader.Connectivity

    # Read node coordinates of a specific region
    reg_1 = reader.get_mesh_region_coordinates(region="S_CAPACITOR")

    # Read all result data for sequence step 2
    reader.set_multi_step(multi_step_id=2)
    results_2 = reader.MultiStepData

    # Read data for a specific quantity and region
    result_1 = reader.get_multi_step_data(multi_step_id=1,
                                          quantities=["elecPotential
                                          regions=["S_CAPACITOR"])
```

I/O (CFSReader)

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    # Print file information
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    # Read the whole mesh
    mesh = reader.MeshData

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    # Read node coordinates of a specific region
    reg_1 = reader.get_mesh_region_coordinates(region="S_CAPACITOR")

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    results_2 = reader.MultiStepData

    # Read data for a specific quantity and region
    result_1 = reader.get_multi_step_data(multi_step_id=1,
                                          quantities=["elecPotential
                                          regions=["S_CAPACITOR"])
```

I/O (`CFSWriter`)

```
from pyCFS.data.io import CFSWriter
```

- Creating new CFS-type HDF5 files
- Writing to existing CFS-type HDF5 files

Usage

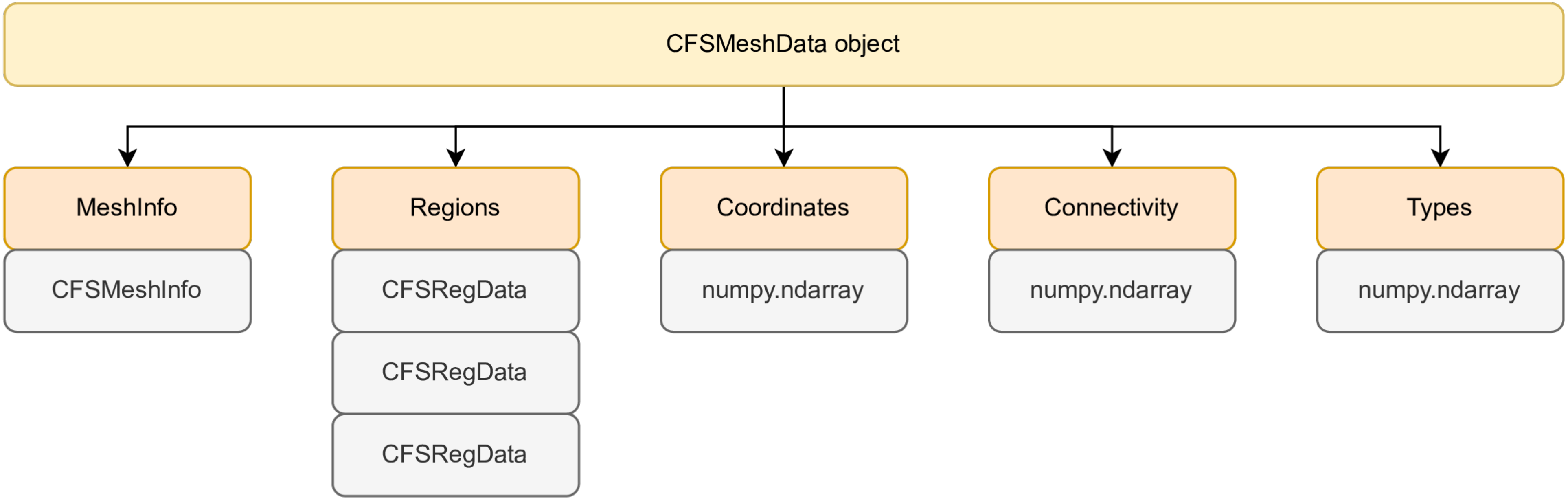
```
with CFSWriter(filename="file.cfs") as writer:
    # Create new file
    writer.create_file(mesh_data=mesh, result_data=result_1)

    # Write additional squence step
    writer.write_multistep(result_data=results_2, multi_step_id=2)
```

I/O (`CFSMeshData`)

```python
from pyCFS.data.io import CFSMeshData
```

- Container object for all mesh related data
- Various mesh operations



I/O (CFSMeshData)

Usage examples

```python
# Create mesh object of point cloud
mesh_points = CFSMeshData.from_coordinates_connectivity(
    coordinates=coordinates,
    region_name="P_measurement"
)

# Create mesh object from coordinates and connectivity
mesh = CFSMeshData.from_coordinates_connectivity(
    coordinates=coordinates,
    connectivity=connectivity,
    element_dimension=2,
    region_name="S_plate"
)

# Merge mesh objects
mesh = mesh + mesh_points

# Print information
print(mesh)

# Compute element normals for a region
mesh.get_region_centroids(region="S_plate")
```

I/O (`CFSMeshData`)

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mesh = mesh + mesh_points

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# Compute element normals for a region
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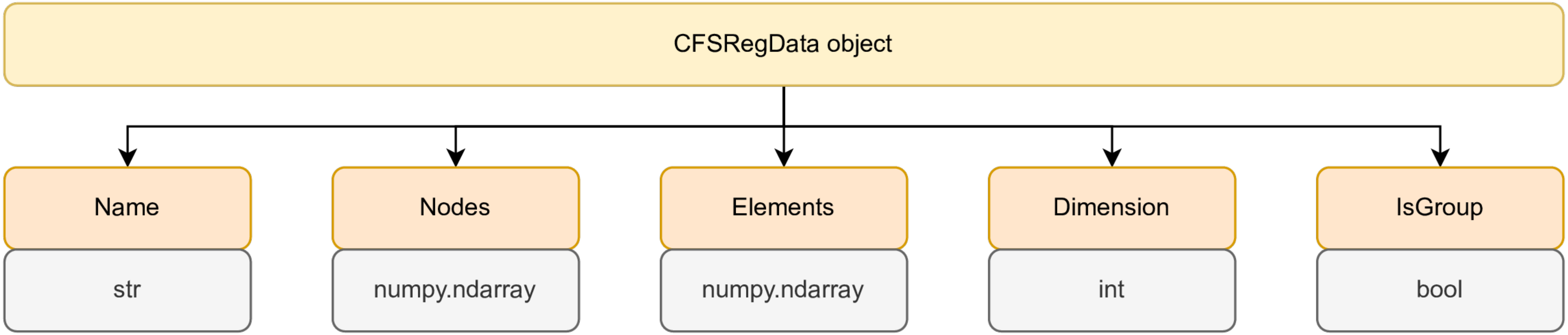
```

I/O (`CFSRegData`)

```
from pyCFS.data.io import CFSRegData
```

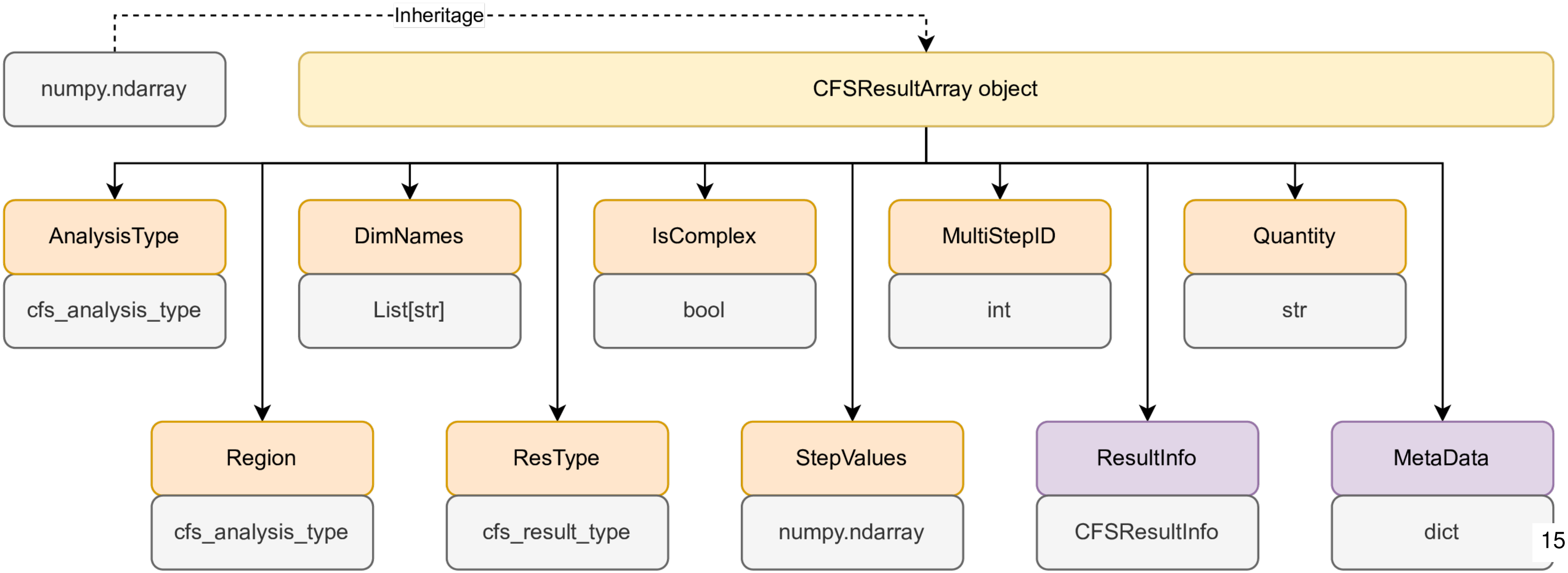
- Container object for all region related data



I/O (CFSResultArray)

```
from pyCFS.data.io import CFSResultArray
```

- Custom numpy array type (compatible with all operations numpy.ndarray is compatible!)
- Including all meta data for write operations



I/O (`CFSResultArray`)

Usage examples

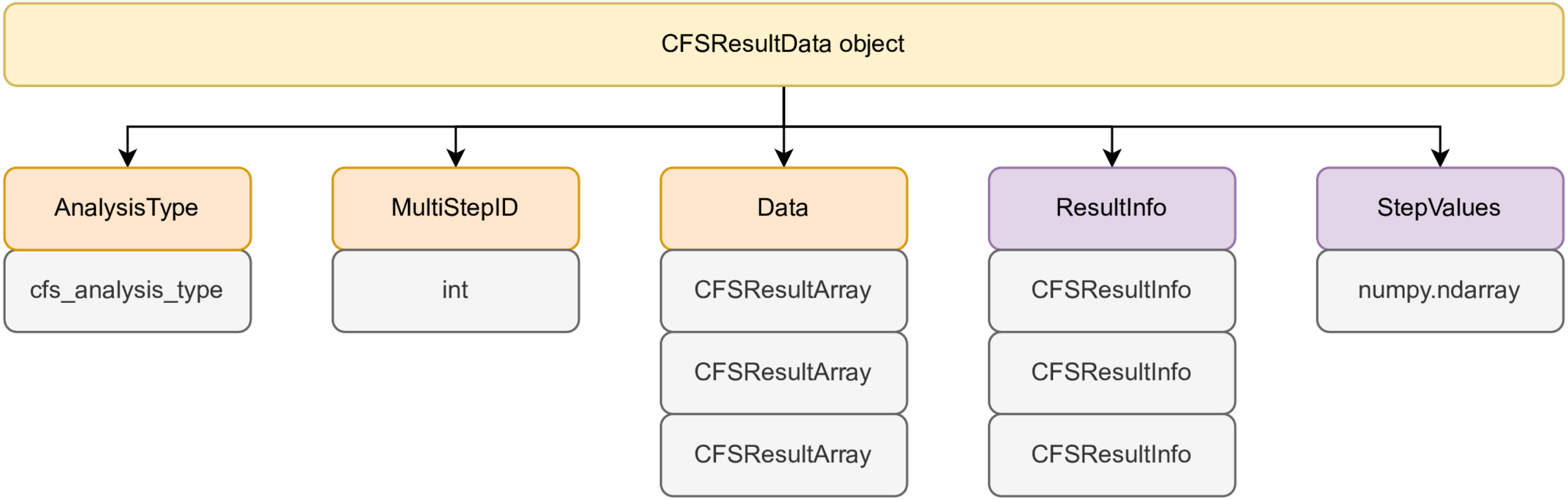
```
# Create a result array object
np_array = np.ones((5, 10, 3))
cfs_array = CFSResultArray(np_array)

# Set meta data for the result array
cfs_array.set_meta_data(
    quantity="elecPotential",
    region="S_CAPACITOR",
    step_values=np.array([0, 1, 2, 3]),
    # dim_names=["-"],
    res_type=cfs_result_type.NODE,
    # is_complex=False,
    # multi_step_id=1,
    analysis_type=cfs_analysis_type.TRANSIENT,
)
```

I/O (`CFSResultData`)

```
from pyCFS.data.io import CFSResultData
```

- Container object for data of a single multistep / sequence step



I/O (CFSResultData)

Usage examples

```
# Create a result container object
result = CFSResultData(analysis_type=cfs_analysis_type.TRANSIENT,
                       multi_step_id=2, data=[array_1, array_2])

# Print information
print(result)

# Extract certain time steps
result_1 = result[0:5]

# Extract certain region and quantity
result_2 = result.extract_quantity_region(quantity="elecPotential",

# Add data to result object (define different multi step ID)
result.add_data_array(data=cfs_array, multi_step_id=2)
```

I/O (CFSResultData)

Usage examples

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# Add data to result object (define different multi step ID)
result.add_data_array(data=cfs_array, multi_step_id=2)
```

I/O (OTHER)

```
from pyCFS.data.io import cfs_types, cfs_util
```

- `cfs_types`
  - Enum definitions based on *openCFS* source code
- `cfs_util`
  - Functions to check object validity

OPERATORS

```
from pyCFS.data.operators import (transformation, interpolators,
                                  projection_interpolation, sngr)
```

- `interpolators`
  - Basic interpolators
    - Node2Cell
    - Cell2Node
    - Nearest Neighbor (bidirectional)
- `projection_interpolation`
  - Projection-based interpolation

OPERATORS

```python
from pyCFS.data.operators import (transformation, interpolators,
                                  projection_interpolation, sngr)
```

- `transformation`
  - Translate / rotate / extrude / revolve mesh
  - Fit mesh onto target mesh
- `sngr`
  - Compute fluctuating flow field from stationary RANS solution

EXTRA FUNCTIONALITY

- Read mesh and data from various formats
  - `ansys_io` (Ansys Mechanical: `.rst`)
  - `ensight_io` (various CFD software: `.case`)
  - `psv_io` (Polytec PSV export: `.unv`)
  - `nihu_io` (NiHu simulation export: `.mat`)
  - *Planned:* `exodus_io` (Cubit mesh export)

EXAMPLE WORKFLOW

I/O

TASKS

1. Read mesh and result data
2. View connectivity array and node coordinates of a specific region
3. Multiply result with factor
4. Add result to existing file as a new sequence step (multi step)

CODE

```
# Import necessary modules
from pyCFS.data import io

# Read file
with io.CFSReader(filename="file.cfs") as f:
    # Read mesh data
    mesh = f.MeshData
    # Read results of sequence step 1
    results = f.get_multi_step_data(multi_step_id=1)

# View connectivity array, get coordinates of V_air
conn = print(mesh.Connectivity)
reg_coord = mesh.get_region_coordinates(region="V_air")

# Get data array of elecPotential in region V_air
elec_pot = results.get_data_array(quantity="elecPotential", region='

# Manipulate result
igte_factor = 1e0
elec_pot *= igte_factor

# Write "corrected" result to new sequence step
```

CODE

```
# Import necessary modules
from pyCFS.data import io

# Read file
with io.CFSReader(filename="file.cfs") as f:
    # Read mesh data
    mesh = f.MeshData
    # Read results of sequence step 1
    results = f.get_multi_step_data(multi_step_id=1)

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conn = print(mesh.Connectivity)
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# Write "corrected" result to new sequence step
```

CODE

```
# Import necessary modules
from pyCFS.data import io

# Read file
with io.CFSReader(filename="file.cfs") as f:
    # Read mesh data
    mesh = f.MeshData
    # Read results of sequence step 1
    results = f.get_multi_step_data(multi_step_id=1)

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# Write "corrected" result to new sequence step
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CODE

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elec_pot = results.get_data_array(quantity="elecPotential", region='

# Manipulate result
igte_factor = 1e0
elec_pot *= igte_factor

# Write "corrected" result to new sequence step
```
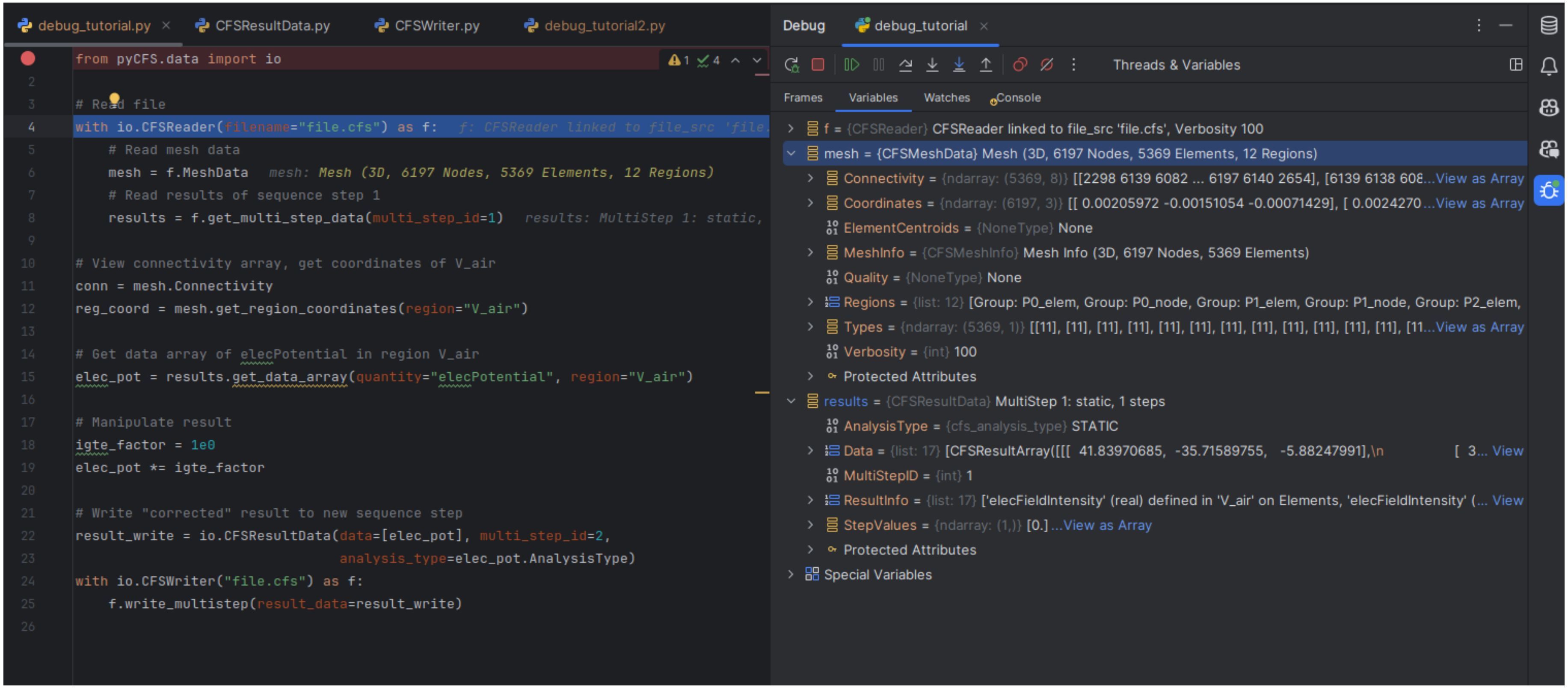
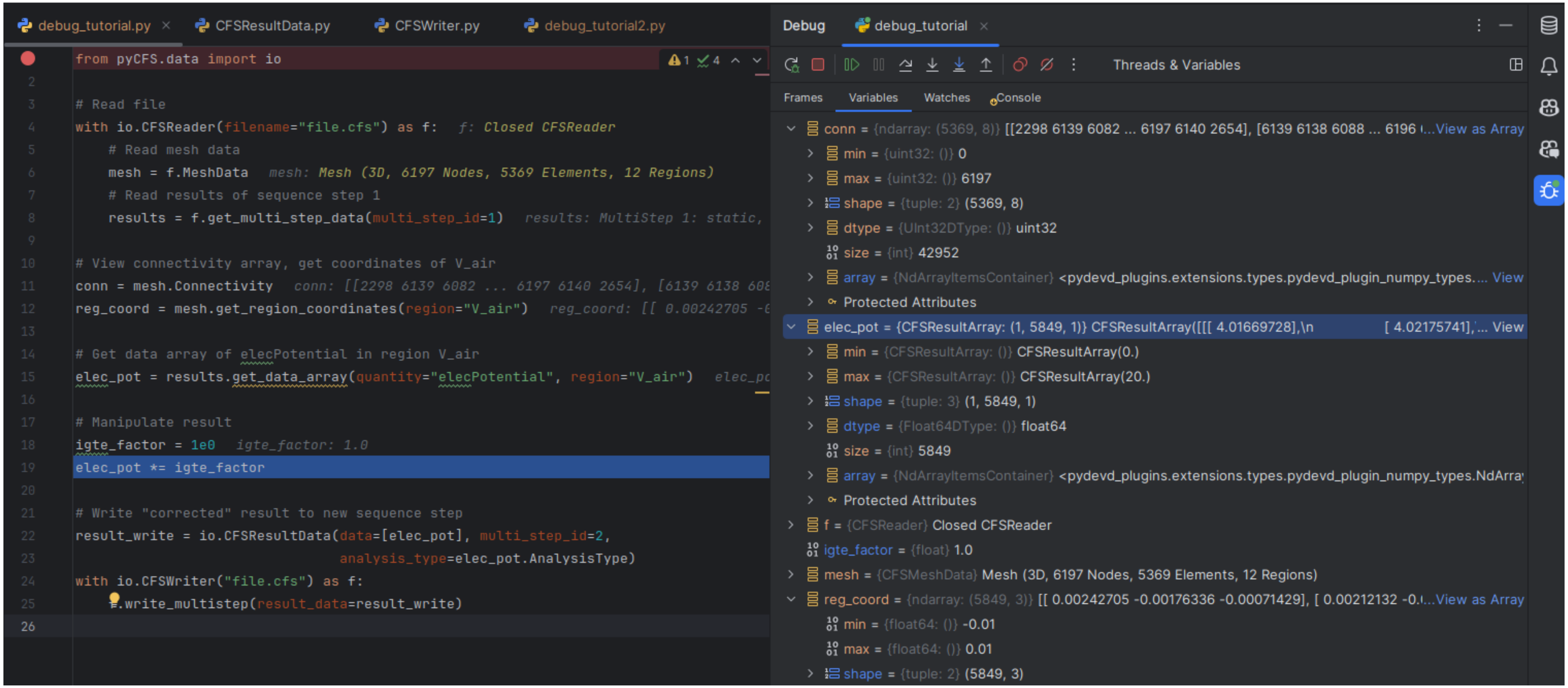

DEBUGGING IN PYCHARM (1)



DEBUGGING IN PYCHARM (2)



EXAMPLE WORKFLOW

`Operators`

TASKS

1. Read mesh and result data
2. Perform Node-to-Cell interpolation
3. Add interpolated data to existing results
4. Write mesh and results to a new file

CODE

```
# Import necessary modules
from pyCFS.data import io
from pyCFS.data.operators import interpolators

# Read source file
with io.CFSReader(filename="file.cfs") as h5r:
    print(h5r)
    mesh = h5r.MeshData
    results = h5r.MultiStepData

# Perform interpolation
results_interpolated = interpolators.interpolate_node_to_cell(
    mesh_data=mesh,
    result_data=results,
    regions=["V_air"],
    quantity_names={"elecPotential": "interpolated_elecPotential"},
)

# Add interpolated result to results container
results.combine_with(results_interpolated)

# Check results container
```

CODE

```python
# Import necessary modules
from pyCFS.data import io
from pyCFS.data.operators import interpolators

# Read source file
with io.CFSReader(filename="file.cfs") as h5r:
    print(h5r)
    mesh = h5r.MeshData
    results = h5r.MultiStepData

# Perform interpolation
results_interpolated = interpolators.interpolate_node_to_cell(
    mesh_data=mesh,
    result_data=results,
    regions=["V_air"],
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)

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    print(h5r)
    mesh = h5r.MeshData
    results = h5r.MultiStepData

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)

# Add interpolated result to results container
results.combine_with(results_interpolated)

# Check results container
```

INTERACTIVE MODE IN VS CODE (1)

debug_tutorial2.py

```python
#%%
# Import necessary modules
from pyCFS.data import io
from pyCFS.data.operators import interpolators

#%%
# Read source file
with io.CFSReader(filename="file.cfs") as h5r:
    print(h5r)
    mesh = h5r.MeshData
    results = h5r.MultiStepData

#%%
# Perform interpolation
results_interpolated = interpolators.interpolate_node_to_cell(
    mesh_data=mesh,
    result_data=results,
    regions=["V_air"],
    quantity_names={"elecPotential": "interpolated_elecPotential"},
)

#%%
# Add interpolated result to results container
results.combine_with(results_interpolated)

# Check results container
print(results)

#%%
# Write output file
with io.CFSWriter("file_out.cfs") as h5w:
    # Write mesh and results to new file
    h5w.create_file(mesh_data=mesh, result_data=results)
```

Interactive-1

Connected to pycfs (Python 3.10.12)

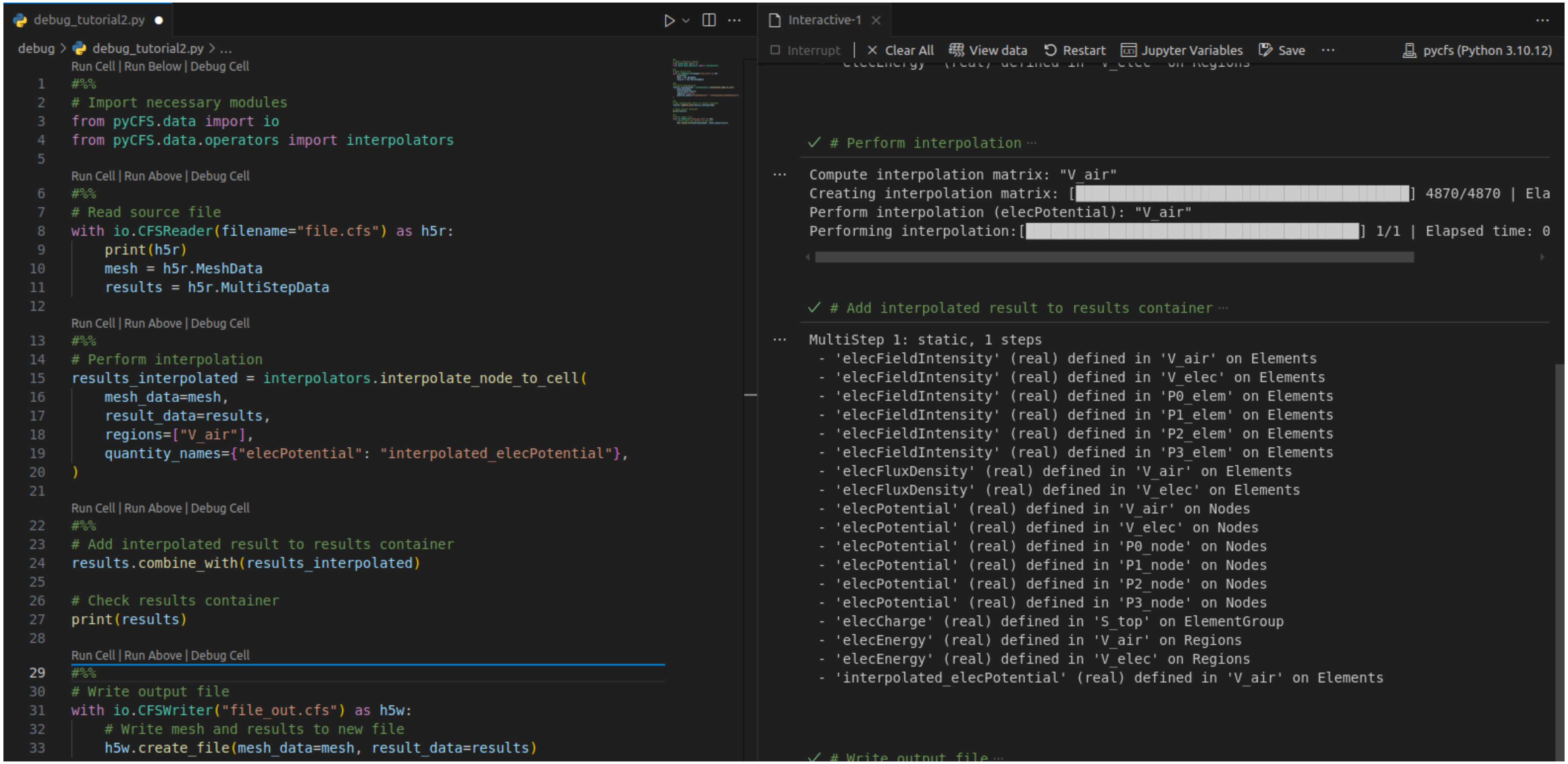
✓ # Import necessary modules

✓ # Read source file

```
File: file.cfs
Mesh
 - Dimension: 3
 - Nodes:     6197
 - Elements:  5369
MultiStep 1: static, 1 steps
 - 'elecFieldIntensity' (real) defined in 'V_air' on Elements
 - 'elecFieldIntensity' (real) defined in 'V_elec' on Elements
 - 'elecFieldIntensity' (real) defined in 'P0_elem' on Elements
 - 'elecFieldIntensity' (real) defined in 'P1_elem' on Elements
 - 'elecFieldIntensity' (real) defined in 'P2_elem' on Elements
 - 'elecFieldIntensity' (real) defined in 'P3_elem' on Elements
 - 'elecFluxDensity' (real) defined in 'V_air' on Elements
 - 'elecFluxDensity' (real) defined in 'V_elec' on Elements
 - 'elecPotential' (real) defined in 'V_air' on Nodes
 - 'elecPotential' (real) defined in 'V_elec' on Nodes
 - 'elecPotential' (real) defined in 'P0_node' on Nodes
 - 'elecPotential' (real) defined in 'P1_node' on Nodes
 - 'elecPotential' (real) defined in 'P2_node' on Nodes
 - 'elecPotential' (real) defined in 'P3_node' on Nodes
 - 'elecCharge' (real) defined in 'S_top' on ElementGroup
 - 'elecEnergy' (real) defined in 'V_air' on Regions
 - 'elecEnergy' (real) defined in 'V_elec' on Regions
```

✓ # Perform interpolation

INTERACTIVE MODE IN VS CODE (2)



INTERACTIVE MODE IN VS CODE (3)