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Postprocessing results from Cardinal using Pyvista

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Outline

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   - What data does Cardinal produce?
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   - What is Pyvista
3. Implementation of readers for Cardinal in Pyvista
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4. Simple example
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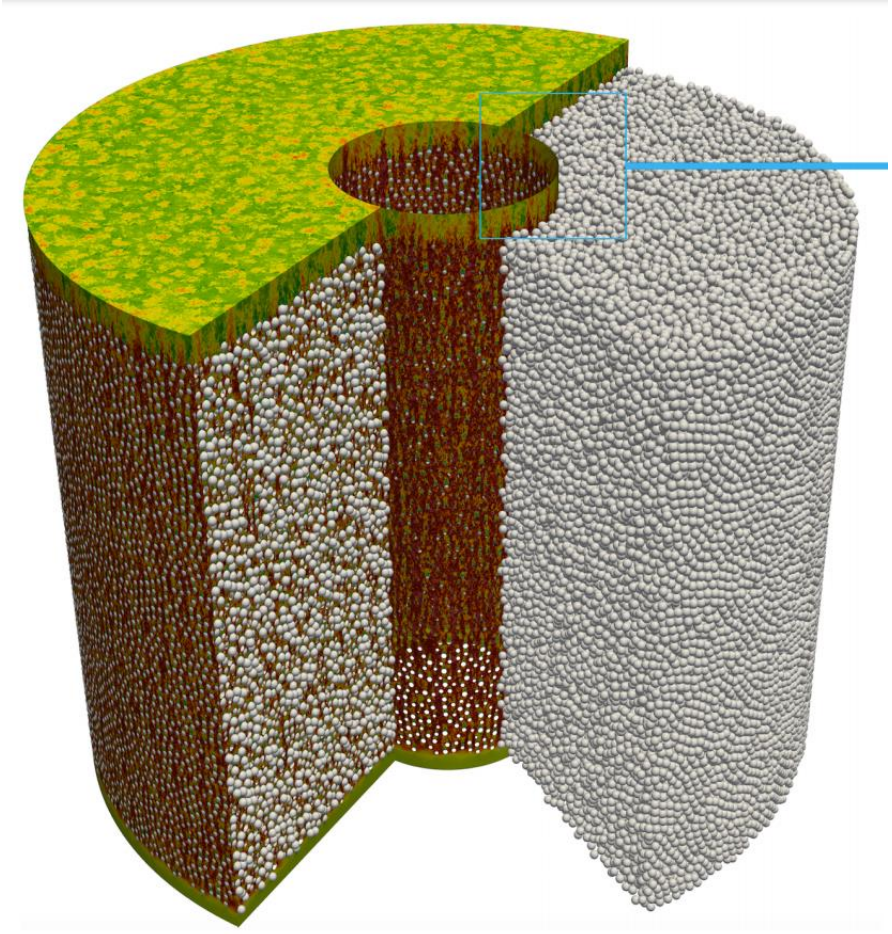
What is Cardinal?



- Wraps nekRS and OpenMC into the MOOSE multiphysics framework.
- Can couple
  - Fluid dynamics
  - Neutron and photon transport
  - Conjugate heat transfer
  - Structural mechanics
  - Any MOOSE app
- Common existing use cases include:
  - Nuclear reactor cores (Fission).
  - Increasingly used for Fusion
    - Breeder blankets.

What data does Cardinal need/produce?

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- Data required:
  - nekRS mesh
    - Bespoke *.re2 format
    - Often exported from Coreform Cubit via Exodus II and converted using exo2nek utility
  - Solid mesh for MOOSE:
    - *.e Exodus II file
  - OpenMC
    - CAD-based geometries for DAGMC (*.h5m)
  - Assorted text files
- Data produced:
  - NekRS output data
    - *.nek5000 metadata file
    - Data file *0.f0001
  - Solid output data
    - *.e Exodus II file
    - *.e.N.p Parallel Exodus II (Nemesis) file
  - OpenMC
    - Has many of its own Python tools
  - Assorted text/CSV files.

What is Pyvista?

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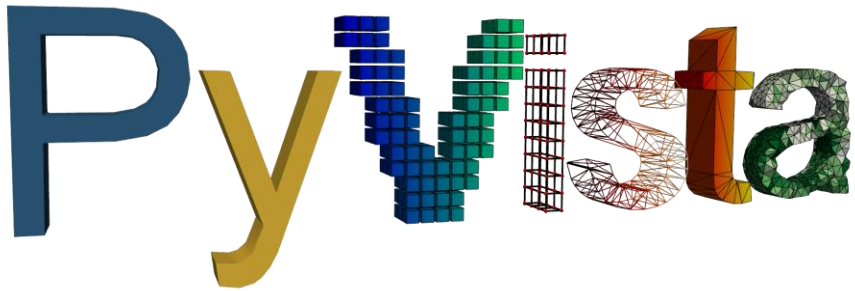
- A Pythonic wrapper to the Visualisation Toolkit (VTK)
- It inherits from the VTK python classes but makes them much more user friendly
  - VTK python classes are mirrors C++ API – very clunky
  - Pyvista classes are *almost* fully compatible with VTK parents so easily extendable
  - Much lower learning curve
- Most filters that you find in Paraview are in Pyvista
  - Both are based on VTK
  - For example:
    - 'Cell data to point data' in Paraview
    - Obj.cell_data_to_point_data() or obj.ctp()
- Easy access to underlying data.



Implementation of readers for Cardinal in Pyvista

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- Two VTK reader classes needed to wrapped to enable visualisation of Cardinal data in Pyvista
- **ExodusIIReader:** wraps the vtkExodusIIReader class from VTK
  - Conveniently exposes blocks/sets and their respective arrays at high level.
  - By default, the element blocks arrays and nodal arrays are enabled.
- **Nek5000Reader:** wraps the vtkNek5000Reader from VTK.
  - Paraview options such as passing the spectral element IDs as cell data and merging element boundary points are available are exposed.
- Note on Nemesis files
  - On the todo list.
    - Wrap vtkPExodusIIReader: cannot get it to work
    - Wrap vtkIOSSReader: requires some donkey work to get into Pyvista
  - As a workaround each file could be read by the ExodusIIReader and merged.

Limitations and comparison with Paraview

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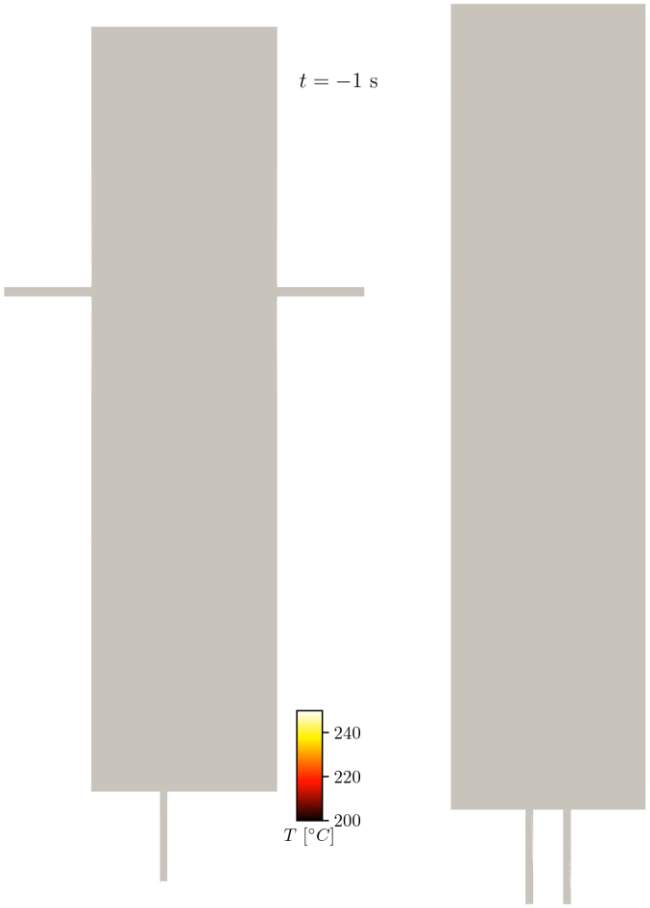
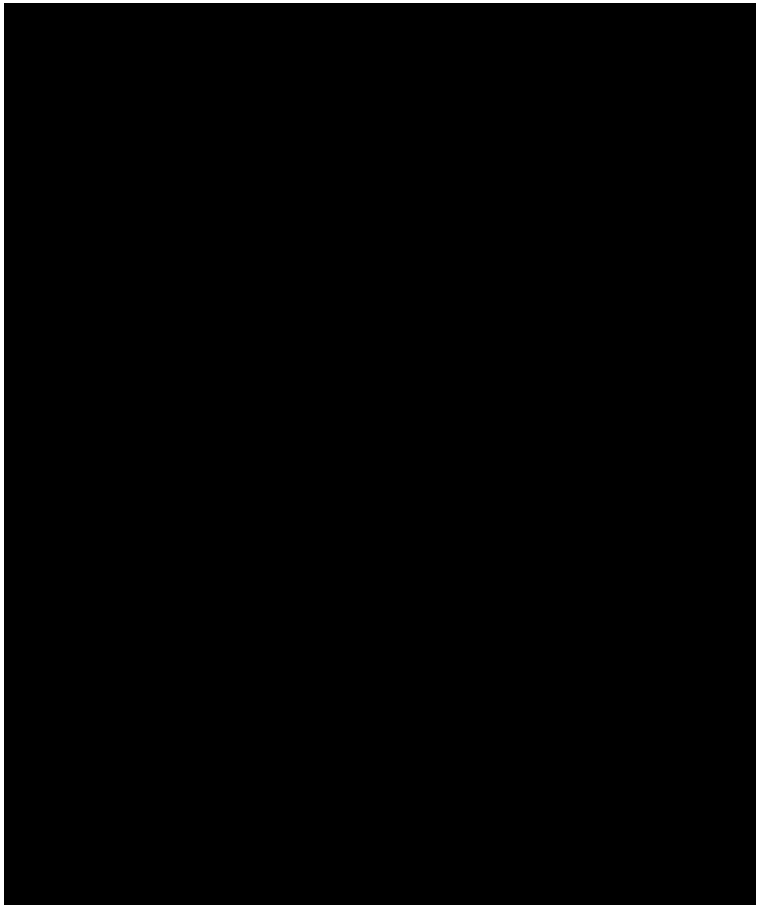
- Pyvista has a similar role in a post-processing pipeline but using both is perfectly possible.
  - Pyvista: scripted repeated postprocessing for producing high-quality plots
  - Paraview: quick look at results using a GUI
- Compared to Paraview, Pyvista has some limitations performance-wise
  - VTK is not by default built with threading or MPI
  - Question: how often do you use Paraview with MPI.
- Pyvista can still run fast:
  - Build VTK from source with OpenMP enabled (I have scripts for this in the repo and a singularity container)
  - Can run it on the HPC for faster file access and use up to a node.
- Now let's look at some examples:

Gallery

- Results from an LES Code_Saturne finite volume simulation of the liquid sodium Thermal Stratification Test Facility at UWM





Discussion

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1. What are trade-offs between using a posteriori and in-situ postprocessing/visualisation including some applications?
   - If you have experience of in-situ visualisation tools such Paraview/VTK Catalyst.
2. How do postprocessing/visualisation workflows change between unstructured and structured datasets?
3. Do you have suggestions about where a scripted high-level tool like Pyvista can be used in the work flows common to the group.