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Postprocessing results from Cardinal using Pyvista

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Outline

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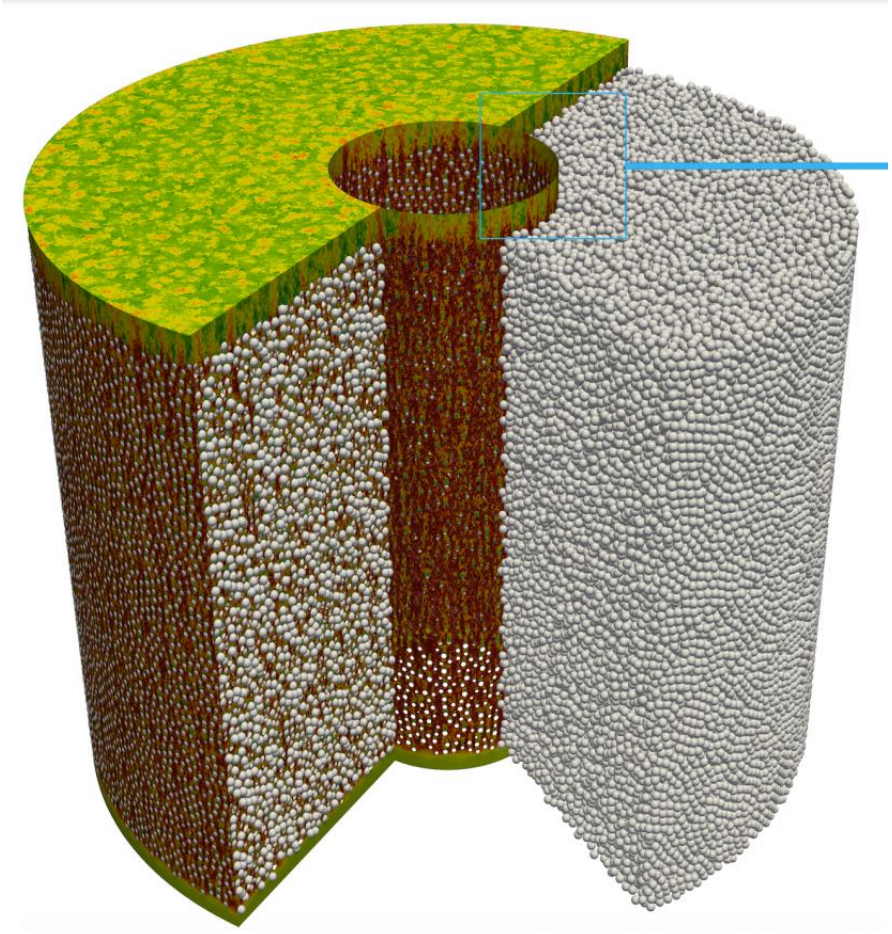
1. Cardinal
   - What is Cardinal?
   - What data does Cardinal produce?
2. Pyvista
   - What is Pyvista
3. Implementation of readers for Cardinal in Pyvista
   - ExodusIIReader and Nek5000Reader
4. Simple example
   - Flow around a pebble Cardinal tutorial
5. Discussion

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
    - *.re2 format often exported from Coreform Cubit via Exodus II
  - Solid mesh for MOOSE:
    - *.e Exodus II file
  - OpenMC
    - CAD geometry
  - Assorted text files

- Data produced:
  - NekRS output data
    - *.nek5000 and associated 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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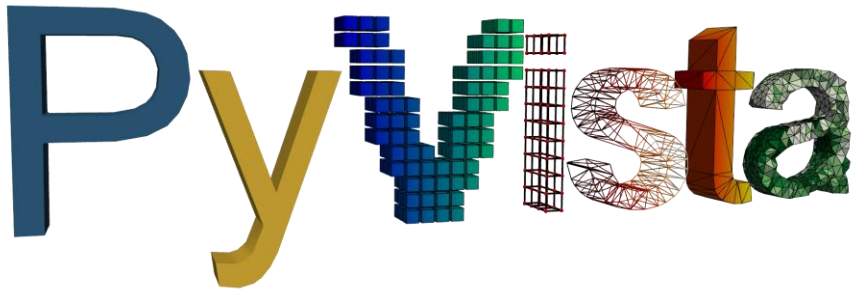
- A Pythonic wrapper to the Visualisation Toolkit (VTK)
- It inherits from the VTK python classes but makes them much more user friendly
  - VTK python classes are mirrors C++ API – very clunky
  - Pyvista classes are fully compatiable with VTK parents so easily extendable
  - Much lower learning curve
- 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.
  - As a workaround each file could be read by the ExodusIIReader and merged.

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Example

Flow over a pebble

Limitations and comparison with Paraview

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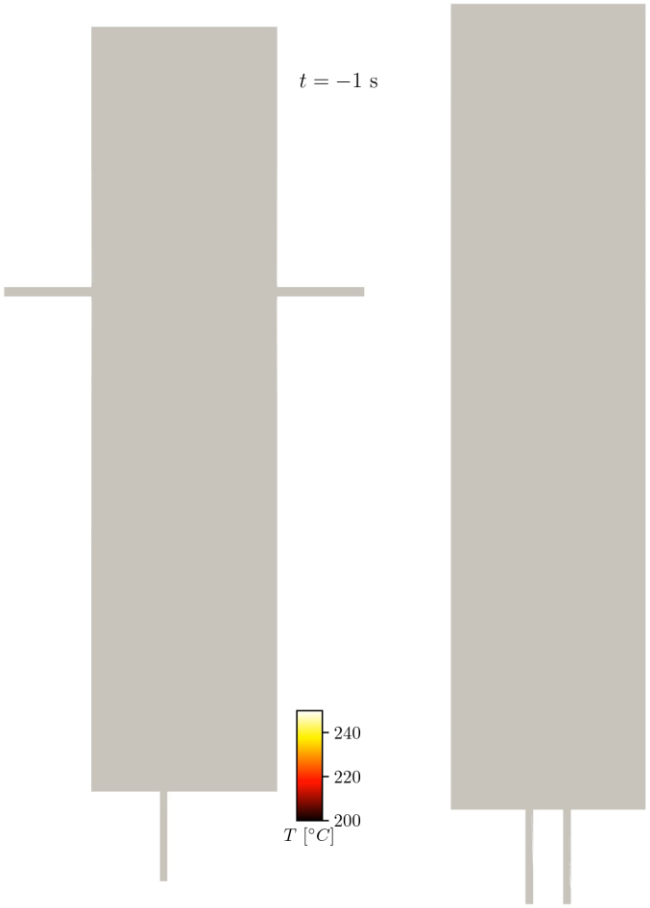
- Pyvista has a similar role in a post-processing pipeline but using both is perfectly possible, so let's compare

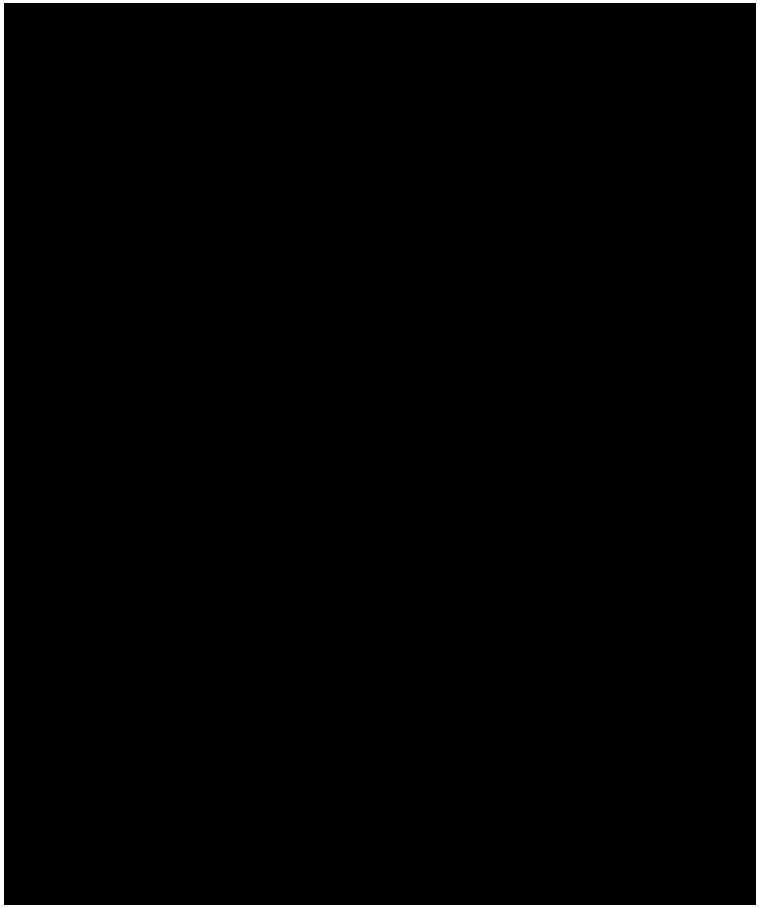
Pyvista	Paraview
Scripted, repeatable post-processing and visualisation	Having a quick look at results (Has a GUI)
Large unstructured meshes (VTK not built with MPI)	Very large unstructured meshes (VTK built with MPI)
Can be combined with matplotlib to produce high quality figures	Use server client mode on an HPC with MPI.
	'Start trace' and 'dump trace' can help with scripting but can be verbose particularly for plotting

- Pyvista can still run very fast:
  - Build VTK from source with OpenMP enabled (I have scripts for this and a singularity container)
  - Can run it on the HPC for faster file access and use up to a node
- Use Paraview to determine slice locations or camera/focal point positions and input them into Pyvista script.

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.