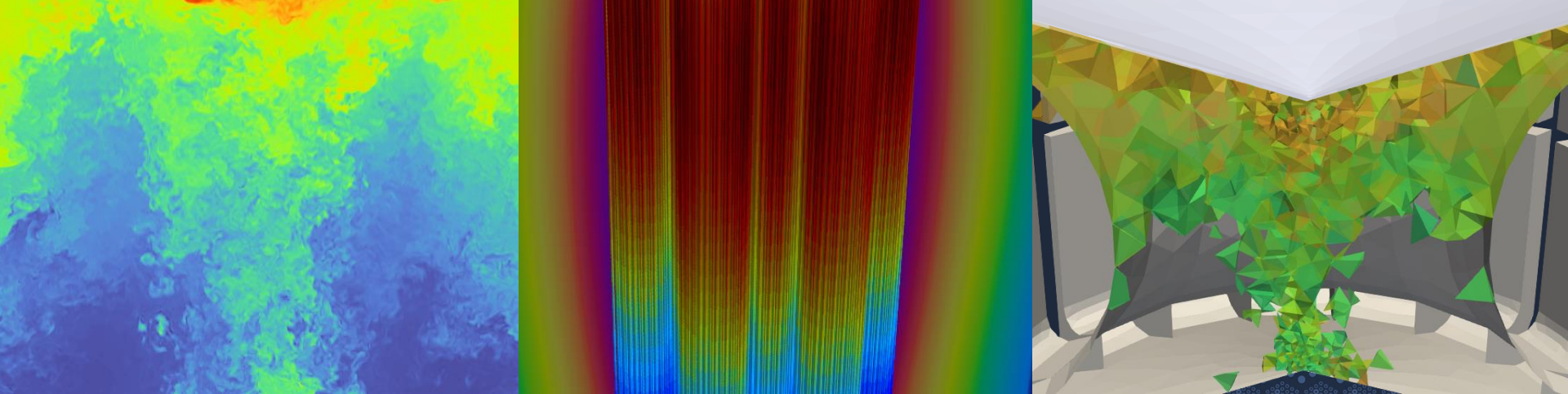




# Cardinal: Multiphysics and Multiscale Simulation for Fusion Applications

A. Novak<sup>1</sup>, A. Hegazy<sup>1</sup>, K. Sawatzky<sup>1</sup>, M. Eltawila<sup>1</sup>, M. Reji<sup>1</sup>, S. Schott<sup>1</sup>, P. Shriwise<sup>2</sup>, P. Romano<sup>2</sup>, W. Ahammed<sup>3</sup>, P. Wilson<sup>3</sup>, H. Brooks<sup>4</sup>, P.C. Simon<sup>5</sup>, G. Giudicelli<sup>5</sup>, C. Icenhour<sup>5</sup>, C. Taylor<sup>5</sup>, J. Pacheco Duarte<sup>3</sup>, B. Lindley<sup>3</sup>, J. Quinn<sup>6</sup>, S. Coleman<sup>7</sup>

<sup>1</sup>University of Illinois, Urbana-Champaign

<sup>2</sup>Argonne National Laboratory

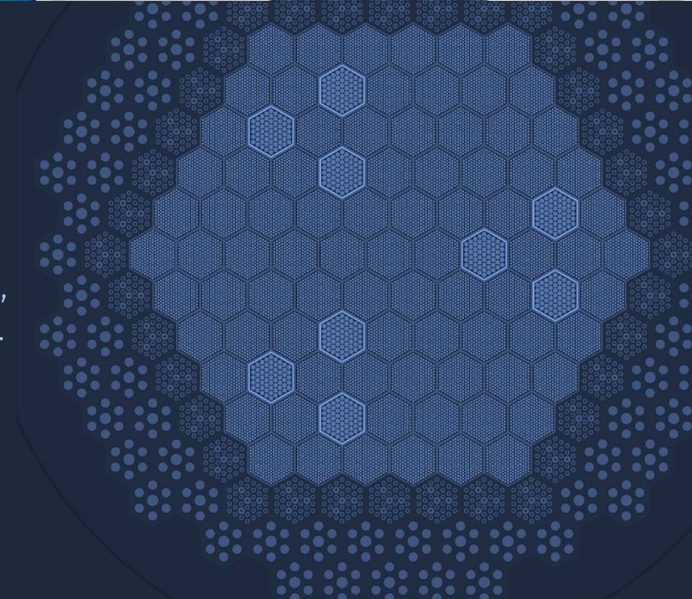
<sup>3</sup>University of Wisconsin, Madison

<sup>4</sup>United Kingdom Atomic Energy Authority

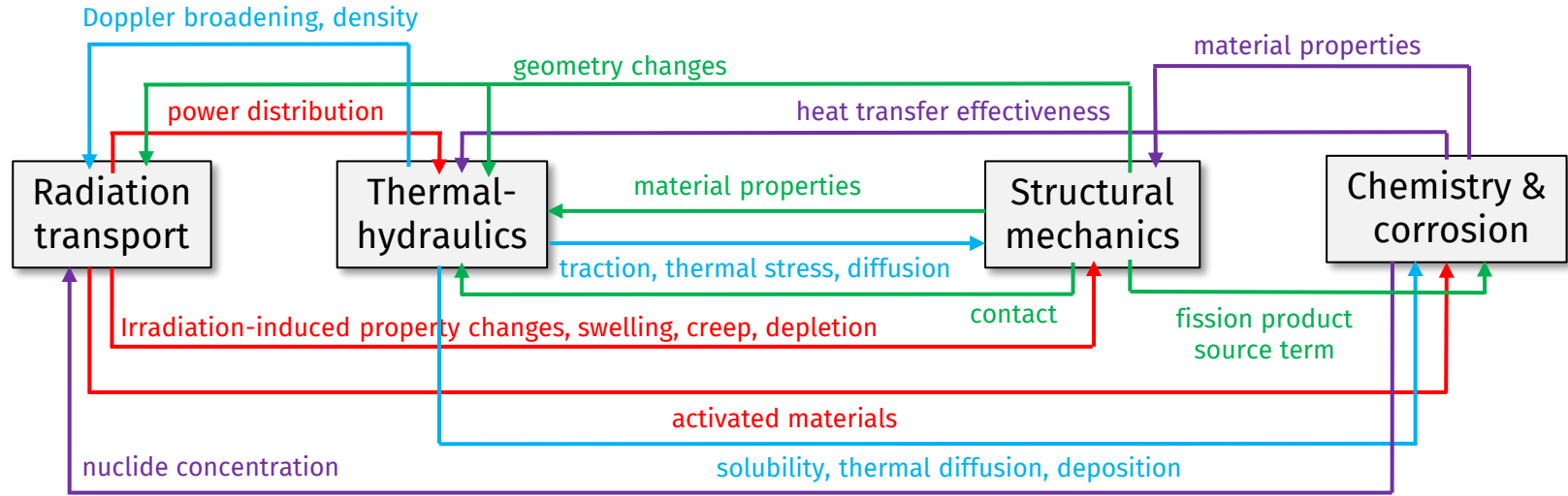
<sup>5</sup>Idaho National Laboratory

<sup>6</sup>Colorado State University

<sup>7</sup>RadiaSoft

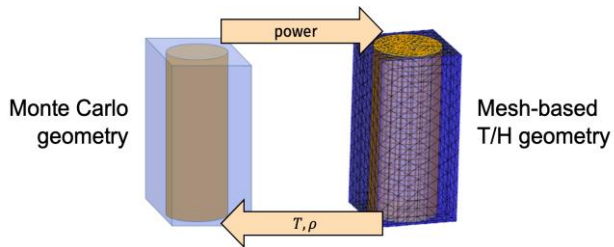


# Multiphysics in Fusion

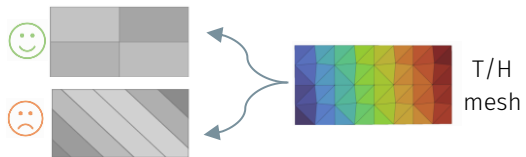


# R&D Challenges

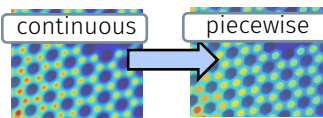
## Data Transfers



Highly manual process to build geometries and exchange data



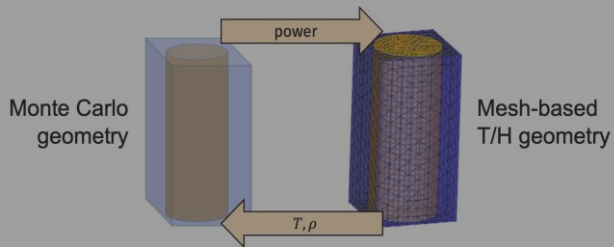
Limitations on distance-to-collision sampling



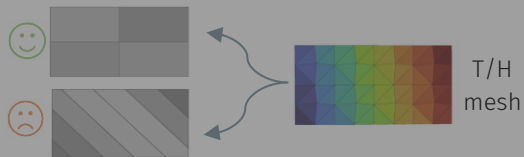
Need a general-purpose capability

# R&D Challenges

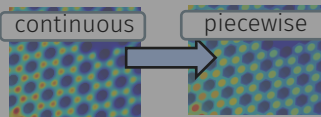
## Data Transfers



Highly manual process to build geometries and exchange data



Limitations on distance-to-collision sampling



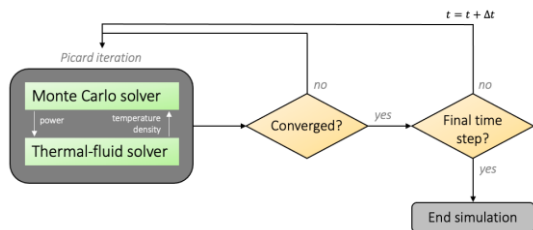
Need a general-purpose capability

## Iterative Methods

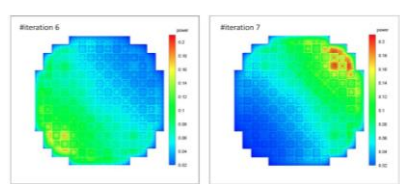
combine stochastic and matrix-based methods

Monte Carlo

$Ax = b$



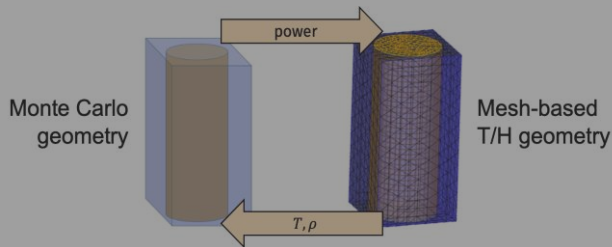
Operator splitting and/or poor statistics can cause instabilities



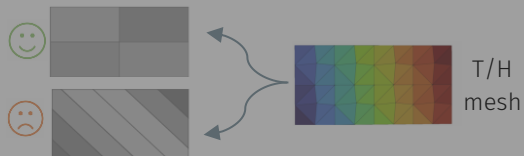
Need control over iteration scheme

# R&D Challenges

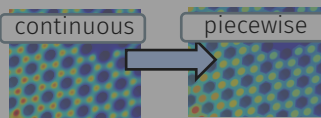
## Data Transfers



Highly manual process to build geometries and exchange data



Limitations on distance-to-collision sampling



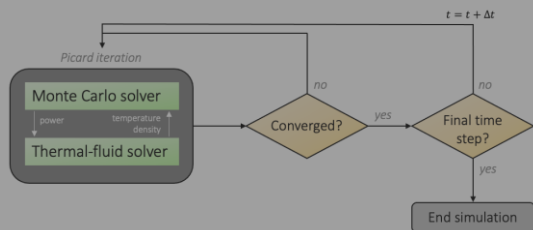
Need a general-purpose capability

## Iterative Methods

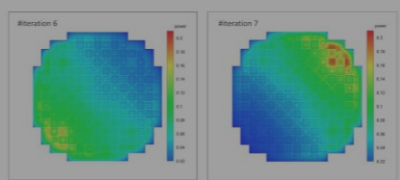
combine stochastic and matrix-based methods

Monte Carlo

$Ax = b$



Operator splitting and/or poor statistics can cause instabilities



Need control over iteration scheme

## Software and Parallelization



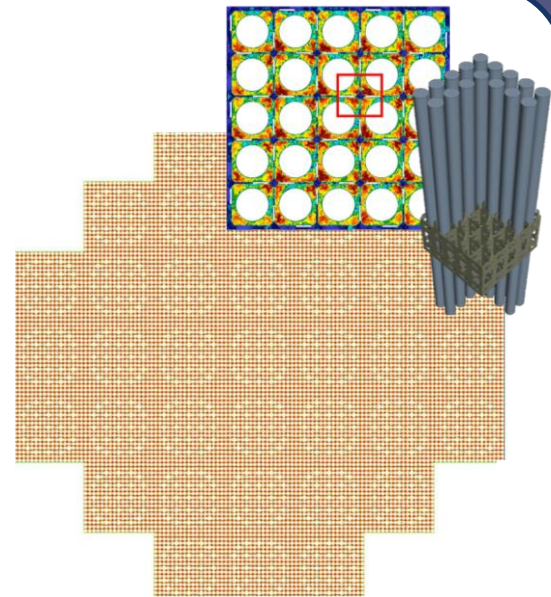
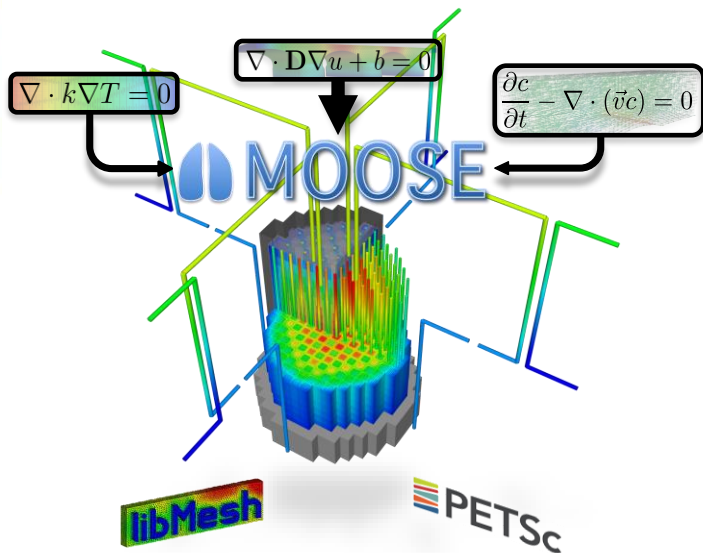
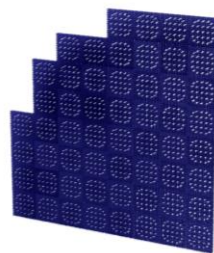
Need to leverage GPUs and be designed with performance in mind

Scarce open-source high-fidelity multiphysics software

Performant & open source important

- Cardinal: High-fidelity Multiphysics for Fusion
- Adaptive mesh refinement for breeder blankets
- Neutronics to accelerate fusion materials development
- Liquid metal MHD experiments
- Reticulated foam extraction systems
- Conclusions

# Cardinal



## OpenMC

C++ Monte Carlo radiation transport + depletion

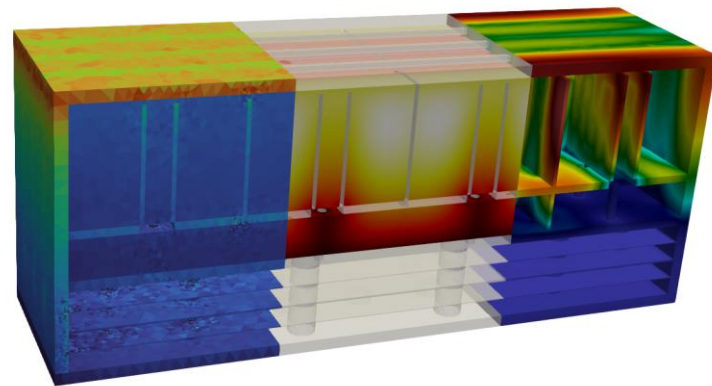
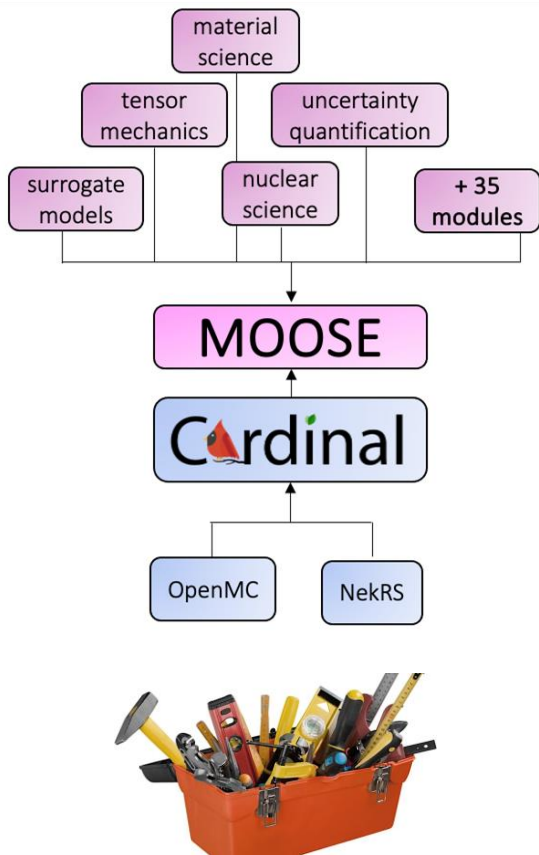
## NekRS

C++ spectral element turbulent incompressible flow; induction & inductionless MHD

## MOOSE: multiphysics framework

Extensible, modular C++ classes to define physics model components  
(parallel communication, mesh-to-mesh data transfers, kernels, materials, ...)

# Big-Picture: *Add OpenMC and NekRS to a large “toolbox” for fusion simulation*



MOOSE framework

**data transfers**

**solution postprocessing**

**mesh adaptivity**

**checkpointing**

MOOSE modules

**solid mechanics**

**heat transfer**

**stochastic tools**

**thermal-hydraulics**

MOOSE applications

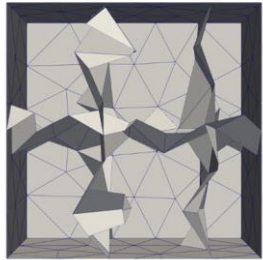
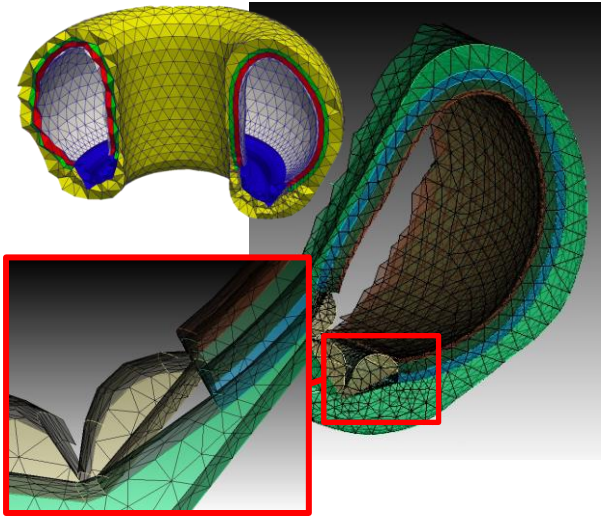
**OpenMC  $n - \gamma$  transport**

**NekRS CFD and MHD**

**TMAP8 tritium**

**SALAMANDER PIC**

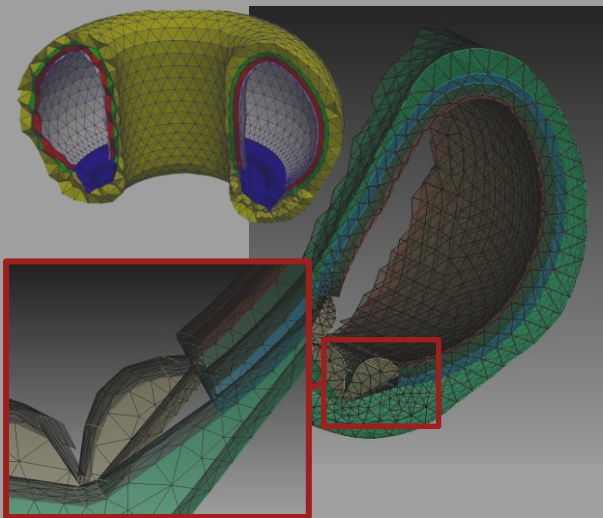
## *Some Notable Software Features*



**Automatic re-generation  
of CAD geometries to  
capture feedback**

surfaces bounding each cell

## Some Notable Software Features



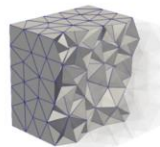
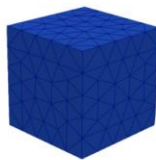
Automatic re-generation  
of CAD geometries to  
capture feedback

surfaces bounding each cell

*Continuous geometry  
deformation is directly  
used in OpenMC*



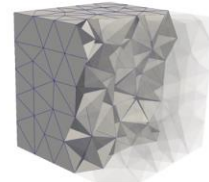
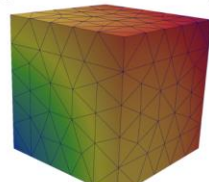
Displacement magnitude  
(from MOOSE thermomechanics)



Cardinal generates OpenMC  
mesh geometry

Initial condition

Displacement magnitude  
(from MOOSE thermomechanics)

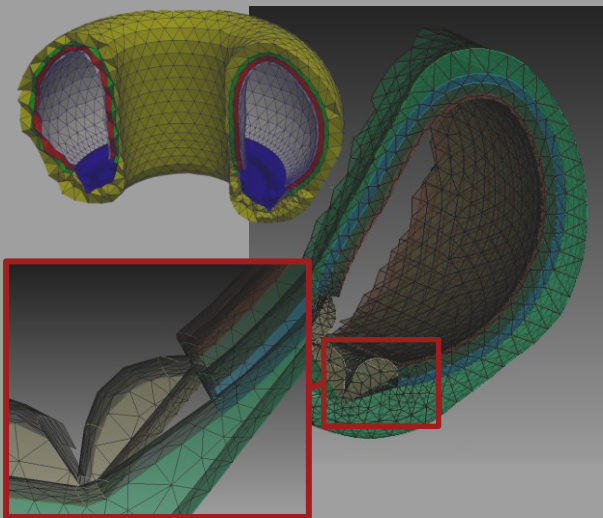


Cardinal generates new OpenMC  
mesh geometry

After Picard iteration 1

**Thermomechanics feedback to Monte  
Carlo neutronics**

## Some Notable Software Features



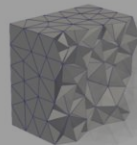
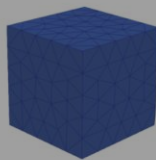
**Automatic re-generation  
of CAD geometries to  
capture feedback**

surfaces bounding each cell

*Continuous geometry  
deformation is directly  
used in OpenMC*



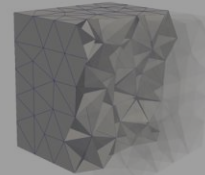
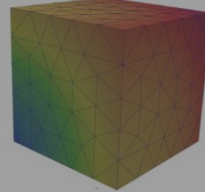
Displacement magnitude  
(from MOOSE thermomechanics)



Cardinal generates OpenMC  
mesh geometry

Initial condition

Displacement magnitude  
(from MOOSE thermomechanics)

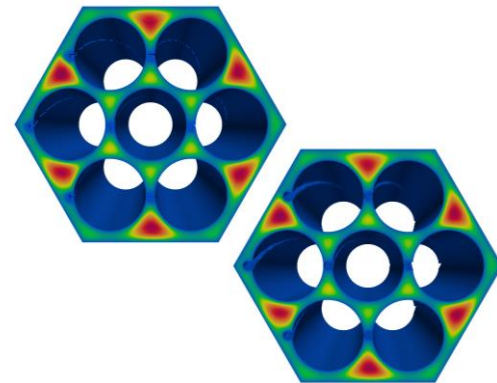
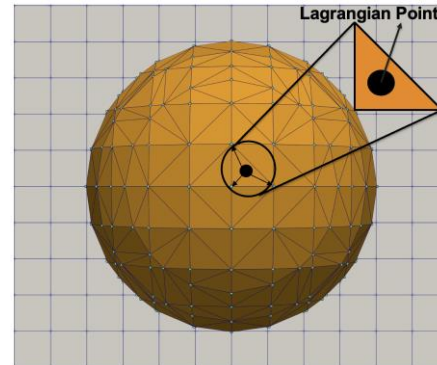


Cardinal generates new OpenMC  
mesh geometry

After Picard iteration 1

**Thermomechanics feedback to Monte  
Carlo neutronics**

*Sandia study quantified ~80% of CFD  
engineers' time spent on mesh generation!*



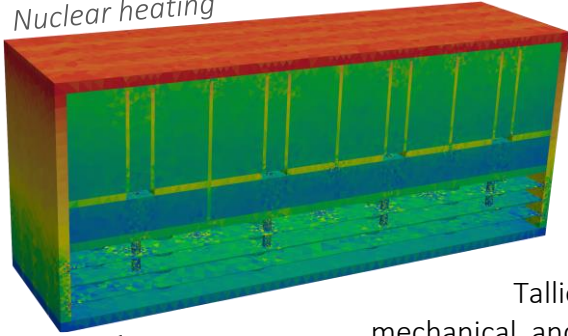
**Immersed boundary methods for CFD of  
complex geometries**

- Cardinal: High-fidelity Multiphysics for Fusion
- Adaptive mesh refinement for breeder blankets
- Neutronics to accelerate fusion materials development
- Liquid metal MHD experiments
- Reticulated foam extraction systems
- Conclusions

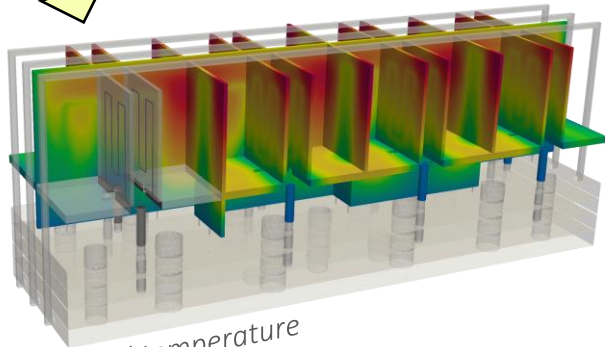
# Monte Carlo Tallies

Spatial resolution

*Nuclear heating*



Tallies are **inputs** to T/H,  
mechanical, and material analysis...  
on **different length scales**

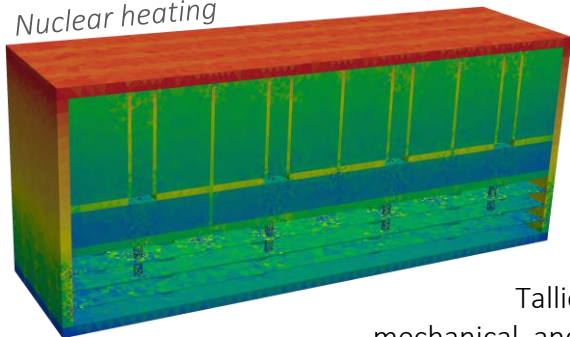


*Solid temperature*

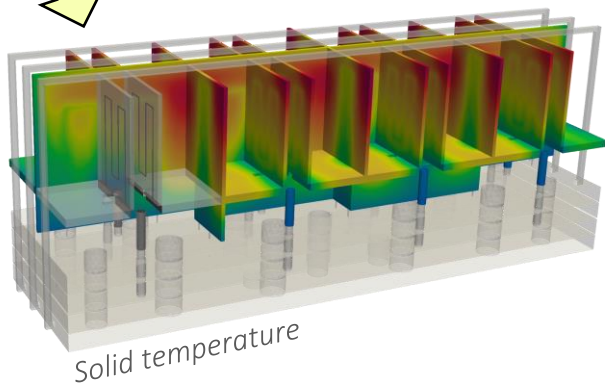
# Monte Carlo Tallies

## Spatial resolution

*Nuclear heating*



Tallies are **inputs** to T/H,  
mechanical, and material analysis...  
on **different length scales**



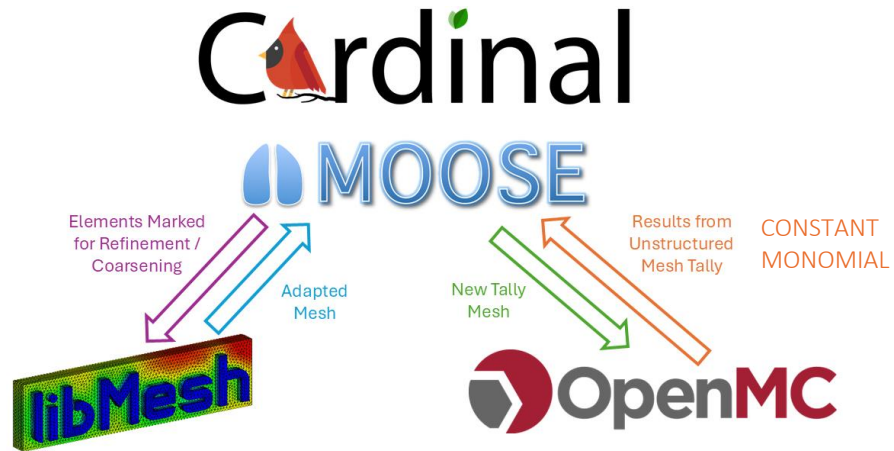
## Runtime, Statistical Error, and Stability



Refinement is penalized by  $\sigma \sim \frac{1}{\sqrt{N}}$

Statistical error and/or finer resolution  
can also destabilize Picard iteration

# Adaptive Mesh Refinement in Cardinal

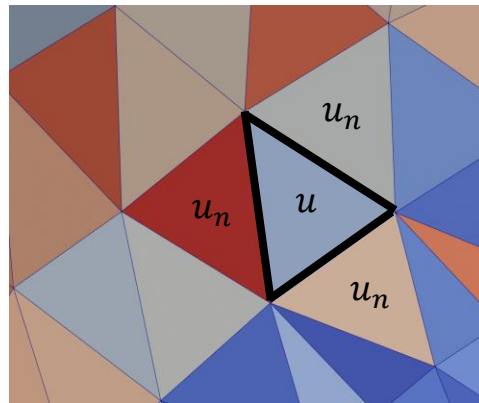
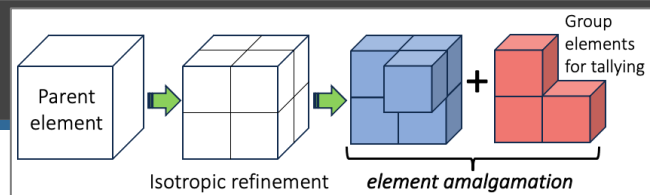
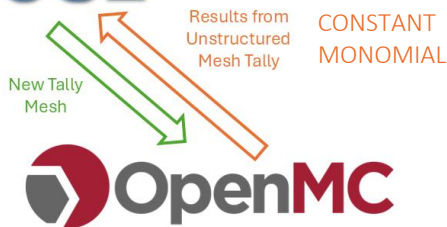
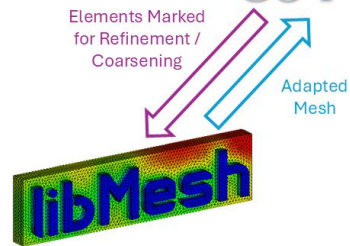


- Indicators: estimate of error in each element
- Markers: decide which elements to refine/coarsen

# Adaptive Mesh Refinement in Cardinal

# Cardinal

## MOOSE



- An OpenMC unstructured mesh tally is re-initialized on each adaptivity cycle
- Any number of adaptivity cycles are allowed within a single Picard iteration – AMR subcycling
- Tallies are constant monomials (for now)

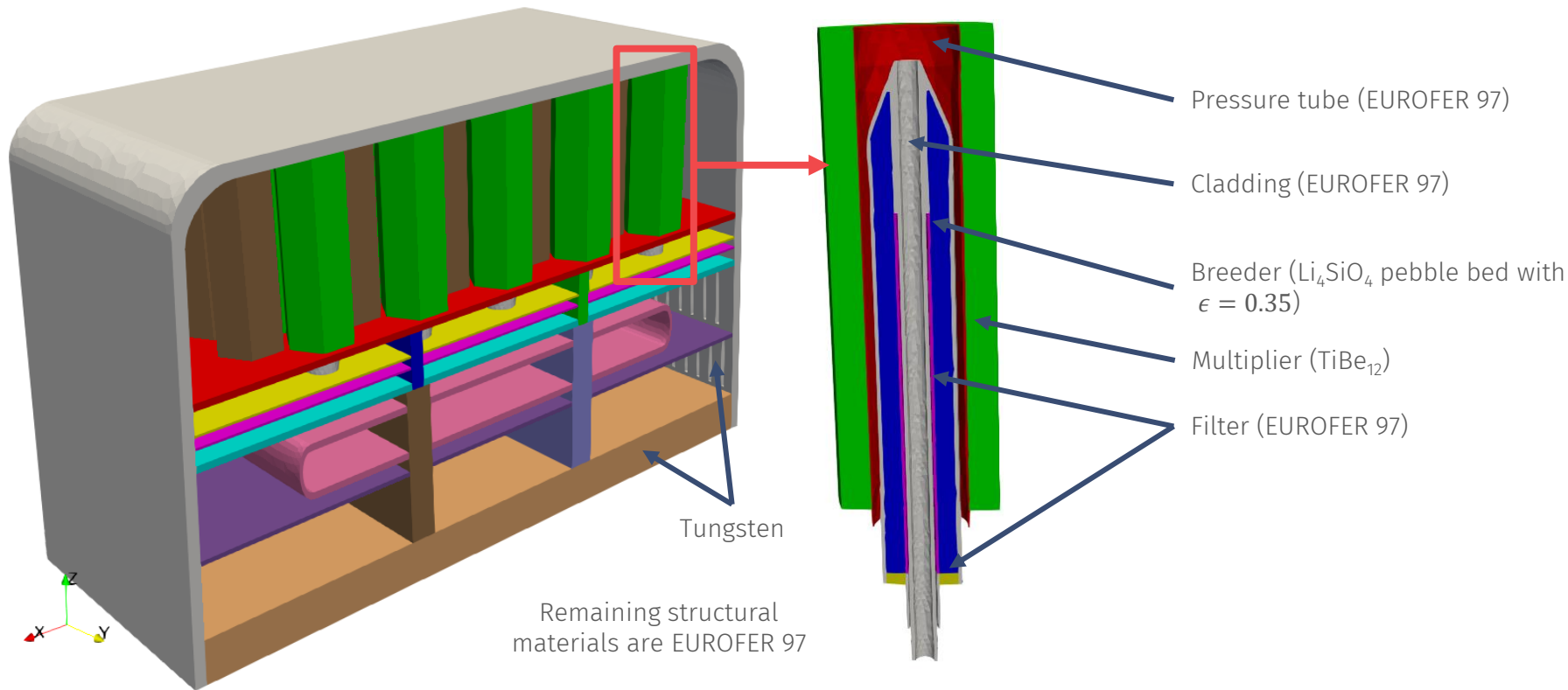
$$\text{ValueJumpIndicator: } \sqrt{h \int (u - u_n)^2 dS}$$

$$\text{VectorMagnitudeIndicator: } \sqrt{h \int \|\vec{u}\| dV}$$

$$\text{VectorJumpIndicator: } \sqrt{h \int (\vec{u} - \vec{u}_n)^2 dS}$$

$$\text{ElementOpticalDepthIndicator: } \Sigma_x h$$

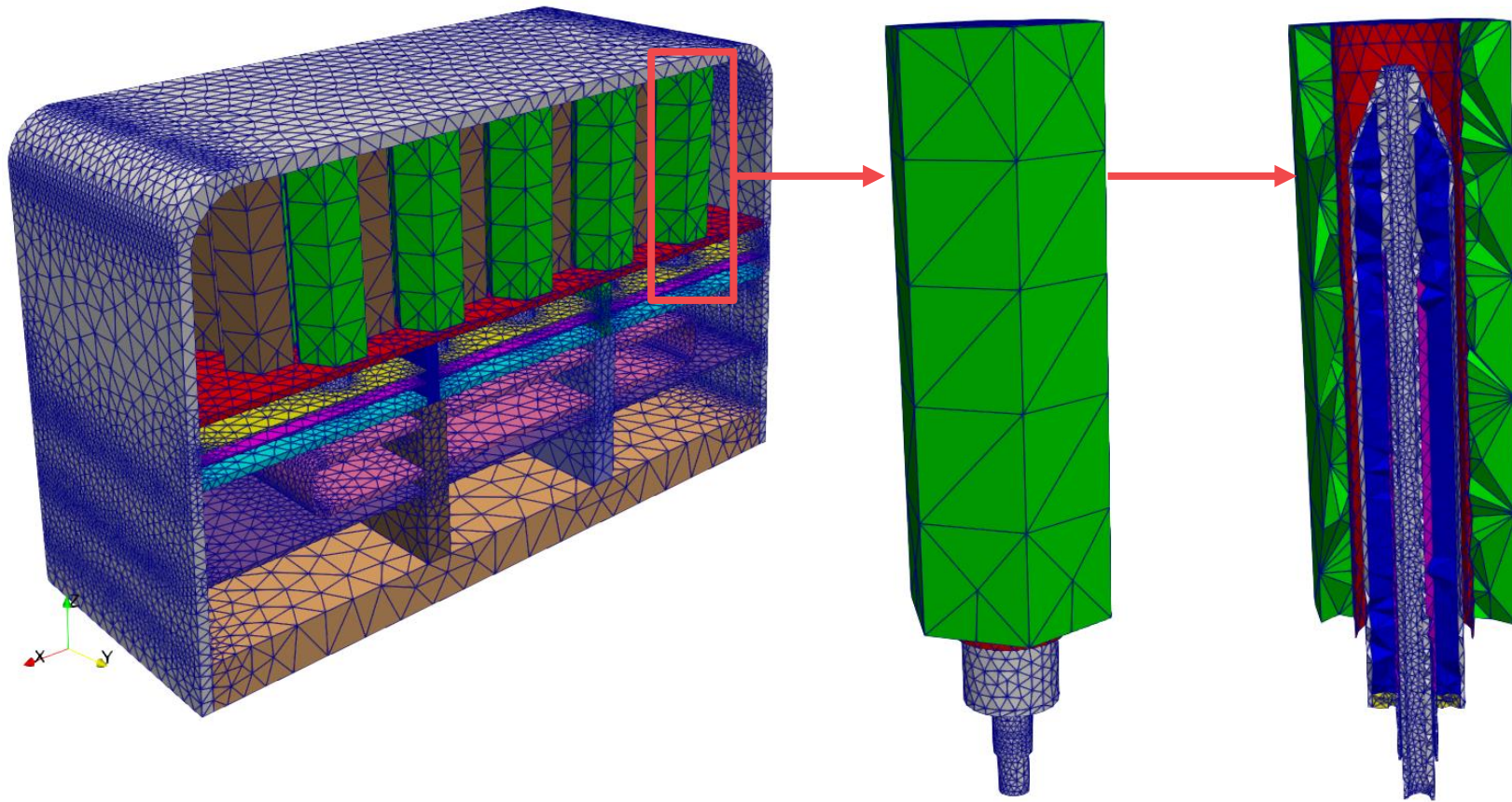
# HCPB Outboard Blanket Module



CAD generated with Hypnos, a parametric geometry engine for blanket design developed by the UKAEA:

<https://github.com/aurora-multiphysics/hypnos>

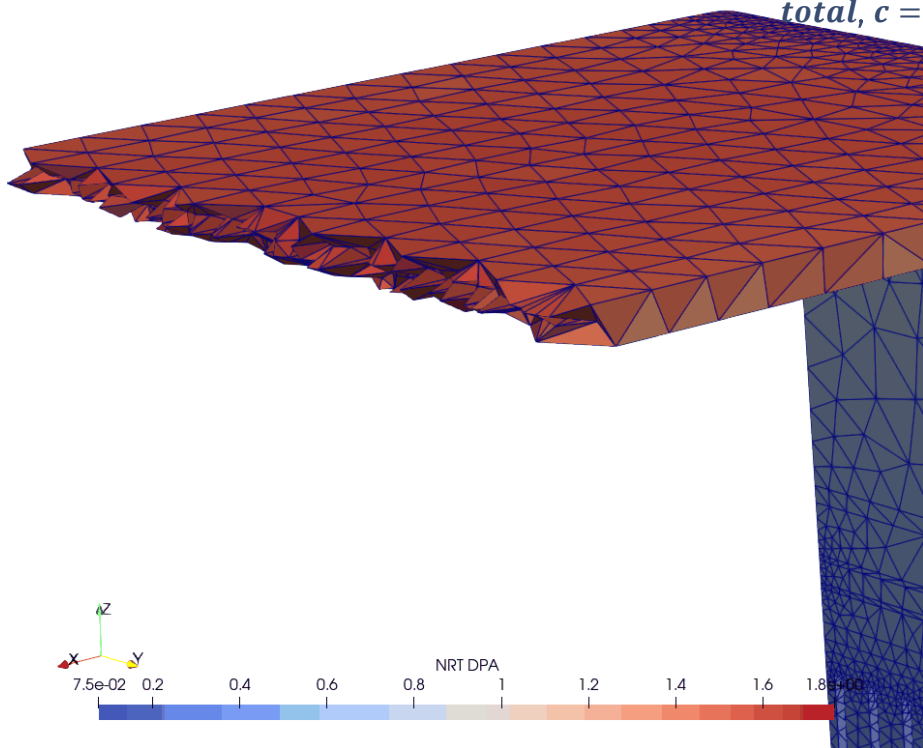
# Initial Mesh



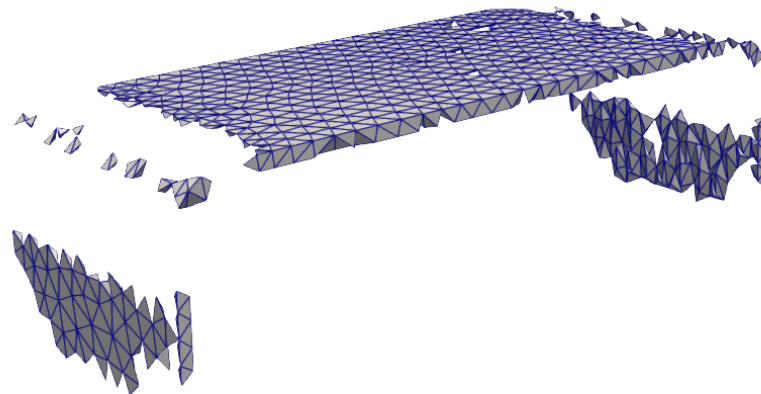
# Applying AMR to DPA on the First Wall

Combining an inverted `ElementOpticalDepthIndicator` with the `ErrorFractionLookAheadMarker`

*total,  $c = 0.3$ ,  $t = 1\%$*



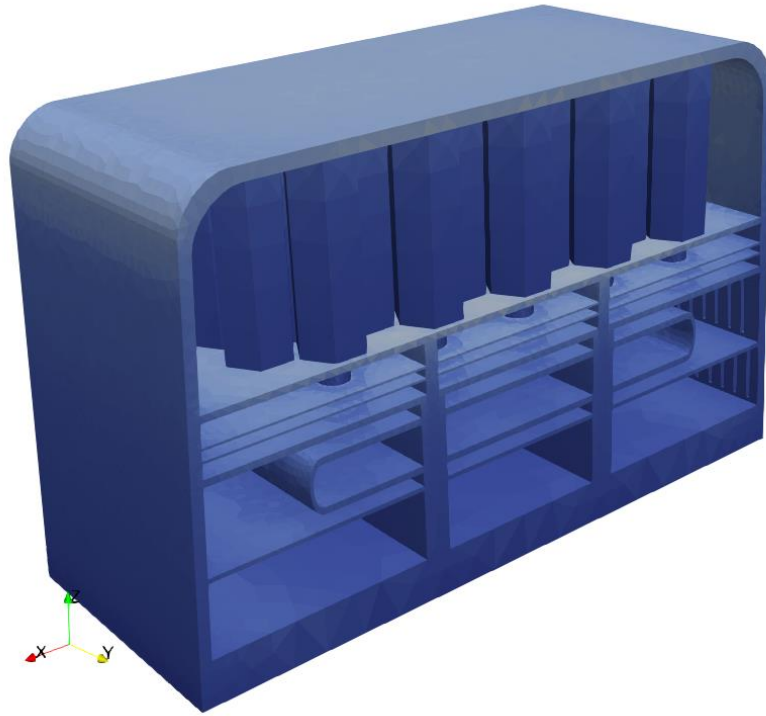
NRT DPA



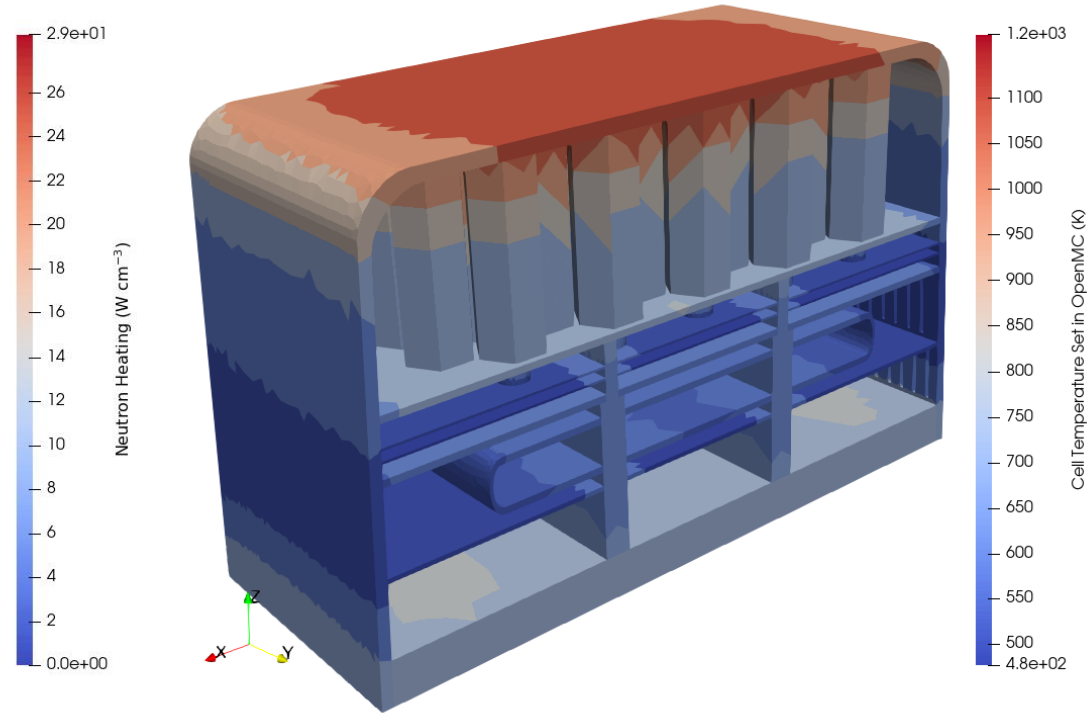
Elements Marked for Refinement

Refinement Cycle: 0.000000

# Next Step: Multiphysics-Driven Adaptivity

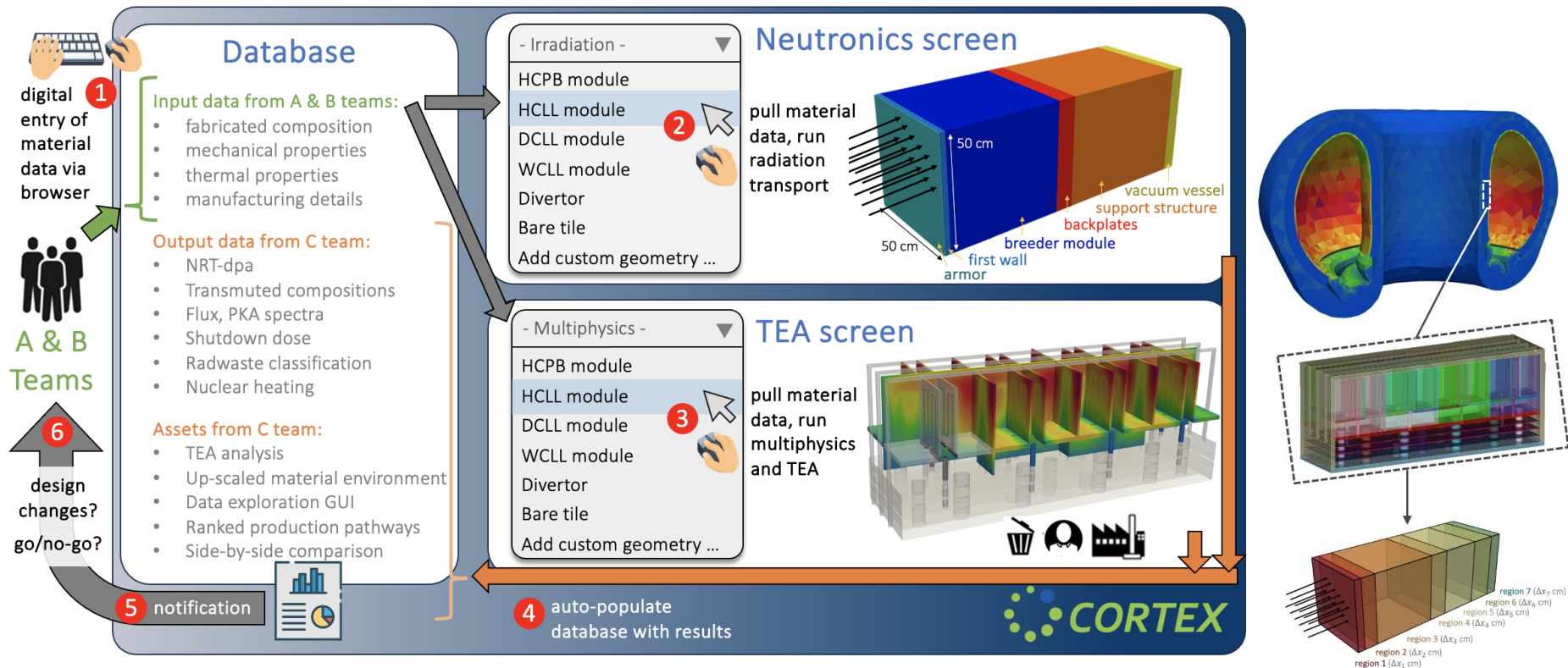


Neutron Heating



Temperature

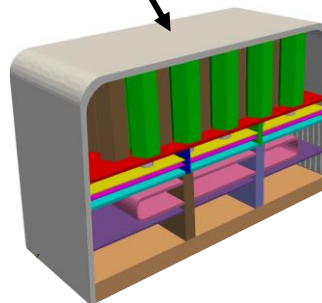
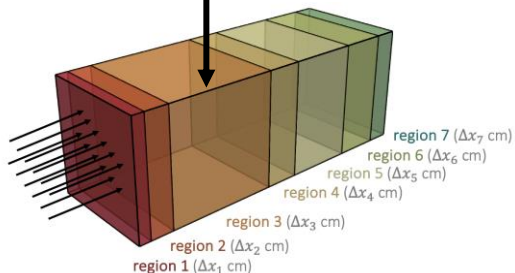
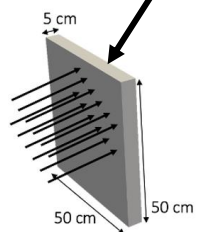
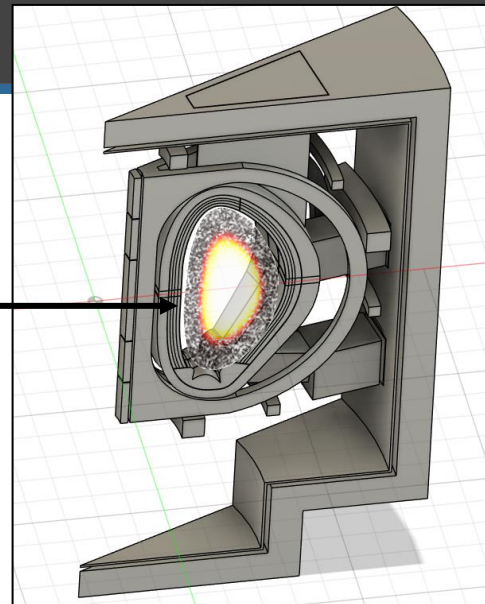
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# CORTEX Materials Database

The screenshot shows the CORTEX Materials Database interface. The main table displays material properties for Eurofer 97. The 'Composition' section provides instructions for entering material data and includes a table for Weight % and Atom %.

| Element or Nuclide | Weight % |     |      | Atom % |     |     |
|--------------------|----------|-----|------|--------|-----|-----|
|                    | Target   | Min | Max  | Target | Min | Max |
| C                  | 0.11     |     |      |        |     |     |
| Cr                 | 9.00     |     |      |        |     |     |
| W                  | 1.10     |     |      |        |     |     |
| Mn                 | 0.40     |     |      |        |     |     |
| V                  |          |     | 0.15 | 0.25   |     |     |
| Ta                 | 0.12     |     |      |        |     |     |
| N                  | 0.03     |     |      |        |     |     |
| P                  | 0.01     |     |      |        |     |     |
| S                  | 0.01     |     |      |        |     |     |
| B                  | 0.00     |     |      |        |     |     |
| O                  | 0.01     |     |      |        |     |     |
| Fe                 | balance  |     |      |        |     |     |
| Nb                 |          |     | 0.00 | 0.01   |     |     |
| Mo                 |          |     | 0.00 | 0.01   |     |     |
| Ni                 |          |     | 0.00 | 0.01   |     |     |
| Cu                 |          |     | 0.00 | 0.01   |     |     |



<https://sirepo.com/cortex>

The screenshot shows a laptop screen displaying a spreadsheet application. The top toolbar includes icons for file operations (Save, Open, Print), editing (Undo, Redo), and viewing (Zoom). Below the toolbar, there are tabs labeled "Materials", "Operating Conditions", and "Geometry".

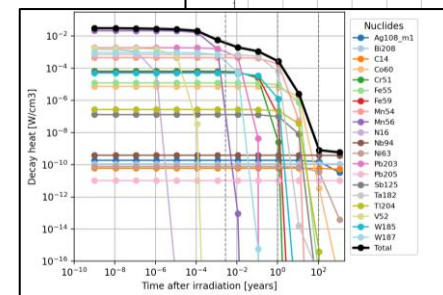
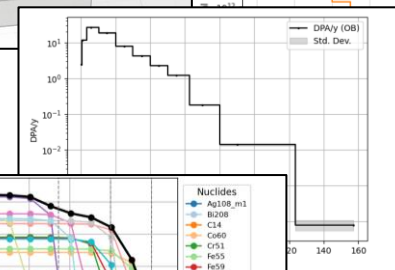
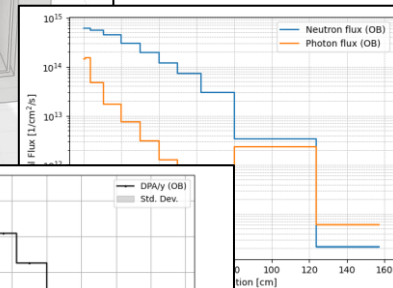
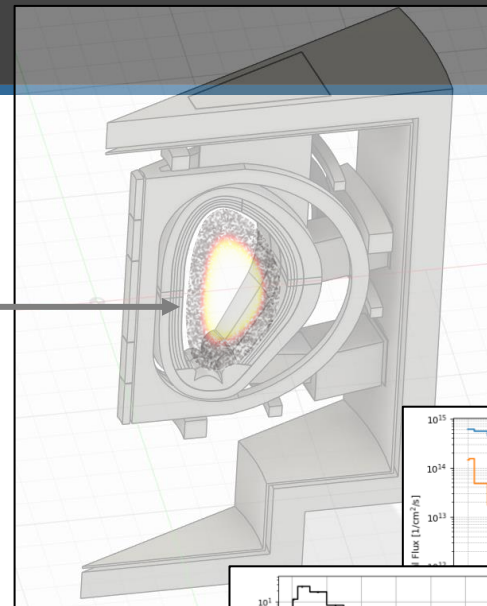
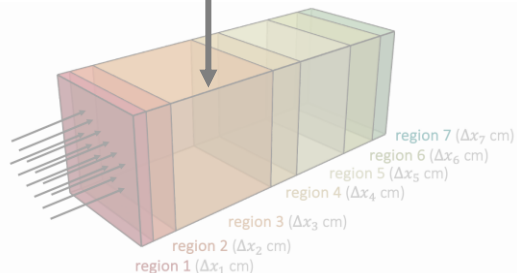
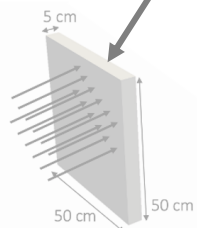
The main area of the spreadsheet contains a form for entering material data:

- Name:** Eurofer 97 string between 1 and 100 characters. A note below says: "Enter the name of your material."
- Density:** 19 number of g/cm<sup>3</sup> between 1 and 25. A note below says: "Enter the density of your material during in-service conditions."
- Composition:** A section titled "Enter the composition of your material. The components of a material must ALL be given in weight % or ALL be given in atomic percent. Neutronics simulations will use the 'target' value if provided. If the 'target' value is not provided, the midpoint of the max/min range will be used, unless the 'min' value is zero in which case the maximum is used (assuming a conservative approach for impurities). One element or nuclide can be indicated as 'balance' in order to fill the remaining material components to 100% weight percent or 100% atomic percent."

Below the composition instructions is a table with columns for Element or Nuclide, Target, Min, Max, Atom %, and another set of Target, Min, Max columns. The table lists various elements and their values:

| Element or Nuclide | Target  | Min  | Max  |      | Atom % | Target | Min | Max |
|--------------------|---------|------|------|------|--------|--------|-----|-----|
| C                  |         | 0.11 |      |      |        |        |     |     |
| Cr                 |         | 9.00 |      |      |        |        |     |     |
| W                  |         | 1.10 |      |      |        |        |     |     |
| Mn                 |         | 0.40 |      |      |        |        |     |     |
| V                  |         |      | 0.15 | 0.25 |        |        |     |     |
| Ta                 |         | 0.12 |      |      |        |        |     |     |
| N                  |         | 0.03 |      |      |        |        |     |     |
| P                  |         | 0.01 |      |      |        |        |     |     |
| S                  |         | 0.01 |      |      |        |        |     |     |
| B                  |         | 0.00 |      |      |        |        |     |     |
| O                  |         | 0.01 |      |      |        |        |     |     |
| Fe                 | balance |      |      |      |        |        |     |     |
| Nb                 |         |      | 0.00 | 0.01 |        |        |     |     |
| Mo                 |         |      | 0.00 | 0.01 |        |        |     |     |
| Ni                 |         |      | 0.00 | 0.01 |        |        |     |     |
| Co                 |         |      | 0.00 | 0.01 |        |        |     |     |

A sidebar on the left side of the screen shows a "Favorites" list with items like AirDrop, Recents, Appicatio, Desktop, Download, Document, ownCloud, coleman, and Sys. Menu2.



OpenMC predictions of  
NRT-dpa, He/H  
production, heating,  
transmutation, ...

# PbLi MHD Experimental Facility: MAGNES



## Engineering significance of MHD:

- MHD pressure drop
- Suppression of turbulence
- Flow distributions: cooling, recirculation, stagnation
- Mass transfer: tritium permeation, plate-out/collection of high-melting point impurities

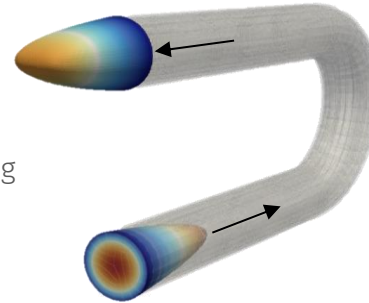
## Computational challenges:

- Hartmann and side layers scale as  $1/Ha$ ,  $1/\sqrt{Ha}$
- Numerical stiffness,  $\Delta t \sim 1/Ha^2$

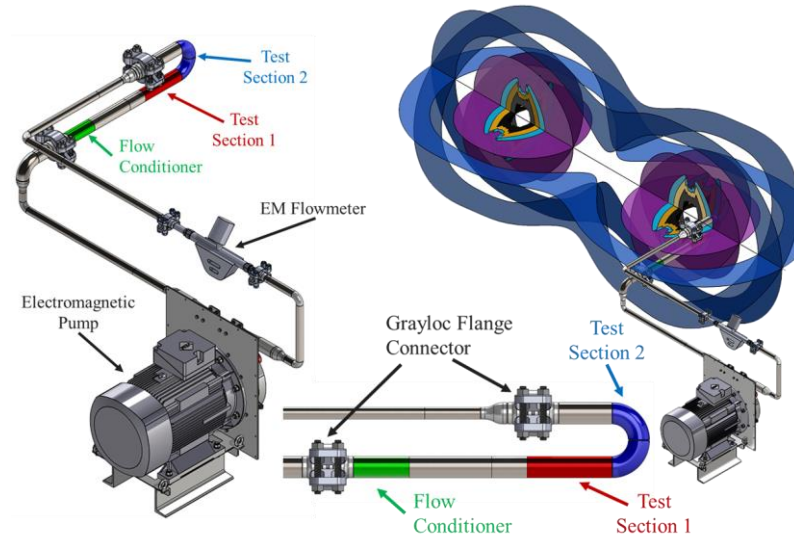
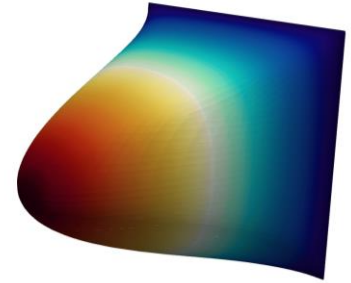
New MHD facility being commissioned at Univ. of Wisconsin, Madison through FIRE using ~5 T field near WHAM magnets.

- Develop open-access benchmark data for isothermal PbLi MHD flows (up to  $Ha \sim 4000$ ): insulations, advanced heat exchange surfaces, ...
- Validate MHD codes
- Develop MHD pressure drop library to facilitate systems-level design

NekRS MHD simulations of experimental test section.



Evolution from hydrodynamic flow to Hunt MHD flow



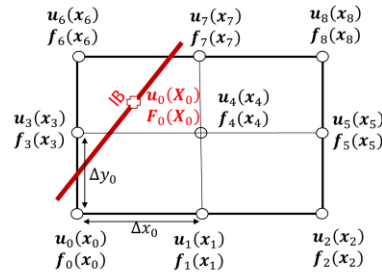
# Reticulated Foams for Tritium Extraction



- High surface area capillary foams for tritium extraction
- NekRS immersed boundary method based on direct forcing approach with overlapping meshes

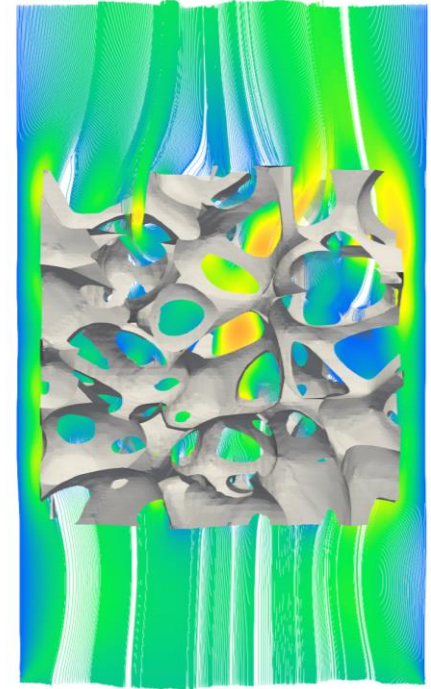
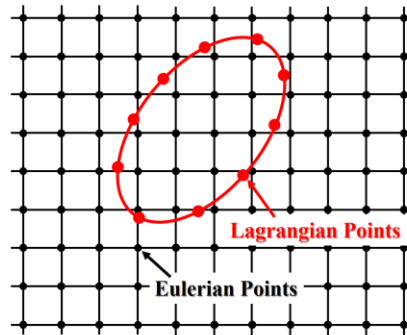
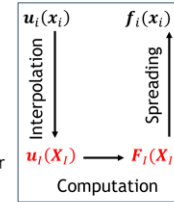


Foam images:  
Chase Taylor (INL)



○ Eulerian Point

⊗ Lagrange Marker



Preliminary NekRS immersed boundary  
simulation of reticulated foam

# Concluding Thoughts

- Code interoperability will benefit multiphysics simulations, multiscale techniques, and UQ/SA. But code-specific workflow challenges remain for
  - CAD-based neutronics modeling
  - Meshing for CFD } *Hard to “parallelize”*
- Software quality assurance (SQA) will be important for fusion and is a huge undertaking – we are QA’ing non-MOOSE codes via MOOSE (e.g. NekRS)
- We are building an open-access fusion materials database (<https://sirepo.com/cortex>) which is linked to fusion neutronics device/component models
  - Suggestions for this tool to support your needs?
  - We welcome material data contributions – do you have datasets you’d like us to upload?
- Community requests for MHD test sections for MAGNES?

# Questions?

<https://cardinal.cels.anl.gov>

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