Updates on Multiphysics Endeavors with OpenMC

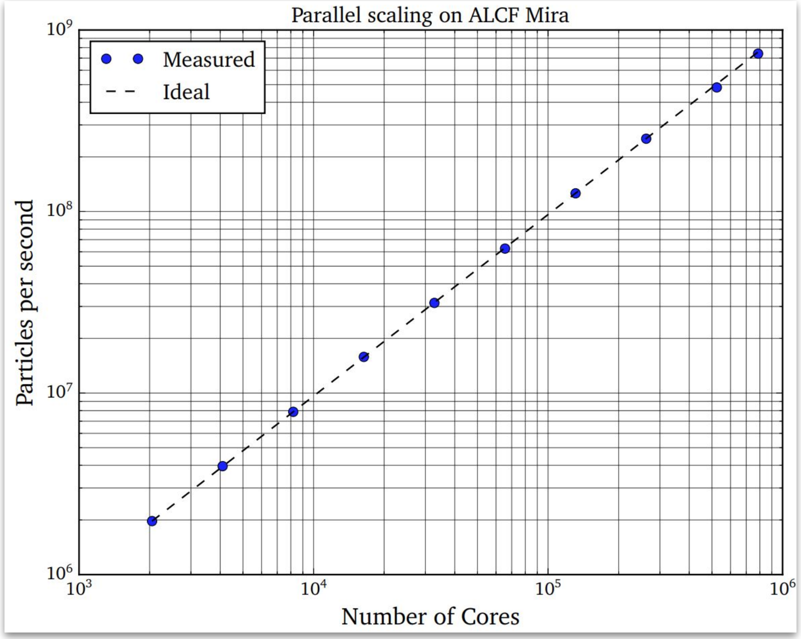
Technical Meeting on the Development and Application of Open-Source Modelling and Simulation Tools for Nuclear Reactors

June 22nd, 2022

OpenMC

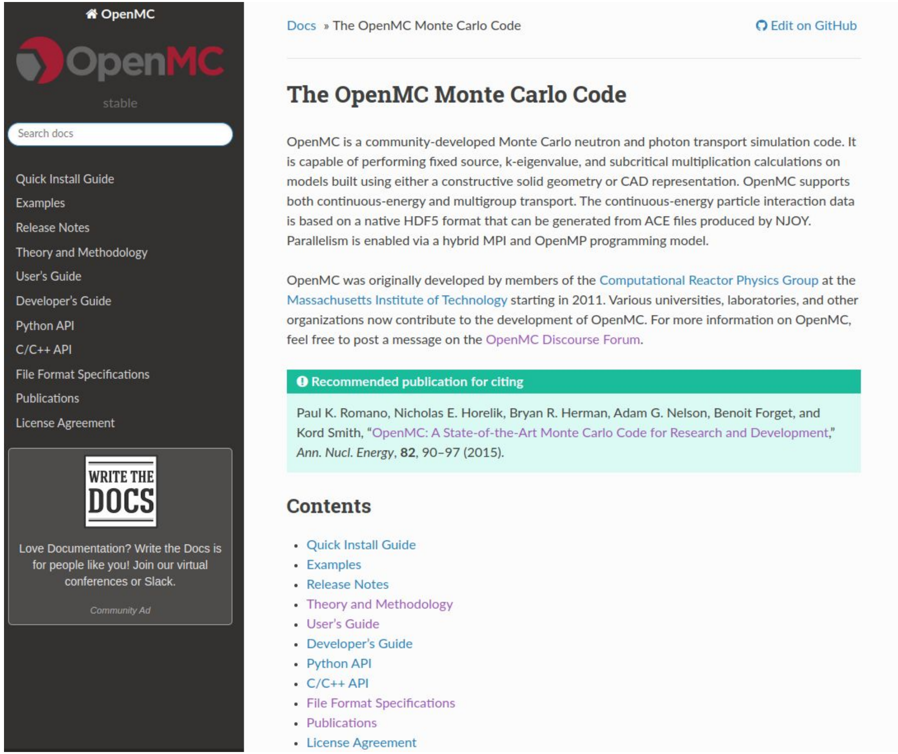
Open-source Monte Carlo Particle Transport

- C/C++ and Python APIs
- Parallel Performance
- Nuclear data interface
- Plotter
- Depletion
- CAD-based geometry
- Community driven
- Technical Committee
    - Paul Romano
    - Ben Forget
    - Adam Nelson
    - Sterling Harper



OpenMC

- Mixed **C++** and **Python** codebase
- **CMake** build system
- Distributed memory parallelism: **MPI**
- Shared memory parallelism: **OpenMP**
- Version control: **git**
- Project management: [GitHub]
- CI: [GitHub actions]
- Documentation: [Read the Docs]



OpenMC C/C++ API for Multiphysics

- Initialize simulation
- Find cell/material at location (domain mapping)
- Create tallies
- Execute simulation
- Extract tally results
- Set cell temperatures and material densities
- Reset tallies/batches
- Re-running simulation
- Finalize simulation

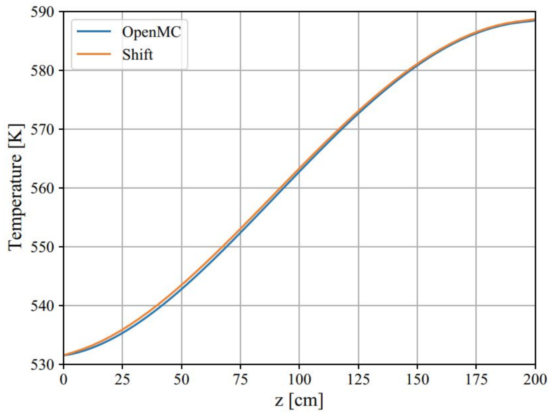
OpenMC Python C-API

Great example written by April Novak

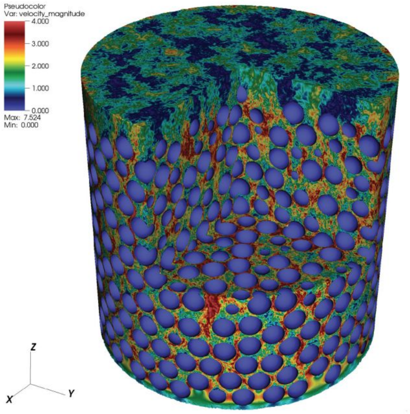
```
with openmc.lib.run_in_memory():
  for i in range(n_iterations):
    openmc.lib.reset()

    openmc.lib.run()

    # ---- Multiphysics feedback part ---- #

    # get the total kappa fission computed by OpenMC over the entire domain
    total_kappa_fission = openmc.lib.tallies[1].mean

    # power (W) in each layer of the solid
    q = np.zeros(N)

    for j in range(N):
      q[j] = openmc.lib.tallies[2].mean[j] / total_kappa_fission

      # to get in units of W, multiply by the total power
      q[j] *= power

      # for greater than the first iteration, relax
      if (i > 0):
        q[j] = (1.0 - alpha) * q_iterations[i - 1][j] + alpha * q[j]

    # compute the fluid temps, fluid densities, and solid temps
    fluid_temps = part3_backend.fluid_temperature(q, T_inlet, N)
    fluid_densities = part3_backend.fluid_density(fluid_temps, N)
    solid_temps = part3_backend.solid_temperature(q, fluid_temps, N, R, Rf, H)
```

Multiphysics Endeavors

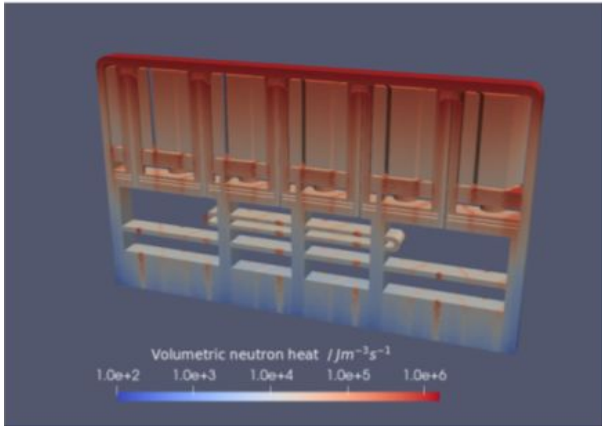
ENRICO



CARDINAL



AURORA



Common Characteristics

- In-memory coupling
- High fidelity
- Highly scalable
- Open-source

ENRICO

Exascale Nuclear Reactor Investigative COde

- DOE Exascale Computing Project
- Collaboration between ANL and ORNL
- Goal:

  Demonstration of a full core SMR multiphysics simulation on an exascale platforms

ENRICO: Solvers

"[A Code-Agnostic Driver Application for Coupled Neutronics and Thermal-Hydraulic Simulations]"
Romano, Hamilton, et. al.

Neutronics:

OpenMC

SHIFT

Thermal Hydraulics:

Nek5000

NekRS

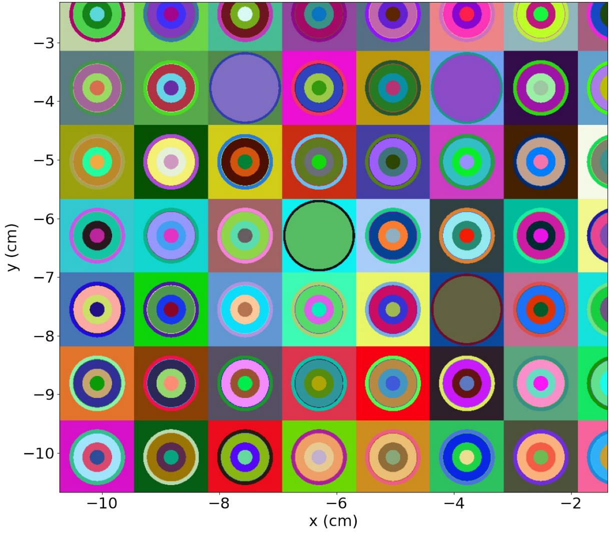
TH Surrogate Model

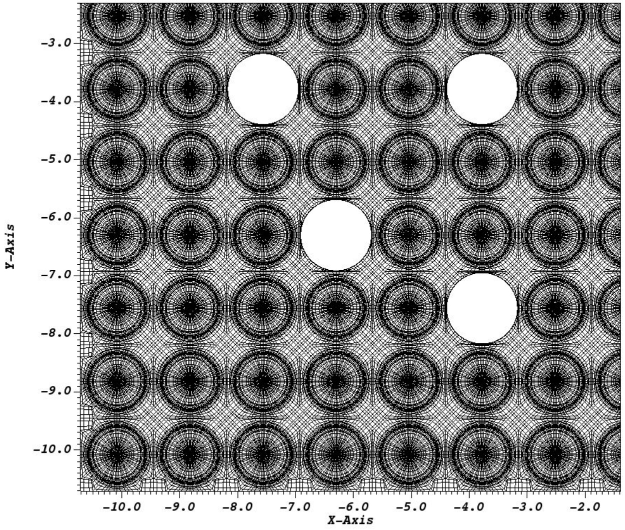
OpenFOAM*

*unmerged

ENRICO: Domain Mapping

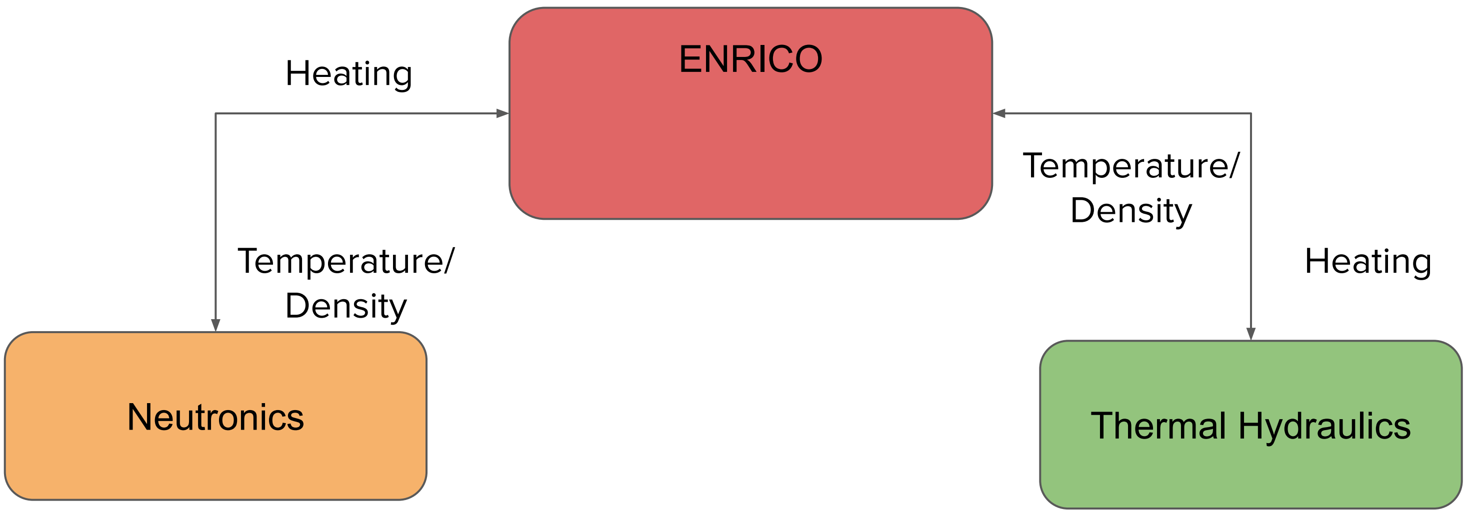
- Expected that CSG and TH mesh regions approx. match
- One CSG cell to many TH element mapping (largely automated)



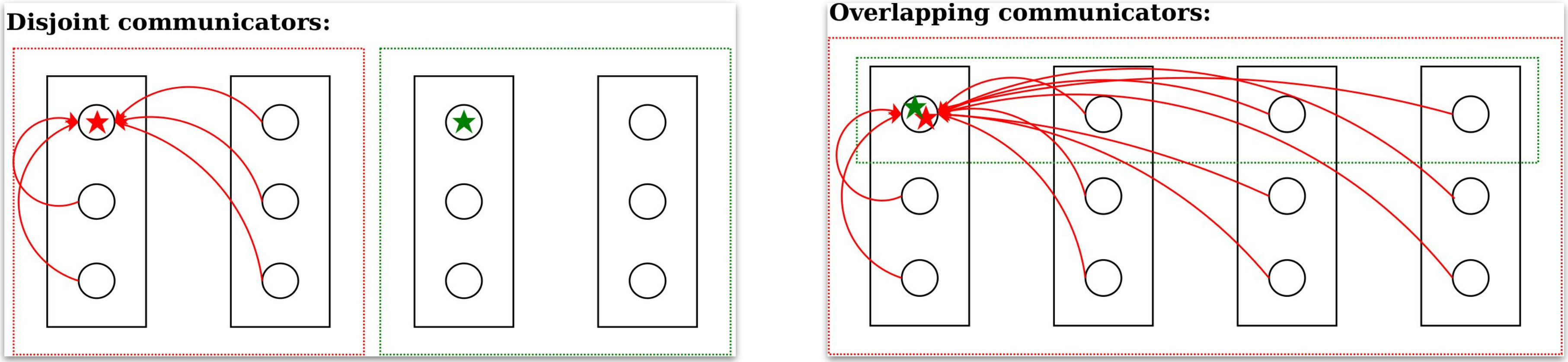


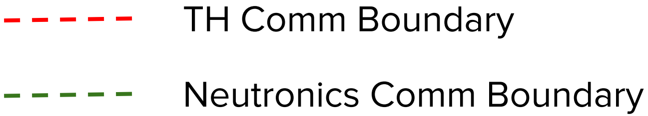
OpenMC Argonne NATIONAL LABORATORY

ENRICO: Information Flow

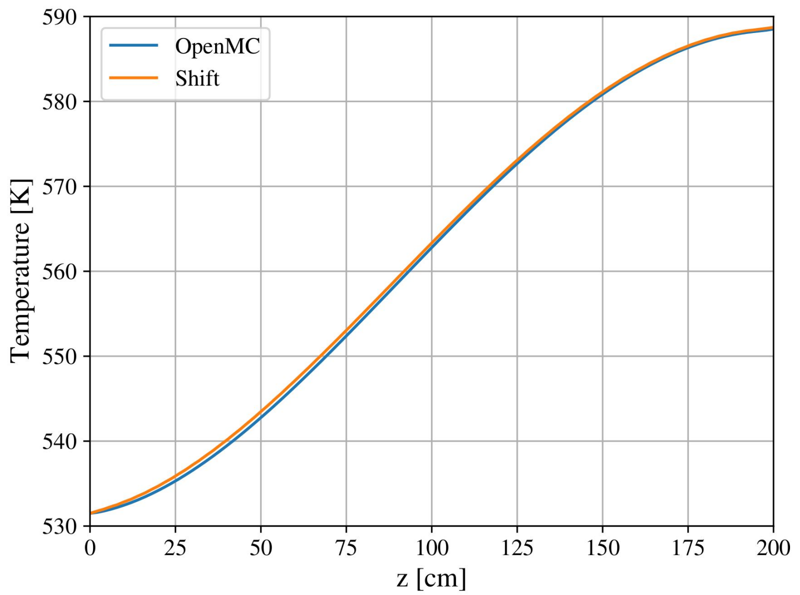


ENRICO: MPI Communication





ENRICO: 17 x 17 Assembly



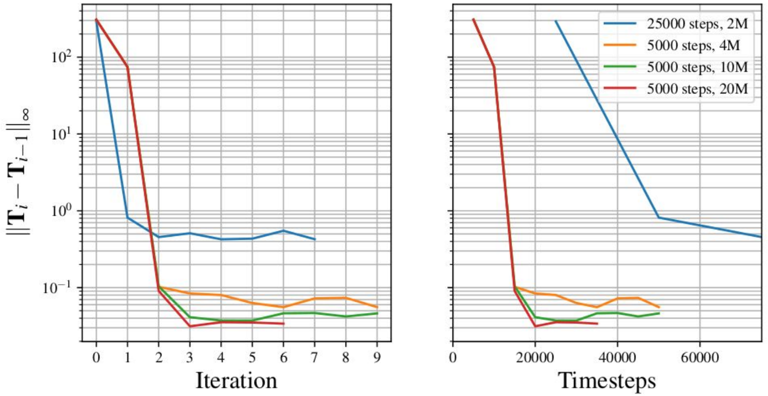


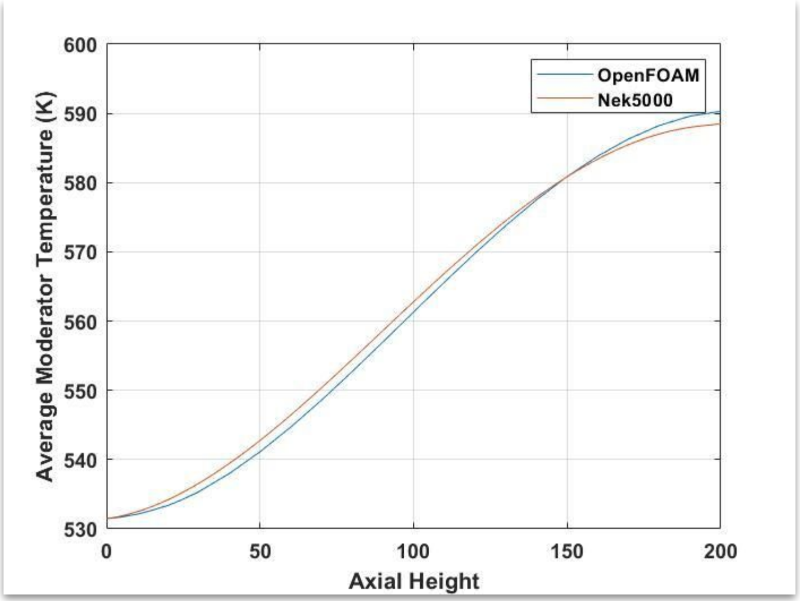
Fig. 6. Convergence of the temperature distribution on the short model as a function of iterations (left) and Nek5000 timesteps (right).

ENRICO: OpenFOAM

"[Coupled OpenFOAM and OpenMC for high-fidelity multiphysics reactor core simulations]"
Bullerwell, Hou, et. al.

Table IV. Global Differences in Heat Generation Rate Distributions

Relative RMS Difference	Absolute RMS Difference (W/cm^3)	Max Relative Difference	Max Absolute Difference (W/cm^3)
0.945721%	2.151217	2.349505 %	5.042066



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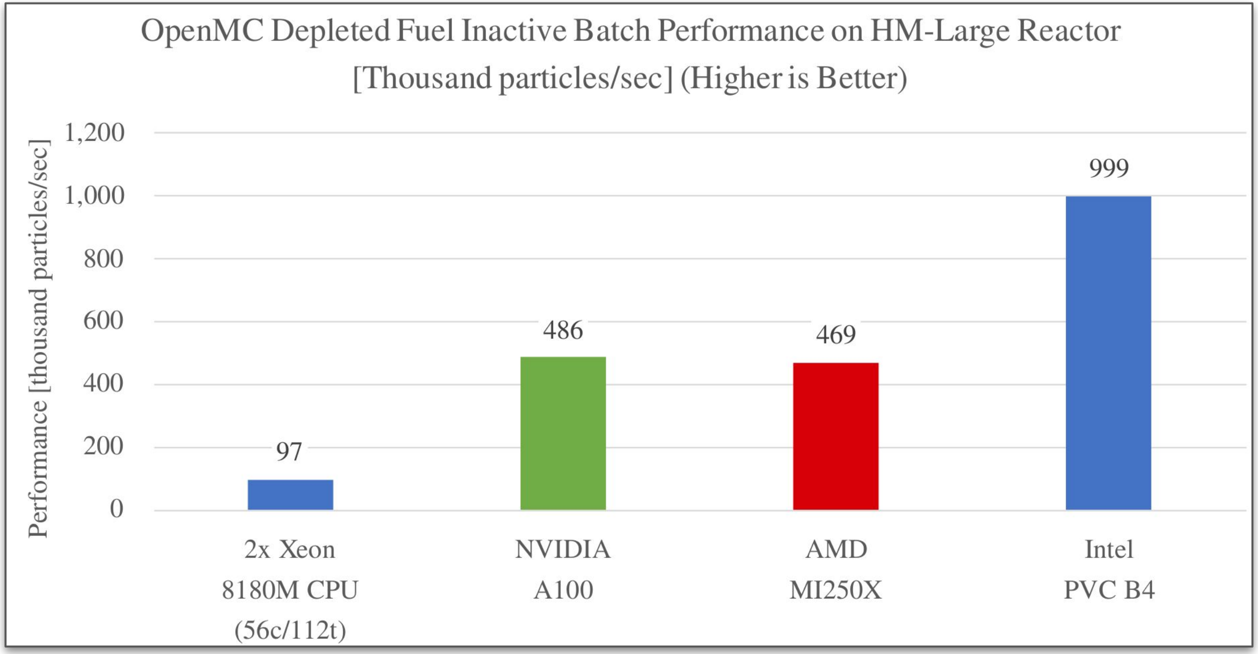
ENRICO: GPU Offloading



"[Toward Portable GPU Acceleration of the OpenMC Monte Carlo Particle Transport Code]"
John Tamm et. al.

Cardinal

CARDINAL

- A MOOSE app
- Collaboration between ANL, INL, UIUC, and Penn. State
- Project Lead: April Novak
- Goal:

  Advanced reactor multiphysics simulator

  - HTGC-PBR
  - SFR
  - PGCR

Cardinal: Solvers

"A Code-Agnostic Driver Application for Coupled Neutronics and Thermal-Hydraulic Simulations"
Romano, Hamilton, et. al.

Neutronics:

OpenMC

Heat Conduction:

MOOSE Heat Conduction

Thermal Hydraulics:

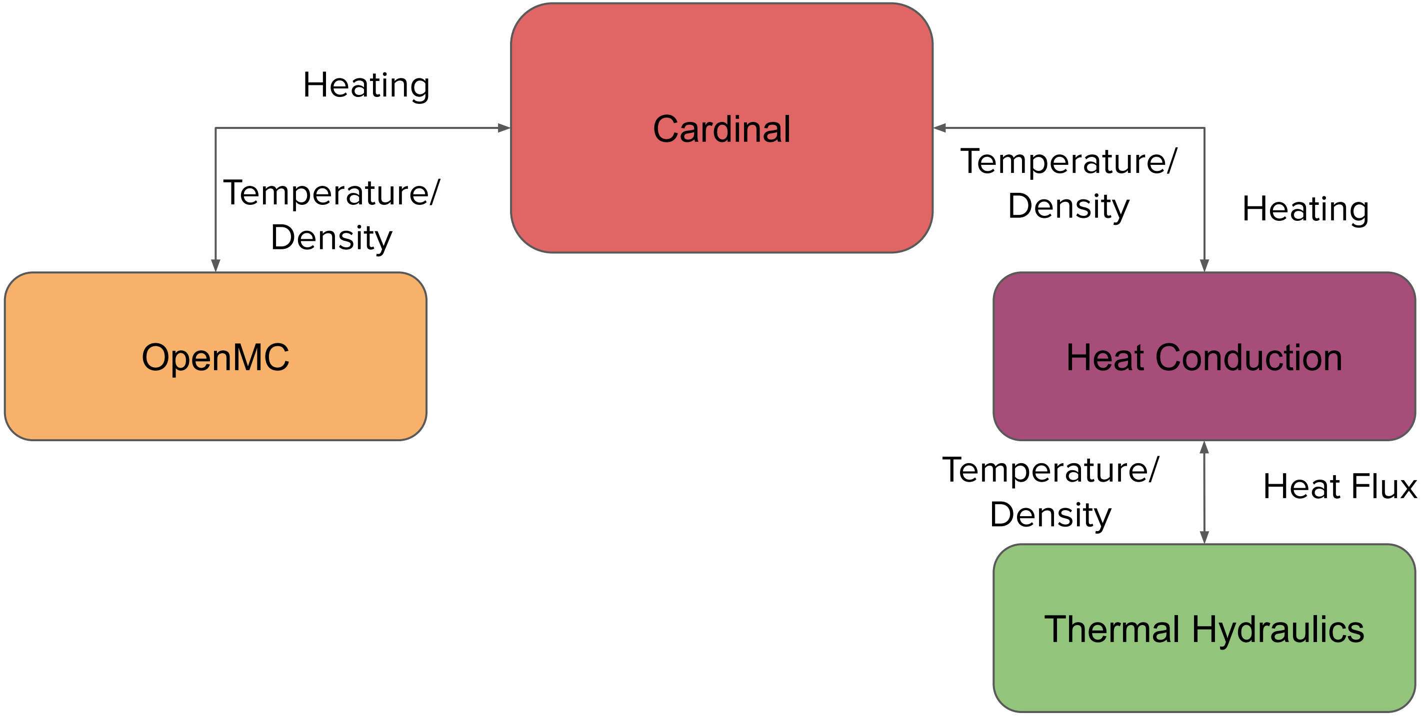
NekRS

MOOSE THM

Other MOOSE Apps:
SAM, Sockeye, BISON, etc.

*unmerged

Cardinal: Information Flow



Cardinal: Domain Mapping

Same as ENRICO – “one neutronics cell to many TH element” approach with automated mapping

- Fluid (T, ρ) vs. solid regions (T) are specified on the MOOSE mesh
- Higher levels in the OpenMC geometry can be specified
- Unstructured mesh tallies to perform one-to-one element transfers

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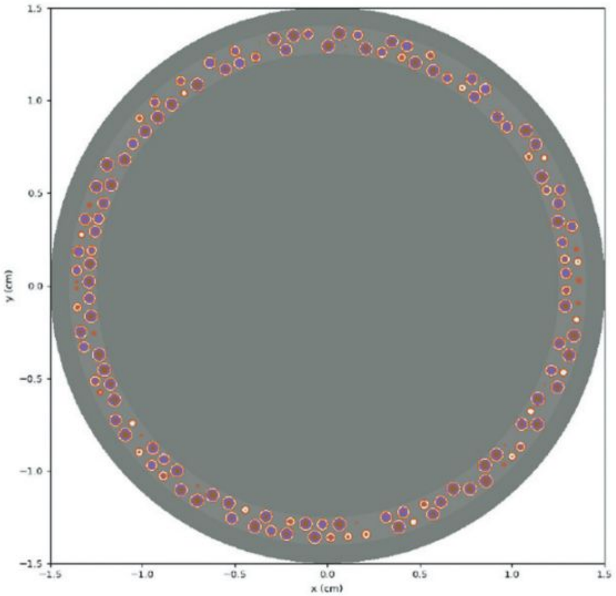
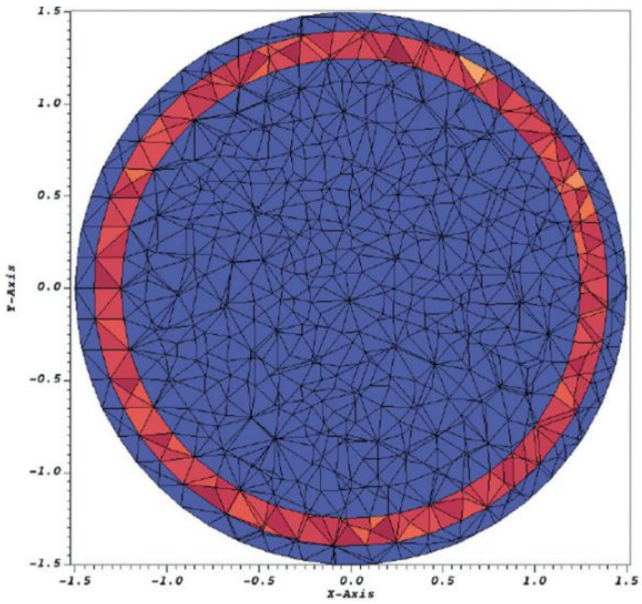
Cardinal: Unstructured Mesh Tallies





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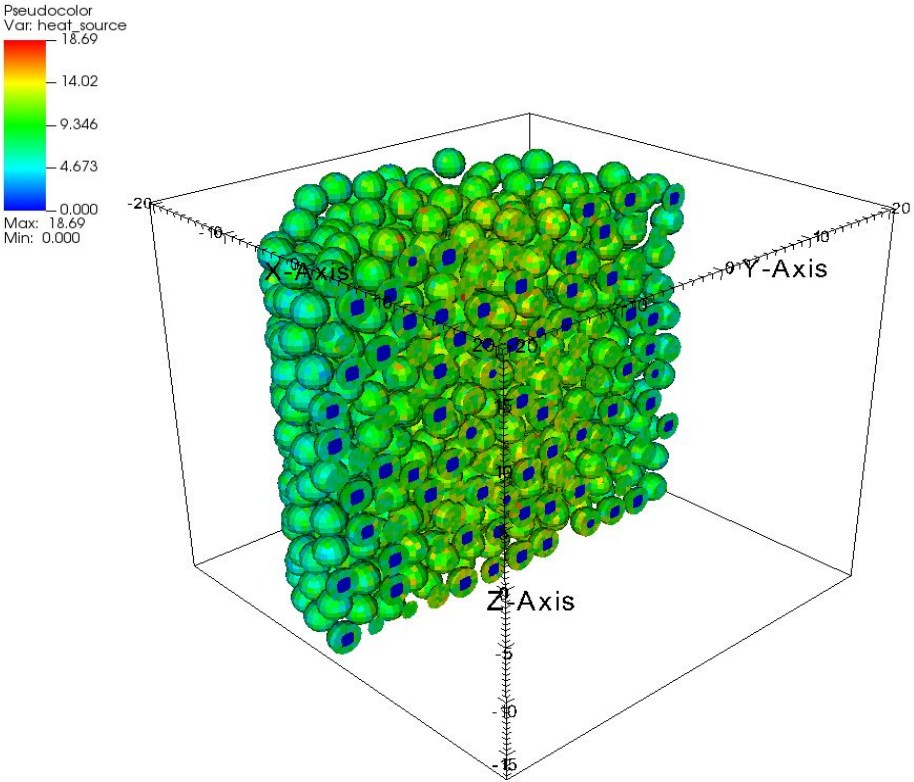
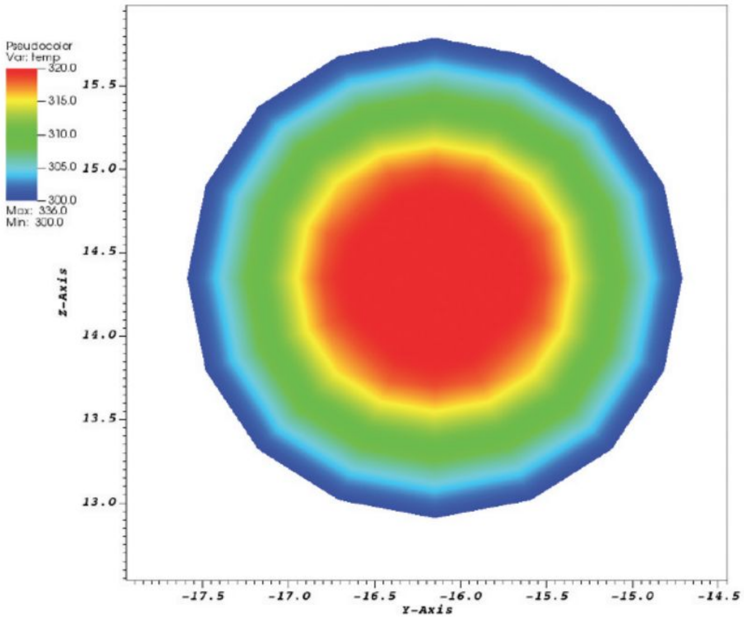
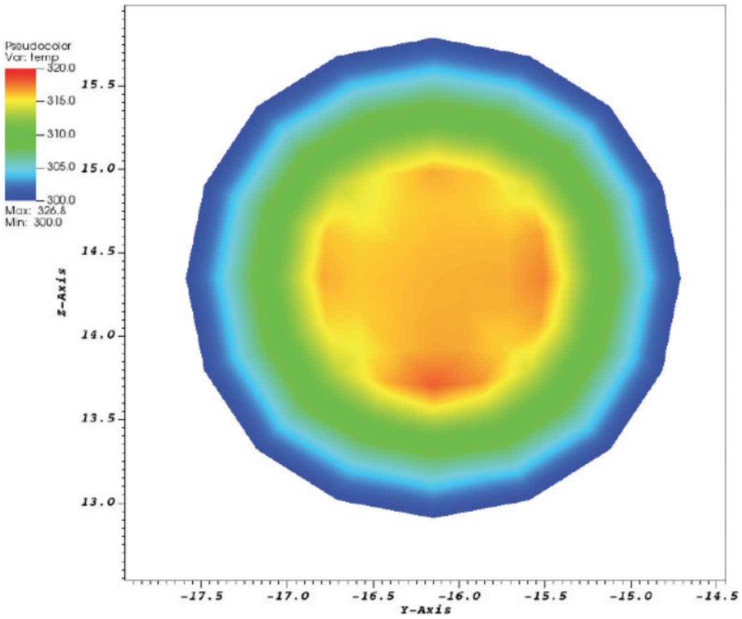
Cardinal: PBR Simulation



Cardinal: Unstructured Mesh Tallies



Cell Tally



Unstructured Mesh Tally

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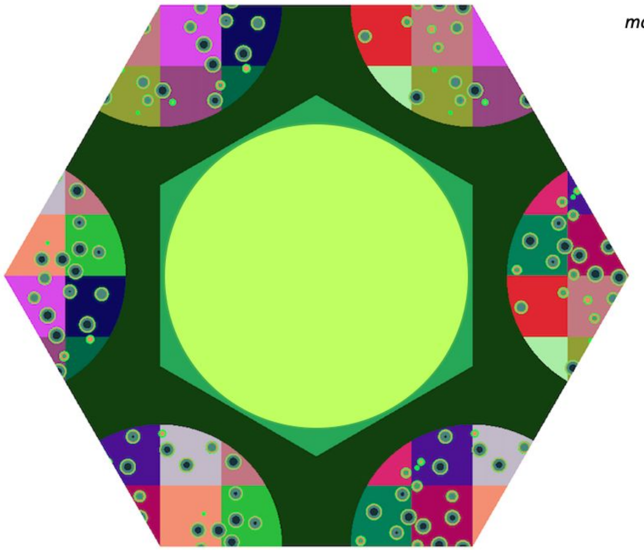
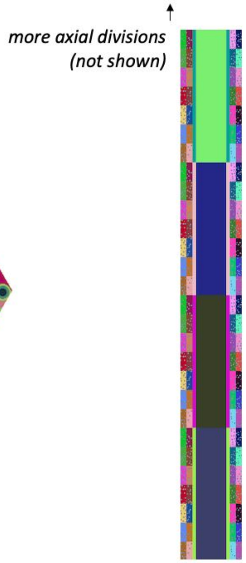
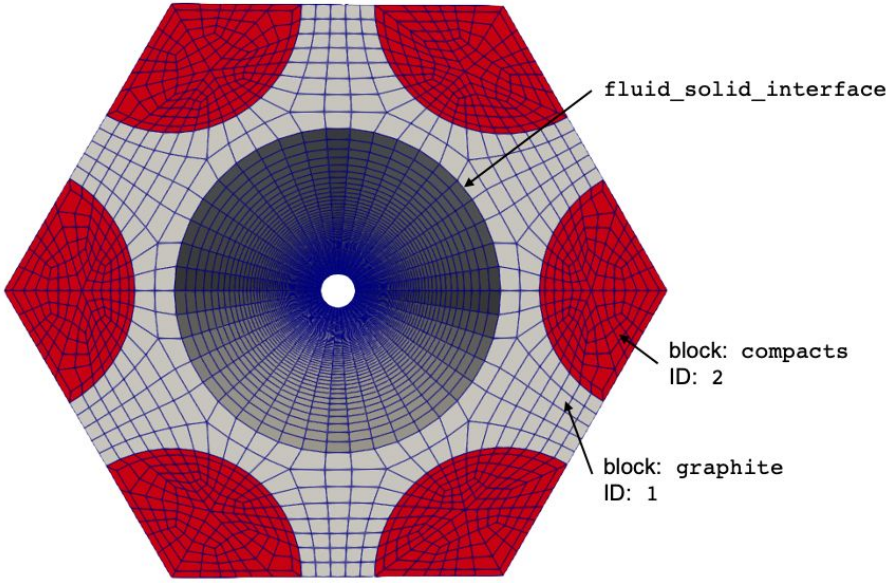
Cardinal: Domain Mapping



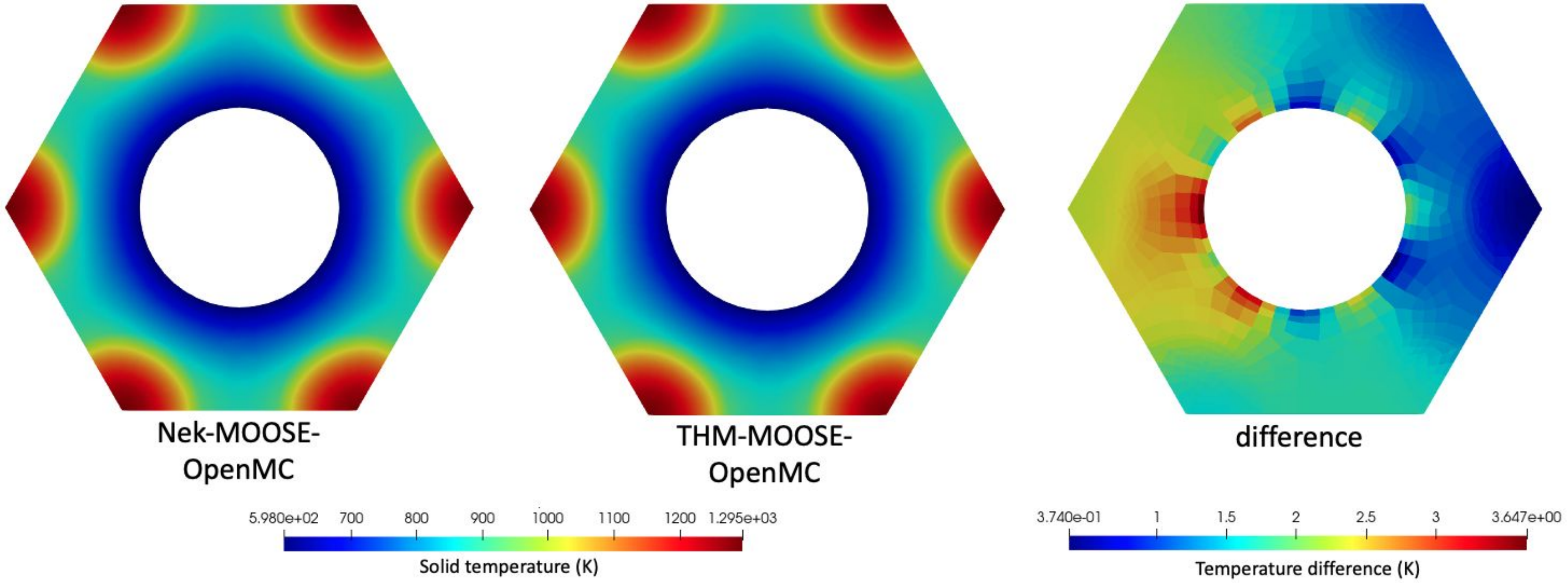
$x - y$ view



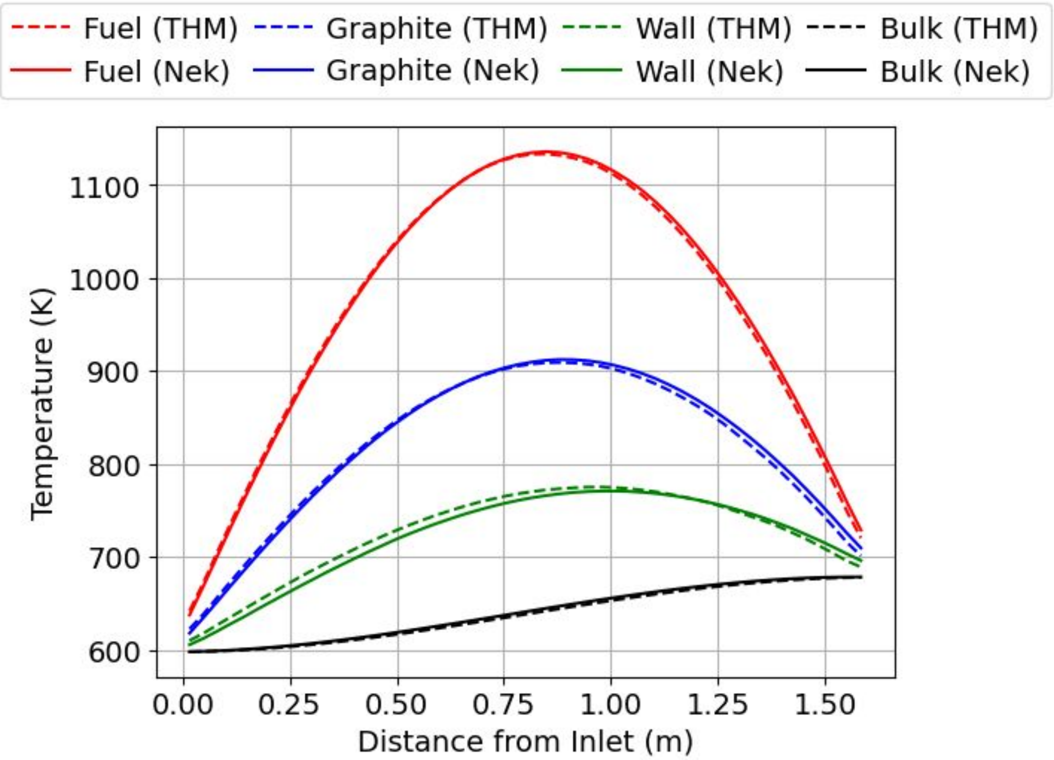
$x - z$ view



Cardinal: Results

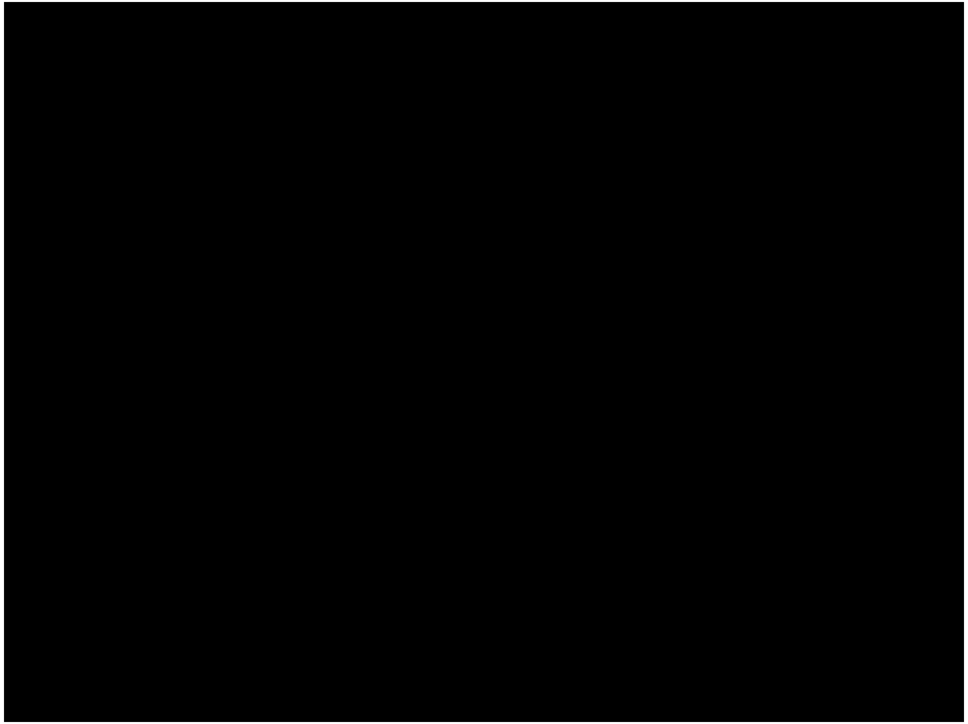


Cardinal: Results



Cardinal: Tracer Simulation

Aaron Huxford
University of Michigan
June 2022



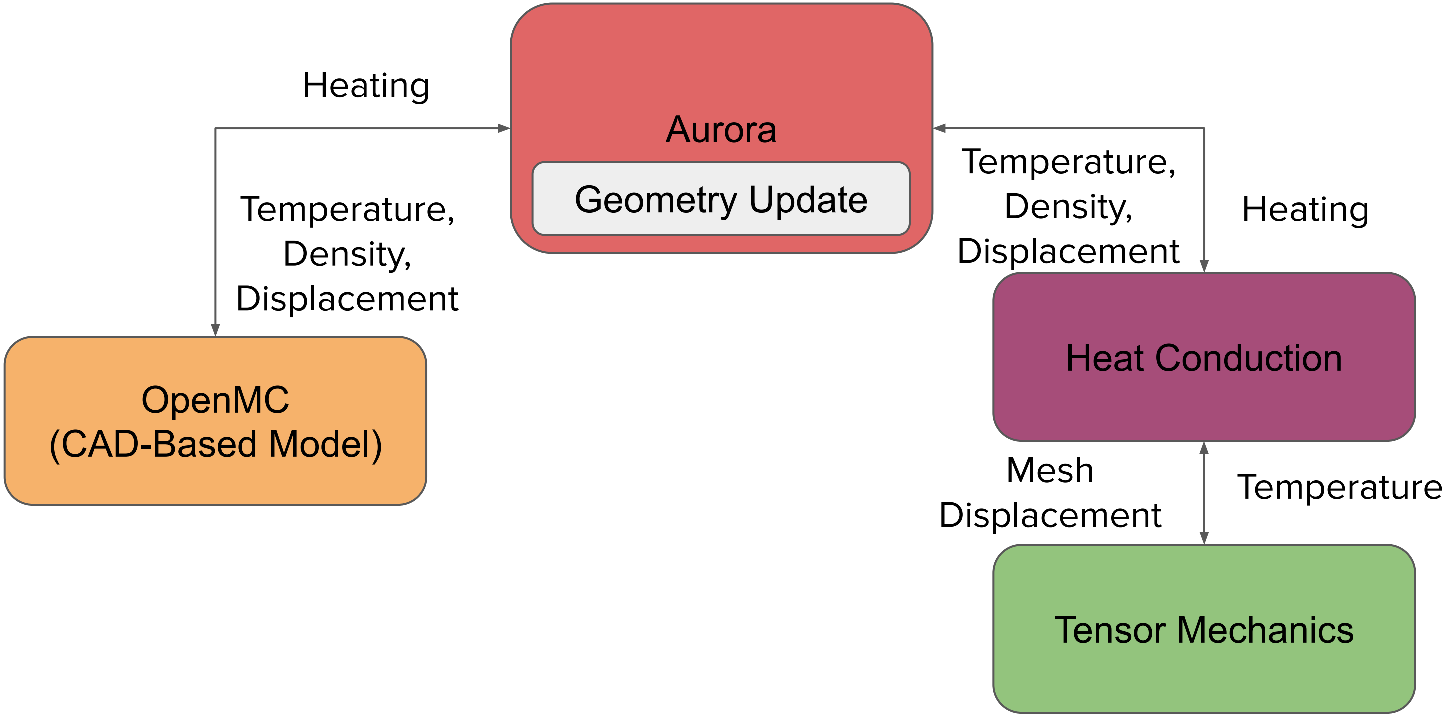
Aurora

AURORA

- A MOOSE app produced by the UKAEA
- Project Leads: Helen Brooks, Andrew Davis
- Goal

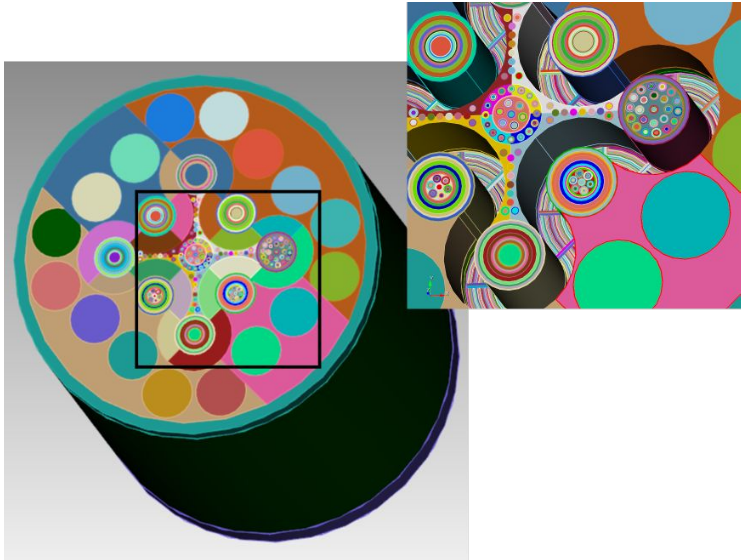
  Multiphysics simulation of components in fusion environments

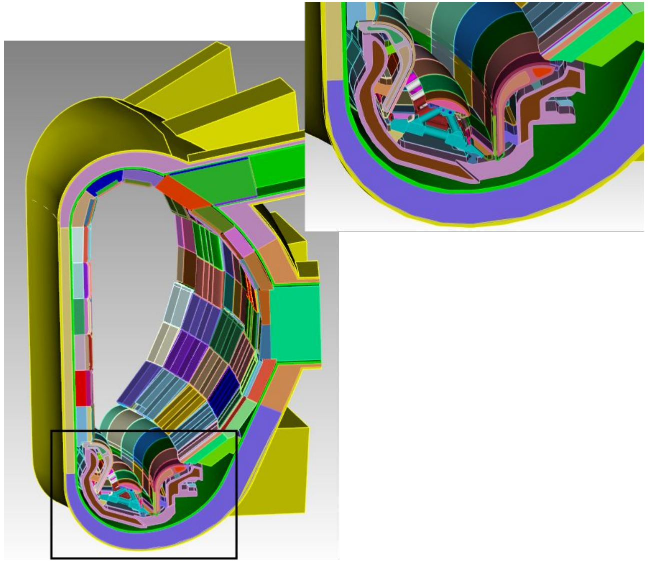
Aurora: Information Flow



Aurora: DAGMC

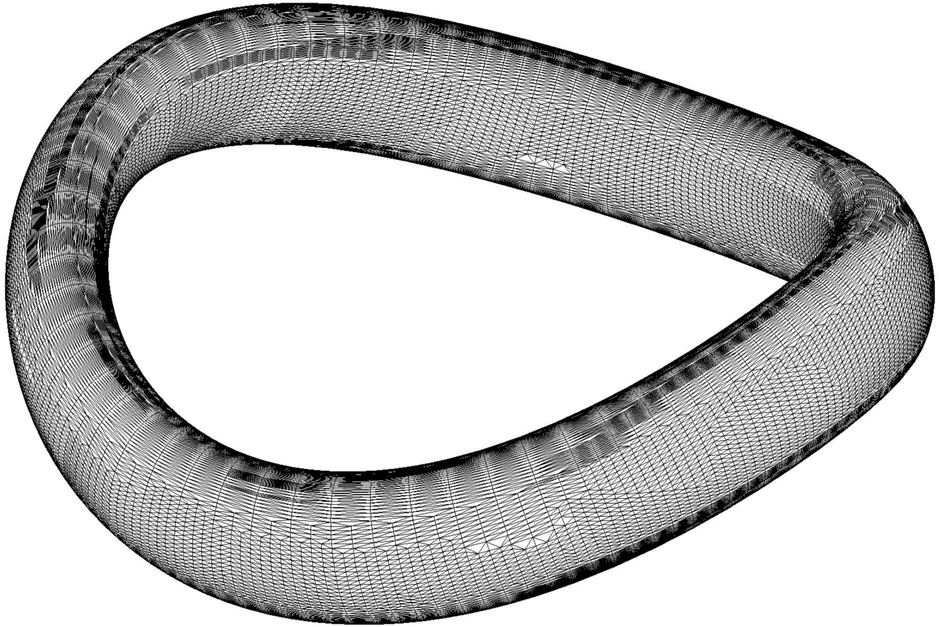
Monte Carlo particle transport on surface tessellations of CAD geometry



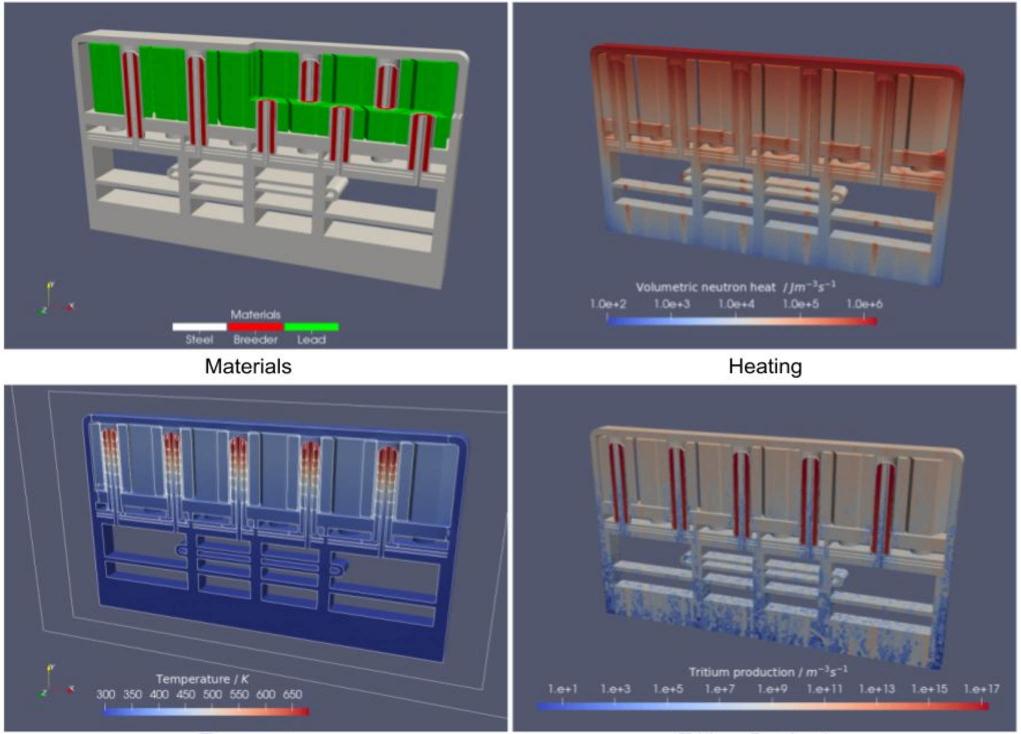


Aurora: DAGMC

Monte Carlo particle transport on surface tessellations of CAD geometry



Aurora: Application



Materials Heating

Temperature Tritium Production

Multiphysics Testing

OpenMC's C/C++ API now contains functions that are purely for multiphysics. Where does testing belong?

Answer is still unclear. Some are tested in OpenMC, some are tested in multiphysics apps themselves.

Acknowledgements

OpenMC

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

WISCONSIN UNIVERSITY OF WISCONSIN–MADISON

Massachusetts Institute of Technology

PennState

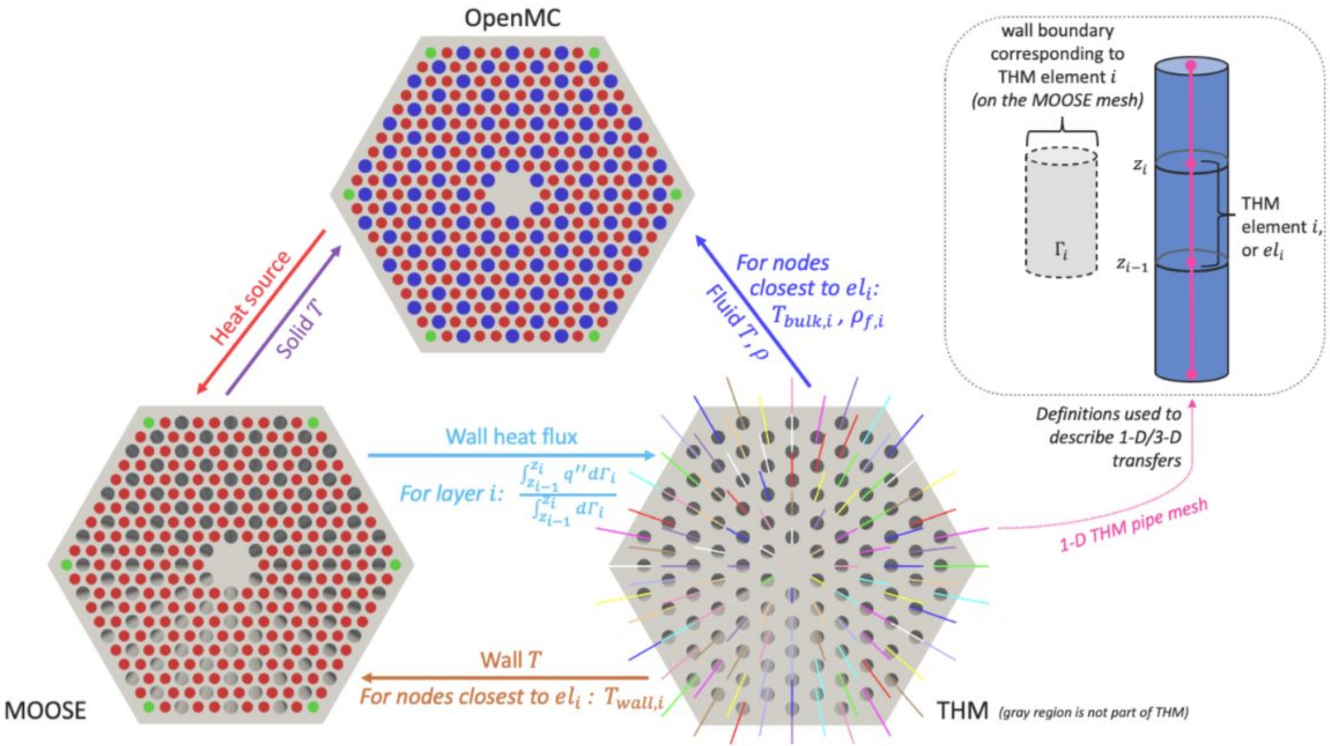
INL Idaho National Laboratory

UK Atomic Energy Authority

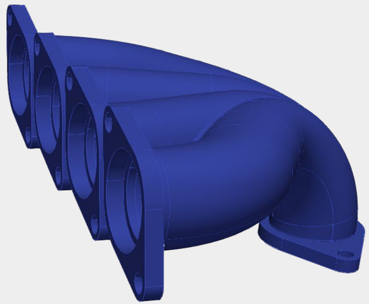
Argonne NATIONAL LABORATORY

Thank you!

Cardinal: Information Flow

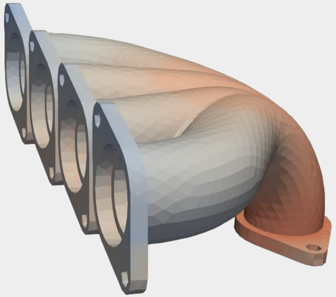


Aurora: Neutronics Model Updates



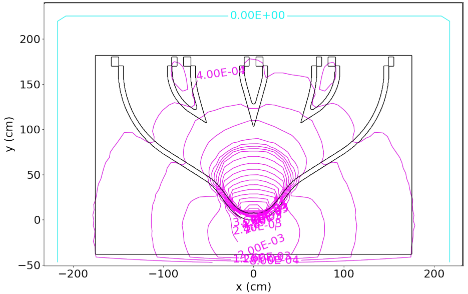
CAD Model

Run OpenMC w/ unstructured mesh tally



Unstructured Mesh Tally Result

External Physics Kernels



Generate new DAGMC Surfaces/Cells