

Cardinal: Integrating OpenMC and NekRS with the MOOSE Ecosystem

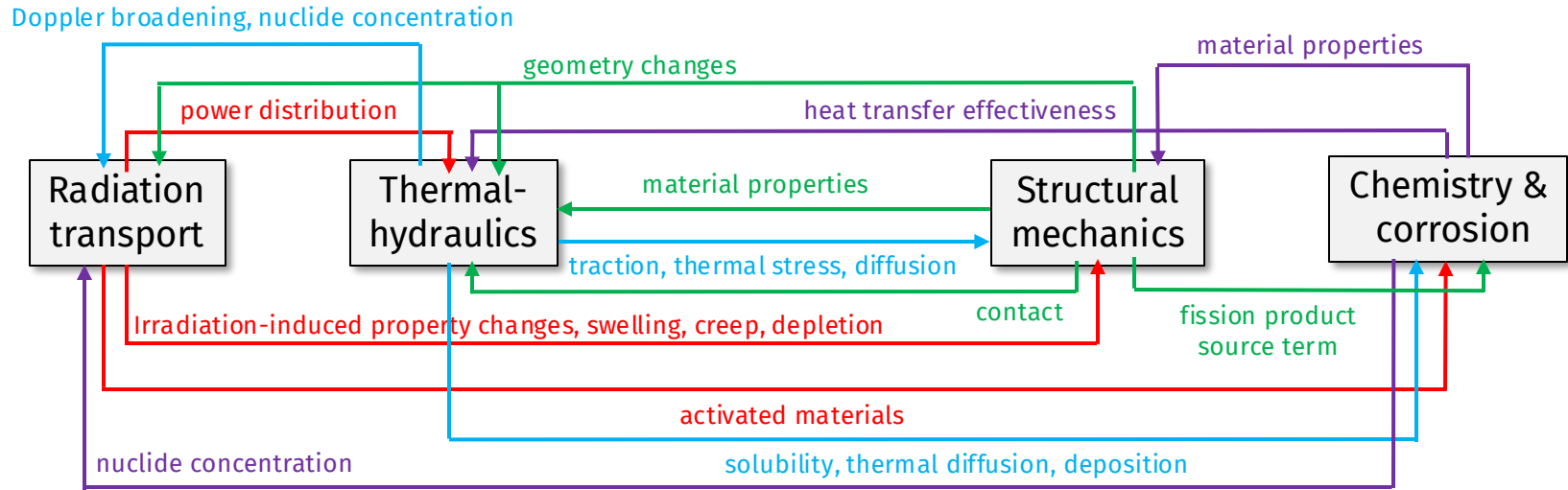
April Novak

Assistant Professor
Nuclear, Plasma, and Radiological Engineering (NPRE)
University of Illinois, Urbana-Champaign

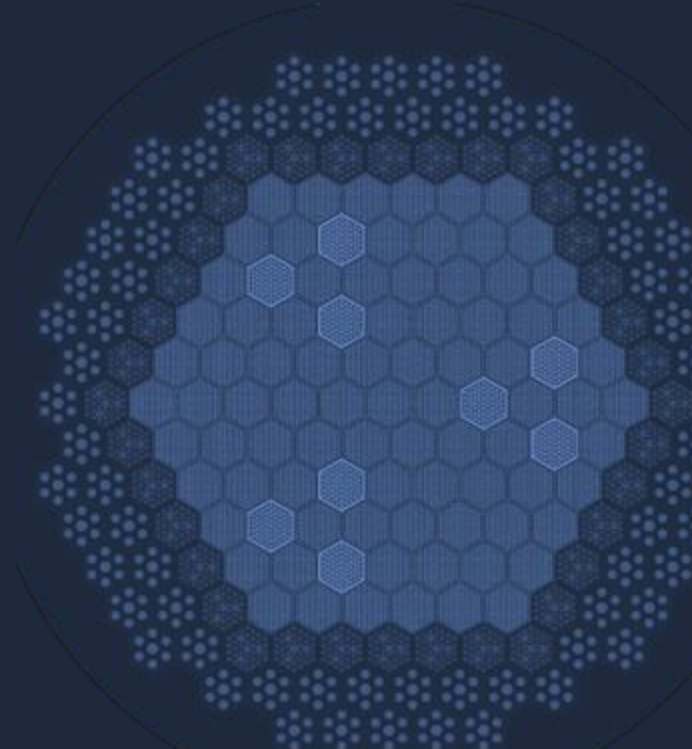
Joint Appointment, Nuclear Science and Engineering (NSE) Division
Argonne National Laboratory

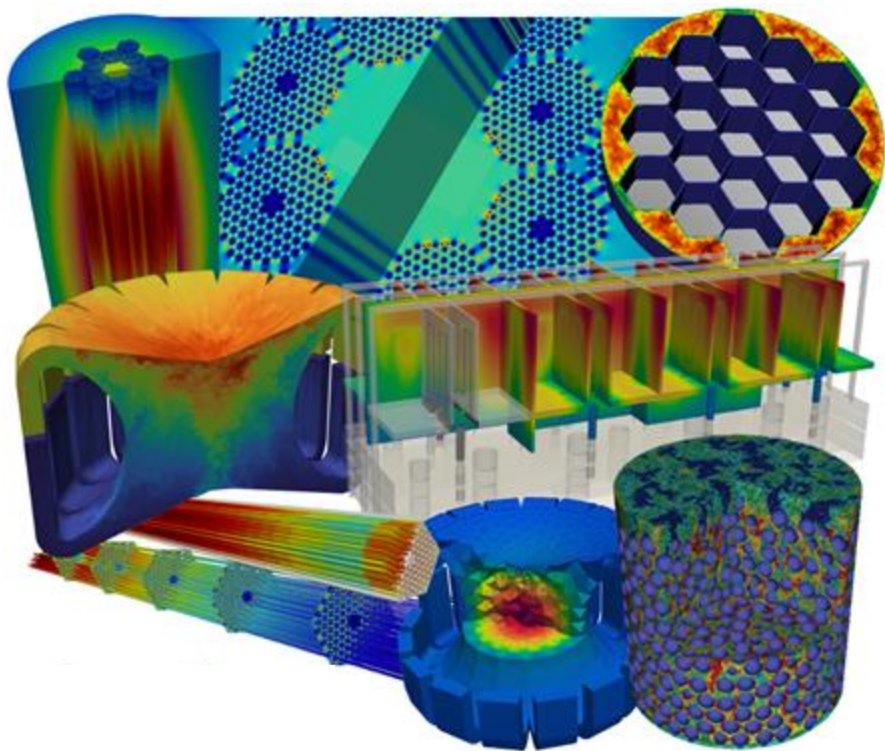


Multiphysics/Multiscale Analysis



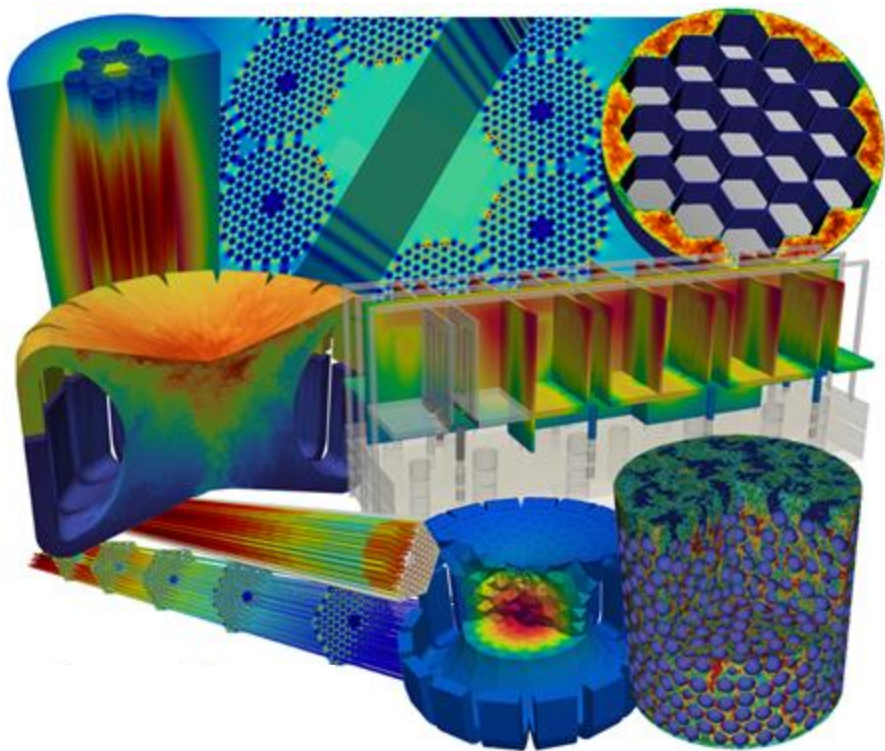
- Introducing the Cardinal software application: MOOSE, NekRS, OpenMC
- Fusion & fission application examples





Cardinal

- Open-source multiphysics coupling of **OpenMC** and **NekRS** with **MOOSE**
- Links high-fidelity radiation transport + CFD to MOOSE fusion ecosystem:
 - Plug-and-play multiphysics/scale coupling
 - Obtain reference solutions for benchmarking
 - Develop constitutive models (e.g., heat transfer coefficients, multigroup cross sections)
 - Advanced postprocessing and visualization



Cardinal

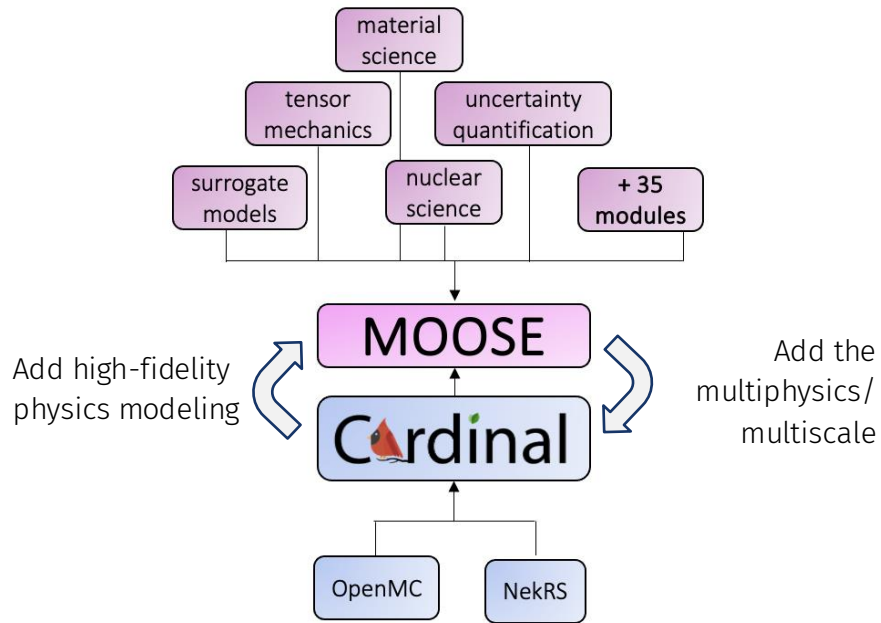
- Nuclear heating (e.g. power deposition)
- Composition changes (e.g. breeding)
- Shielding requirements
- Material activation, radioactive waste classification
- Material damage (dpa), gas production
- Non-proliferation analyses
- Diagnostics, sensor responses

OpenMC

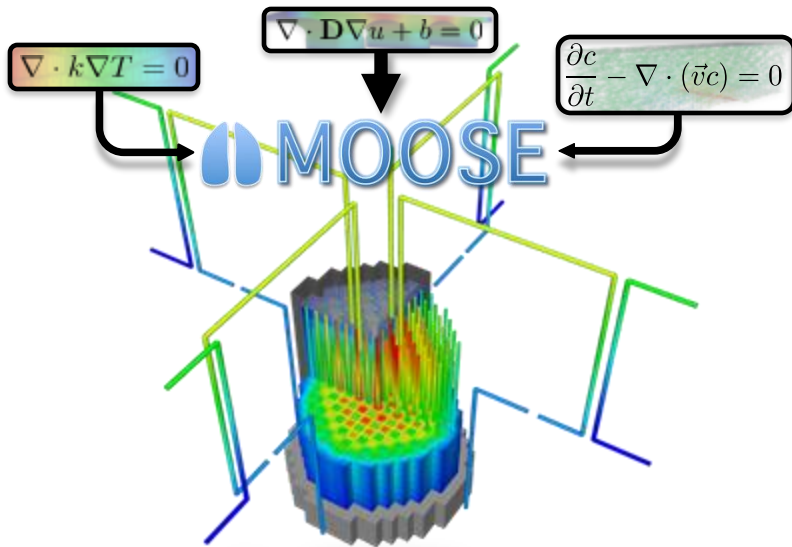
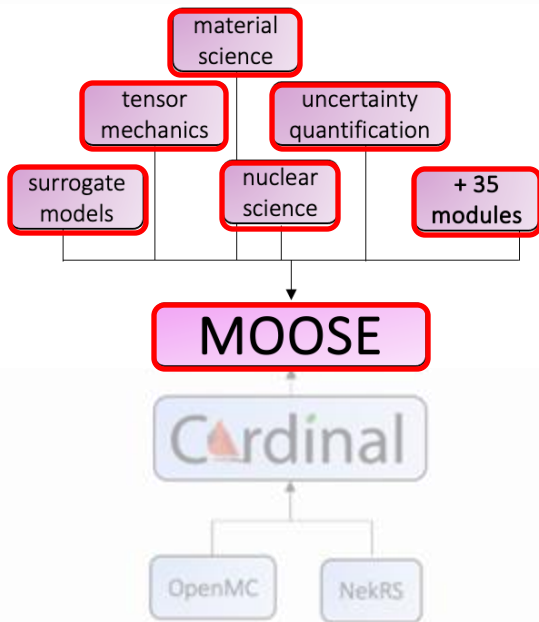
- Heat transfer and fluid flow
- Temperature and heat flux thermal limits
- Pressure losses and pumping power
- Passive scalar transport (e.g., mass transport)
- Magnetohydrodynamics
- Fluid-structure interaction

NekRS

Big-Picture: *Make OpenMC and NekRS seamlessly interoperable with MOOSE*

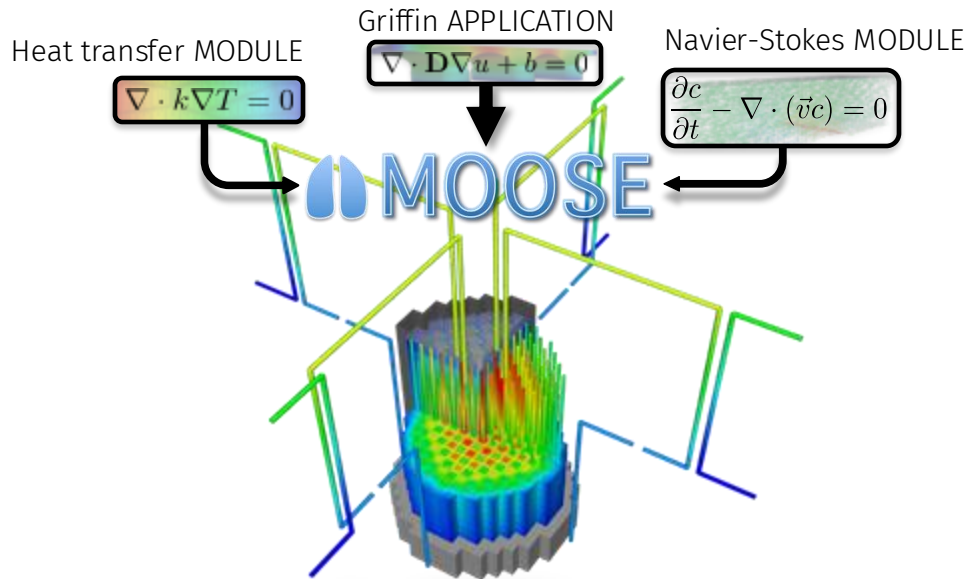
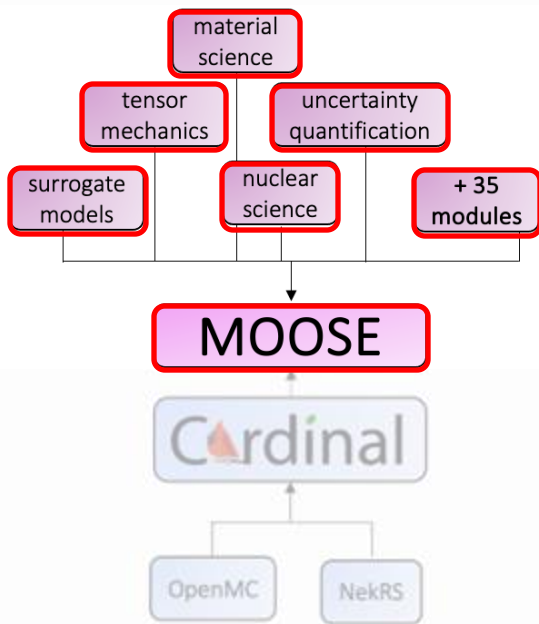


MOOSE



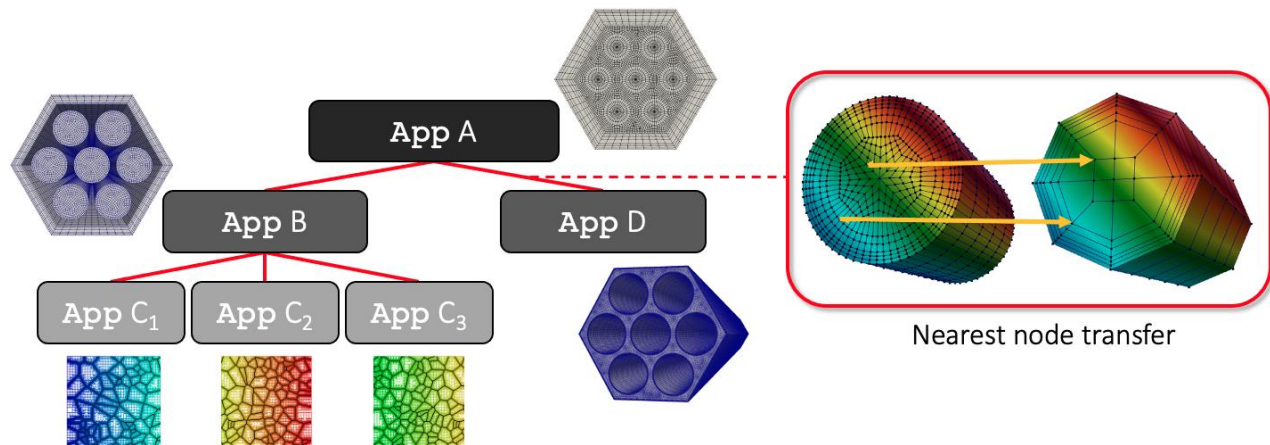
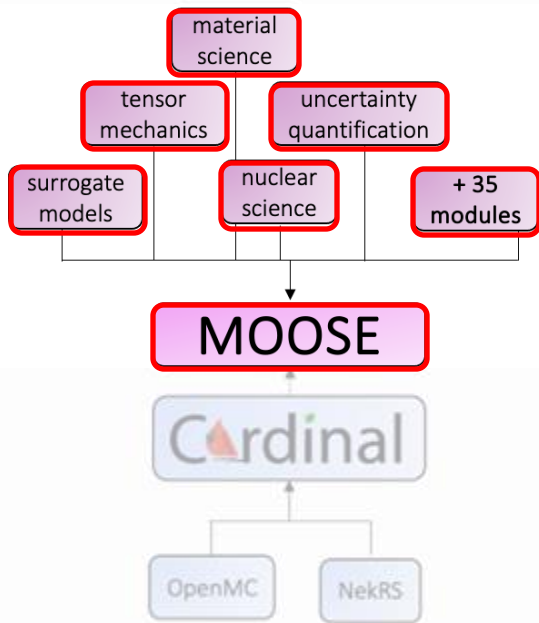
- Finite element/volume framework (Idaho National Lab)
- Plug-and-play framework for multi-scale/physics analysis
- NQA-1 (Nuclear Quality Assurance Level 1) compliant
- Used by numerous entities for nuclear analysis (private companies, R&D, U.S. Nuclear Regulatory Commission)

MOOSE



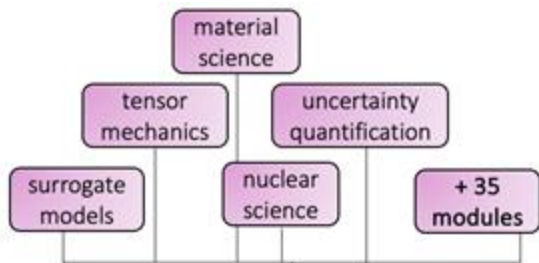
- **Framework:** complete platform of 40+ modular systems
 - Define the governing equation(s) of interest, with boundary/initial conditions
 - Specify constitutive models/closures
 - Couple equations together
 - Postprocess the solution
- **Modules:** common physics/engineering capabilities
- **Applications:** special-purpose physics capabilities

MOOSE MultiApps and Transfers



- Automatically parallel
- In-memory data transfers
- Arbitrary tree for simulations
- Flexible synchronization (unique time steps)

Big-Picture: *Add OpenMC and NekRS to the MOOSE “toolbox”*

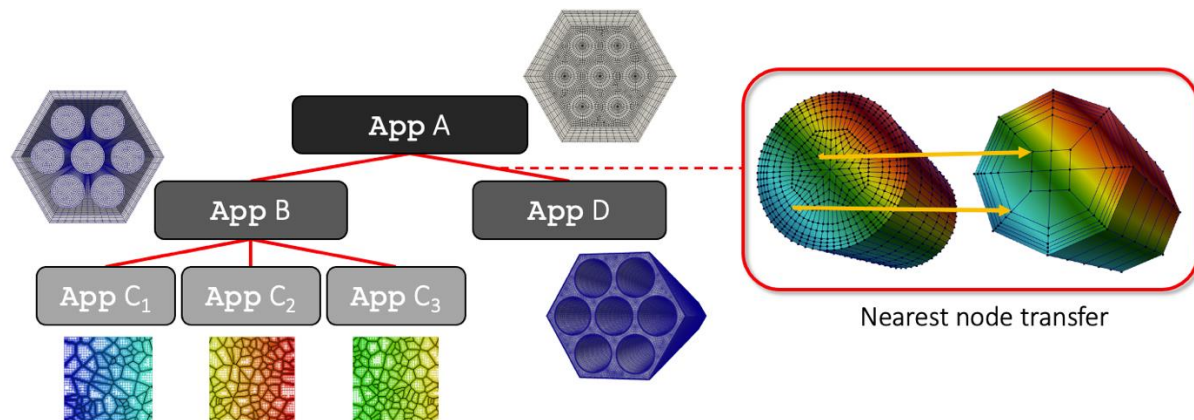


MOOSE

Cardinal

OpenMC

NekRS



Coupling framework



Physics applications

mesh-to-mesh data transfers

OpenMC neutron-photon transport

solution postprocessing

software QA

NekRS Navier-Stokes

mesh adaptivity

uncertainty quantification

TMAP8 tritium

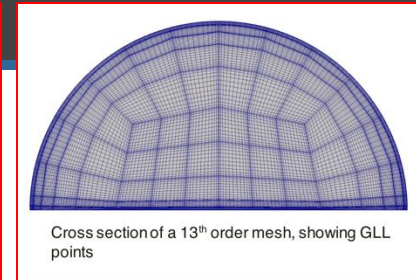
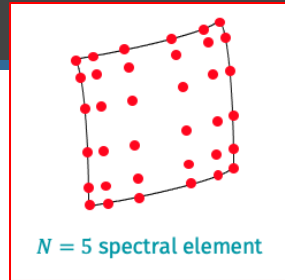
checkpointing

timestep control

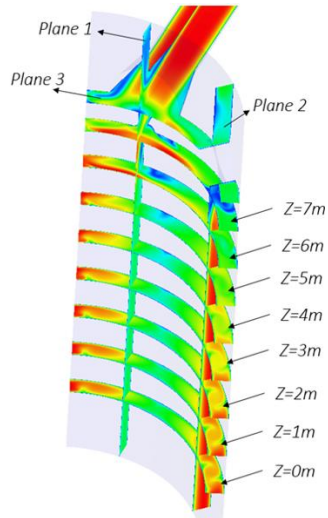
MOOSE thermomechanics

NekRS: *Physics and Numerical Method*

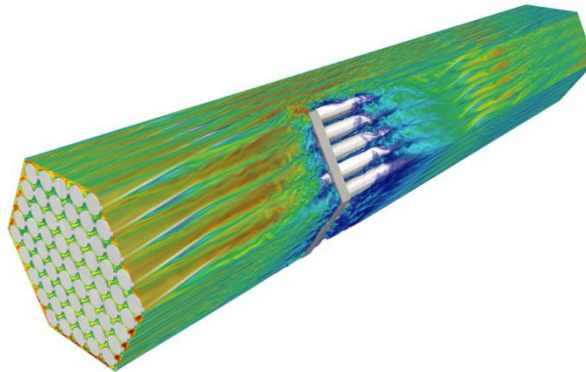
- Navier-Stokes solver for incompressible and low-Mach flows
 - **Turbulence:** $k - \tau$ RANS, High/low-pass LES filters, and DNS
 - **Runs on both CPU and GPU** and is **massively parallel**
 - New physics and solvers are under active development



- **Spectral element method:** nodal interpolants of GLL quadrature
 - Mesh with curvilinear hexahedral elements, typically use order 5–7
 - High-order has low numerical dissipation/dispersion well-suited to long time integrations and turbulence



RANS simulation of cold water injection
in a downcomer
image: Yiqi Yu



LES of a wire-wrapped pin bundle
image: Dezhi Dai

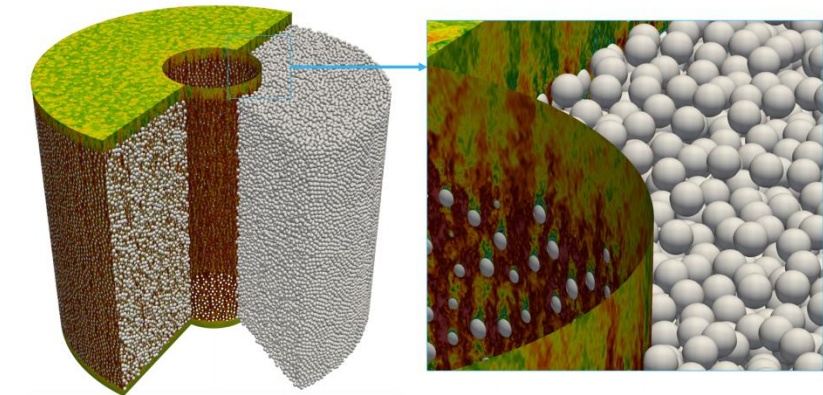
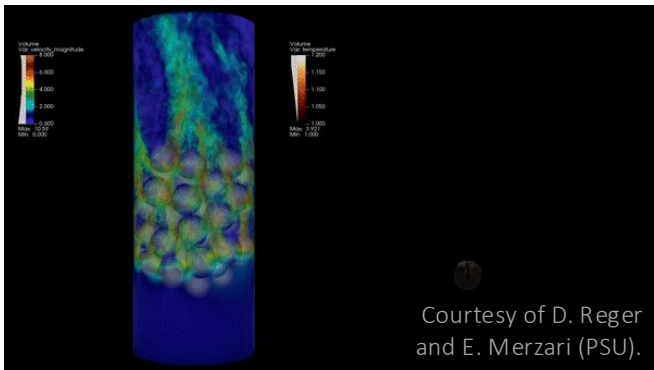
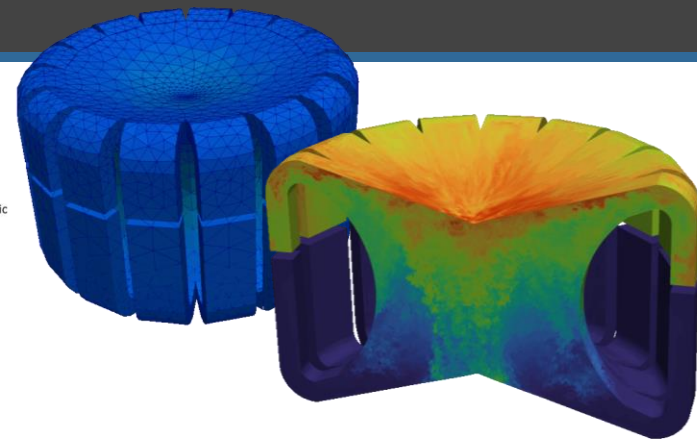
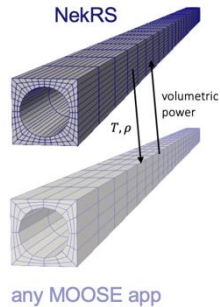
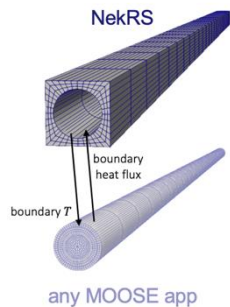


image: Misun Min (<https://ieeexplore.ieee.org/document/10046048>),
funded through the CEED program

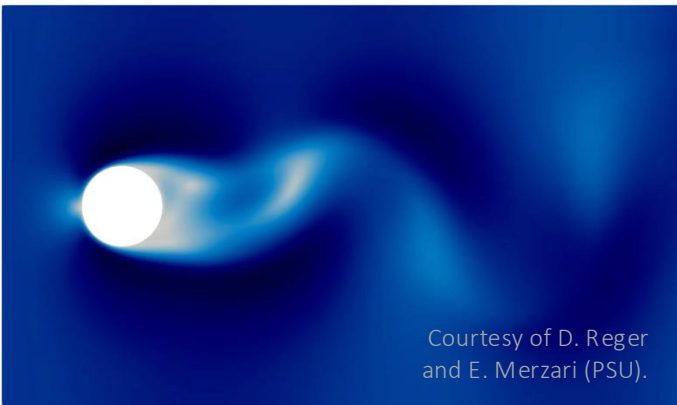
NekRS Coupling Modes



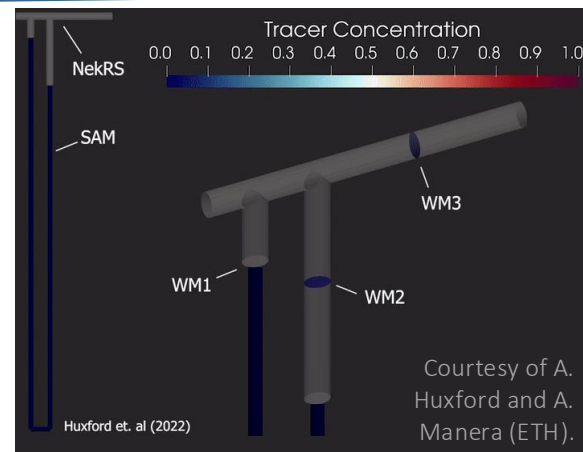
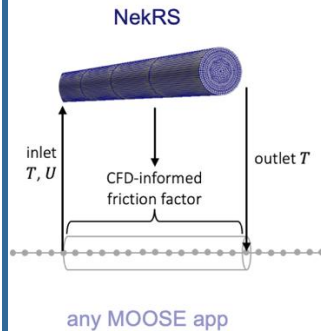
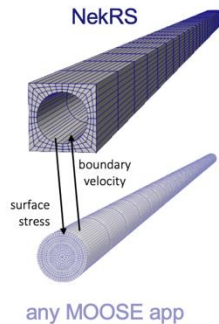
Conjugate heat transfer (NekRS + MOOSE heat transfer)



Neutronics coupling (NekRS + OpenMC)



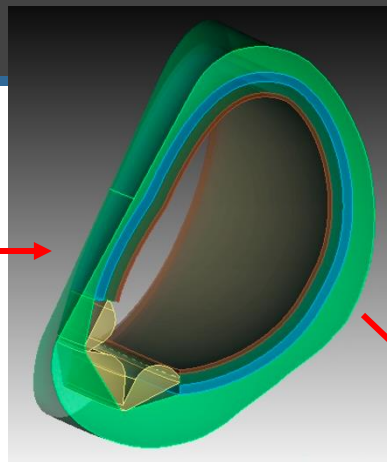
Fluid-structure interaction (NekRS + MOOSE solid mechanics)



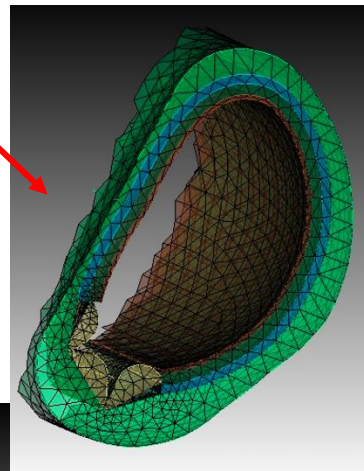
CFD-systems coupling (NekRS + SAM)

OpenMC

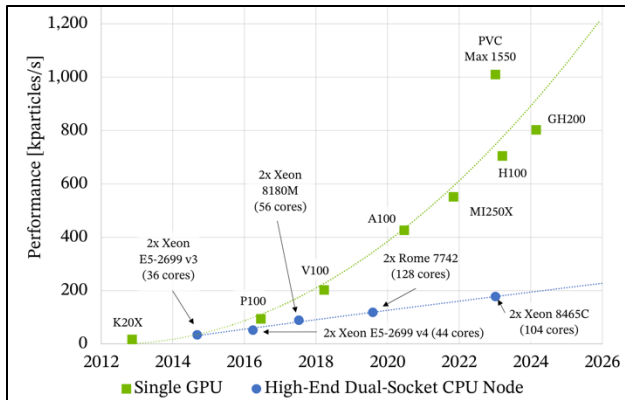
- **Monte Carlo neutron and photon** transport for k-eigenvalue and fixed source calculations; built-in depletion capabilities
- Geometry can be specified in either **unstructured mesh** (surface, volume) or **Constructive Solid Geometry** (CSG)
- **Runs on both CPU and GPU** and is **massively parallel**, scales from laptops to supercomputers
- First published Monte Carlo code to perform 1 million particles/s/GPU with transmuted/depleted materials



Section of a tokamak built using CAD.

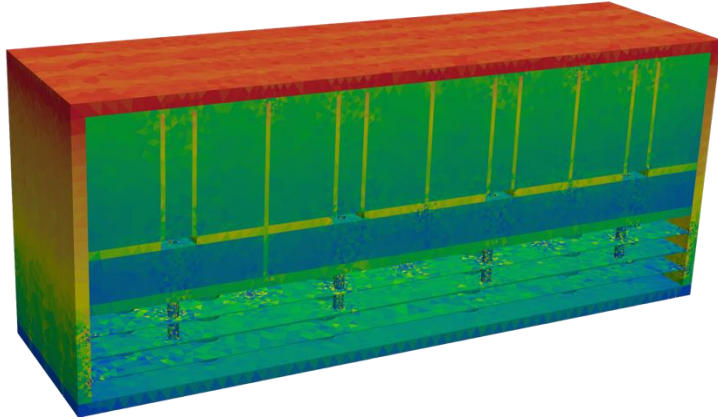


Facet the surfaces.

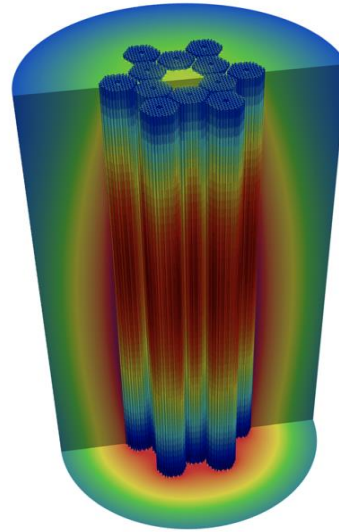


Cardinal

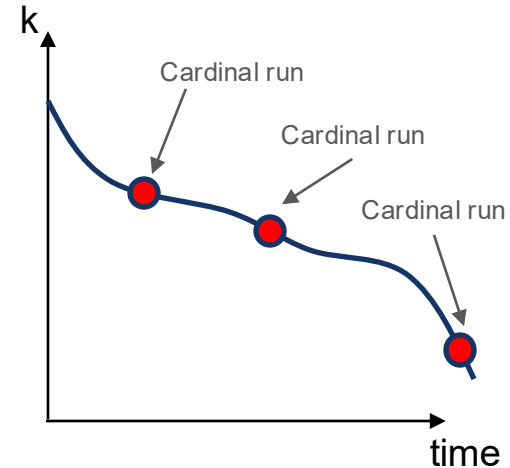
- **Modes/solvers:** Fixed-source, k -eigenvalue, depletion, volume calculation



Fixed source neutron-photon transport
Breeder blanket module



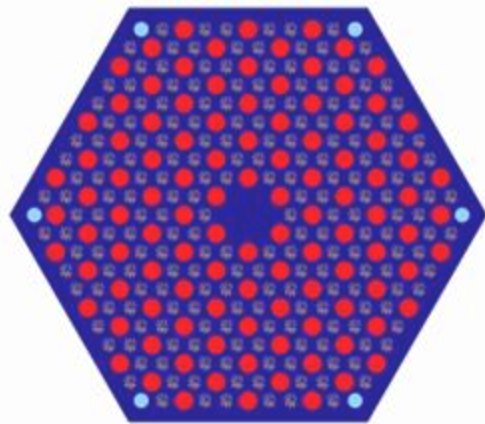
k -eigenvalue neutron transport
Fission reactor



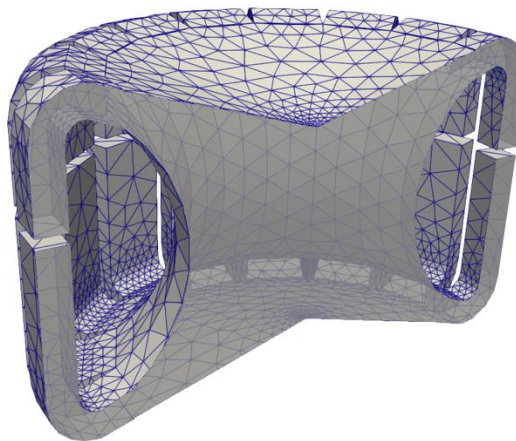
Depletion/activation

Cardinal

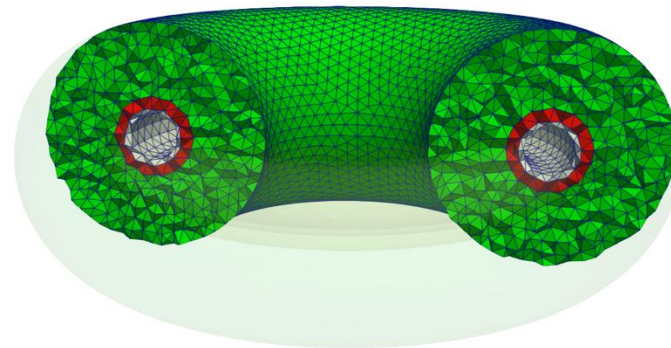
- **Modes/solvers:** Fixed-source, k -eigenvalue, depletion, volume calculation
- **Geometry:** Constructive solid geometry, CAD surface mesh, unstructured mesh*



Constructive Solid Geometry (CSG)



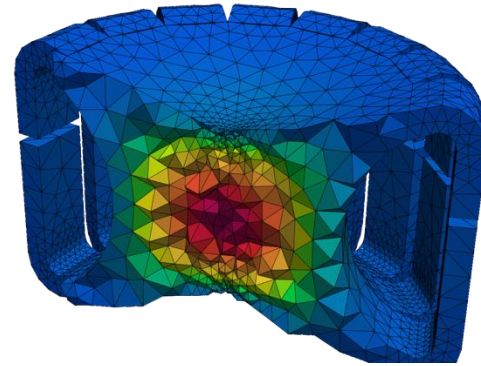
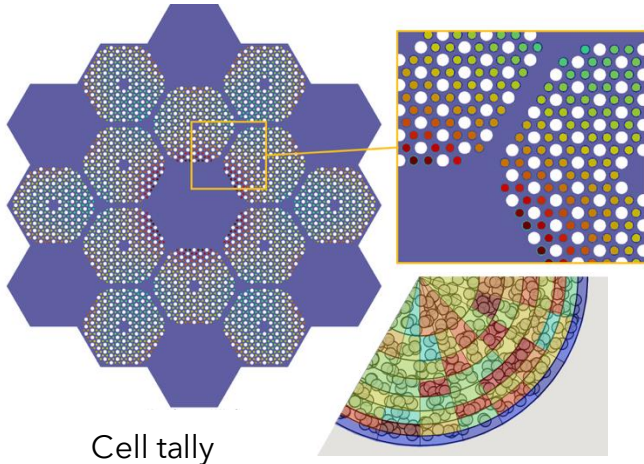
DAGMC surface meshes



libMesh unstructured volume mesh
(*coming soon)

Cardinal

- **Modes/solvers:** Fixed-source, k -eigenvalue, depletion, volume calculation
- **Geometry:** Constructive solid geometry, CAD surface mesh, unstructured mesh
- **Tallies:** cell tallies, unstructured mesh tallies



Unstructured mesh tally

Cardinal

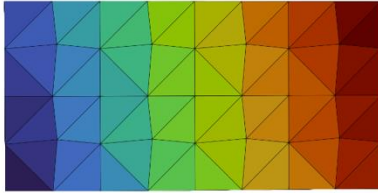
- **Modes/solvers:** Fixed-source, k -eigenvalue, depletion, volume calculation
- **Geometry:** Constructive solid geometry, CAD surface mesh, unstructured mesh
- **Tallies:** cell tallies, unstructured mesh tallies
- **Physics Feedback:** temperature (Doppler), density, composition, geometry, on-line multigroup cross section generation

Cardinal

- **Data transfer:**

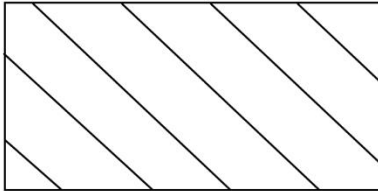
- **CSG:** element-cell mapping based on element centroids
- **CAD:** mesh-to-mesh mapping

Temperature



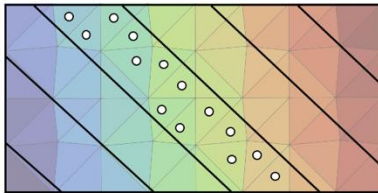
element ↔ cell
mapping

OpenMC
cells



Temperature applied
to OpenMC

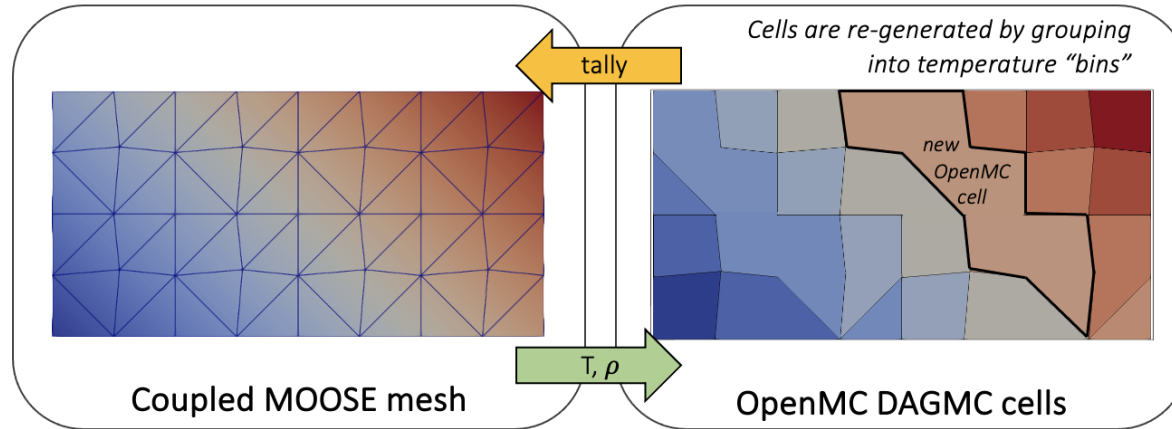
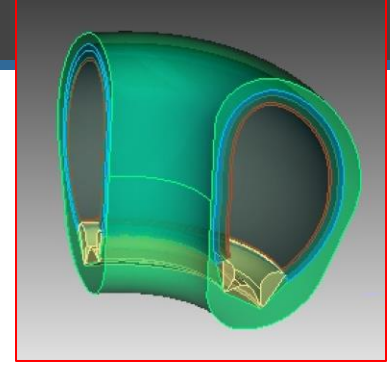
cells
overlapped
on mesh



Cardinal

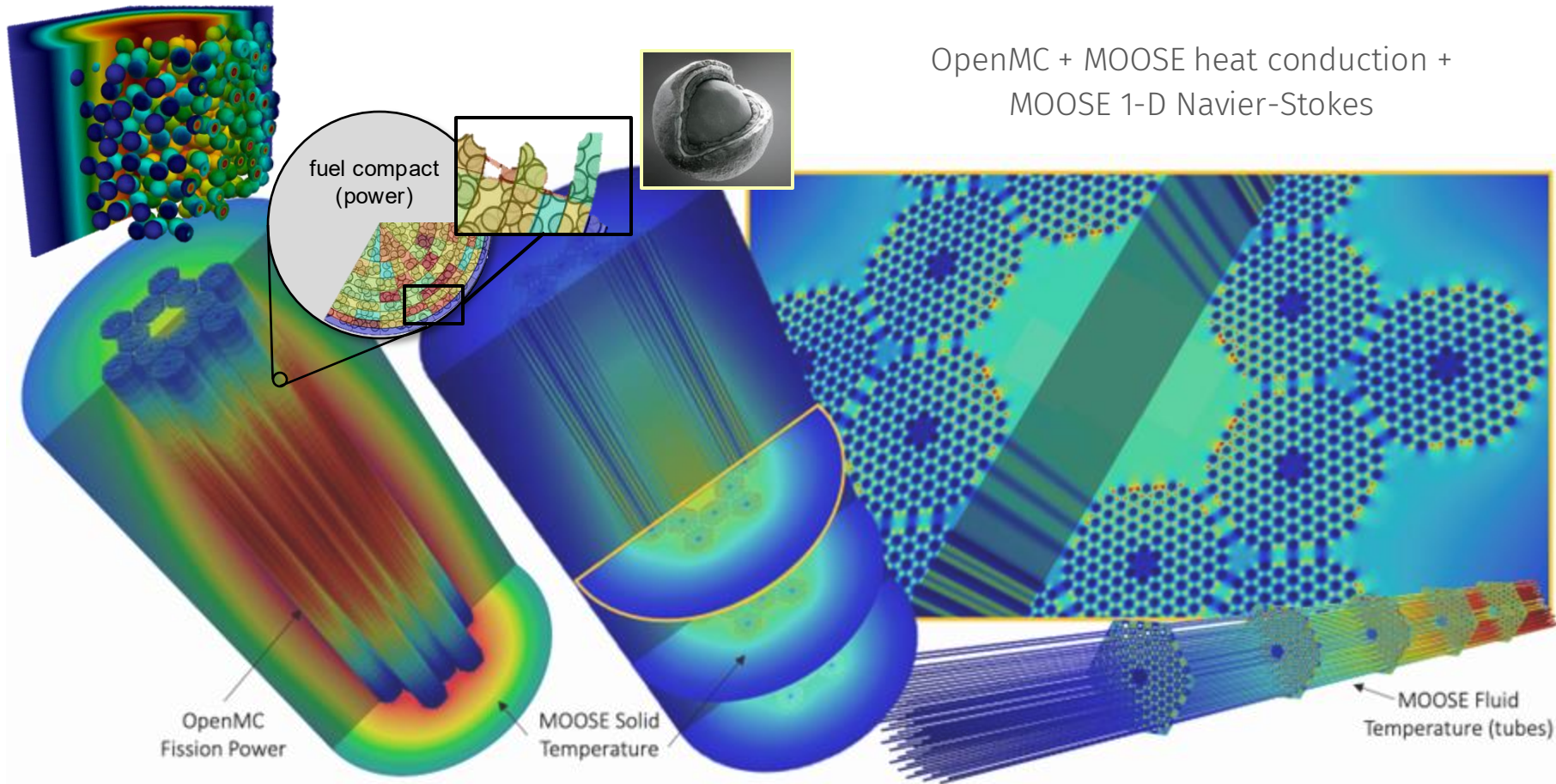
- **Data transfer:**

- **CSG:** element-cell mapping based on element centroids
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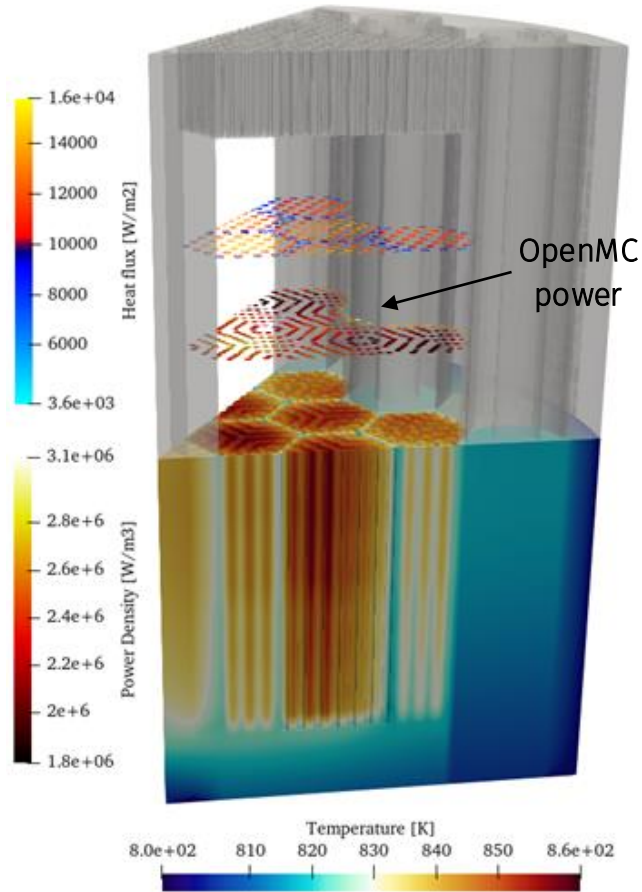


On-the-fly geometry refinement to resolve temperature, density fields (developed by Dr. Helen Brooks, UKAEA)

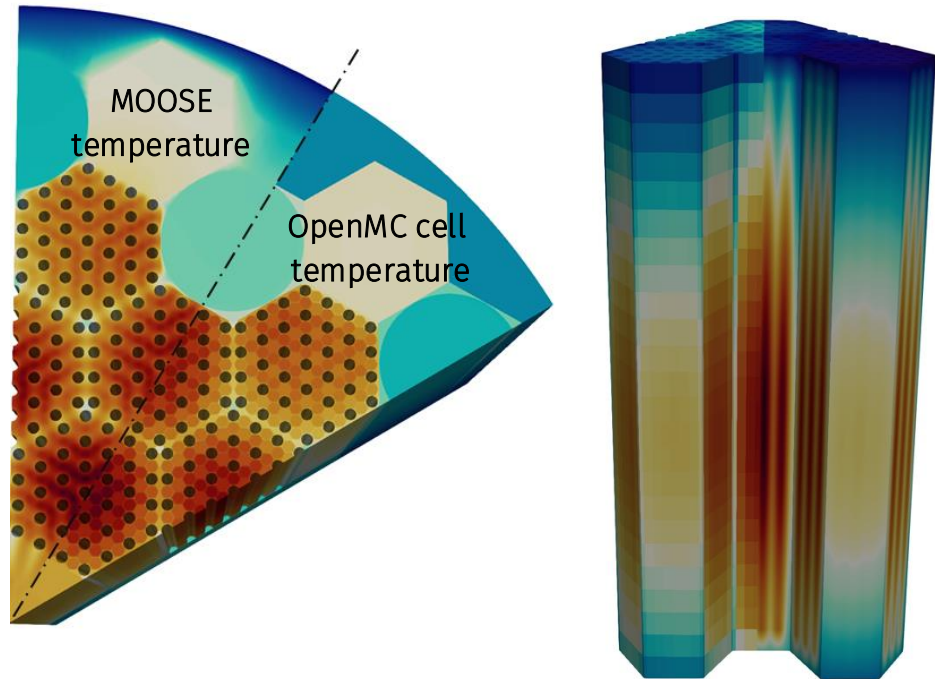
High Temperature Gas Reactors



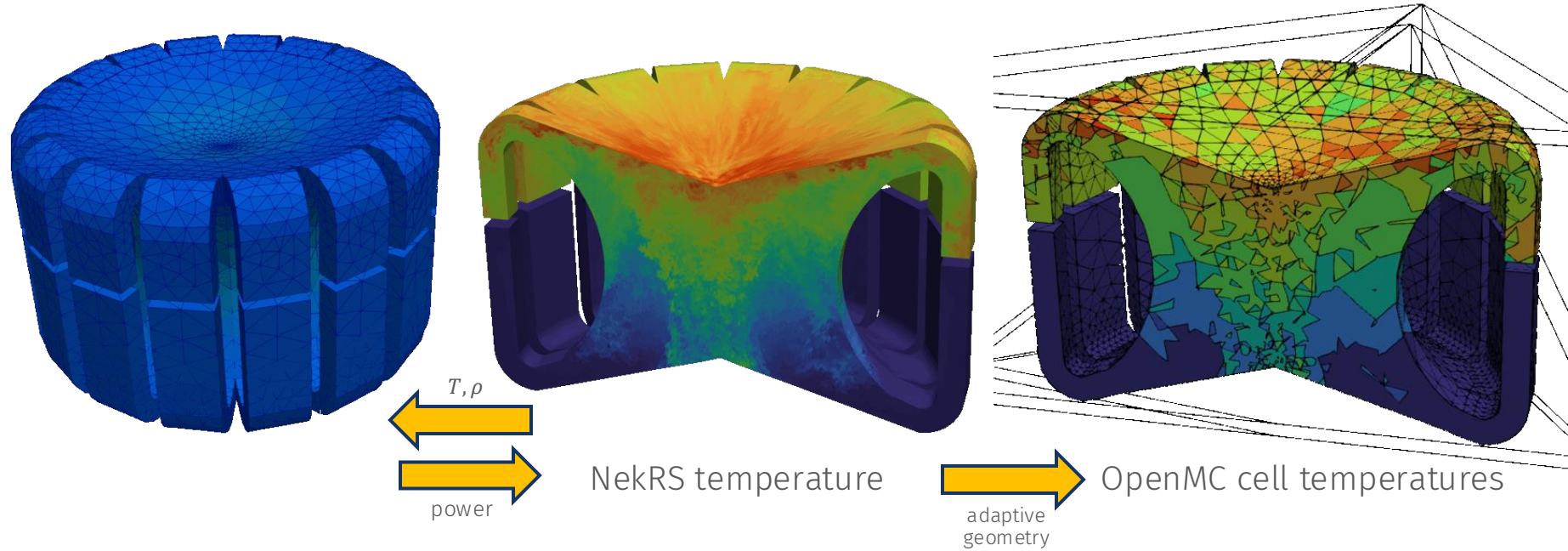
Heat Pipe Microreactors



OpenMC + MOOSE heat conduction +
MOOSE 1-D heat pipes



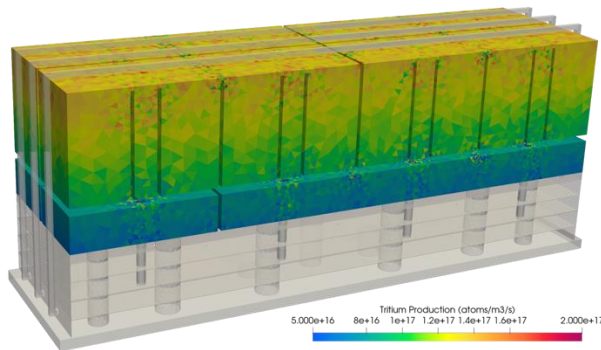
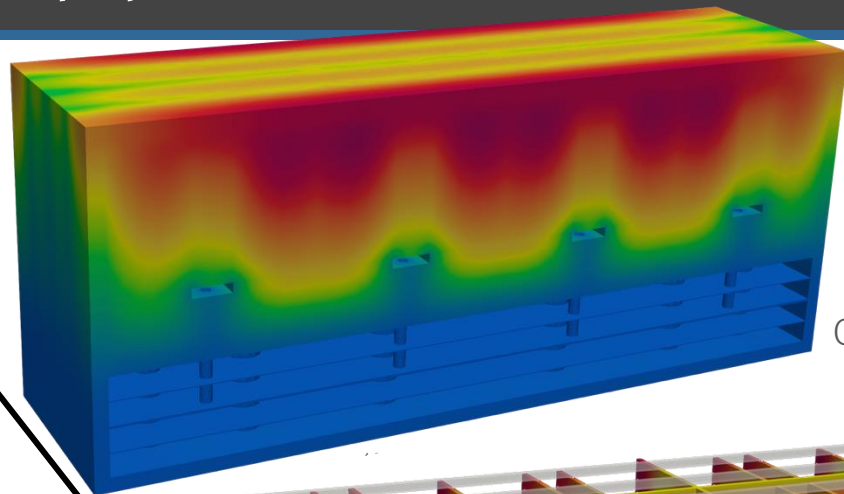
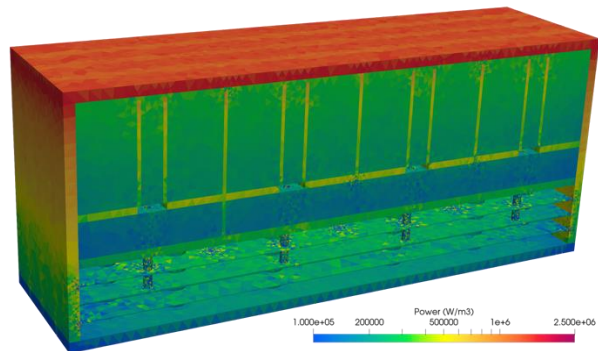
Molten Salt Reactors



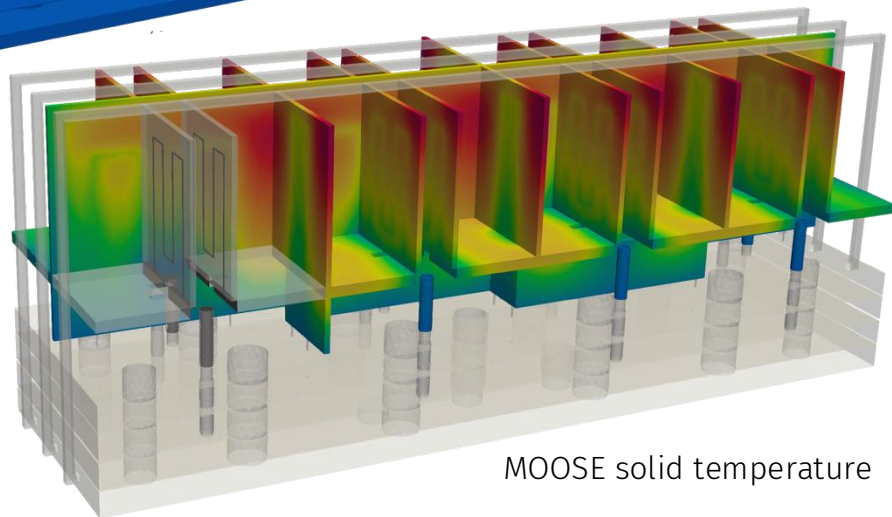
Fusion Breeder Blanket Multiphysics

CAD geometry and mesh provided by UKAEA
(Helen Brooks, Andrew Davis)

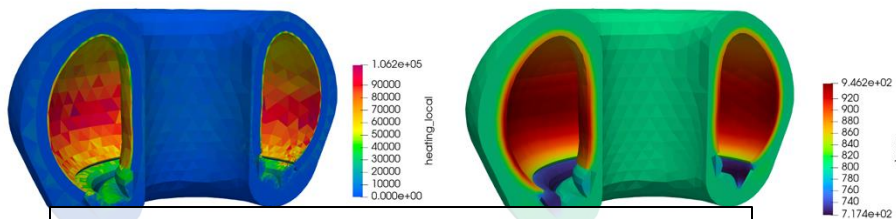
OpenMC nuclear heating distribution



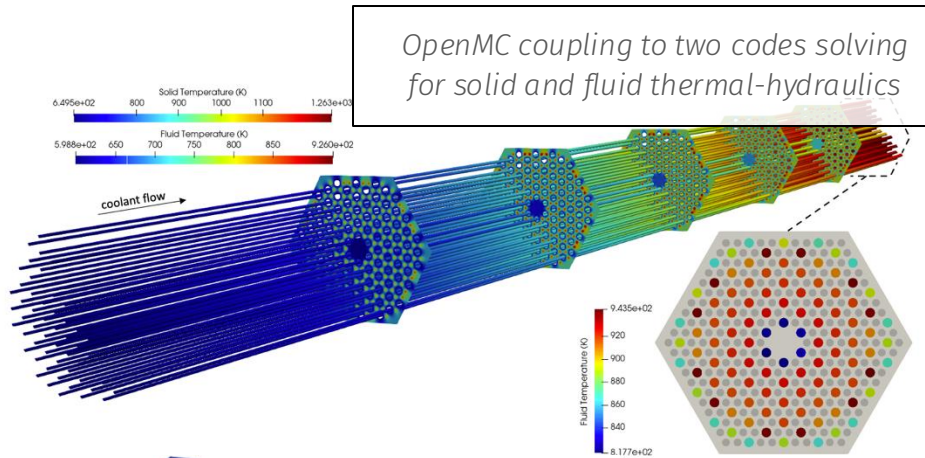
OpenMC tritium production rate



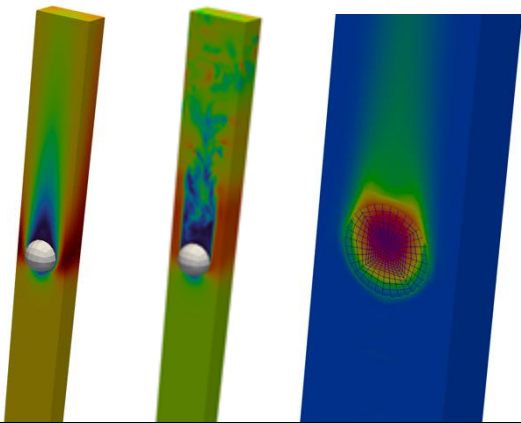
25 Tutorials on the Cardinal Website: <https://cardinal.cels.anl.gov>



OpenMC coupling to MOOSE on CAD geometries

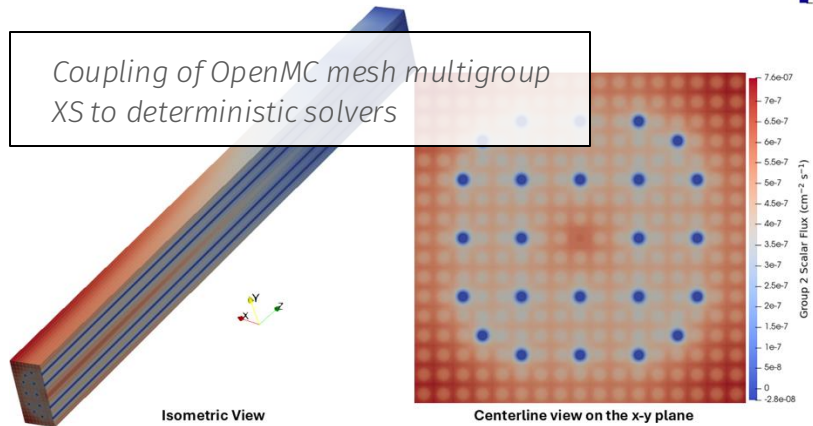


OpenMC coupling to two codes solving for solid and fluid thermal-hydraulics



Introduction to NekRS turbulence modeling, conjugate heat transfer coupling to MOOSE

Coupling of OpenMC mesh multigroup XS to deterministic solvers



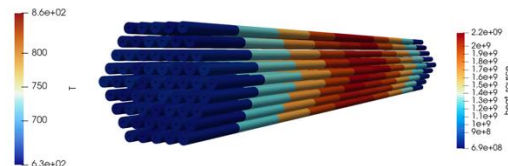
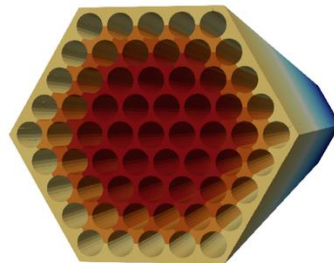
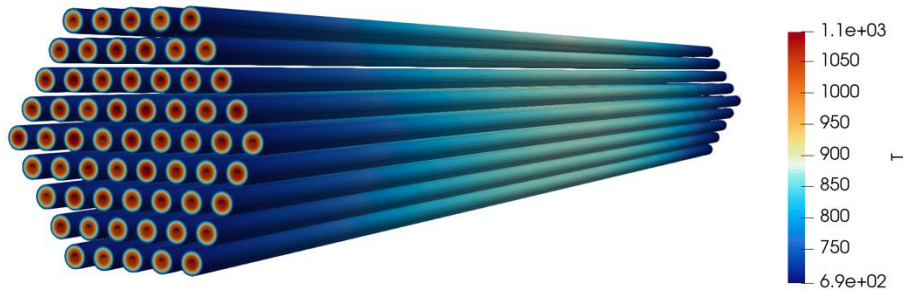
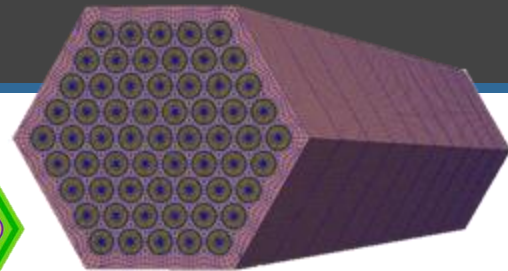
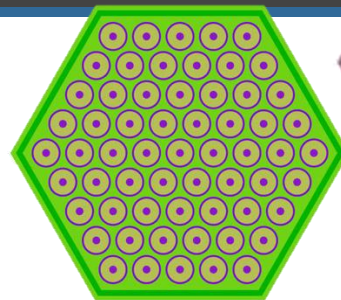
Isometric View

Centerline view on the x-y plane

Workshop Schedule

cardinal.cels.anl.gov/tutorials/subchannel.html

- **Step 1:** Build OpenMC and MOOSE heat conduction model of CEFR fuel assembly
- **Step 2:** Multiphysics coupling of OpenMC and MOOSE heat conduction
- **(time permitting) Step 3:** Coupled OpenMC, heat conduction, and a subchannel solver



Take-Home Activity: `all_coupled` folder

- Vary the number of axial layers in the mesh (10, 20, 30 layers)
 - Plot the temperature in the center fuel pin as a function of z as the mesh is refined ([plot the data in `openmc_out_conduction0_T_0005.csv`](#))
 - How many axial layers would you recommend for use in this model?
- Change the thermal conductivity of the fuel (k from 1.0 to 10.0 W/m/K)
 - Plot the maximum fuel temperature and the multiplication factor as the thermal conductivity is varied and explain the trends you see ([these values are printed to the screen as postprocessors](#))
- Vary the power level (power from 500 KWth to 1000 KWth)
 - Compute a power reactivity coefficient as a function of power (be sure to increase the number of particles and inactive batches to have sufficiently low statistical noise and a converged source)
 - What important physical process is missing from this model? Explain what effect you think including it will have on the power reactivity coefficient

Questions?

ajnovak2@illinois.edu

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

