High-Fidelity Multiphysics in Fission

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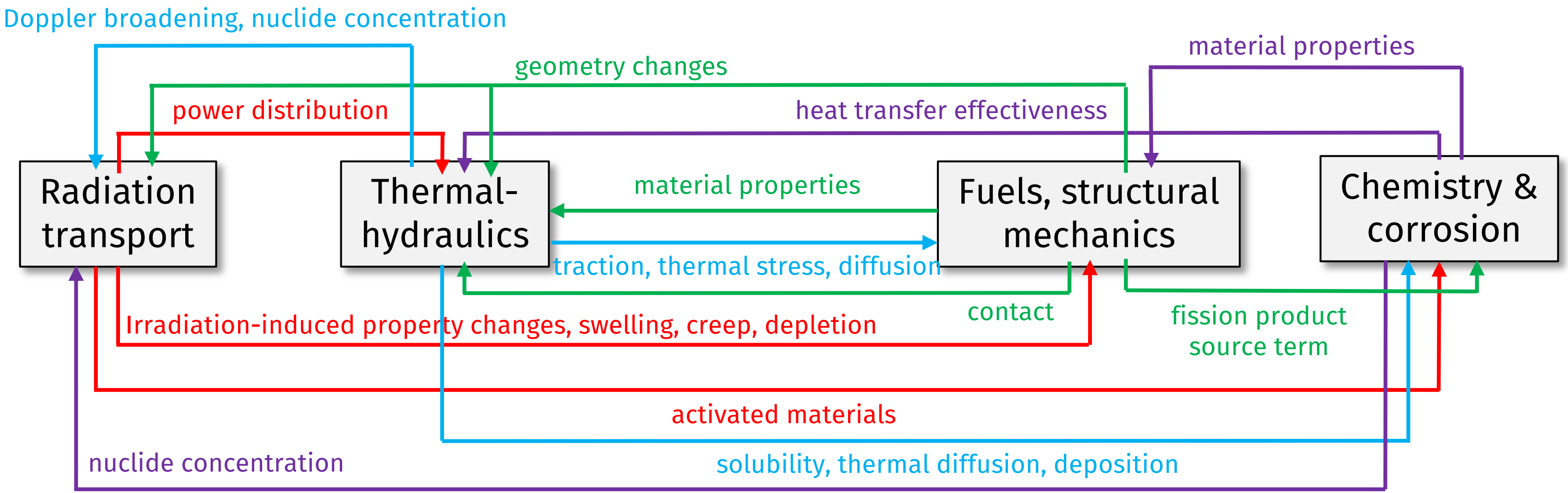
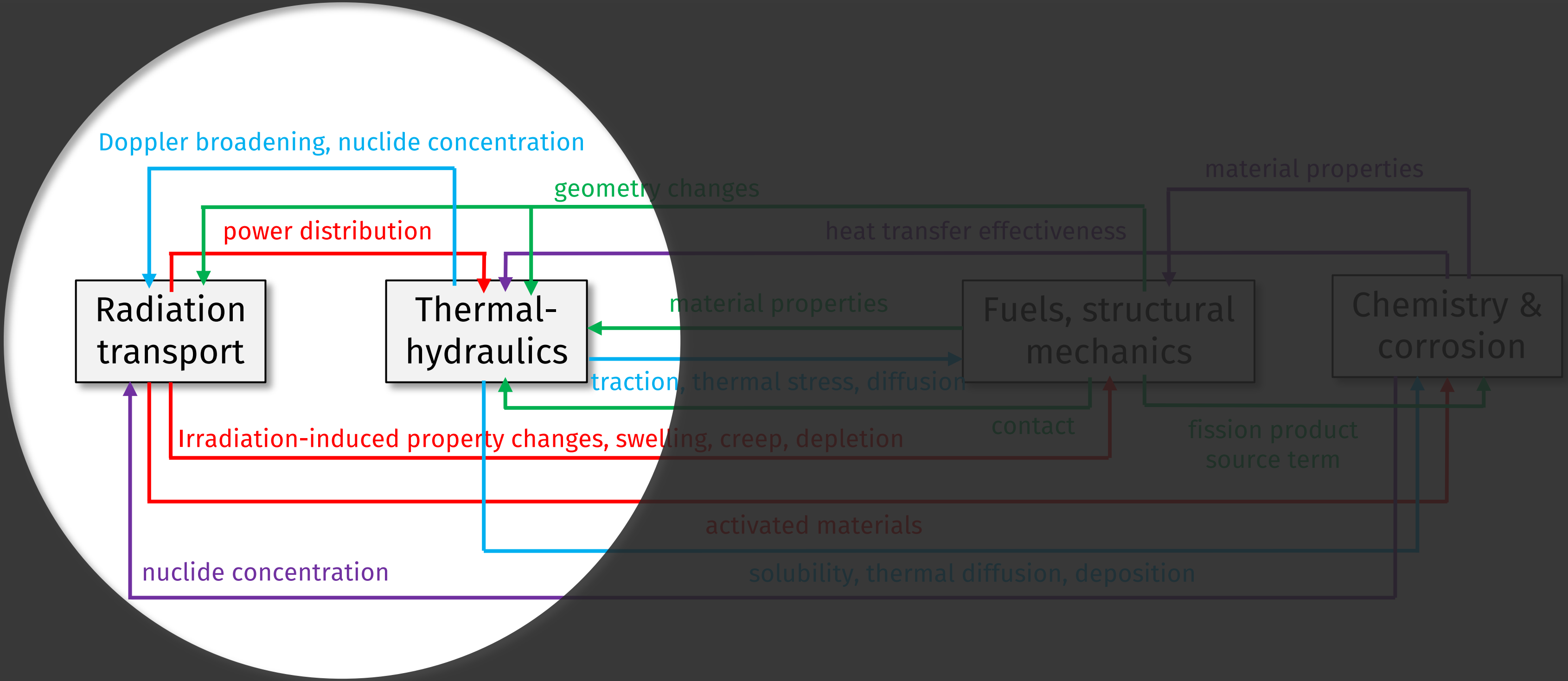
Multiphysics in Nuclear Engineering

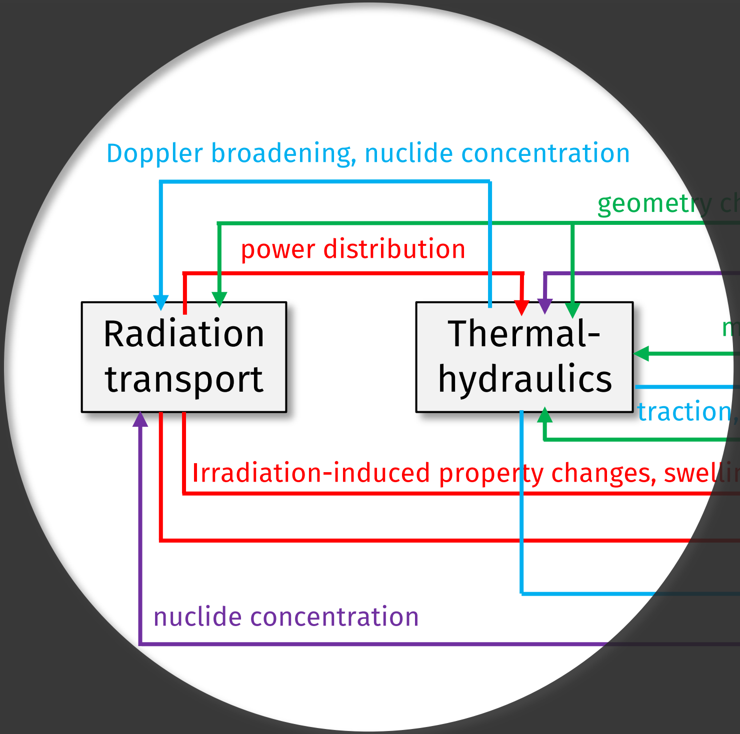


Focus Areas



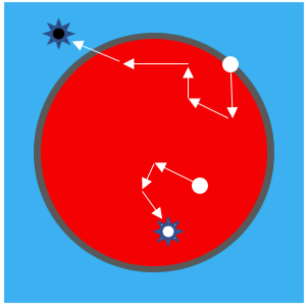
Doppler broadening, nuclide concentration
geometry changes
power distribution
material properties
heat transfer effectiveness
Radiation transport
Thermal-hydraulics
material properties
Fuels, structural mechanics
Chemistry & corrosion
traction, thermal stress, diffusion
contact
fission product source term
Irradiation-induced property changes, swelling, creep, depletion
activated materials
nuclide concentration
solubility, thermal diffusion, deposition

Modeling & Simulation: “Virtual Experiments”

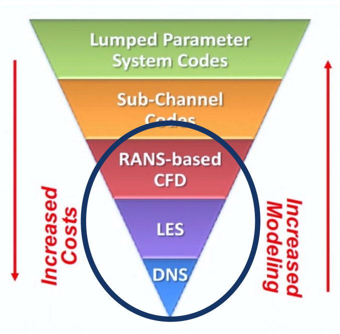


- Enables studies that would otherwise be impractical due to:
  - Cost/timeframe
  - Personnel/environmental risk
  - Limits of instrumentation technology
- Advanced reactors have scarce experimental data
- Complementary to experiments

High-Fidelity Multiphysics



Monte Carlo radiation transport



Computational Fluid Dynamics

- Limited physics/numeric approximations
  - May reduce conservatism
  - Provide additional context to experiments
  - Benchmark and inform coarse-mesh methods

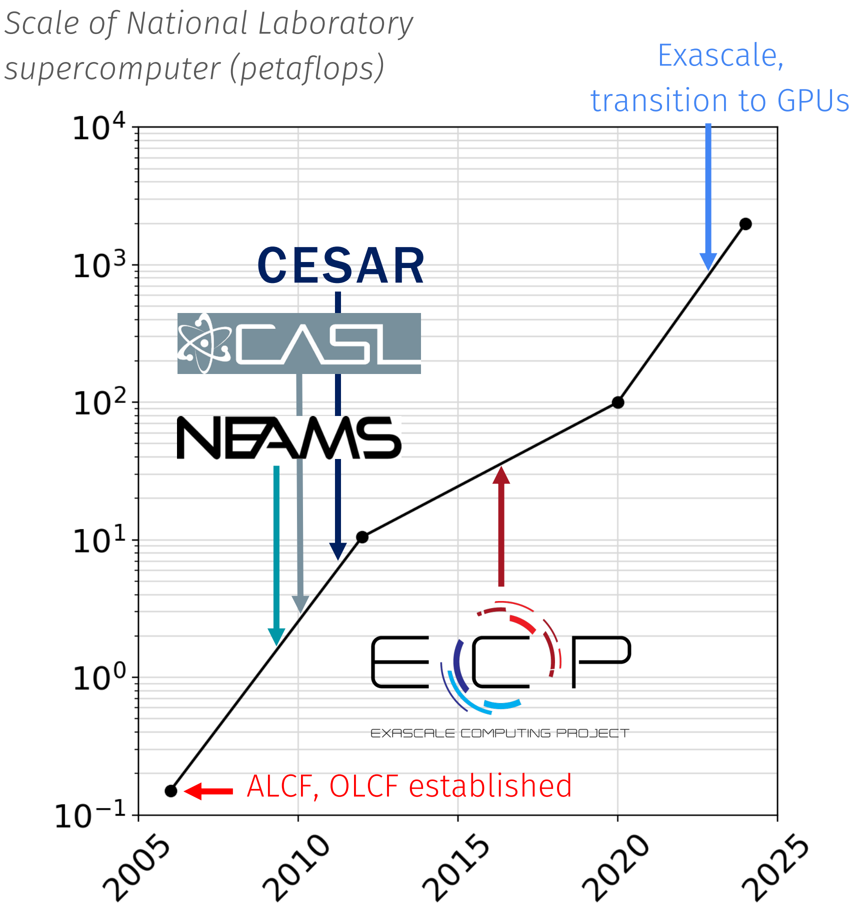
History and Challenges

Cardinal: High-Fidelity Multiphysics

History and Challenges

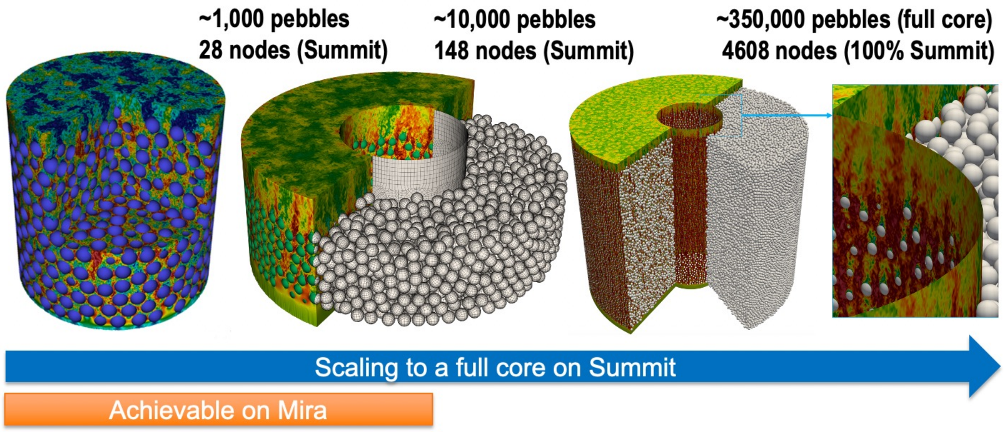
Cardinal: High-Fidelity Multiphysics

An Abridged U.S. History

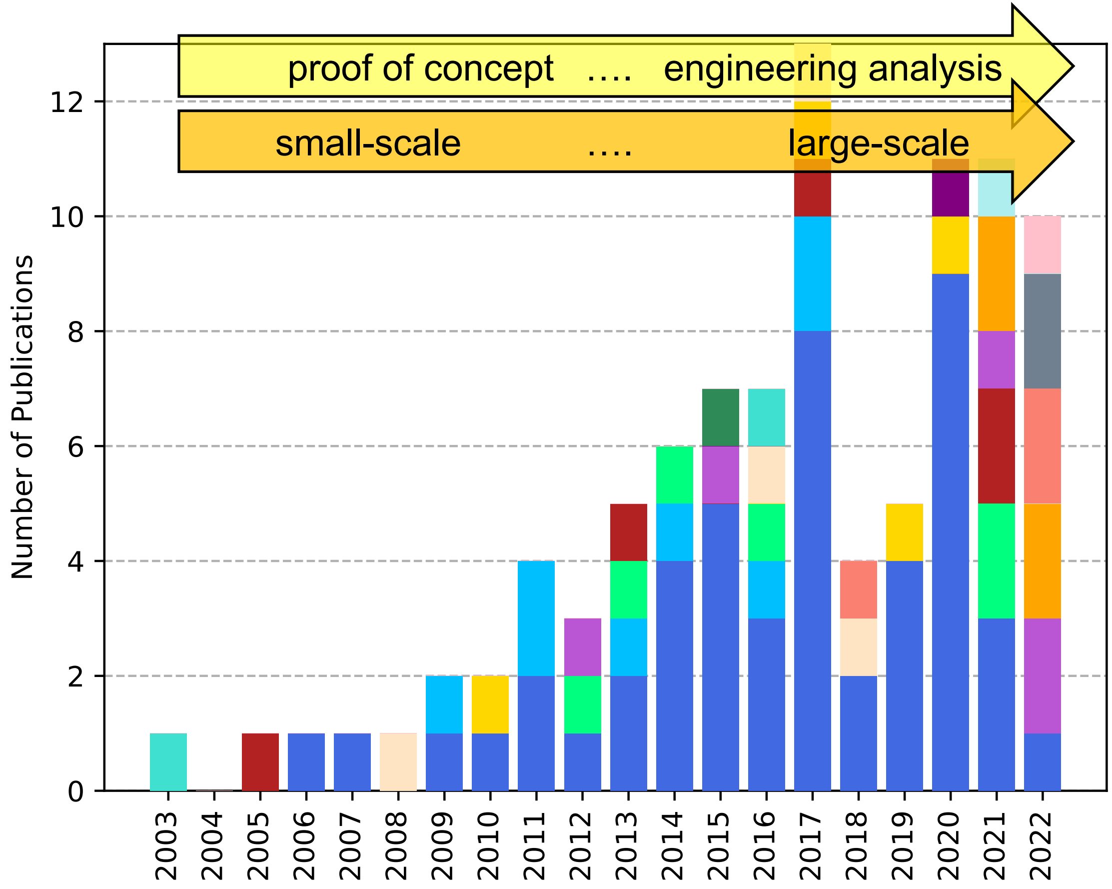


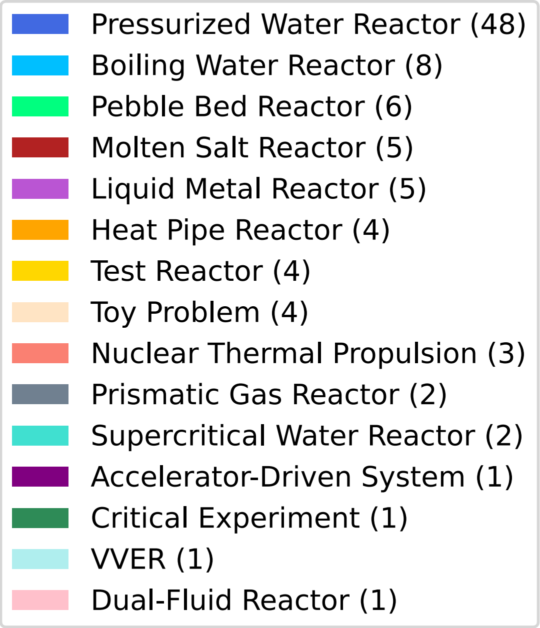
Nuclear reactors exhibit many challenges to computational modeling.

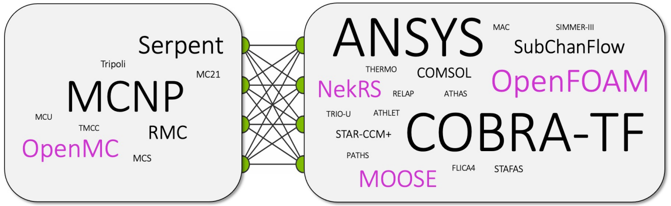
- Extreme range of scales in length and time
- Tightly-coupled physics (higher-temperature, smaller sizes, load following, longer core life, …)
- (Sometimes) difficult to construct “unit cells”



High-Fidelity History



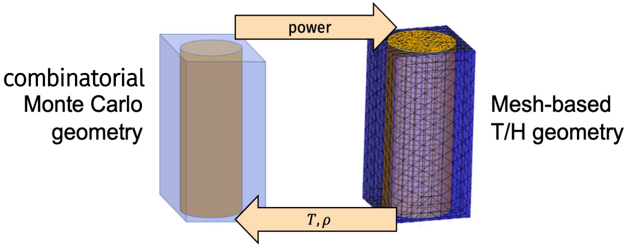




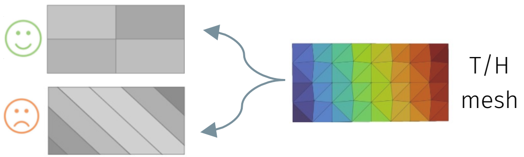
R&D Challenges

R&D Challenges

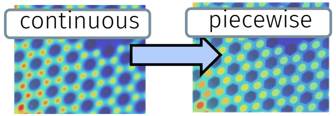
Data Transfers



Highly manual process to build geometries and exchange data



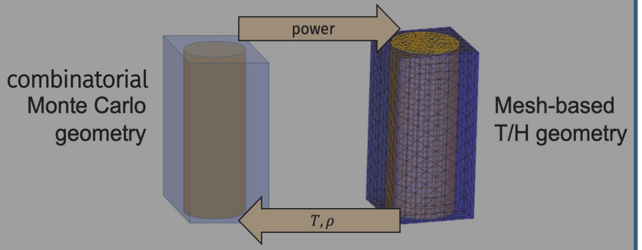
Limitations on distance-to-collision sampling



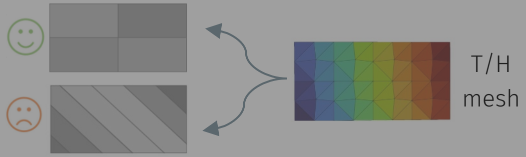
Challenges "general purpose" use

R&D Challenges

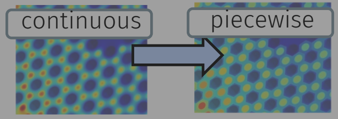
Data Transfers



Highly manual process to build geometries and exchange data



Limitations on distance-to-collision sampling



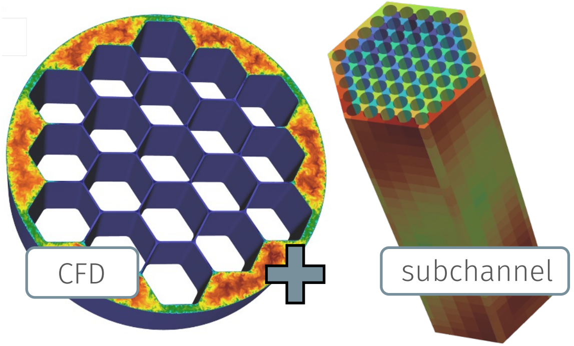
Challenges "general purpose" use

Iterative Methods

combine stochastic and matrix-based methods

stochastic → Monte Carlo; matrix-based → $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$

Inflexible algorithms excluded multiscale methods

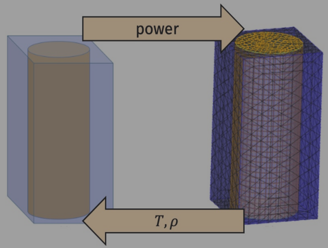


Challenges effective reactor simulation

R&D Challenges

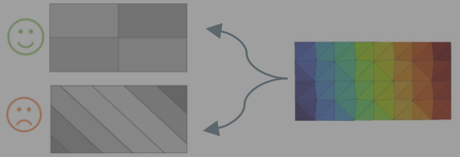
Data Transfers

combinatorial Monte Carlo geometry

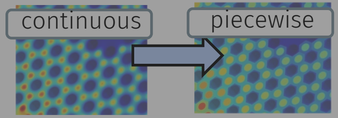


Mesh-based T/H geometry

Highly manual process to build geometries and exchange data



Limitations on distance-to-collision sampling



Challenges "general purpose" use

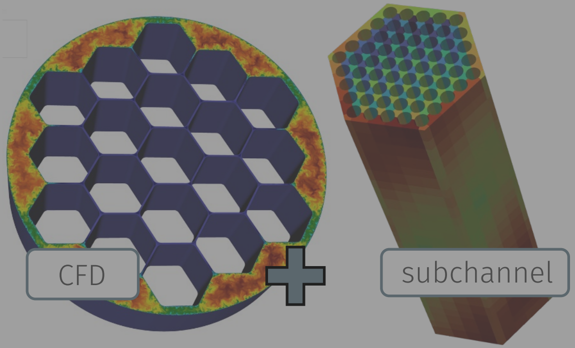
Iterative Methods

combine stochastic and matrix-based methods

Monte Carlo

$Ax = b$

Inflexible algorithms excluded multiscale methods



Challenges effective reactor simulation

Software and Parallelization

GitHub

image credit: OLCF

Prior work largely limited to CPUs

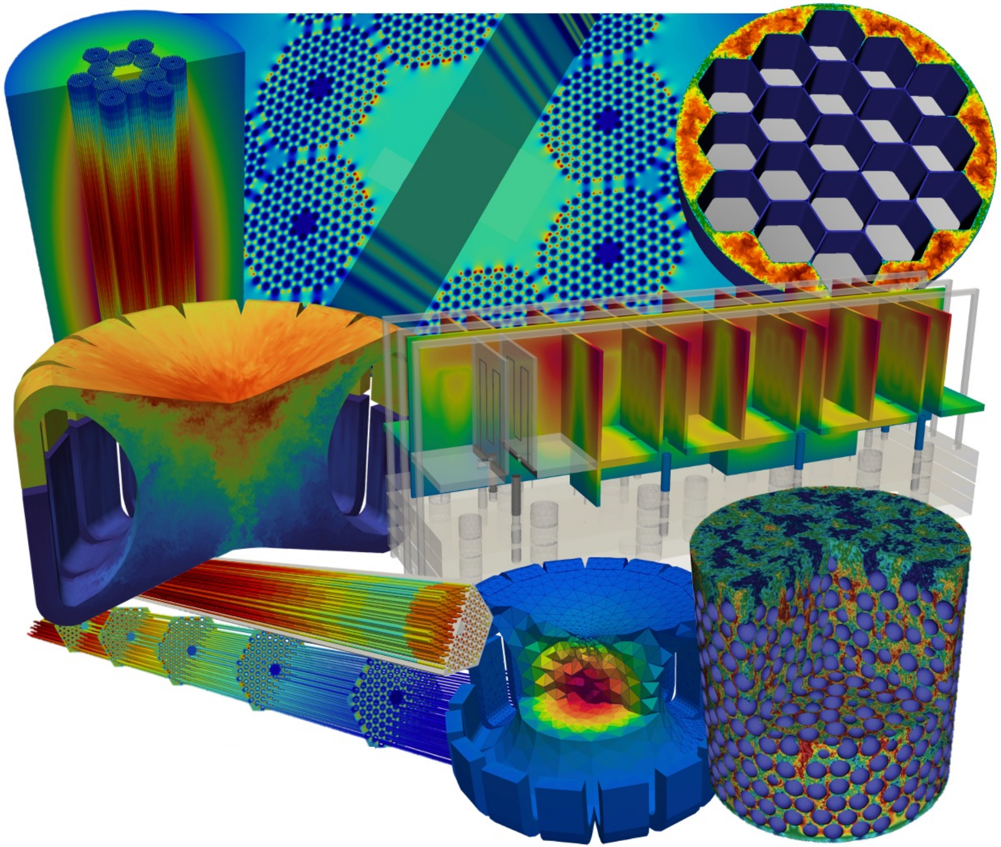
Near-total lack of open-source high-fidelity multiphysics software

Challenges large-scale simulation

History and Challenges

Cardinal: High-Fidelity Multiphysics

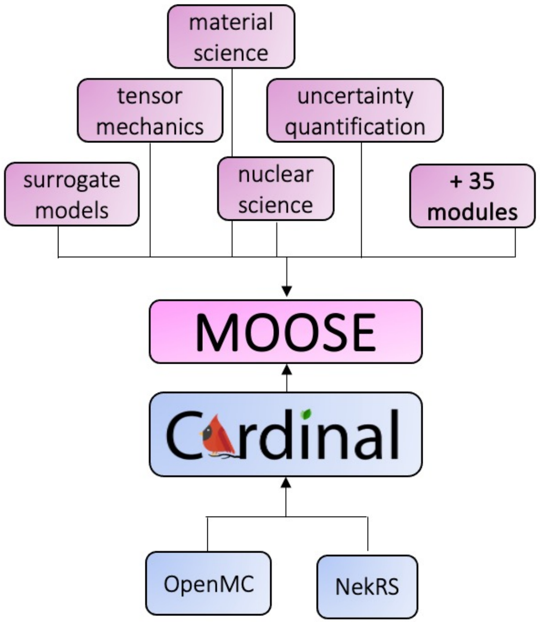
Argonne National Laboratory | Idaho National Laboratory | University of Illinois Urbana-Champaign | PennState | UK Atomic Energy Authority

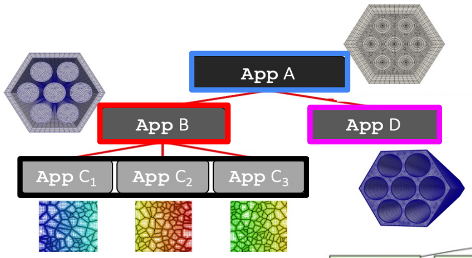


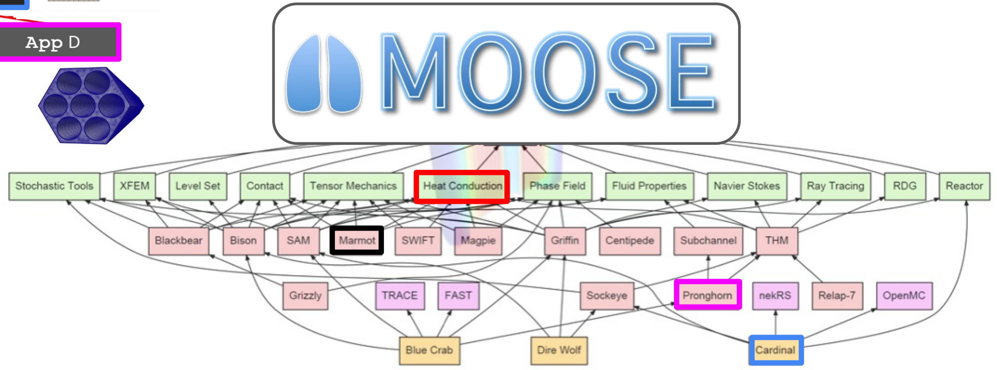
Cardinal

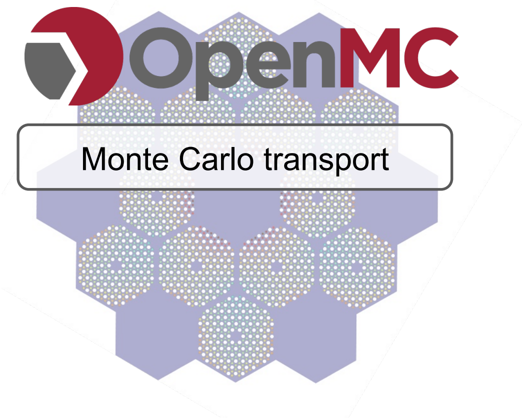
- MOOSE (framework)
- OpenMC (Monte Carlo)
- NekRS (CFD)

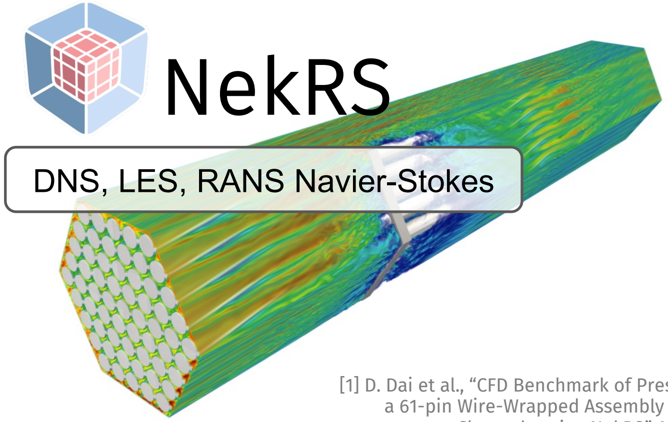
Cardinal





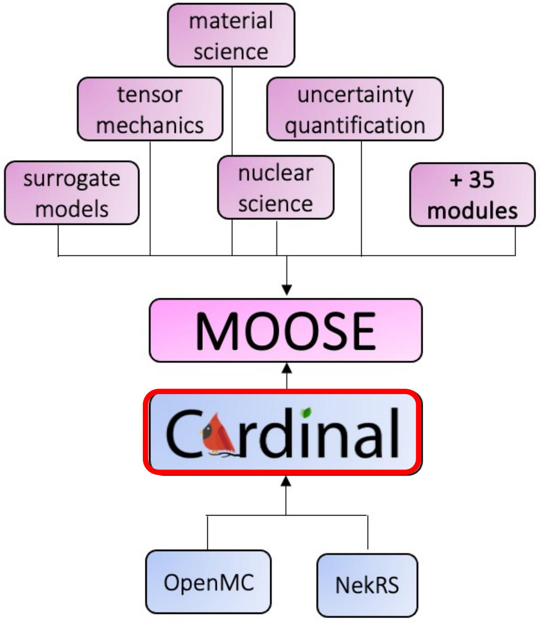


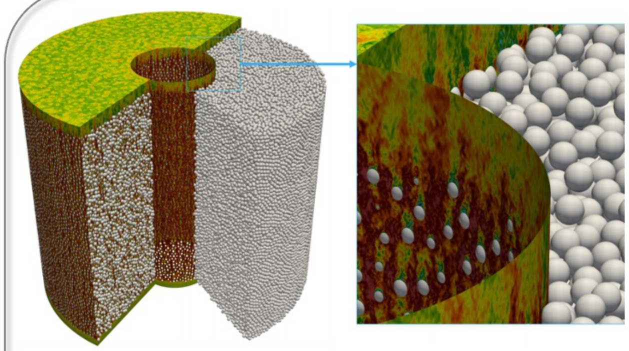




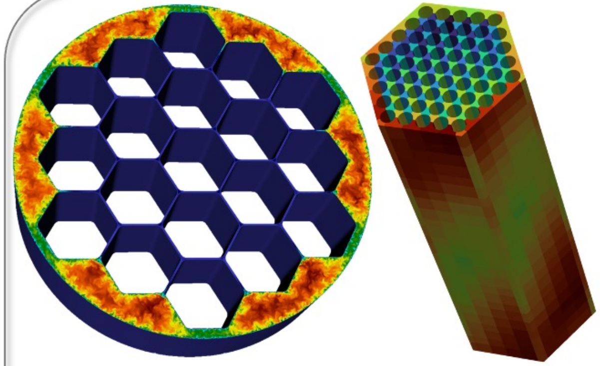
[1] D. Dai et al., “CFD Benchmark of Pressure Drop in a 61-pin Wire-Wrapped Assembly with Blocked Channels using NekRS” ANL/NSE-23/6

Cardinal

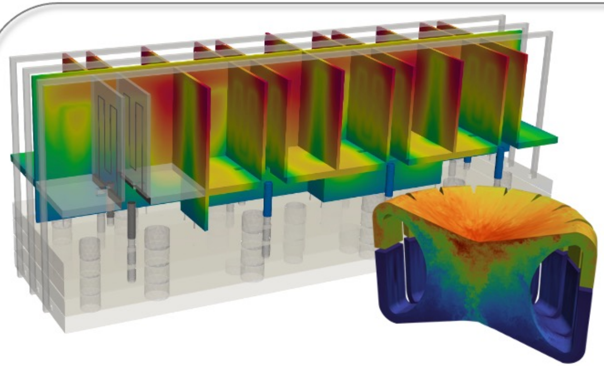




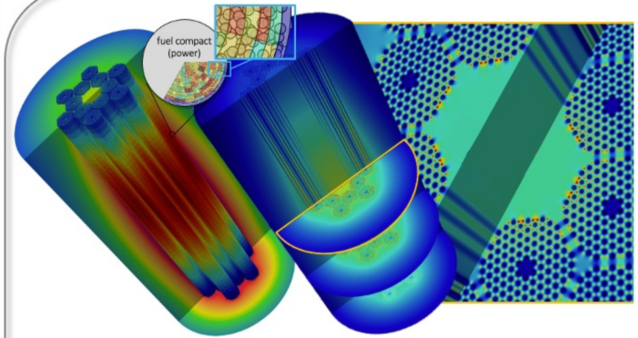
Scalable Mixed CPU-GPU codes
In-memory coupling



Flexible Pluggable into entire MOOSE ecosystem
Geometry-agnostic mesh transfers

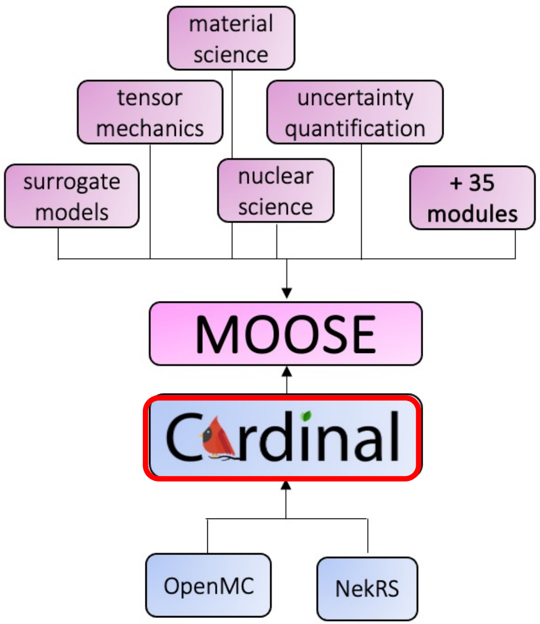


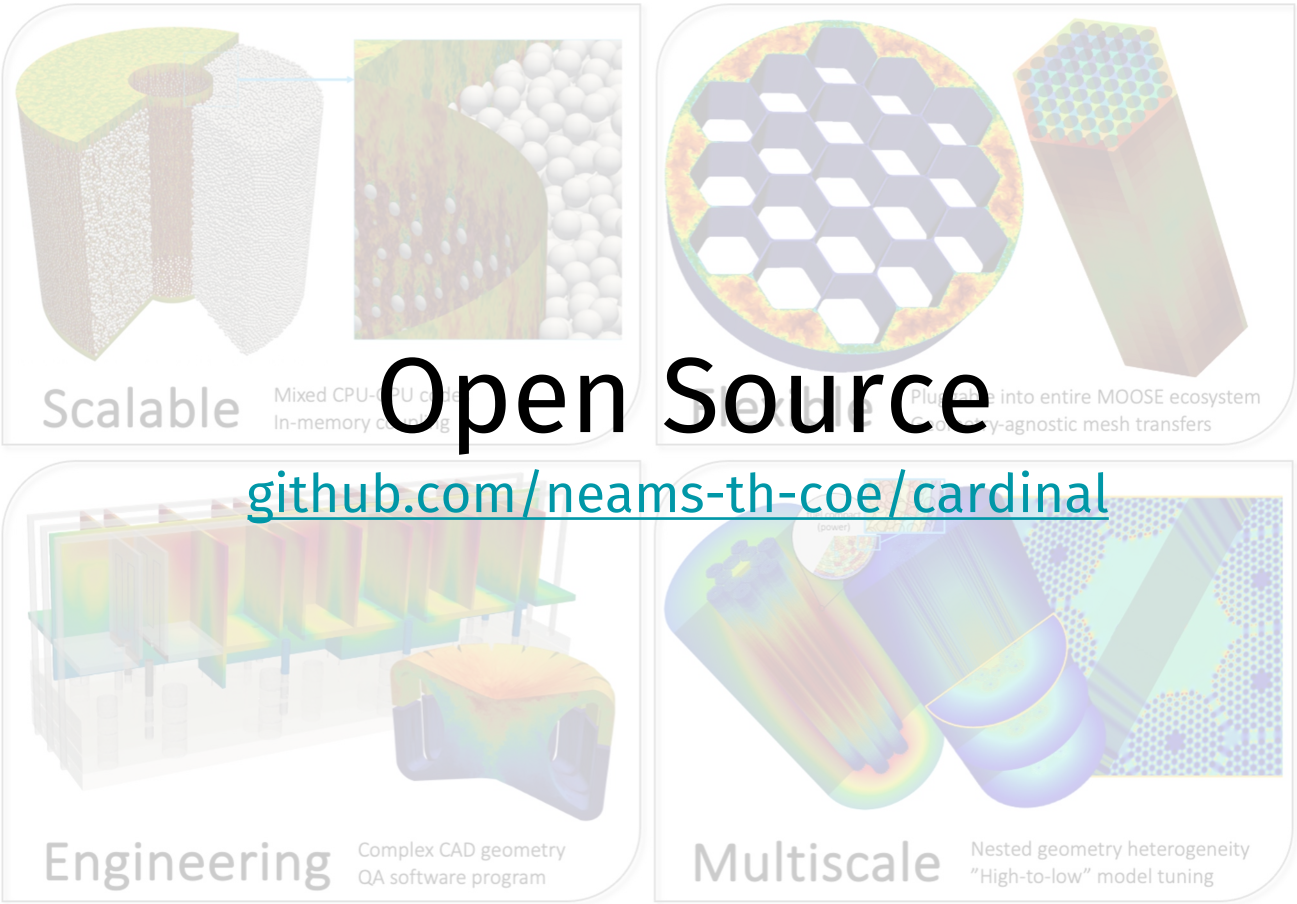
Engineering Complex CAD geometry
QA software program



Multiscale Nested geometry heterogeneity
"High-to-low" model tuning

Cardinal





Open Source

github.com/neams-th-coe/cardinal

Applications

- High Temperature Gas Reactors
- Pebble Bed Reactors
- Molten Salt Reactors
- Sodium Fast Reactors
- Lead Fast Reactors
- 3D/1D Multiscale Coupling
- Pressurized Thermal Shock
- Fluid-Structure Interaction
- Fusion Components
- Physics-Informed Machine Learning

NEAMS Nuclear Energy Advanced Modeling and Simulation

NEUP Nuclear Energy University Program U.S. Department of Energy

U.S.NRC

GAIN Gateway for Accelerated Innovation in Nuclear

Argonne NATIONAL LABORATORY

INL Idaho National Laboratory

Applications

High Temperature Gas Reactors

Pebble Bed Reactors

Molten Salt Reactors

Sodium Fast Reactors

Lead Fast Reactors

3D/1D Multiscale Coupling

Pressurized Thermal Shock

Fluid-Structure Interaction

Fusion Components

Physics-Informed Machine Learning

multiscale, combining 1-D and 3-D methods

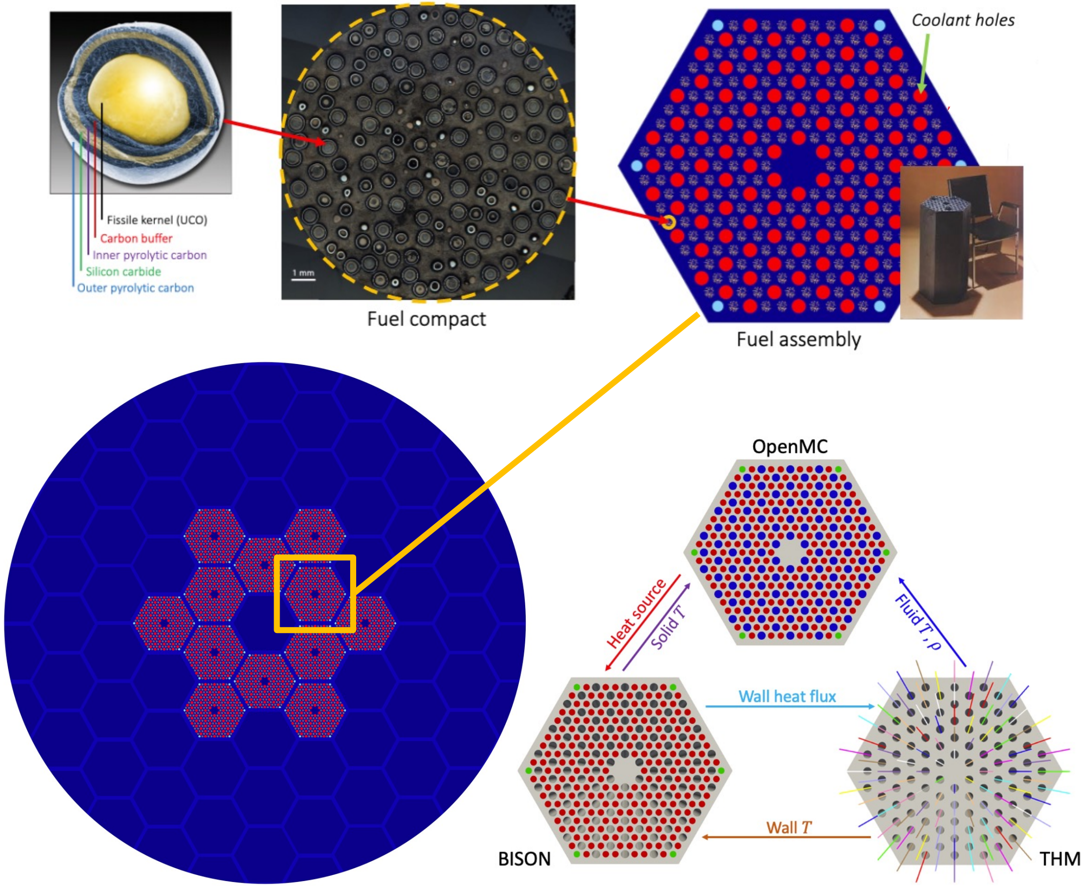
advanced adaptive geometry

High Temperature Gas Reactors (HTGRs)

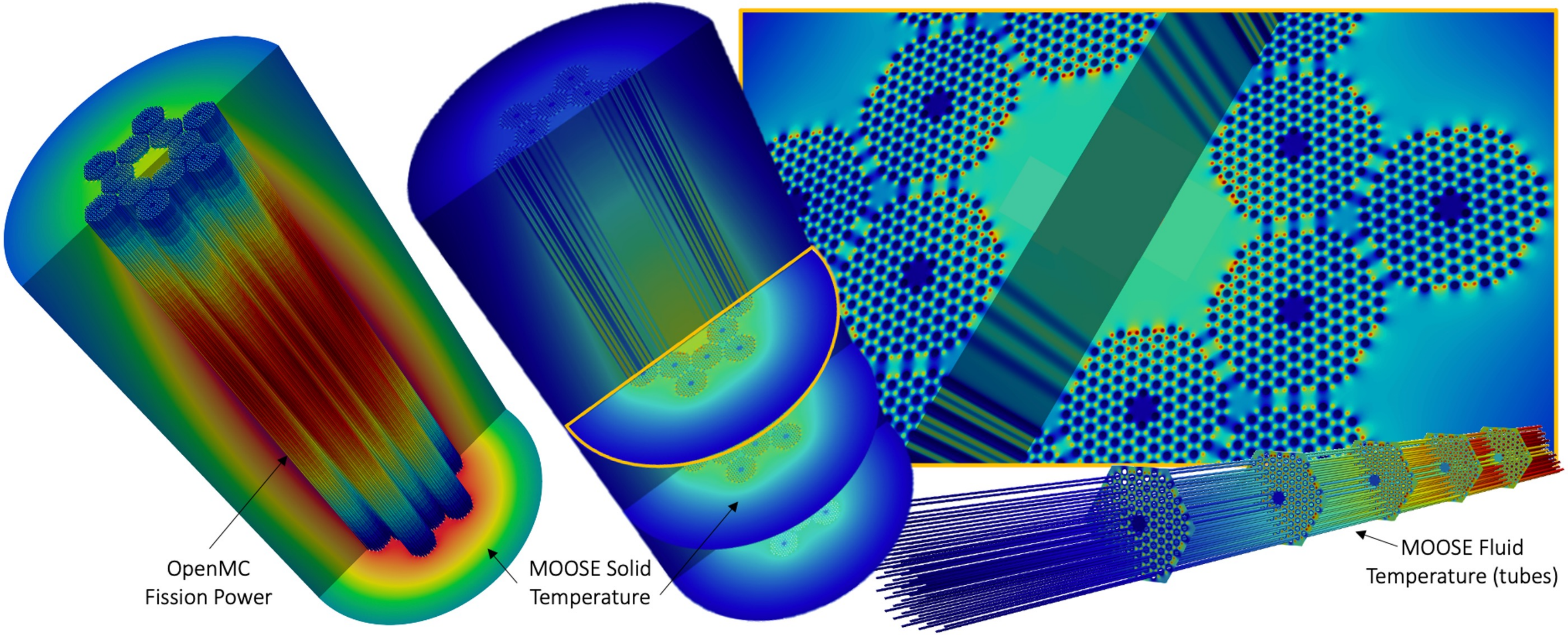
High Temperature Gas Reactors | 3D/1D Multiscale Coupling
Pebble Bed Reactors | Pressurized Thermal Shock
Molten Salt Reactors | Fluid-Structure Interaction
Sodium Fast Reactors | Fusion Components
Lead Fast Reactors | Physics-Informed Machine Learning

Particle fuel requires special considerations to:

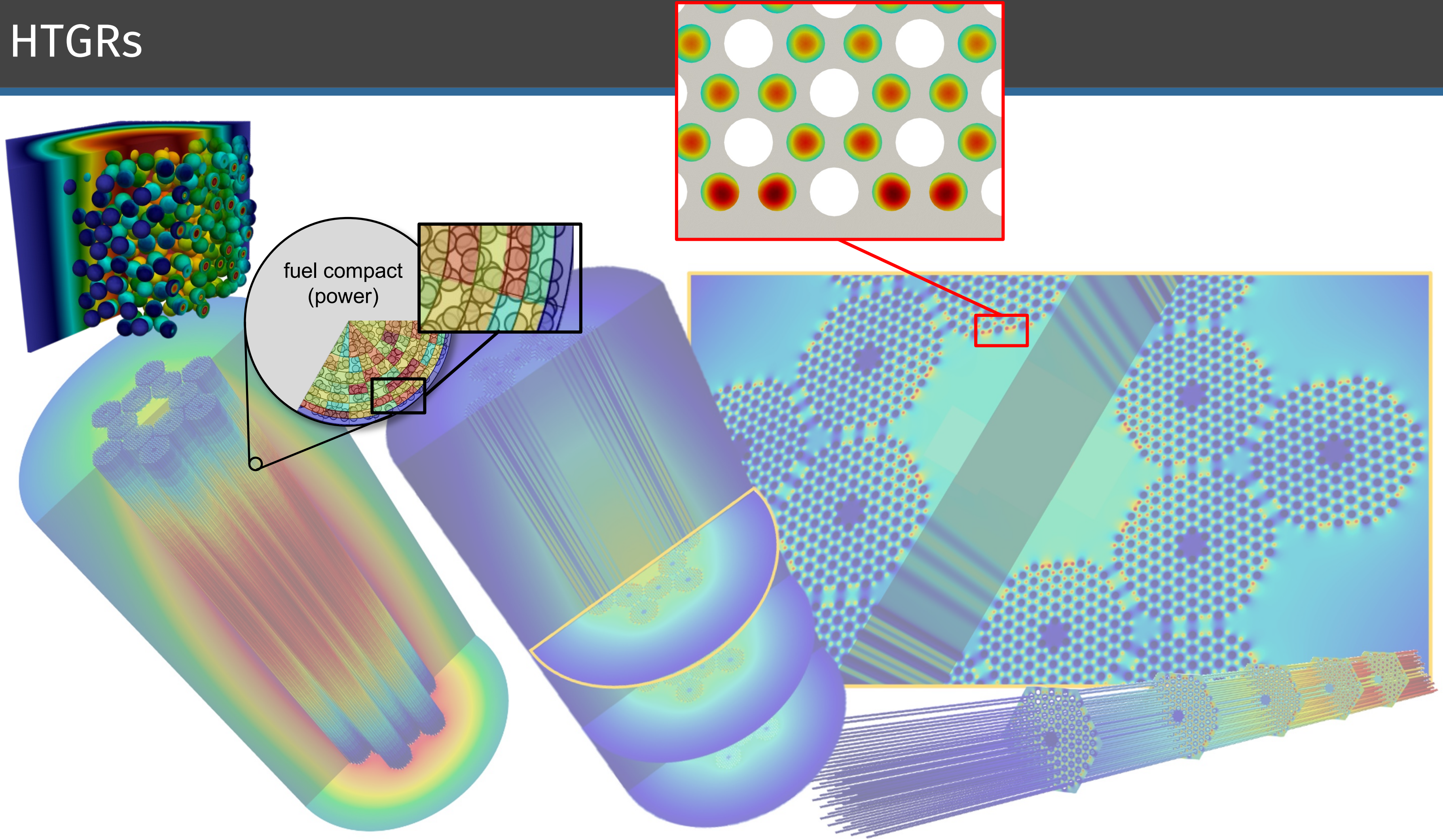
- Generate multigroup cross sections, Σ
- Apply temperature feedback



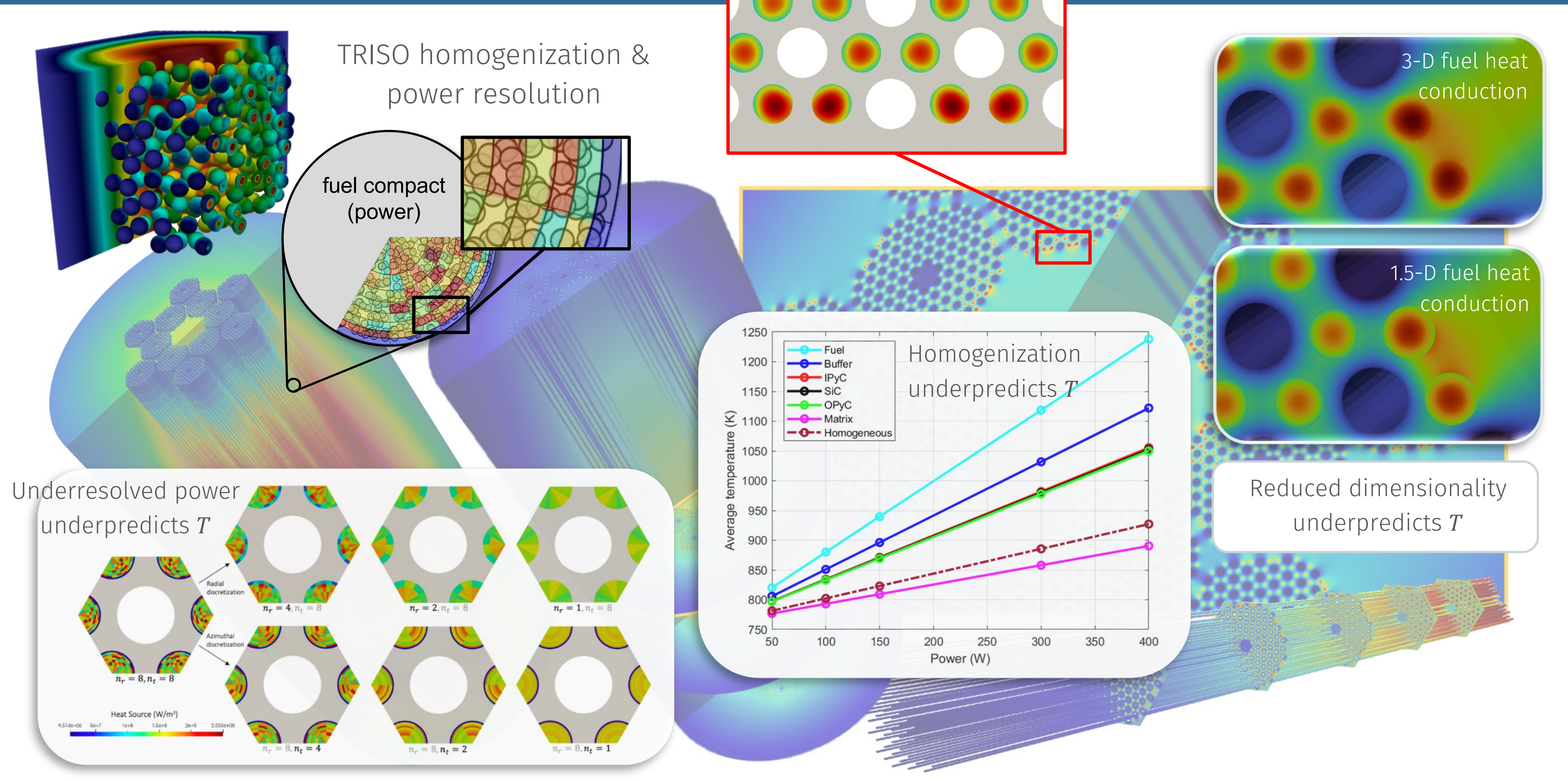
HTGRs


OpenMC
Fission Power
MOOSE Solid
Temperature
MOOSE Fluid
Temperature (tubes)

HTGRs

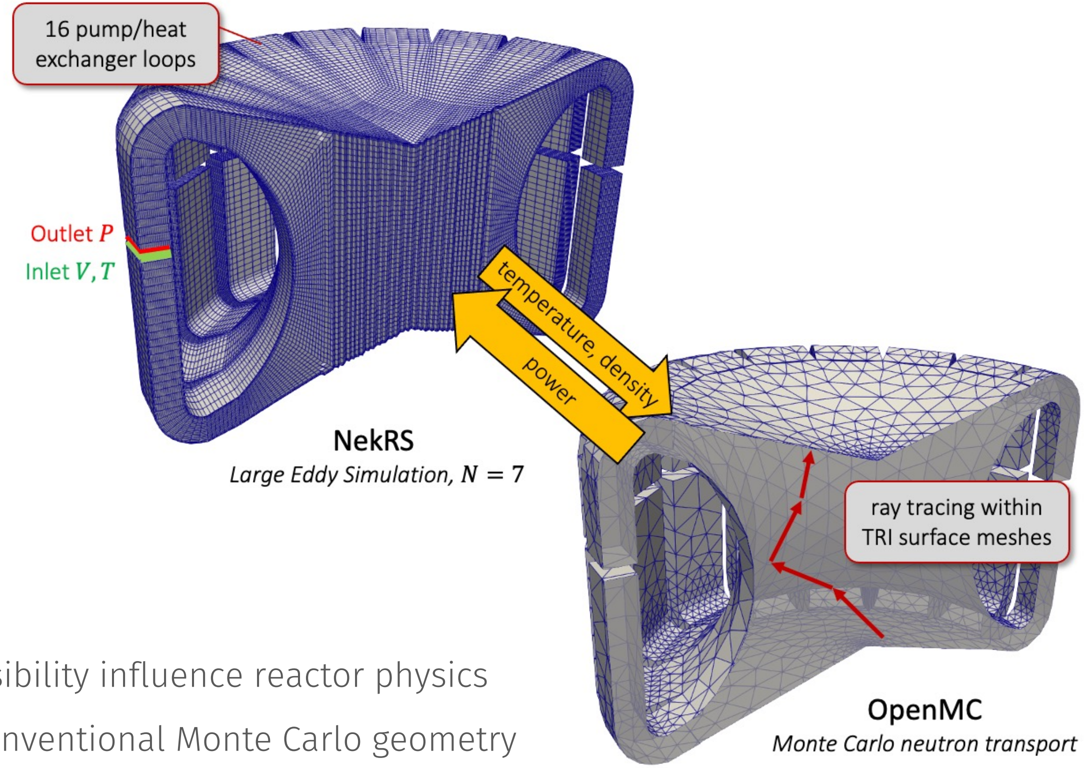


HTGRs


TRISO homogenization &
power resolution
fuel compact
(power)
3-D fuel heat
conduction
1.5-D fuel heat
conduction
Reduced dimensionality
underpredicts T
Homogenization
underpredicts T
Fuel
Buffer
IPyC
SiC
OPyC
Matrix
Homogeneous
Average temperature (K)
Power (W)
1250
1200
1150
1100
1050
1000
950
900
850
800
750
50
100
150
200
250
300
350
400
Underresolved power
underpredicts T
Radial
discretization
Azimuthal
discretization
$n_r = 8, n_t = 8$
$n_r = 4, n_t = 8$
$n_r = 2, n_t = 8$
$n_r = 1, n_t = 8$
$n_r = 8, n_t = 4$
$n_r = 8, n_t = 2$
$n_r = 8, n_t = 1$
Heat Source (W/m³)

Applications

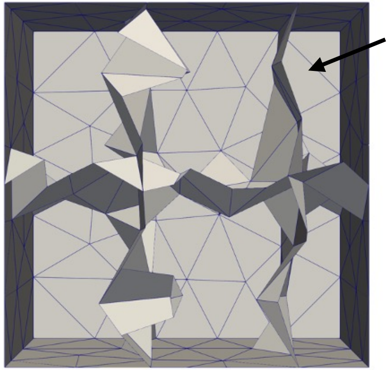
High Temperature Gas Reactors	3D/1D Multiscale Coupling
Pebble Bed Reactors	Pressurized Thermal Shock
Molten Salt Reactors	Fluid-Structure Interaction
Sodium Fast Reactors	Fusion Components
Lead Fast Reactors	Physics-Informed Machine Learning



- Flow recirculation, stagnation, and compressibility influence reactor physics
- Vessel shape is difficult to construct with conventional Monte Carlo geometry

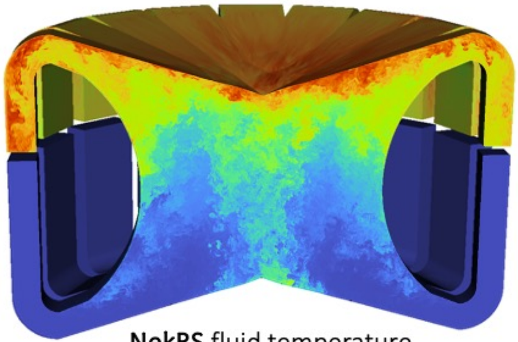
Adaptive Geometry

In collaboration with UKAEA; originally developed in Aurora (github.com/aurora-multiphysics/aurora)



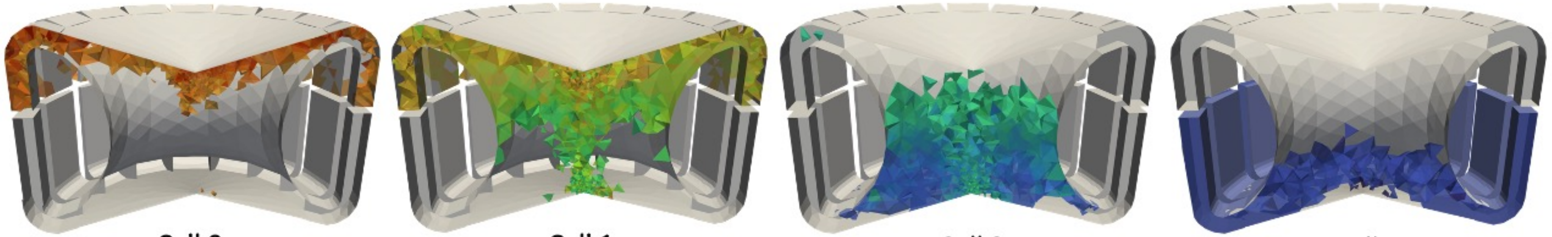
surfaces bounding each cell

Each region has constant temperature and density



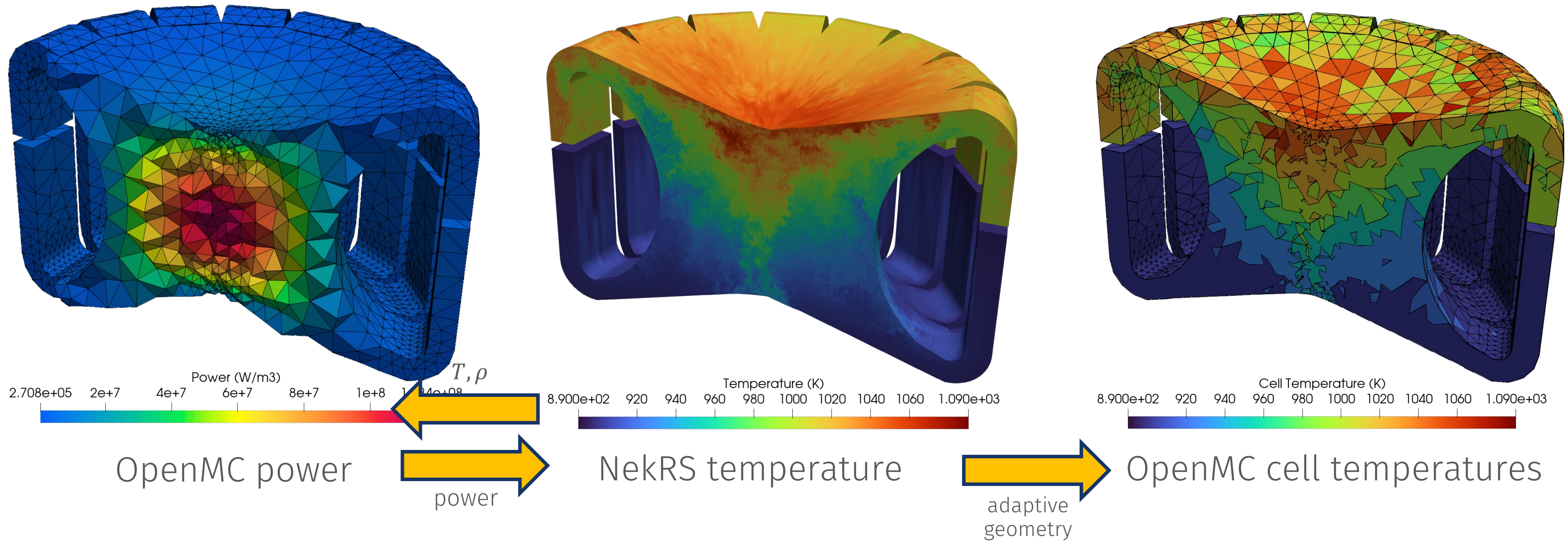
NekRS fluid temperature

Re-generate OpenMC geometry



Cell 0	**Cell 1**	**Cell 2**	**Cell 3**
elements with $T_0 < T < T_1$	elements with $T_1 < T < T_2$	elements with $T_2 < T < T_3$	elements with $T_3 < T < T_4$

Molten Salt Fast Reactor



- Unsteady turbulence coupled to neutron transport
- Dynamic on-the-fly geometry re-generation
- Straightforward refinement studies enhance robustness of multiphysics

Conclusions

- Multiphysics simulation can accelerate nuclear technology development

- Cardinal is designed to address challenges in high-fidelity multiphysics simulation:
    - Improved robustness and flexibility to reduce barrier-to-entry
    - Streamlined integration of multiscale techniques
    - Mixing CPU-GPU codes
    - Open source

- Many needs remain:
    - Experimental validation data!

Thank you!

Website: cardinal.cels.anl.gov

Cardinal

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Gateway for Accelerated Innovation in Nuclear (GAIN)
Nuclear Energy University Programs (NEUP)
Nuclear Regulatory Commission (NRC)

Innovative and Novel Computational Impact on Theory and Experiment (INCITE)
Argonne Laboratory Computing Resource Center (LCRC)
ASCR Leadership Computing Challenge (ALCC)
Idaho National Laboratory HPC
SummitPLUS (OLCF)

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