High-Fidelity Multiphysics in Fission

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Multiphysics in Nuclear Engineering

- Radiation transport
- Thermal-hydraulics
- Fuels, structural mechanics
- Chemistry & corrosion

Interactions:
- Doppler broadening, nuclide concentration
- Power distribution
- Geometry changes
- Heat transfer effectiveness
- Material properties
- Contact
- Fission product source term
- Activation
- Nuclide concentration
- irradiation-induced property changes, swelling, creep, depletion
- traction, thermal stress, diffusion
- activated materials
- 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

Radiation transport

Thermal-hydraulics

- Doppler broadening, nuclide concentration
- power distribution
- Irradiation-induced property changes, swelling, creep, diffusion
- nuclide concentration

Chemistry & corrosion

- material properties
- solubility, thermal diffusion, deposition
- activated materials

Material properties

- traction, thermal stress, diffusion
- irradiation-induced property changes, swelling, creep, diffusion
High-Fidelity Multiphysics

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

Monte Carlo radiation transport

Computational Fluid Dynamics
History and Challenges

Cardinal: High-Fidelity Multiphysics
History and Challenges

Cardinal: High-Fidelity Multiphysics
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

- Proof of concept to engineering analysis
- Small-scale to large-scale

Number of Publications

- Pressurized Water Reactor (48)
- Boiling Water Reactor (8)
- Pebble Bed Reactor (6)
- Molten Salt Reactor (5)
- Liquid Metal Reactor (5)
- Heat Pipe Reactor (4)
- Test Reactor (4)
- Toy Problem (4)
- Nuclear Thermal Propulsion (3)
- Prismatic Gas Reactor (2)
- Supercritical Water Reactor (2)
- Accelerator-Driven System (1)
- Critical Experiment (1)
- VVER (1)
- Dual-Fluid Reactor (1)
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

Iterative Methods

- Combine stochastic and matrix-based methods
  - Monte Carlo
  - $Ax = b$

- Inflexible algorithms excluded multiscale methods

Challenges “general purpose” use

Challenges effective reactor simulation
R&D Challenges

Data Transfers

- Highly manual process to build geometries and exchange data
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Iterative Methods

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- Inflexible algorithms excluded multiscale methods

Software and Parallelization

- Challenges "general purpose" use
- Challenges effective reactor simulation
- Challenges large-scale simulation

Prior work largely limited to CPUs

Near-total lack of open-source high-fidelity multiphysics software
History and Challenges

Cardinal: High-Fidelity Multiphysics
Cardinal

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

MOOSE

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

material science
tensor mechanics
uncertainty quantification
surrogate models
nuclear science
+ 35 modules

OpenMC
NekRS
Cardinal

Open Source

github.com/neams-th-coe/cardinal

MOOSE

Cardinal

material science

tensor mechanics

uncertainty quantification

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+ 35 modules

Scalable

Mixed CPU/GPU in-memory solvers

Plug into entire MOOSE ecosystem

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Multiscale

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OpenMC

NekRS
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Applications

High Temperature Gas Reactors
Pebble Bed Reactors
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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
Particle fuel requires special considerations to:

- Generate multigroup cross sections, $\Sigma$
- Apply temperature feedback
HTGRs
HTGRs

TRISO homogenization & power resolution

Fuel heat conduction methods

3-D fuel heat conduction

1.5-D fuel heat conduction

Underresolved power underpredicts $T$

Reduced dimensionality underpredicts $T$

Homogenization underpredicts $T$
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

- Flow recirculation, stagnation, and compressibility influence reactor physics
- Vessel shape is difficult to construct with conventional Monte Carlo geometry
Each region has constant temperature and density.
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

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