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Title: One Click Multiphysics for Nuclear Reactors

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One Click Multiphysics for Nuclear Reactors

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2024 MCNP User Symposium
August 19-22, 2024

Outline

- Code Development:
  - Coupling MCNP and Abaqus
  - LANL’s computational code for nuclear reactor modeling and simulations
- Neutronics/Heat Transfer Results:
  - Godiva Sphere
  - Godiva Refracted with Water
  - ZEBRA
  - DEIMOS
- Conclusions and future work

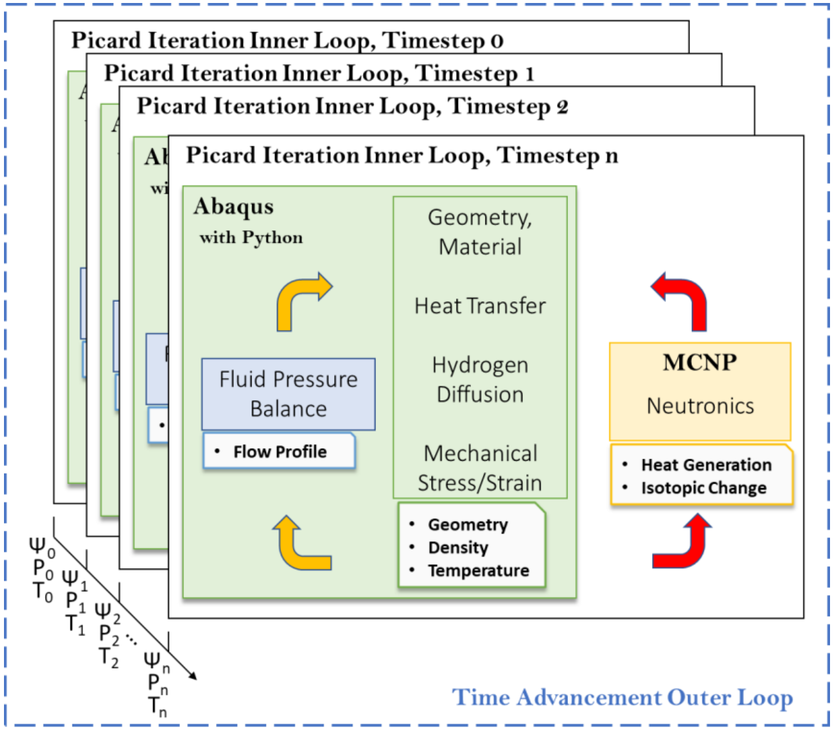
Project Description

- We are developing a multiphysics framework for advanced reactor design and analysis.

- Four physics are performed in a fully automated time-dependent sequence for nuclear reactor design tasks.
  - neutronics, heat transfer, thermomechanics, and mass diffusion

- A Python code is developed to loosely couple two gold standard codes for multiphysics reactor simulations.
  - **MCNP**:
    - Monte Carlo particle transport; LANL code
    - neutronics
  - **Abaqus**:
    - Finite Element Analysis; commercial code
    - heat transfer, thermosmechanics, and mass diffusion

One Click MCNP/Abaqus Multiphysics for Nuclear Reactors



- The MCNP and Abaqus capabilities have been proven for many years to be reliable, robust, and accurate in various mission-critical applications.
- MCNP and Abaqus are heavily utilized and routinely **validated** for many real-world applications.

Loosely Couped Multiphysics Approach

- Pros:
  - Existing single-physics codes can be reused, saving time and resource in code development.
  - By using well-validated individual codes that are known to produce accurate results in their respective domains, the overall confidence in the multiphysics simulation results is increased. This ensures that each part of the simulation is reliable, contributing to the credibility and trustworthiness of the final integrated outcome.
- Cons:
  - The needs to transfer data between different codes can introduces significant overhead, impacting performance and computational efficiency.
  - Different finite element mesh models are used in different codes, requiring data mapping and resulting in reduced efficiency.

The same finite element mesh model is used in both MCNP and Abaqus, ensuring compatibility and streamlines data exchange between the two codes. MCNP and Abaqus are well-validated codes.

R&D Goals

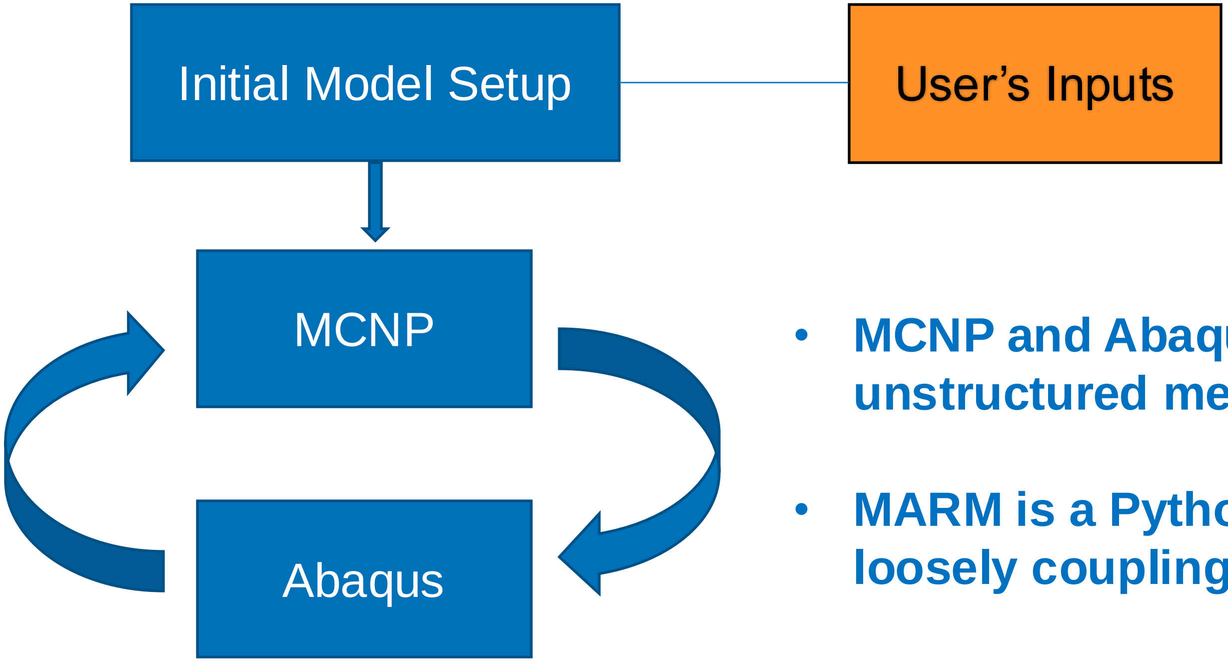
- FY24 (October 2023 – September 2024)
  - Develop a computational tool for neutronics & heat transfer multiphysics reactor simulations.
  - Create test problems (unstructured mesh models).

- FY25 (October 2024 – September 2025)
  - Add thermomechanics and mass diffusion
  - Code verification (comparison with another code -- NEAMS)
  - Code validation (comparison with experiment data)
    - SNAP-10, Clementine, KRUSTY, Deimos

Expected Results: A computational tool that can be used to execute nuclear reactor design tasks with high-fidelity results but with minimal user intervention.

MARM Framework

MARM = **M**CNP and **A**baqus based **R**eactor **M**ultiphysics

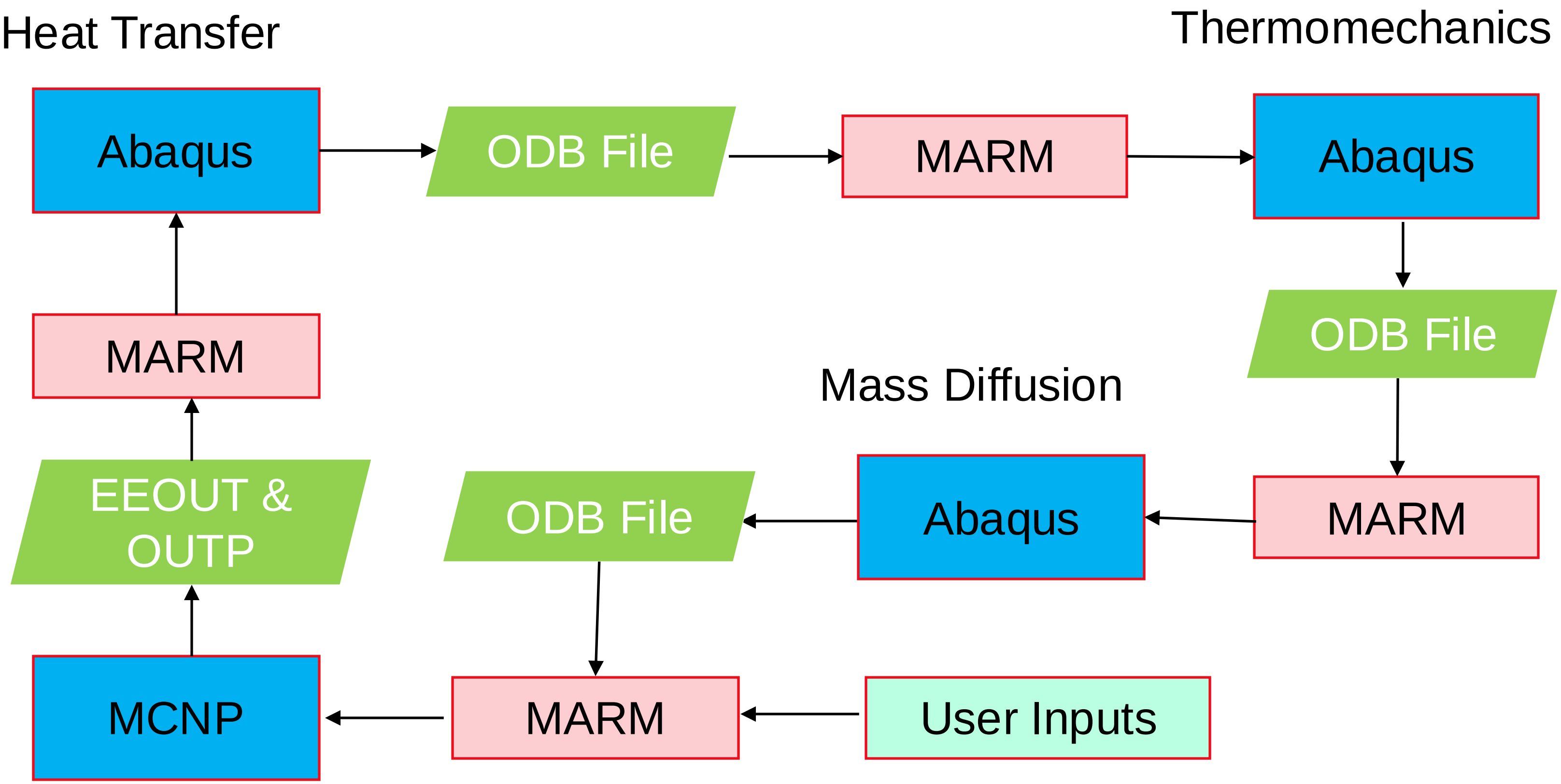


One-Click

- **MCNP and Abaqus use the same unstructured mesh geometry models.**
- **MARM is a Python code developed for loosely coupling MCNP/Abaqus.**

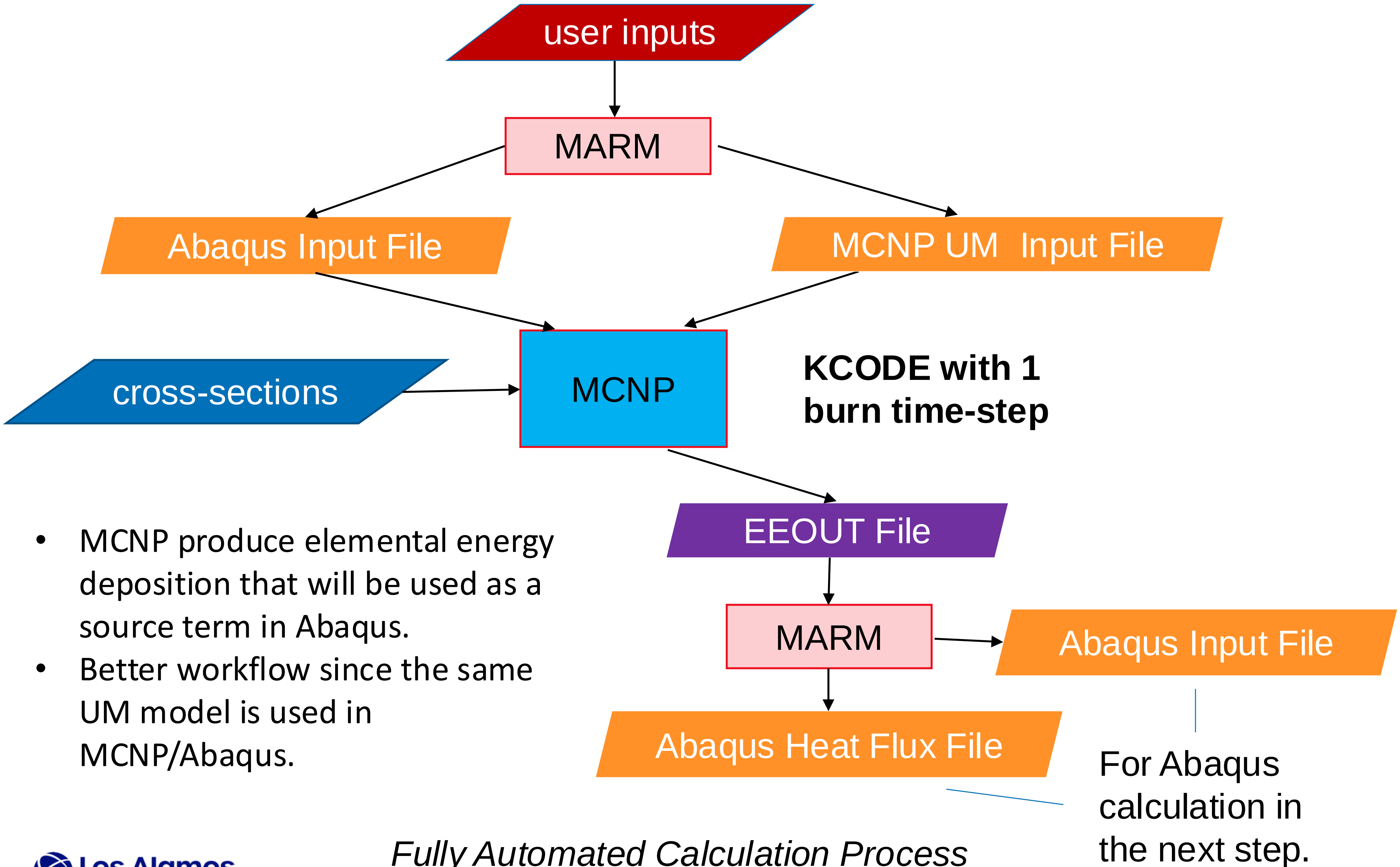
MARM is EAR export controlled and is available for government use.

Loosely Coupled MCNP and Abaqus Codes



- Coupled neutron-photon transport and depletion/burnup are in MCNP.
- Heat transfer, thermomechanics, and mass diffusion physics are in Abaqus.

Neutronics/Heat Transfer Coupling: Initial Step



- MCNP produce elemental energy deposition that will be used as a source term in Abaqus.
- Better workflow since the same UM model is used in MCNP/Abaqus.

Fully Automated Calculation Process

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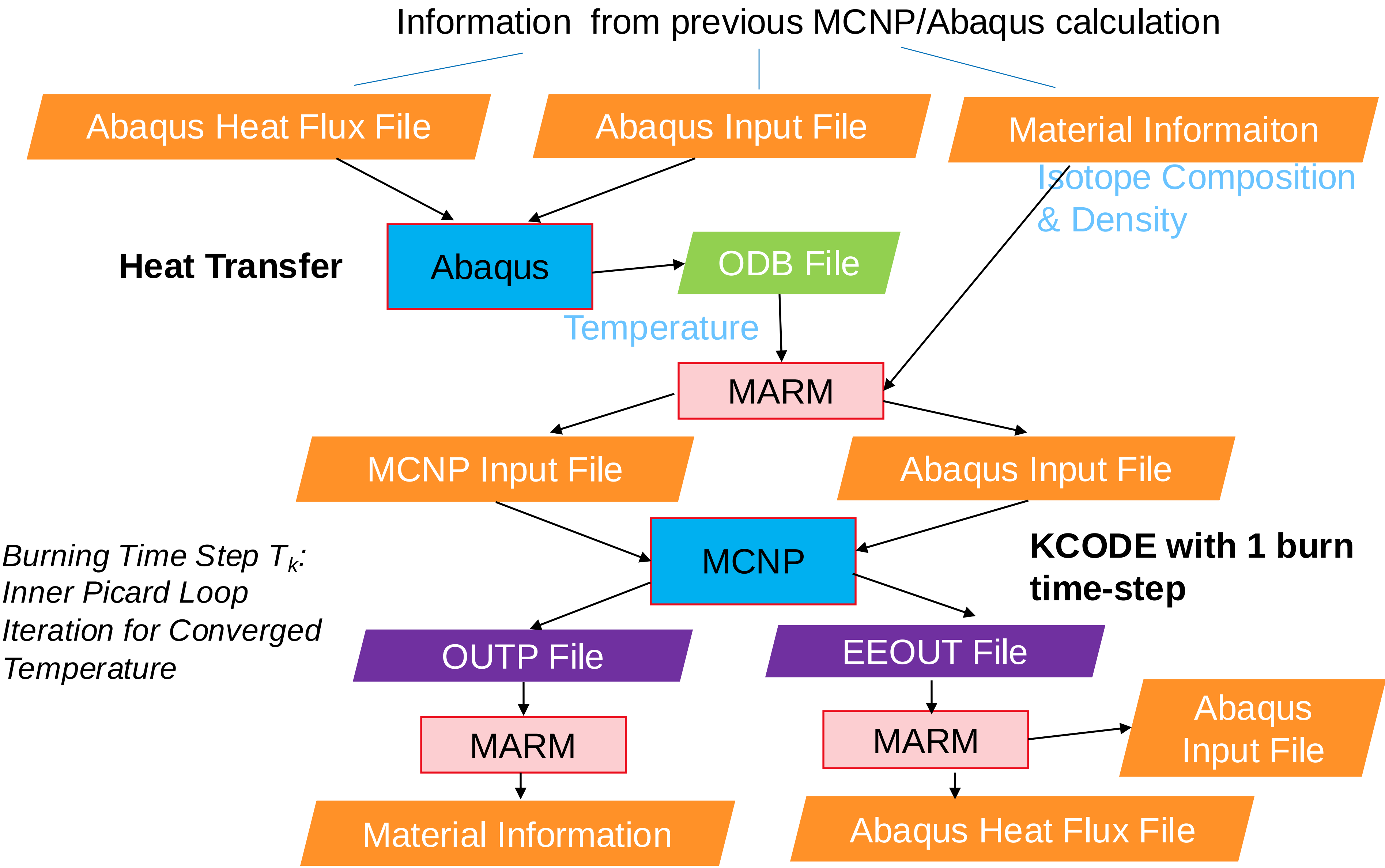
Neutronics/Heat Transfer Coupling: Inner Picard Loop



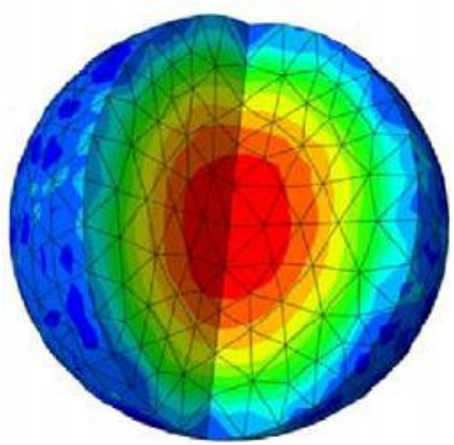
Fully Automated Calculation Process

GODIVA

Godiva

Godiva, high-enriched Uranium sphere used for criticality experiments

- Sphere is separated into different masses and is turned critical by an assembly joining all parts
- Produces short bursts on the MW scale



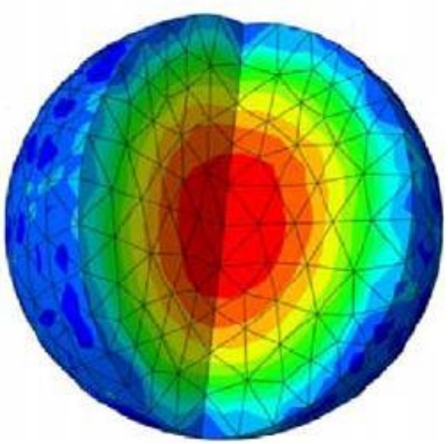
Modeling Godiva w/ MARM

MCNP Model

- KCODE : 130 cycles w/ 10,000 particles
- Burnup for 1 day at 75 W
- Begin w/ XS at 300 K

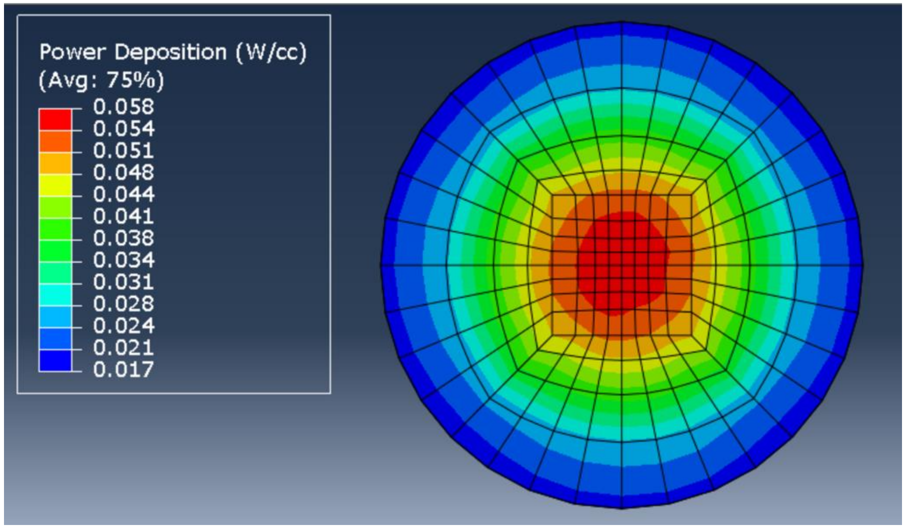
Abaqus HT Model

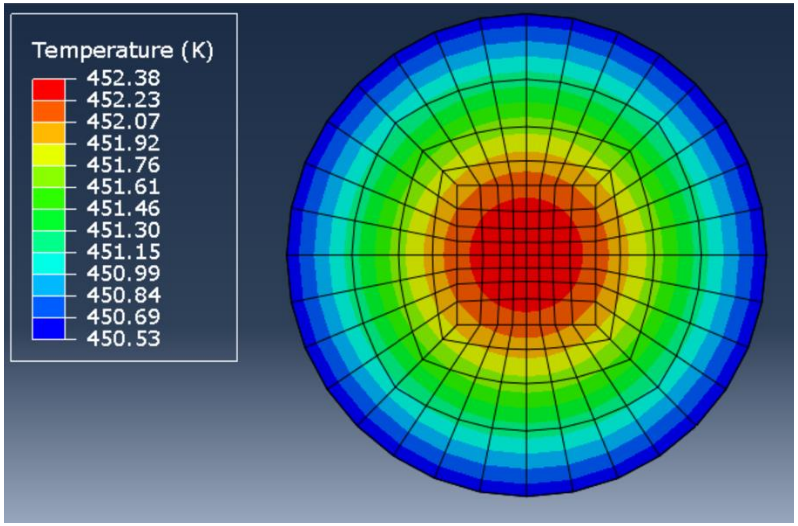
- Steady-state analysis
- Convection B.C of 5 W/m-K at outer surface
- I.C of 293 K



MCNP Power Deposition and Abaqus Temperature Profile

- Power deposition results w/ room temperature XS
- Profile is passed to Abaqus heat transfer simulation as the source term

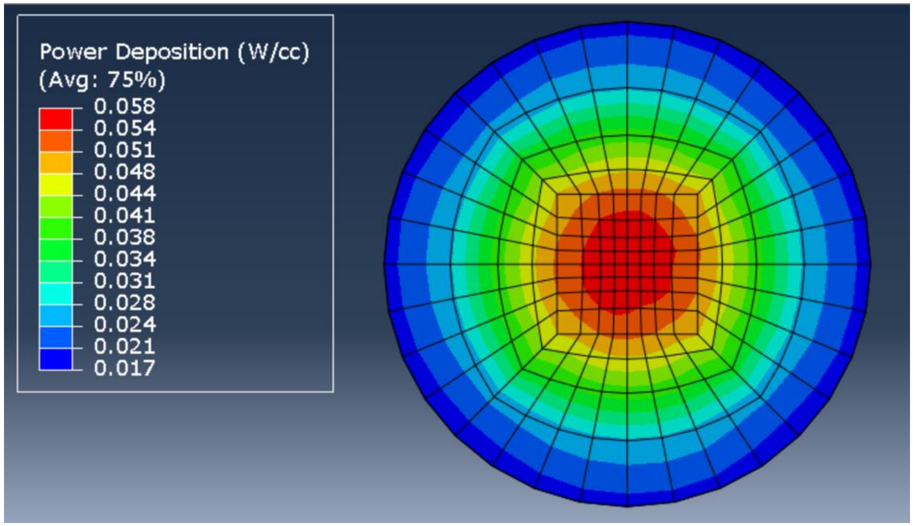


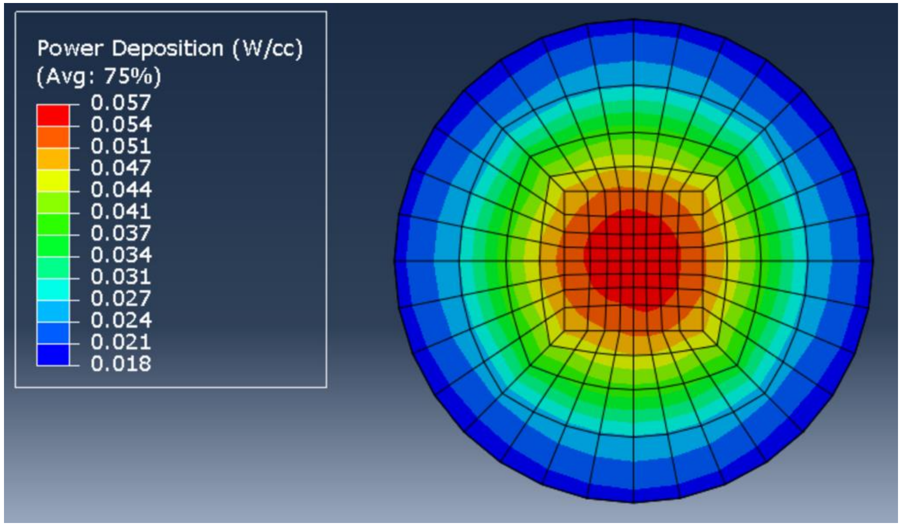


Neutronic/Thermal Feedback

- After the XS were updated with the new temperature profile, a new power deposition and keff result is found

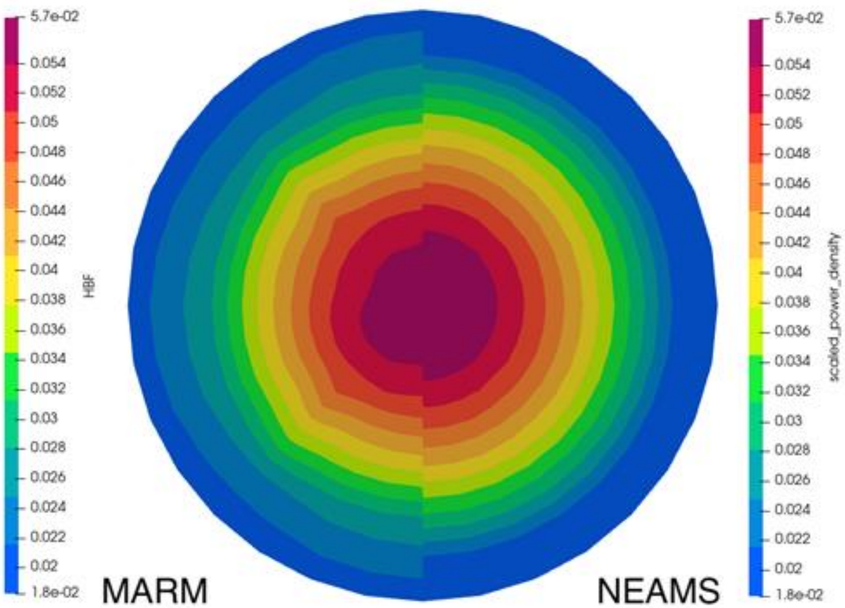
Keff for Iteration 1	Keff for Iteration 2
0.99815 ± 0.00058	0.99743 ± 0.00064

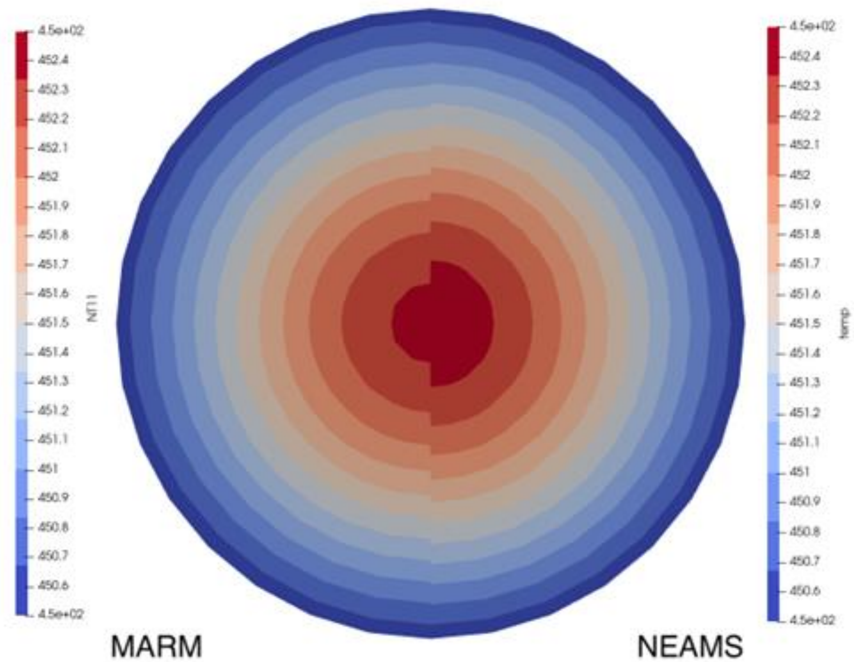




Comparing MARM and NEAMS

- Compare results of MARM model to NEAMS model that couples GRIFFIN and BISON
  - NEAMS (Nuclear Energy Advanced and Simulation) Workbench





Modeling Godiva Refracted with Water w/ MARM

Smaller HEU sphere surrounded by water.

MCNP Model

- KCODE : 130 cycles w/ 10,000 particles
- Burnup for 1 day at 7.5 kW
- Begin w/ XS at 300 K

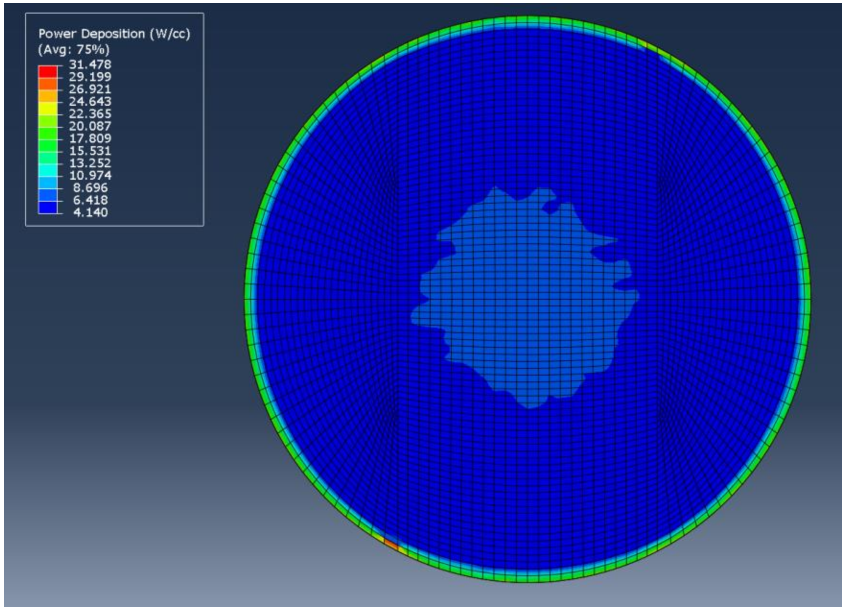
Abaqus HT Model

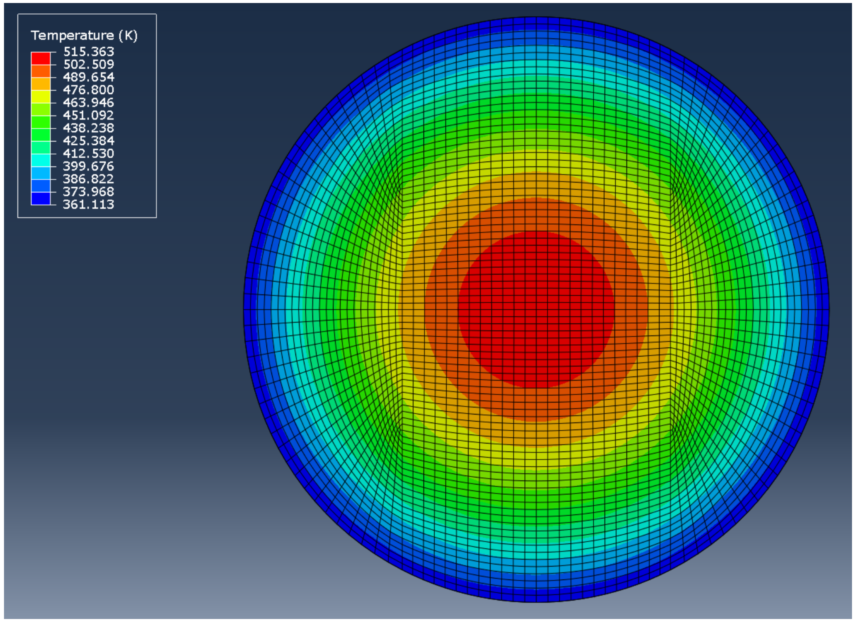
- Steady-state analysis
- Convection B.C of 5 W/m-K at outer surface
- I.C of 293 K

MCNP Power Deposition and Abaqus Temperature Profile

- Power deposition results w/ room temperature XS

- Profile is passed to Abaqus heat transfer simulation as the source term

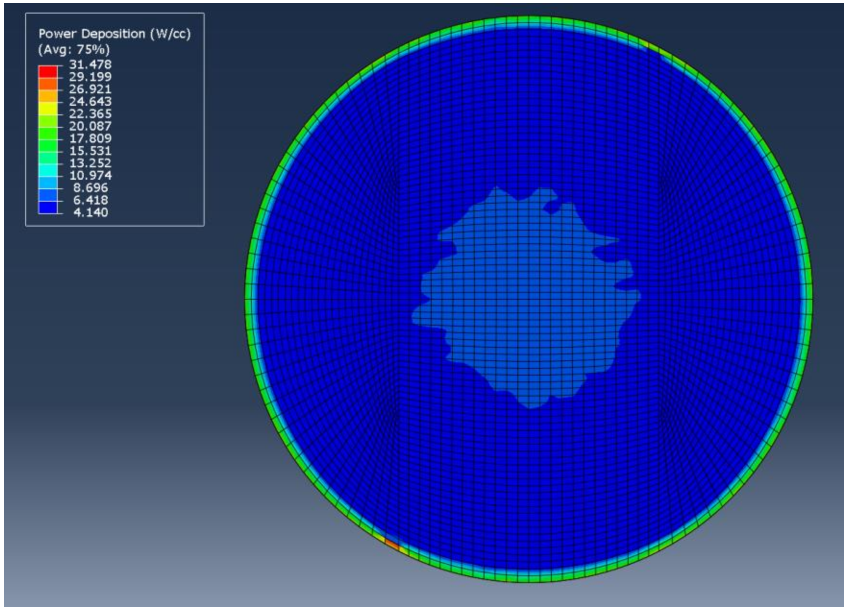


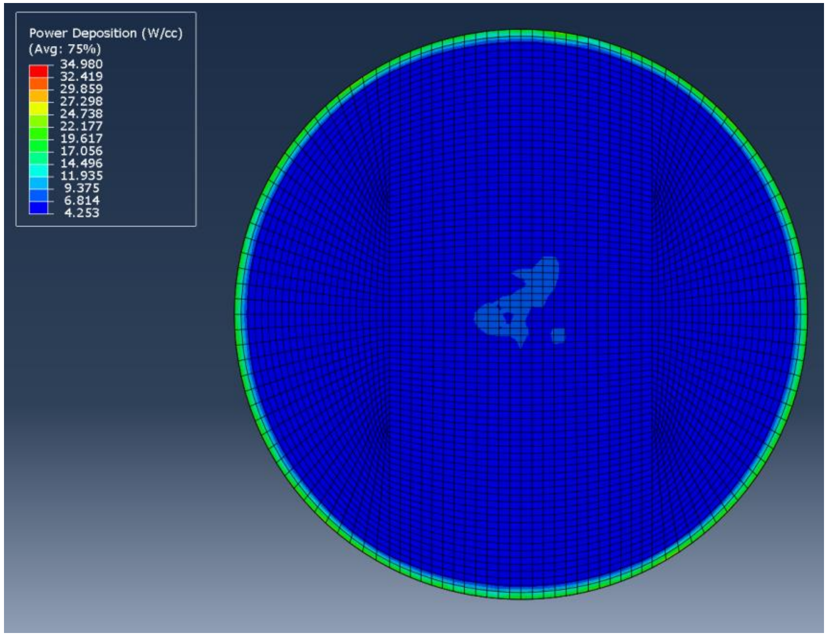


Neutronic/Thermal Feedback

- After the XS were updated with the new temperature profile, a new power deposition and keff result is found

Keff for Iteration 1	Keff for Iteration 2
0.99821 ± 0.00073	1.00224 ± 0.00073





Comparing MCNP UM to Experimental and CSG Results

Godiva

	Volume (cm^3)	Keff
UM	2,750.67	0.99815 ± 0.00058
CSG	2,797.22	0.998775 ± 0.000624
Experimental	--	1.000 ± 0.0010

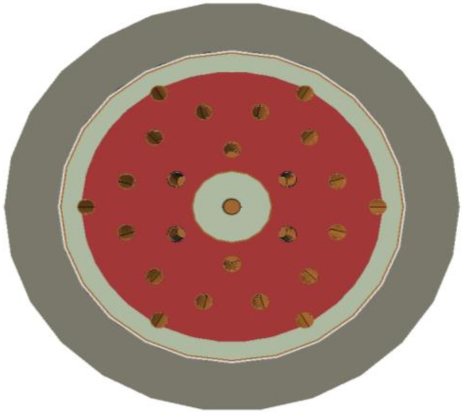
Godiva/ Water

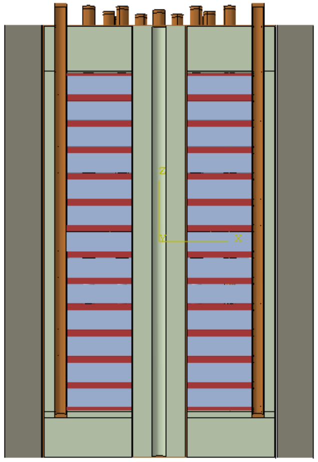
	Volume (cm^3)	Keff
UM	1,177.23	0.99821 ± 0.00073
CSG	1,179.10	0.99868 ± 0.00084
Experimental	--	0.9985 ± 0.0011

ZEBRA

ZEBRA

LANL's paper advanced reactor.





Materials:

- 14 fuel (U-$12.5Mo$) plates (in red)
- 13 moderator ($YH_{1.8}$) plates (in blue)
- Moly heat pipes (in orange)
- Inner and outer reflector (in gray)

Geometry:

- Active core weight: 425 kg
  - Fuel: 125 kg
- Diameter: 45 cm
- Height: 70 cm

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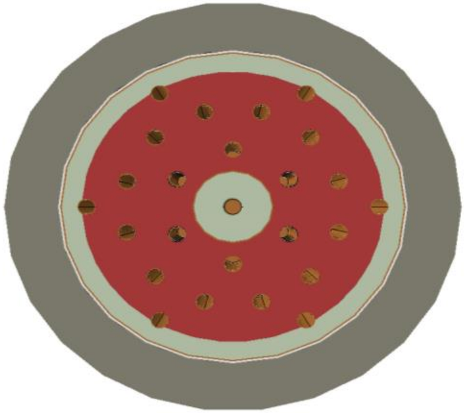
Modeling Zebra w/ MARM

MCNP Model

- KCODE : 130 cycles w/ 10,000 particles
- Burnup for 1 day at 50 kW
- Begin w/ XS at 300 K

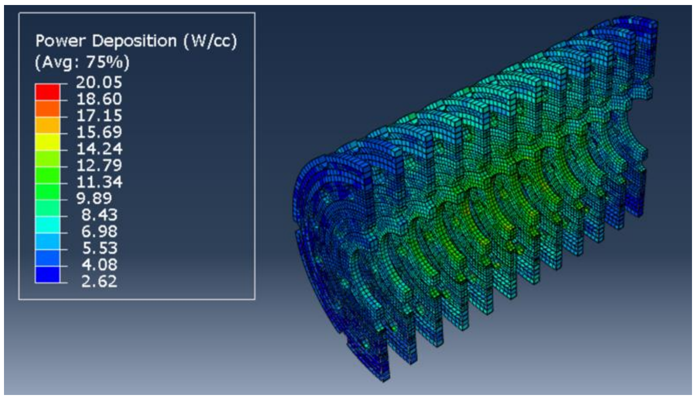
Abaqus HT Model

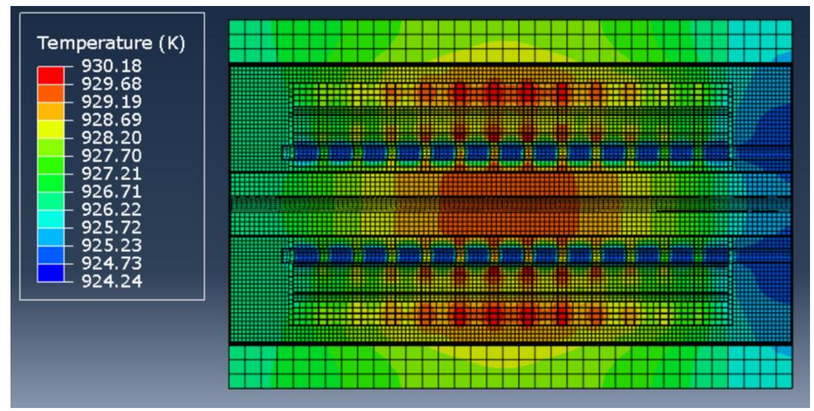
- Steady-state analysis
- Fixed temperature B.C of 925 K at heat pipes
- I.C of 293 K

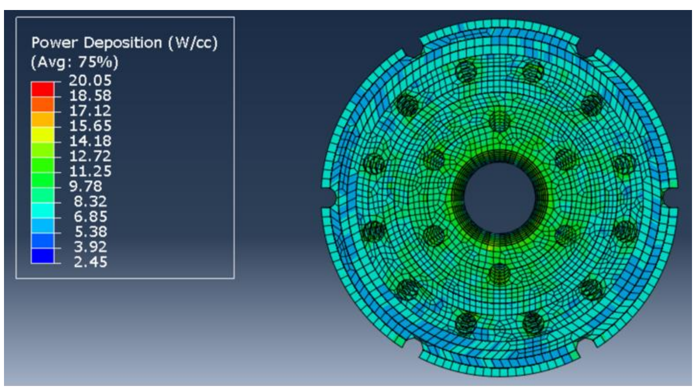


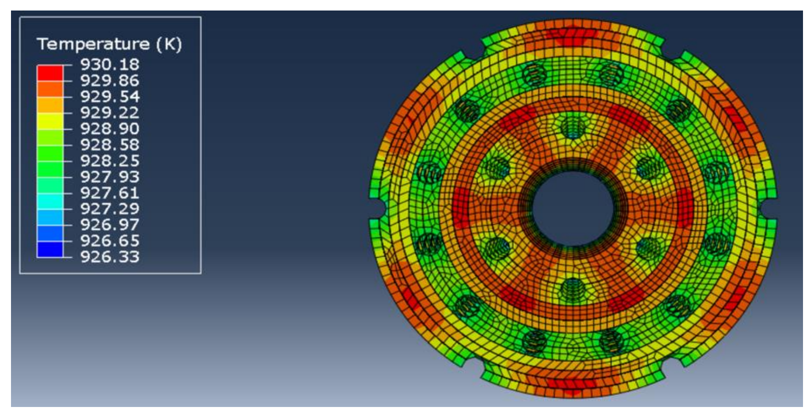
MCNP Power Deposition and Abaqus Temperature Profile

- Power deposition results w/ room temperature XS
- Profile is passed to Abaqus heat transfer simulation as the source term





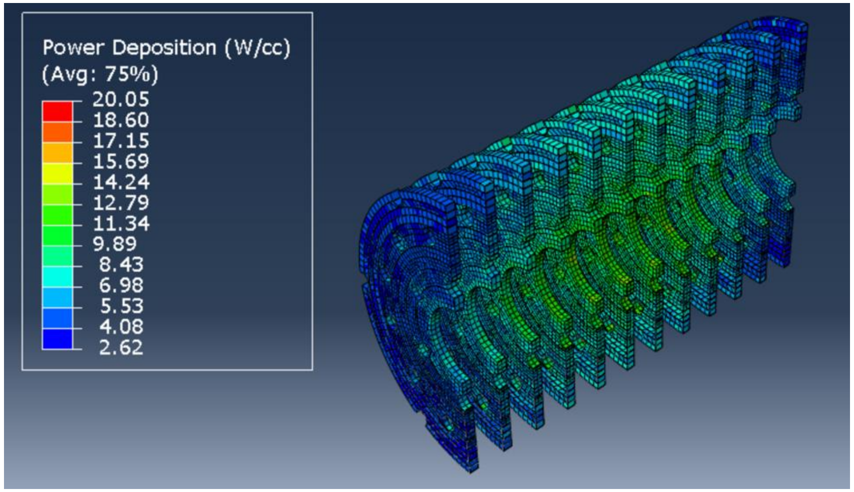


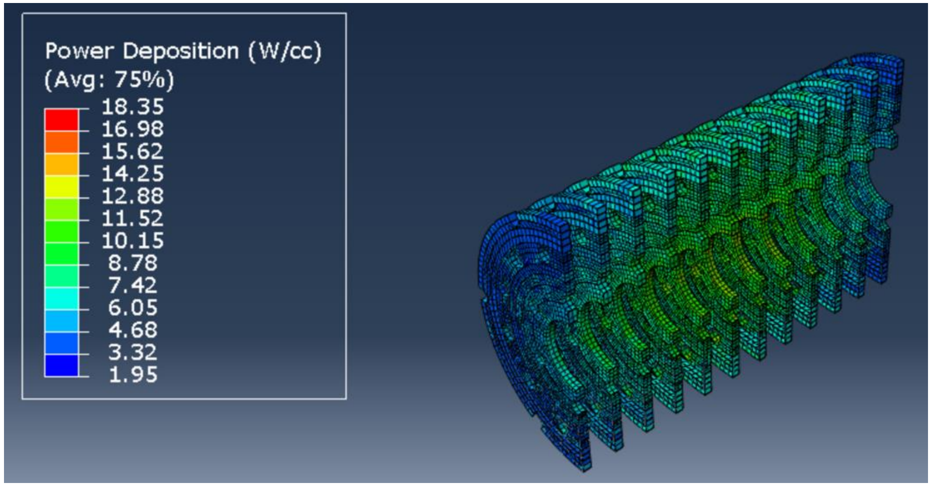


Neutronic/Thermal Feedback

- After the XS were updated with the new temperature profile, a new power deposition and keff result is produced

Keff for Iteration 1	Keff for Iteration 2
1.06418 ± 0.00077	1.05391 ± 0.00083

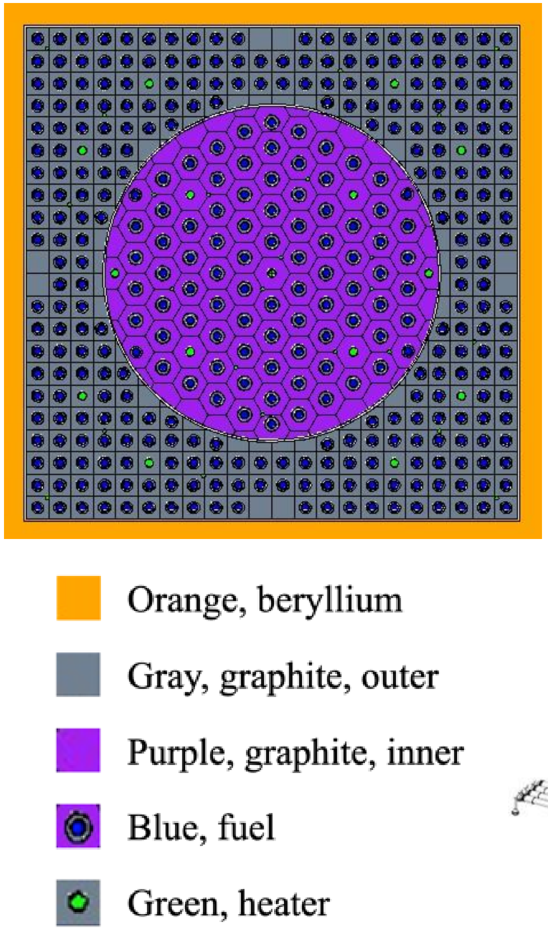


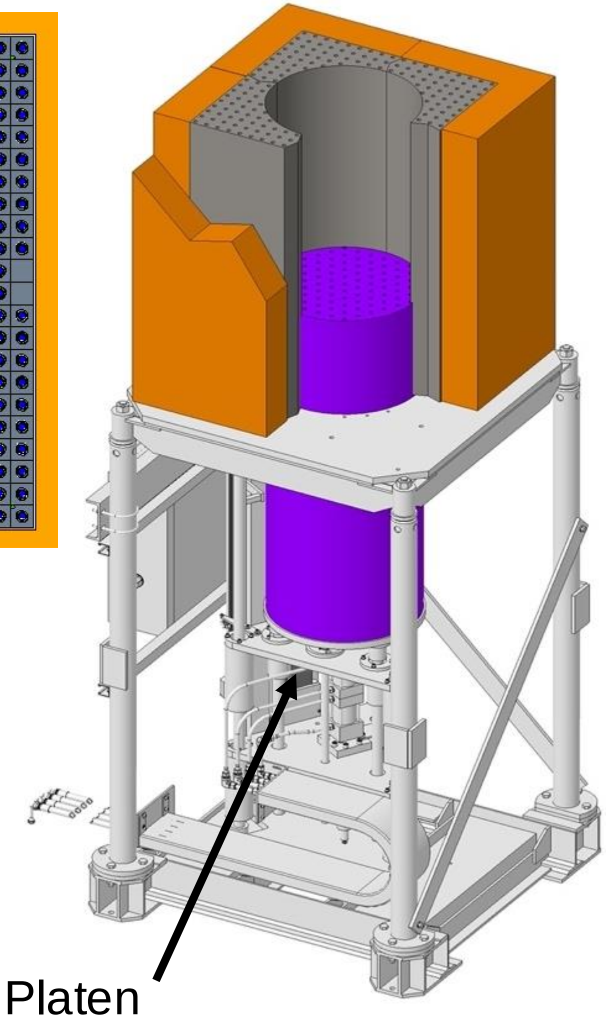


DEIMOS

DEIMOS

- Deimos, proposed critical experiment
  - Thermal/epithermal spectrum
  - Existing high-assay low-enriched uranium (HALEU) tri-structural isotropic (TRISO) particle fuel form in NCERC inventory
  - Reactivity temperature coefficient measurements via electric heating and control system designed at LANL
  - Predictive multiphysics modeling and simulation has been conducted





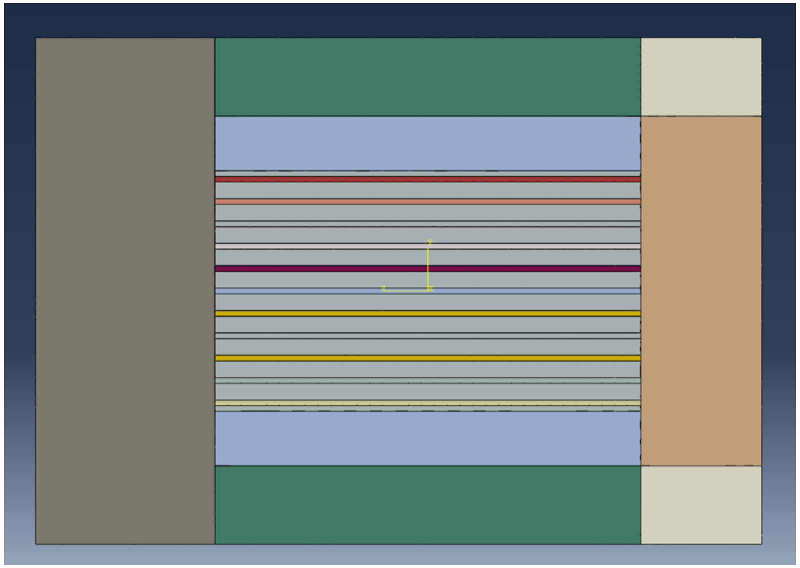
Modeling Deimos w/ MARM

MCNP Model

- KCODE : 130 cycles w/ 10,000 particles
- Burnup for 1 day at 5.5 kW
- Begin w/ XS at 300 K

Abaqus HT Model

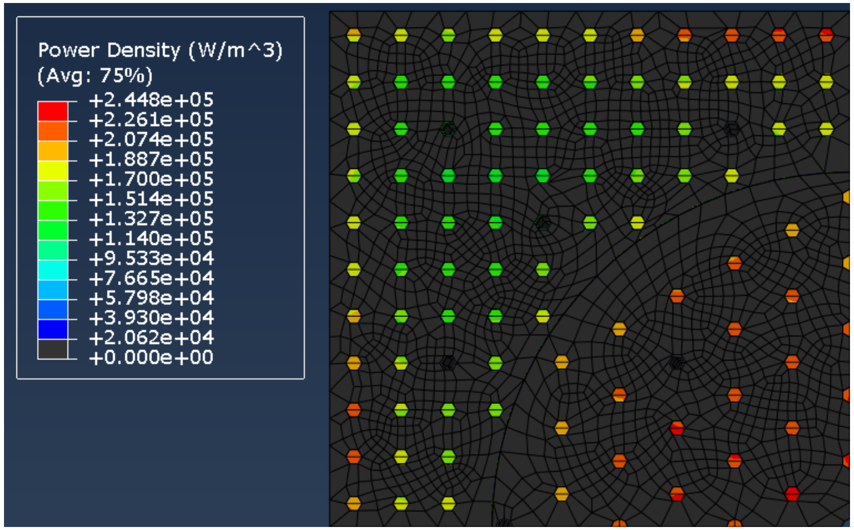
- Steady-state analysis
- Convection B.C of 5 W/m-K at outer surface
- I.C of 293 K

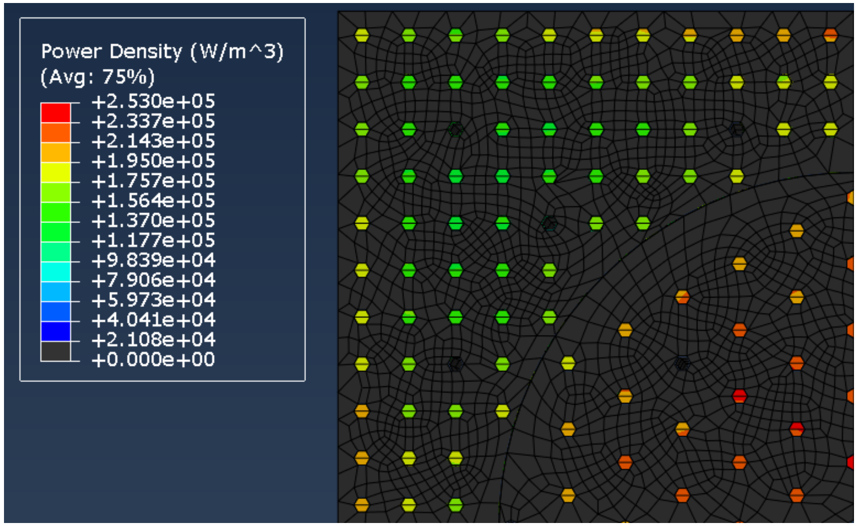


Neutronic/Thermal Feedback

- After the XS were updated with the new temperature profile, a new power deposition and keff result is produced

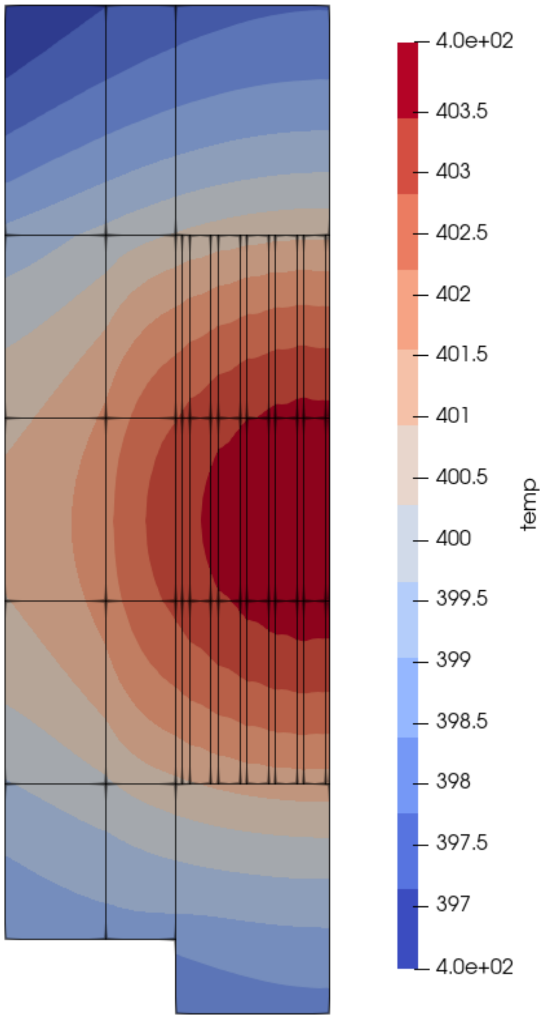
Keff for Iteration 1	Keff for Iteration 2
1.05700 ± 0.00081	1.05305 ± 0.00094



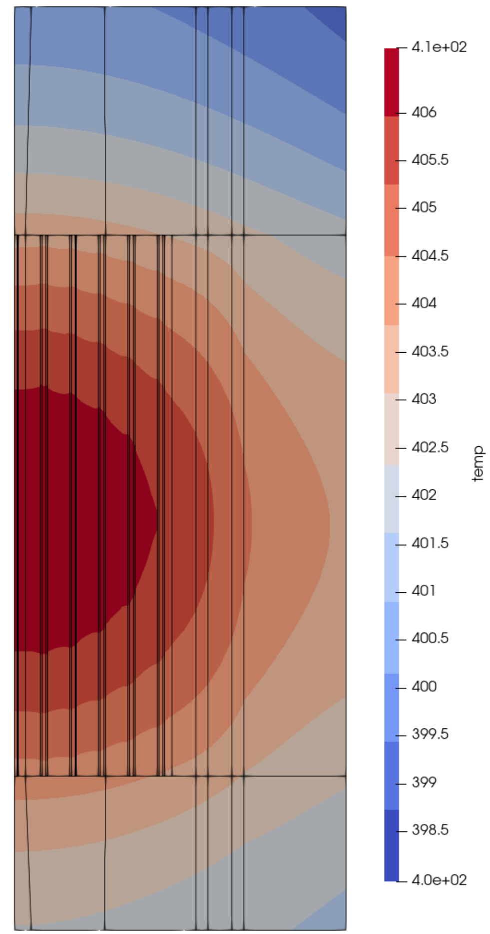


Deimos Temperature [K] Distributions

- 5.5 kW total fission power, steady-state simulation

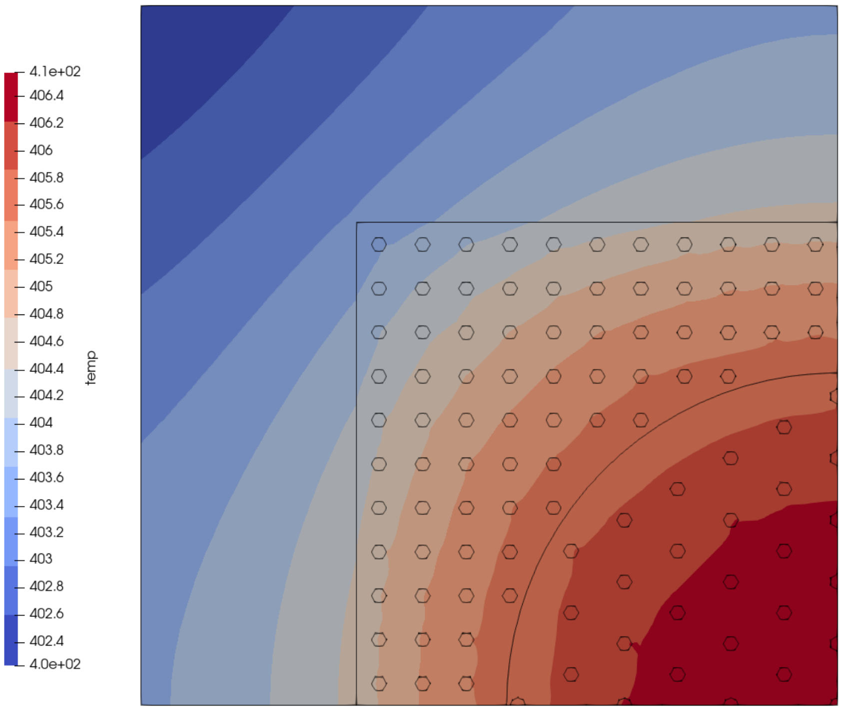


NEAMS

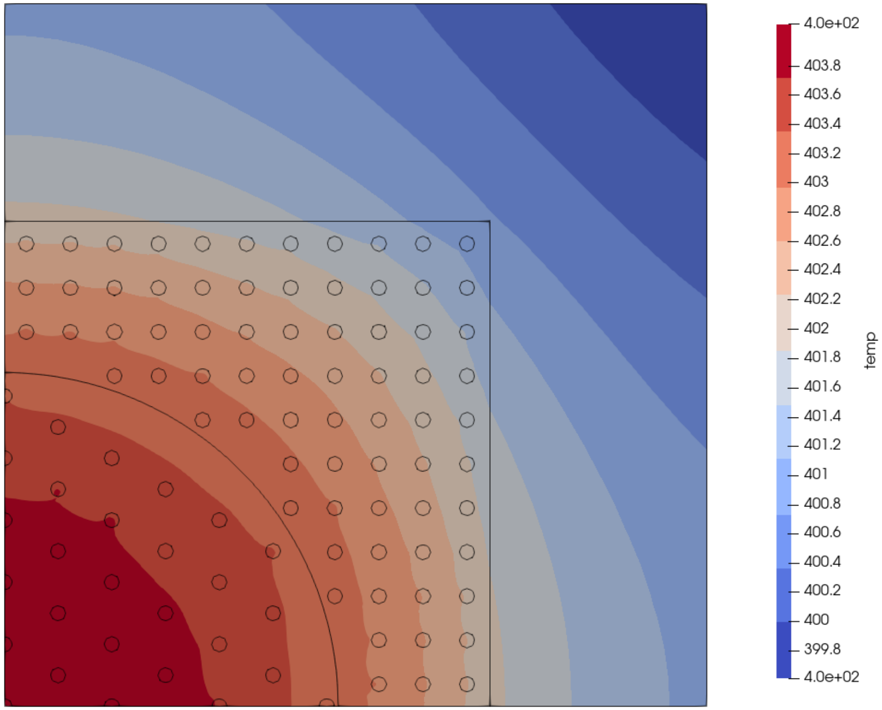


MARM

Deimos Temperature [K] Distributions

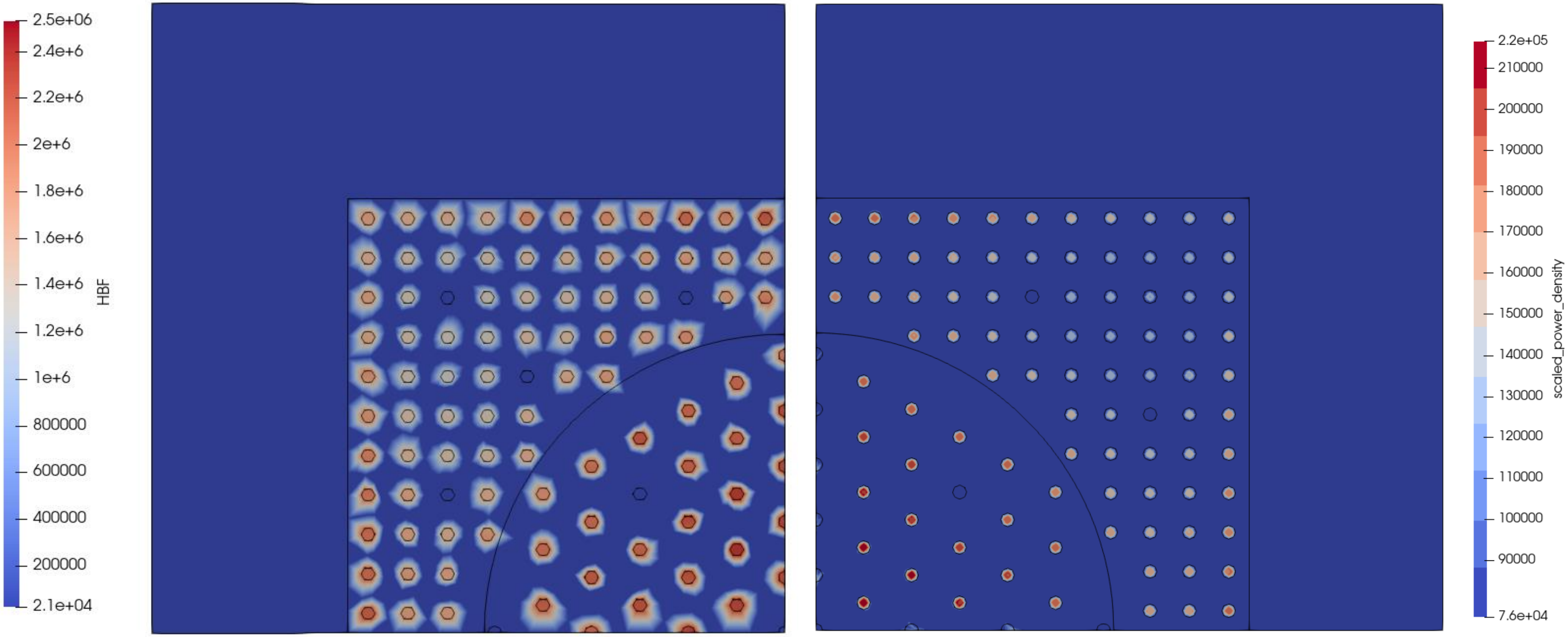


MARM



NEAMS

Deimos Power Density [W/m^3] Plots



MARM

NEAMS

White circles around each pin due to Paraview interpolation when plotting csv data

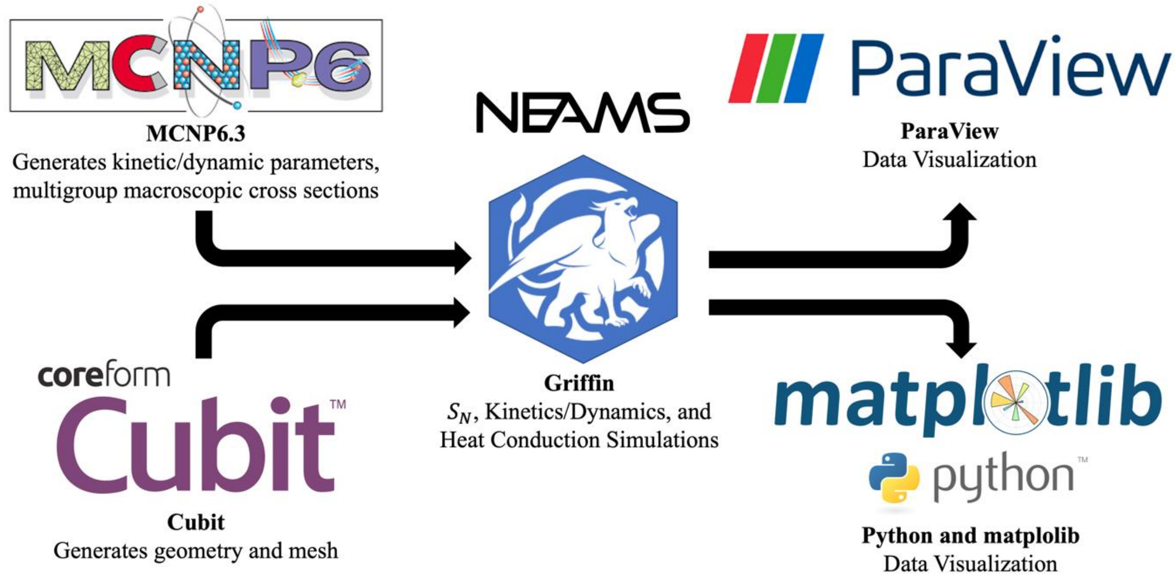
Conclusions and Future work

- We are developing a loosely coupling MCNP/Abaqus framework for advanced reactor design and analysis.
- Neutronics and heat transfer multiphyiscs were coupled. The code was tested for Godiva, Godiva refracted with water, ZEBRA, DEIMOS.

- Future Work:
  - Implement additional physics: thermosmechanics and mass diffusion.
  - Code-to-code verification (MCNP/Abaqus vs MCNP/BISON)
  - Full system validation: SNAP-10, Clementine, KRUSTY, DEIMOS

Backup Slides

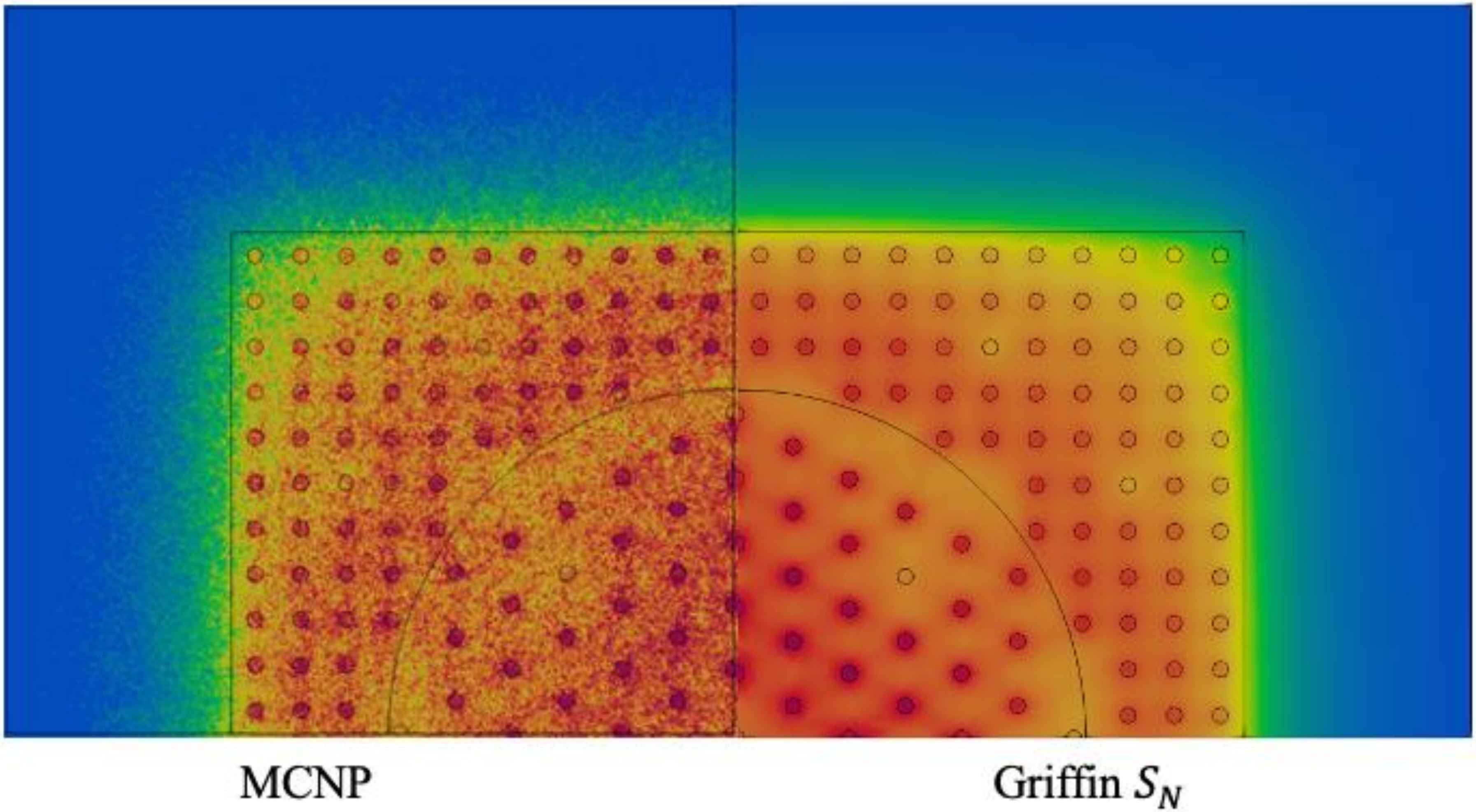
NEAMS Framework



Nuclear Energy Advanced Modeling & Simulation (NEAMS) Framework

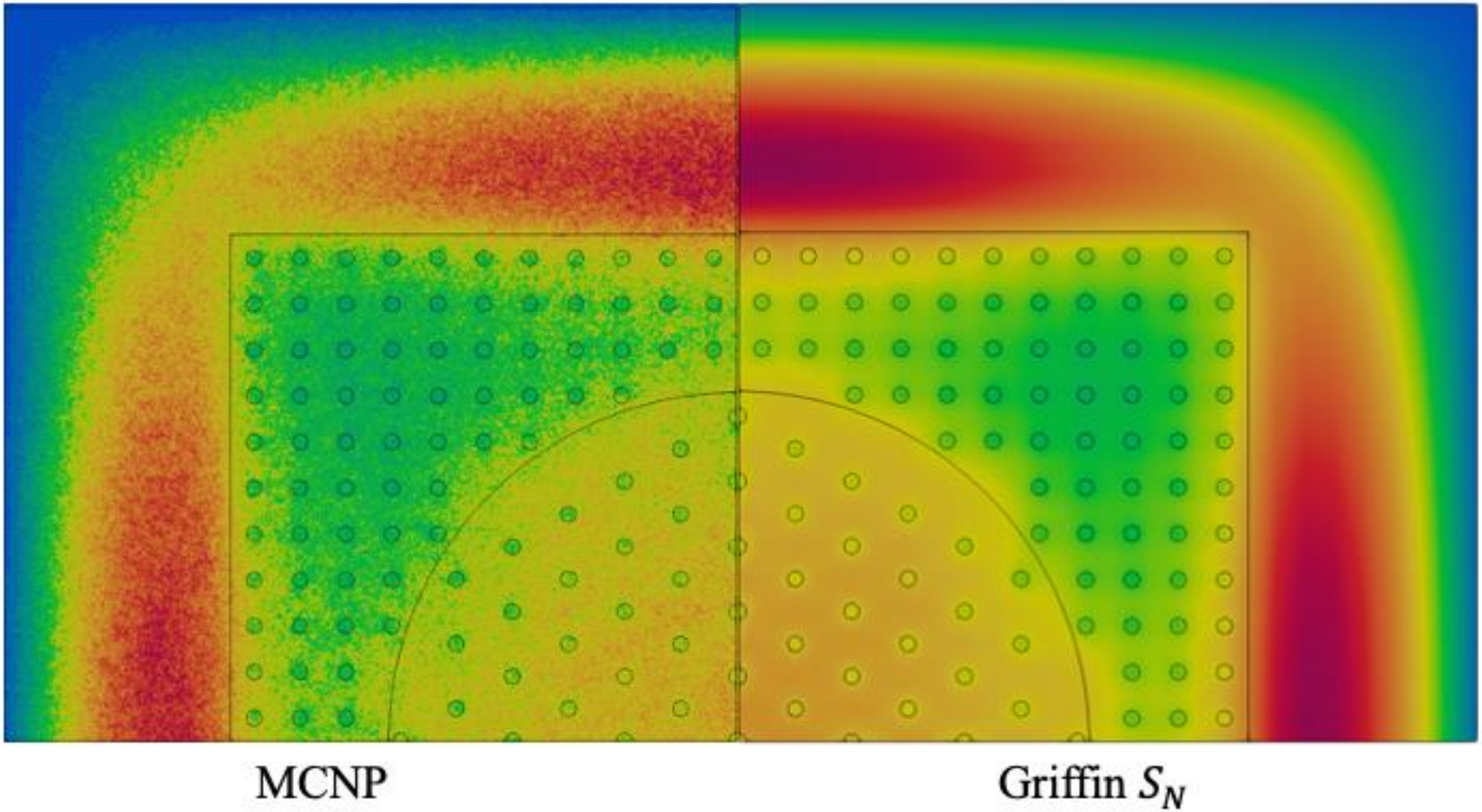
Tool for Optimization and Group-structure Analysis (TOGA)

MCNP CSG and Griffin Fast Flux Comparison for DEIMOS



(2.2313 MeV < E < 19.64 MeV)

MCNP CSG and Griffin Thermal Flux Comparison for DEIMOS



($\boldsymbol{E}$ < 0.54 eV)