



U.S. DEPARTMENT OF
ENERGY

Nuclear Energy

SHARP Multiphysics

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**Advanced Reactor Modeling and Simulation Workshop
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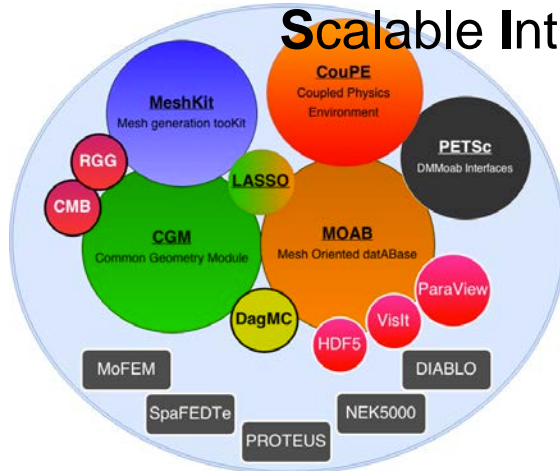
Interrelated Phenomena over a range of Length and Time Scales

- Among all of reactor technologies being pursued by industry and DOE-NE R&D programs, modeling & simulation needs vary
- Reactor design and safety performance requires analysis of a wide range of length and time scales of interrelated physics
 - Reactivity response to minor geometric changes during transients in SFRs
 - Analysis of inherent safety and passive decay heat removal for large pebble bed or prismatic block HTGRs
 - Intrinsic connection between neutronics and flow field in liquid fueled MSR
- Need for a **mission-agile toolkit** for reactor core analysis
 - **Multiphysics, multiresolution, multiscale**



SHARP Multiphysics Interface: SIGMA

Scalable Interfaces for Geometry and Mesh-based Applications



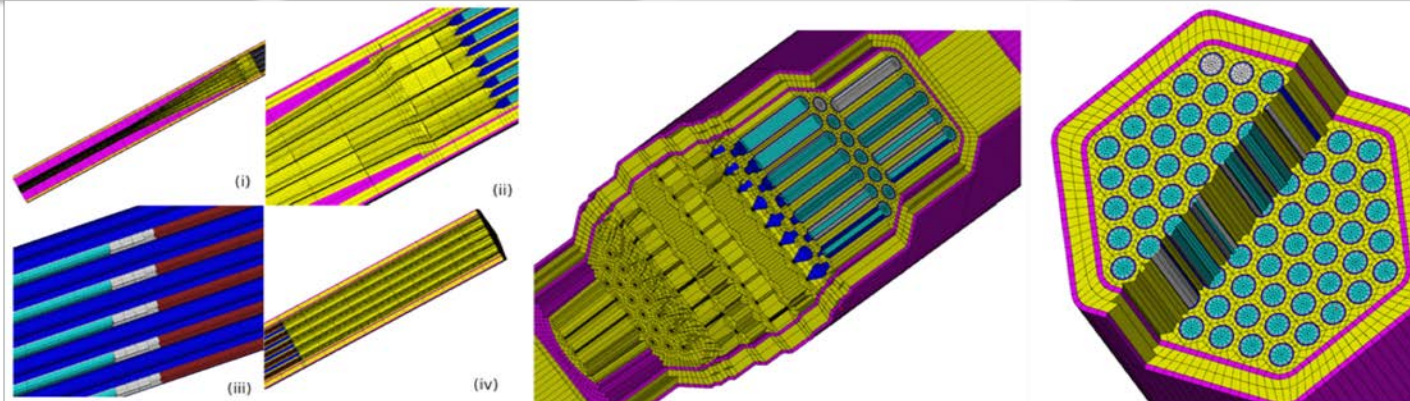
- CGM: ACIS and OCC geometry models
- MeshKit: Optimal mesh for complex geometries with extensions to use Cubit/Tetgen/Netgen
- MOAB: Scalable array based for access and storage of mesh data on entities
- CouPE: Coupled physics global nonlinear solvers based on PETSc for multiphysics solutions

Define
Geometry
(**CGM**)

Generate
Mesh
(**MeshKit**)

Discrete
Mesh
(**MOAB**)

Coupled
Physics
(**CouPE**)

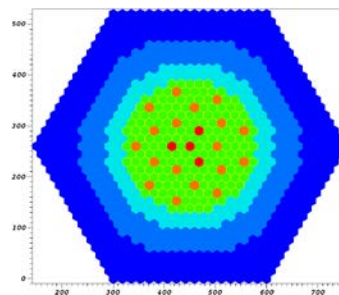




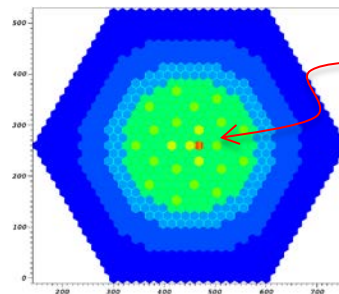
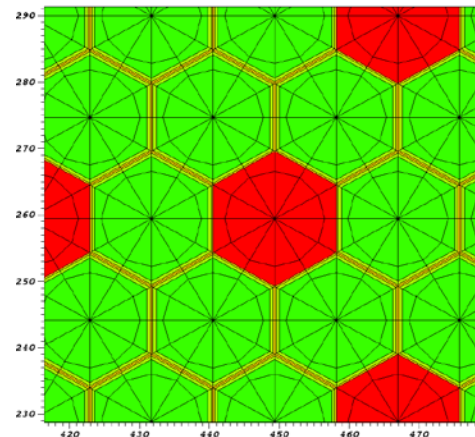
SHARP – Multiresolution

■ Neutronics with mixed local resolutions

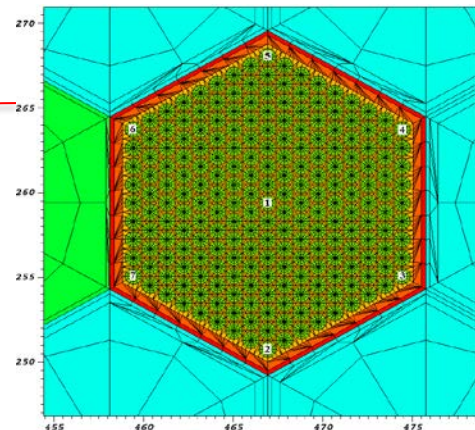
- Model A - Homogenized assembly model (as generally considered in applications of current deterministic codes, notably DIF3D-VARIANT)
- Model B - Explicit representation of wrapper tube and inter-assembly sodium gap for all fuel regions
- Model C - Explicit pin by pin representation of a single assembly in the inner core, leaving a full material homogenization in all other assemblies



Model B

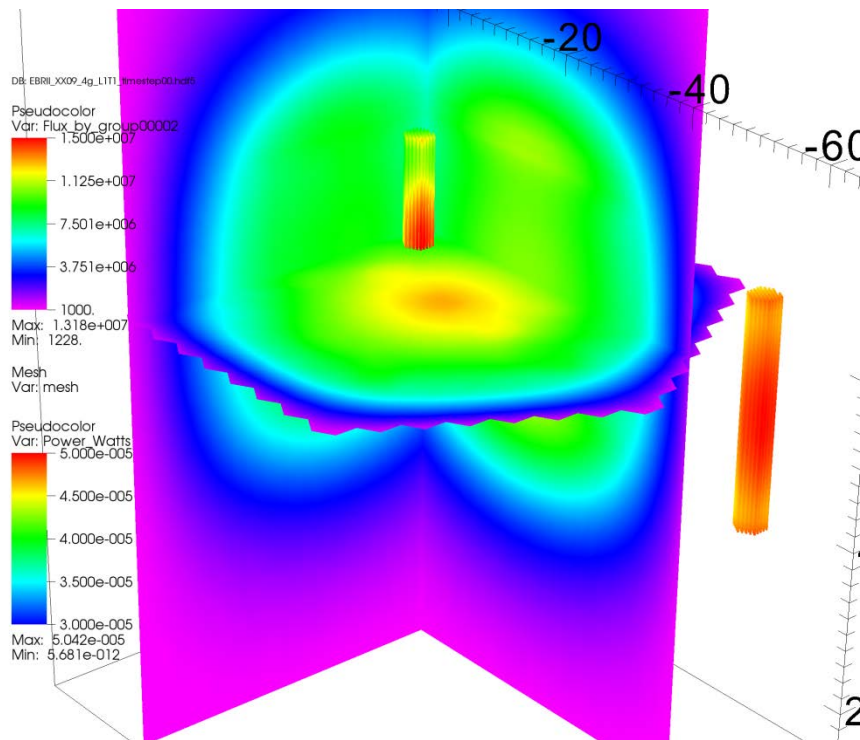


Model C

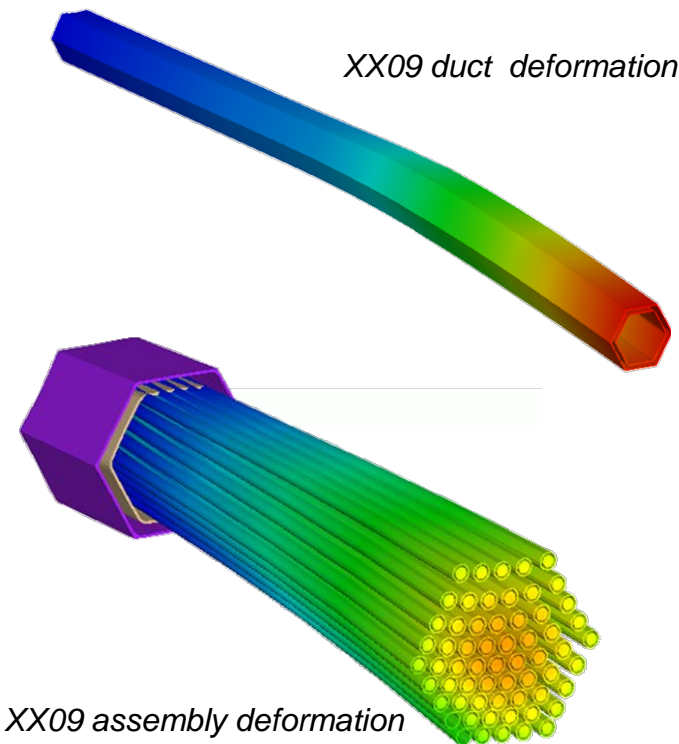




SHARP – Multiresolution (cont.)



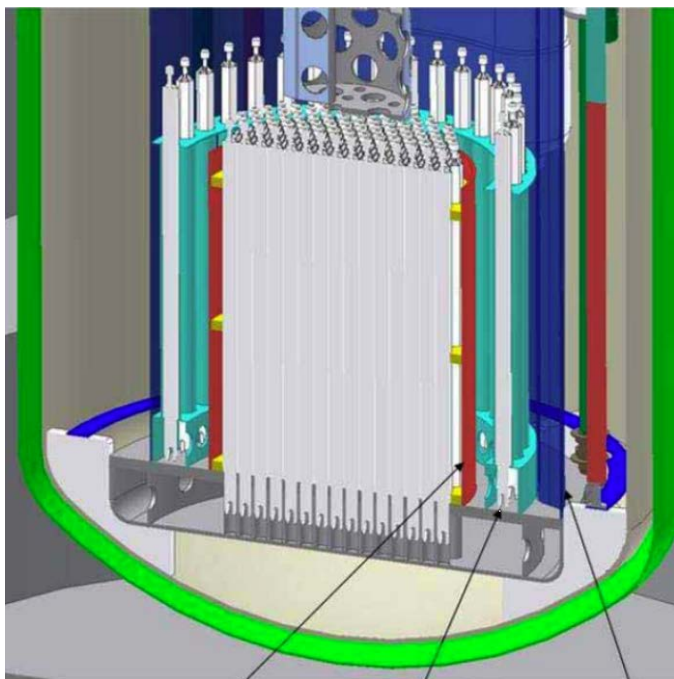
EBR-II power distribution, note XX09 assembly in the middle



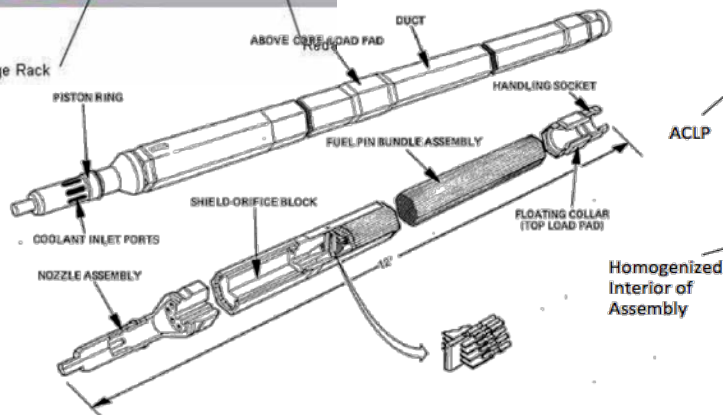
EBR-II simulations have demonstrated capability to mix fully heterogeneous regions (“pin-by-pin”) with homogenized assemblies.



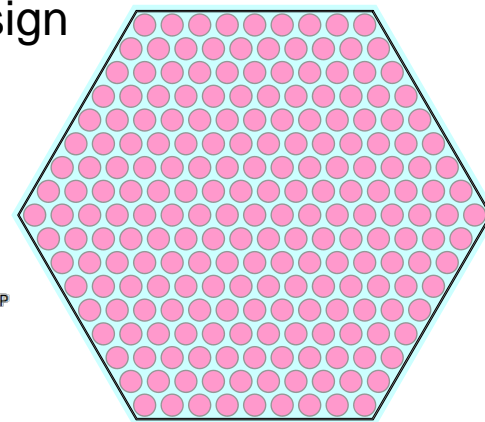
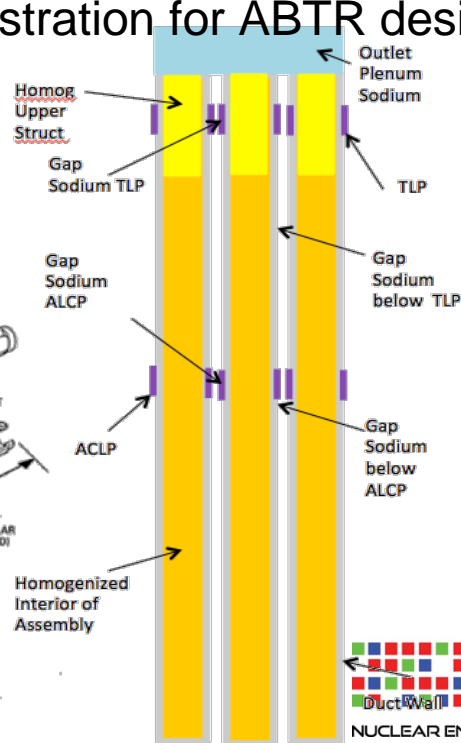
SHARP – Multiphysics SFR Core Deformation



*CAD model and
drawing of the
Advanced Burner
Test Reactor
(ABTR) core*



- Core thermal expansion is one of the primary reactivity feedback mechanisms for FR safety
- Geometry deforming due to temperature gradients in the presence of restraining contacts
- By appropriate design of the core restraint system, neutron leakage is enhanced
- Demonstration for ABTR design



Section of BB'



SFR Core Deformation: Neutronics Homogenization

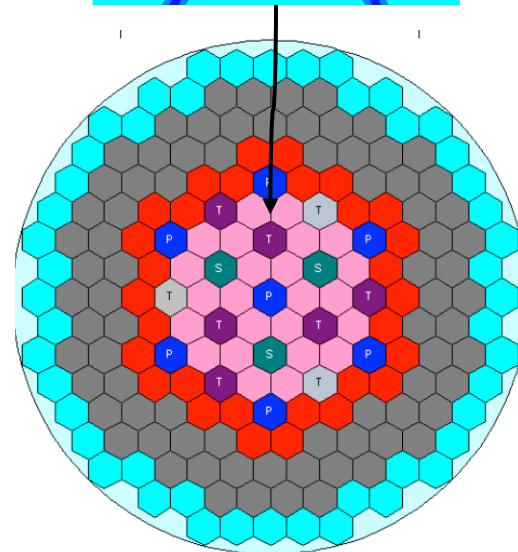
■ For the SHARP simulations of core structural deformations, want to:

- Explicitly model the duct walls
- Homogenize the interior pin bundle to reduce computational cost
- Not possible with conventional nodal transport tools (e.g. DIF3D)

■ Approach cross-verified by comparing to MCNP for various homogenization approaches

	Sum of All Control Rod Worths (Δk)
MCNP (1σ)	0.12061 \pm 0.00015
PROTEUS (33 groups)	0.12042
PROTEUS (70 groups)	0.12036
PROTEUS (116 groups)	0.12065

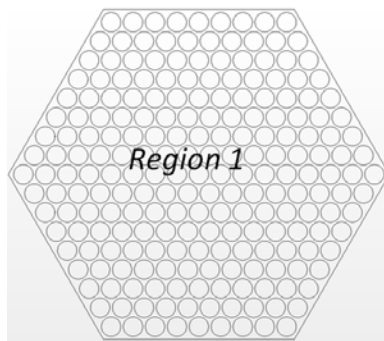
Heterogeneous Duct



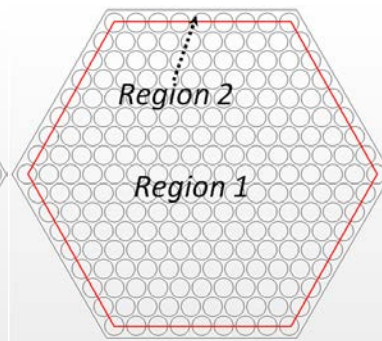


SFR Core Deformation: T/H Homogenization

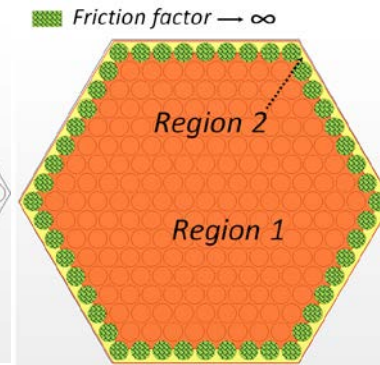
- Deformation is driven by thermal expansion of the duct walls
- Explicit-geometry CFD is prohibitively expensive computationally
- Need to develop porous media models (~300x faster):
 1. Single-region: Uniform q''' , porosity, and inlet velocity
 2. Two regions: Different volumetric heat generation rates
 3. Two regions: Distinct q''' , porosity, and inlet velocity



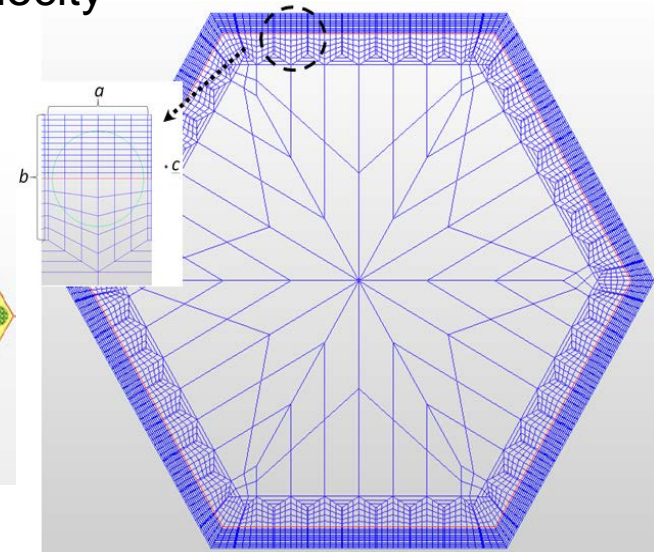
Porous Media 1



Porous Media 2

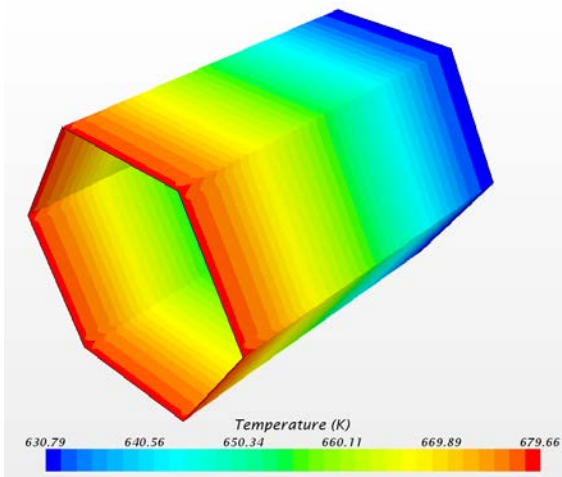


Porous Media 3

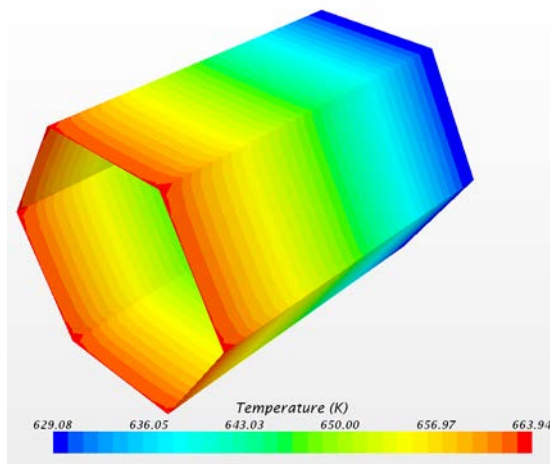




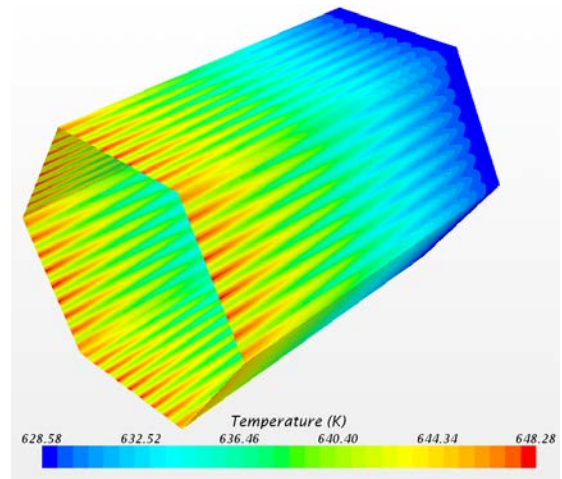
SFR Core Deformation: Temperature Prediction



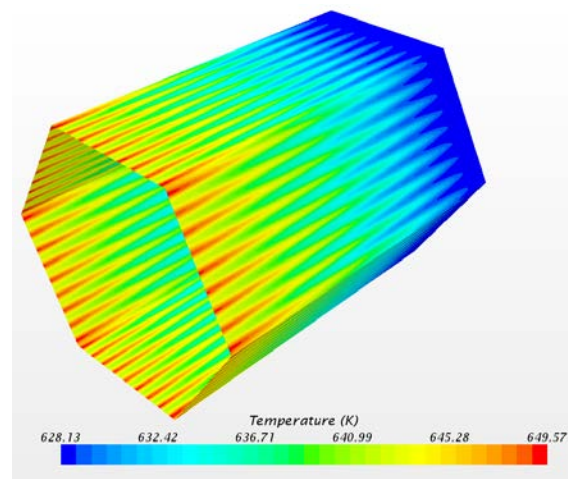
Porous Media 1



Porous Media 2



Porous Media 3



Reference CFD (pin-by-pin)

■ Peak wall temperature rise above 630K:

1. 50 K (off by 2.5x)
2. 34 K
3. 18 K

Reference CFD: 19 K

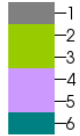


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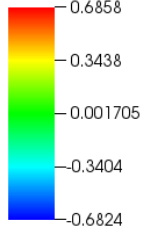
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Full ABTR coupled calculations

Filled Boundary
Var: materials1(mesh1)

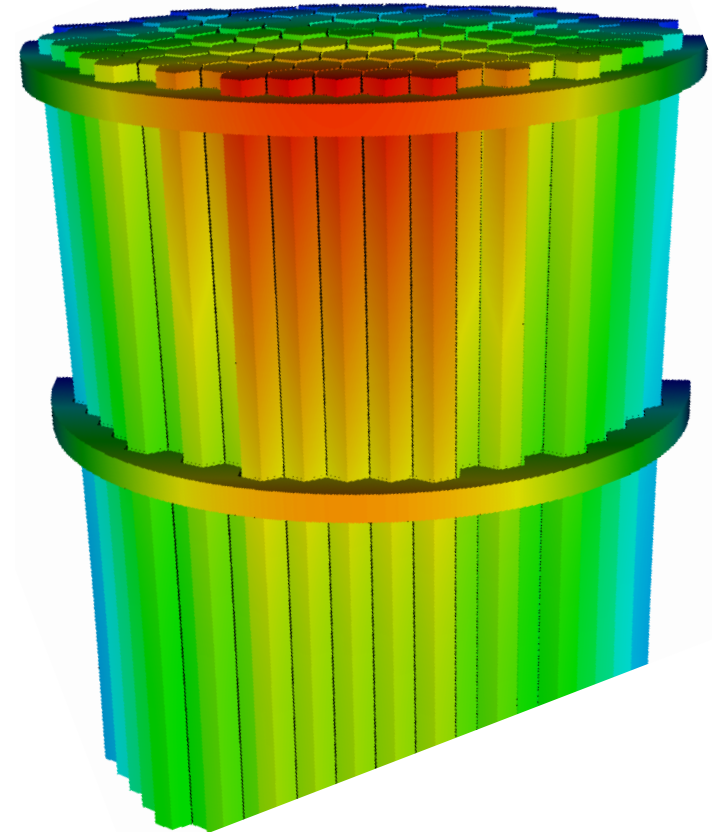
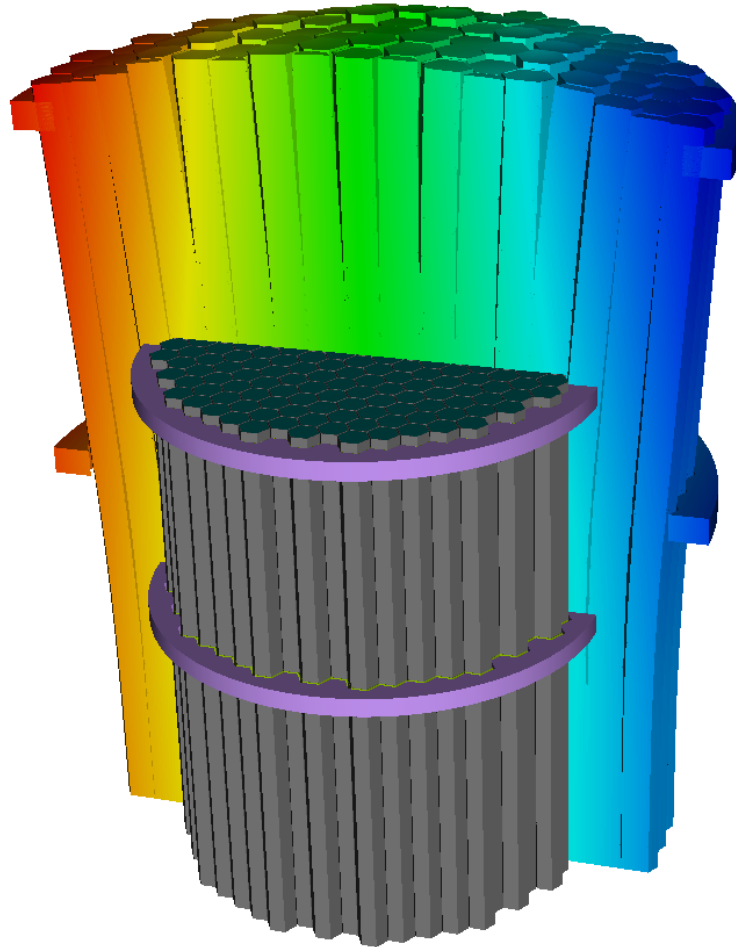


Pseudocolor
Var: derived/displacement/y



Max: 0.6858
Min: -0.6824

Filled Boundary
Var: materials1(mesh1)



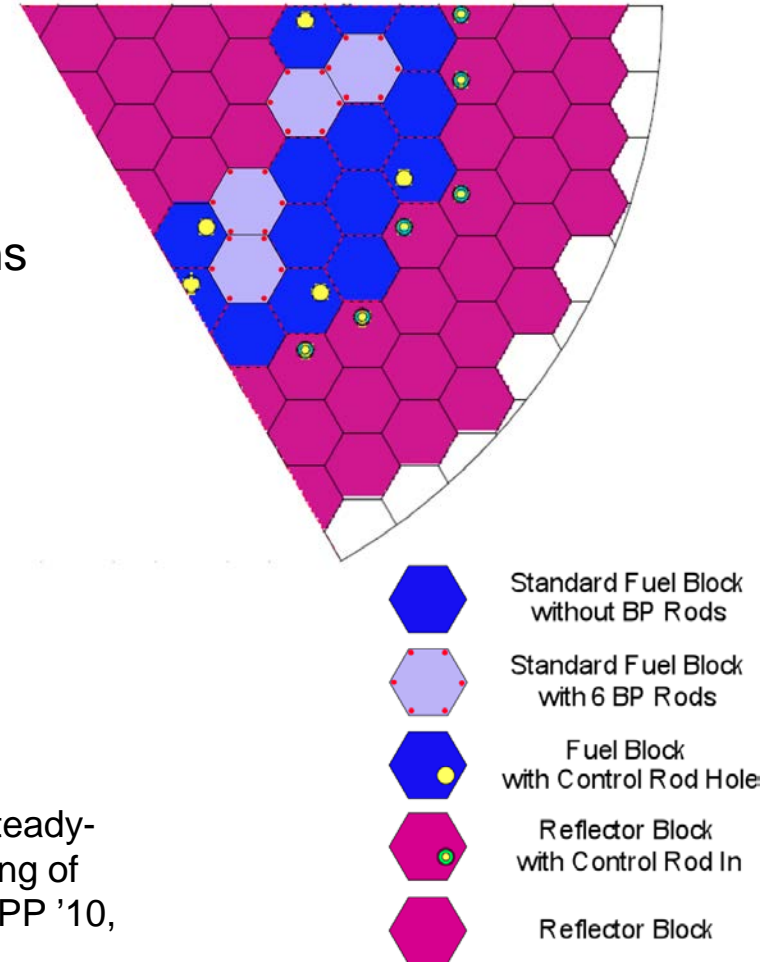
ABTR full core displacement in the y direction magnified by 100 x



VHTR Model

■ Benchmark model based on GT-MHR

- 60° periodic boundaries
- 3 rings of fuel columns
- Control rod channels open in fuel columns
- Control rods fully inserted into reflector columns (“operating rods in”)
- Burnable poisons biased towards inner ring to flatten power shape



J. W. Thomas, C. H. Lee, W. D. Pointer, and W. S. Yang, “Steady-State, Whole-Core VHTR Simulation with Consistent Coupling of Neutronics and Thermo-Fluid Analysis”, Proceedings of ICAPP '10, San Diego, CA, USA, June 13-17, 2010



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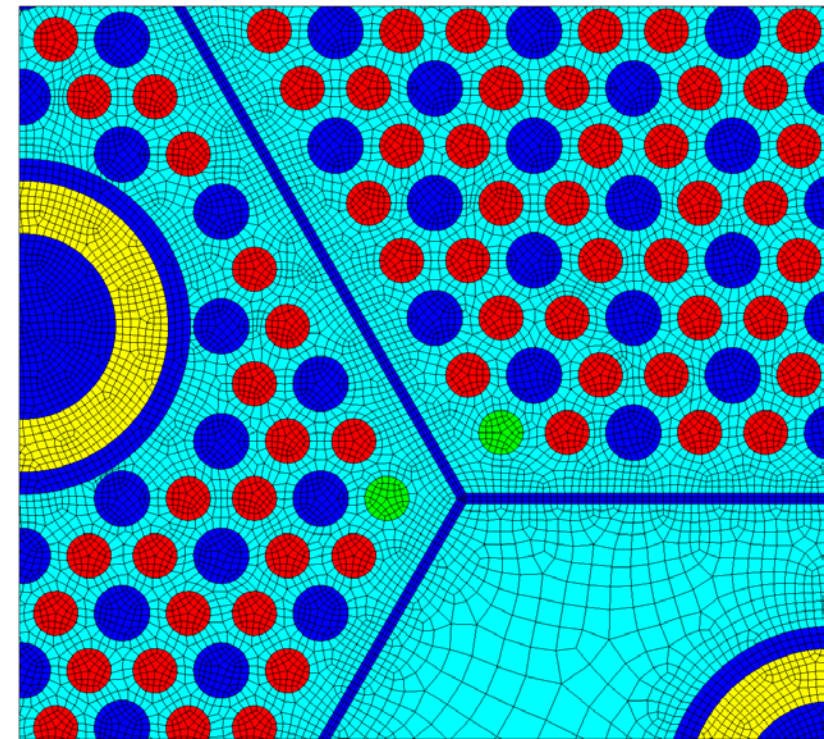
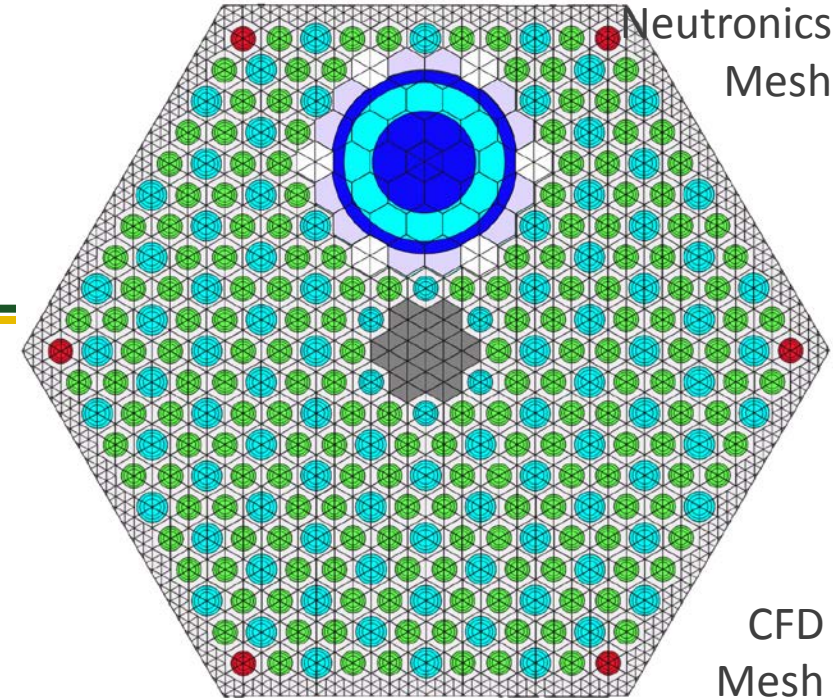
VHTR Model (cont.)

■ Neutronics model

- Global k-eff solution from multigroup CMFD problem with pin-cell mesh
- Coupled to 2-D planar MOC
 - Provides multigroup cross sections (equivalence theory)
 - Gets axial source from global CMFD
- Subgroup resonance treatment

■ CFD model

- Geometry includes fuel compacts, flow channels, and bypasses through gaps
- Coolant flow paths connected by common inlet and outlet plena
- 20M cells
- High-Re Realizable k-epsilon RANS

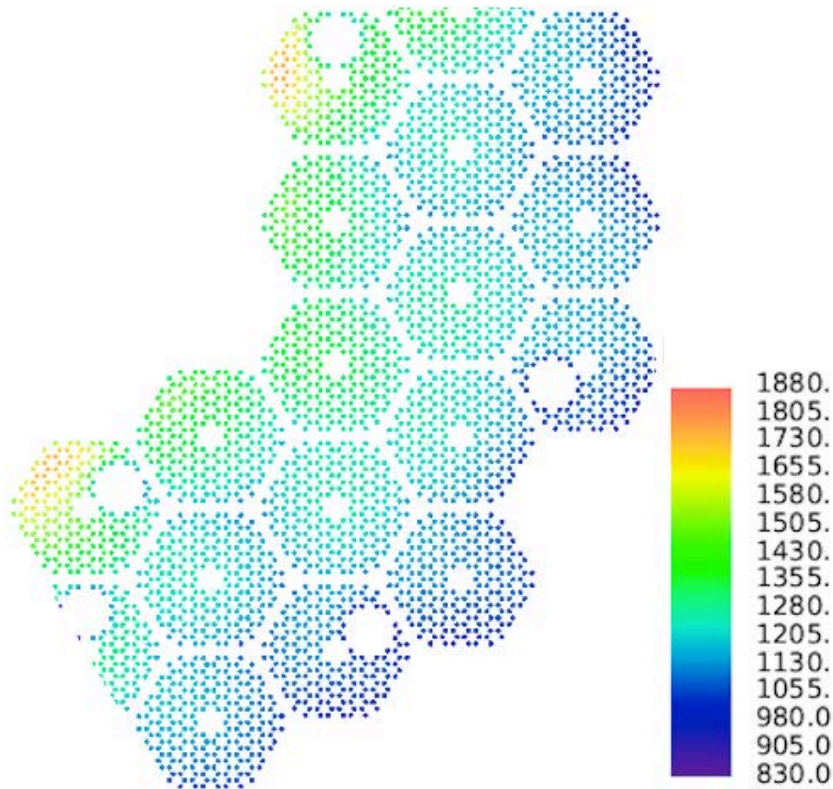




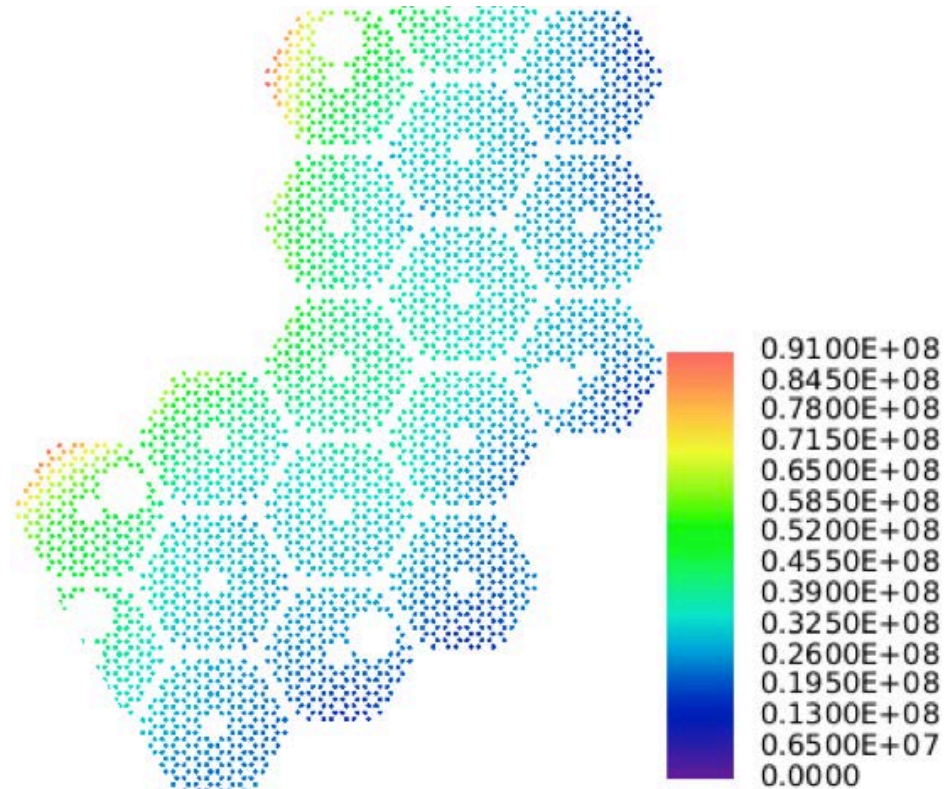
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VHTR Multi-Physics Demonstration



CFD Prediction of
Temperature at Midplane




Neutronics Prediction of
Heat Source at Midplane

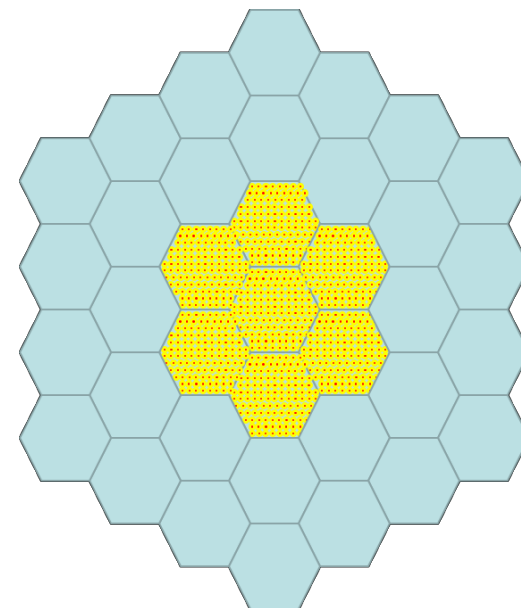
J. W. Thomas, C. H. Lee, W. D. Pointer, and W. S. Yang, "Steady-State, Whole-Core VHTR Simulation with Consistent Coupling of Neutronics and Thermo-Fluid Analysis", Proceedings of ICAPP '10, San Diego, CA, USA, June 13-17, 2010



Ongoing Projects

- After release of SHARP in March 2016, RPL focus shifted to assessment and V&V of its component and multi-physics analysis capabilities
 - Systematic approach for DOE-NE ART program engagement in M&S
 - Joint modeling and experiment design with ART analysts (cultivate user base)
 - Set the foundation for future work based on assessed strengths/shortcomings

- SFR challenge problems and V&V opportunities
 - Hot-channel/pin factor analysis for AFR-100
 - **SHARP-zoom (analytic magnifier)** 
 - Coupled system-CFD analyses (to support bilaterals with Japan, France, China)
 - Wire-wrapped SFR pin bundle benchmarks (ART FOA with Areva/TerraPower, EU-Sesame, bilateral/trilateral with Japan and France)
 - Reduced-order thermal stratification modeling for SAM



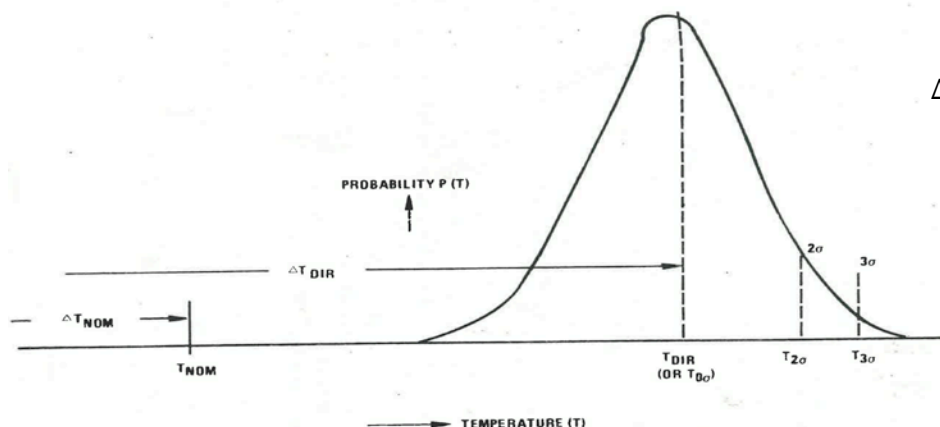


SFR Hot Channel Factors

■ Corrections of nominal values to account for uncertainties on M&S, experiments, instrumentation, manufacturing tolerance, correlations, etc.

- J. Muraoka, et al, *Assessment of FFTF Hot Channel Factors*, HEDL-TI-75226 (1976)
- F. Bard, et al, *FFTF Hot Channel Factors and Other Uncertainties Used in Safety Analysis and Life-Time Prediction for Fuel Pin Performance*, WHC-SP-0608 (1990) – Applied Technology
- A. Friedland, *CRBRP Core Assemblies Hot Channel Factors Preliminary Analysis*, CRBRP-ARP-0050 (1980)
- M. D. Carelli, et al, *Hot Channel Factors for Rod Temperature Calculations in LMFBR Assemblies*, Nucl. Eng. Design 62 (1980)
- L. Briggs, *Safety Analysis and Technical Basis for Establishing an Interim Burnup Limit for Mark-V & Mark-VA Fueled Subassemblies in EBR-II*, ANL (1995)
- R. Villim, *Reactor Hot Spot Analysis*, ANL, FRA-TM-152 (1985)
- W. Yang, et al, *Potential Gains through Reduced Hot Spot Factors*, ANL Intra-laboratory memo (2005)

■ Semi-statistical horizontal methods: Direct and statistical HCFs



$$\Delta T_{cool} = (\Delta T_{cool}^{nom}) \prod_{i=HCFs} DH_{cool}^i + \sqrt{\sum_{i=HCFs} (\Delta T_{cool}^{non} \times SH_{cool}^i)^2}$$



SFR Hot Channel Factors: Direct HCFs

Factor	Description
Power level measurement uncertainty	<ul style="list-style-type: none">Defined as system design requirement
Inlet Flow Maldistribution	<ul style="list-style-type: none">Uncertainties in assembly flow distribution due to flow maldistribution in lower plenum, manufacturing tolerances in internal structures and orifice, etc.
Intra-assembly Flow Maldistribution	<ul style="list-style-type: none">Uncertainties of flow distribution within assembly, which are due to the simplified model and applied empirical factors of sub-channel codes.
Cladding Circumferential Temperature	<ul style="list-style-type: none">Due to wire-wrap, the axial velocity and temperature around a fuel pin have strongly azimuthal dependence.HCF was measured at ORNL 7 and -19 pins tests and firstly evaluated by FATHOM-360 code (NSE. 64, 1977).
Physics Modeling	<ul style="list-style-type: none">There are many sub-factors under this category such as flux solver approximation, 2D synthesis method), etc.In CRBR, the lumped uncertainty of the power distribution was estimated using the ZPPR mockup of CRBRP (the C/E error is about +/-2% except for specific locations)
Control Rod Banking	<ul style="list-style-type: none">Control rods are grouped and there is manufacturing tolerance (i.e., insertion depth is not identical), which introduces asymmetric power.

- Highlighted in yellow are targeted HCFs that will be reevaluated via high-fidelity multi-physics methods



SFR Hot Channel Factors: Stochastic HCFs

Factors	Description
Reactor ΔT and Inlet Temp. Variation	<ul style="list-style-type: none">Uncertainties of inlet, outlet and ΔT due to deterioration of primary components
Inlet Flow Maldistribution	<ul style="list-style-type: none">Uncertainties of pressure measurement, manufacturing tolerance, orifice flow rate, assembly flow rate, etc.
Loop Temperature Imbalance	<ul style="list-style-type: none">Loop temperature imbalance affects inlet temperature distribution.CRBR allows cold leg loop-to-loop temperature imbalance of 34 F, which results in 4.9 F (2-sigma) uncertainty in inlet temperature
Wire Wrap Orientation	<ul style="list-style-type: none">Analyzed by sub-channel code, COTEC, which is 1% uncertainty
Subchannel Flow Area	<ul style="list-style-type: none">Uncertainties of rod dimension tolerance, bow, etc.
Film Heat Transfer Coefficient	<ul style="list-style-type: none">Uncertainties of correlation, etc.
Cladding thickness and conductivity	<ul style="list-style-type: none">Uncertainties of correlation, etc.
Coolant Properties	<ul style="list-style-type: none">Uncertainties of correlation, etc.
Intra-assembly flow maldistribution	<ul style="list-style-type: none">Flow and temperature distributions were calculated using sub-channel code of COBRA, COTEC, and THI-3D.
Nuclear Data	<ul style="list-style-type: none">Evaluation nuclear data library uncertainties
Criticality	<ul style="list-style-type: none">Control rod depth error due to uncertainty in the prediction of criticality
Fissile Maldistribution	<ul style="list-style-type: none">Fuel manufacturing uncertainties
Fuel Thermal Conductivity	<ul style="list-style-type: none">Uncertainties due to pellet diameter, fresh and irradiated fuel conductivity, porosity of swollen fuel, redistribution, etc.
Power level measurement	<ul style="list-style-type: none">Instrument uncertainties (flow rate, temperature, etc.) and control systems.



SFR Hot Channel Factors: Impact on MW Temperature

■ Potential impact of improved HCFs on peak mid-wall temperature estimation using CRBR HCFs, assuming:

- No uncertainties on direct HCFs when they are evaluated via SHARP simulations
- 50% reduction of statistic HCFs when they are evaluated via SHARP simulations

For AFR-100, 17°C MW temperature drop (5-7% power increase)

Factors		Coolant	Film	Clad	Peak MW Temperature
Inlet coolant temp. °C		395.0			
Nominal temperatures at peak MW temperature, °C		566.1	570.0	581.1	581.1
CRBR HCFs	Direct, °C	+198.3	+10.9	+11.7	632.4
	Statistical (2σ)	21.6			
With improved CRBR HCFs (tentative)	Direct, °C	+188.7	+4.7	+13.3	615.1
	Statistical (2σ)	18.4			



Planned activities: HTGR Challenge Problems

Steam Cycle HTR Primary Circuit Layout

- Core Power (200-600 MWt)
- Coated particle (TRISO) fuel embedded in graphite blocks (or pebbles)
- Helium coolant at ~4-7MPa –forced convection under normal ops

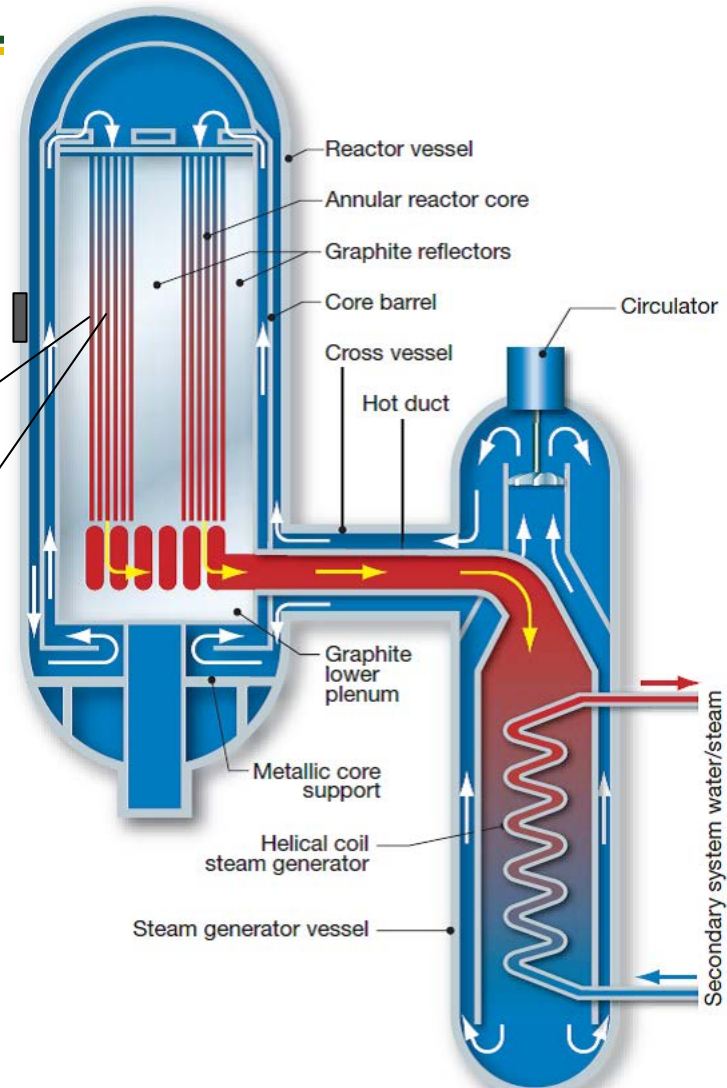
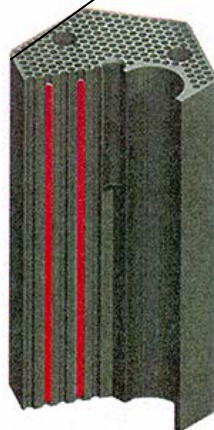
Particle



Compact



Block



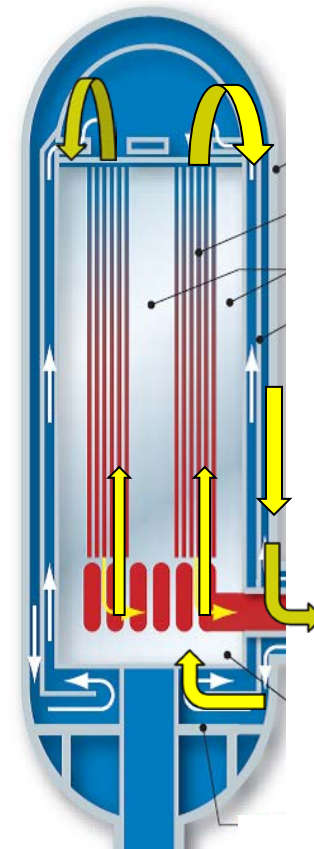
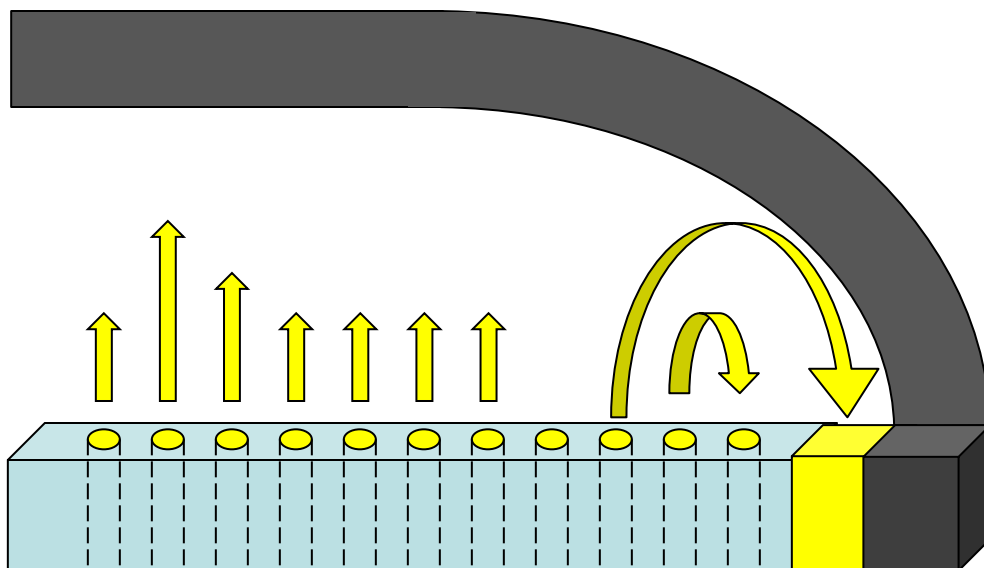
(1 of 2 steam generators shown)



HTGR Challenge Problems (cont.)

Buoyancy-driven Core Channel-to-Plenum Flow Mixing

- Blower trip leads to loss of forced flow through core
- Buoyancy drives natural circulation through channels and riser
- Flow can be complex, unstable, and may, if unmitigated, lead to hot plumes impinging on upper plenum structures (fuel integrity is not threatened)
- Objective: Investigate the sensitivity of the plenum flows to channel geometry, number of channels, heating profiles, etc.





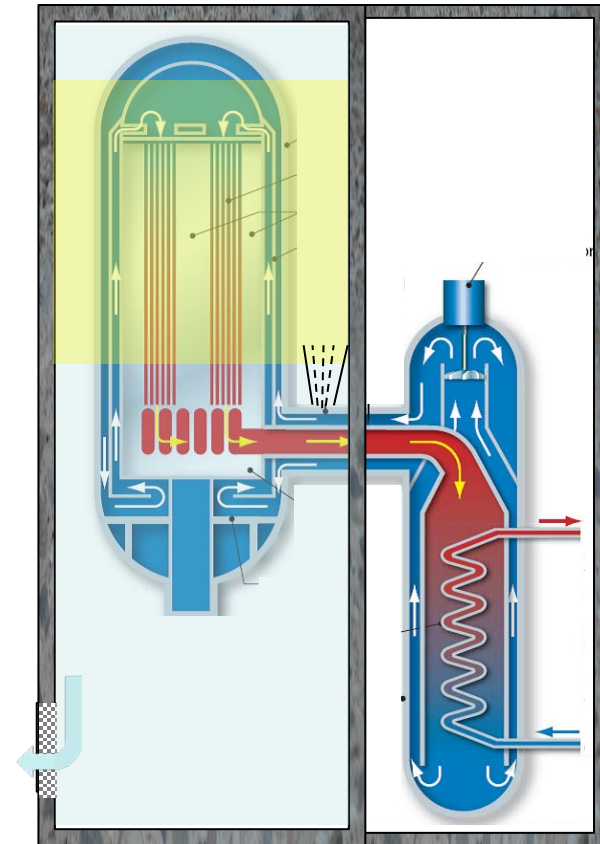
HTGR Challenge Problems (cont.)

Break in primary boundary

- Leak or break leads to depressurization
- Helium displaces air; air may leak into the RPV, causing erosion of graphite (oxidation)
- Objective: Investigate mixing of helium and air in the cavity and the extent to which air can enter the RPV

Performance of Reactor Cavity Cooling System

- RCCS rejects parasitic heat losses and decay heat to the atmosphere
- Water-based systems exhibit complex flow behavior including boiling
- Objective: Investigate fluid-structure interactions and the sensitivity of fluid behavior to the number of riser channels per chimney





Planned activities: MSR Challenge Problems

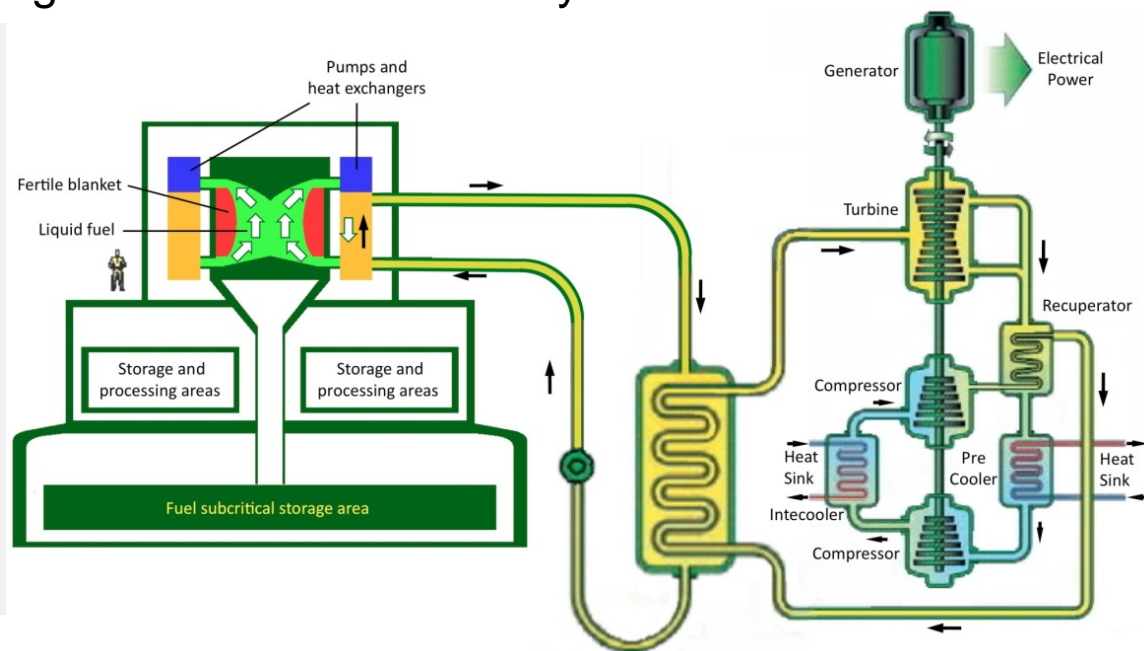
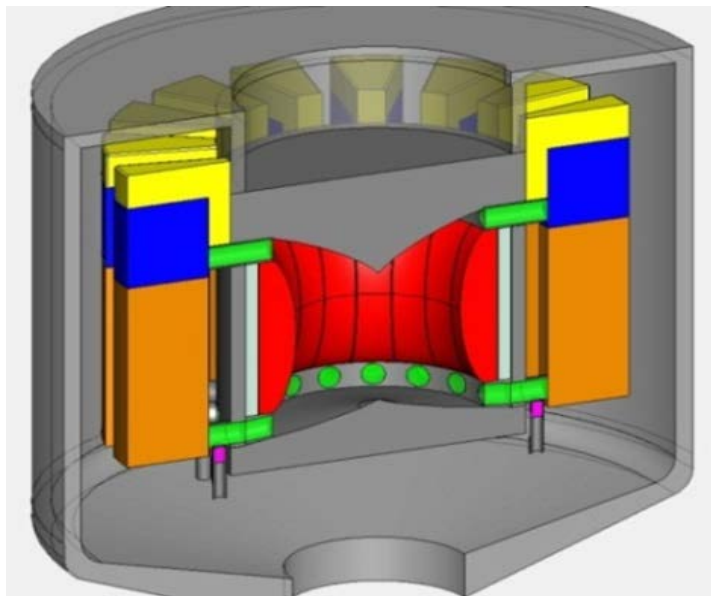
MSR designs with dissolved fuel have unique M&S needs that may not be met with systems analysis codes alone

- Heat is produced directly in the “coolant”
- Unique design with fuel circuit, an intermediate circuit, and the power conversion system
- Unique core configurations with potential recirculation and stagnation zones
- Reactivity management challenges (fissile/fertile inventory, sensitivity to local minor density variations in MSFR)
- Fission product/gas management, potential for online reprocessing
- No control rods in the core
 - Reactivity control by the IHX heat transfer rate, fuel-salt feedback coefficients, continuous fissile loading, and the core geometry
 - No requirement for controlling the flux shape
- Quick reconfiguration of the core geometry (gravitational draining) for passive safety



MSR Challenge Problems (cont.)

- Design and fissile inventory optimization (power vs. fuel salt volume and core geometry)
- Multi-physics modeling of thermo-chemico-fluid dynamics
- Limiting factors:
 - Heat exchanger capacity
 - Irradiation damage to the structural materials
 - For fast spectrum, breeding ratio vs. fissile inventory



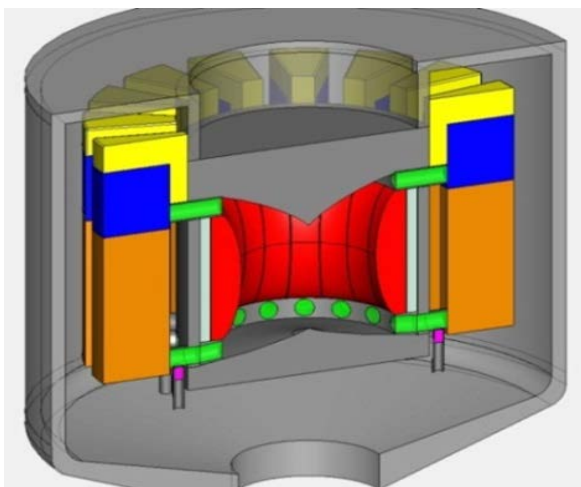


MSR Challenge Problems (cont.)

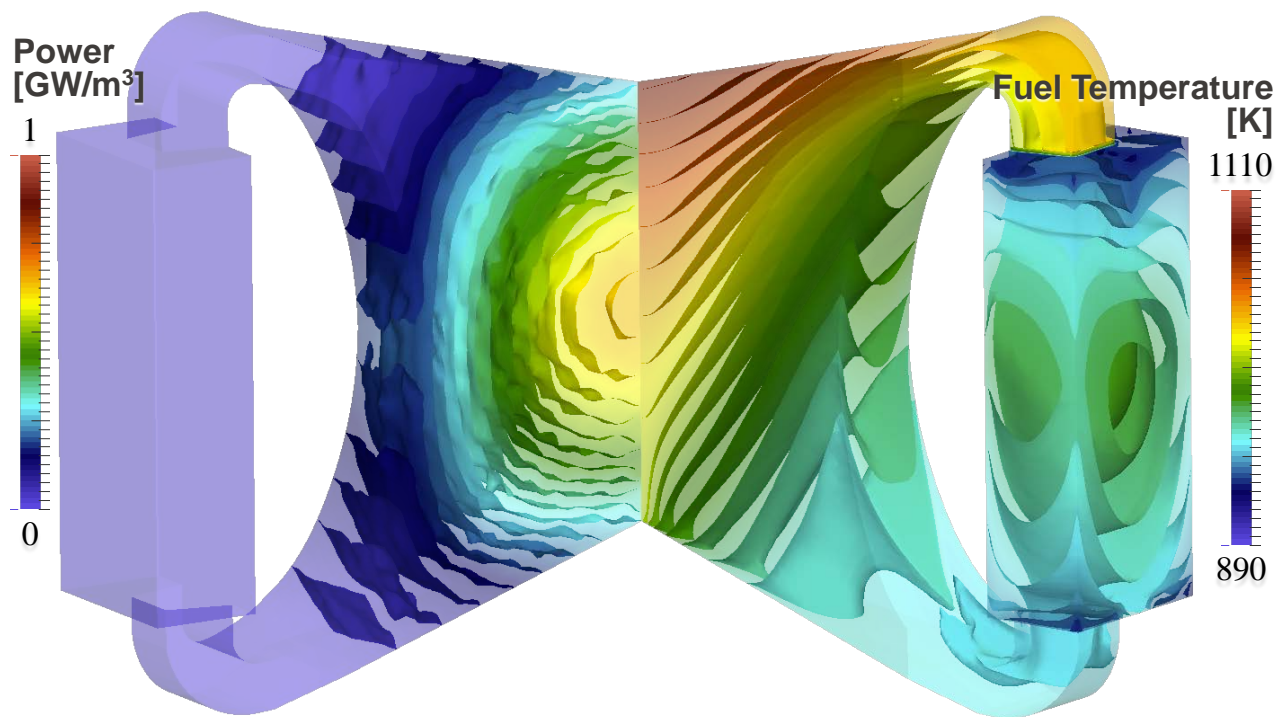
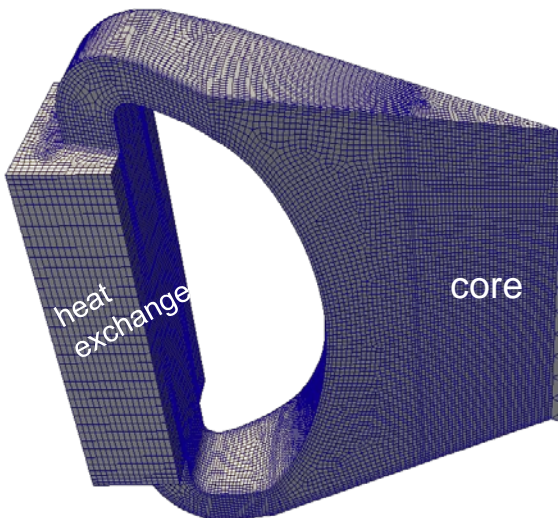
- Opportunities to leverage SHARP toolkit for MSR M&S: Coupled neutronics + thermal-hydraulics simulations
 - High-fidelity, high-resolution T&H modeling for flow and temperature distributions using CFD
 - MC²-3 for thermal and fast fission cross sections
 - PROTEUS for neutronics with full-spatial resolution of potentially complex core geometry
 - REBUS or ORIGEN to support depletion analysis toward an equilibrium cycle
 - PERSENT for calculation of kinetic parameters and reactivity feedback
 - Delayed neutron source
 - Doppler feedback effect
 - Density feedback effect
 - System Analysis Module (SAM) for the intermediate circuit and power conversion system response.



MSR Challenge Problems (cont.)



Results for CEA Samofar MSFR design using
coupled Monte-Carlo and OpenFoam codes
(<http://samofar.eu/project>)





MSR Challenge Problems (cont.)

Potential support for MSR accident analysis needs:

■ Fuel circuit accidents

- Loss of Heat Sink
- Loss of Fuel Flow
- Station blackout
- Overcooling
- Reactivity anomalies

■ Draining system accidents (draining blockage)


■ Balance of plant upsets

- Steam generator tube rupture




Overview of Warthog

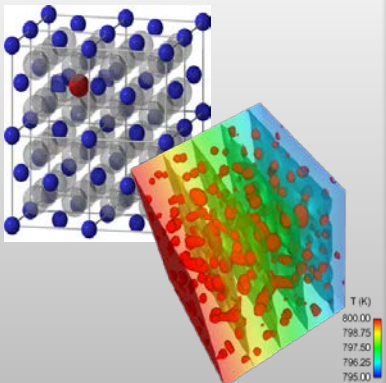
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MOOSE
Multiphysics Object-Oriented Simulation Environment

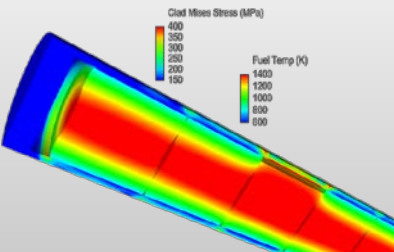


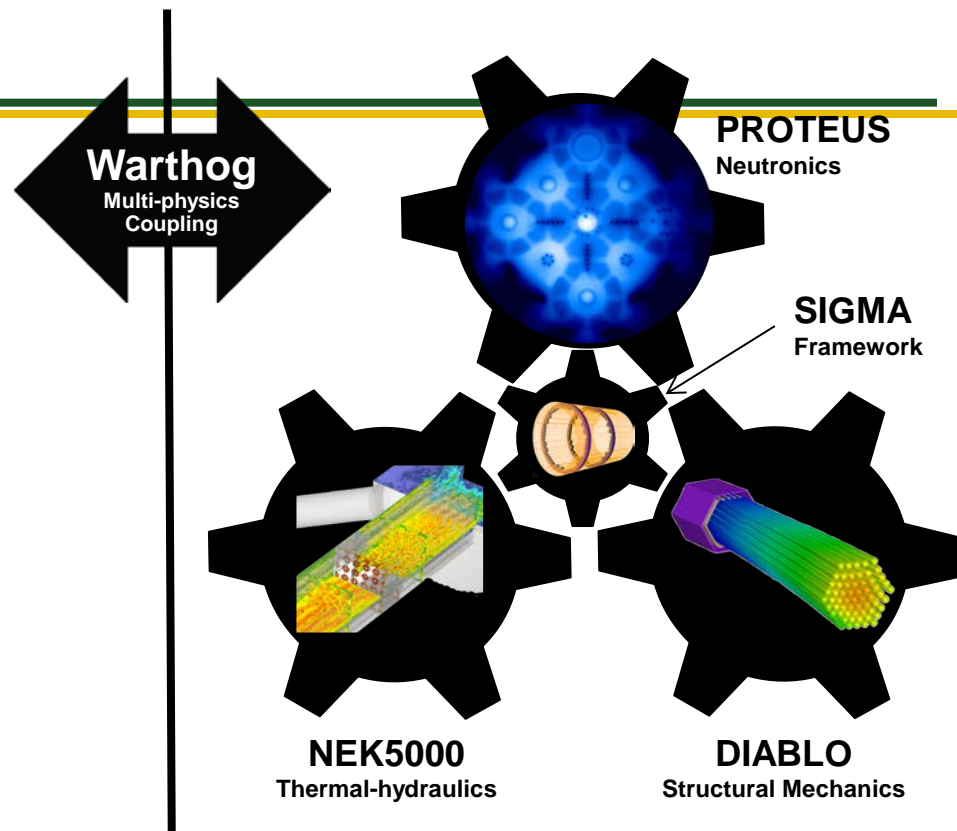
MARMOT
Atomistic-Mesoscale
Material Model





BISON
Fuel Performance





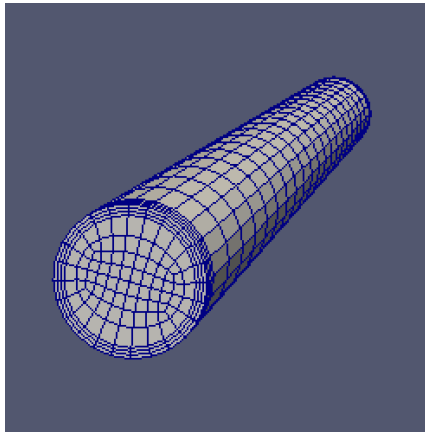
Warthog serves to couple tools in the SHARP suite with those using the MOOSE Framework



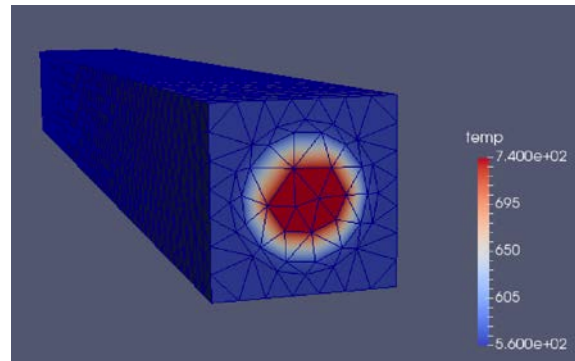
Status on Warthog

■ Currently supports PROTEUS -> BISON coupling

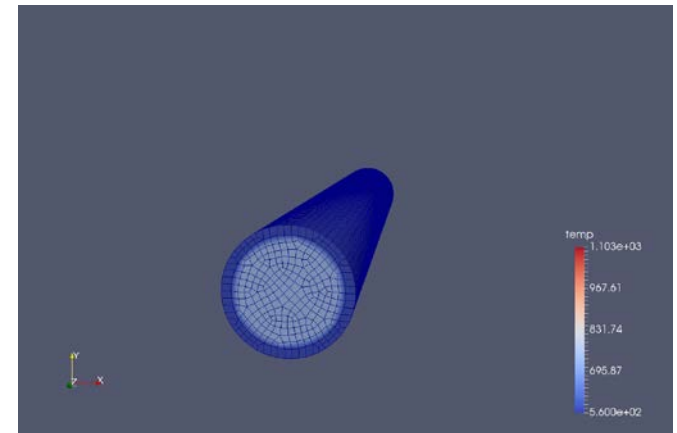
- Pin cell coupling has been demonstrated
- Assembly model work ongoing



BISON Mesh



PROTEUS Mesh
with Initial Temp.



Temperature from BISON
over one hour



Summary

Nuclear Energy

- SHARP leverages advanced single-physics computational tools to solve multiphysics problems in a manner closer to first-principles
 - Provide insight into core/component design that can't be easily measured or accounted for with conventional tools/methods
- Aims is to capture the integral effects with multiresolution when the system codes provide information on key parameters with large uncertainty
 - Thermal-stratification in upper plena
 - Thermal-striping leading to thermal fatigue induced failures
 - Thermo-structural analysis of primary coolant boundary during accidents
 - Flow-induced vibrations
- High-fidelity multiphysics approaches are of interest for mature concepts to support commercial deployment
 - System codes coupled with appropriate sub-grid physics or higher-fidelity tools can also meet the needs of an advanced concept (**next presentation**)