

DireWolf: MOOSE-based Multiphysics Simulator for Megawatt Scale Micro-Reactor

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Presentation Overview



- DireWolf
- Sockeye Heat Pipe – Preliminary Effort and Future Development Plans
- Preliminary Design-A DireWolf Results
- LANL/INL Joint DireWolf Efforts on Monolith Micro-Reactor under ARPA-E MEITNER Award



What is DireWolf?



1. The dire wolf is an extinct species of the genus *Canis*. It is one of the most famous prehistoric carnivores in North America, along with its extinct competitor, the saber-toothed cat *Smilodon fatalis*. The dire wolf lived in the Americas during the Late Pleistocene and Early Holocene epochs.
2. Multi-Physics Micro-Reactor Simulator Using the NEAMS HPC MOOSE Framework and MultiApps and Transfers

MOOSE: The Cornerstone of INL's High Performance Computing Modeling and Simulation Effort



MOOSE (Multiphysics Object-Oriented Simulation Environment): HPC Development and Runtime Computational Framework (NQA-1 compliant)

- Started in May of 2008 (LDRD).
- *MOOSE* is an C++ object-oriented software framework allowing rapid development of new simulation tools.

- 1D, 2D or 3D FEM (CG, DG and XFEM) with both mesh and time step adaptivity.
- Subjected to multiple peer-reviews, NQA-1 compliant.
- Application development focuses on implementing physics (PDEs) rather than numerical implementation issues.
- Leverages multiple DOE and university developed scientific computational tools (MPI, PETSc, LibMesh, Hypr, etc.).
- Seamlessly couples native (*MOOSE*) applications using *MOOSE MultiApps and Transfers*.
- Efficiently couples non-native (and non-C++) codes using *MOOSE-Wrapped Apps*.
- Obtained Free Software Foundation, Inc.'s Lesser General Public License Version 2.1 on February 12, 2014. *MOOSE* also received a 2014 R&D 100 Award.
- Two PECASE awards, Derek Gaston (2012) and Michael Tonks (2017).

DireWolf Heat-Pipe-Cooled Micro-Reactor Projects

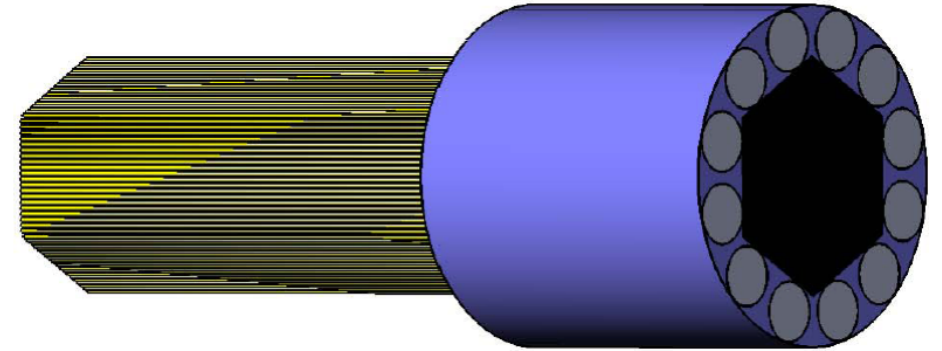
Heat-pipe-cooled reactors are nearly “solid-state” and avoid many of the complexities and issues arising from the traditional reactor concepts that rely on a coolant pumped through the reactor core.

Micro-Reactor projects include:

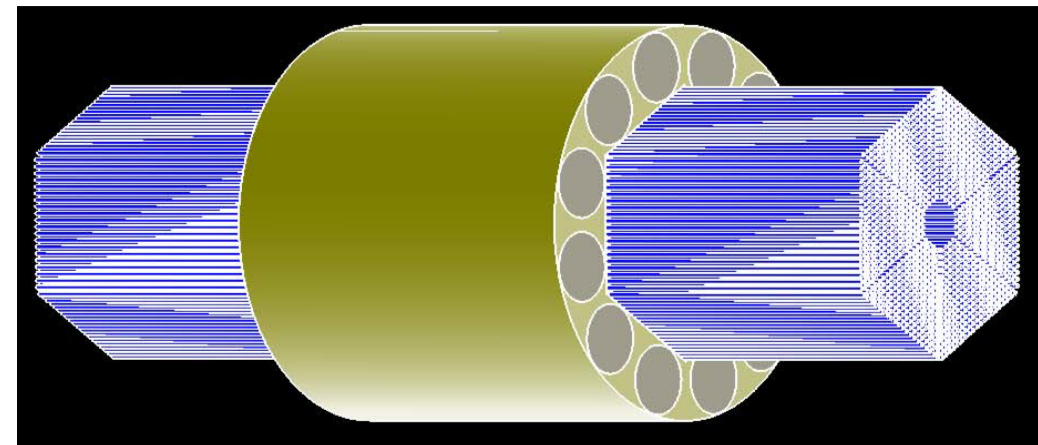
- MEITNER ARPA-e *Solid Core Block “SCB” for an Inherently Safe Heat Pipe Reactor*
- Special Purpose Reactor (SPR) is a small 5 MWt, heat pipe-cooled, fast reactor based on the Los Alamos National Laboratory (LANL) Mega-Power concept.
- Oklo fast reactor.

DireWolf Simulation Approach:

- *MAMMOTH* (reactor physics)
- *Rattlesnake* (transient radiation transport)
- *BISON* (nuclear fuel performance)
- *Grizzly* (structural mechanics)
- *Sockeye* (advanced heat pipe technology)
- *RELAP-7* (Open-air and SC CO₂ Brayton cycles)



Sockeye will support the simulation of both single- and double-ended heat pipe configurations



Radiation Physics for Irradiated Nuclear Fuel & Materials



Rattlesnake (NEAMS and NRC): *Multi-scale multi-level radiation transport*

- Multi-scale: Assembly homogenized, pin-homogenized, fuel-resolved simultaneously in one simulation.
- CFEM-Diffusion, DFEM-Diffusion, SAAF-CFEM-SN, SAAF-CFEM-PN, LS-CFEM-SN, LS-CFEM-PN, DFEM-SN, and DFEM-PN).
- **Designed to support tightly coupled nonlinear multiphysics simulations, primarily focused on fuel performance analysis, both locally and core-wide for safety issues (strong transients).**



MAMMOTH (NEAMS): *Advanced multi-scale nuclear physics*

- State-of-the-art depletion solver with CRAM and nonlinear Eigensolver.
- Isotopic composition to → BISON and MARMOT (fuel performance) to update local fuel thermal-mechanical-chemical property evolution and fission gas inventories
- Isotope, density, and temperature feedback for cross-sections.
- Pin-wise power and burnup distributions.
- Provides fluence calculations for radiation damage predictions (dpa).

Multi-scale Nuclear Fuels and Materials Modeling



BISON (NEAMS, CASL, AFC): Block-Implicit Simulation of Nuclear fuels (BISON)
Engineering-scale fuel performance application

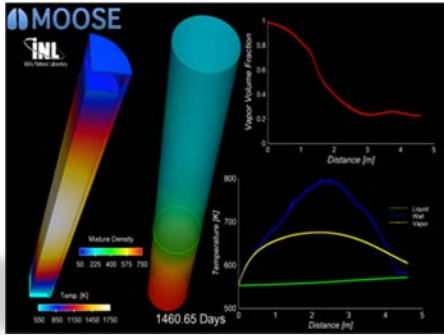
- All-fuels: Models LWR, TRISO, plate, and metal fuels in 1D, 2D and 3D.
- Material models are empirically derived. **Tight coupling with Marmot to provide lower length-scaled informed "science-based" predicative capabilities.**
- **Designed to support tightly coupled nonlinear multi-scale multiphysics simulations with MAMMOTH, Rattlesnake, and Marmot, to address both locally and core-wide for safety issues for HBS and ATF design (strong transients).**



Grizzly (LWRS and NEAMS): Structural mechanics for component aging and irradiation damage evolution (NQA-1 compliant)

- Supports LWR R&D to safely operate NPPs beyond original design life.
- Structural mechanics for reactor pressure vessel (RPV), containment vessels, fuel assemblies, etc.
- Reactor Metals (embrittlement, fatigue, corrosion, etc.), e.g. RPV, core internals, and weldments.
- Long-term concrete degradation (mechanical, chemical, and irradiation).
- High fluence phase transformations (multi-scale template).

Reactor System and Structural Mechanics



RELAP-7 (LWRS and NEAMS): RELAP-7 is *INL's Next Generation Reactor System Analysis Tool (NQA-1 compliant)*

- The overall design goal of RELAP-7 development is to leverage 35 years of advancements in software design, numerical integration methods, and physical models.
- All-speed, all-fluid (vapor-liquid, gas, liquid metal) flow – agnostic of reactor concept (PWR, BWR, SMR, SFR, MSR, FHR, HTGR, etc.).
- Multi-physics integration with other MOOSE-based applications (BISON, MASTODON, MAMMOTH, Rattlesnake)

Sockeye (NEAMS and GAIN): *Advanced heat pipe application, primarily for micro-reactors.*



- Multiple approaches: Simple heat balance, intermediate two-phase FEM approximation, and a more sophisticated two-phase, two-channel FEM approximation.
- Derived from **FlowChannel2Phase** component in RELAP-7 using 7-equation two-phase flow model.
- Designed for both single and double-ended operation.
- Tightly coupled to MOOSE thermomechanics (BISON).

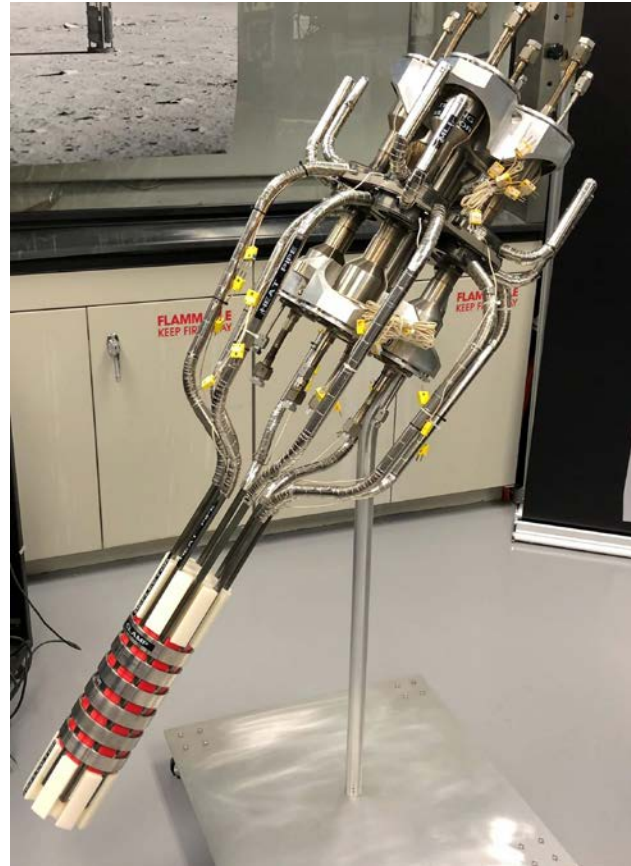
Sockeye Heat Pipe – Preliminary Effort and Future Development Plans

Sockeye: NEAMS Advanced Heat Pipe simulation capability for heat pipe-cooled micro-reactors

Sockeye is designed to support heat pipe-cooled micro-Reactor concepts. Heat pipes are efficient heat transport devices, and their use in nuclear reactors to transport fission heat out of the reactor core is a novel application.



- Funding Sources: NEAMS and GAIN
- Collaborators:



The KRUSTY (Kilopower Reactor Using Stirling Technology) prototype unit on display in the Stirling Research Lab at the NASA Glenn Research Center in Cleveland, Ohio

Heat Pipe-Cooled Reactors:

- A heat-pipe reactor is typically a solid-block core with the fuel in holes inside the solid block.
- The heat pipes remove the heat from the block as the liquid in the heat pipe is vaporized.
- The heat is deposited in the condenser region of the heat pipe.
- The condenser region can be sized to accommodate multiple heat exchangers, such as one for power conversion and two for redundant decay heat removal.

Proof of Concept: Simplified Sockeye Model based on LANL Heat Pipe Technology

Heat Pipe Transient Response Approximation

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Initial development of the MOOSE-based Sockeye Heat Pipe application began in June 2017 in anticipation of INL/LANL collaboration on 5MW Megapower micro-reactor concept.

First version of Sockeye is based upon LANL HP-Approx Heat Pipe code and coupled to BISON nuclear fuels performance code for proof of concept purposes.

Abstract. A simple and concise routine that approximates the response of an alkali metal heat pipe to changes in evaporator heat transfer rate is described. This analytically based routine is compared with data from a cylindrical heat pipe with a crescent-annular wick that undergoes gradual (quasi-steady) transitions through the viscous and condenser boundary heat transfer limits. The sonic heat transfer limit can also be incorporated into this routine for heat pipes with more closely coupled condensers. The advantages and obvious limitations of this approach are discussed. For reference, a source code listing for the approximation appears at the end of this paper.

INTRODUCTION

Heat pipe transient response has been well studied, (Ambrose, 1991), (Bowman, 1994), (Cao, 1992), (Colwell, 1992), (Hall, 1994), (Issacci, 1991), (Jang, 1995), (Tournier, 1995), and (Tournier, 2001). The physical mechanisms are numerous and involved, especially if frozen startup is examined in any detail. Physics related to transient heat pipe operation can include: transition from free molecule to continuum flow in the vapor space, the migration of the melt front in capillary structures, mass transfer between the liquid and vapor regions, and compressibility effects. Entrainment of fluid from the wick, freezing of condensed vapor preventing fluid return to the evaporator, dewetting, and inadequate capillary pumping forces can limit heat pipe startup. Analytical techniques have been used to calculate frozen startup characteristics. Cao (1992) developed a heat pipe startup solution using analytical relations and a flat front assumption that is in some respects similar to the approach taken in this paper. Silverstein (1992) described a calculation approach that divides a heat pipe into evaporator, active, and inactive regions to find temperature history as the continuum front moves through the condenser.

Sockeye Heat Pipe Theory

The unsteady one dimensional diffusion equation with a heating source term and radiation to the surroundings can be written:

$$C \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + \dot{q} - G_R(T^4 - T_\infty^4)$$

In difference form about the cartridge heaters, fuel tubes, and evaporator node:

$$C_{CH} \frac{T_{CH} - T_{CH}^P}{\Delta t} = \dot{q}_{ELECT} - G_{RI}(T_{CH}^4 - T_{FT}^4)$$

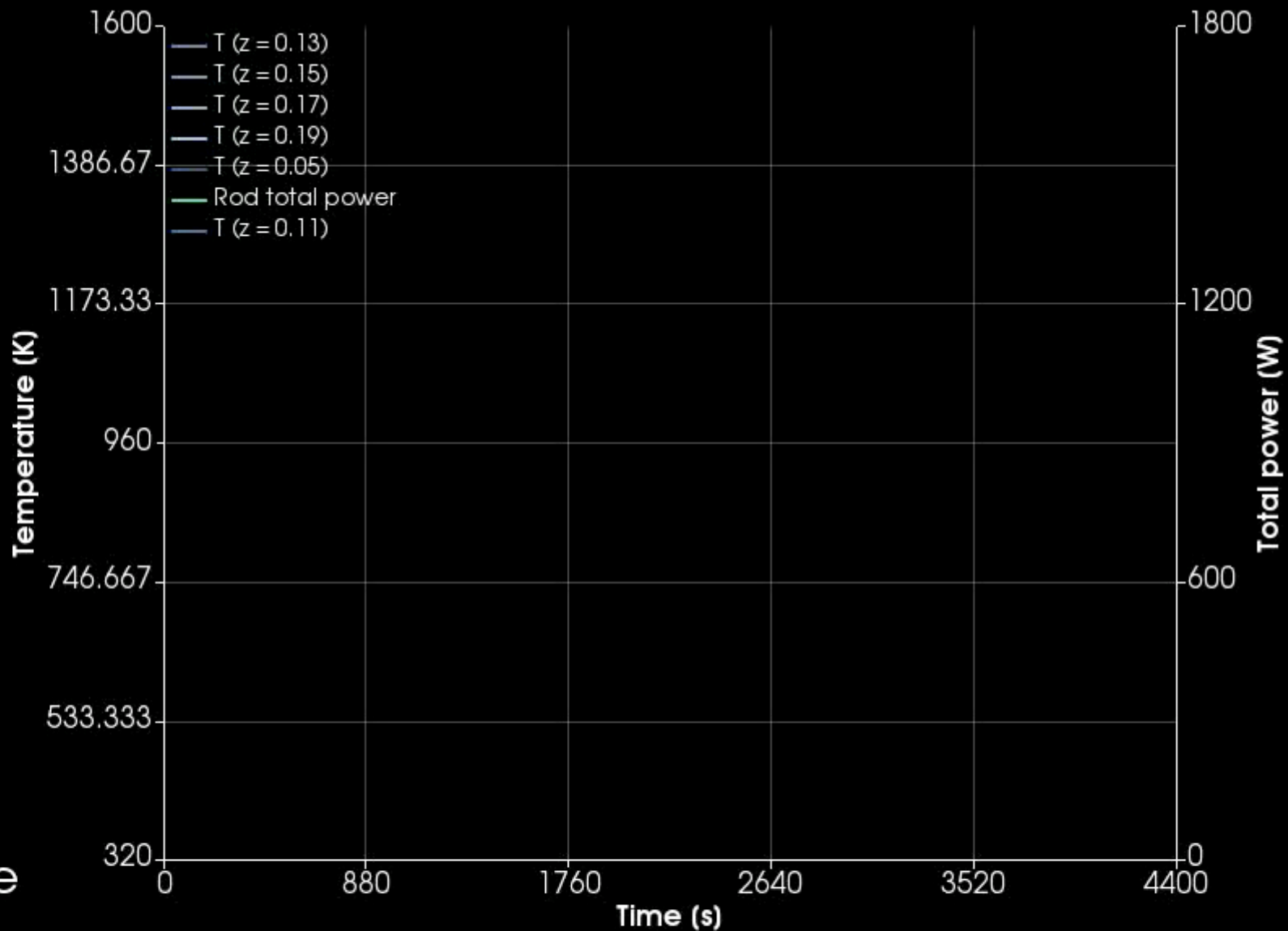
$$C_{CH} \frac{T_{CH} - T_{CH}^P}{\Delta t} = G_{RI}(T_{CH}^4 - T_{FT}^4) - G_{RO}(T_{FT}^4 - T_\infty^4) - G_C(T_{FT} - T_1)$$

$$C_{CH} \frac{T_{CH} - T_{CH}^P}{\Delta t} = G_C(T_{FT} - T_1) - G_{R,1}(T_1^4 - T_\infty^4) - \dot{q}_{LIM}$$

BISON

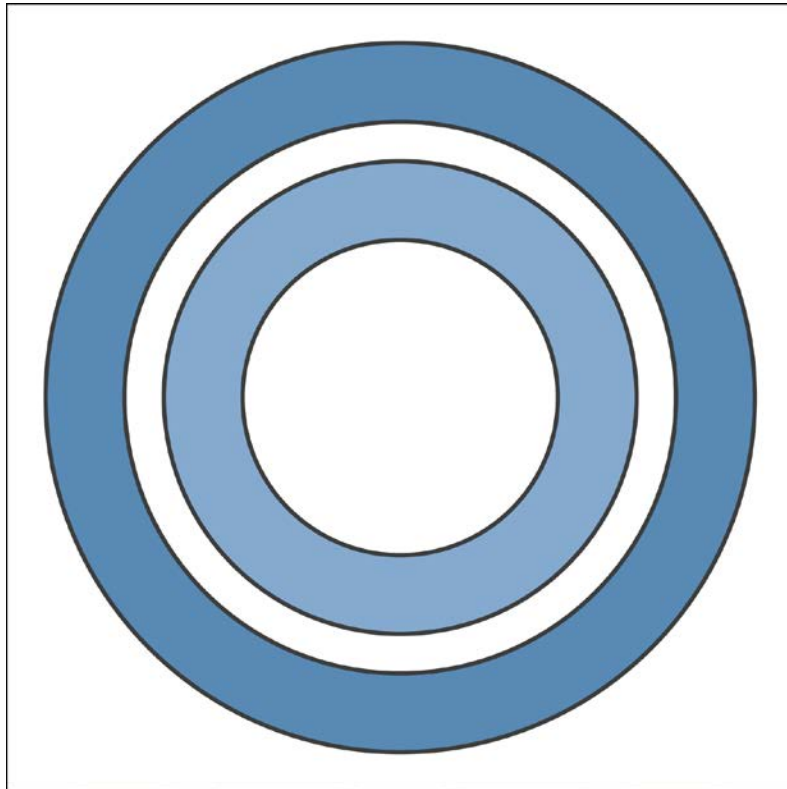


Sockeye

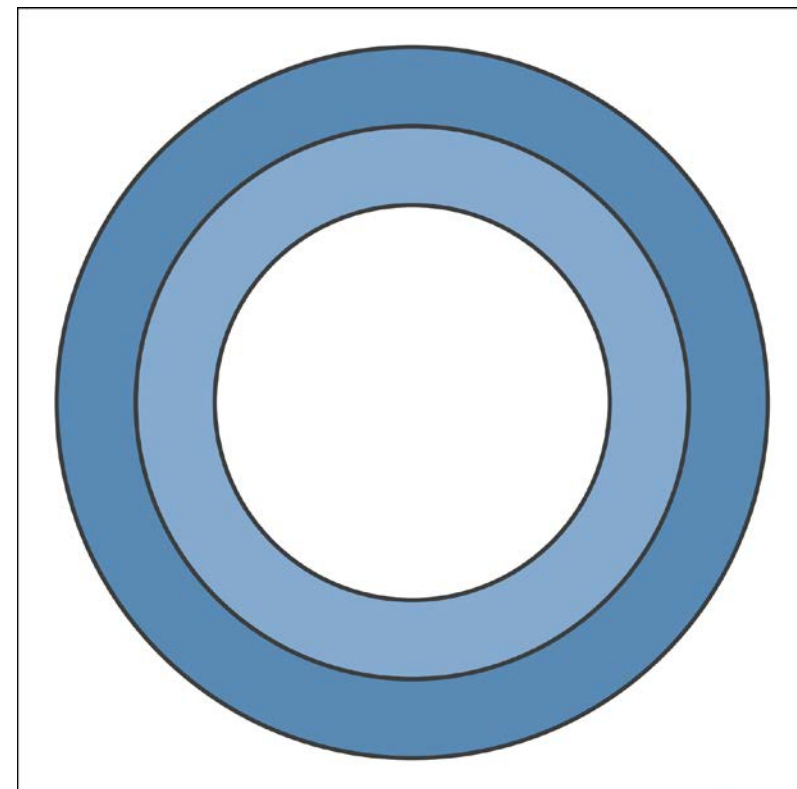


Preliminary heat-pipe/fuel coupling results

Wick Configurations for an Advanced Sockeye



Concentric Annular Wick



Screen Wick

Simplified 7-equation two-phase flow model for heat pipes

$$\frac{\partial \alpha_k A}{\partial t} = \mu A (p_k + \Delta p_{k \rightarrow j}^{cap} - p_j) - \frac{\Gamma_{k \rightarrow j}^{int} a_{int} A}{\rho_{int}}$$

Volume fraction for phase k

$$\frac{\partial (\alpha_k \rho_k A)}{\partial t} + \frac{\partial (\alpha_k \rho_k u_k A)}{\partial x} = -\Gamma_{k \rightarrow j}^{int} a_{int} A$$

Phasic mass conservation

$$\frac{\partial (\alpha_k \rho_k u_k A)}{\partial t} + \frac{\partial \alpha_k (\rho_k u_k^2 + p_k) A}{\partial x} = p_{int} \frac{\partial \alpha_k}{\partial x} A - F_k^{wall} A + \alpha_k \rho_k g_x A$$

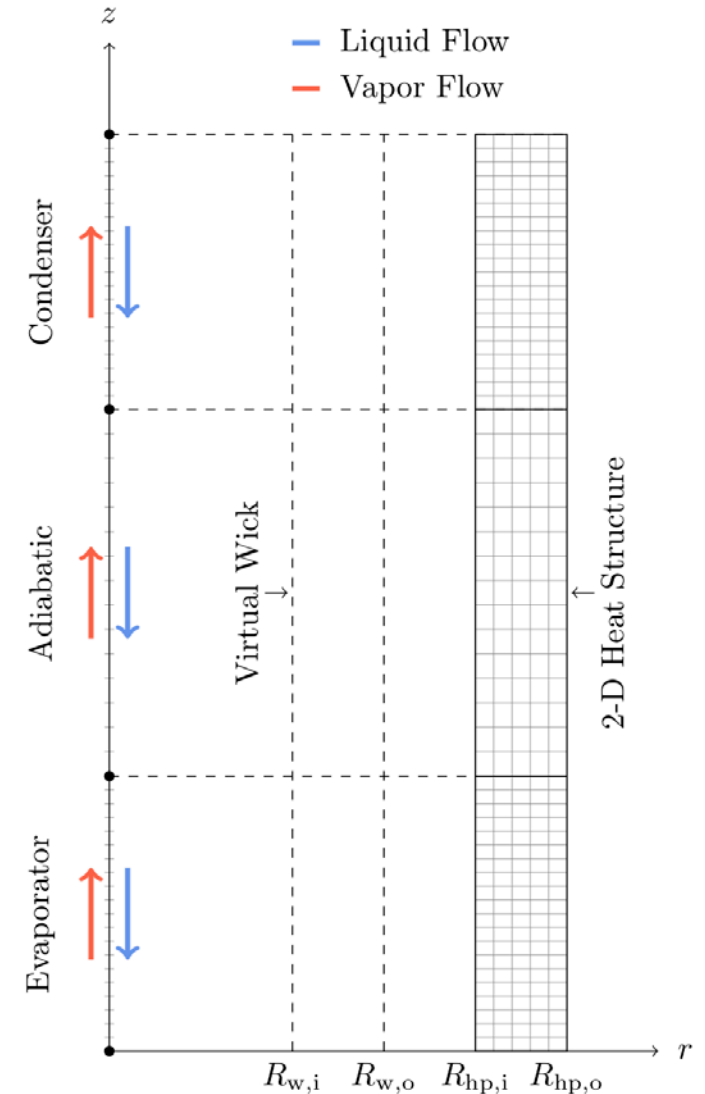
Balance of momentum

$$\begin{aligned} \frac{\partial (\alpha_k \rho_k E_k A)}{\partial t} + \frac{\partial \alpha_k u_k (\rho_k E_k + p_k) A}{\partial x} = & -p_{int} \mu (p_k + \Delta p_{k \rightarrow j}^{cap} - p_j) A \\ & - F_k^{wall} u_k A + \alpha_k \rho_k g_x u_k A + q_{wall \rightarrow k} P_{wall} \\ & + q_{int \rightarrow k} a_{int} A - \Gamma_{k \rightarrow j}^{int} E_k a_{int} A \end{aligned}$$

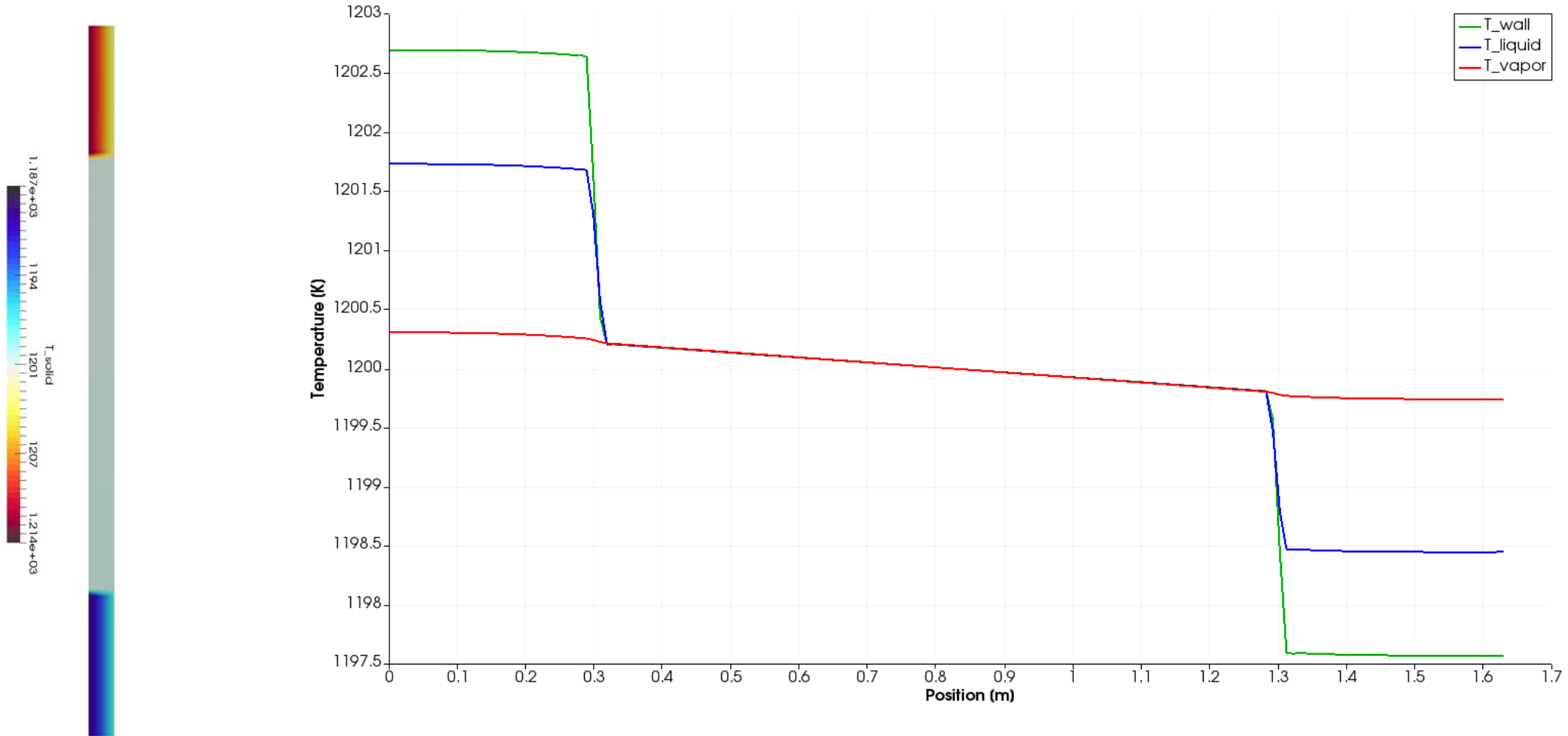
Phasic energy conservation

Intermediate Two-phase Approach: Collocated Heat Pipe Model

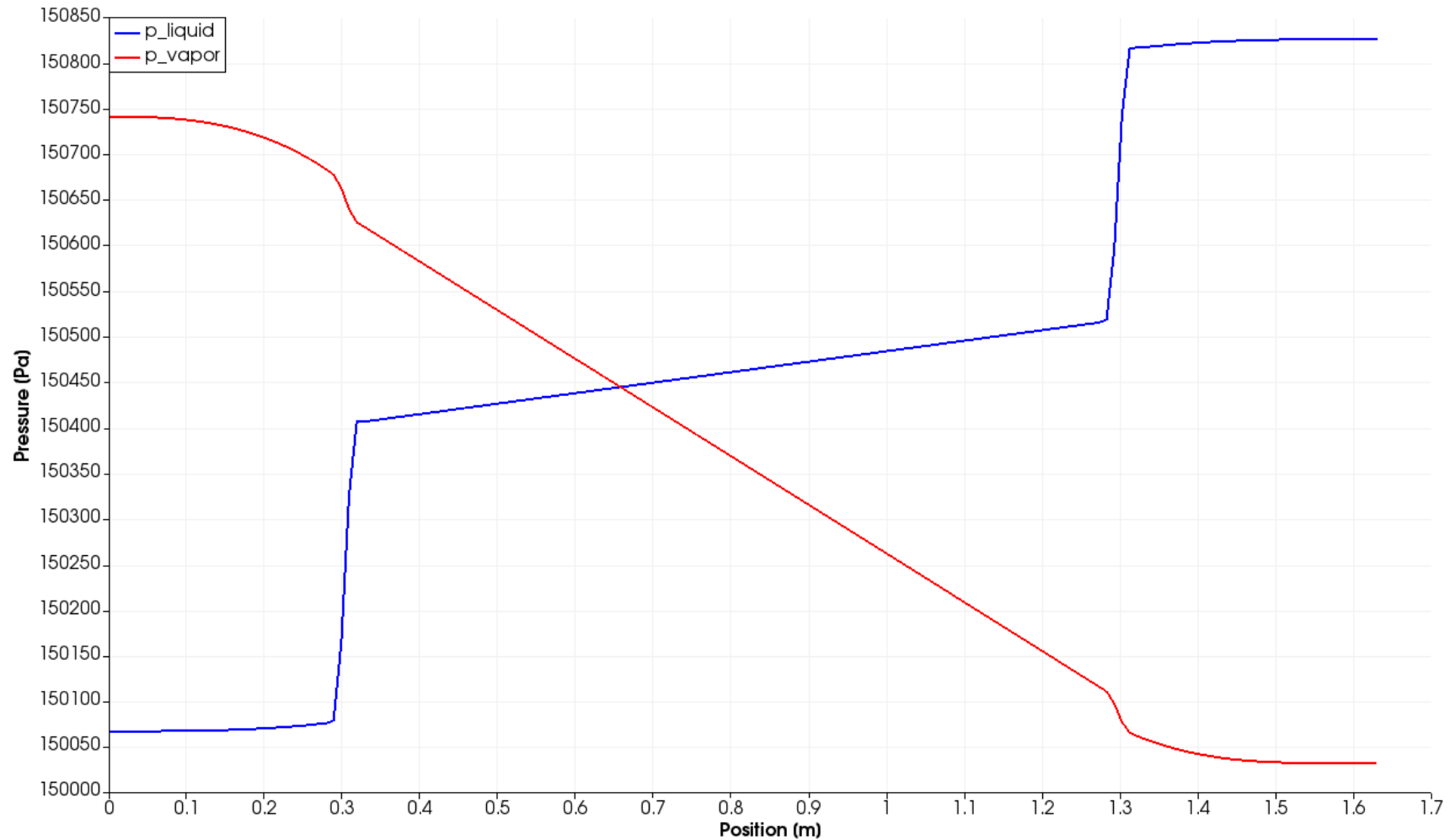
- Designed for normal reactor operation.
- Aggregate melting model – the two-phase flow model is not actually simulated until the onset of boiling. Prior to boiling, solid-phase melting and liquid-phase heating are simulated for step simulation.
- Assumes:
 - 1D two-phase independent flow.
 - Virtual wick, is fully saturated at all operating regimes.
 - Thus, phasic interface is fixed and the interfacial velocity is zero.
 - Velocity relaxation turned off.
 - Pressure relaxation modified with capillary pressure.
 - Wall heat flux deposited in the liquid phase only (wick is always saturated).
- Use reconstructed discontinuous Galerkin (rDG) finite elements to model the flow.
- 2D heat structure (CG-FEM) for improved thermal transient accuracy. In the future the 2D heat structure will have mechanics for thermal expansion and mechanical contact.



Preliminary Collocated Heat Pipe Model Results



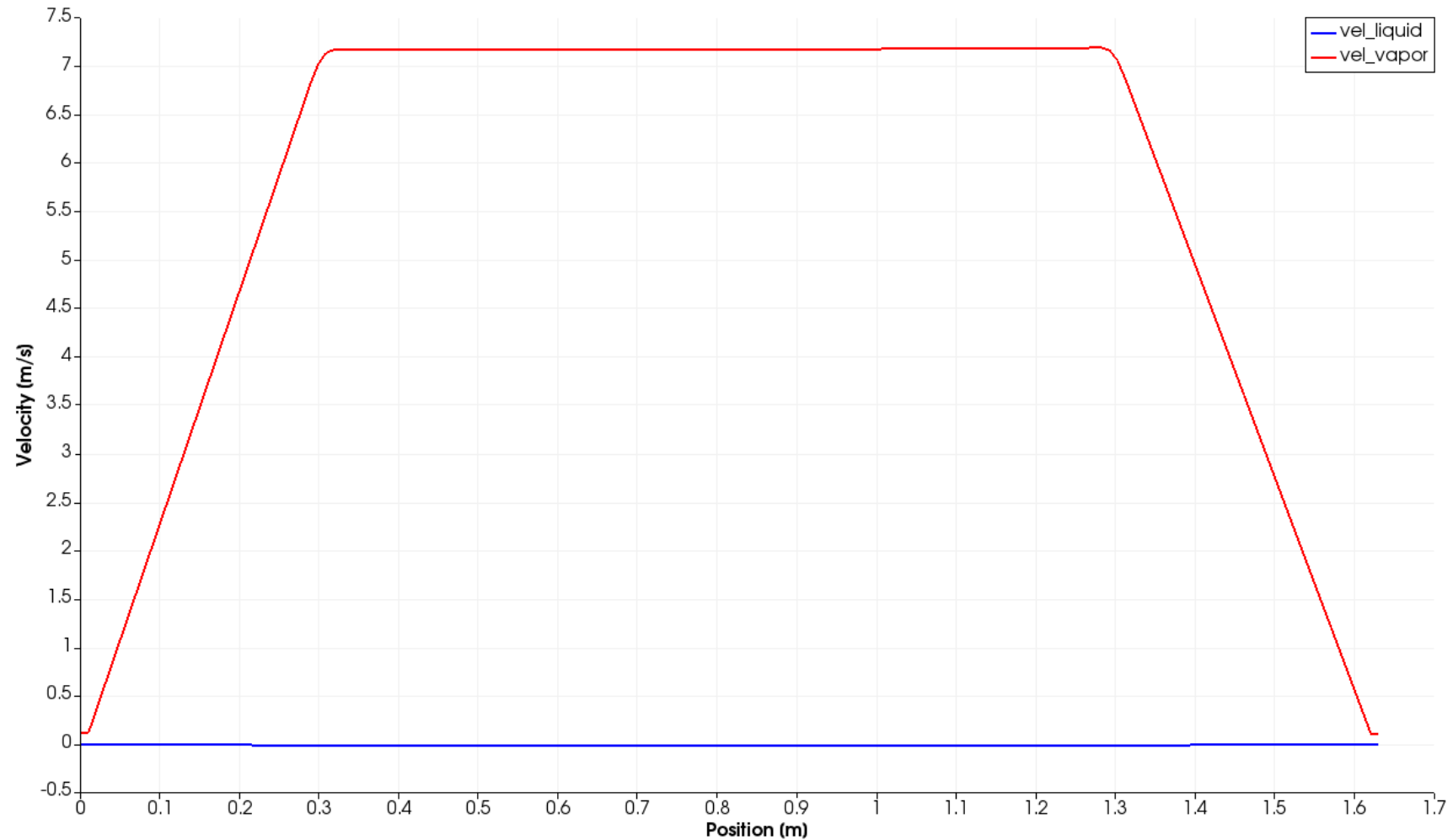
Preliminary Collocated Heat Pipe Model Results (cont'd)



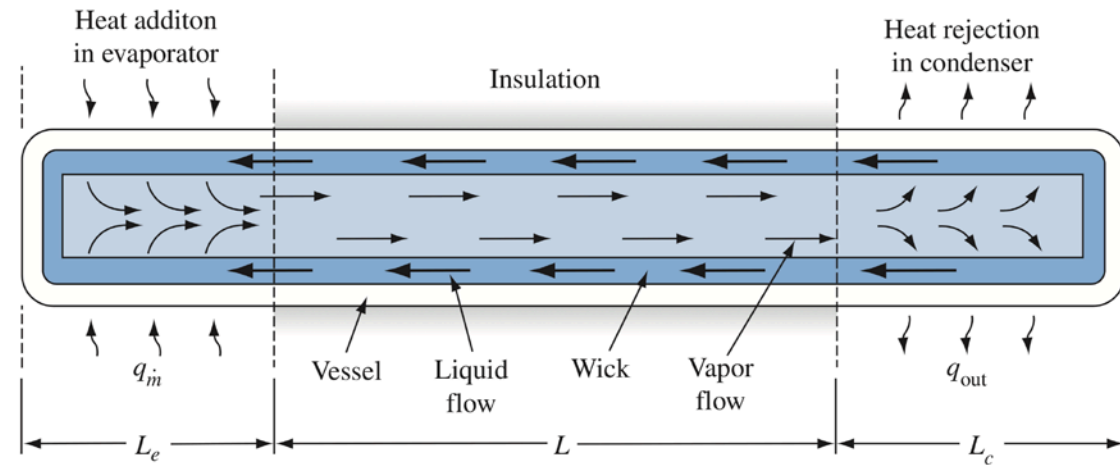
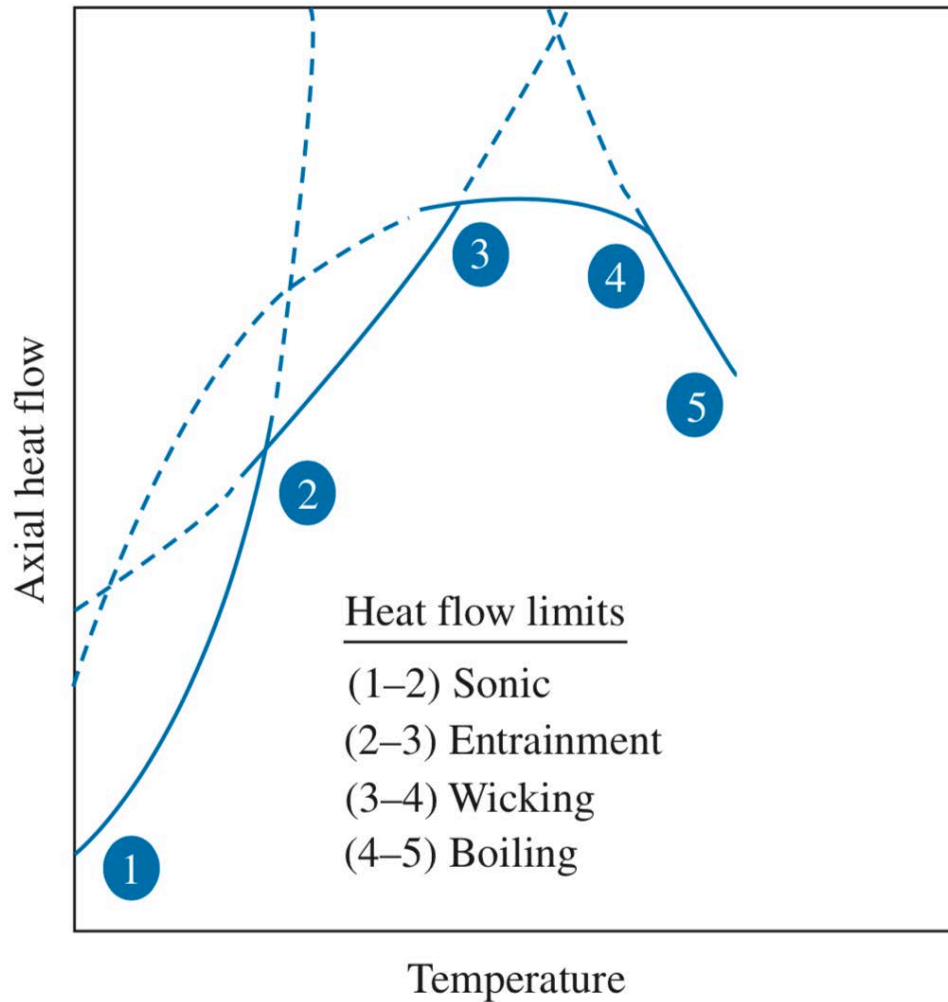
Preliminary Collocated Heat Pipe Model Results (cont'd)



Preliminary Collocated Heat Pipe Model Results (cont'd)



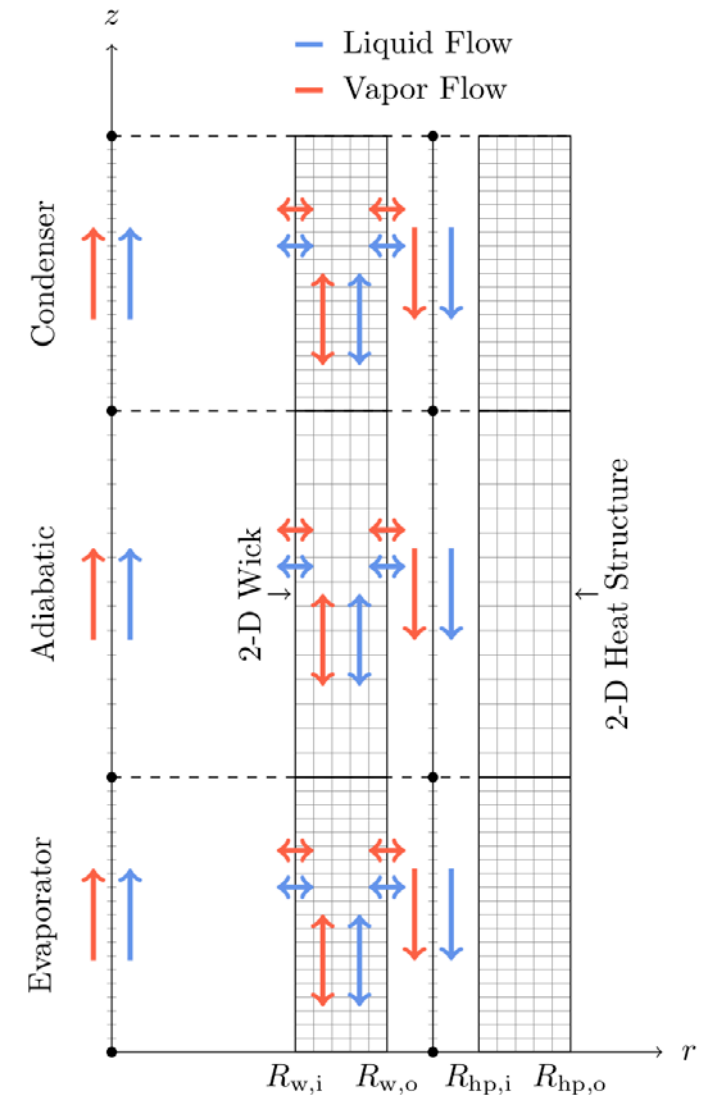
Advanced Design Goal: Predict Operating Limits



- **Viscous:** Viscous friction in the vapor flow limits the circulation of the working fluid.
- **Sonic:** The velocity of the vapor at the exit of the evaporator reaches the speed of sound -- choking the flow.
- **Entrainment:** The vapor moves so fast that it steals liquid from the wick. Dry out in the evaporator occurs.
- **Wicking:** The capillary action of the wick is not strong enough to sufficiently circulate the working fluid.
- **Boiling:** Nucleate boiling occurs in the evaporator. Vapor bubbles block the wick pores.

Advanced Two-phase, Two-channel Heat Pipe Model (FY-2020)

- Designed for investigating the defined five potential operating limits.
- Also capable of normal reactor operation.
- Separate 1D flow channels for vapor core channel and liquid annular channel. Channels are discretized with 1st or 2nd order rDG.
- Flow channels are separated by a resolved 2D wick structure.
- 2D wick structure models assume:
 - 2D two-phase porous flow model based upon pore diameter and capillary action (surface tension)
 - 2D variation in volume fraction
- Aggregate melting.
- Na and K working fluids properties.
- 2D heat (CG-FEM) for improved thermal transient accuracy and thermomechanics (thermal expansion and mechanical contact).

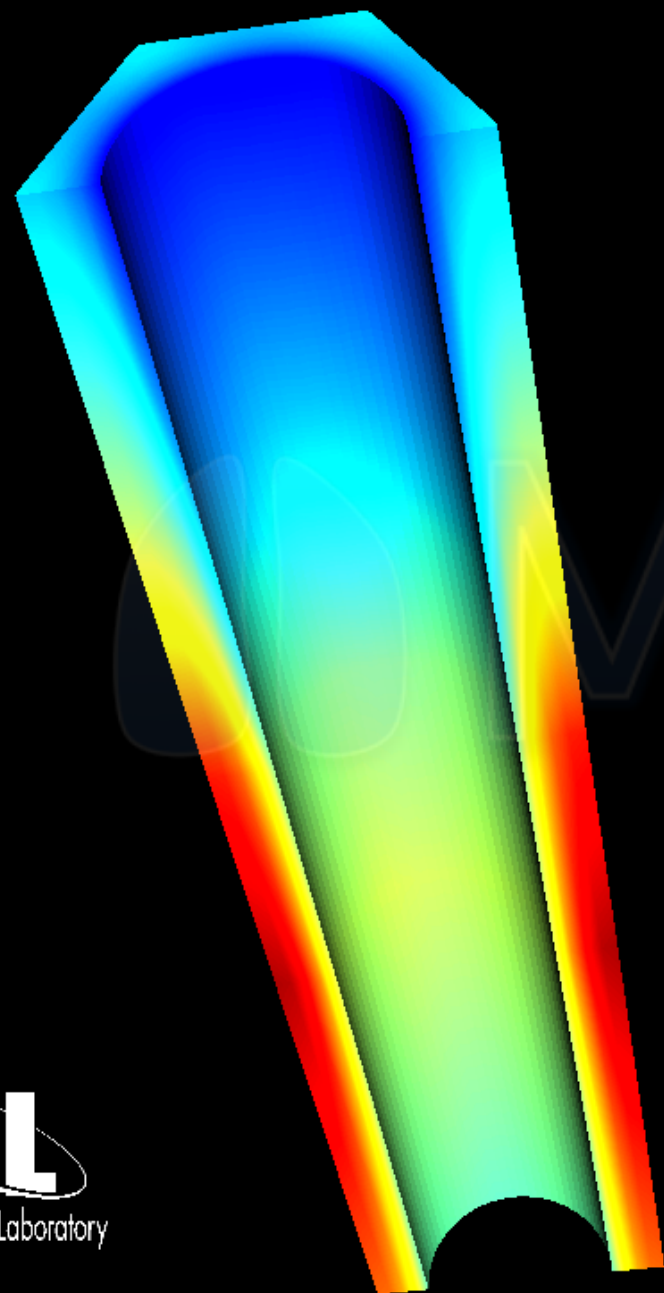


Preliminary Design-A* DireWolf Results

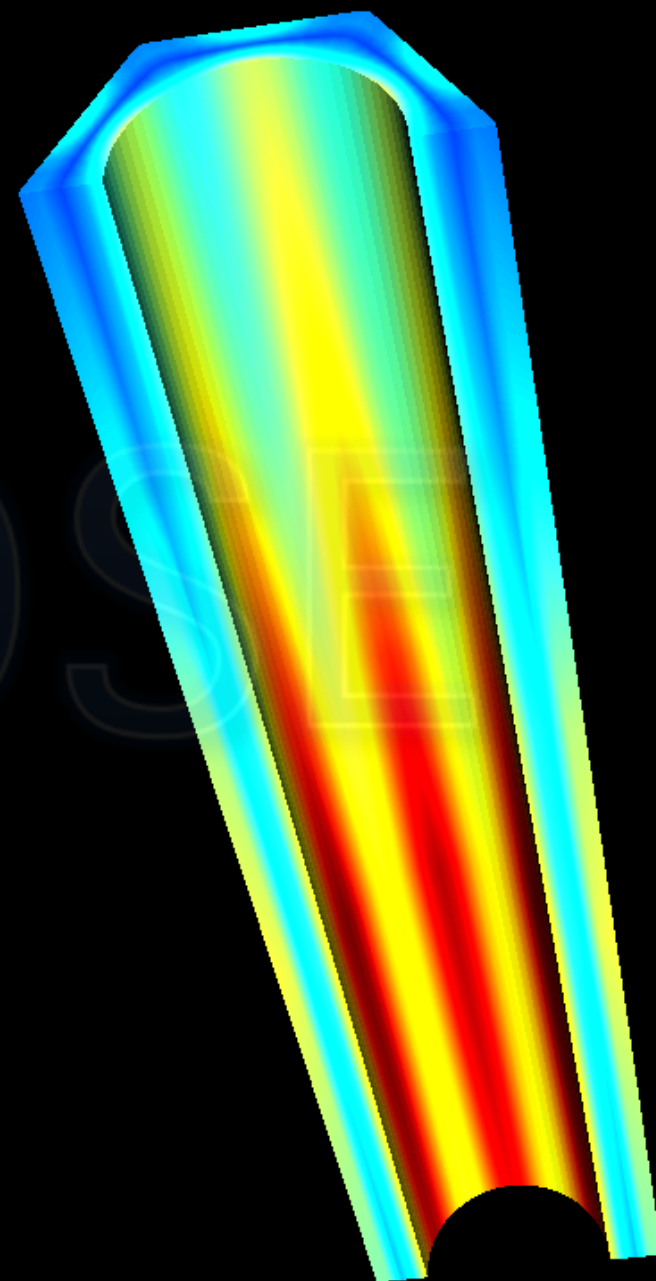
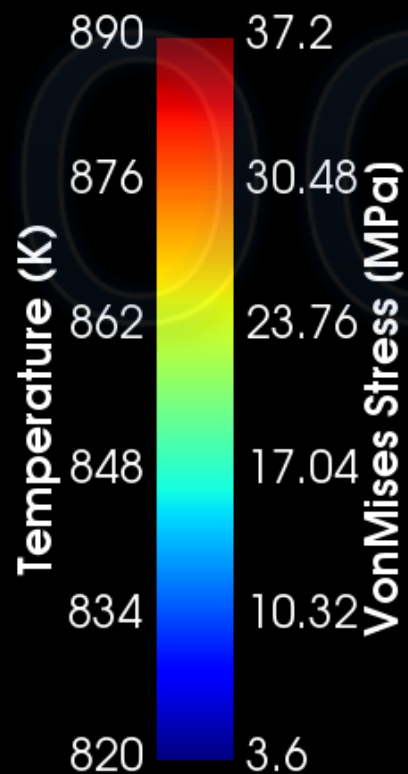
*James W. Sterbentz James E. Werner Andrew J. Hummel John C. Kennedy Robert C. O'Brien Axel M. Dion Richard N. Wright Krishnan P. Ananth, ***Preliminary Assessment of Two Alternative Core Design Concepts for the Special Purpose Reactor***, INL/EXT-17-43212, 2017.

Microreactor Simulation

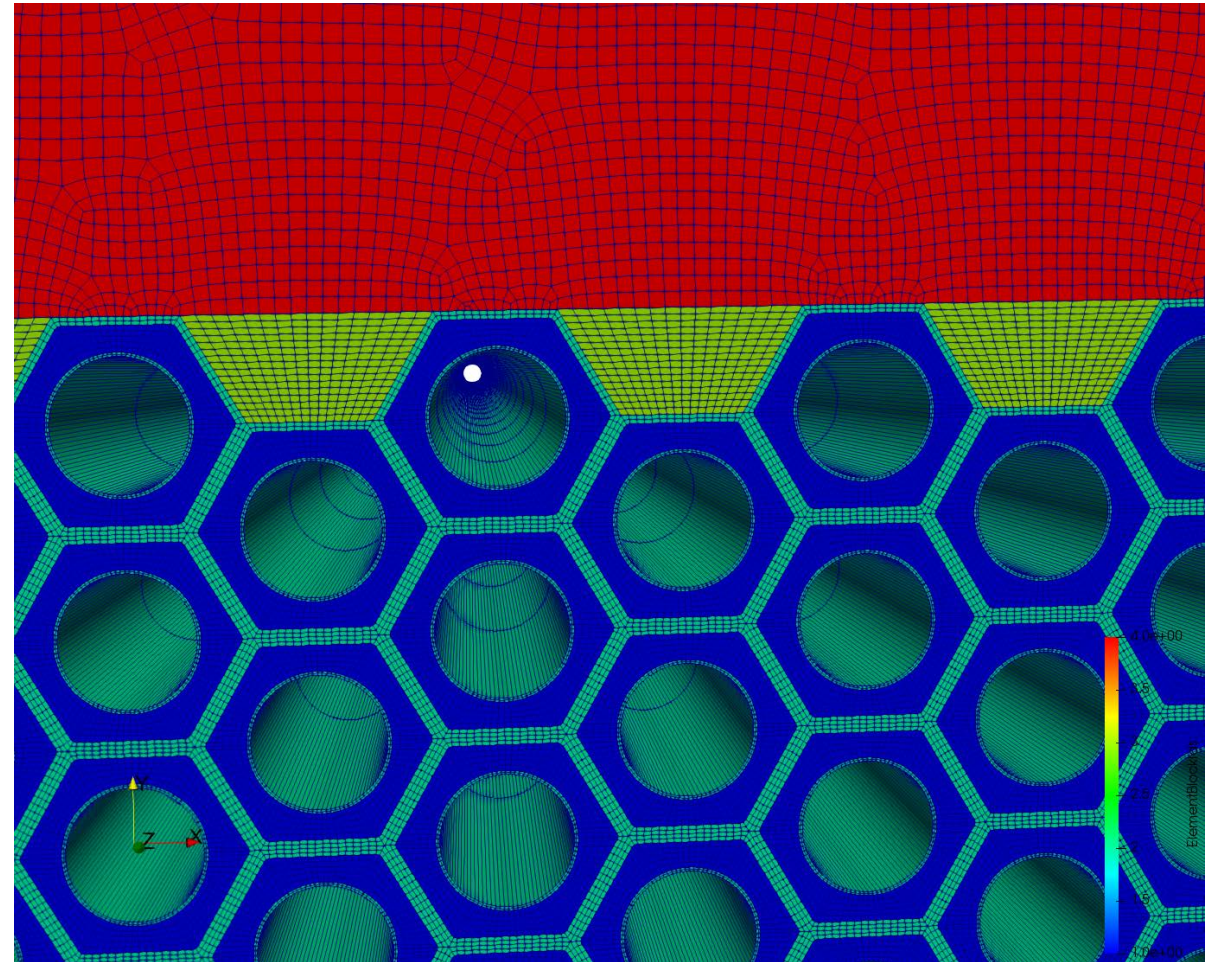
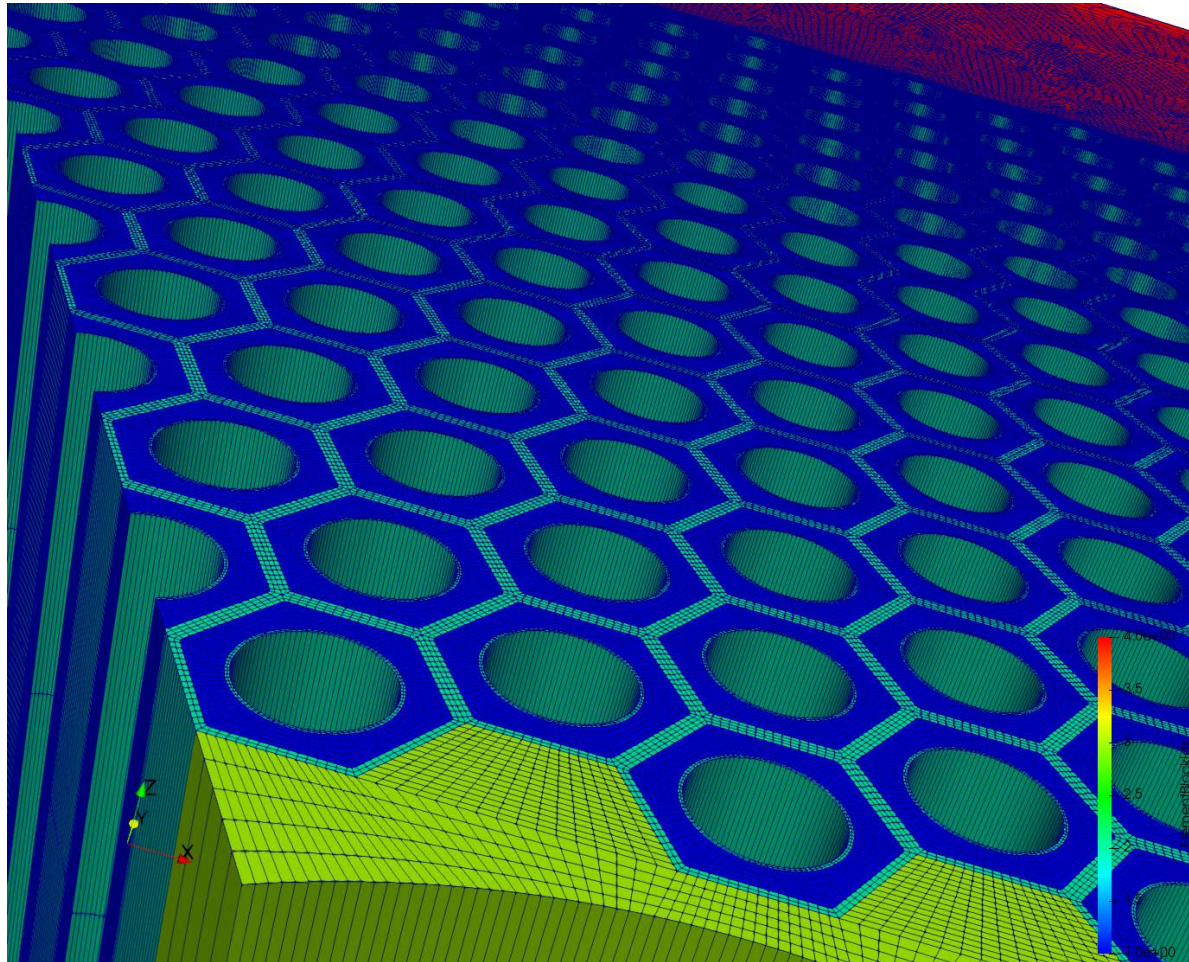
10x scale in x and y axis



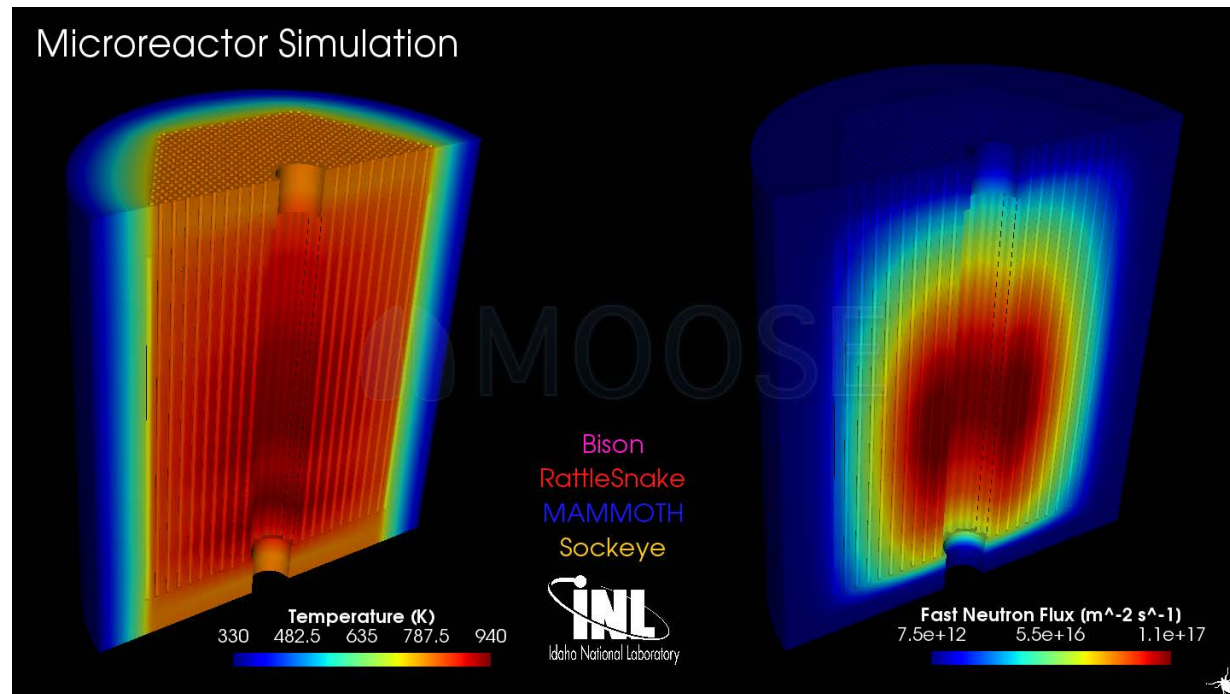
MAMMOTH
Rattlesnake
Sockeye
Bison



Micro-Reactor Full Core Mesh (Hexagonal Fuel Design)



Preliminary Heat-Pipe-Cooled Micro-Reactor (Hexagonal Fuel Design) Transient (7.25 hour power up)



- **Applications:**
 - MAMMOTH
 - BISON
 - Sockeye
- **Transient Scenario:** 7.25 hr linear ramp to 100% power
- **Number of FEs:**
 - MAMMOTH = 2,287,656 (3D)
 - BISON = 1,506,168 (3D)
 - Sockeye = 732,042 (1D)
- **MPis =**
 - 256 BISON
 - 1080 MAMMOTH
- **Run time = ~3 hours**





Micro-Reactor and Sockeye Contributors

DireWolf:

- Mark DeHart
- Javier Ortensi
- Vincent Labouré
- Steve Novascone
- Sebastian Schunert
- David Andrs
- Topher Mathews (LANL)
- Miklaela Blood (LANL)
- Vendant Mehta (LANL)
- Blake Wilkerson (LANL)
- Will Hoffman

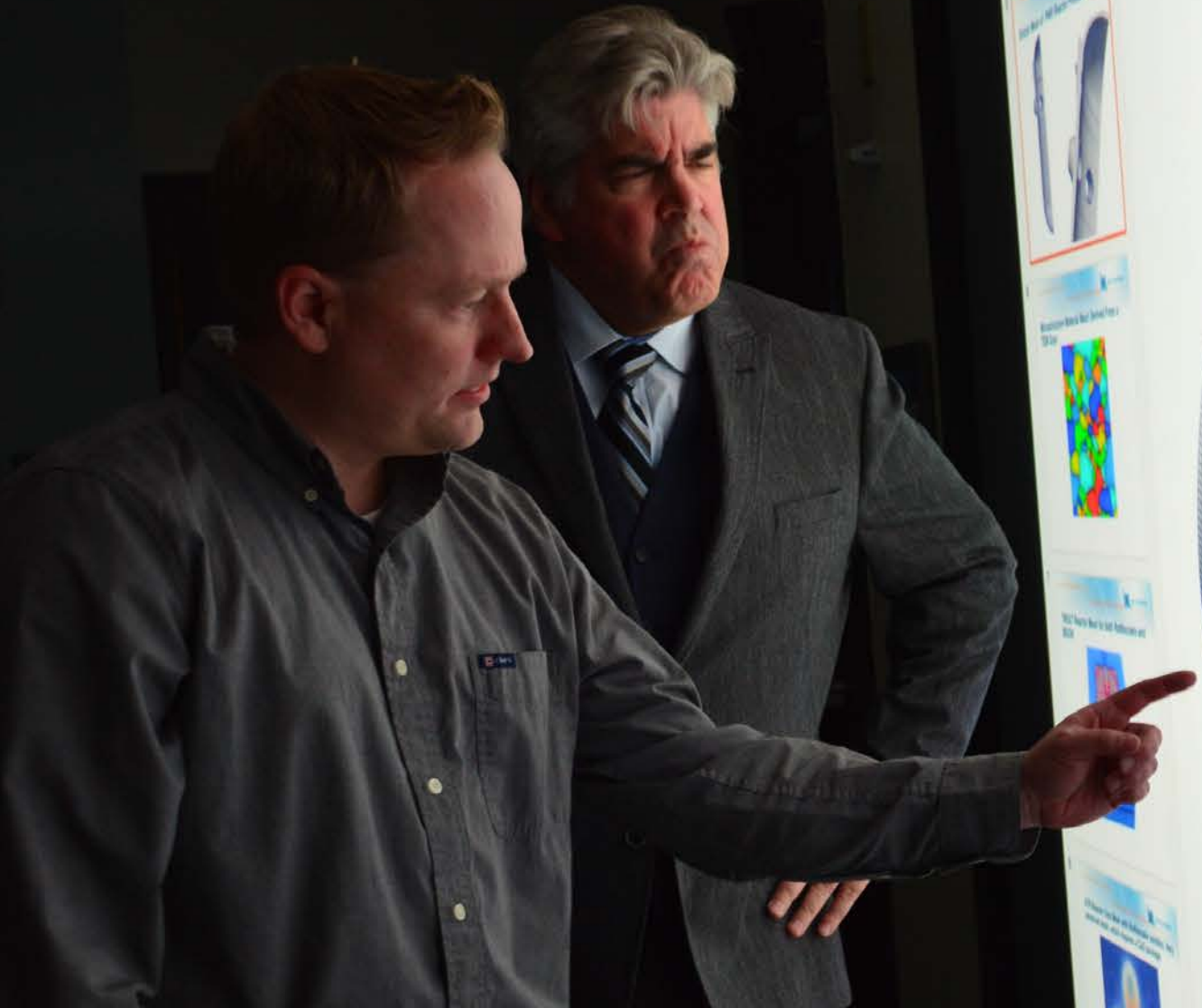
Sockeye:

- Rich Martineau
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- David Andrs
- Russell Johns (LANL)
- Valerie Lawdensky (LANL)
- Ray Berry
- Robert Ried (LANL)



Questions?

I didn't think so!



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Application Access Control (Source Code)

- The following are levels of access that are available:
- Level 0: **Restricted** (default) - No access granted to binaries or source. This means that it is not made available in source or binary format to unauthorized individuals.
- Level 1: **Executable only** - Access is granted to pre-built binaries built and maintained by the application owners. No source code access is granted.
- Level 2: **Header only access** - Access to application headers is made available to facilitate the development of “pluggable” objects. New objects may be built and compiled by the end user and linked at runtime to the application.
- Level 3: **Read-only source access** - Full read-only access to the application repository is granted, giving the developer access to all source code and tools for building binaries.
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