An Intro to Moltres,
An MSR Multiphysics Code

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1) Conclusions

- A MOOSE-based code for multiphysics simulation of molten salt reactors has been developed.
- The code can model salient physics required for multiphysics simulations of MSRs, namely, many group neutron diffusion, delayed neutron precursor advection, salt buoyancy, and incompressible Navier-Stokes.
- The code was found to successfully simulate the MSRE for both statics and transients. Work is underway to simulate fast spectrum MSRs in the MOOSE framework.
- Code is FOSS, sustainably developed with continuous integration. Find it here:

2) Introduction

What are the bare minimum physics required to model a fluid-fueled reactor?

Multigroup diffusion:

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} = \nabla \cdot D_g \nabla \phi_g + \sum_{g\neq g'}^{G} \Sigma^s_{g'\to g}\phi_{g'} + \chi^p_g \sum_{g'=1}^{G}(1-\beta)\nu\Sigma^f_{g'}\phi_{g'} + \chi^d_g \sum_i^I \lambda_i C_i - \Sigma^r_g \phi_g$$

A modified version of the delayed neutron precursor production/decay equation that accommodates advection:

$$\frac{\partial C_i}{\partial t} = \sum_{g'=1}^{G} \beta_i \nu \Sigma^f_{g'}\phi_{g'} - \lambda_i C_i - u \cdot \nabla C_i$$

An equation to describe heat generation, transport, and conduction must be solved too:

$$\rho_f c_{p,f}\frac{\partial T_f}{\partial t} + \nabla \cdot (\rho_f c_{p,f}\vec{u} \cdot T_f - k_f \nabla T_f) = \sum_g \phi_g \Sigma_{f,g} E_{f,g}$$

The above colors illustrate the strong coupling:
Red = function of temperature
Blue = neutron fluxes
Green = precursor concentrations

The Moltres code is built on the MOOSE framework from INL, a flexible toolkit for solving partial differential equations via the finite element method.

MOOSE, by default, will solve PDE weak forms using continuous Galerkin FEM. Let's see what happens when continuous Galerkin gets applied to a simple, 1D problem with a convective term.

Solve this equation via CG on the domain (0,1] with BC u(0)=0:

$$\frac{\mathrm{d}u}{\mathrm{d}x} + \lambda u = \mathrm{e}^{\lambda x}$$

Idea of finite elements: substitute a basis of functions to approximate the problem by. Substituting a linear Lagrange basis gives:

$$\sum_j \xi_j \int_0^1 \phi_i \phi'_j \mathrm{d}x + \lambda \sum_j \xi_j \int_0^1 \phi_i \phi_j \mathrm{d}x = \int_0^1 \phi_i \mathrm{e}^{\lambda x}\mathrm{d}x$$

Where the test space leads to a system of linearly independent equations of the form Ax=b. Numerically solving with lambda=3 and 100 nodal values yields an unphysical solution:

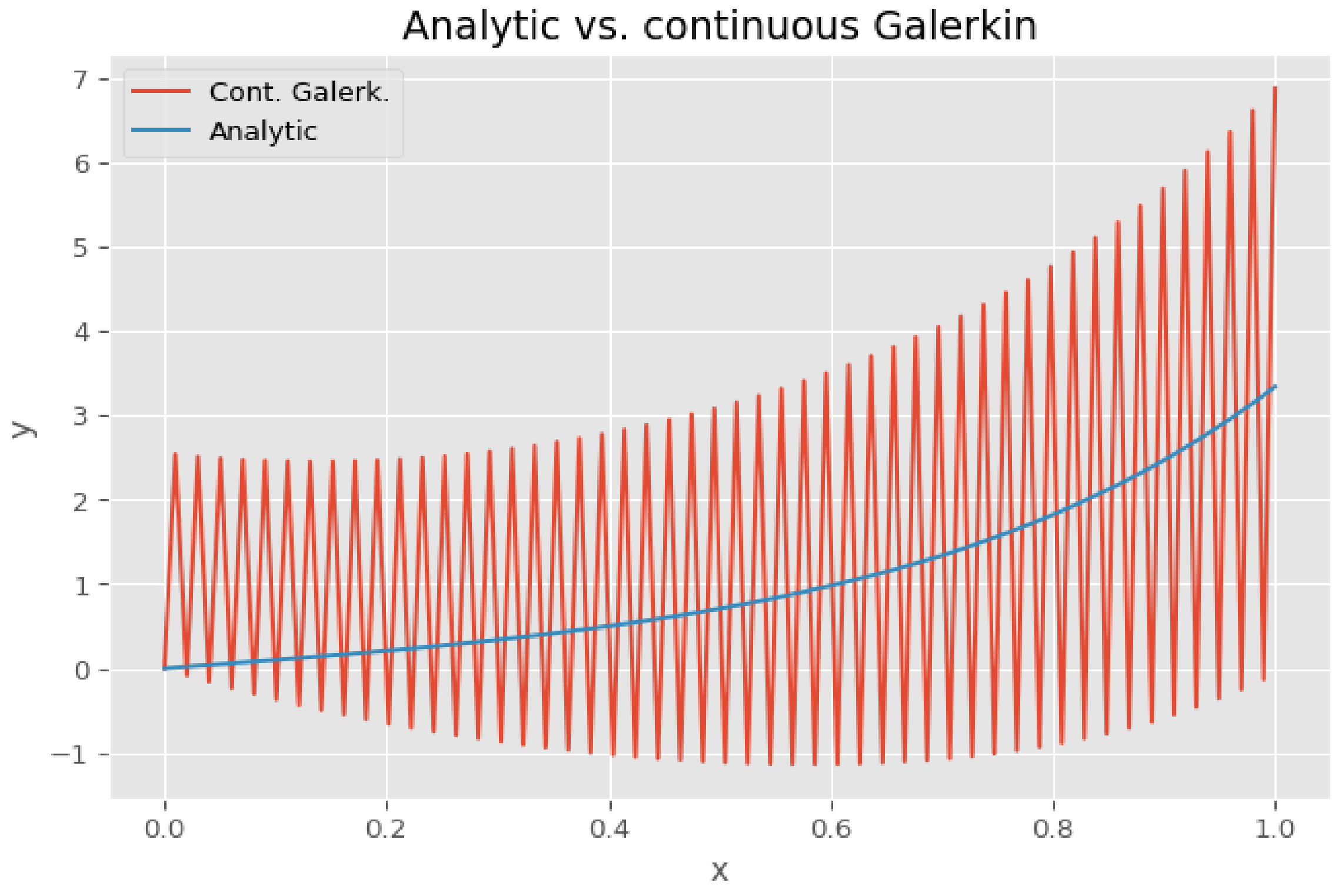


Figure (1): continuous Galerkin fails to approximate transport. Moltres automatically makes discontinuous Galerkin [2] solutions to delayed neutron precursor transport.

3) Benchmark case: MSRE

- Documented in [3], the molten salt reactor experiment began construction at ORNL in 1960, went critical in 1964, and concluded experiments in 1969.
- Transient and steady state measurements were made on neutronics: for transients, time-series power level was measured. For steady state, some measurements of core flux and temperature distribution can be found. Can Moltres match the experiment?

Table (1): some reactor parameters

Moder. height	162.56 cm
Moder. radius	70.1675 cm
Avg volumetric heat rate	4 W / ccm
Total power	8 MW(th)
Channel hydraulic diameter	1.524 cm
Channel Re #	858

Table (2): MSRE materials

Moderator	Nuclear graphite
Fuel	FliBe-ZrF4-UF4 eutectic
Vessel	Hastelloy-N

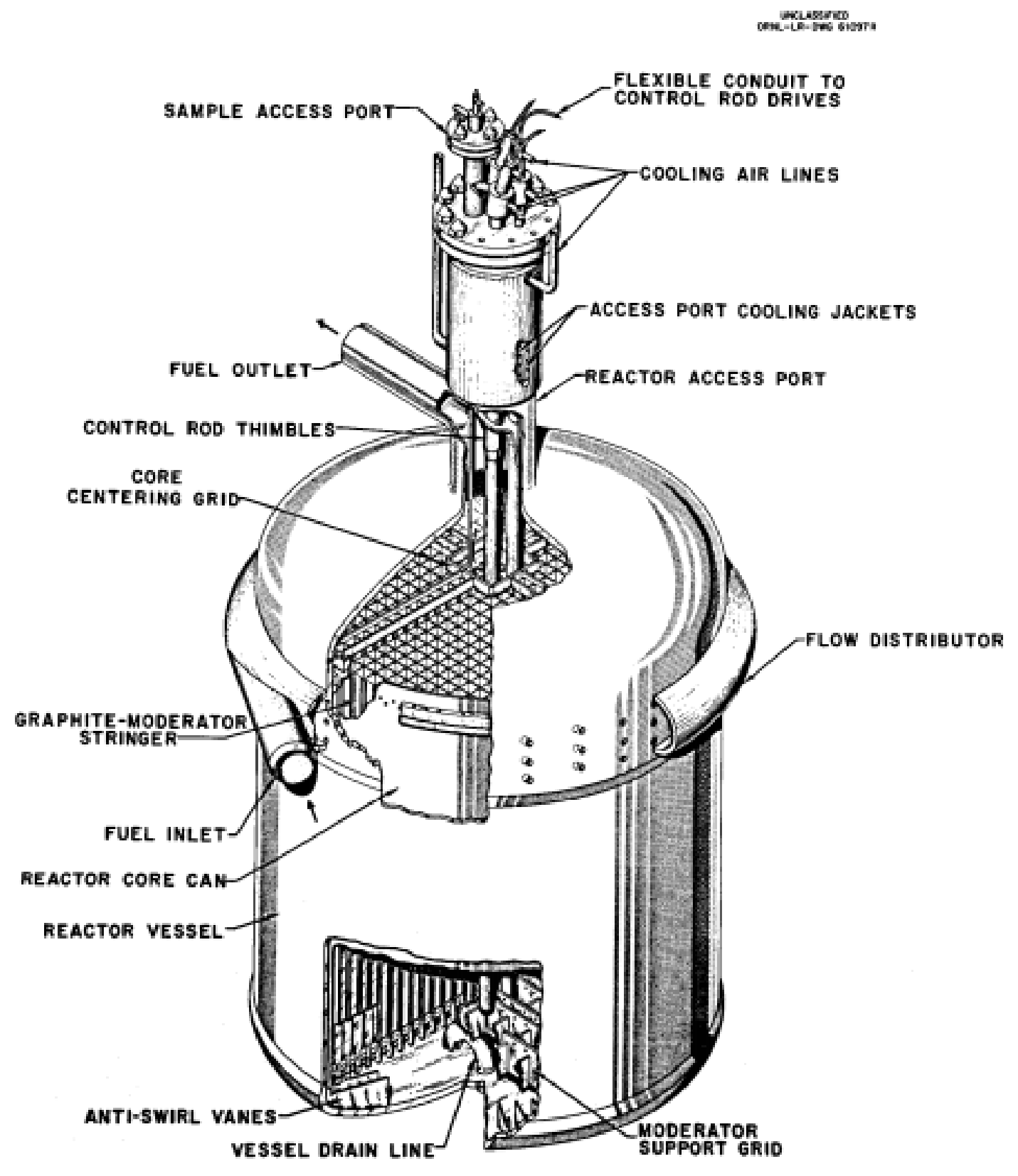
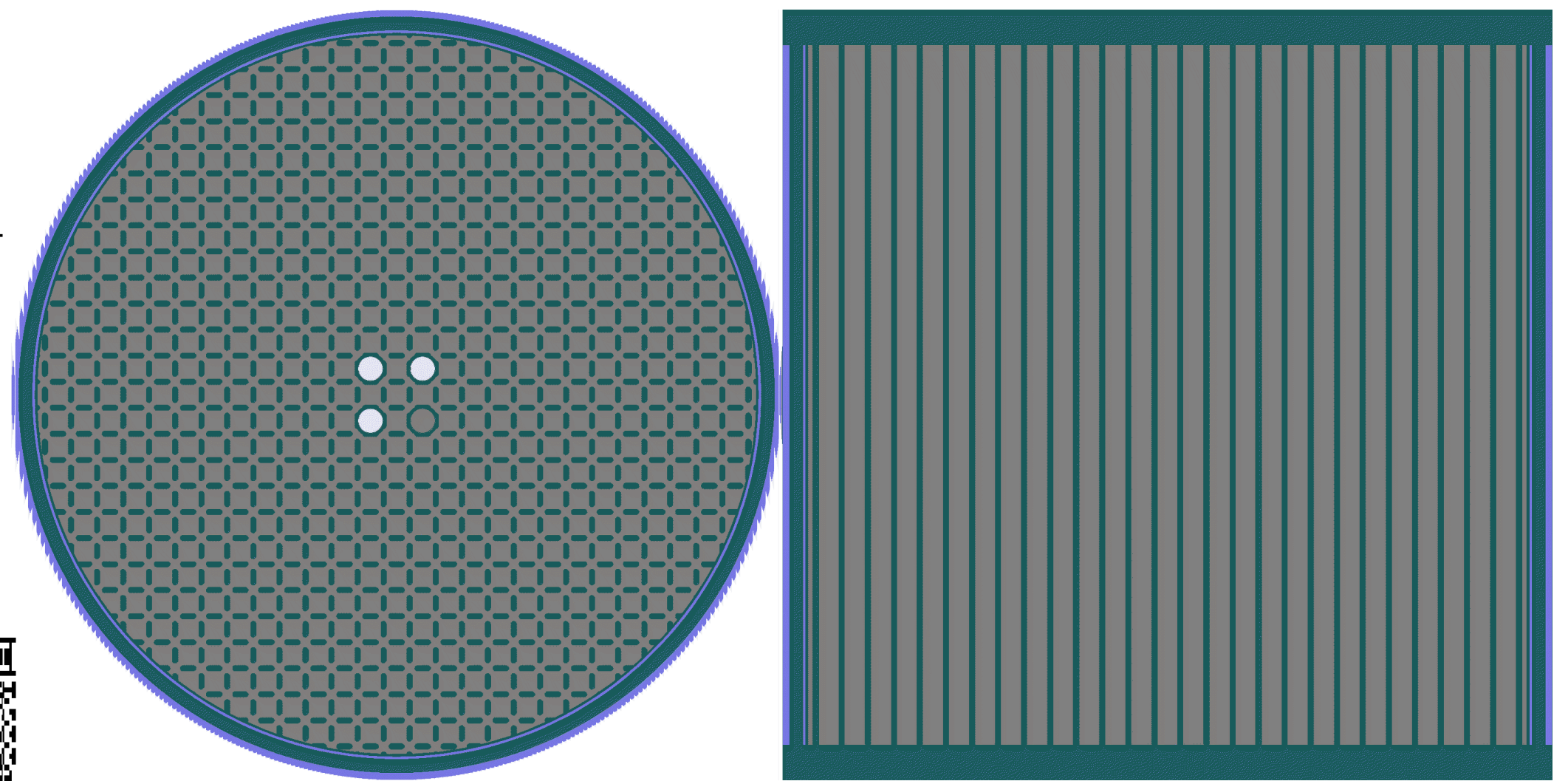


Figure (2): ORNL MSRE diagram.

3.1) MSRE group constants

- Since we have access to the Blue Waters supercomputer, we solve for heterogeneous flux in a few-group setting.
- Relatively little documentation on group constant generation for molten salt reactors, so Serpent 2 calculates a spectrum in both graphite and fuel. After that, cross sections are condensed into a four group structure originally intended for FHRs with B1 critical spectrum adjustment.

Figure (3): MSRE geometry used in Serpent 2. Notice: exact channel geometry and control rod guide tubes.



- Group constants were generated separately for both fuel and graphite, with each material individually heated or cooled from the nominal temperature of 900 K in increments of 100K from 700-1600K.
- Whether cross terms in heating seriously affect reactivity should be determined in a followup study.

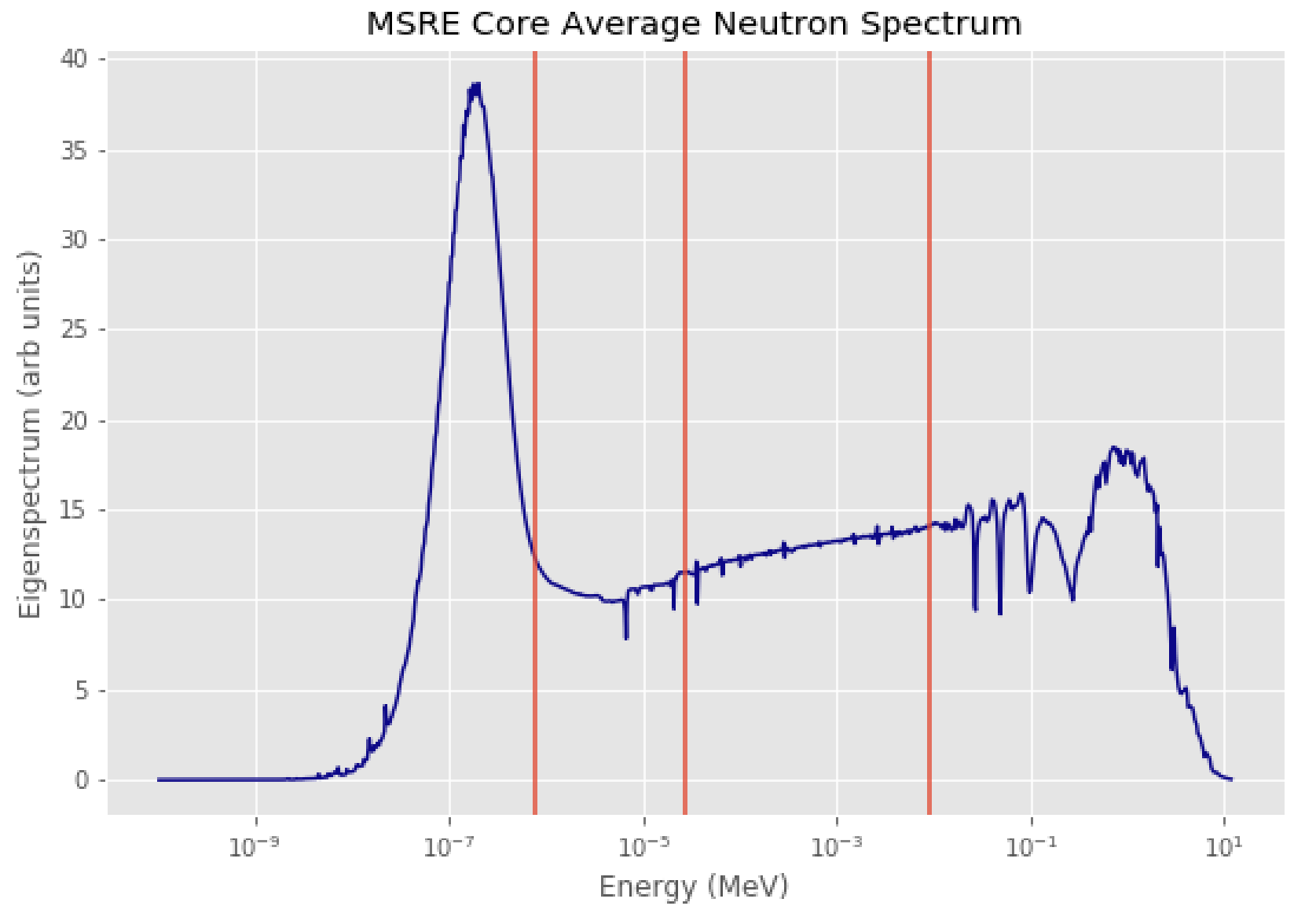


Figure (4): MSRE spectrum with no control rod insertion from Serpent 2, energy group boundaries in four group structure drawn.

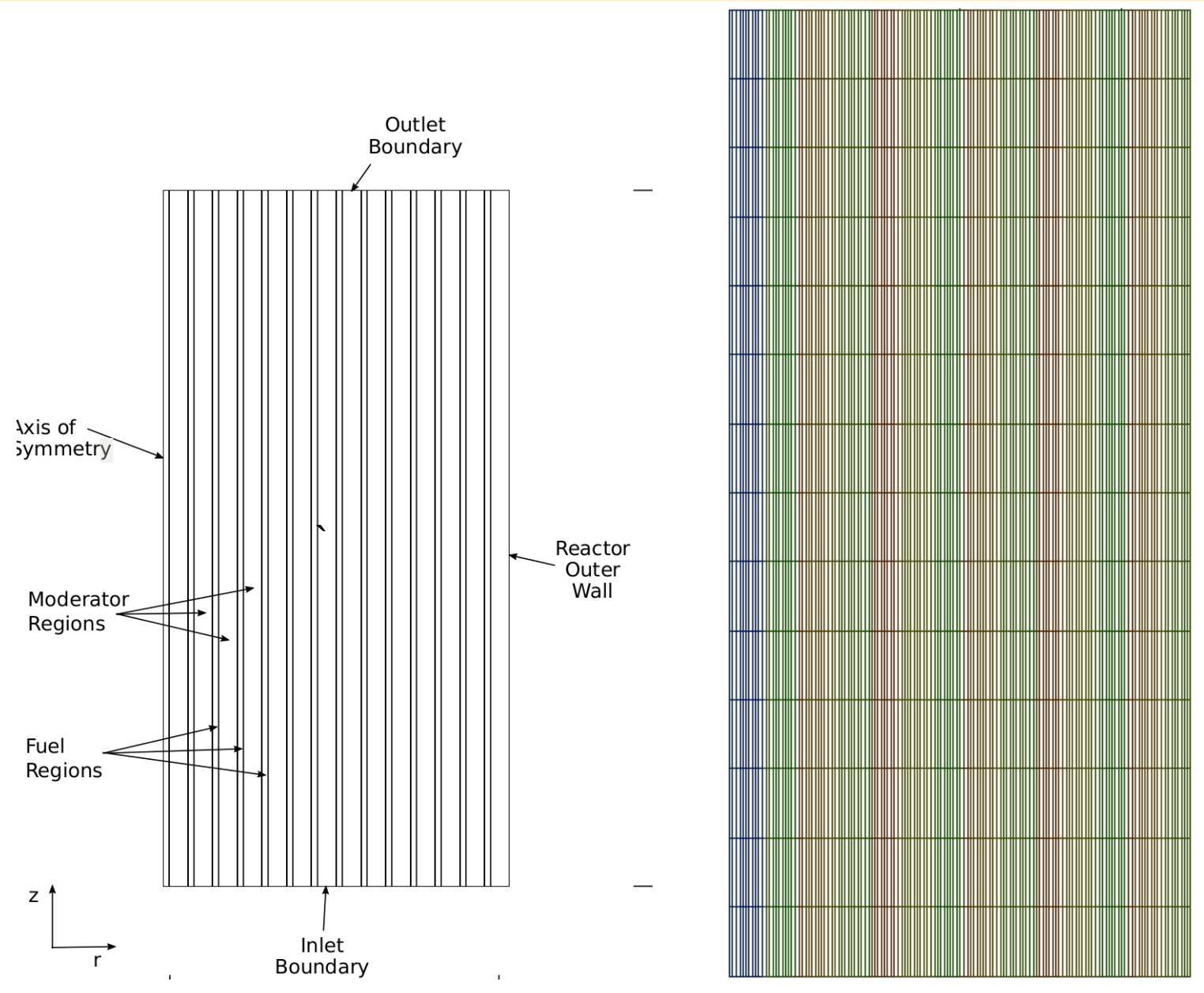
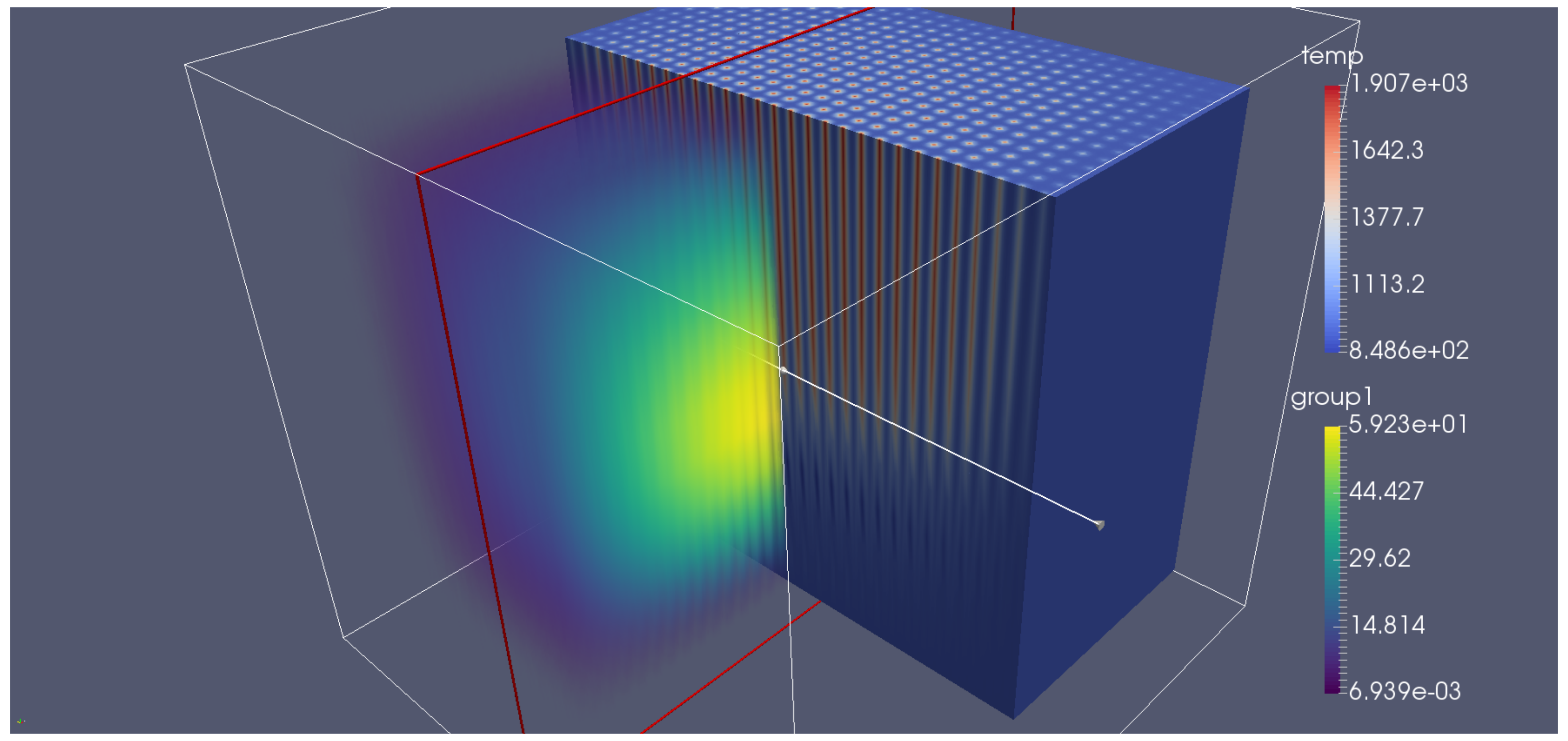


Figure (5): salt-fraction preserving computational mesh in axisymmetric RZ coordinates, used for transient calculations.

4) Results

Figure (6): cuboidal MSRE steady-state result with gamma heating. Fast neutron flux was volume rendered. Slug flow used in channels. Flux eigenmode solution was used with power normalized to 8 MW(th).



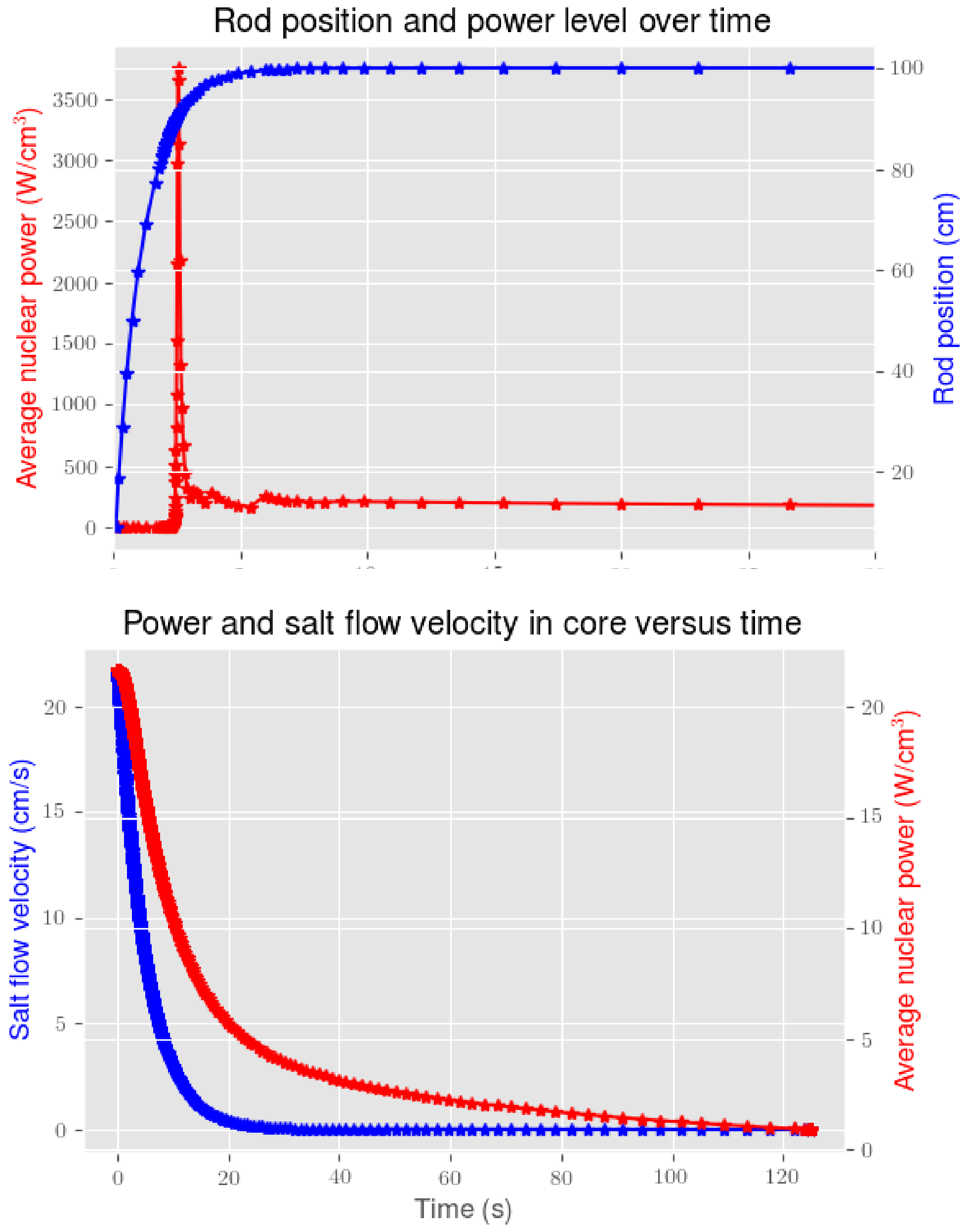
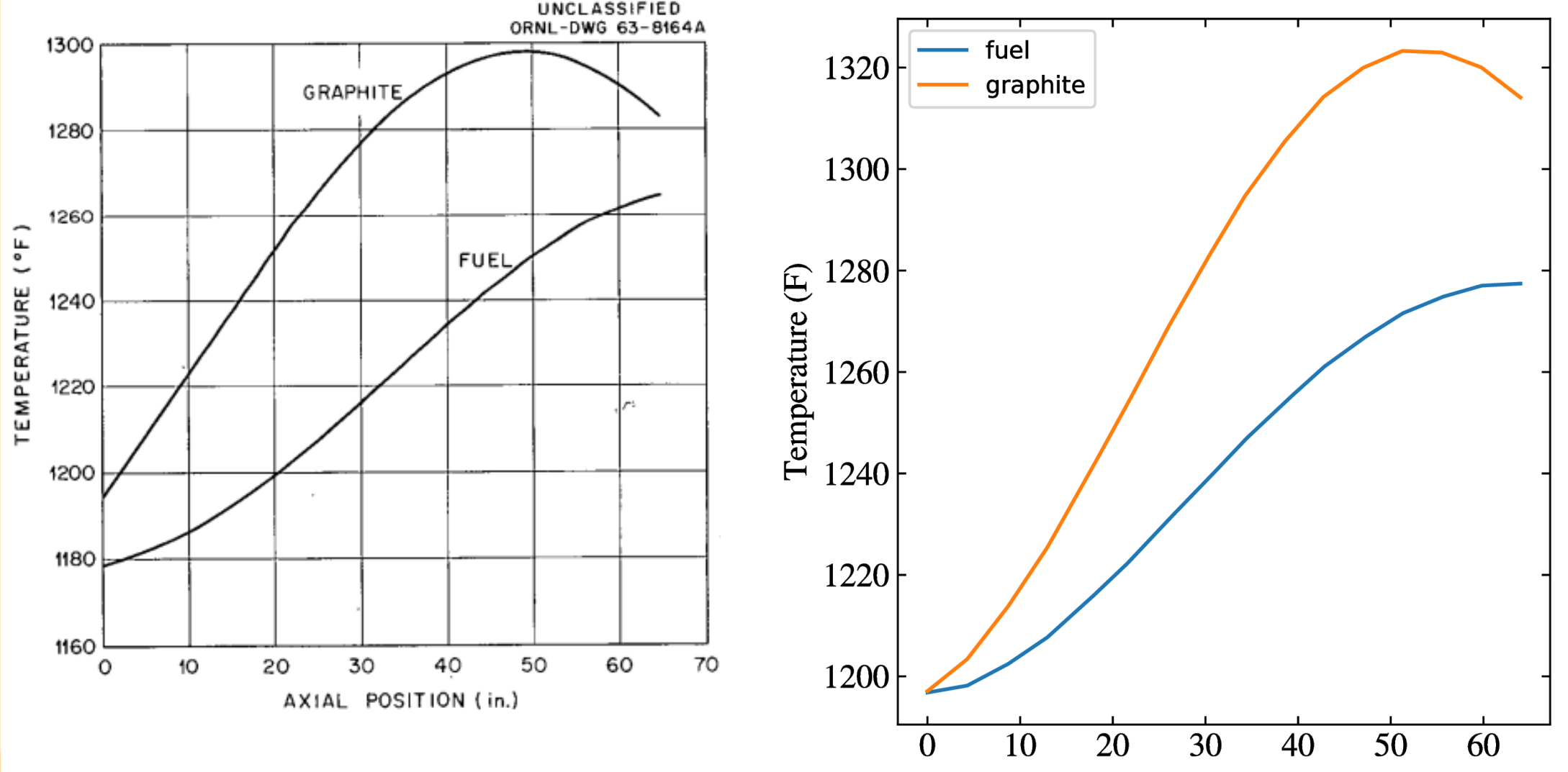


Figure (7): 2D axisymmetric MSRE transient responses. (above) reactor approaches prompt supercriticality due to control rod jerk. (below) salt pump coastdown causes negative thermal feedback to bring reactor subcritical.

Axial Temperature distribution: exp. And calculated



Radial flux distribution: exp. and calculated

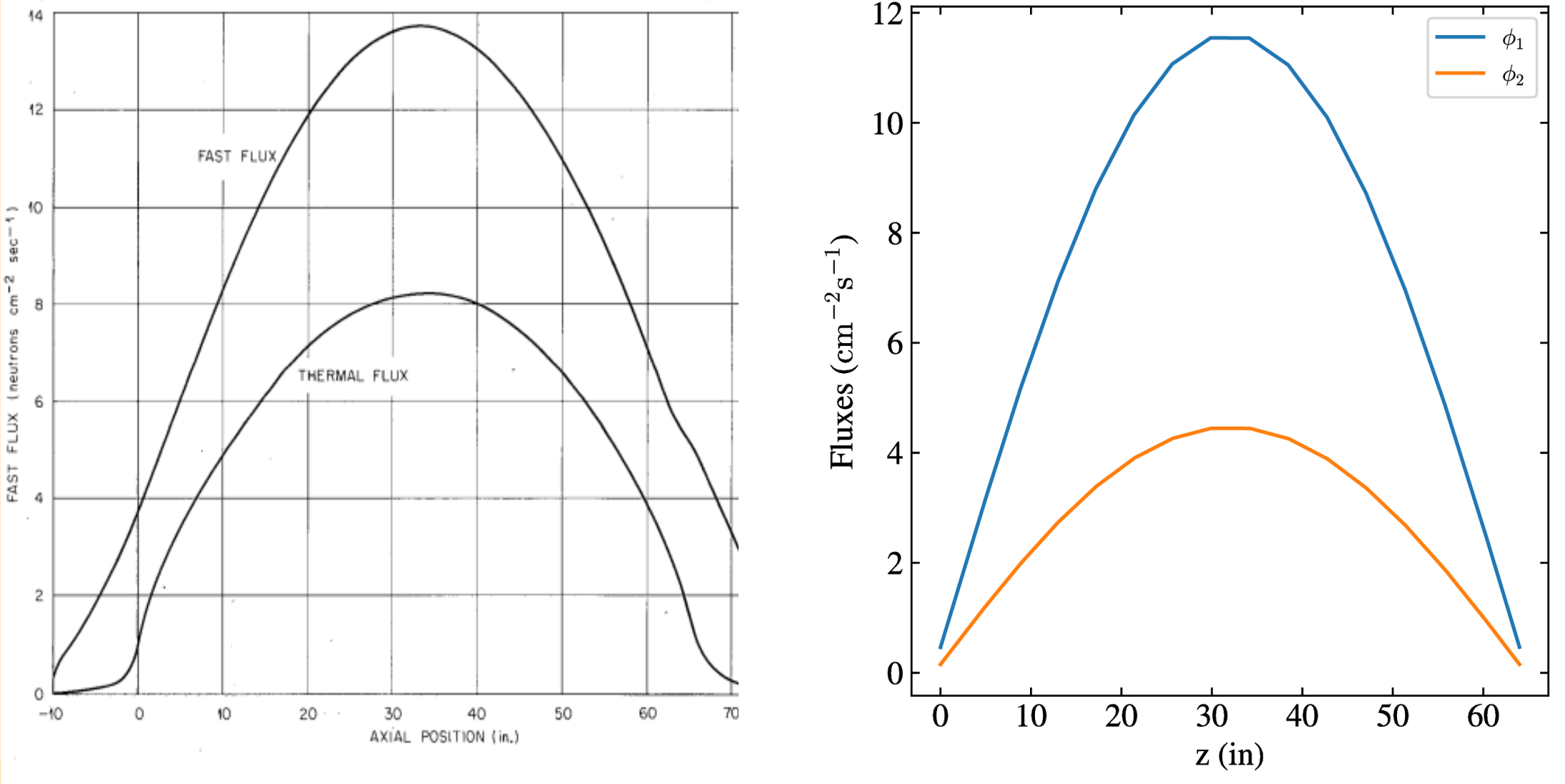
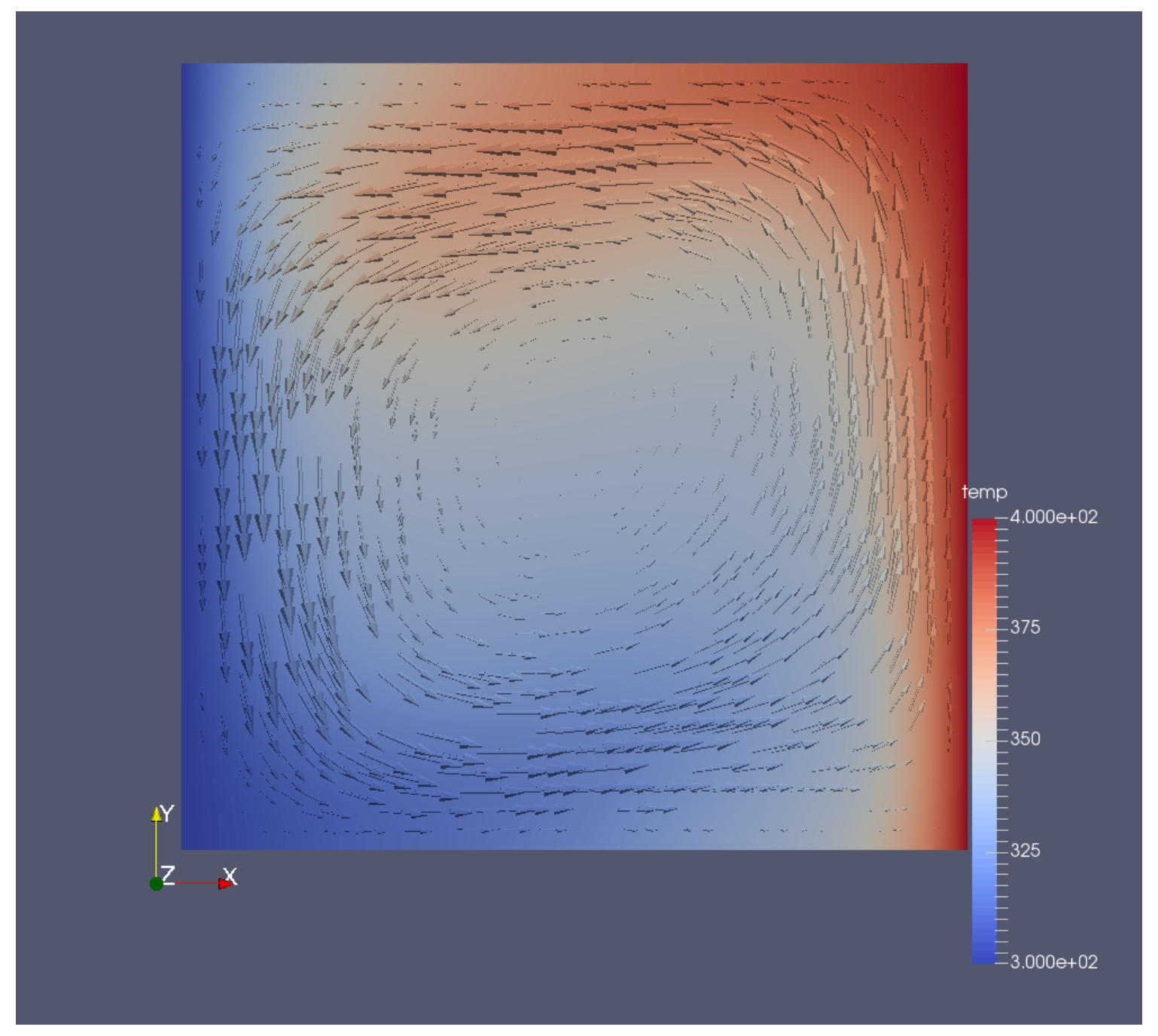


Figure (8): steady-state cuboidal MSRE calculations compare well to MSRE data. Moltres overpredicts MSRE peak temperature by 1.54% from experimental 1300 °F. Fast flux was underpredicted by 17% from the experimental 13.9*10^13 n/cm^2/s, however.

5) Future Work

- Work underway to coupled multigroup diffusion and discontinuous Galerkin precursor transport to Navier-Stokes modules.
- Effects of salt/graphite temperature change cross terms yet to be quantified.
- Scaling studies underway.
- Moltres opens research ability for high power MSR transients unexplored at the MSRE.

Figure (9), right. Salt buoyancy can be approximated using the Boussinesq approximation. Moltres can couple into MOOSE Navier-Stokes modules for simulation of molten salt fast reactors.



6) References

[1] Gaston, Derek, Chris Newman, Glen Hansen, and Damien Lebrun-Grandie. 2009. "MOOSE: A Parallel Computational Framework for Coupled Systems of Nonlinear Equations." Nuclear Engineering and Design 239 (10):1768–78. https://doi.org/10.1016/j.nucengdes.2009.05.021.
[2] Ern, Alexandre, and Jean-Luc Guermond. 2004. 159: Theory and Practice of Finite Elements. 2004 edition. New York: Springer.
[3] Robertson, R. C. 1965. "Msre Design and Operations Report. Part I. Description of Reactor Design." ORNL-TM-728. Oak Ridge National Lab., Tenn. http://www.osti.gov/scitech/biblio/4654707.
[4] Gentry, Cole. 2016. "Development of a Reactor Physics Analysis Procedure for the Plank-Based and Liquid Salt-Cooled Advanced High Temperature Reactor." Doctoral Dissertations, May. http://trace.tennessee.edu/utk_graddiss/3695.