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Initial Coupling of the RELAP-7 and PRONGHORN Applications

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Abstract

Modern nuclear reactor safety codes require the ability to solve detailed coupled neutronics and thermal fluids problems. For larger cores, this implies fully coupled higher dimensionality spatial dynamics with appropriate feedback models that can provide enough resolution to accurately compute core heat generation and removal during steady and unsteady conditions. In this work, the reactor analysis code PRONGHORN is coupled to RELAP-7 as a first step to extend RELAPs current capabilities. This report details the mathematical models, the type of coupling, and the testing results from the integrated system. RELAP-7 is a MOOSE-based application that solves the continuity, momentum, and energy equations in 1-D for a compressible fluid. The pipe and joint capabilities enable it to model parts of the power conversion unit. The PRONGHORN application, also developed on the MOOSE infrastructure, solves the coupled equations that define the neutron diffusion, fluid flow, and heat transfer in a full core model. The two systems are loosely coupled to simplify the transition towards a more complex infrastructure. The integration is tested on a simplified version of the OECD/NEA MHTGR-350 Coupled Neutronics-Thermal Fluids benchmark model.

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Nomenclature

$\varepsilon =$ material porosity

$\rho_f =$ density of the fluid

$\mu =$ dynamic viscosity of the fluid

$K =$ permeability

$P =$ static pressure

$W =$ isotropic friction coefficient

$\phi_g =$ neutron flux for group g

$\vec{g} =$ gravity

$\vec{u} =$ intrinsic phase averaged velocity vector

$\varepsilon\vec{u} =$ superficial averaged or Darcy velocity vector

$T =$ temperature

$R =$ gas constant

$C_p =$ specific heat at constant pressure

$C_v =$ specific heat at constant volume

$\gamma =$ ratio of specific heats (C_p/C_v)

$e =$ internal energy

$\langle f, \Psi \rangle_\Gamma =$ surface integral of $f\Psi$

$(\vec{f}, \nabla\Psi) =$ volume integral of $\vec{f} \cdot \nabla\Psi$ over the whole domain

$d_h =$ hydraulic diameter

$\hat{n}_x =$ the x-component of the "outward unit normal" of the domain

$E =$ total energy

$\beta =$ delayed neutron fraction

$\chi_g =$ fraction of fission neutrons born in energy group g

$\lambda_k =$ decay coefficient for delayed neutron precursor group k

$D_g =$ diffusion coefficient for neutron energy group g

$\Sigma_{Rg} =$ removal cross section for neutron energy group g

$\Sigma_{fg} =$ fission cross section for neutron energy group g

$\Sigma_s^{g' \to g} =$ scattering cross section from neutron energy group g' to group g

$\alpha_p =$ steady state core power

$k_{eff} =$ dominant eigenvalue for the neutron diffusion k-eigenvalue problem

1 Introduction

The RELAP-7 code is part of the next generation of nuclear reactor system safety analysis codes being developed at the Idaho National Laboratory (INL). The current capabilities of RELAP-7 include single phase fluid flow in 1-D pipes and joints. The pipe is the fundamental component of the RELAP-7 code, and all problems modeled with RELAP-7 consist of networks of these pipes. For non-isothermal cases, three equations are solved: continuity, momentum and energy equations (continuity and momentum only, if isothermal). Wall friction factors and convective heat transfer coefficients are calculated through closure laws or provided by user inputs. The effect of gravity is taken into account through pipe orientation and flow direction. The latest model includes heat removal from a fixed power distribution [1]. However, the current version of RELAP-7 does not contain a nuclear reactor module to perform the necessary coupled core power generation and heat removal computations. The next step in the evolution of the code is the addition of thermal-fluid feedback from a full core coupled neutronics-thermal fluids solver.

The PRONGHORN code, which was initially developed to model gas cooled pebble bed reactors [2], is being extended for the modeling of prismatic high temperature reactors. The code solves the neutron diffusion equation, with a Darcy fluid flow model, and a conjugate heat transfer model for solid and fluid energy transfer. Some of the improvements in PRONGHORN include an extension to 3-D geometry and the use of a homogenized stationary two-phase flow model (extended Hazen-Depuit-Darcy).

Both RELAP-7 and PRONGHORN are applications developed on the MOOSE system. MOOSE (Multiphysics Object-Oriented Simulation Environment) is a framework for solving computational engineering problems in a well-planned, managed, and coordinated way. By leveraging open source software packages, such as PETSC [3] (a nonlinear solver developed at Argonne National Laboratory) and LibMesh [4] (a Finite Element Analysis package developed at University of Texas), MOOSE significantly reduces the expense and time required to develop new applications. Numerical integration methods and mesh management for parallel computation are provided by MOOSE. Therefore, RELAP-7 and PRONGHORN code developers only need to focus on physics and user experience. By using the MOOSE development framework, the RELAP-7 and PRONGHORN codes can take advantage of all contributions made to MOOSE by other application developers which follows the paradigm for efficient modern software design. Multiphysics and multiple dimensional analyses capabilities can be obtained by coupling RELAP-7 and other MOOSE based applications and by leveraging with capabilities developed by other DOE programs such as PRONGHORN. These capabilities strengthen the focus of RELAP-7 to systems analysis-type simulations and gives priority to retain and significantly extend RELAP5s capabilities.

2 Governing Equations

2.1 RELAP-7 Model

A simplified flow model for compressible flow is used in this work as an initial step towards more complex models. The equations for an non-isothermal fluid in a one-dimensional pipe are

- *Fluid Continuity Equation*

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \tag{1}$$

- *Momentum Equation*

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + P_{\text{EOS}})}{\partial x} - \rho g_x + f \frac{\rho}{2 d_h} |u| u = 0 \tag{2}$$

  where g_x is the component of the gravity vector in the x-direction and f is a dimensionless friction factor. An equation of state (EOS) of the general form $P_{\text{EOS}} = P(\rho, \rho u)$ completes the definition of the model.

- *Energy Conservation Equation*

$$\frac{\partial (\rho E)}{\partial t} + \frac{\partial (\rho u H)}{\partial x} + H_w a_w (T - T_w) + u \left(f \frac{\rho}{2 d_h} |u| u - \rho g_x \right) = 0 \tag{3}$$

  where $H \equiv E + \frac{P_{\text{EOS}}}{\rho}$ is the total enthalpy, and H_w, a_w are generic heat-transfer coefficients intended to model heat loss/addition along the length of the one-dimensional pipe. The total energy $E \equiv e + \frac{u^2}{2}$, where e is the internal energy of the fluid. The equation of state is required to close the system.

For this initial work, the ideal gas equation of state should suffice and produce reasonable results. This can be enhanced in the future by adding a compressibility factor or using a more sophisticated equation of state, like Redlich-Kwong. The following EOS was implemented in the RELAP-7 application:

- *Equation of State*

$$P_{\text{EOS}} = (\gamma - 1) \rho e \tag{4}$$

  The correlation between temperature and internal energy is

$$T = \frac{e}{C_v} \tag{5}$$

2.2 Pronghorn Model

The Pronghorn multi-physics equation set includes: 1) a Darcy fluid flow model, 2) a conjugate model for heat transfer, and 3) a neutron diffusion model for neutron interactions.

The conservation of fluid mass with no phase change and a single fluid species in a homogenized porous medium is expressed by [5]

- *Fluid Continuity Equation*

$$\frac{\partial \varepsilon \rho_f}{\partial t} + \nabla \cdot \left(\varepsilon \rho_f \vec{u}\right) = 0, \tag{6}$$

The Darcy flow model is a currently accepted engineering representation of flow in HTGRs [6, 2]. The Darcy-law assumes the fluid momentum is proportional to a gradient of pressure. This assumption holds when changes in momentum develop rapidly in response to changes in pressure. Darcy's Law or viscous drag term is represented by an empirical friction factor W. The governing equation for momentum in the Darcy flow model with a gravitational term is presented as

- *Darcy Momentum Equation*

$$\varepsilon \nabla P - \varepsilon \rho_f \vec{g} + W \rho_f \vec{u} = 0, \tag{7}$$

The governing equation for pressure in the Darcy flow model is obtained by solving Eq. (7) for $\rho_f \vec{u}$ and substituting into Eq. (6):

- *Pressure Poisson Equation*

$$\frac{\partial \varepsilon \rho_f}{\partial t} + \nabla \cdot \left(\frac{\varepsilon^2}{W}(-\nabla P + \rho_f \vec{g})\right) = 0 \tag{8}$$

The ideal gas law is then used to substitute the gas density and obtain an equation in terms of pressure. The resulting equation is a special form of the pressure Poisson equation

$$\frac{1}{R}\frac{\partial}{\partial t}\left(\frac{\varepsilon P}{T_f}\right) - \nabla \cdot \frac{\varepsilon^2}{W}\nabla P + \nabla \cdot \frac{\varepsilon^2}{WR}\frac{P\vec{g}}{T_f} = 0. \tag{9}$$

The governing equations for heat transfer in the fluid:

- *Fluid Energy Equation*

$$\frac{\partial}{\partial t}\left[\varepsilon \rho_f c_{pf} T_f\right] + \nabla \cdot (\varepsilon \rho_f c_{pf} \vec{u} T_f) - \nabla \cdot \varepsilon \kappa_f \nabla T_f + \alpha (T_f - T_s) = 0, \tag{10}$$

The governing equation for heat transfer in the solid medium

- *Solid Energy Equation*

$$\frac{\partial}{\partial t}\left[(1-\varepsilon)\rho_s c_{ps} T_s\right] - \nabla\cdot\left(\kappa_{s,\text{eff}}\nabla T_s\right) + \alpha(T_s - T_f) - Q = 0, \tag{11}$$

The governing equations for time dependent neutron diffusion:

- *Neutron Diffusion Equation*

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} - \nabla\cdot D_g\nabla\phi_g + \Sigma_{Rg}\phi_g - Q_g = 0, \tag{12}$$

where

$$Q_g = -(1-\beta)\chi_g\sum_{g'}\nu\Sigma_{fg'}\phi_{g'} - \sum_{g',g'\neq g}\Sigma_s^{g'\to g}\phi_{g'} - \sum_k \chi_{d_{g,k}}\lambda_k C_k$$

The governing equation for the k^{th} delayed neutron precursor

- *Delayed Neutron Precursor Equation*

$$\frac{\partial C_k}{\partial t} + \lambda_k C_k - \sum_{g'}\beta_{k,g'}\nu\Sigma_{fg'}\phi_{g'} = 0 \tag{13}$$

Before we can solve the time dependent system we need a reference steady state solution. A nuclear reactor operating at steady state is said to be critical meaning that the neutron population that is consumed due to absorption or leaked out of the system is identically replaced either fission. Since design of a perfectly critical reactor is both physically and numerically impossible, the multiplication factor or critical Eigenvalue k_{eff} is introduced into the mathematically "steady state" diffusion equation shown here

- *Neutron Diffusion Eigenvalue Equation*

$$-\nabla\cdot D_g\nabla\phi_g + \Sigma_{Rg}\phi_g - \frac{\chi_g}{k_{eff}}\sum_{g'}\nu\Sigma_{fg'}\phi_{g'} - \sum_{g',g'\neq g}\Sigma_s^{g'\to g}\phi_{g'} = 0. \tag{14}$$

Solving 14 for the fundamental mode gives the relative shape of the neutron fluxes and the dominant Eigenvalue. In order to smoothly couple to other physics the flux solutions are normalized by the neutron fission source such that:

$$\int_V dV\, \kappa_g \Sigma_{fg} \phi_g = 1 \tag{15}$$

This formulation allows the heat source term to be independent of the neutron flux scaling by enforcing the steady state reactor power level

$$\begin{aligned} P &= \int_V dV\, \alpha_p \kappa_g \Sigma_{fg} \phi_g \\ &= \alpha_p \int_V dV\, \Sigma_{fg} \phi_g, \end{aligned} \tag{16}$$

where α_p is the core power in MW_{th}.

The neutron diffusion approximation Eq.(14) is implicitly coupled to the heat conduction equation Eq.(11) through the material properties which are functions of temperature. Additionally, the normalized fission heat sourced calculated from the neutron diffusion eigenvalue problem is scaled by the steady state core power and is the source term for the solid temperature equation.

3 Geometry Description

The original testing plan [7] specified the use of the OECD/NEA Coupled Neutronics-Thermal Fluids Benchmark model [8] for PRONGHORN. Significant modifications to the original model were required to perform this initial coupling study due to the complexity of the benchmark and shortcomings in both PRONGHORN and the RELAP-7 applications. It is worth noting that these applications are still in the early stages of development. The simplified models retains the essential features of the General Atomics MHTGR-350 MW_{th} design.

3.1 Pronghorn Geometry and Data

The original benchmark provides a full specification including a set of 26 neutron energy group and temperature dependent cross sections in addition to temperature, burn-up, and fluence dependent thermophysical properties. Instead, a 2 neutron energy group binary library was developed by collapsing the 26 group structure from the benchmark. The collapsed cross sections were calculated using the fluxes provided in the benchmark cross section file for each cross section set. With two groups there is a loss of accuracy in the neutronic calculations for HTRs unless neutron leakage corrections are employed. Leakage corrections are currently not available in PRONGHORN. The expected error is near 2000 pcm (per cent mil), nevertheless, the lower number of groups decreases the calculation time by a factor of ten or more and greatly simplifies debugging, which is the primary focus of this initial coupling .

The original 3-D geometry with $1/3^{rd}$ core symmetry was also simplified to a 2-D cylindrical (R-Z) model. The layout of this simplified MHTGR-350 model is shown in Figure 1. The core includes an inner reflector region, annular active core, top and bottom reflectors, and an outer reflector region. The model is 11.1 m tall and 2.97 m in radius. The active core measures 7.9 m in height and radially 0.92 m for the annular region width. The coolant flows directly into the top reflector, followed by the active core, and, finally, the bottom reflector. Non-local heating effects and radiation heat transfer are neglected.

From the pronghorn perspective the simulation entails a multi-physics steady state problem. Therefore, given a set of boundary conditions from RELAP-7 the code solves a non-linear eigenvalue problem. The cross sections for this model include the effects of the variations in fuel and moderator temperature. The tracked parameters include: system pressure, core inlet temperature, core outlet temperature, core fuel temperature distribution, core moderator temperature distribution, core fluid temperature distribution, core power distribution, and local static pressure distribution.

3.2 RELAP-7 Geometry

The RELAP-7 model is entirely based on 1-D pipes and junctions. Figure 2 shows an schematic of the system. The boundary conditions for temperature and velocity (or momentum) are specified at the inlet junction. This is followed by the 5 m hot duct which carries the hot helium from the

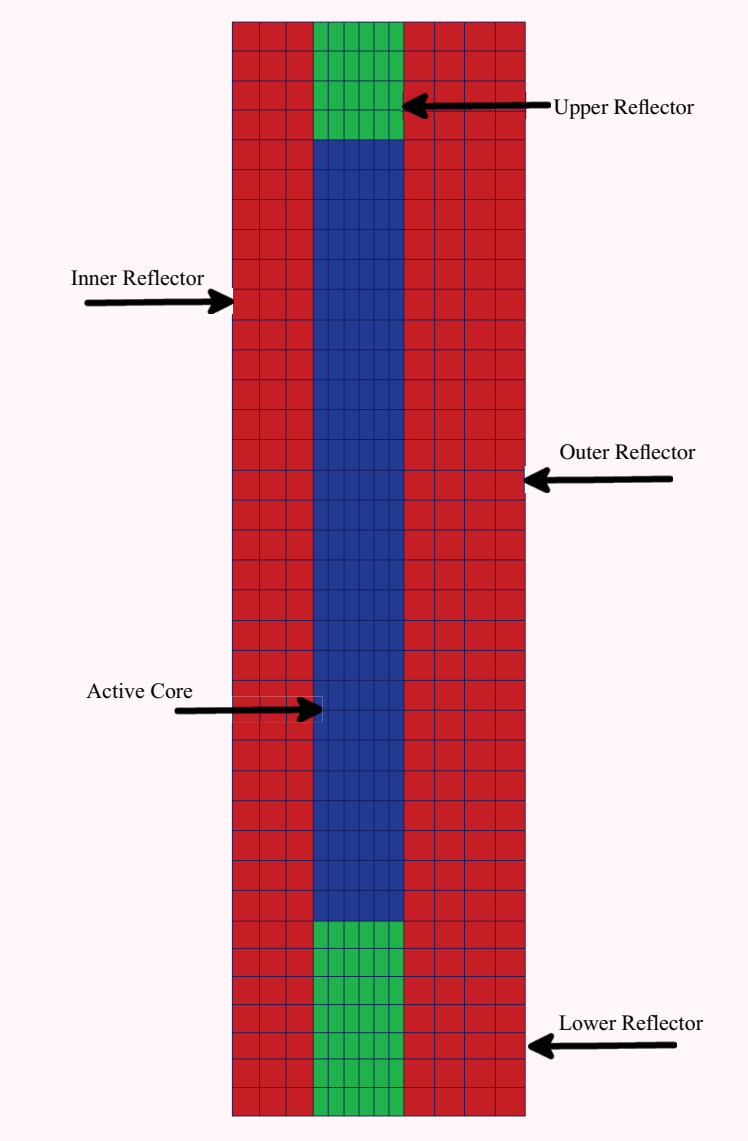


Figure 1: Simplified R-Z MHTGR-350 MW Reactor Geometry

reactor outlet to the steam generator. The steam generator tube bundle is modeled as a 8.0 m pipe capable of removing approximately 350 MW_{th}. After the the tube bundle the flow continues into the steam generator vessel annulus, which corresponds to the pipe labeled "sg2cir." This component carries the cold helium to the circulator. Unfortunately, the circulator model in RELAP-7 is not currently working properly, therefore is shown here as a pipe. Finally, the cold duct carries the gas from the circulator outlet to the reactor inlet. The pressure boundary condition is specified at the outlet junction.

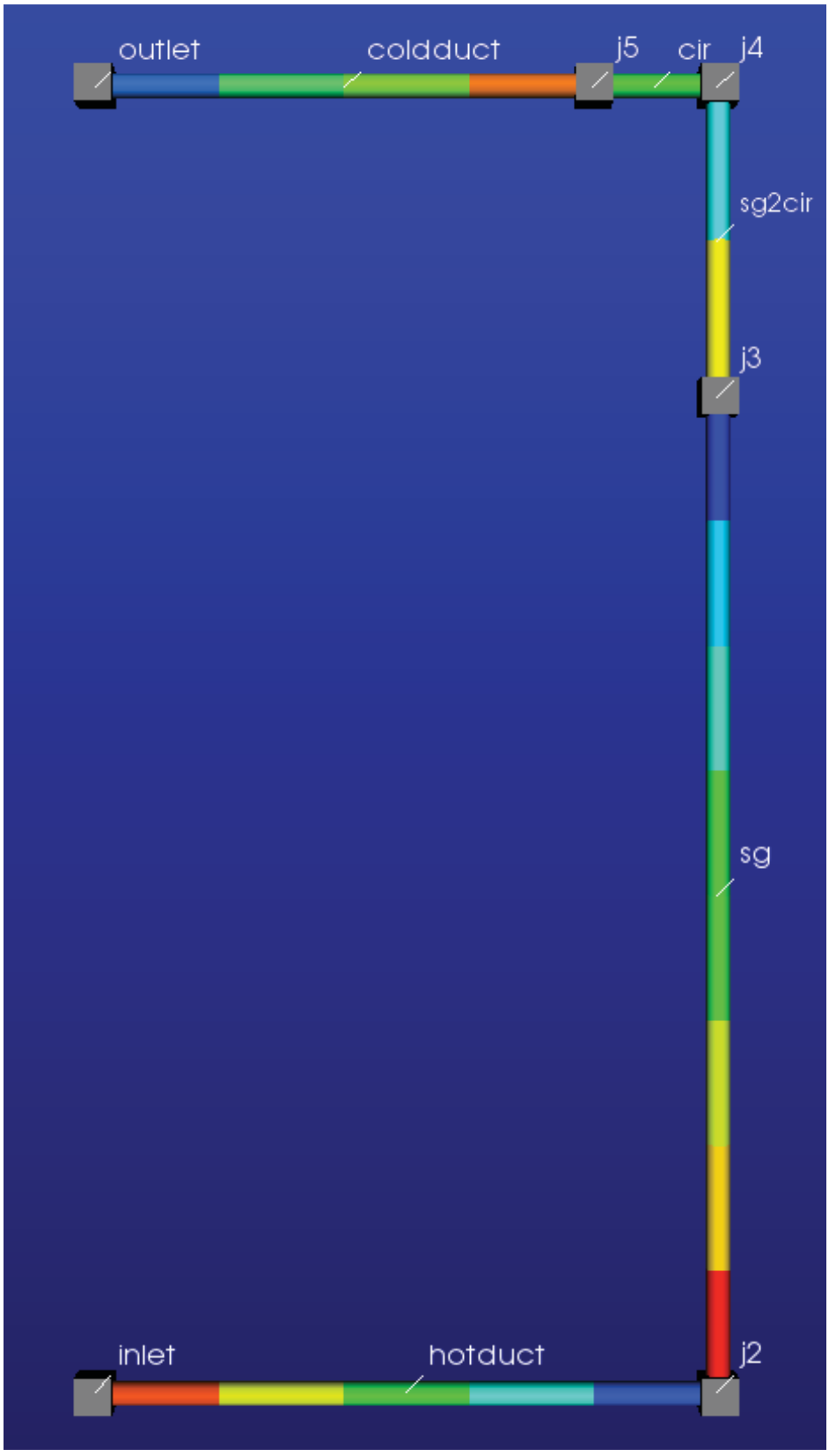


Figure 2: Relap-7 Plant System Layout

4 Numeric Method

The method of weighted residuals (or Galerkin procedure) is used to obtain the approximation to the integral form of the PDEs. The weighted residual form of the equations is derived by multiplying each term of the differential equations by a test function Ψ and integrating over the volume. The final weak formulation is obtained by trading differentiation with the product rule. The method of weighted residuals is used to formulate a nonlinear system of the form

$$\mathbf{F}(\mathbf{U}) = 0. \tag{17}$$

This system is then solved iteratively via the JFNK method [9, 10]. The JFNK method is a combination of the quadratically convergent Newton method and a Krylov subspace iterative method. The first-order Taylor expansion of Eq. (17) about $\mathbf{U}^m$ gives the following linear system,

$$\mathbb{J}^m \delta\mathbf{U}^m = -\mathbf{F}(\mathbf{U}^m), \tag{18}$$

where $\mathbb{J}^m_{i,j} \equiv \frac{\partial \mathbf{F}_i(\mathbf{U}^m)}{\partial \mathbf{U}^m_j}$ is the i,j element of Jacobian matrix for the m^{th} Newton iteration. The linear system (18) is solved using a Krylov subspace method and the solution is updated as

$$\mathbf{U}^{m+1} = \mathbf{U}^m + d\,\delta\mathbf{U}^m, \tag{19}$$

where $0 < d \leq 1$ is a scalar damping parameter chosen adaptively to avoid unphysical solutions.

Because Krylov methods merely require matrix-vector products, a Jacobian-Free Newton-Krylov (JFNK) method can be used to alleviate the explicit formation of the expensive Jacobian matrix. In JFNK the matrix-vector product is approximated by the finite difference form,

$$\mathbb{J}\mathbf{v} \approx \frac{\mathbf{F}(\mathbf{U} + h\mathbf{v}) - \mathbf{F}(\mathbf{U})}{h}, \tag{20}$$

where h is the perturbation parameter and $\mathbf{v}$ is provided by the Krylov method.

In PRONGHORN, the JFNK method is used to replace the upscattering iterations (the thermal and fast neutron flux vectors are solved simultaneously), additionally a nonlinear Eigenvalue solver is implemented in Pronghorn. This solver is "pre-conditioned" with the power iteration method in which the fission source and Eigenvalue are fixed during the Krylov iterations. Previous work used JFNK to treat coupled neutronics and thermal fluids problems or to solved the nonlinear scattering problem in neutronics [11, 12].

5 Finite Element Discretization

5.1 RELAP-7 Model

The weak formulation that is associated with the RELAP-7 Model ((1), (2), and (3)) leads to the following nonlinear residual functions:

- *Fluid Continuity Nonlinear Residual Function*

$$\mathbf{F}_{\rho}(\boldsymbol{U}) = \left(\frac{\partial \rho}{\partial t}, \Psi\right) - \left(\rho u, \frac{\partial \Psi}{\partial x}\right) + \langle \rho u \hat{n}_x, \Psi \rangle_{\Gamma} \tag{21}$$

- *Momentum Nonlinear Residual Function*

$$\begin{aligned}\mathbf{F}_{\rho u}(\boldsymbol{U}) = &\left(\frac{\partial (\rho u)}{\partial t}, \Psi\right) - (\rho g_x, \Psi) + \left(f\frac{\rho}{2d_h}|u|u, \Psi\right) - \left(\rho u^2, \frac{\partial \Psi}{\partial x}\right) + \left(P, \frac{\partial \Psi}{\partial x}\right) \\ &+ \left\langle \rho u^2 \hat{n}_x, \Psi \right\rangle_{\Gamma} + \langle P \hat{n}_x, \Psi \rangle_{\Gamma}\end{aligned} \tag{22}$$

- *Energy Conservation Nonlinear Residual Function*

  Substituting $\rho u H = \rho u(E + \frac{P}{\rho}) = u(\rho E + P)$ in (3) and applying the Galerkin procedure yields

$$\begin{aligned}\mathbf{F}_{\rho E}(\boldsymbol{U}) = &\left(\frac{\partial (\rho E)}{\partial t}, \Psi\right) + (H_w a_w (T - T_w), \Psi) + \left(f\frac{\rho}{2d_h}|u|u^2, \Psi\right) - (u\rho g_x, \Psi) \\ &- \left(\rho u E, \frac{\partial \Psi}{\partial x}\right) - \left(uP, \frac{\partial \Psi}{\partial x}\right) + \langle \rho u E \hat{n}_x, \Psi \rangle_{\Gamma} + \langle uP \hat{n}_x, \Psi \rangle_{\Gamma}\end{aligned} \tag{23}$$

  where

  $\mathbf{F}$ = nonlinear residual function

  $\mathbf{U} = (\rho, \rho u, \rho E)^T$

  Ψ is a scalar test function

5.2 Pronghorn Model

The weak formulation that is associated with the Pronghorn equation set is obtained by applying the method of weighted residuals to equations (7), (9), (10), (11), (12), and (13), respectively.

- *Momentum Nonlinear Residual Function*

$$\mathbf{F}_{\rho \vec{u}}(\boldsymbol{U}) = (\varepsilon \nabla P, \Psi) - \left(\varepsilon \rho_f \vec{g}, \Psi\right) + \left(W \rho_f \vec{u}, \Psi\right) \tag{24}$$

- *Pressure Poisson Nonlinear Residual Function*

$$\mathbf{F}_P(\boldsymbol{U}) = \left(\frac{\partial}{\partial t}\left(\frac{\varepsilon P}{RT_f}\right), \Psi\right) + \left(\frac{\varepsilon^2}{W}\nabla P, \nabla\Psi\right) - \left(\frac{\varepsilon^2}{W}\rho_f \vec{g}, \nabla\Psi\right) - \left\langle \frac{\varepsilon^2}{W}\nabla P, \Psi\right\rangle + \left\langle \frac{\varepsilon^2}{W}\rho_f \vec{g}, \Psi\right\rangle \tag{25}$$

- *Fluid Energy Nonlinear Residual Function*

$$\mathbf{F}_{T_f}(\boldsymbol{U}) = \left(\frac{\partial \varepsilon \rho_f c_{pf} T_f}{\partial t}, \Psi\right) - \left(\varepsilon \rho_f c_{pf} \vec{u} T_f, \nabla\Psi\right) + \left(\varepsilon \kappa_f \nabla T_f, \nabla\Psi\right) + \left(\alpha(T_f - T_s), \Psi\right) + \left\langle \varepsilon \rho_f c_{pf} \vec{u} T_f, \Psi\right\rangle - \left\langle \varepsilon \kappa_f \nabla T_f, \Psi\right\rangle \tag{26}$$

- *Solid Energy Nonlinear Residual Function*

$$\mathbf{F}_{T_s}(\boldsymbol{U}) = \left(\frac{\partial (1-\varepsilon)\rho_s c_{ps} T_s}{\partial t}, \Psi\right) + \left(\kappa_{seff} \nabla T_s, \nabla\Psi\right) + \left(\alpha(T_s - T_f), \Psi\right) - (Q, \Psi) - \left\langle \kappa_{seff} \nabla T_s, \Psi\right\rangle \tag{27}$$

- *Neutron Diffusion Nonlinear Residual Function*

$$\mathbf{F}_{\phi_g}(\boldsymbol{U}) = \left(\frac{1}{v_g}\frac{\partial \phi_g}{\partial t}, \Psi\right) + (D_g \nabla\phi_g, \nabla\Psi) - \left\langle D_g \nabla\phi_g, \Psi\right\rangle + (\Sigma_r \phi_g, \Psi) - \left((1-\beta)\chi_g \sum_{g'} \nu\Sigma_{fg'}\phi_{g'}, \Psi\right) - \left(\sum_{g', g'\neq g} \Sigma_s^{g'\to g}\phi_{g'}, \Psi\right) - \left(\sum_k \chi_{d_{g,k}} \lambda_k C_k, \Psi\right) \tag{28}$$

- *Delayed Neutron Precursor Nonlinear Residual Function*

$$\mathbf{F}_{C_k}(\boldsymbol{U}) = \left(\frac{\partial C_k}{\partial t}, \Psi\right) + (\lambda_k C_k, \Psi) - \left(\sum_{g'} \beta_{k,g'} \nu\Sigma_{fg'}\phi_{g'}, \Psi\right) \tag{29}$$

where

$\mathbf{F}$ = nonlinear residual function

$\mathbf{U} = (\rho\vec{u}, P, T_f, T_s, \phi_g, C_k)^T$

Ψ is a scalar test function

6 System Integration

6.1 Direct Coupling with Boundary Conditions

The integration of RELAP-7 and PRONGHORN is based on a loose coupling of the system, whereby each application will use an independent mesh. A data exchange will be implemented to couple the codes. This type of direct coupling has been successfully used in the past with the TINTE time dependent core solver and the Flownex systems code[13, 14, 15]. To determine the required parameters for the exchange we will look at the fluid boundary terms.

For the RELAP-7 model the coupling arises from the boundary terms of the fluid continuity, momentum, and fluid energy equations

$$\langle \rho u \hat{n}_x, \Psi \rangle_\Gamma$$
$$\langle \rho u^2 \hat{n}_x, \Psi \rangle_\Gamma + \langle P \hat{n}_x, \Psi \rangle_\Gamma$$
$$\langle \rho u E \hat{n}_x, \Psi \rangle_\Gamma + \langle u P \hat{n}_x, \Psi \rangle_\Gamma$$

The corresponding boundary conditions for the RELAP-7 fluid medium are expressed as

$$\begin{aligned} P &= P_{PH_{inlet}} && \in \Gamma_{R7_{outlet}} \\ \vec{n} \cdot \left[-\frac{\varepsilon}{W} \nabla P + \frac{\varepsilon \rho_f \vec{g}}{W} \right] &= (\vec{n} \cdot \rho \vec{u})_{PH_{outlet}} && \in \Gamma_{R7_{inlet}} \\ T_f &= T_{PH_{outlet}} && \in \Gamma_{R7_{inlet}} \end{aligned}$$

where

$P_{PH_{inlet}}$ is the inlet pressure pressure computed in PRONGHORN that will be imposed on the RELAP-7 outlet boundary , $\Gamma_{R7_{outlet}}$

a fixed, uniform mass flow rate condition is set at the inlet boundary, $\Gamma_{R7_{inlet}}$

a fixed, uniform temperature from the PRONGHORN model, $T_{PH_{outlet}}$, is set at the RELAP-7 inlet boundary, $\Gamma_{R7_{inlet}}$

For the PRONGHORN model the coupling arises from the boundary terms of the fluid pressure and fluid energy equations

$$\left\langle \frac{\varepsilon^2}{W} \nabla P, \Psi \right\rangle + \left\langle \frac{\varepsilon^2}{W} \rho_f \vec{g}, \Psi \right\rangle$$
$$\left\langle \varepsilon \rho_f c_{pf} \vec{u} T_f, \Psi \right\rangle - \left\langle \varepsilon \kappa_f \nabla T_f, \Psi \right\rangle$$

Note that the momentum equation in the PRONGHORN model does not contain any boundary terms. The conditions for this equation are imposed via the pressure Poisson equation. The corresponding boundary conditions for the fluid medium are expressed as

$$
\begin{aligned}
P &= P_{R7_{inlet}} && \in \Gamma_{PH_{outlet}} \\
\vec{n} \cdot \left[-\frac{\varepsilon}{W} \nabla P + \frac{\varepsilon \rho_f \vec{g}}{W} \right] &= (\vec{n} \cdot \rho \vec{u})_{R7_{outlet}} && \in \Gamma_{PH_{inlet}} \\
T_f &= T_{R7_{outlet}} && \in \Gamma_{PH_{inlet}}
\end{aligned}
$$

where

$P_{R7_{inlet}}$ is the inlet pressure computed in RELAP-7 that will be imposed on the PRONGHORN outlet boundary, $\Gamma_{PH_{outlet}}$

a fixed, uniform mass flow rate condition is set at the inlet boundary, $\Gamma_{PH_{inlet}}$

a fixed, uniform temperature from RELAP-7 model, $T_{R7_{out}}$, is set at the inlet boundary, $\Gamma_{PH_{inlet}}$

6.2 Helium Circulator

A helium circulator model is necessary to maintain system flow rate. Unfortunately, RELAP-7 does not currently include a circulator model. A simplified circulator was modeled by modifying the boundary conditions.

The direct coupling boundary conditions for pressure in RELAP-7 are modified to

$$
P = \frac{P_{PH_{inlet}}}{C_R} \qquad \in \Gamma_{R7_{outlet}}
$$

where C_R is the compression ratio of the helium circulator.

The direct coupling boundary conditions for temperature and inlet mass flow rate in PRONGHORN are modified to

$$
\vec{n} \cdot \left[-\frac{\varepsilon}{W} \nabla P + \frac{\varepsilon \rho_f \vec{g}}{W} \right] A_p = (\vec{n} \cdot \rho \vec{u})_{R7_{outlet}} A_p \qquad \in \Gamma_{PH_{inlet}}
$$

$$
T_f = T_{R7_{outlet}} C_R{}^{\gamma - 1/\gamma} \qquad \in \Gamma_{PH_{inlet}}
$$

where

A_p is the cross sectional area of the pipe at the pronghorn inlet

$\gamma = \frac{C_p}{C_v}$, the ratio of specific heats

7 System Testing

7.1 Pronghorn Testing

Testing for the PRONGHORN calculation was done by solving for each physics (neutronics, heat conduction, pressure and momentum, and fluid energy) separately. This was done by holding the coupled values for the independent physics constant for each calculation. Once adequate convergence behavior was achieved the convergence behavior of the tightly coupled problem was examined. The final mesh and the order of the Lagrange shape functions used in the coupled RELAP-7/PRONGHORN calculation were chosen such that reasonable spatial convergence of the k-eigenvalue would be achieved in a minimal time for each PRONGHORN solve. To that end, a spatial convergence study for the k-eigenvalue with first and second order shape functions was done. After some preliminary studies, it was found that better convergence with a lower calculation time cost was obtained by using a finer mesh in the fluid flow areas which include the core and the reflector regions directly above and below the core more than in the rest of the geometry. The results of the spacial convergence study are presented in Figure 3. Second order Lagrange functions showed much better convergence behavior with refinement at less time per degree of freedom than first order Lagrange functions. The coupled RELAP-7/PRONGHORN calculation was solved with two uniform refinements on the base mesh, which consistently produced eigenvalues within a relative error of $1E-6$ compared to a highly refined reference solution with the same initial conditions.

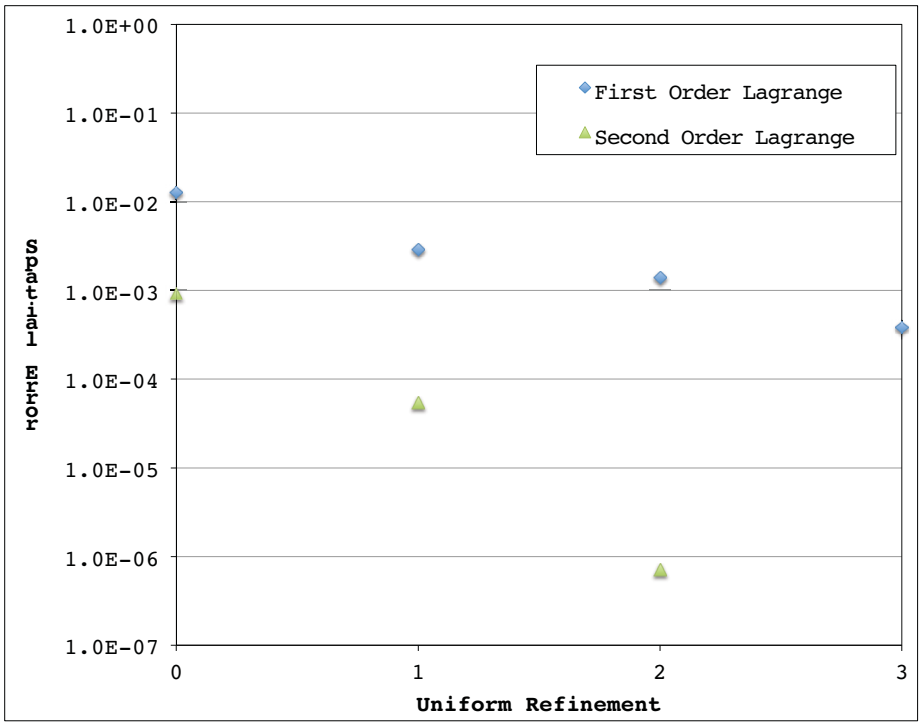


Figure 3: Spatial Convergence of the k-Eigenvalue for First and Second Order Lagrange Functions

The convergence behavior of the eigenvalue and thermal fluid properties was examined as a function of the nonlinear or Newton steps taken. The average values for the average solid core temperature, fluid temperature, inlet pressure, and eigenvalue are compared to the final solution converged solution for or chosen reference solution. For each of the initial power iteration steps taken there was one nonlinear or Newton solve. It was found heuristically for this model and geometry that a minimum of 7 power iterations led to more consistent convergence than if fewer power iterations steps were taken. The convergence rates for the different parameters are the quite similar past the initial power iterations steps as can be seen in Figure 4. This convergence behavior gives us some confidence that we have indeed reached an adequately converged solution for the different primary variables. For this study, the each PRONGHORN calculation was done without consideration of the solution from the previous cycle. This is done to avoid biasing the coupled RELAP-7/PRONGHORN calculation. Future work would likely use the converged solution from the previous cycle as an initial guess in place of the initial the power iteration steps and would likely speed up the convergence of the PRONGHORN coagulation since we would likely be within the Newton convergence radius.

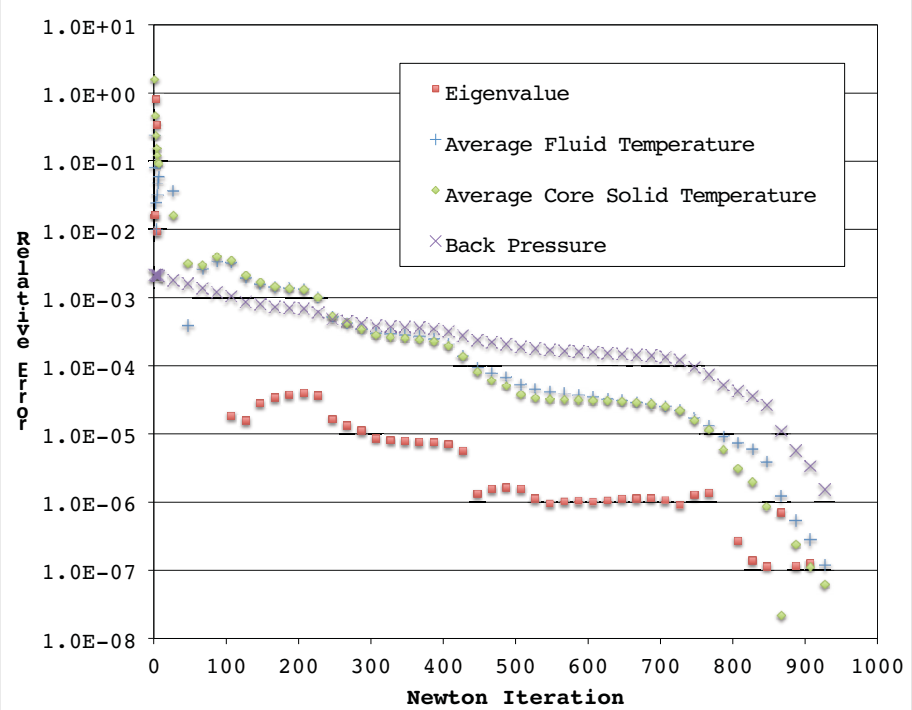
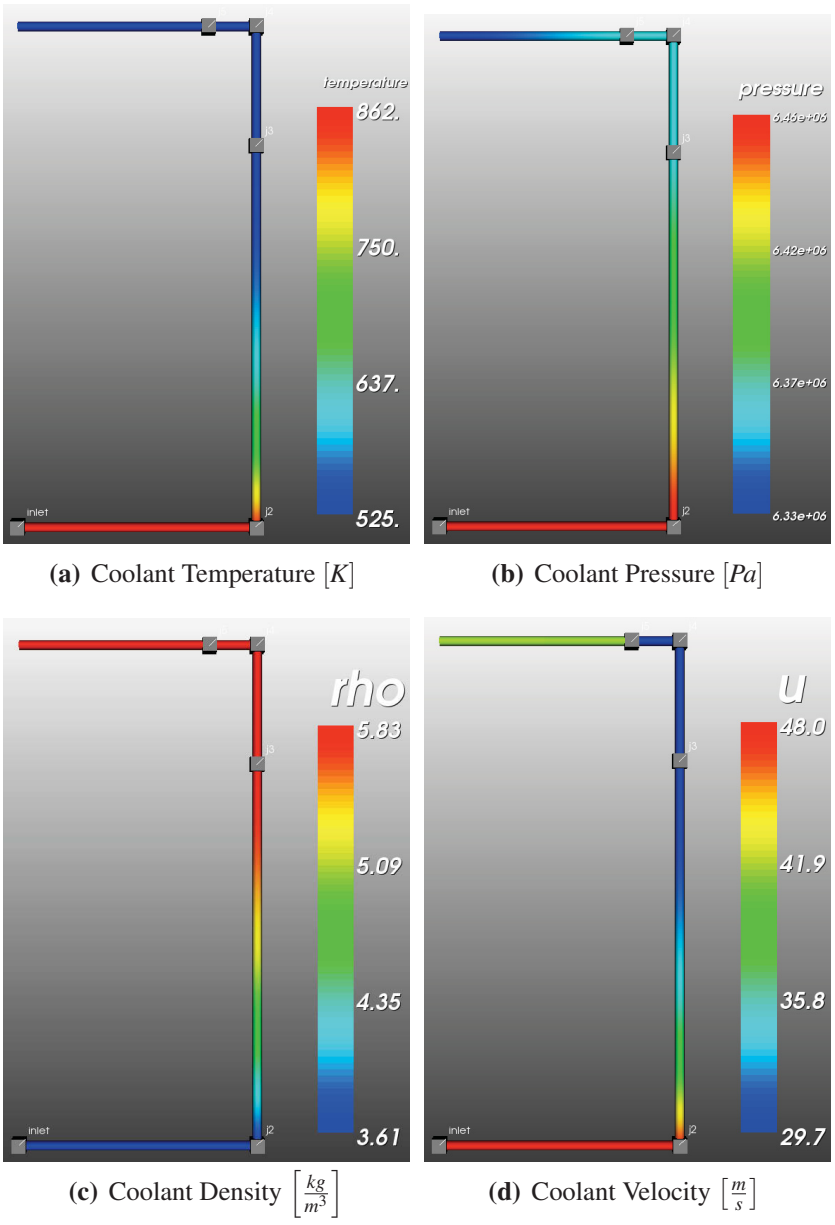


Figure 4: Relative Error of Selected Parameters compared to a Fully Coupled Thermal Fluid-Neutronics PRONGHORN Calculation as a function of Newton Iterations

7.2 RELAP-7 Testing

A null transient (steady state) solution was obtained in RELAP-7 to ensure the proper function of the various components, including the circulator, which is modeled via the pressure boundary condition. The equation of state was also checked out with this first case. A fluid temperature of 862 K and a velocity 48 m/s were fixed at the inlet. The system pressure was fixed at the outlet to 6.42 MPa and the compression ratio for the circulator was set to 1.01422. Results from this simulation are included in Figure 5.



(a) Coolant Temperature $[K]$ **(b)** Coolant Pressure $[Pa]$

(c) Coolant Density $\left[\frac{kg}{m^3}\right]$ **(d)** Coolant Velocity $\left[\frac{m}{s}\right]$

Figure 5: Thermal-Physical Results from a RELAP7 System Calculation with a Null Transient

A simulation time of 1.07 seconds was more than necessary to achieve the steady state condition. The execution time was 141 seconds on 7 processors. The fluid temperature remains constant until it reaches the steam generator section after which it drops to 525 K. The system pressure, which was set to 6.42 MPa at the boundary is decreased by the circulator model to 6.33E6. The pressure drop across the loop, from the inlet to the circulator, is 0.13 MPa. The density reaches its peak in the cold duct with a value of 5.83 kg/m^3. The fluid velocity slows in the steam generator as the fluid is cooled, but experiences a sudden increase in the cold duct section, due to the change in the pipe area.

7.3 Integrated System Testing

The convergence pattern for the principal PRONGHORN variables during the coupled calculation is shown in Figure 6. The coupled system converges approximately after 80 coupled cycles. Both the solid and fluid temperatures are the slowest converging parameters, whereas pressure and eigenvalue show a faster convergence behavior. The fluctuations in the pressure can emerge from a number of initiators (circulator model, large temperature changes, coupled system instabilities) and have not been resolved yet. Nevertheless, the coupled solution reaches the steady state condition.

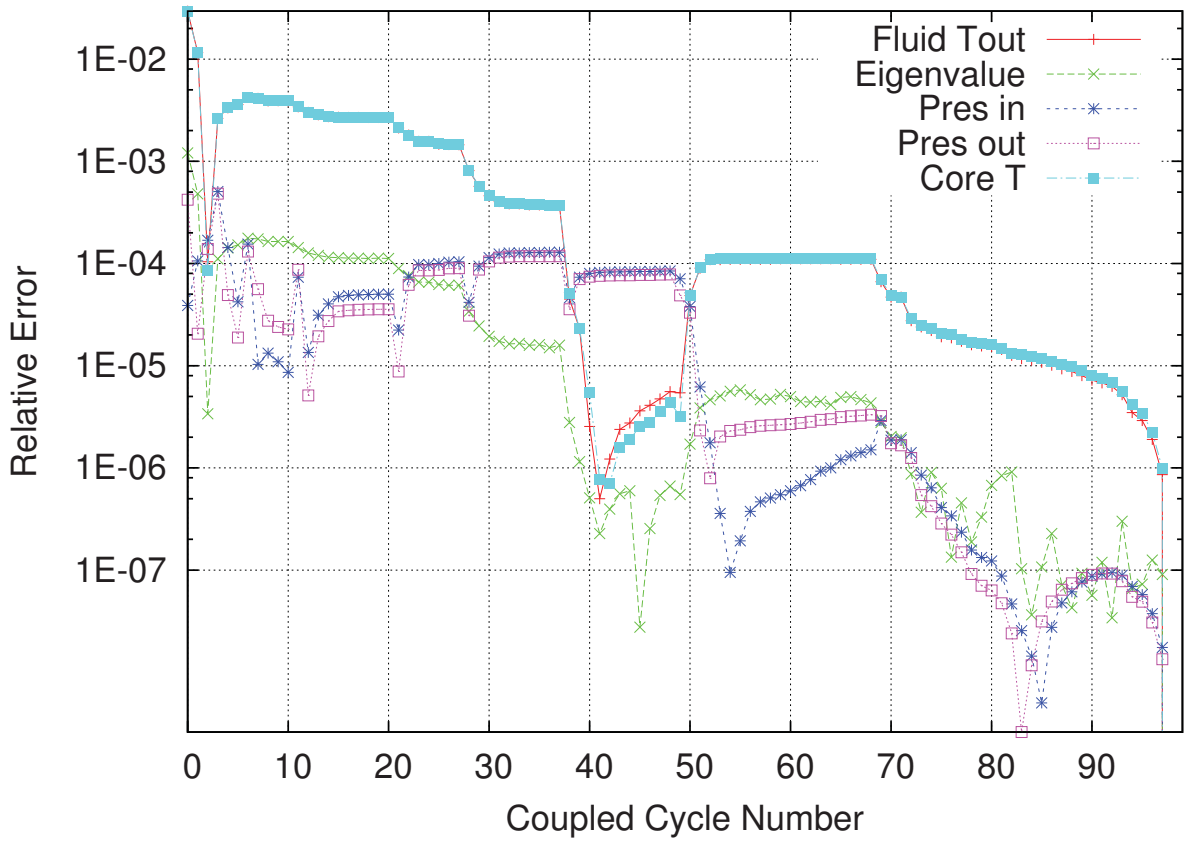
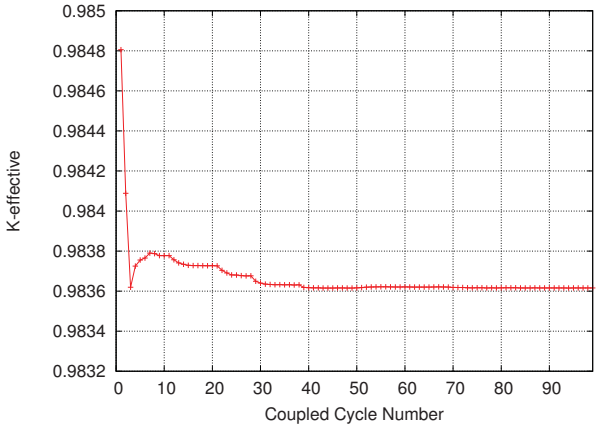
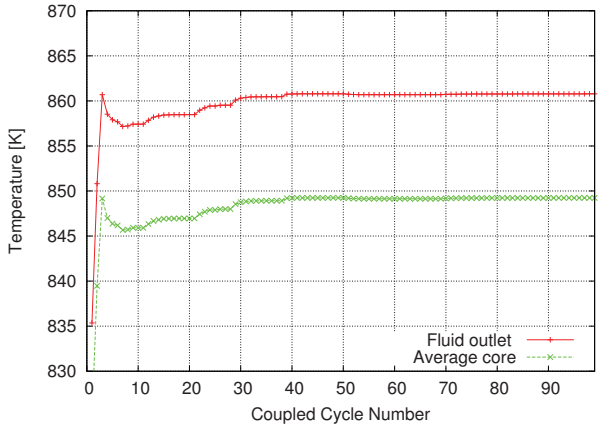


Figure 6: Convergence Pattern of the Coupled Calculation

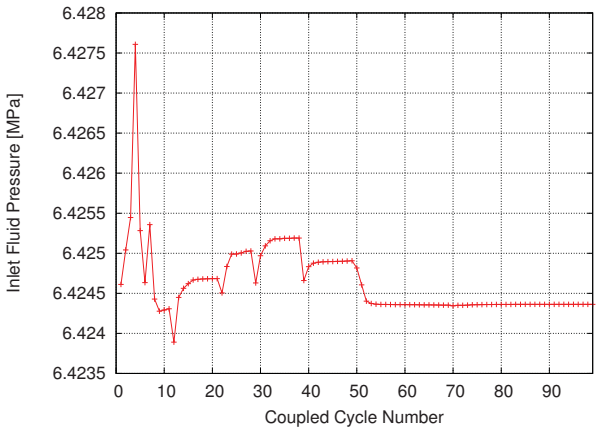
Figure 7 includes the PRONGHORN results as a function of coupled cycle and Figure 8 shows the RELAP-7 results as a function of simulation time. The final eigenvalue is 0.983616 with an average core temperature of 849 K. The strong negative feedback of the reactor can be seen in the first cycles where the average core temperature increases and, consequently, produces a sharp decrease in the core eigenvalue. The calculated temperature coefficient of reactivity for these first cycles is $-5x10^{-5}\Delta k/k/^{o}C$, which is consistent with that of the MHTGR design at the end of equilibrium cycle [16]. The average fluid temperature exiting the core is low, 860 K, and probably due to low heat transfer coefficients. The RELAP-7 pressure plot in Figure 8(c) seems to indicate that the sudden temperature increase in the early cycles induces an oscillation in the pressure solution in the system. The oscillation dampens over time and the system finally reaches a stable point.



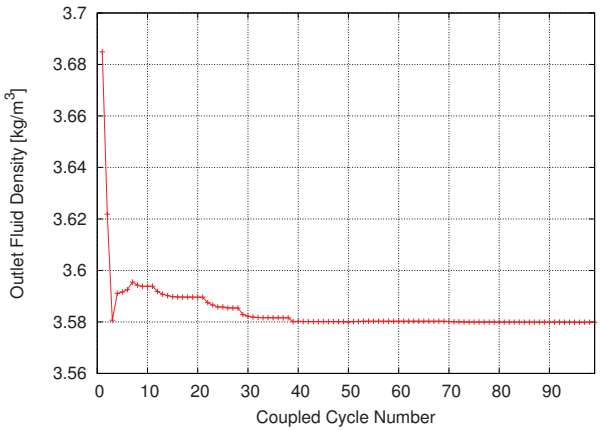
(a) Eigenvalue



(b) Coolant and Core Temperatures $[K]$



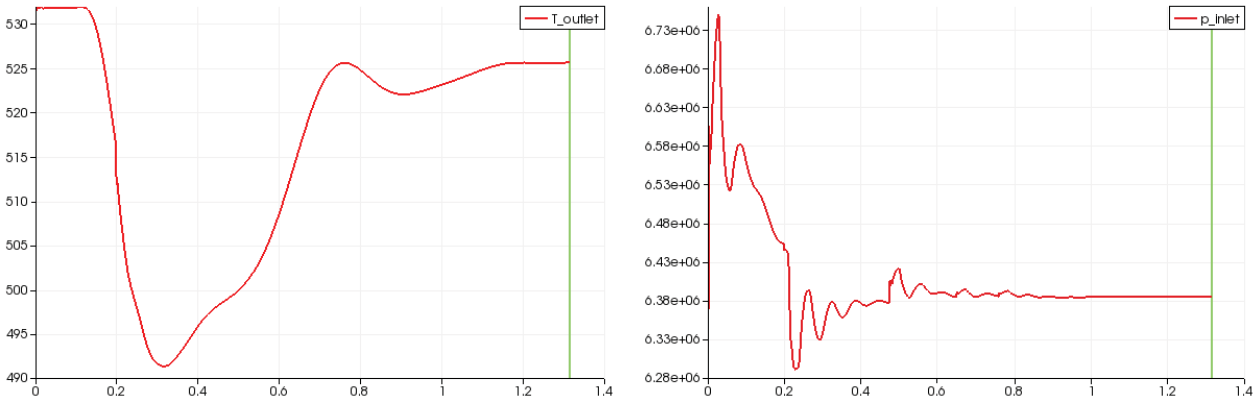
(c) Coolant Inlet Pressure $[MPa]$



(d) Coolant Outlet Density $\left[\frac{kg}{m^3}\right]$

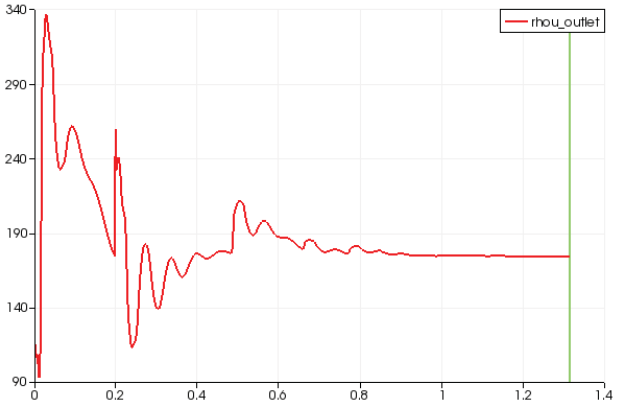
Figure 7: PRONGHORN Coupled Calculation Results

The flux and heat source distributions are included in Figure 9. The fast flux in Figure 9(a) is mainly constraint near the active core region whereas the thermal flux in Figure 9(b) displays the typical double radial hump, that is characteristics of the MHTGR's annular core with inner and



(a) Coolant Outlet Temperature $[K]$

(b) Coolant Inlet Pressure $[Pa]$

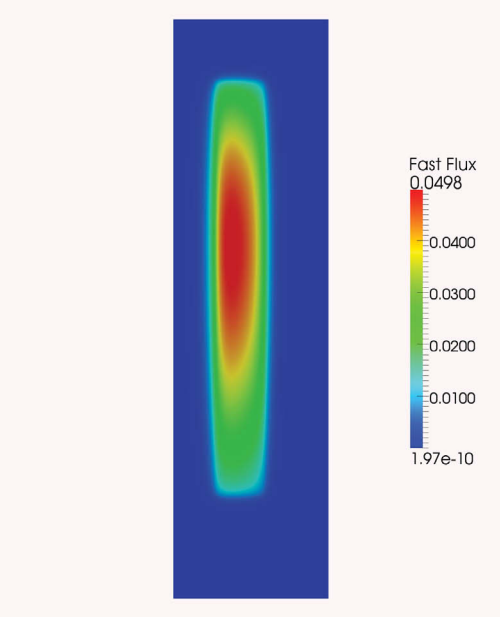


(c) Coolant Outlet Momentum $\left[\frac{kg}{m^2 s}\right]$

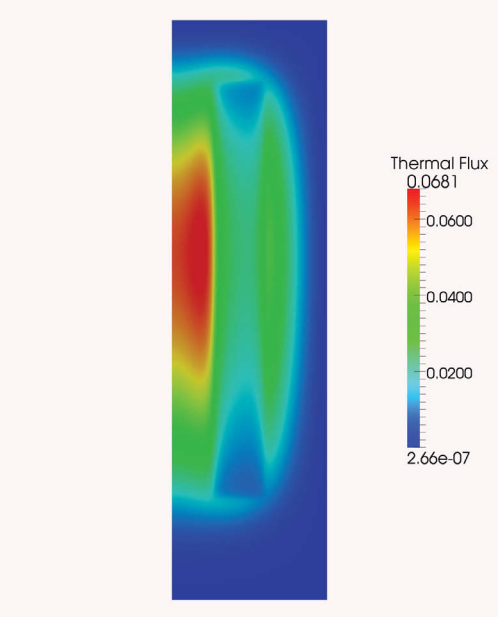
Figure 8: RELAP-7 Coupled Calculation Results

outer reflectors. The fission heat source in Figure 9(c) shows a peak near the inner reflector, which corresponds to the large thermal flux peak in the reactor core caused by the inner reflector region. In addition, the flux and fission heat source distributions display a top peaked shape that is driven by the temperature distribution (shown in 10(b)). Since the flow in the reactor originates at the top and proceeds down through the core it creates a cooler fuel region in upper portion of the core. Other relevant thermo-physical distributions of the MHTGR R-Z core model are shown in Figure 10. As previously mentioned, the coolant temperature distribution is low for the reactor design. The pressure drop across the reactor 40 kPa, which is 15 percent higher than the nominal 34 kPa.

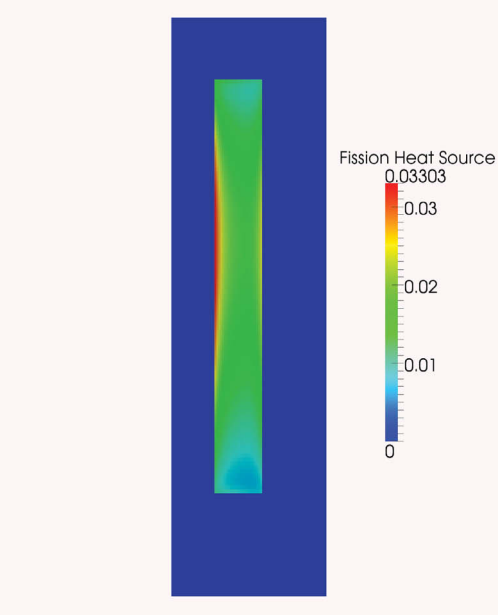
The RELAP-7 time dependent results are included in Figure 8. The plots show similar patterns to those in PRONGHORN. All of the coupling variables (outlet temperature, inlet pressure and outlet momentum) appear to stabilize. The RELAP-7 distributions shown in Figure 11 are very similar to those obtained with the original null transient problem used during stand alone testing.



(a) Scaled Fast Flux

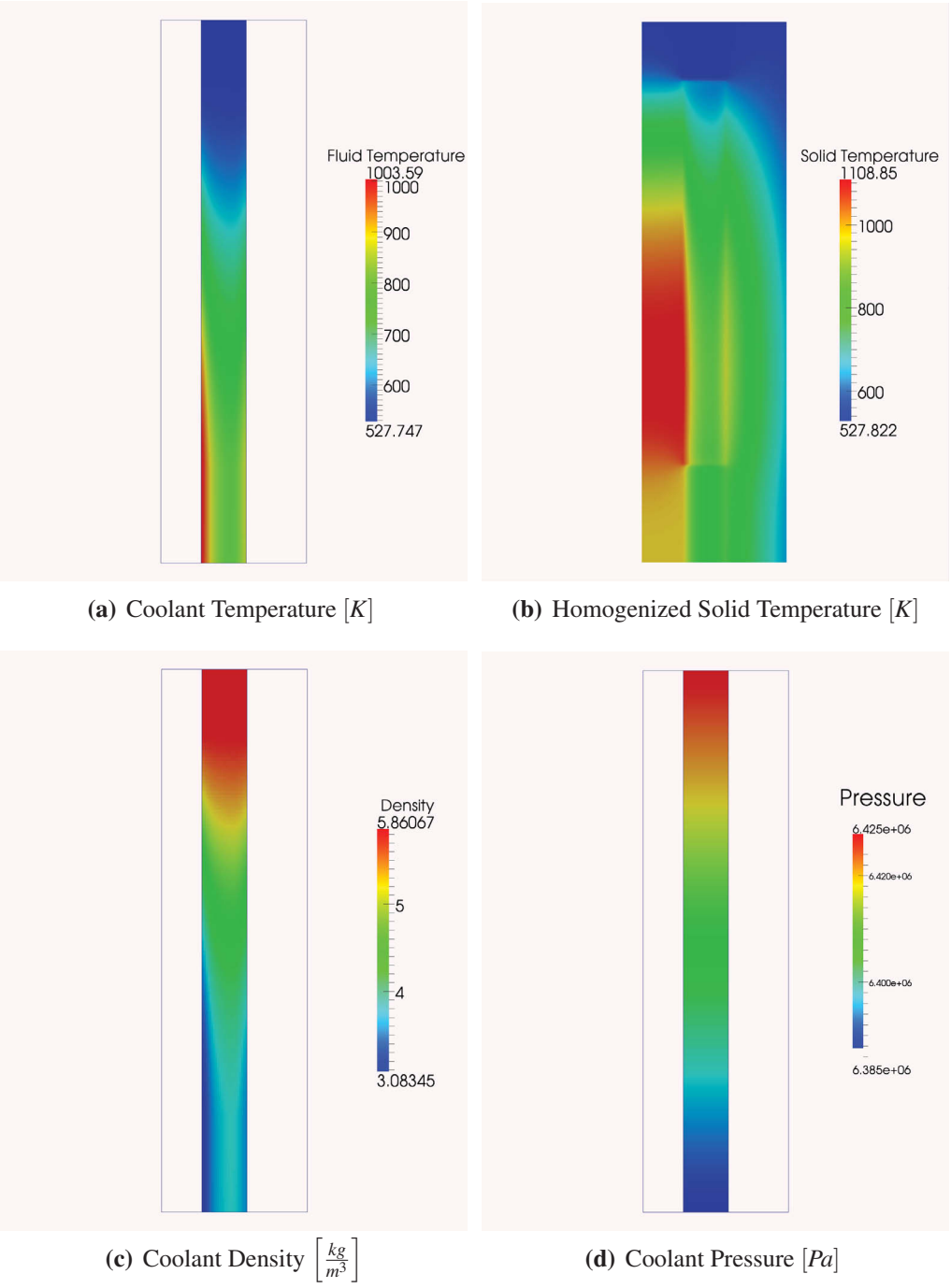


(b) Scaled Thermal Flux



(c) Normalized Fission Heat Source

Figure 9: Neutronics Results From the Final PRONGHORN Core Calculation



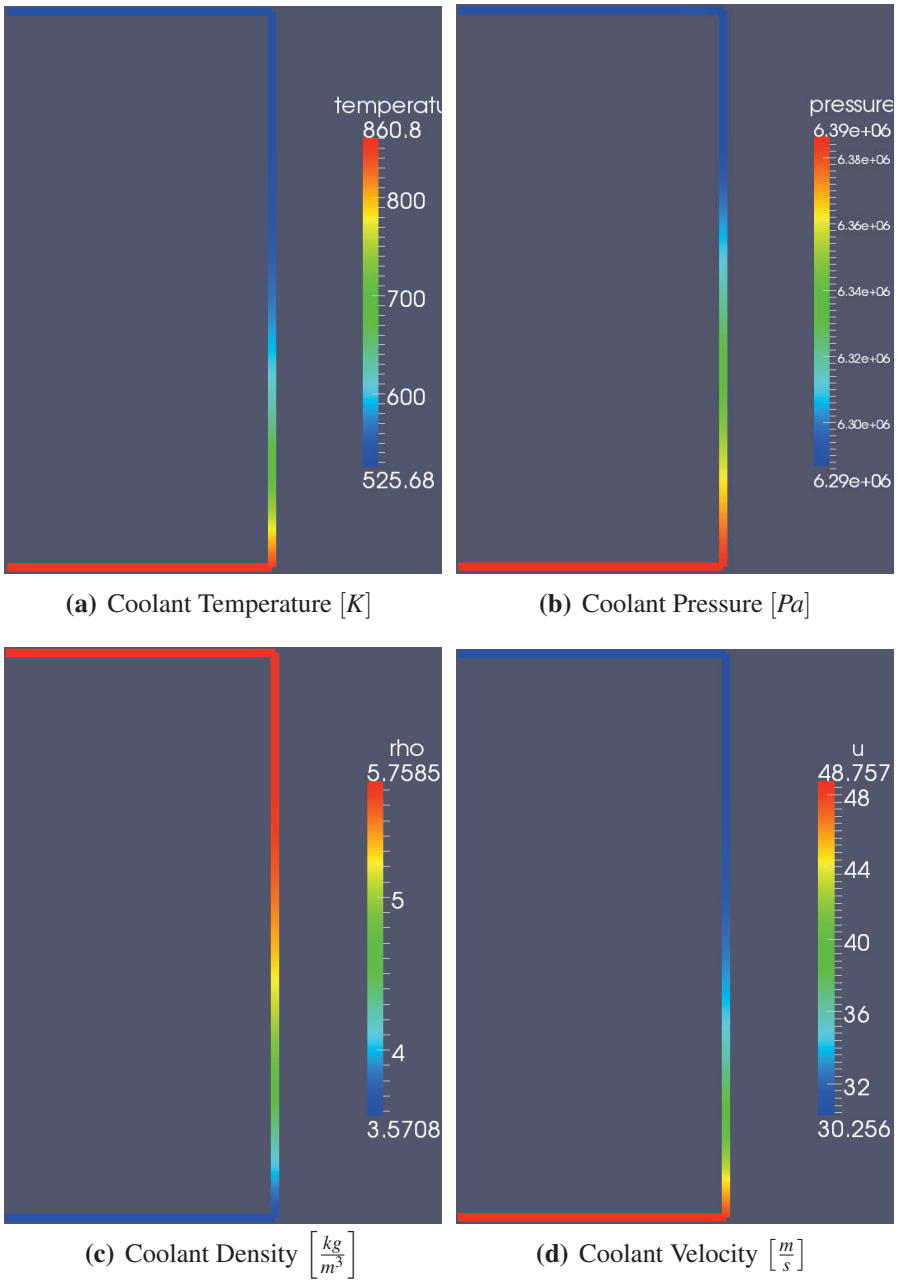
(a) Coolant Temperature $[K]$

(b) Homogenized Solid Temperature $[K]$

(c) Coolant Density $\left[\frac{kg}{m^3}\right]$

(d) Coolant Pressure $[Pa]$

Figure 10: Thermal Physical Results from the Final PRONGHORN Core Calculation



(a) Coolant Temperature $[K]$

(b) Coolant Pressure $[Pa]$

(c) Coolant Density $\left[\frac{kg}{m^3}\right]$

(d) Coolant Velocity $\left[\frac{m}{s}\right]$

Figure 11: RELAP-7 Distributions from the Coupled Calculation

8 Conclusion

The RELAP-7 and PRONGHORN applications have been successfully coupled using an operator split approach. The results show that the coupled system correctly converges to the steady state condition. All final distributions contain the characteristics of the MHTGR design. The convergence pattern shows good behavior for the exception of some initial pressure oscillations that eventually dampen. The source of the oscillations is currently undetermined, but various possibilities have been identified. There were significant difficulties with the modeling of a circulator in RELAP-7 and the effects of the component were simulated by use of modified boundary conditions in the coupled system.

9 Future Work

The successful coupling of RELAP-7 and PRONGHORN code was possible because of the use of the MOOSE framework. However, the code used to couple RELAP7 and PRONGHORN is currently available only as a prototype which demonstrates how to tie the codes together and exchange the information between them. More work is required to turn this prototype into a production code, which is possible given available funds and personnel within a short period of time.

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