

Solving the neutron transport equation on unstructured mesh and its application on high-fidelity multi-physics analysis of micro reactors

Authors: Hu, Dr. Tianliang, Jiang, Dr. Duoyu, Zhang, Dr. Xinyi, Dr. Lipeng Wang, Cao, Dr. Lu, Dr. Huaqi Li, Li, Mr. Da, Dr. Lixin Chen, Dr. Tianliang Hu

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Abstract

High-fidelity unstructured mesh based neutron transport method is necessary to accurately model the behavior of micro reactors considering high neutron leakage, the thermal-hydraulics and geometry deformation feedback effects. Based on the MOOSE framework, the multi-group self-adjoint angular flux neutron transport equation is solved. The unstructured mesh modeling capability provides flexibility in representing irregular shapes and boundaries in micro reactors, while the combination of finite element and discrete ordinate methods ensures efficient and accurate solution of the neutron transport equation. The neutron transport solver was then applied for the neutronics analysis of Xi' an Pulsed Reactor, steady-state multi-physics analytical benchmark problem and coupled neutronics/heat transfer/thermal expansion analysis of the Godiva prompt critical transient. The ability of treating the nonlinearity including source-term coupling between different physics, material nonlinearity and geometric nonlinearity are proved in our analysis. Future work will be conducted on more realistic micro reactor designs like heat pipe cooled reactors and gas cooled reactors.

Full Text

Preamble

Solving the Neutron Transport Equation on Unstructured Mesh and Its Application to High-Fidelity Multi-Physics Analysis of Micro Reactors

Tianliang Hu,¹ Duoyu Jiang,¹ Xinyi Zhang,¹ Lipeng Wang,¹ Lu Cao,¹ Huaqi Li,¹ Da Li,¹ and Lixin Chen^{1,*} ¹Northwest Institute of Nuclear Technology, Xi'

an 710024, China

A high-fidelity unstructured mesh-based neutron transport method is necessary to accurately model the behavior of micro reactors, considering high neutron leakage and the feedback effects of thermal-hydraulics and geometry deformation. Based on the MOOSE framework, the multi-group self-adjoint angular flux (SAAF) neutron transport equation is solved. The unstructured mesh modeling capability provides flexibility in representing irregular shapes and boundaries in micro reactors, while the combination of finite element and discrete ordinate methods ensures efficient and accurate solution of the neutron transport equation. The neutron transport solver was then applied to the neutronics analysis of the Xi'an Pulsed Reactor, a steady-state multi-physics analytical benchmark problem, and coupled neutronics/heat transfer/thermal expansion analysis of the Godiva prompt critical transient. Our analysis demonstrates the ability to treat nonlinearities including source-term coupling between different physics, material nonlinearity, and geometric nonlinearity. Future work will focus on more realistic micro reactor designs such as heat pipe cooled reactors and gas cooled reactors.

Keywords: Neutron transport; unstructured mesh; micro reactor; MOOSE; multi-physics

INTRODUCTION

The International Atomic Energy Agency classifies nuclear reactors with electric power less than 300 MW as small nuclear reactors, while the US Department of Energy recently defined small nuclear reactors in the MW range as microreactors. Micro reactors offer technological advantages such as excellent portability, high thermal efficiency, and inherent safety, attracting increasing attention from the nuclear industry. Their potential lies not only in meeting growing global energy needs and combating climate change, but also in providing emergency power supply on land, as well as in deep sea, deep space, and other specialized areas in the future [1, 2].

Micro-reactors are characterized by their compact size and unique design features, such as control mechanisms with rotational control drums. Accurately modeling high neutron leakage and complex geometry is crucial for simulating the neutronics of advanced micro reactors [3, 4]. Traditional methods like neutron diffusion-based nodal methods and finite difference methods are unsuitable for this task due to the intricate nature of micro-reactor cores. Instead, a high-fidelity unstructured mesh-based neutron transport method enables more detailed representation of core geometry, leading to more accurate predictions of nuclear reactions and power generation within these small-scale reactors.

Another critical aspect of micro reactor simulation is the necessity of accurately considering multi-physics coupling effects. Micro reactors are strongly heterogeneous systems where interactions between neutron transport, thermal heat transfer, and structural mechanics can significantly impact each other, leading

to complex and interdependent behaviors. Furthermore, the heterogeneity of micro reactors introduces additional challenges in modeling these multi-physics coupling phenomena. The varying spatial and temporal scales of different physical processes require a comprehensive approach that accounts for their individual characteristics while capturing their interconnected nature [5, 6]. For accurate modeling of complex neutronics-thermal-structure mechanics coupling phenomena in micro reactors, it is essential to solve the partial (ordinary) differential equations describing different physics. The key is to accurately solve the nonlinearity caused by multi-physical coupling. For micro reactors, these nonlinearities include: (1) nonlinearity caused by source-term coupling between different physics—the power distribution calculated from neutronics simulation serves as the heat source for heat transfer calculations, and the temperature distribution obtained from heat transfer simulation serves as the load for structural mechanics calculations; (2) material nonlinearity—the neutron cross sections in neutronics calculations and the physical properties in thermal-hydraulic and mechanical calculations are influenced by state parameters such as temperature, density, and pressure; (3) geometric nonlinearity—deformation caused by temperature or external load strongly influences neutron leakage and heat transfer characteristics, thus providing another significant feedback effect. This feedback effect needs to be properly handled, especially for micro reactors. Traditional analysis tools are developed individually with fixed mesh, and this effect can only be treated implicitly by modification of atom density.

These two simulation demands have combined to challenge the capabilities of traditional analysis tools. To address these modeling challenges, various efforts have been conducted based on both commercial and open-source multi-physics coupling environments like MOOSE [7], OpenFOAM [8], MFEM [9], and COMSOL [10] in recent years. Tom et al. studied the neutronics characteristics of the CROCUS experimental reactor using the multi-physics coupling analysis code GenFOAM, developed based on OpenFOAM, employing unstructured mesh to precisely describe the complex geometry of the reactor core [11]. Hu et al. developed a multi-physics coupling code using the OpenFOAM platform to analyze steady and transient states in fast-spectrum molten salt reactors [12–14]. To investigate shockwave compression of solid fissile materials, Cervi et al. developed a coupled neutronics-shock physics model using an arbitrary Lagrangian-Eulerian approach based on the OpenFOAM platform [15]. Wang et al. developed the multi-physics and multi-scheme radiation transport applications Rattlesnake and Griffin on the MOOSE platform [16, 17]. Various reactors, including Empire, SNAP, ATR, NTP, and TREAT, have been analyzed using these codes, proving them to be promising tools for advanced micro-reactor analysis [18–22]. To support modeling and safety analysis of micro-reactors, a code named MEZCAL was developed based on the MFEM library, capable of accurately and effectively solving the multi-group neutron transport equation with unstructured mesh modeling capability [23]. Wang et al. developed a neutron transport solver using the finite element method within the commercial multi-physics coupling environment COMSOL for hexagonal-z reactor simulation [10].

Jiang et al. developed a three-dimensional space-time kinetics neutron transport code SAAFCGSN based on the MOOSE platform and demonstrated that it achieves high computational accuracy while effectively managing the cusping effect of control rods [24]. The Monte Carlo method with unstructured mesh capability [25, 26] is also widely adopted in multi-physics simulation of micro reactors. Mehta et al. demonstrated the significance of capturing multiphysics effects in a hydride-moderated reactor system using MCNP and Abaqus-based Reactor Multiphysics software package [27]. Jaeuk et al. performed multiphysics analysis of the 60-degree symmetrical sector model of the MegaPower three-dimensional core for normal operation and heat pipe-failed conditions using the GPU-based continuous-energy Monte Carlo code PRAGMA [28]. Novak et al. implemented an adaptive, on-the-fly mesh-based Monte Carlo geometry algorithm in Cardinal to reduce the barrier-to-entry for high-fidelity multiphysics of reactors [29]. Jiang et al. investigated the coupling calculation of a three-dimensional steady-state neutronics and thermal-hydraulics model for the XAPR by utilizing Cardinal [30]. Wang et al. studied the thermal deformation simulation, expansion reactivity feedback, and density feedback of KRUSTY under unified unstructured mesh using MCNP and Abaqus [31]. Leppanen et al. implemented the multi-physics coupling scheme in Serpent, which supports various interface types, including an unstructured OpenFOAM format polyhedral mesh and a special interface type for fuel performance coupling [32]. All these efforts present an alternative and promising way for high-fidelity analysis of micro-reactors.

In this work, we present an attempt to solve the SAAF (self-adjoint angular flux) neutron transport equation on unstructured mesh based on the MOOSE framework and its application to multi-physics analysis of micro-reactors. The structure of this paper is as follows: Section 2 presents a detailed description of the physics models, including neutron transport, heat transfer, structural mechanics, and the coupling method. In Section 3, preliminary multi-physics simulations of micro-reactors are demonstrated. Finally, Section 4 summarizes the conclusions.

II. MODELS AND METHODS

A. Unstructured Mesh Neutron Transport Method

To accurately estimate the spatial distribution and time evolution of neutron flux and power density in micro reactors, the neutron transport model is adopted in this work. The transient neutron transport equation is a differential-integral equation with seven degrees of freedom, including space, energy, angle, and time. To solve the equation numerically, it must be discretized in energy, angle, space, and time. We prefer using discrete ordinates discretization for angular discretization in reactor-like geometries as it provides a good balance between accuracy and efficiency. By combining multi-group and discrete ordinates discretization, we can characterize the neutron transport equation with isotropic scattering as Eq. (1).

$$\frac{d}{dt} \int_V \phi_{g,n}(\mathbf{r}) dV + L_{g,n}(\mathbf{r}) + R_{g,n}(\mathbf{r}) = S_s(\mathbf{r}) + (1 - \beta) \sum_g \int_V \phi_{p,g}(\mathbf{r}) dV + \sum_i \lambda_i C_i - \sum_i \beta_i \lambda_i C_i$$

where:

$$\begin{aligned} L_{g,n}(\mathbf{r}) &= -\nabla \cdot \mathbf{\Omega}_{g,n} \phi_{g,n}(\mathbf{r}) \\ R_{g,n}(\mathbf{r}) &= -\Sigma_{t,g} \phi_{g,n}(\mathbf{r}) \\ S_s(\mathbf{r}) &= \sum_{s,g} \int_{\Omega} \Sigma_{s,g} \phi_{s,n}(\mathbf{r}) d\Omega \end{aligned}$$

\mathbf{r} is the neutron position defined in the spatial domain; Ω is the neutron travel direction; t is the time; g is the index of neutron energy group; $\phi_{g,n}$ is angular neutron flux; k_{eff} is the multiplication factor; v_g is the speed of neutrons within energy group g ; $\Sigma_{t,g}$ is the total cross section for neutrons in energy group g ; $\Sigma_{s,g}$ is the scattering cross section for neutrons going from energy group g to g and from direction n to n ; $\nu \Sigma_{f,g}$ is the product of the fission cross section and the average number of neutrons generated per fission event for neutrons in energy group g ; $p_{g,i}$ is the prompt neutron energy spectrum; $d_{g,i}$ is the delayed neutron energy spectrum; C_i is the concentration of delayed neutron precursor of group i ; λ_i is the decay constant for delayed neutron precursor of group i ; β_i is the fraction of neutrons from fission going into delayed neutron precursor group i .

In this study, we use the finite element method to discretize Eqn. (1), which is commonly used in solid mechanics, heat conduction, and other areas. The flexibility of the finite element method in handling unstructured meshes makes it well suited for simulating complex geometries in microreactors. However, directly applying continuous FEM to Eq. (1) can lead to instability due to its representation of a system of hyperbolic PDEs. Continuous finite element method is only stable for elliptic PDEs [23]. Therefore, the SAAF equation has been considered in this work. The SAAF equation can be derived by introducing the Auxiliary Flux Equation, which can be defined as:

$$\frac{d}{dt} \int_V \phi_{g,n}(\mathbf{r}) dV = \int_V (S_s(\mathbf{r}) + (1 - \beta) \sum_g \int_V \phi_{p,g}(\mathbf{r}) dV + \sum_i \lambda_i C_i - L_{g,n}(\mathbf{r}) - R_{g,n}(\mathbf{r})) dV$$

The initial stage of the discretization process involves dividing the geometric domain D into separate, non-overlapping elements. Following this, the discretized version of Eq. (1) for the neutron transport equation is multiplied by a test function $v(\mathbf{r})$ and integrated across the problem domain D to derive the weak form:

$$\int_V v(\mathbf{r}) \left(\frac{d}{dt} \int_V \phi_{g,n}(\mathbf{r}) dV + L_{g,n}(\mathbf{r}) + R_{g,n}(\mathbf{r}) \right) dV = \int_V v(\mathbf{r}) \left(S_s(\mathbf{r}) + (1 - \beta) \sum_g \int_V \phi_{p,g}(\mathbf{r}) dV + \sum_i \lambda_i C_i - \sum_i \beta_i \lambda_i C_i \right) dV$$

where $(L_{g,n}(\mathbf{r}), v(\mathbf{r})) = - \int_V \nabla \cdot \mathbf{\Omega}_{g,n} \phi_{g,n}(\mathbf{r}) v(\mathbf{r}) dV$ represents volume integration.

$$\int_{\Gamma} g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma = \int_{\Gamma} g_n(\mathbf{r}) \Omega_n \cdot \mathbf{n} d\Gamma$$

Using fractional integral and Gaussian theorem, the second term in Eqn. (4) can be translated to:

Then the Auxiliary Flux Equation is inserted into Eq. (7):

$$\int_{\Gamma} L g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma = \int_{\Gamma} L^* g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma + \int_{\Gamma} g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma$$

$$\int_{\Gamma} (L^* g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma) = \int_{\Gamma} L(\mathbf{r}) (-S_s(\mathbf{r}) \int_{\Gamma} g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma - \beta \int_{\Gamma} p_{gSp}(\mathbf{r}) \mathbf{n} \cdot d\Gamma + L g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma)$$

The weak form of the SAAF equation then can be derived \langle, \rangle represents surface integration. as Eqn. (10) and Eqn. (11):

$$\int_{\Gamma} (L g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma) = \int_{\Gamma} S_s(\mathbf{r}) \mathbf{n} \cdot d\Gamma + \int_{\Gamma} L(\mathbf{r}) \int_{\Gamma} L g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma$$

$$\int_{\Gamma} L(\mathbf{r}) \int_{\Gamma} L g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma + \int_{\Gamma} g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma = \int_{\Gamma} (R g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma) - \beta \int_{\Gamma} p_{gSp}(\mathbf{r}) \mathbf{n} \cdot d\Gamma$$

$$\int_{\Gamma} L(\mathbf{r}) \int_{\Gamma} L g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma = \int_{\Gamma} (-\lambda_i C_i(\mathbf{r})) \mathbf{n} \cdot d\Gamma$$

Regarding the boundary conditions, the SAAF equation's boundary condition can be separated into terms for outflow and inflow, which can be represented as follows:

$$\int_{\Gamma} g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma = \int_{\Gamma} g_n(\mathbf{r}) \Omega_n \cdot \mathbf{n} > 0 \int_{\Gamma} g_n(\mathbf{r}) \Omega_n \cdot \mathbf{n} < 0 \int_{\Gamma} g_n(\mathbf{r}) \Omega_n \cdot \mathbf{n} d\Gamma$$

In Eqn.(12), \mathbf{n} denotes the unit vector that points outward in the normal direction from the boundary. The vacuum boundary condition is expressed as:

$$\int_{\Gamma} g_n(\mathbf{r}) \mathbf{n} \cdot d\Gamma = \int_{\Gamma} g_n(\mathbf{r}) \Omega_n \cdot \mathbf{n} > 0 \int_{\Gamma} g_n(\mathbf{r}) \Omega_n \cdot \mathbf{n} < 0$$

In this study, we have developed the kernels for each term in Eq. (10) and (11), as well as the boundary conditions for Eqn. (12) and (13) using the MOOSE platform. The MOOSE platform, developed by Idaho National Laboratory, is an open-source computing platform designed for solving multi-physics numerical problems. It utilizes the finite element method and PJFNK algorithm to efficiently solve partial differential equations in a modular manner. In MOOSE terminology, kernels and boundary conditions are implemented as C++ classes with methods for calculating residual and Jacobian contributions corresponding to specific parts of governing equations. The static neutron transport equation is an eigenvalue problem, which can be solved using the built-in Eigenvalue Executioner in MOOSE. Additionally, various time schemes are available for transient simulations.

B. Heat Transfer and Structure Mechanics Model

The Doppler effect and mesh deformation feedback effect are crucial factors that influence the steady-state and dynamic behavior of micro reactors. These effects can impact neutron leakage within the reactor, ultimately affecting its

performance. To obtain the temperature distribution in micro reactors, it is necessary to apply the energy balance equation with internal heat generation, as shown in Eqn. (14):

$$= \cdot (k T (r, t)) + qf (r, t)$$

The mechanical model solves the conservation of momentum for solid mechanics:

$$- \cdot \sigma = F$$

We utilize the theory of infinitesimal small strain, which establishes a linear relationship between stress and displacement tensors. This theory is based on the assumption that displacement is significantly smaller than any relevant dimensions, allowing us to consider unchanged geometry and constitutive properties of materials at each point in space during deformation. This approach enables accurate analysis and prediction of material behavior under various loading conditions, providing valuable insights for engineering design and structural analysis. By considering infinitesimally small strains, we can simplify complex problems and make accurate predictions about material behavior without needing to account for large deformations or non-linear effects:

$$(X u + T$$

The symmetric strain tensor and the thermal expansion for isotropic materials are directly linked to the nominal stress tensor σ :

$$\sigma_{ij} = C_{ijkl} \epsilon_{kl} + \beta T \Delta T \delta_{ij} = 2G \epsilon_{ij} + \lambda \epsilon_{kk} \delta_{ij} + \beta T \Delta T \delta_{ij}$$

C. Multi-Physics Coupling Method

Equations (1), (14), (16), (17) and the corresponding initial conditions and boundary conditions constitute the multi-physics coupling system. The distribution of neutron flux, power, temperature, displacement, and other physical quantities can be obtained by solving these equations. After space and time discretization, all based on the MOOSE platform, the partial differential equations describing neutronics, heat transfer, and structure mechanics can be transformed into non-linear equation systems:

$$\begin{matrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{matrix}$$

Where ϕ , T and u are neutron angular flux, temperature, and displacement respectively, and K_{ij} and P are problem-dependent coupling coefficients.

Methods to solve the multi-physics coupling system can be divided into two main categories: strong coupling method and weak coupling method. All the nonlinear equation systems are assembled in a single matrix through a strong coupling approach as shown in Eqn. (18) for the strong coupling method. The discretized nonlinear equations are then solved directly, and solutions for all

physical quantities are updated simultaneously during iteration. The advantage of the strong coupling method is its intuitiveness and simplicity. Based on the MOOSE multi-physics coupling framework, the strong coupling method can be easily implemented. At the same time, the strong coupling method can directly use the Newton iteration method to update all solution variables synchronously, with variables converging simultaneously. Moreover, the local convergence rate of the Newton iteration method is second order. However, the strong coupling method has the following problems: (1) the properties of partial (ordinary) differential equations describing different physics are different, and direct simultaneous solution of all equations may lead to a large condition number of the matrix, even ill-conditioned, resulting in slow convergence or even non-convergence of solutions; (2) because all nonlinear equations are solved together, the direct simultaneous solution consumes large amounts of memory and computational resources, generally limiting its application to one-dimensional or two-dimensional problems. In the multi-physics coupling analysis of micro reactors, full three-dimensional strong coupling calculation cannot be easily realized at present; (3) in time-dependent problems, there is a problem of time scale inconsistency. Physics with slow temporal changes may need to adopt the same time step as physics with fast changes, increasing computational burden.

Unlike the strong coupling method, the core idea of the weak coupling method is to transform the multi-physics coupling problem into several sub-problems by operator splitting, with sub-problems coupled by data transfer. Thus, the solution between different physical models in the weak coupling method is completely decoupled, as shown in Eqns. (19), (20), and (21). By designing different iterative methods, the weak coupling method can be further divided into loose coupling method or tight coupling method. The weak coupling method offers the advantage of maximizing the utilization of developed single-physics models and codes. The disadvantage is that only first-order convergence can be achieved, and for some cases, the convergence rate is slow.

$$\begin{aligned} \text{K11}(\text{Tf uel}, \text{Tf luid}) \cdot \phi &= \tilde{\text{P}}\phi(\phi, \text{Tf uel}, \text{Tf luid}) \\ \text{K22}(\phi, \text{Tf uel}, \text{Tf luid}) \cdot \text{Tf uel} &= \tilde{\text{P}}\text{f uel}(\phi, \text{Tf uel}, \text{Tf luid}) \\ \text{K33}(\text{Tf uel}, \text{Tf luid}) \cdot \text{Tf luid} &= \tilde{\text{P}}\text{f luid}(\text{Tf uel}, \text{Tf luid}) \end{aligned}$$

Based on the above methods, a multi-physics coupling analysis code has been developed in this paper. Currently, there are two main strategies for developing multi-physics coupling codes. The traditional strategy is to couple mature and widely validated codes together by developing data exchange interfaces. Since these single-physics codes are often developed with different spatial and temporal numerical discretization methods, the resulting multi-physics code is usually very complex and can only be applied to specific cases. The other approach is to develop a multi-physics code based on a multi-physics coupling environment with a unified architecture. Representative environments include MOOSE, COMSOL, and OpenFOAM. Using a multi-physics coupling environment can unify grid processing, discretization of partial differential equations, solution of linear equation systems, parallel computing, etc., under a framework for all

codes developed based on the platform to share. This approach can improve code utilization and avoid redundant development. However, since platforms generally use a single numerical discretization method, the same spatial and temporal numerical discretization methods must be used for different physical phenomena. For certain specific problems, computational efficiency may be lower than that of the first approach.

In this work, the MOOSE framework is chosen as the development platform. Although MOOSE supports the strong coupling method, it often resulted in solve failures from our experience. Therefore, the majority of our simulations rely on the weak coupling method, with the inclusion of the strong coupling method for thermo-mechanical simulations of Godiva prompt critical transients. The MultiApp and Transfer system in MOOSE allows for weak coupling, enabling the neutronics solver to naturally connect with other physics codes developed on the MOOSE framework, thus enhancing multi-physics capabilities. This integration of different physics codes within the MOOSE framework provides a seamless platform for simulating complex physical phenomena across multiple disciplines.

III. APPLICATION

A. XAPR Case

The XAPR is a light water-cooled reactor with graphite reflection. It has two core configurations: one for steady-state operation at 2 MW thermal power and another for pulsed operation with peak power up to 4300 MW. This study focuses on steady-state operation conditions, as shown in Fig. 1 Figure 1: see original paper. The steady-state core consists of 9 hexagonal rings containing 101 fuel elements, 82 graphite elements, 6 control rod elements, 2 stainless steel elements, 2 running rabbit irradiation tubes, a neutron source element, and a central water chamber. The central water chamber occupies the center of the core with water-filled middle channels while graphite reflector elements surround the perimeter. Standard fuel rods occupy 99 channels, while two channels are for thermometric fuel rods. One channel is used by the neutron source rod, and two channels each are occupied by stainless steel elements and running rabbit irradiation tubes. The standard fuel rod consists of thick stainless-steel cladding, three fuel pellets, three Zr-4 mandrels, and two graphite reflectors, along with upper and lower plugs. The space between the fuel pellet and cladding is filled with 0.1 MPa helium to improve thermal conductivity. The XAPR fuel is a uniform combination of enriched uranium and zirconium hydride.

Incorporating UZrH1.6 in the XAPR leads to a significant immediate negative temperature feedback coefficient, thus providing the core with exceptional inherent safety. In previous studies, the limitations of either unstructured-mesh neutron diffusion method [35, 36] or nodal transport method [38] have been evident in their inability to accurately account for neutron leakage and geometric modeling simultaneously. To address this issue, a detailed unstructured-

mesh model was developed for neutron transport simulation using the MOOSE Reactor module, as depicted in Fig. 1(b). This approach allows for a more comprehensive and precise representation of neutron behavior within complex geometries, leading to improved accuracy in nuclear reactor simulations. By incorporating advanced computational techniques and sophisticated modeling tools, this work aims to overcome the shortcomings of previous methods and provide a more reliable platform for studying micro reactors.

The XAPR core simulation with 224,910 elements and S8 level symmetric angular quadrature allows for detailed analysis of neutron transport within the reactor. Multi-group cross sections for the XAPR reactor model are generated from our previous work and use a 7-group energy structure as shown in Table 1 [38, 39]. Neutron scattering is treated using transport-corrected P0 cross sections, ensuring accurate representation of neutron behavior within the reactor core.

Comparison is made between the calculated core criticality and the referenced keff at various control rod positions. The power density distribution of the reactor core can be seen in Fig. 2 [Figure 2: see original paper]. The core integral parameter keff at different control rod positions is compared in Table 2. The results from this realistic micro-reactor model indicate that our neutron transport method developed in this paper can properly treat neutron leakage and complex geometry in micro reactors.

B. Multi-Physics Analytical Benchmark Problem

Currently, with increasing computing capabilities, there is growing demand for high-fidelity reactor simulation using multi-physics coupling models. However, few relevant benchmark problems and experimental results exist for neutronics/thermal/mechanical multi-physics coupling codes at present, limiting verification of related codes. In this paper, a one-dimensional nuclear-thermal-mechanical coupling analytical problem proposed by the US Naval Nuclear Laboratory was used to preliminarily verify the multi-physics coupling program based on MOOSE [40]. Although this analytical problem is not based on real reactor design or experimental measurement results, it has the ability to verify the nonlinearity caused by source term coupling in solving multi-physics coupled codes as well as material nonlinearity and geometric nonlinearity.

The benchmark problem involves multiplicative 1-D neutron transport (Eqn. (22)) combined with thermal conduction, convection, Doppler broadening (Eqn. (23)), and expansion effects (Eqn. (24)) along the length of the slab. This benchmark presents a highly nonlinear challenge due to nonlinearity caused by coupling of source terms between different physics, materials, and geometric deformations.

$$\begin{aligned} \text{(cid:20)} \quad & \Sigma_t(x) \frac{d\phi(x)}{dx} + (\lambda - 1)\Sigma_t(x)\phi(x) = 0 \\ \text{(cid:20)} \quad & k(T) \frac{dT(x)}{dx} + q\Sigma_t(x)\phi(x) = 0 \\ \text{(cid:90)} \quad & T = a(T) \frac{dT}{dx} \end{aligned}$$

The neutron transport model consists of one-speed neutrons traveling with directions $\mu = \pm 1$ in a 1-D slab with initial length L_0 , mass density ρ , and zero-incident-flux boundary conditions on both sides. For the structure mechanics simulation, the slab is mechanically constrained and perfectly insulated in the transverse dimensions (y and z-axes) but free to expand along the x-axis as the temperature changes. The thermal expansion coefficient is defined as:

$$\alpha(T) =$$

The steady-state temperature distribution is solved by the thermal conductivity equation. The thermal conductivity is a linear function of temperature as described in Eqn. (26). The boundary condition is convective with heat transfer coefficient h at the ends.

$$T(x) = T_0 + \alpha T(x)$$

The neutronics-heat transfer-mechanics coupling simulation is achieved based on the MOOSE MultiApp and Transfer system. The heat transfer simulation is the MasterApp and has two MultiApps: neutron transport simulation (MultiApp1) and thermal expansion simulation (MultiApp2). The converged solution is achieved by Picard iteration. The power distribution obtained from neutron transport simulation is transferred to heat conduction simulation, and the temperature distribution obtained from heat conduction simulation is then used in the thermal stress calculation. The displacement obtained from thermal stress simulation is further utilized in heat conduction simulation, which in turn affects neutron transport simulation. In the simulation, all three models use the same mesh for calculation, so the MultiAppCopyTransfer in MOOSE is adopted for data transfer.

Because the heat transfer simulation is the MainApp, the initial nonlinear residual of the temperature solution in each Picard iteration step is used as the criterion to judge convergence of Picard iteration. In the case with mesh number of 100, the residual variation with Picard iteration number is shown in Fig. 3(a) [Figure 3: see original paper]. Firstly, a mesh independence study was performed using different numbers of elements in the x-direction. As shown in Fig. 3(b) and 3(c), the effective multiplication factor, central temperature ($x = 0$), and boundary node displacement are calculated and analyzed. The simulation results converge gradually with increasing element number. It can be concluded that convergent solution can be achieved when the number of grids is 100.

According to the mesh independence analysis results, the numerical solution with mesh number of 100 is compared with the analytical solution. The numerical solution of k_{eff} is 0.29630, the analytical solution is 0.29557, and the derivation is 73 pcm. The boundary node displacement is 6.48 cm in our numerical simulation, demonstrating strong alignment with the analytical solution of 6.47 cm. The central maximum temperature is 343.15 K, and the numerical solution is 343.07 K. The temperature distribution along the x-direction is compared with analytical solutions as shown in Fig. 4 [Figure 4: see original paper]. The maximum difference is at the center point, less than 0.03%. In general, the

numerical results obtained by the MOOSE-based multi-physics coupling code are in good agreement with analytical solutions in neutronics, heat transfer, and mechanics. It is proved that the multi-physical coupling strategy can deal with complex nonlinearity existing in reactor simulation.

In micro reactors, thermal expansion is a significant factor in the feedback mechanism. Changes in reactor geometry directly impact neutron leakage and heat transfer characteristics. The effect of mesh deformation on neutronics and heat transfer is analyzed as shown in Table 3. The derivations of our numerical results and analytical solutions are large under all three cases, especially when neutronics simulation does not consider mesh deformation. In these cases, the deviation of k_{eff} is large, with maximum difference of 1905 pcm. It is also found that the number of Picard iterations changes significantly if mesh deformation is not taken into account. Under conditions 1 and 3, the number of Picard iterations is reduced to 8, and the nonlinear coupling effect is obviously weakened. The number of Picard iterations is reduced by 2 in case 2, indicating that the main nonlinear effects are caused by geometric nonlinearity of neutron transport.

In summary, although this case is not a real micro reactor problem, the analytical solution can effectively test the modeling and computing capability of existing multi-physical coupling programs, particularly the capability of treating geometric nonlinearity.

C. Godiva Prompt Critical Transient Problem

Godiva I is the world's first fast neutron pulse reactor built by LANL. It is an unshielded bare spherical U-235 assembly without reflecting layers. The radius is 8.7407 cm. The critical mass is about 52 kg with density about 18.75 g/cm^3 [41]. The fast neutron pulsed reactor can run in the instantaneous supercritical state when the burst pulse occurs. The fission rate increases several orders of magnitude in a few milliseconds, and the relative volume of the core changes, which has the mechanism of thermal expansion and self-extinguishing. The pulse process involves reactor dynamics, unsteady heat transfer, mechanical analysis, and coupling processes. Therefore, transient analysis of fast neutron pulse reactors can verify not only the accuracy of neutronics calculation but also validate nuclear thermodynamic coupling calculation and mechanical deformation feedback models.

As shown in Fig. 5 [Figure 5: see original paper], three-dimensional geometry is used for simulation. The heat transfer and mechanical parameters used in the calculation are shown in Table 4 [42]. In heat transfer simulation, the adiabatic boundary condition is adopted because the temperature rise of the system during the transient is relatively small. The Doppler feedback effect on reactivity can be ignored, so only changes in atom density are considered in our simulation. In this paper, the mechanics calculation adopts the infinitesimal small strain theory, and the volume strain of the computational element can be

expressed as:

$$V(t) - V_0 = \det(X u(t) + I) - 1$$

Assuming that the neutron energy spectrum remains unchanged during the transient, the change in neutron macroscopic cross-section is mainly caused by the change in atom density due to element volume change. The method for updating neutron cross sections is shown as:

$$\Sigma(t) = \Sigma_0 V(t) / V_0$$

The explicit temporal coupling between neutronics and thermomechanics is illustrated in Fig. 7 [Figure 7: see original paper]. The transient simulation follows this calculation flow at every time step: (1) the internal heat source is calculated from the neutron flux distribution provided by the previous time step; (2) the thermal-mechanics equations are solved by the HeatTransfer and SolidMechanics modules in MOOSE framework; (3) the volume strain of each element is calculated according to nodal displacement using Eqn. (27), then the multi-group macro cross-sections are updated according to atom density change using Eqn. (28), and displacements are transferred to the meshes of neutronics dynamics calculation for deformation; (4) the neutronics dynamics simulation is performed according to updated macroscopic cross-section and mesh. The coupled solution of neutronics dynamics and thermo-mechanics problem is realized by the MultiApp and Transfer systems of MOOSE, with the thermo-mechanics solver as the MainApp and the neutronics solver as the MultiApp.

Before transient simulation, a steady-state neutronics simulation is performed followed by normalizing the reactor core power to 500W. The three-dimensional distribution of power density is shown in Fig. 6 [Figure 6: see original paper]. Notably, the temperature distribution exhibits a similar spatial pattern (with contour shapes mirroring those of power distribution). The normalized neutron flux acts as the initial condition for transient calculation. The duration of transient calculation is 0.001 s and the time step is 1×10^{-7} s in the simulation.

Fig. 8 Figure 8: see original paper and Fig. 8(b) illustrate changes in power and average temperature over time during a prompt critical transient. With introduction of step positive reactivity, there is only slight rise in average temperature as a result of gradual increase in system power in the initial stage. Then system power rises rapidly and temperature increases rapidly. The accumulated fission energy leads to thermal expansion of uranium metal. Neutron leakage is enhanced due to deformation and introduces negative reactivity. The core then enters sub-critical state, resulting in rapid decrease in core power. As a result of rapid fluctuation in fission power, it is evident that the uranium metal sphere undergoes both compression and expansion, as depicted in Fig. 8(c) and Fig. 8(d), leading to a thermal inertia effect. The oscillation of surface displacement, velocity, and acceleration closely matches the experimental scenario. Since the negative feedback effect was introduced totally by geometry deformation in this transient, the numerical results prove that the method developed in this paper is capable of handling this complicated multi-physics coupling process.

IV. SUMMARY AND CONCLUSIONS

The current study involved development of a second-order SAAF equation-based neutron transport solver within the MOOSE framework. The neutronics solver has capability for modeling complex geometry as well as explicit treatment of mesh deformation, thus providing an efficient tool for neutronics simulation of advanced micro reactors. Since the neutronics solver is built on MOOSE, it naturally couples to other physics models by either strong coupling or weak coupling method.

As applications, the neutronics solver has been used for high-fidelity analysis of micro reactors. The XAPR steady-state neutronics simulation was performed first. Numerical results demonstrate that the neutron transport method proposed in this study effectively handles complex geometry in micro reactors. Then, two multi-physics coupling cases with neutron transport and thermo-mechanics coupling were analyzed based on the method proposed in this work. The ability to handle nonlinearity caused by source-term coupling, material nonlinearity, and geometric nonlinearity was proved by both steady-state and transient multi-physics analysis. Our results indicate that the impact of mesh deformation on reactor core contributes significantly to the behavior of micro reactors. More efforts need to be devoted to multi-physics modeling of more complex micro reactor designs like heat pipe reactors and gas cooled reactors in the future.

- [1] A. Peakman, Z. Hodgson, B. Merk, et al. Advanced micro-reactor concepts [J]. *Progress in Nuclear Energy*, 107: 61-70 (2018).
- [2] X.Y. Kang, H.Q. Li, S. Chen, et al. Conceptual core schemes and thermal analysis for 5 MWt Heat pipe cooled micro reactor [J]. *Modern Applied Physics*, 13(2): 020401 (2022).
- [3] Q.Z. Sun, X.J. Liu, X. Chai, et al. A discrete-ordinates variational nodal method for heterogeneous neutron Boltzmann transport problems [J]. *Computers & Mathematics with Applications*, 170: 142-160 (2018).
- [4] H. Yin, X.J. Liu, T.F. Zhang, et al. An efficient parallel algorithm of variational nodal method for heterogeneous neutron transport problems [J]. *Nuclear Science and Techniques*, 35: 69 (2024).
- [5] A. G. Mylonakis, M. Varvayanni, N. Catsaros, et al. Multi-physics and multi-scale methods used in nuclear reactor analysis [J]. *Annals of Nuclear Energy*, 72: 104-119 (2014).
- [6] C. Demaziere. Multi-physics modelling of nuclear reactors: current practices in a nutshell [J]. *International Journal of Nuclear Energy Science & Technology*, 7(4): 288-318 (2013).
- [7] D. Gaston, C. Newman, G. Hansen, et al. MOOSE: A parallel computational framework for coupled systems of nonlinear equations [J]. *Nuclear Engineering and Design*, 239(10): 1768-1778 (2009).
- [8] C. Fiorina, I. Clifford, S. Kelm, et al. On the development of multi-physics tools for nuclear reactor analysis based on OpenFOAM®: State of the art, lessons learned and perspectives [J]. *Nuclear Engineering and Design*, 111604

(2021).

- [9] R. A. Robert, MFEM: A modular finite element methods library [J]. *Computers & Mathematics with Applications*, 81: 42-74 (2021).
- [10] Y.H. Wang, J.C. Chen, D. Li, et al. Simulation of SN transport equation for hexagonal-z reactor using the COMSOL Multiphysics software [J]. *Nuclear Engineering and Design*, 111604 (2021).
- [11] M. Tom, C. Fiorina, H. Mathieu, et al. Investigation and Validation of Unstructured Mesh Methodologies for Modeling Experimental Reactors [J]. *Energies*, 15: 1512 (2022).
- [12] T.L. Hu, L.Z. Cao, H.C. Wu, et al. Coupled neutronics and thermal-hydraulics simulation of molten salt reactors based on OpenMC/TANSY [J]. *Annals of Nuclear Energy*, 31: 107322 (2017).
- [13] C.H. Wan, T.L. Hu, L.Z. Cao, et al. Multi-physics numerical analysis of the fuel-addition transients in the liquid-fuel molten salt reactor [J]. *Annals of Nuclear Energy*, 14: 104987 (2022).
- [14] T.L. Hu, L.Z. Cao, S.H. Yang, et al. Analysis of the thermal feedback effect and nuclides flow effect on the fuel-cycle characteristics of Molten Salt Reactors [J]. *International Journal of Energy Research*, 45: 11677-11688 (2021).
- [15] E. Cervi, A. Cammi. An Arbitrary Lagrangian-Eulerian, coupled neutronics-shock physics model for the analysis of shockwave implosion of solid fissile materials [J]. *Annals of Nuclear Energy*, 141: 107322 (2020).
- [16] Y.Q. Wang, S. Chunert, J. Ortensi, et al. Rattlesnake: A MOOSE-Based Multi-physics Multi-scheme Radiation Transport Application [J]. *Nuclear Technology*, 1047-1072 (2021).
- [17] Y.Q. Wang, C. Lee, Y.S. Jung, et al. Performance Improvements for the Griffin Transport Solvers [R]. US: Idaho National Laboratory, 2023.
- [18] T. Martin, B. Friederike, J. Matthew, et al. Two-step neutronics calculations with Shift and Griffin for advanced reactor systems [J]. *Annals of Nuclear Energy*, 173: 11031 (2022).
- [19] H. Khang, M. D. Modeling of the Advanced Test Reactor Using OpenMC, Cubit, and Griffin [R]. US: Idaho National Laboratory, 2023.
- [20] O. Havier, A. Benjamin, P. Matthew, et al. Validation of the Griffin application for TREAT transient modeling and simulation [J]. *Nuclear Engineering and Design*, 385: 111478 (2021).
- [21] N. A. Isaac, G. Sam, L. Ben, et al. Verification of the Serpent-Griffin Workflow using the SNAP 8 Experimental Reactor [R]. US: Idaho National Laboratory, 2023.
- [22] M. Vincent, S. Sebastian, T. Stefano, et al. Automated Power-following Control for Nuclear Thermal Propulsion Startup and Shutdown Using MOOSE-based Applications [J]. *Progress in Nuclear Energy*, 161: 104710 (2023).
- [23] W. C. Dawn, S. Palmtag. Solving the Neutron Transport Equation for Microreactor Modeling Using Unstructured Meshes and Exascale Computing Architectures [J]. *Nuclear Engineering and Design*, 111604 (2021).
- [24] D.Y. Jiang, P. Xu, X.B. Jiang, et al. Application Research on Whole-Core Three-Dimensional Space-Time Kinetics Neutron Transport Code SAAFCSN [J]. *Nuclear Power Engineering*, 46(01): 13-23 (2024).

- [25] X. Zhang, S.C. Liu, Z.Y. Wang, et al. Development of unstructured mesh tally capability in cosRMC and application to shutdown dose rate analysis [J]. *Fusion Engineering and Design*, 181: 113211 (2022).
- [26] Z.Y. Wang, S.C. Liu, X.K. Zhang, et al. Research on Monte Carlo Particle Transport Method Directly Using CAD Geometry [J]. *Atomic Energy Science and Technology*, 55: 88–91 (2021).
- [27] V.K. Mehta, J. Armstrong, D.V. Rao, et al. Capturing multiphysics effects in hydride moderated microreactors using MARM [J]. *Annals of nuclear energy*, 172: 109067 (2022).
- [28] J. Lm, M.J. Jeong, J. Choi, et al. Multiphysics Analysis System for Heat Pipe-Cooled Micro Reactors Employing PRAGMA-OpenFOAM-ANLHTP [J]. *Annals of nuclear energy*, 197(8): 1743–1757 (2023).
- [29] A.J. Novak, H. Brooks, P. Shriwise, et al. Monte Carlo multiphysics simulation on adaptive unstructured mesh geometry [J]. *Nuclear Engineering and Design*, 429: 113589 (2024).
- [30] D.Y. Jiang, P. Xu, T.L. Hu, et al. Coupled Monte Carlo and Thermal-Hydraulics Modeling for the Three-Dimensional Steady-State Analysis of the Xi' an Pulsed Reactor [J]. *Energies*, 16(16): 6046 (2024).
- [31] L.P. Wang, L. Cao, S. Chen, et al. Study of KRUSTY Thermal Expansion Negative Feedback Calculation Based on Unstructured-Mesh MCNP [J]. *Nuclear Power Engineering*, 44(02): 286–294 (2024).
- [32] J. Leppanen, V. Valtavirta, A. Rintala, et al. Status of Serpent Monte Carlo code in 2024 [J]. *EPJ Nuclear Sciences Technologies*, 11: 3 (2025).
- [33] Q. Zhang, S. Cen. *Multiphysics Modeling: Numerical Methods and Engineering Applications: Tsinghua University Press Computational Mechanics Series* [M]. Elsevier, 2015.
- [34] N. Martin, R. Stewart, S. Bays, et al. A multiphysics model of the versatile test reactor based on the MOOSE framework [J]. *Annals of Nuclear Energy*, 172: 109066 (2022).
- [35] D.Y. Jiang, P. Xu, T.L. Hu, et al. Transient multi-physics coupling analysis of the Xi' an Pulsed Reactor under pulsed condition [J]. *Annals of Nuclear Energy*, 200: 110379 (2024).
- [36] T.L. Hu, D.Y. Jiang, X.Y. Zhang, et al. Steady-state analysis of Xi' an Pulse Reactor based on the multi-physics coupling method [J]. *Annals of Nuclear Energy*, 211: 110922 (2025).
- [37] H.W. Guo, Y.N. Zhu, X.Y. Zhang, et al. Calculation and Experiment of Differential Worth of Adjuster Rod for Xi' an Pulsed Reactor [J]. *Modern Applied Physics*, 7(2): 020201 (2016).
- [38] X.Y. Zhang, X.B. Jiang, Y.Q. Zheng, et al. Three-dimensional Transient analysis of Xi' an pulsed reactor by the coupled neutronics and thermal-hydraulics code [J]. *Annals of Nuclear Energy*, 175: 109254 (2022).
- [39] X.Y. Zhang, L.P. Wang, Y.P. Wang, et al. Influence of Depletion on Reactivity Insertion Transients for Xi' an Pulsed Reactor [J]. *Nuclear Power Engineering*, 44(5): 30–38 (2023).
- [40] D. P. Griesheimer, G. Kooreman. Analytical benchmark solution for 1-D neutron transport coupled with thermal conduction and material expansion [R].

American Nuclear Society-ANS, La Grange Park, IL 60526 (United States), 2022.

[41] R. E. Peterson. Lady Godiva: An unreflected uranium-235 critical assembly, LA-1614 [R]. US: Los Alamos National Laboratory, 1953.

[42] Y.Q. Wang, S. Schunert, J. Ortensi, et al. Demonstration of MAMMOTH Fully Coupled Simulation with the Godiva Benchmark Problem [C]// International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, 2017.

[43] J.M. Wang, W.F. Liang, S. Chen, et al. Dynamic behavior in fast burst reactor with three-dimensional coupled multiphysics method [J]. Nuclear Engineering and Design, 338: 16-22 (2018).

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