# Development and Verification of a General-Purpose Nuclear-Thermal Coupling Program Based on preCICE and Its OpenFOAM-adapter

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## Abstract

To address the issues of low efficiency and insufficient accuracy in traditional programs for multi-physics coupling simulation of nuclear reactors, a general three-dimensional neutronics-thermal-hydraulic coupling program is constructed based on the open-source coupling library preCICE and its adapter OpenFOAM-adapter. The neutron physics module employs a finite volume method neutron transport program developed by our research group, while the thermal-hydraulic module integrates three-dimensional solid heat conduction (laplacianFoam) and fluid convection heat transfer models (buoyantPimpleFoam). Through secondary development, the volume coupling functionality of the conjugate heat transfer module is extended to achieve cross-mesh data exchange between the neutronics and thermal-hydraulic modules. A single-rod benchmark problem of a pressurized water reactor is selected to conduct mesh independence analysis, comparing data transfer methods including nearest-neighbor mapping, nearest-projection mapping, and radial basis function mapping. The results demonstrate that the program can accurately output three-dimensional power distribution, neutron flux density, temperature field, and velocity field, with the relative error of the coolant outlet average temperature being less than 0.1% and the relative error of the cladding maximum temperature being 0.14%. The calculated results agree well with literature values. This program breaks through the traditional customized development paradigm, supports heterogeneous mesh differential configuration and large-scale parallel computing, and can provide a reference tool for reactor safety analysis, optimization design, etc.

## Full Text

# Development and Validation of a General-Purpose Neutronics-Thermal-Hydraulics Coupling Code Based on preCICE and the OpenFOAM-Adapter

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## Abstract

**Background:** The safe operation of nuclear reactors relies on precise simulation of multi-physics couplings, including neutron transport, conjugate heat transfer, and fluid dynamics. Traditional customized coupling programs often suffer from low efficiency and insufficient accuracy, struggling to meet the demands of complex scenarios in advanced reactor designs, such as high-resolution digital twin simulations. **Purpose:** This study aims to develop a general-purpose three-dimensional neutronics-thermal-hydraulics coupling code with high precision, leveraging the open-source multi-physics coupling library preCICE and its adapter OpenFOAM-adapter. The goal is to enable accurate prediction of safety parameters and in-depth analysis of multi-physics interactions within reactor cores. **Methods:** The proposed framework integrates a neutron transport module and a thermal-hydraulic module. The neutron physics module employs a self-developed neutron transport solver based on the finite volume method, validated against benchmark problems. The thermal-hydraulics module combines a 3D solid heat conduction model (laplacianFoam) and a buoyant turbulent flow model (buoyantPimpleFoam) for detailed analysis of temperature and velocity fields. Through secondary development of the preCICE adapter, the conjugate heat transfer (CHT) module is enhanced to support volume coupling and bidirectional data exchange between neutron and thermal-hydraulics solvers. A typical pressurized water reactor (PWR) single-rod benchmark is used for validation, involving grid independence analysis and comparison of three data mapping methods: nearest-neighbor, nearest-projection, and radial basis function (RBF) interpolation. **Results:** The program accurately outputs key parameters, including 3D power distribution, neutron flux density, velocity fields, and temperature fields. Quantitative verification shows a relative error of less than 0.1% for the coolant outlet temperature and 0.14% for the maximum cladding temperature, satisfying the precision requirements of reactor design codes. Grid independence analysis confirms that a medium-fidelity thermal-hydraulic grid combined with a coarse neutron grid balances accuracy and computational efficiency. Among data mapping methods, nearest-neighbor mapping provides acceptable precision with the lowest computational cost, while RBF interpola-

tion, though more accurate, incurs higher computational overhead. **Conclusions:** The developed program breaks through the limitations of traditional customized coupling approaches, supporting heterogeneous grid configurations and large-scale parallel computing. It offers a robust tool for high-resolution neutronics-thermal-hydraulics coupling simulations, facilitating safety analysis, design optimization, and digital twin modeling of reactor cores.

**Keywords:** preCICE, OpenFOAM-adapter, reactor neutronics, thermal-hydraulics, neutronics-thermal-hydraulics coupling

## 1. Physical Models

### 1.1 Three-Dimensional Neutron Transport Spatio-Temporal Kinetics Model

The Boltzmann transport equation describes the neutron transport balance within a system, with each term representing neutron production, transport, and loss mechanisms. The three-dimensional Boltzmann equation in unit volume, unit solid angle, and unit energy interval is expressed as:

$$\cdot\nabla\psi(\mathbf{r},E,\ ,t)+\Sigma_t(\mathbf{r},E,t)\psi(\mathbf{r},E,\ ,t)=\int_0^\infty dE'\int_{4\pi}d\ '\Sigma_s(\mathbf{r},E'\to E,\ '\to\ ,t)\psi(\mathbf{r},E',\ ',t)+\frac{\chi(E)}{4\pi}\int_0^\infty dE'\nu\Sigma_f$$

where $t$ is the time variable, $\mathbf{r}$ denotes the neutron position vector, is the neutron direction vector, $\psi(\mathbf{r},E,\ ,t)$ is the angular neutron flux density per unit energy, per unit solid angle, and per unit volume; $\Sigma_t(\mathbf{r},E,t)$ is the total neutron cross-section, $\Sigma_s(\mathbf{r},E'\to E,\ '\to\ ,t)$ represents scattering from initial energy $E'$ and direction $'$ to energy $E$ and direction , and $\nu\Sigma_f(\mathbf{r},E,t)$ is the fission neutron production cross-section. The discrete ordinates method (SN) is employed for angular discretization, offering high numerical efficiency and flexible control of angular quadrature order. Spatial discretization follows the finite volume method, consistent with OpenFOAM' s numerical framework. Energy discretization adopts the multi-group approximation, dividing the neutron energy spectrum into several energy groups and performing weighted averaging of material properties (e.g., reaction cross-sections, neutron velocities) within each group to obtain multi-group parameters. Detailed computational procedures for the neutron transport solver can be found in reference [18].

### 1.2 Three-Dimensional Solid Heat Conduction Model

Heat conduction in fuel and cladding regions is described by the three-dimensional heat conduction equation:

$$\rho C_p\frac{\partial T}{\partial t}=\nabla\cdot(k\nabla T)+Q$$

where $\rho$ is material density, $C_p$ is specific heat capacity at constant pressure, $T$ is the temperature field distribution, $k$ is thermal conductivity, and $Q$ is the volumetric heat source term.

The heat source term in the fuel region is obtained from neutron transport calculations:

$$Q(\mathbf{r}) = \sum_{g=1}^{G} \kappa_g \Sigma_{f,g}(\mathbf{r}) \phi_g(\mathbf{r})$$

where $\kappa_g$ is the energy release per fission in group $g$, $\Sigma_{f,g}$ is the fission cross-section, and $\phi_g$ is the neutron flux density for group $g$.

### 1.3 Three-Dimensional Fluid Convective Heat Transfer Model

Energy released from nuclear fission reactions heats the fuel, and this heat is transferred to the coolant through conduction and convection. The coolant flow and heat transfer processes are governed by the following equations:

**Continuity:**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$$

**Momentum:**

$$\frac{\partial (\rho \mathbf{U})}{\partial t} + \nabla \cdot (\rho \mathbf{U}\mathbf{U}) = -\nabla p + \nabla \cdot \tau + \rho \mathbf{g}$$

**Energy:**

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{U} h) = \nabla \cdot (k_{eff} \nabla T) + \frac{\partial p}{\partial t} + \mathbf{U} \cdot \nabla p + \tau : \nabla \mathbf{U}$$

where $\rho$ is fluid density, $\mathbf{U}$ is velocity vector, $p$ is static pressure, $\tau$ is stress tensor, $k_{eff}$ is effective thermal conductivity, and $h$ is specific enthalpy. This model assumes forced convection dominance and neglects radiation heat transfer, making it suitable for strong convection scenarios such as cladding-coolant interfaces.

## 2. preCICE Open-Source Coupling Library and Its Secondary Development

### 2.1 preCICE Core Framework and Adapter Principle

[Figure 1: see original paper]

preCICE (Precise Code Interaction Coupling Environment) is an open-source multi-physics coupling library jointly developed by the Technical University of Munich and the University of Stuttgart. Its core design philosophy is modular

decoupling, aiming to establish a generalized multi-physics coupling paradigm for complex engineering scenarios. As shown in Figure 1, the technical framework operates through a two-stage collaborative mechanism: preprocessing and solution coupling. During preprocessing, multiple data mapping algorithms [19] (e.g., nearest-neighbor, nearest-projection, radial basis function) complete geometric matching and data synchronization at coupling boundaries, establishing interface consistency between heterogeneous solvers. The solution coupling stage employs iterative convergence strategies to dynamically update cross-field data.

For coupling scheme design, preCICE provides various combinations of serial/parallel and explicit/implicit coupling. In parallel coupling, unified time windows enable independent solving of each physics solver. Within each time window, solvers perform sub-cycling based on their own time steps, with data exchange completed through interpolation at each time point. For numerical stability, explicit coupling should always be used for unidirectional data transfer, while implicit coupling with convergence acceleration schemes [20] (constant under-relaxation, Aitken adaptive under-relaxation, and quasi-Newton variants such as IQN-ILS and IQN-IMVJ) is recommended for strongly coupled bidirectional problems like conjugate heat transfer. When coupling more than two solvers, two options exist: configuring coupling schemes for each solver pair individually, or treating them as an integrated system. For multi-solver strong coupling scenarios in thermal-hydraulic modules, fully implicit multi-coupling schemes [19] can be employed to achieve dynamic equilibrium through iterative solving, significantly enhancing efficiency for large-scale multi-physics problems while maintaining accuracy.

As shown in Figure 2 [Figure 2: see original paper], preCICE provides official adapters for mainstream solvers (e.g., OpenFOAM, CalculiX) [21] and supports API bindings for C, Fortran, and Python. Adapters "glue" each solver to the preCICE library, functioning either as modules/classes within solver code or as standalone software using solver callback interfaces. preCICE enables collaborative simulation of heterogeneous solvers through efficient data exchange and iterative algorithms. This design supports coupling among multiple solvers while significantly reducing code intrusiveness and development complexity, allowing developers to focus on single-physics solver optimization without restructuring underlying communication logic.

### 2.2 Functional Extension of the Conjugate Heat Transfer Module

In coupled simulations, solvers exchange data through coupling meshes, which can be either common coupling interfaces (surface coupling) or common coupling volumes (volume coupling). This study extends the conjugate heat transfer (CHT) module in the official OpenFOAM adapter by first adding read/write support for heat source terms. Second, the interface is expanded from surface coupling at mesh boundaries to volume coupling for specified volumetric data (temperature and heat source), providing computational support for coupling

thermal-hydraulic and neutron physics modules.

Typically, preCICE handles data transfer between interfaces of two solvers, with coupling interfaces specified via the `patches` field in the `preciceDict` configuration file. The extended adapter supports both surface coupling at domain boundaries and volume coupling for complete domains or subdomains. This work implements dynamic configuration of coupling domains using OpenFOAM's `topoSet` tool. For whole-domain coupling, boundary `patches` need not be specified; instead, enabling `volumeCenters` mode in the `locations` field of `preciceDict` incorporates the entire domain into volume coupling (temperature and heat source data transfer operate in this mode by default). For local coupling scenarios, `cellSet` classes define specific subdomains, supporting division by geometric location or material properties. Given the uniform material property distribution in this model (no complex scenarios like fuel enrichment gradients), geometric topology serves as the basis for `cellSet` partitioning (e.g., cladding region, coolant channel). The configuration process involves two key steps: first, enabling `volumeCenters` mode in the `locations` field of `preciceDict` and explicitly declaring the target `cellSet` name; second, using `topoSet` to generate cell sets for specified geometric regions to achieve coupling binding. Typical configuration examples are shown in Figure 3 [Figure 3: see original paper].

## 3. Coupling Architecture Design

### 3.1 Unified Computational Platform Architecture

This study proposes a heterogeneous mesh coupling architecture based on a unified computational platform. The architecture integrates neutron transport, 3D solid heat conduction, and 3D fluid convection solvers within the OpenFOAM framework to construct a multi-physics collaborative platform. This single-platform approach effectively avoids redundant computations from cross-platform data conversion and achieves high-precision data transfer between heterogeneous meshes through the preCICE library, while leveraging parallel architectures of both preCICE and OpenFOAM to enhance overall computational efficiency. Compared to traditional single-mesh coupling methods, a typical heterogeneous mesh mapping strategy is adopted where each physics solver employs independent mesh systems with resolution differentiated according to physical characteristics. Data transfer follows physical conservation principles, with cross-mesh data achieved through preCICE's various mapping methods.

### 3.2 Multi-Solver Coupling Mechanism

The bidirectional feedback mechanism of neutronics-thermal-hydraulics coupling constitutes the core of reactor multi-physics analysis. Before calculation, the Monte Carlo code OpenMC [22] generates few-group macroscopic cross-sections at different temperatures and densities, expressed as polynomial functions fitted to temperature and density. The thermal-hydraulics module

outputs temperature fields $T$ and density fields $\rho$ for fuel, cladding, and coolant through conjugate heat transfer calculations. Based on these fields, multi-group macroscopic cross-sections $\Sigma(\mathbf{r}, T, \rho)$ (e.g., fission cross-section $\Sigma_f$, scattering cross-section $\Sigma_s$) in the neutronics model are updated to reflect dynamic material property changes. The neutronics module solves for neutron flux $\phi(\mathbf{r}, E)$ using updated cross-sections and calculates fission heat source term $Q$, which feeds back as input boundary conditions to the thermal-hydraulics module, driving the next iteration of heat transfer and flow calculations. Coupling strength (e.g., data exchange frequency, convergence tolerance) directly affects key parameters such as core power peaking factors and coolant temperature gradients, and determines the spatio-temporal evolution of reactivity feedback (Doppler effect, moderator temperature effect). Explicit coupling strategies may cause numerical oscillations, while implicit coupling enhances stability through iterative correction but requires trade-offs in computational cost.

The neutronics-thermal-hydraulics coupling control equation system consists of equations (1)-(8) with corresponding initial and boundary conditions. The solution flow is shown in Figure 4 [Figure 4: see original paper], where ST denotes sink temperature and HTC denotes heat transfer coefficient.

## 4. Code Validation and Results Analysis

The neutron transport solver employed in this study has been developed and validated in previous work [18], with its computational accuracy and reliability confirmed. The thermal-hydraulic module integrates mature official OpenFOAM solvers, including verified heat conduction and flow heat transfer modules. Given the independent reliability of each single-physics solver, this validation focuses on verifying the logical correctness of the adapter-based coupling framework and assessing multi-physics data transfer reliability.

### 4.1 Benchmark Geometry, Material Properties, and Boundary Conditions

A typical PWR single-rod model is selected as the validation case, referenced from literature [23]. The authors coupled MCNP5 Monte Carlo particle transport code with STAR-CCM+ CFD software to develop a high-fidelity coupling tool called MULTINUKE for PWR steady-state analysis. The fuel rod diameter is 1.0 cm, Zircaloy-4 cladding thickness is 0.1 cm, and water channel half-width is 1.5 cm. To optimize computational efficiency, the axial height is compressed to 20 cm to control mesh scale. Detailed geometry is shown in Figure 5 [Figure 5: see original paper].

Fuel uses 5% enriched $UO_2$, and the moderator is liquid water. Specific geometric parameters and material configurations are listed in Table 1 , and thermal property parameters for each material are provided in Table 2 .

The boundary condition system covers both neutronics and thermal-hydraulics dimensions, with Robin mixed boundary conditions [24] applied at coupling in-

terfaces. Detailed configurations are shown in Table 3 . Neutronics calculations employ a two-group energy structure (0.625 eV threshold).

### 4.2 Mesh Independence Analysis and Parameter Sensitivity Study

To evaluate the impact of mesh discretization on results, a multi-resolution mesh study is conducted. Both coolant and neutronics modules employ coarse, medium, and fine mesh levels (Table 4 ), with the fuel cell axially divided into 20 layers.

Figure 6 [Figure 6: see original paper] shows mesh sensitivity analysis results. Coolant temperature remains relatively stable across different mesh combinations, with a maximum deviation of 0.0024%. Solution time increases stepwise with coolant mesh refinement, while maximum cladding temperature stabilizes with medium mesh (maximum deviation 0.173%). Each neutronics mesh refinement approximately doubles solution time but has relatively minor impact on results (maximum deviation 0.347%). Considering both computational efficiency and accuracy, medium coolant mesh combined with coarse neutronics mesh is selected as the optimal configuration.

The computational platform uses an Intel Core i9-14900KF processor (32 physical cores), employing a task-division strategy for optimal resource allocation: fuel/cladding heat conduction uses single-core serial processing, coolant convection uses 20-core parallel computation, and the neutron transport module uses 4-core parallel computation. Under this heterogeneous architecture, single-core serial execution requires 955 seconds, while the multi-core parallel scheme reduces total computation time to 509 seconds, improving efficiency by nearly 50% with a speedup ratio of 1.88. This quantitatively demonstrates that targeted parallel resource scheduling with heterogeneous mesh configurations significantly enhances computational efficiency while maintaining accuracy, validating the program' s parallel computing capability.

### 4.3 Key Physical Parameter Validation

Literature [23] provides coupling results from MCNP5 and STAR-CCM+, including axial power distribution, axial centerline fuel temperature, maximum cladding temperature, coolant outlet temperature, and coolant velocity distribution. As shown in Figure 7 [Figure 7: see original paper], the axial power and temperature distributions calculated by our coupling code agree well with reference values. Normalized power is slightly lower than literature values in the middle section of the fuel cell and shows larger deviations near the inlet and outlet. This discrepancy partly stems from turbulence model differences: literature STAR-CCM+ used a two-layer k-epsilon model (which directly resolves the viscous sublayer and offers advantages in predicting wall heat transfer), while this study employs standard k-epsilon and k-Omega SST models for sensitivity analysis. The fundamental difference in near-wall treatment, particularly in wall heat flux prediction accuracy, constitutes an important source of deviation in

fuel rod temperature (especially in the latter half). K-Omega SST, through its cross-model design combining near-wall fine simulation (k-Omega) with far-field efficiency (k-Epsilon), more accurately characterizes turbulent momentum/heat transport in near-wall regions, strong gradient zones, and separated flows, yielding temperature distributions closer to reference values. K-epsilon, applicable only to fully developed turbulence, suffers from isotropic assumptions and wall function deficiencies in low-Reynolds near-wall and separated regions, resulting in approximately 10 K mean absolute temperature deviation as shown in Figure 7(b). Additionally, literature employed coarser meshes compared to our finer discretization, contributing to error sources. However, as shown in Figure 7(a), power distribution shows low sensitivity to turbulence model selection.

Table 5 presents quantitative comparison of important parameters. Coolant outlet average temperature shows only 0.03% error compared to reference values, while maximum cladding temperature is 0.14% lower than the reference. These results demonstrate that our coupling program achieves accuracy comparable to literature values, confirming the correctness of the coupling process and reliability of computational results.

### 4.4 Performance Comparison of Data Mapping Methods

This section compares three preCICE mapping methods: nearest-neighbor, nearest-projection, and radial basis function (RBF). preCICE requires each mapping to provide constraint conditions ensuring physically consistent and numerically stable data exchange between solvers, including conservative constraint (global conservation of physical quantities like mass, energy, momentum across coupling interfaces) and consistent constraint (geometric and field continuity at coupling interfaces).

Nearest-neighbor mapping calculates Euclidean distances at output mesh nodes and copies values from the nearest geometric vertex. This method is computationally fast and simple but has numerical defects: under consistent constraints, some input values may be unused while others are reused; under conservative constraints, output vertices may receive no values or multiple values that are accumulated.

Nearest-projection mapping extends nearest-neighbor by performing orthogonal projection of output nodes onto the nearest input mesh element, using barycentric coordinates as interpolation weights. While relatively fast and numerically superior to nearest-neighbor according to preCICE documentation, it requires explicit mesh connectivity information.

RBF mapping assembles and solves a global (potentially sparse) linear system constructed on one mesh and evaluated on another, using linear combinations of radially symmetric basis functions centered at each vertex plus a linear polynomial. It is generally more accurate with higher-order convergence rates but computationally more demanding. Reference [20] provides detailed RBF theory. This study employs global direct RBF mapping (RBF-global-direct) with

thin-plate spline basis functions $\phi(r) = r^2 \ln(r)$ (where $r$ is Euclidean distance between nodes), which eliminates shape parameter and support radius tuning uncertainties. Numerically, an $N \times N$ dense matrix (where $N$ is source mesh node count) is constructed during initialization. Due to thin-plate splines' non-strict positive definiteness, QR decomposition is automatically triggered instead of Cholesky decomposition, implemented via Eigen' s Householder transformations to orthogonalize the column space and avoid zero eigenvalue perturbations.

Figure 8 [Figure 8: see original paper] shows the impact of different mapping methods on results. Compared to nearest-neighbor mapping, nearest-projection and RBF mapping show significantly increased time costs, with RBF mapping requiring approximately twice the time of nearest-neighbor mapping. In this calculation, nearest-projection did not demonstrate its documented speed advantage over nearest-neighbor. For temperature calculations, all three methods show minimal impact on coolant outlet average temperature. However, for maximum cladding temperature prediction, nearest-neighbor and RBF mapping produce highly consistent results, while nearest-projection shows approximately 3% deviation, likely due to geometric connectivity information processing errors.

## 5. Conclusions and Outlook

Addressing the scarcity of high-fidelity multi-physics analysis tools for numerical reactors, development difficulties, and the demand for versatile, broad-spectrum, multi-combination coupling capabilities, this study develops and validates a general-purpose neutronics-thermal-hydraulics coupling program based on preCICE and OpenFOAM-adapter.

1. **Adapter Extension:** The official OpenFOAM-adapter provided by preCICE was extended by adding heat source term read/write functionality to the CHT module and implementing volume-coupling data exchange interfaces. This breaks through traditional surface coupling limitations, enabling temperature field and neutron flux mapping on non-matching meshes within volume coupling domains, ultimately forming a hybrid surface-volume coupling architecture for general multi-physics neutronics-thermal-hydraulics coupling support.

2. **Coupling System Implementation:** Using the extended adapter, a fuel-cladding-coolant triple coupling system was established, implementing surface-coupling-based conjugate heat transfer calculations. Further coupling with the previously developed neutron transport solver achieved heterogeneous mesh neutronics-thermal-hydraulics coupling based on volume coupling. The partitioned solving strategy supports differentiated coarse/fine mesh configurations between solvers.

3. **Validation and Performance:** Mesh independence analysis identified the optimal discretization scheme (coarse neutronics mesh + medium thermal-hydraulics mesh). Key parameter validation demonstrated 0.03% relative error in coolant outlet temperature and 0.14% deviation in peak

cladding temperature. Systematic evaluation of preCICE' s three mapping algorithms quantitatively revealed that nearest-neighbor mapping offers optimal accuracy-efficiency trade-offs for the current application.

Future research will focus on multi-physics functional expansion and uncertainty analysis. Current work primarily addresses neutronics-thermal-hydraulics coupling; incorporating structural mechanics modules such as fuel rod deformation to build a "neutronics-thermal-mechanics" multi-physics system would better capture complex physical processes in actual reactor operation. Linking with uncertainty analysis code DAKOTA for uncertainty quantification and sensitivity analysis of parameters like coolant outlet temperature, inlet flow rate, and cladding temperature would more comprehensively reflect program reliability and credibility.

**Author Contributions:** Tan Liangkang: program development, validation, data analysis, and manuscript writing; Deng Junjie: data collection; Li Wei: guidance throughout program development, validation, and data analysis; Zhao Pengcheng: funding acquisition, manuscript review and revision; Liu Zijing: manuscript revision and theoretical guidance.

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*Note: Figure translations are in progress. See original paper for figures.*