# Multiphysics Simulations for Heat Pipe Cooled Micro Reactors Using PRAGMA-OpenFOAM-ANLHTP

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### 1. Introduction

A heat pipe cooled micro reactor (HPR) is a small nuclear reactor that passively transports heat from the reactor core using heat pipes. The design concepts of HPRs target generating power ranging from a few kilowatts to megawatts scale. These micro reactors have advantages in a compact design, transportability, and self-adjustment enough for fully autonomous operation, which is suitable for remote areas, military bases, etc.

In this regard, the Kilopower project was started in 2015 to demonstrate a fission nuclear power system in a space-simulated environment, and successful test results were released for the Kilopower Reactor Using Stirling TechnologY (KRUSTY) experiment [1]. With this remarkable achievement, several HPR design concepts were suggested, but the progress is still in the development stage [2][3][4].

Considering the design status of HPRs, multiphysics simulation capability can provide the performance guideline for developing design concepts. Thus, several research groups constructed advanced simulation frameworks based on various physics applications [4][5]. More recently, Seoul National University (SNU) developed a multiphysics analysis system that couples Monte Carlo (MC) neutron transport, thermo-mechanics, and heat pipe thermal analysis. The preliminary research was conducted within practical time and resources [6].

This paper describes the multiphysics simulation capability of the code coupling system at SNU for heat pipe cooled micro reactors. The simulation framework including coupled codes and coupling methodology will be introduced. And the comprehensive results for steady-state operation of HPRs will be presented to demonstrate the capability of the more improved system.

### 2. Simulation Framework

## 2.1. PRAGMA

PRAGMA is a GPU-based continuous-energy MC code developed by SNU, which was dedicated to power reactors at first [7]. To retain general applicability for advanced reactors, a tracking module employing GPU-accelerated ray tracing engine OptiX [8] is developed, and a geometry module is extended to the unstructured mesh geometry. For efficient neutron transport in unstructured mesh geometry, zone-wise delta-tracking

was introduced, which is a variation of the Woodcock delta-tracking algorithm. Further detailed features of PRAGMA are presented in [6] or will be published.

#### 2.2. OpenFOAM

OpenFOAM is an open-source-based CFD tool for thermomechanical analysis [9]. It uses the finite volume method and provides a basic solid mechanics solver. This solver conducts a thermomechanical analysis of small deformation conditions with the linear elasticity assumption. For the analysis the of HPR core, the solver was extended to handle multiple materials and temperature dependencies of each material property.

### 2.3. ANLHTP

ANLHTP is a one-dimensional steady-state thermal analysis code for a sodium heat pipe developed by Argonne National Laboratory [10]. ANLHTP can predict heat transfer rate, temperatures at each region, and several operation limits using a thermal resistance network. The FORTRAN-based source codes are open in the literature, and the codes are reconstructed to couple with OpenFOAM [11]. Recently, for efficient data communication the in coupling process, the codes are ported using C++ language.

### 2.4. Coupling Methodology

The multiphysics coupling algorithm is built on the MPI dynamic process management (DPM) model. The MPI DPM model enables a parent process to spawn child processes and provides a communication model between parent and children. It has the advantage that child processes can use different MPI launch parameters. Fig. 1 illustrates a schematic diagram of the PRAGMA-OpenFOAM-ANLHTP coupling system with Manager-Worker parallelism. This parallelism indicates that worker programs become the actual physics codes, and an independent manager program controls the iteration and data transfer of the workers. PRAGMA and OpenFOAM communicate power, temperature, and density through in-memory access. OpenFOAM and ANLHTP communicate heat flux and heat pipe interface temperature through file-based I/O. A heat pipe worker is newly developed using C++ language, which eliminates pipeline I/O communication

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# 3. Comprehensive Results

This section demonstrates the multiphysics solutions for steady-state conditions and computing performance using PRAGMA-OpenFOAM-ANLHTP. The problems solved throughout this section are Empire 3D assembly benchmark [2] and MegaPower 3D 60° symmetrical sector and full core [3]. All the problems are solved with the computing cluster specified in **Table 1**. The core design parameters of both problems are listed in **Table 2**, and the mesh discretization of the problems is illustrated in **Fig. 2** and **Fig. 3**, which consist of 571 thousand and 6 million mesh elements, respectively. The computing resource allocations are described in **Table 3** and the calculation conditions of PRAGMA are listed in **Table 4**.

Table 1. Computing cluster specifications.

CPU / Node	$2 \times$ Intel Xeon Gold 6230 R
GPU / Node	$8 \times NVIDIA RTX A5000$
Memory / Node	512 GB DDR4
Interconnect	Mellanox Infiniband
	EDR 100 Gbps

Tuble 2. Core design parameters.			
Parameter	Empire 3D	MegaPower 3D	
	Assembly	Core	
E IM. (	UN	UO2	
Fuel Material	(19.75 w/o <sup>235</sup> U)	(19.75 w/o <sup>235</sup> U)	
Heat Pipe	Sodium (We	Sodium (Working fluid)	
Material	SS316 (Heat pipe wall)		
Moderator	VU2	-	
Material	1 112		
Monolith	SS316	SS316	
Material			
Gap Material	Не		
Number of	(0)	2,112	
fuel rods	00		
Number of	61	1,224	
heat pipes	01		
Number of	96	-	
moderator rods			

 Table 2. Core design parameters.



Fig. 2. Mesh discretization of Empire 3D Assembly.



Fig. 3. Mesh discretization of MegaPower 3D core.

	Table 3. Computir	g resource allocations.
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PRAGMA	1 Node (Empire)
	3 Nodes (MegaPower)
OpenFOAM	1 Node (52 CPU Cores)
Manager and ANL HTP	1 Node (2 CPU Cores)

Number of Cycles25 (Inactive), 50 (Active)Number of Neutrons / Cycle20,000,000 (Empire) 200,000,000 (MegaPower)Ramp-upOn (Exponential, Factor: 20)Delta-tracking FeedbackOnCore Power111.11 kWth (Empire) 5 MWth (MegaPower)Libraries (K)700 / 800 / 900 / / 1300 / 1400Total Number of Histories1.15E+09 (Empire) 1.15E+10 (MegaPower)		
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Total Number of1.15E+09 (Empire)Histories1.15E+10 (MegaPower)	Libraries (K)	700 / 800 / 900 / / 1300 / 1400
Histories 1.15E+10 (MegaPower)	Total Number of	1.15E+09 (Empire)
	Histories	1.15E+10 (MegaPower)

Table 4. Calculation conditions of PRAGMA

#### 3.1. Multiphysics Solutions

**Fig. 4** illustrates element-wise solutions calculated by PRAGMA: normalized power distribution and flux distributions of fast, intermediate, and thermal flux at the center plane for the Empire problem. In addition, OpenFOAM and ANLHTP solutions are illustrated in **Fig. 5**: temperature (K) distribution and density (kg/m<sup>3</sup>) distributions of moderator, monolith, and fuel at the center plane for the Empire problem. The fast flux peaks at fuel rods, while the intermediate and thermal ones reach their peaks at moderator rods. The reflective boundary condition in the radial direction leads to higher peripheral power and temperature in the innermost regions.

Fig. 6 and Fig. 7 illustrate 3D element-wise power and temperature distribution for MegaPower 3D full core problem. The peripheral power is high due to the solid reflector, but the same tendency is not observed in the peripheral temperature. This is because there are fewer heat sources around the heat pipes in the peripheral region compared to the center region. Fig. 8 illustrates monolith density distribution. There is little axial variation due to the high thermal conductivity of stainless steel.



Fig. 4. Coupling solutions of Empire: power and fluxes.



Fig. 5. Coupling solutions of Empire: temperature and densities



Fig. 6. Normalized power distribution of MegaPower.



Fig. 7. Temperature (K) distribution of MegaPower.



**Fig. 8.** Monolith density (kg/m<sup>3</sup>) distribution of MegaPower.

### 3.2. Performance Evaluation

The total computing time of the Empire problem is about 20 minutes, most of which is taken by the thermomechanical calculation. The computing time breakdown of the assembly problem is omitted here to focus on the more large-scale problem. **Fig. 9** indicates the computing time breakdown of the MegaPower 3D 1/6 sector and full core problems. PRAGMA does not depend on the problem size, whereas the number of elements affects the performance of OpenFOAM and communication between OpenFOAM and ANLHTP. Nevertheless, both simulations could be completed in about an hour. These results demonstrate that PRAGMA attains scalability through the hardware-accelerated ray tracing library and the delta-tracking approach.



**Fig. 9** Computing time breakdown for MegaPower 1/6 sector and full core.

## 4. Conclusions

Multiphysics simulation capability was demonstrated by coupled solutions for steady-state conditions using the PRAGMA-OpenFOAM-ANLHTP coupling system. The simulation framework was described with composing codes and coupling methodology. The representative HPR problems were analyzed, which shows that the PRAGMA-OpenFOAM-ANLHTP coupling system can consider complicated physical phenomena. Moreover, these multiphysics solutions can be obtained in about an hour, even though employing the MC transport calculation with a tremendous amount of particles. More research for transient conditions will be followed to capture the self-regulating behavior of HPRs within practical resources and time.

#### ACKNOWLEDGMENTS

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#### REFERENCES

[1] M. A. GIBSON *et al.*, "Kilopower Reactor Using Stirling TechnologY (KRUSTY) Nuclear Ground Test Results and Lessons Learned," NASA/TM-2018-219941, U.S. National Aeronautics and Space Administration (2018).

[2] M. D. DEHART *et al.*, "NEAMS FY20 Assessment Problem Draft," INL/MIS-21-62472, Idaho National Laboratory (2020).

[3] P. R. MCCLURE *et al.*, "Design of Megawatt Power Level Heat Pipe Reactors," LA-UR-15-28840, Los Alamos National Laboratory (2015).

[4] N. STAUFF *et al.*, "Detailed Analyses of a TRISO-fueled Microreactor," ANL/NEAMS-21/3, Argonne National Laboratory (2021).

[5] C. H. LEE, Y. S. JUNG, and H. K. CHO, "Micro Reactor Simulation Using the PROTEUS Suite in FY19," ANL/NSE-19/33, Argonne National Laboratory (2019).

[6] J. IM *et al.*, "Multiphysics Analysis System for Heat Pipe Cooled Micro Reactors Employing PRAGMA-OpenFOAM-ANLHTP," Nuclear Science and Engineering, (2023); https://doi.org/10.1080/00295639.2022.2143209.

[7] N. CHOI, K. M. KIN, and H. G. JOO, "Optimization of Neutron Tracking Algorithms for GPU-based Continuous Energy Monte Carlo Calculation," Ann. Nucl. Energy, 162, 108508 (2021).

[8] S. G. PARKER *et al.*, "OptiX: A General Purpose Ray Tracing Engine," ACM Trans. Graphics, 29, 4, 1 (2010).

[9] H. JASAK, "OpenFOAM: Open Source CFD in Research and Industry," Int. J. Nav. Archit. Ocean Eng., 1, 2, 89 (2009). [10] G. A. MCLENNAN, "ANL/HTP: A Computer Code for the Simulation of Heat Pipe Operation," ANL-83-108, Argonne National Laboratory (1983).

[11] M. J. JEONG, S. LEE, and H. K. CHO, "Verification and Validation of the OpenFOAM Stress Analysis Solver for Heat Pipe Cooled Micro Reactor Simulation," Proc. 19th Int. Top; Mtg. on Nuclear Reactor Thermal Hydraulics (NURETH-19), March 6, (2022).