한국원자력학회 2022 추계학술대회 워크샵
창원컨벤션센터, 6층 600A호

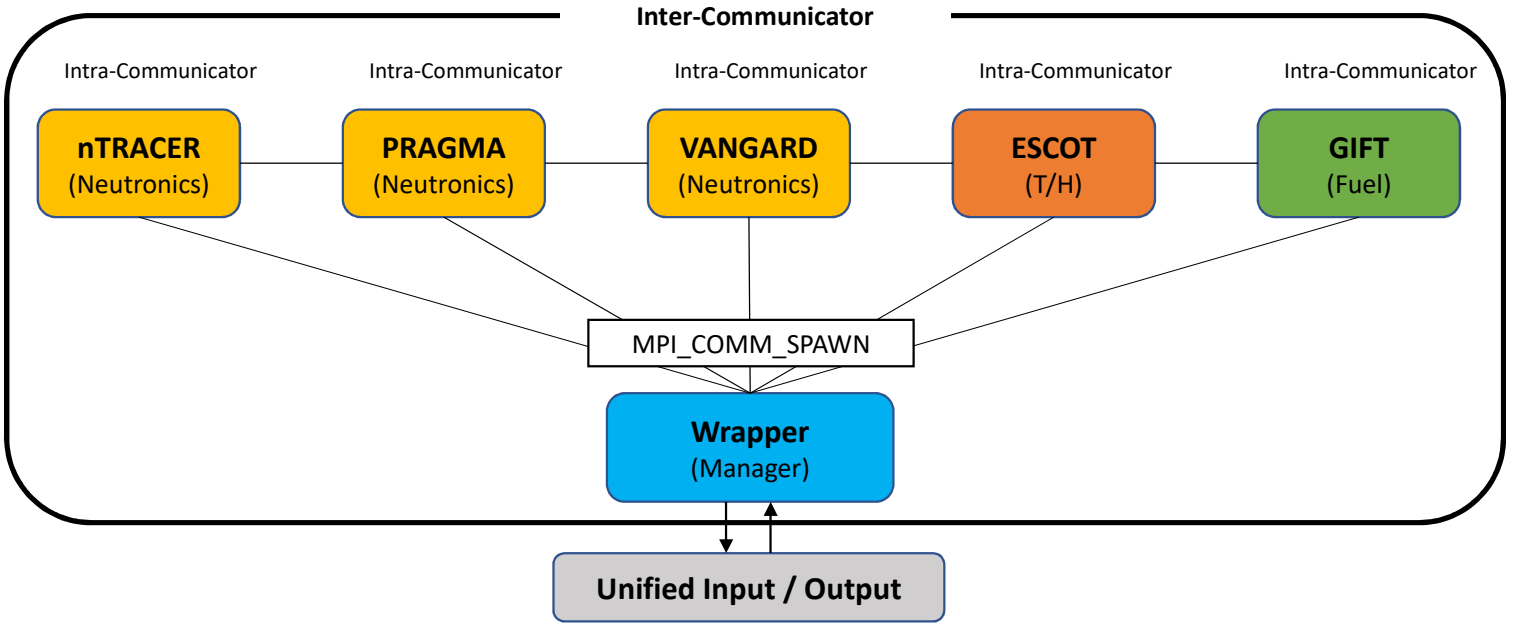
서울대학교 고신뢰도 원자로 다물리 통합 전산해석 플랫폼 개발 현황

권성준
서울대학교

2022년 10월 19일

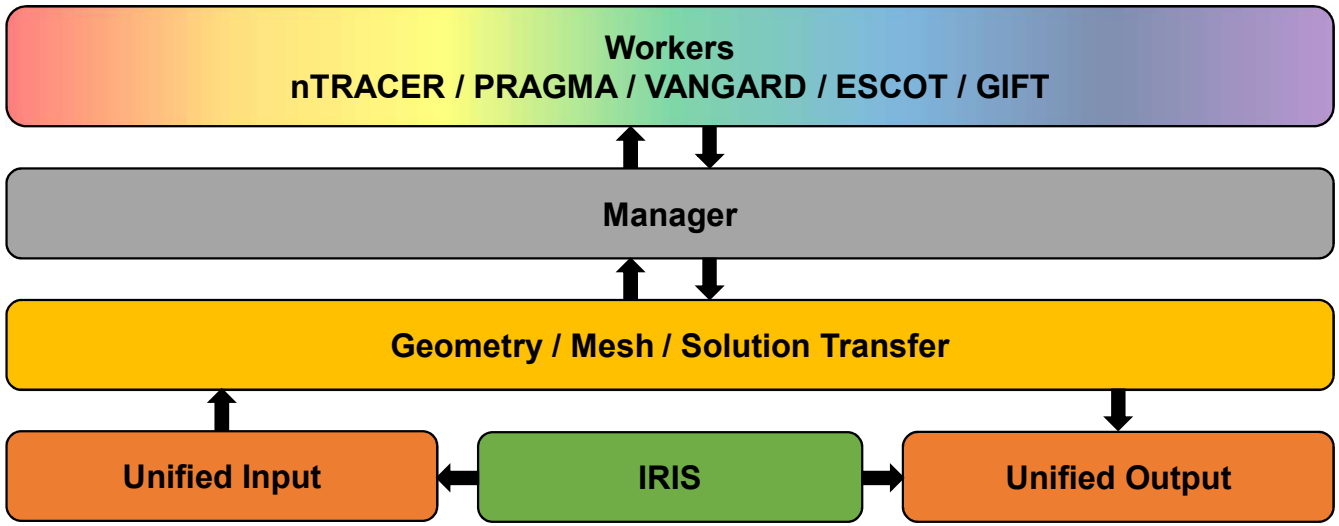
ENGINEERING
COLLEGE OF ENGINEERING
SEOUL NATIONAL UNIVERSITY
서 울 대 학 교 공 과 대 학

- **고신뢰도 다물리 원자로 해석용 초고성능 통합 전산플랫폼 구축**
  Establishment of an Integrated High Performance Computing Platform for High-fidelity Multi-physics Reactor Analyses
  - Project Period : 2021.06 ~ 2023.12
  - **Development of an extensible multi-physics solution framework optimized for PWR analysis** incorporating nTRACER, PRAGMA, VANGARD, ESCOT, and GIFT (with Prof. Youho Lee).
  - **Coupling of PRAGMA, OpenFOAM, and ANLHTP for heat pipe reactor analysis** (with Prof. Hyoung Kyu Cho).



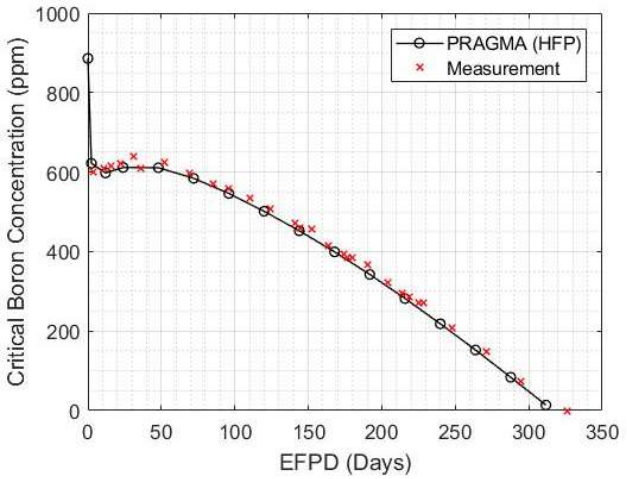
- **IRIS (Innovative Reactor Integrated Simulator)**
  - **An extensible, Python-based code integration framework for multi-physics reactor simulation for PWR analysis.**
    - Focus on steady state non-linear multiphysics calculations.
  - **Aims to provide flexible all-to-all coupling with a unified IO system.**
  - **Employs the MPI Dynamic Process Management (DPM) for code coupling.**

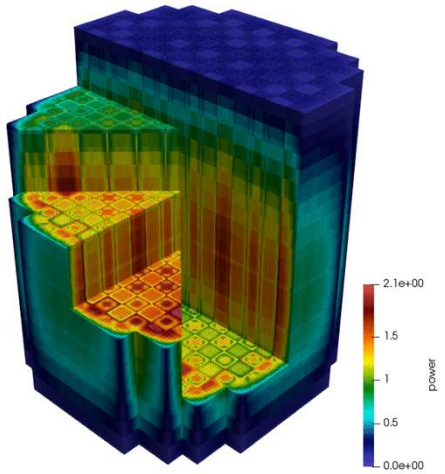
Structure of the IRIS Framework



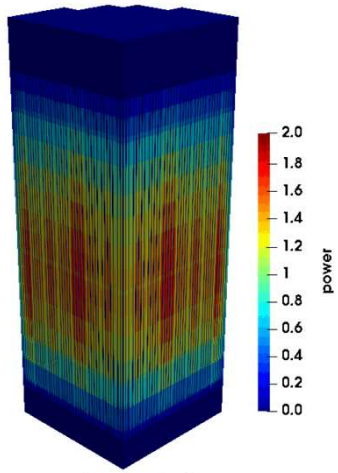
- **Neutronics Calculation Code : nTRACER, PRAGMA and VANGARD**
  - **The three different neutronics calculation codes have been developed in SNURPL.**
    - nTRACER is a 2D/1D MOC method based on the whole core calculation code.
    - PRAGMA is a GPU-based continuous-energy Monte-Carlo code funded by KHNP.
    - VANGARD is a pinwise nodal core analysis code characterized by GPU acceleration.
  - **Every neutronics calculation code adopts a GPU acceleration for an efficient calculation.**

Whole Core Depletion Calculation with Massive Particles by PRAGMA (MIT BEAVRS Benchmark Cycle 1)

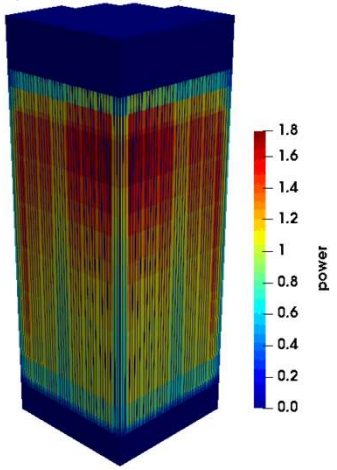




Whole Core Depletion Calculation by VANGARD (MIT BEAVRS Benchmark Cycle 1 & Cycle 2)



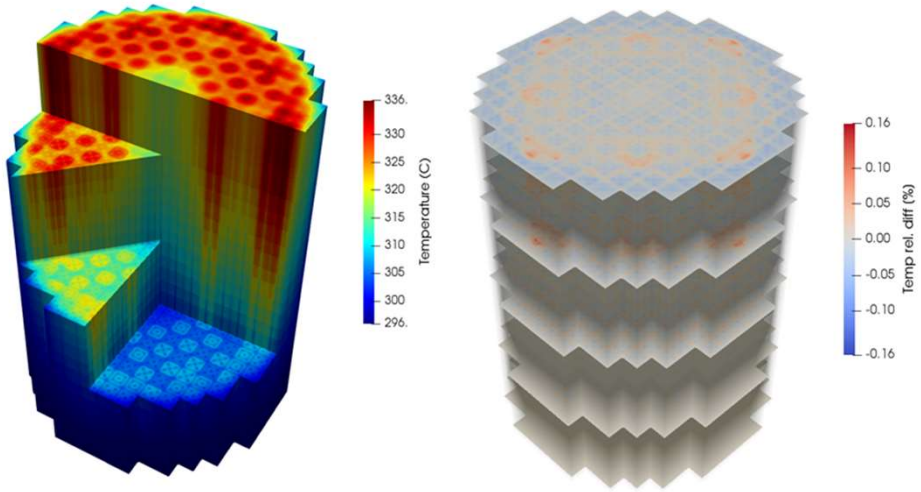
Cycle 1 Power



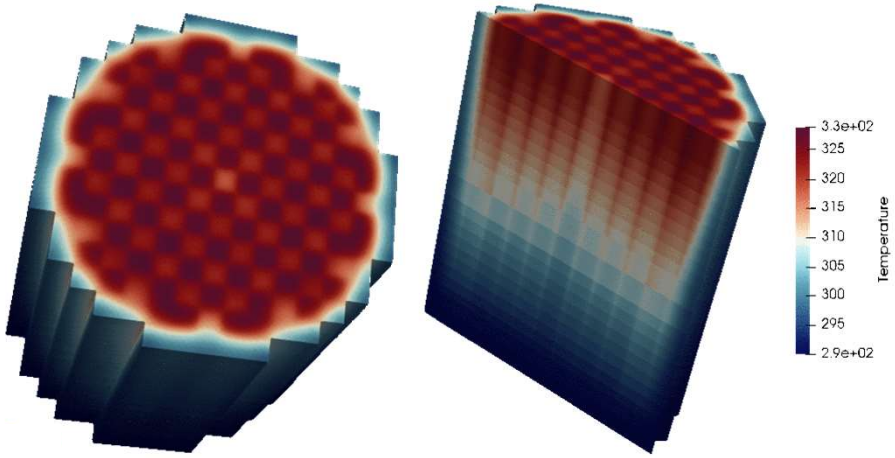
Cycle 2 Power

- **Thermal-Hydraulics (T/H) Calculation Code : ESCOT**
  - ESCOT is a pin-level nuclear reactor core T/H code that employs the drift-flux model.
  - ESCOT adopted GPU acceleration and MPI planar and assembly-wise domain decomposition.

Profile of Temperature and Relative Difference with CTF (OPR 1000 Full Core Problem)



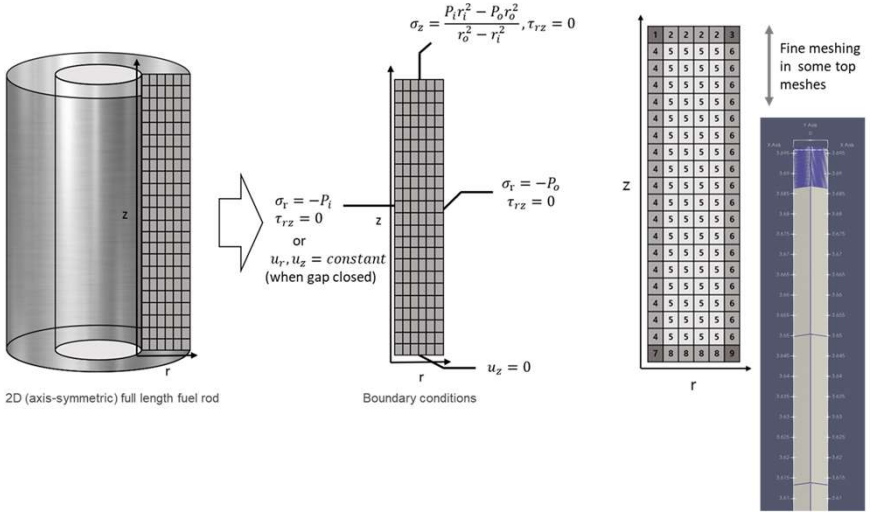
MSLB Analysis by ESCOT (OECD/NEA PWR MSLB Benchmark Phase II)



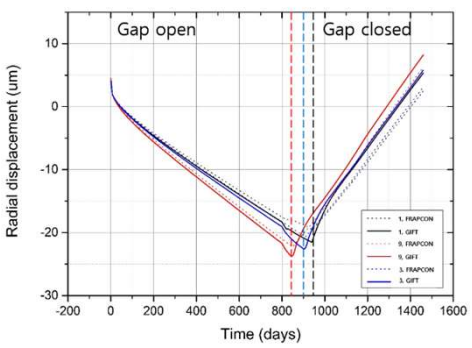
Fuel Performance Calculation Code : GIFT

- **Generalizable Integrated Fuel life Tracker (GIFT) is an integral fuel performance simulation code developed by the SNU fuel lab (Prof. Youho Lee).**
  - It was confirmed that the results of GIFT and FRAPCON were consistent.
- **An axial cladding interaction can be simulated by GIFT since its structural model is based on a 2D model.**
- **The mechanical model of GIFT can simulate a multi-layer cladding structure.**

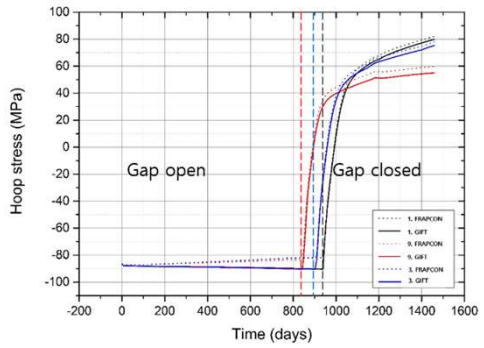
2D Axis-symmetric Full-length Cladding Mechanical Model



Cladding Performance Comparison with FRAPCON



<Open Gap>

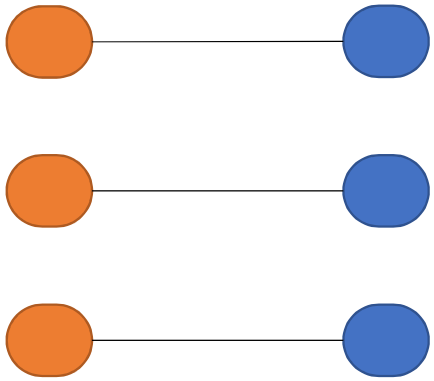


<Closed Gap>

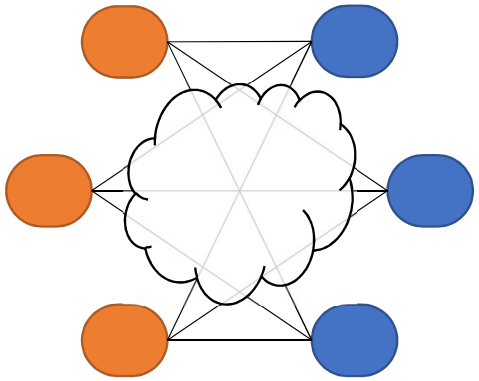
Extensible Code Coupling System of IRIS

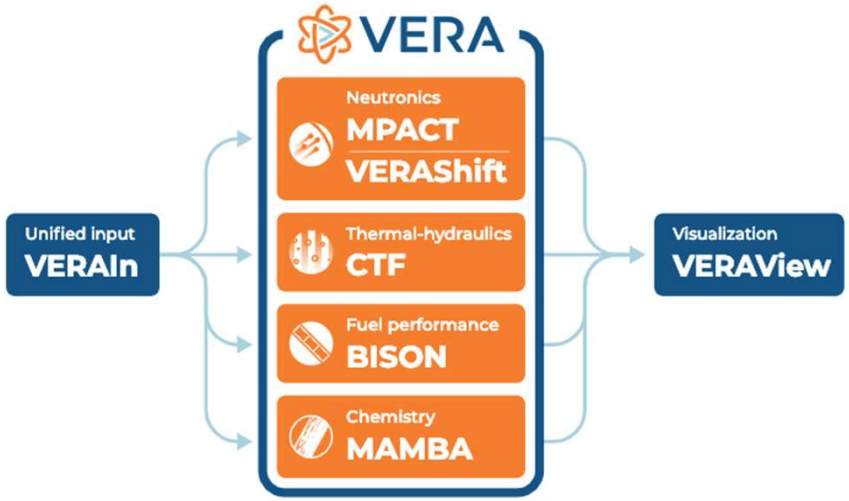
- **All-to-all Coupling Concept and Unified Input System**
  - So far, the coupling works for the multi-physics reactor simulation have been done by directly connecting two or more codes, which lacks extensibility (one-to-one coupling).
  - IRIS aims to provide a common environment ("universe") and driver through which multiple codes can be connected with one another (all-to-all coupling).
  - To construct this "universe", a unified input system that can be interpreted by every code is necessary.
    - VERA adopts a representative unified input system.

One-to-one Coupling (Conventional)



All-to-all Coupling (IRIS)



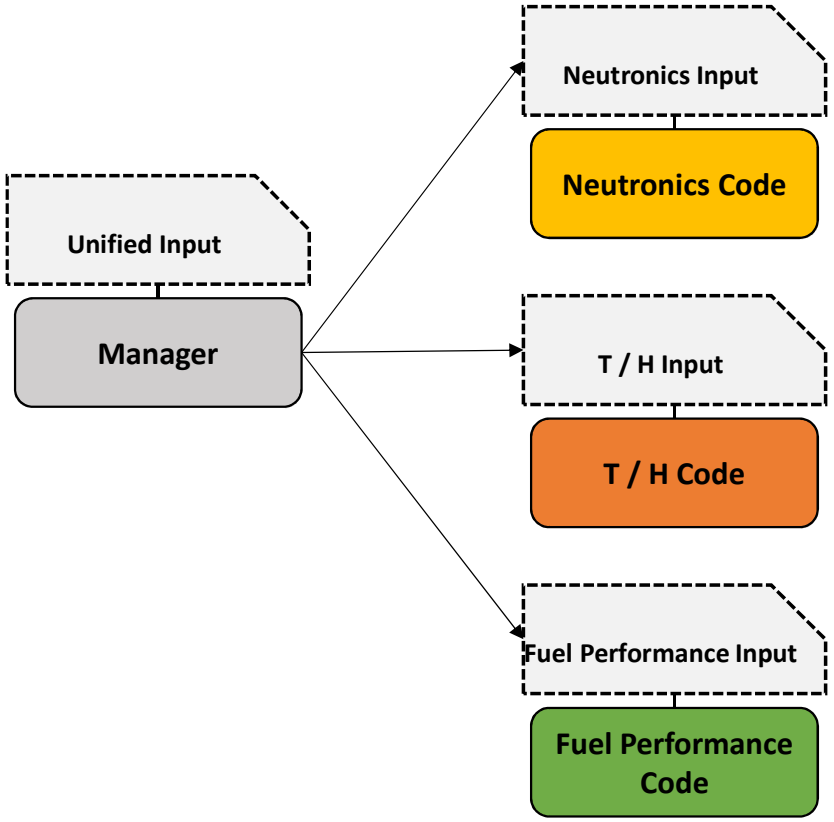


▪ Unified Input System of IRIS

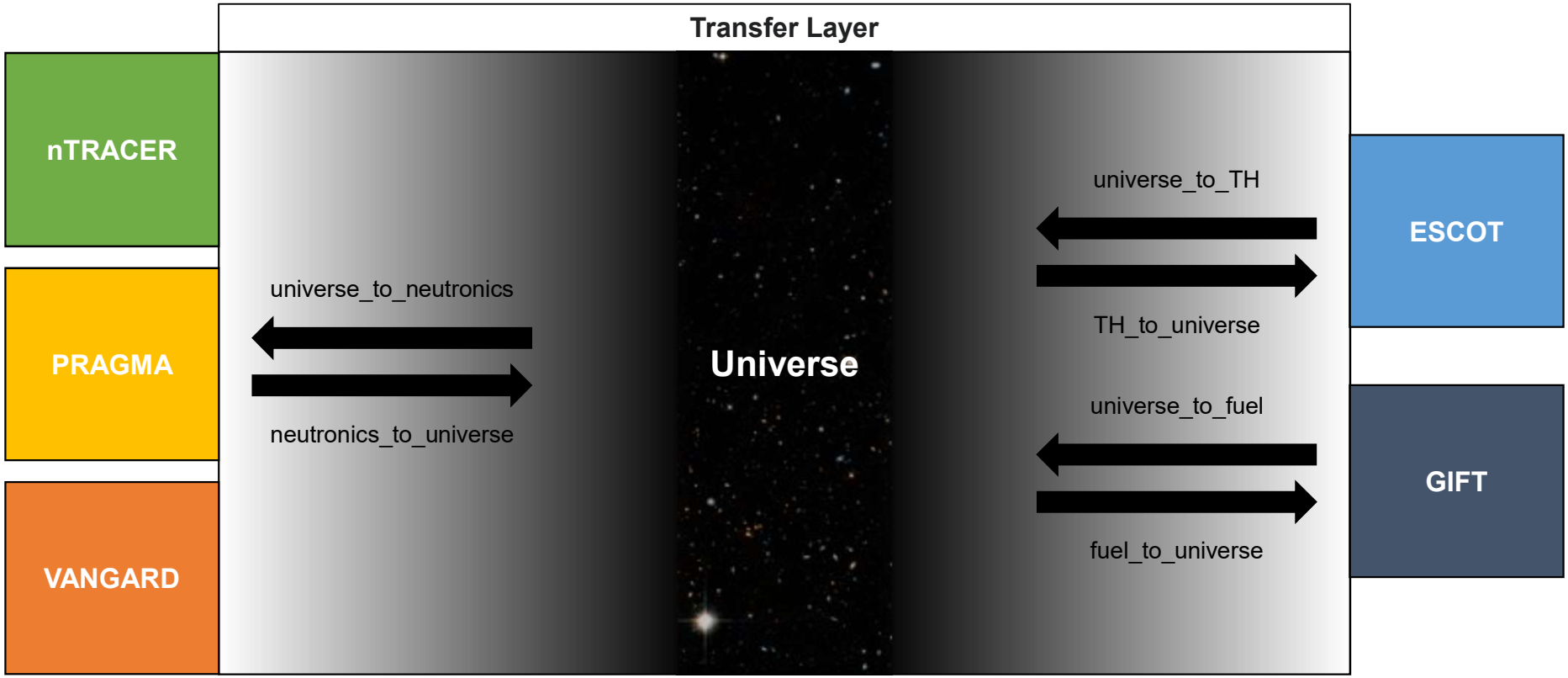
< Unified Input Structure >

CASEID			
STATE	TH_Cond	CORE_POWER	DEPLETE DAYS
MATERIAL / GC	MIXTURE	CLAD	FUEL
	REFL		
GEOM	NPINS	PITCH	PIN_DIM
	CELL	AXIAL	PIN
	ASSEMBLY	RAD_CONF	ALBEDO
	ASSEMBLY	RAD_CONF	ALBEDO
Neutronics Code	HOSTFILE	NUM_PROCS	Info
T/H Code	HOSTFILE	NUM_PROCS	Info
Fuel Calculation Code	HOSTFILE	NUM_PROCS	Info

< Program Execution Process by Unified Input >

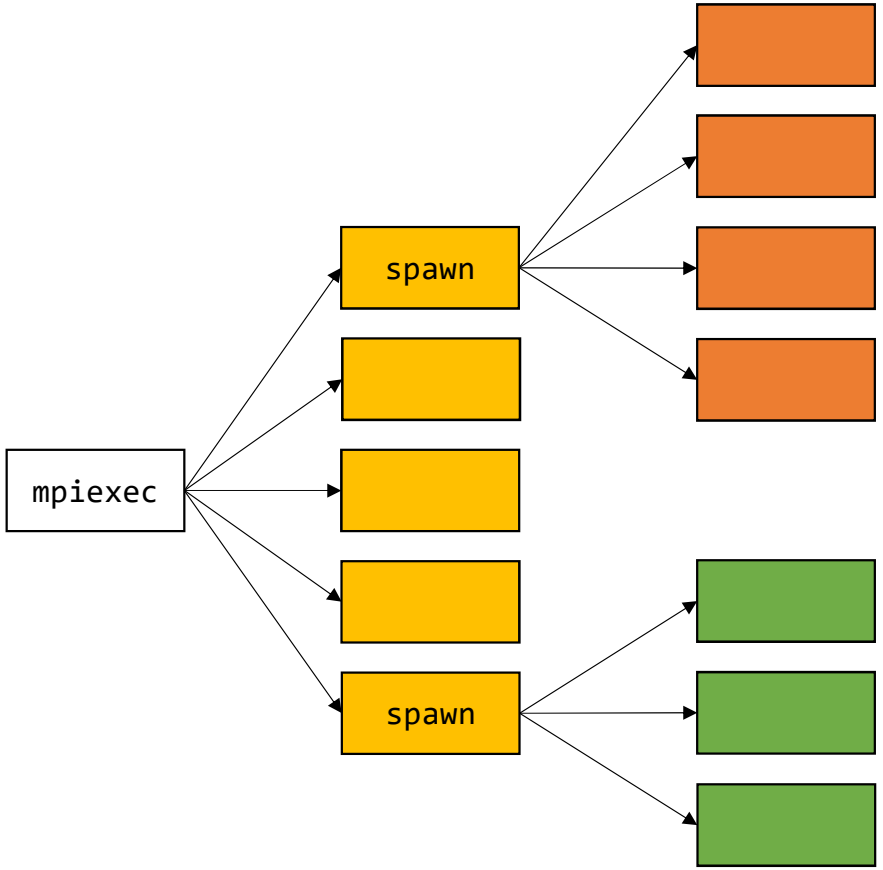


- Coupling Through the “Universe”



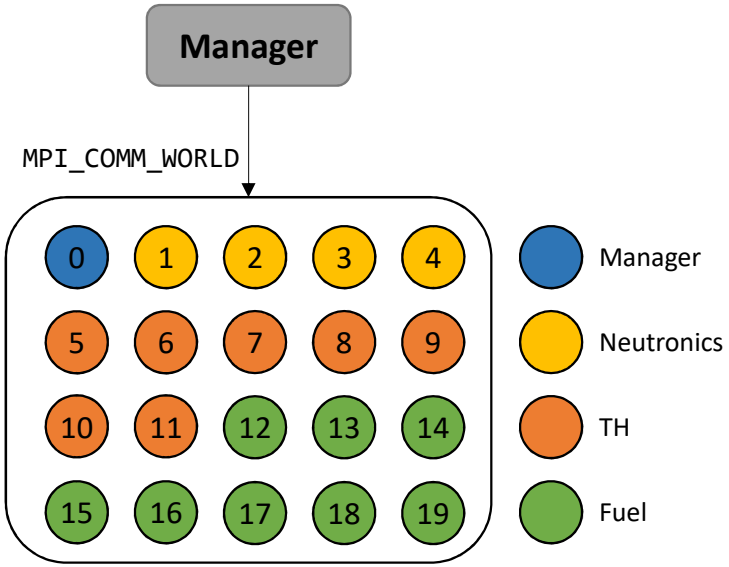
Coupling by MPI Dynamic Process Management

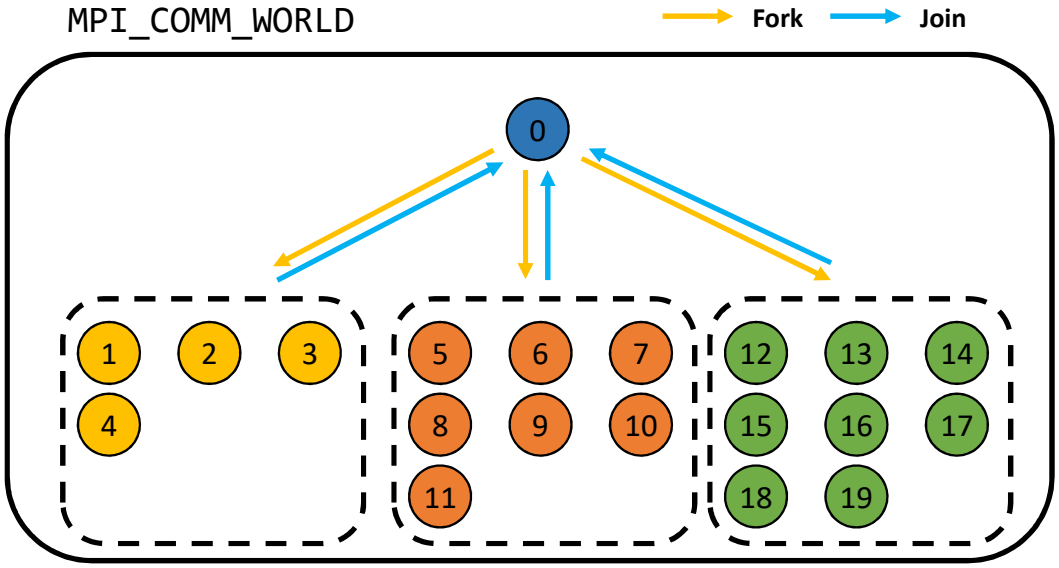
- **MPI Dynamic Process Management (DPM) Model**
  - **With `mpiexec`, only a single program can be launched at a time, and the number of processes is fixed at launch.**
  - **The DPM model in MPI-2 addresses this limitation by allowing for the spawning of new processes via a running program and connecting to existing processes.**
    - A communication model between the parent and children is provided.
    - Child processes can use MPI launch parameters that are different from the parent; e.g., program, number of processes, binding policies, etc.
  - **Namely, multiple MPI-based programs employing different parallelization schemes can establish an interconnection using the MPI DPM model.**
  - **Coupling with Manager – Worker Parallelism**
    - Worker programs (children) become the actual physics codes, and an independent manager program (parent) controls iteration and data transfer of the workers.



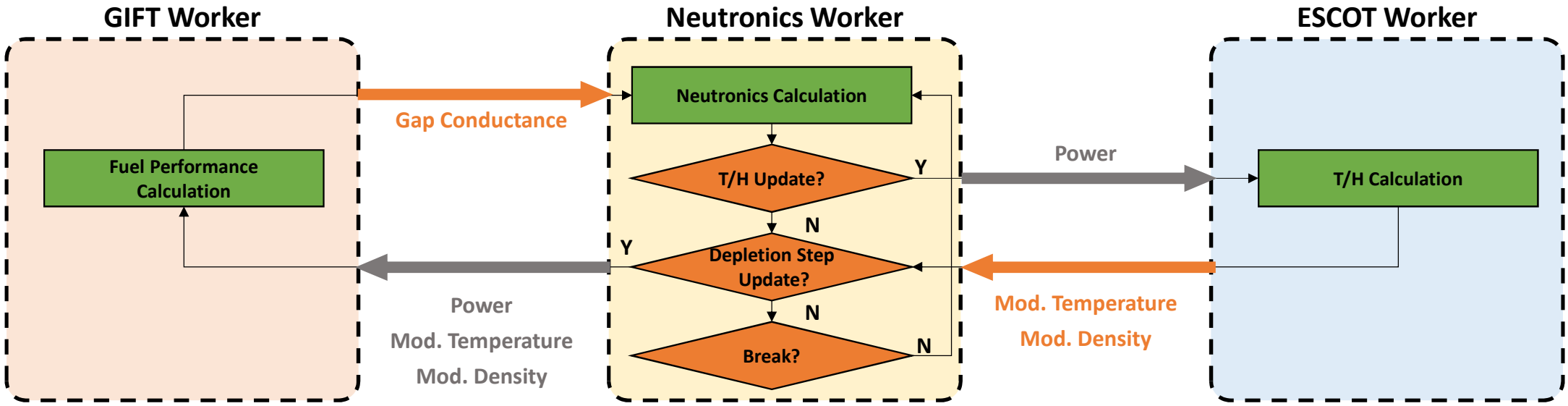
Coupling by MPI Dynamic Process Management

- **MPI Dynamic Parallelization Management in IRIS**
  - The manager program implements a neutronics code, a T/H code and a fuel performance code at once with a **single inter-communicator encompassing the manager program and all the worker programs.**
  - The manager process communicates with a master process among multiple processes of each code.
    - Each code is implemented with a different parallelization scheme.

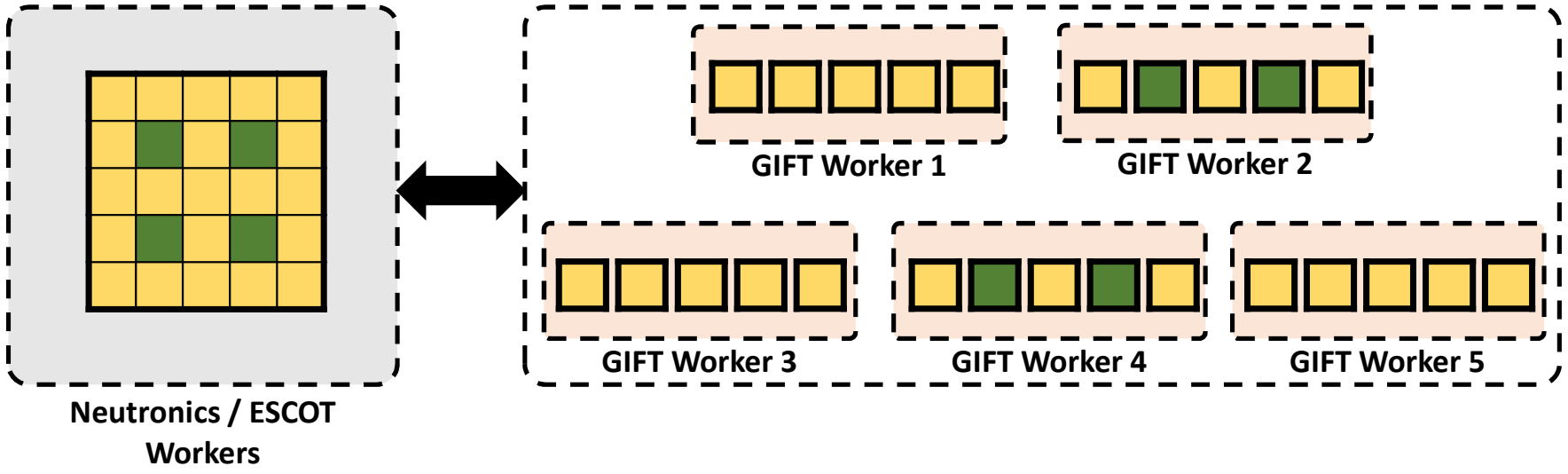




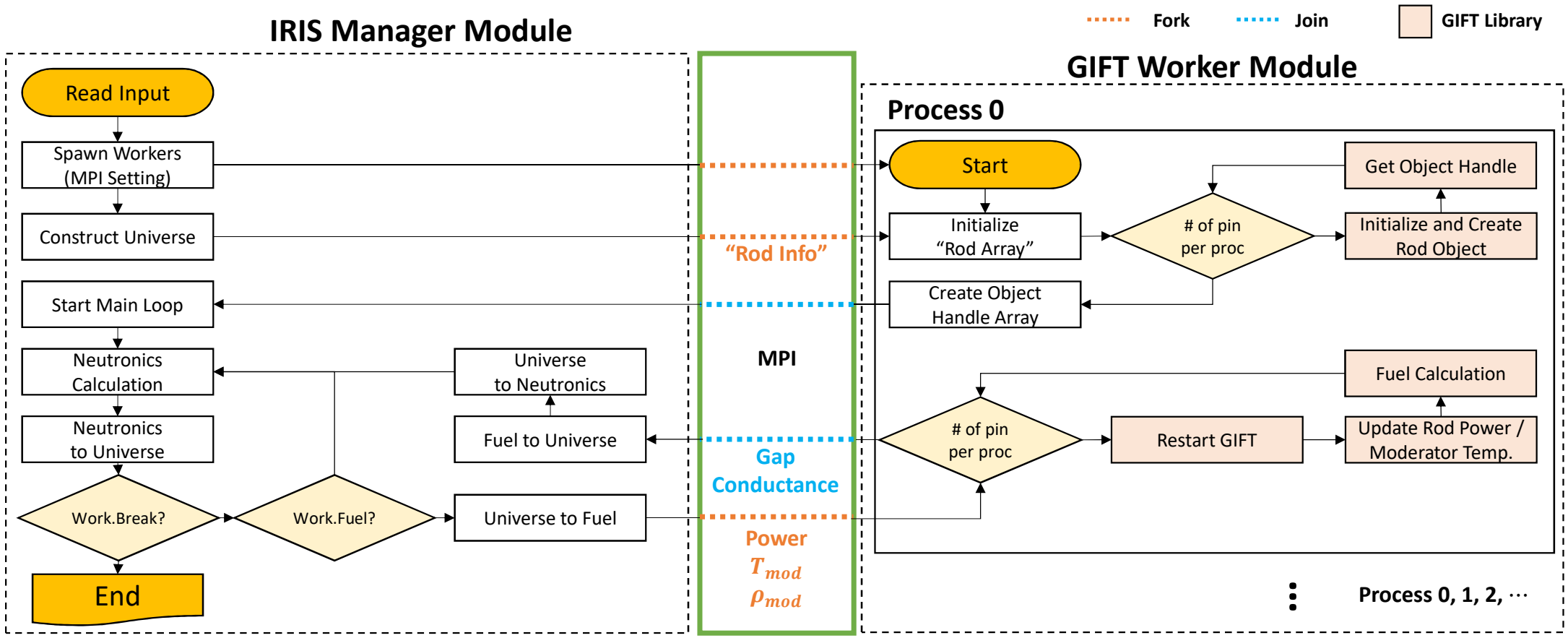
- **Code Coupling System of IRIS**
  - IRIS implements each coupled code with each input file generated from a unified input file.
  - At every T/H update, ESCOT calculates the temperature and density of moderator based on the power calculated by the neutronics calculation codes.
  - At every depletion step, GIFT calculates a gap conductance for each fuel rod based on the power, moderator temperature and density that is calculated by PRAGMA and ESCOT.



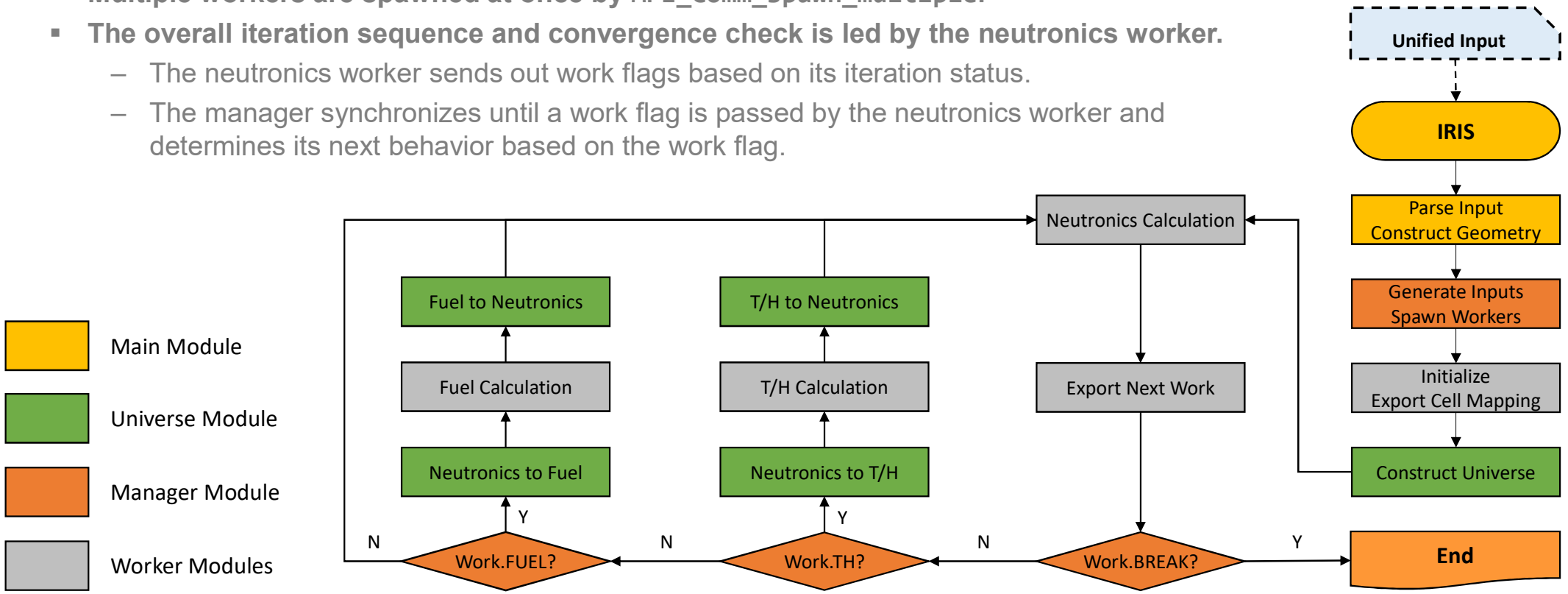
- **Treatment for Different Geometry Scale**
  - **There is a target geometry inconsistency between GIFT and the other codes.**
    - GIFT can only calculate a single fuel rod while the other codes can calculate a core or assembly with multiple rods.
  - **Each GIFT worker should manage multiple fuel rod simulations.**
    - Multiple fuel rods are allocated separately to several GIFT workers for parallelization of GIFT simulations.
    - Each GIFT worker implements the allocated fuel rod simulations sequentially.



- **IRIS / GIFT Coupling Algorithm**



- **IRIS Simplified Algorithm**
  - **Multiple workers are spawned at once by `MPI_Comm_spawn_multiple`.**
  - **The overall iteration sequence and convergence check is led by the neutronics worker.**
    - The neutronics worker sends out work flags based on its iteration status.
    - The manager synchronizes until a work flag is passed by the neutronics worker and determines its next behavior based on the work flag.



Problem Description

- **BEAVERS** Benchmark for Evaluation And Validation of Reactor Simulations
  - ESCOT coupling was verified for the 2D core at BOC.
  - GIFT coupling was verified for depletion calculation of a 3D single assembly.

Core Lattice	
# of Fuel Assemblies	193
Loading Pattern	w/o ^{235}U
Region 1 (Cycle 1)	1.60
Region 2 (Cycle 1)	2.40
Region 3 (Cycle 1)	3.10
Region 4A (Cycle 2)	3.20
Region 4B (Cycle 2)	3.40

Fuel Assemblies	
Pin Lattice Configuration	17 x 17
Active Fuel Length	365.76 cm
# of Fuel Rods	264
# of Grid Spacers	8

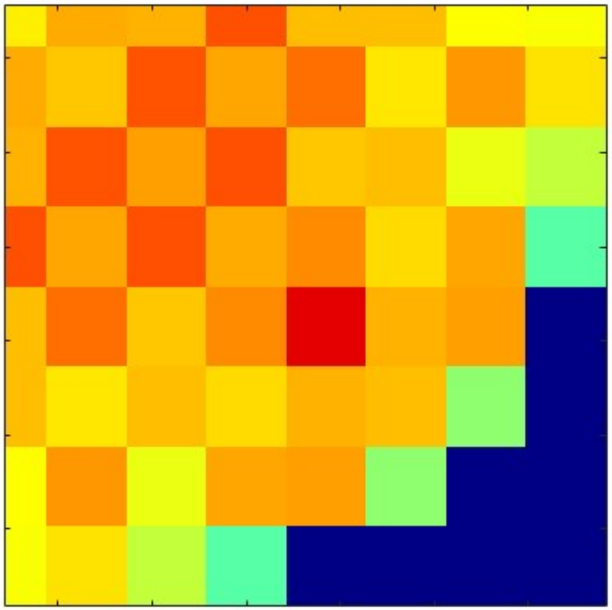
Performance	
Core Power	3411 MWth
Operating Pressure	2250 psia
Core Flow Rate	61.5 x 10^6 kg/hr (5% bypass)

Control	
Burnable Poison Material	Borosilicate Glass 12.5 w/o B_2O_3
# of Burnable Poison Rods	1266

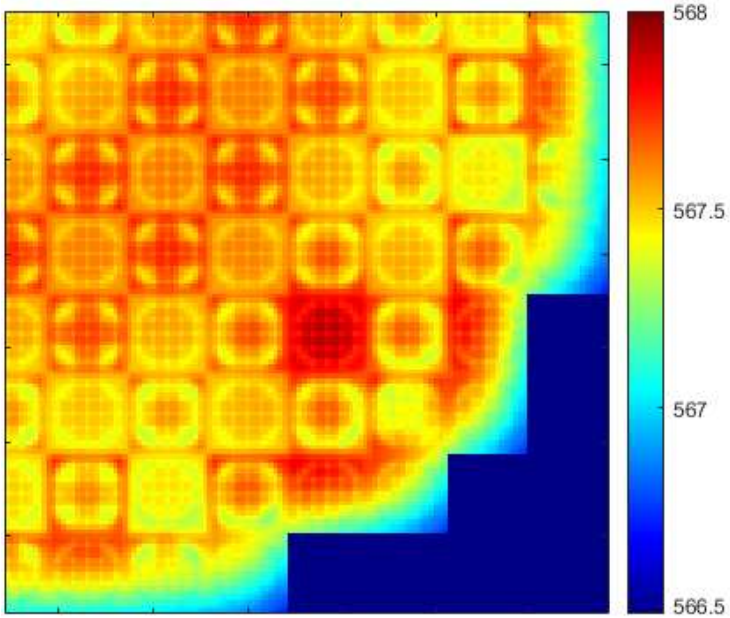
ESCOT Coupled Calculation Results

- **nTRACER – ESCOT Coupled Simulation on IRIS**
  - BEAVRS 2D Core (20cm Height, Nominal Flow Rate)
  - nTRACER – 1 MPI Process / ESCOT – 56 MPI Processes

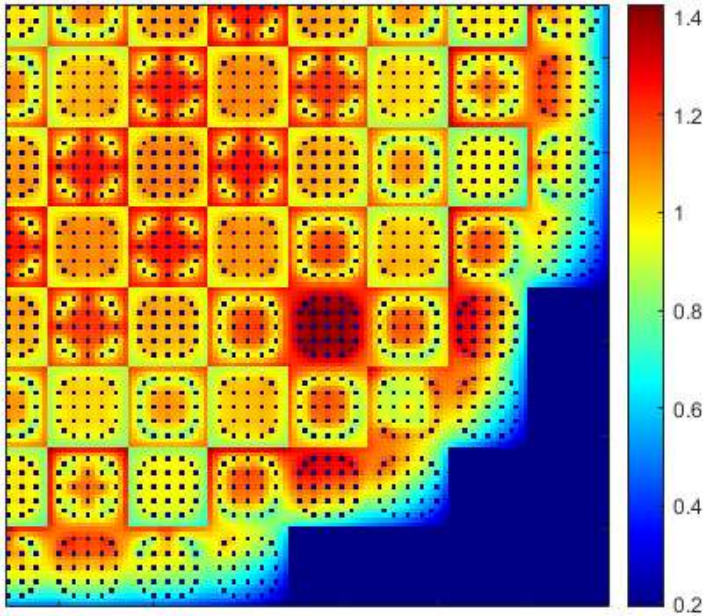
Internal T/H



ESCOT T/H



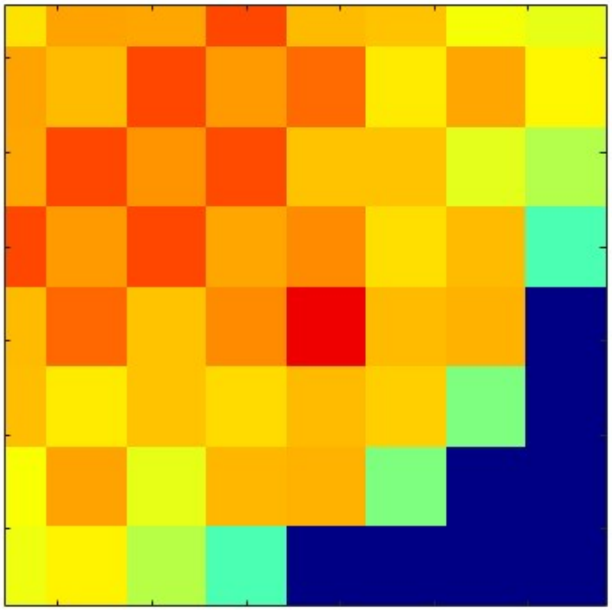
Pin Power



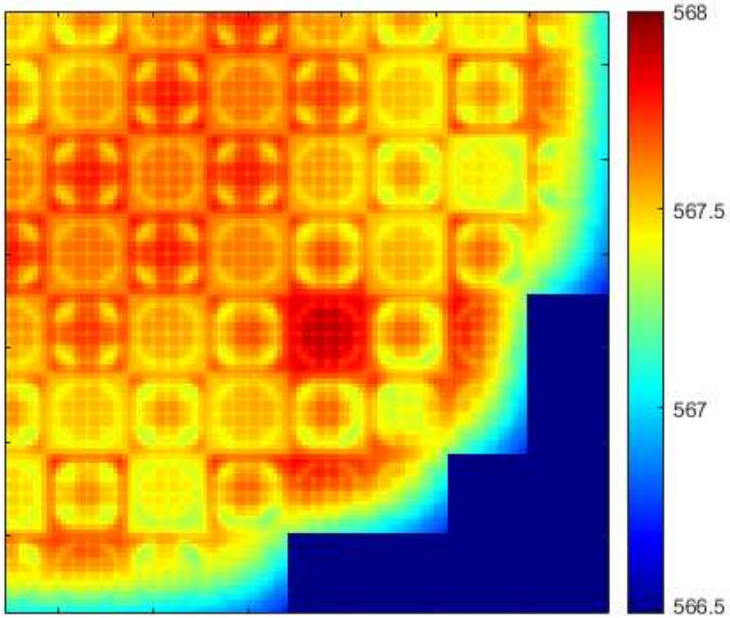
ESCOT Coupled Calculation Results

- **PRAGMA – ESCOT Coupled Simulation on IRIS**
  - BEAVRS 2D Core (20cm Height, Nominal Flow Rate)
  - PRAGMA – 4 MPI Processes / ESCOT – 56 MPI Processes

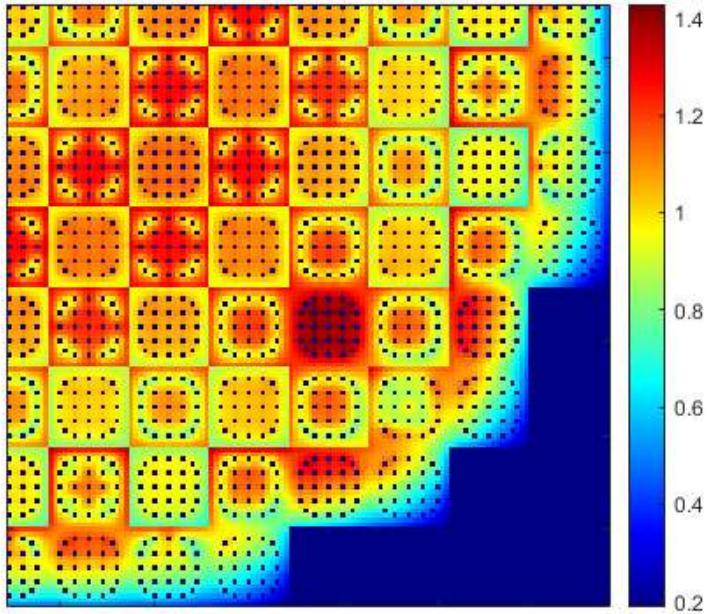
Internal T/H



ESCOT T/H



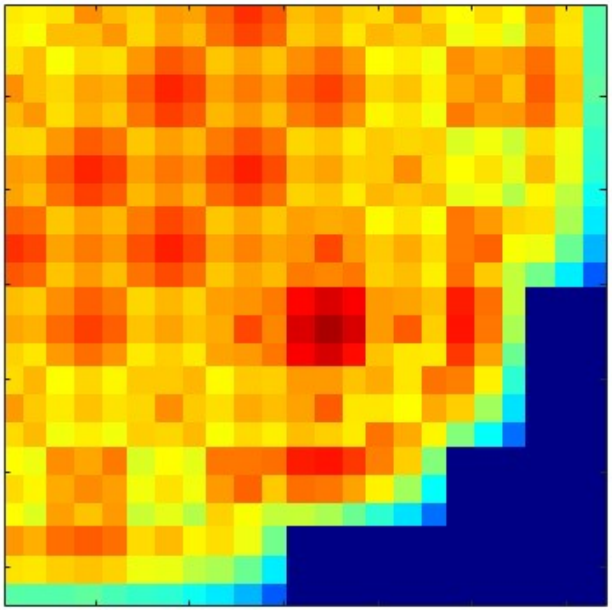
Pin Power



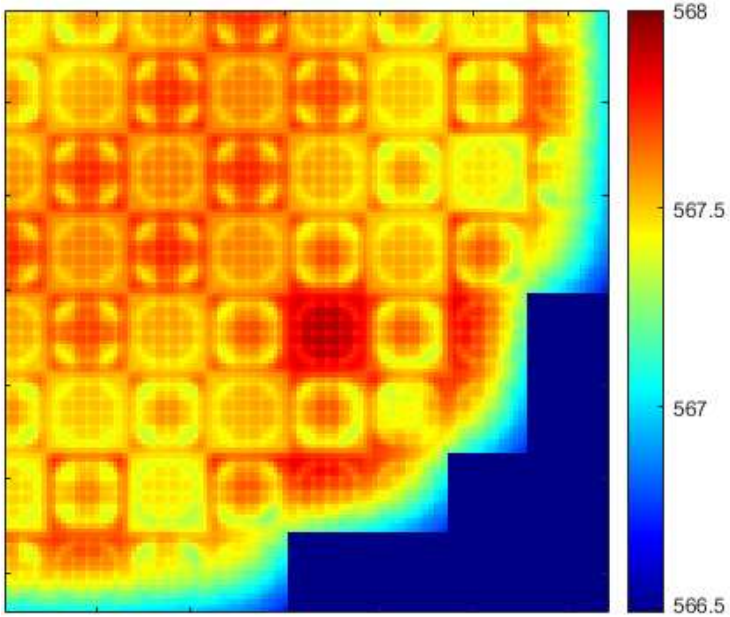
ESCOT Coupled Calculation Results

- **VANGARD – ESCOT Coupled Simulation on IRIS**
  - BEAVRS 2D Core (20cm Height, Nominal Flow Rate)
  - VANGARD – 1 MPI Process / ESCOT – 56 MPI Processes

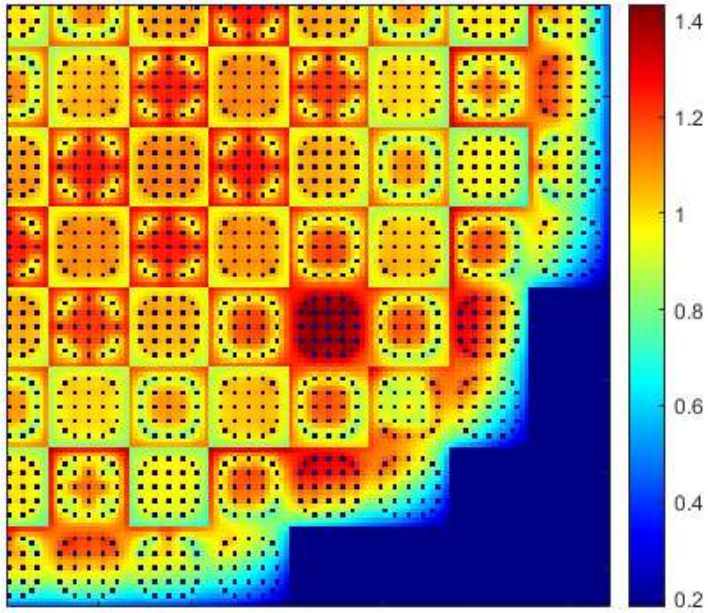
Internal T/H (3 x 3 Macro Channel)



ESCOT T/H



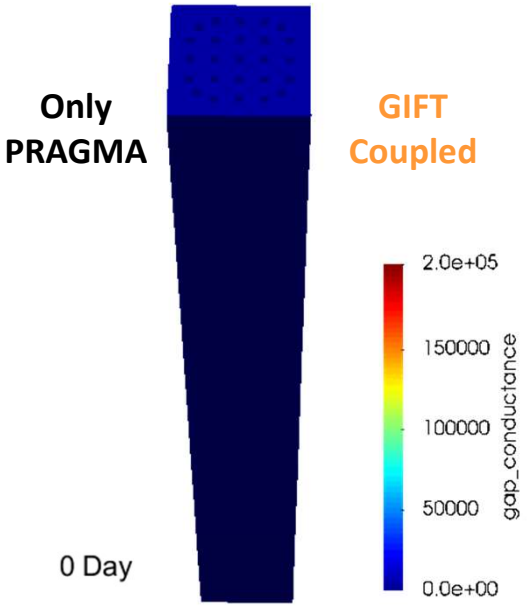
Pin Power



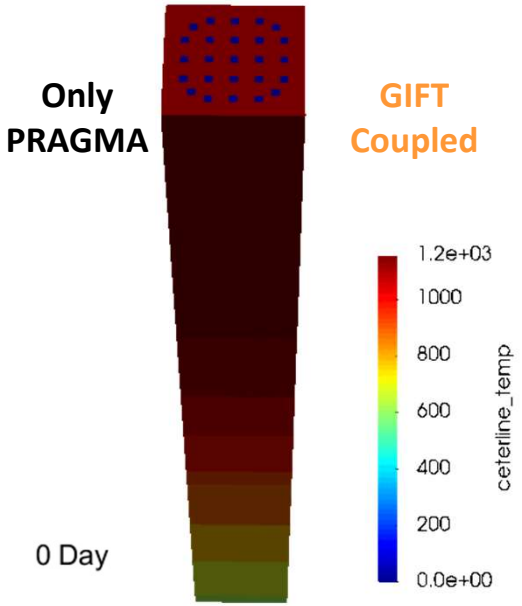
GIFT Coupled Calculation Results

- **GIFT Coupled Single Assembly Calculation Results**
  - GIFT can only be coupled to PRAGMA among neutronics codes due to specific data necessary for GIFT calculation.
  - PRAGMA – 4 MPI Processes / ESCOT – 1 MPI Process / GIFT – 20 MPI Processes

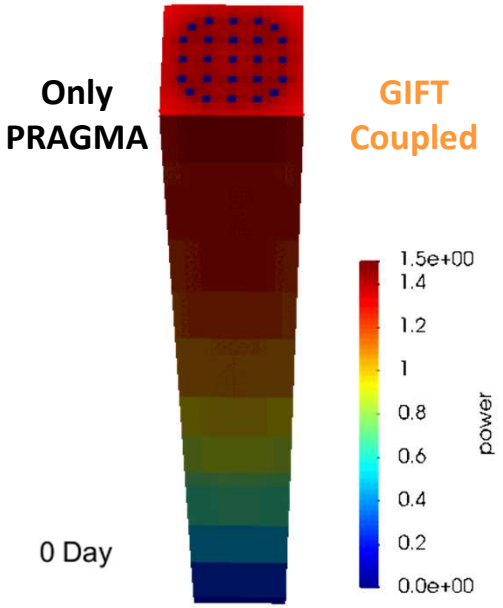
< Gap Conductance >



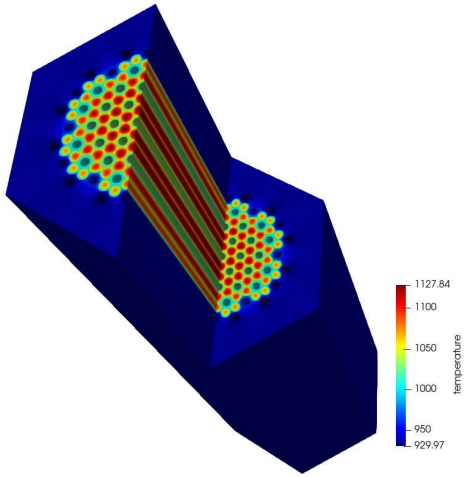
<Centerline Temperature>

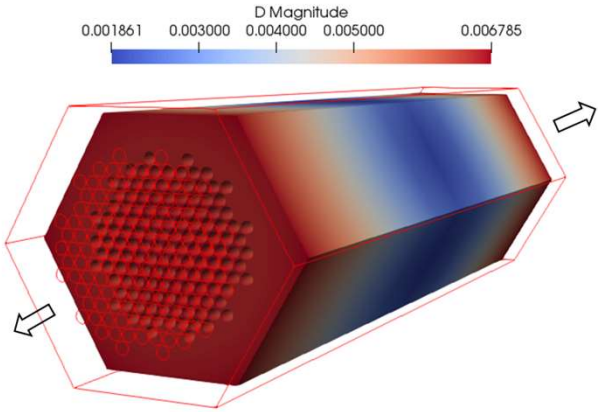


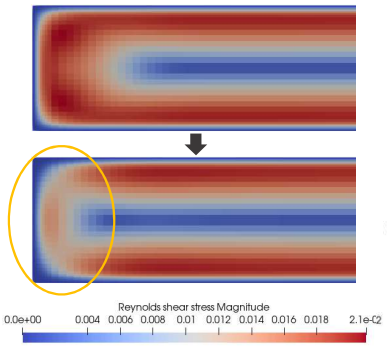
< Power >

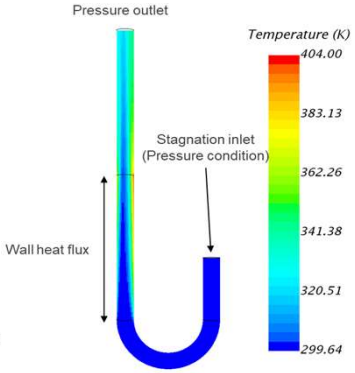


- **PRAGMA-OpenFOAM-ANLHTP Coupling System**
  - **The system aims to analyze a heat pipe cooled micro reactor with high-fidelity multiphysics simulation.**
    - There are no MC solutions with fine-grain thermo-mechanical feedback analysis of Heat-Pipe Cooled Micro Reactors.
  - **An independent multiphysics system is needed to simulate the unstructured geometry of heat pipe reactors since IRIS is optimized for a lattice-based geometry treatment.**
    - An unstructured geometry treatment is necessary for the heat pipe reactor analysis.
  - **It employs the MPI Dynamic Process Management (DPM) and File I/O system for code coupling.**



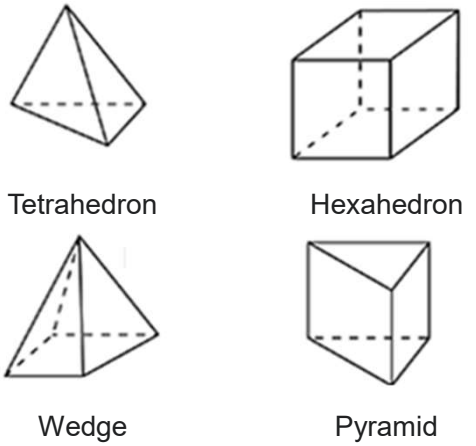


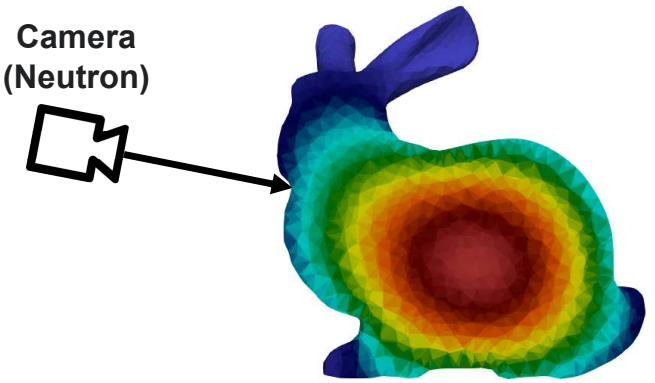




- **Unstructured Geometry Treatment in PRAGMA**
  - **PRAGMA supports general unstructured mesh geometry treatment powered by graphics ray tracing technology.**
  - **PRAGMA uses a CAD design model for treating an unstructured geometry.**
  - **PRAGMA reconstructs an unstructured geometry based on a mesh file generated by ANSYS or CUBIT.**
    - A mesh generator generates meshes of a geometric design model using four basic cells.
    - A mesh file includes information about nodes, edges and volumes.
  - **PRAGMA adopts OptiX for neutron tracking in an unstructured geometry.**
    - OptiX is a CUDA-based ray tracing API optimized for NVIDIA GPUs.
    - Neutron tracking is substituted by ray tracing that treats a neutron as a camera.

Basic Cells in the ANSYS FLUENT

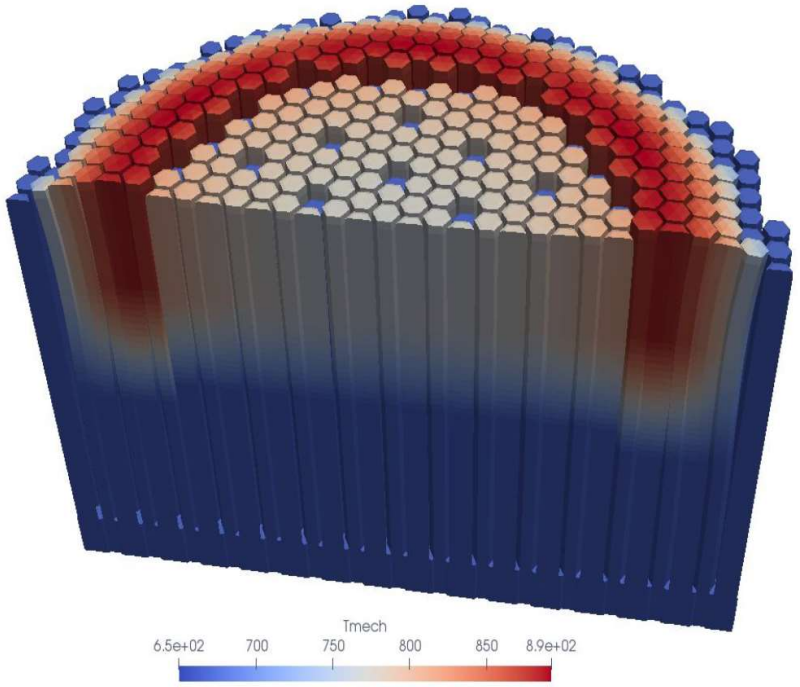




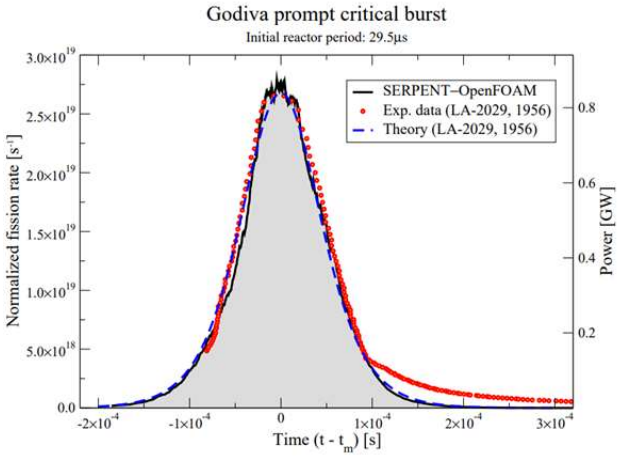
- **OpenFOAM**
  - OpenFOAM is a free, open-source CFD software developed by OpenCFD.
  - It has an extensive range of features to solve all problems associated with complex fluid flows involving chemical reactions, turbulence, and heat transfer.
  - **Based on the momentum equation, displacement results could be fed back to neutronics application, thereby deforming the mesh.**

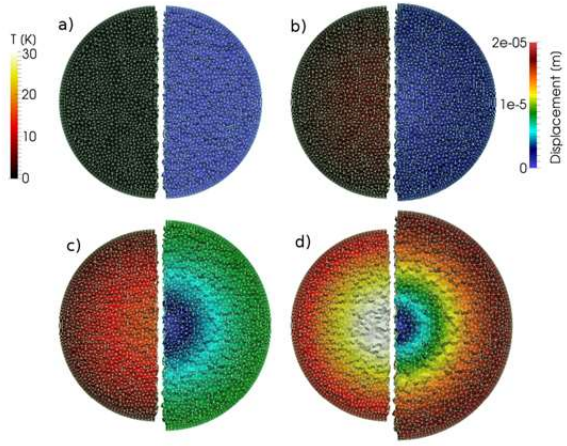
OpenFOAM®

Gen-FOAM Multi-Physics Analysis



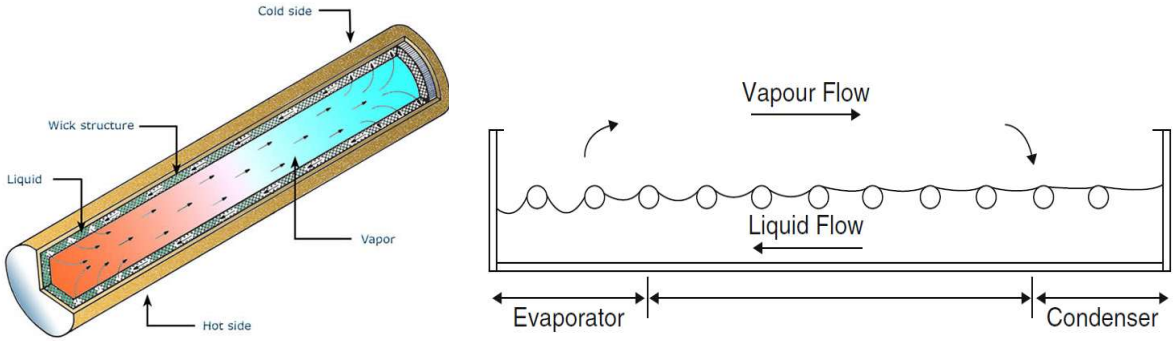
Serpent-OpenFOAM Coupling Transient Analysis



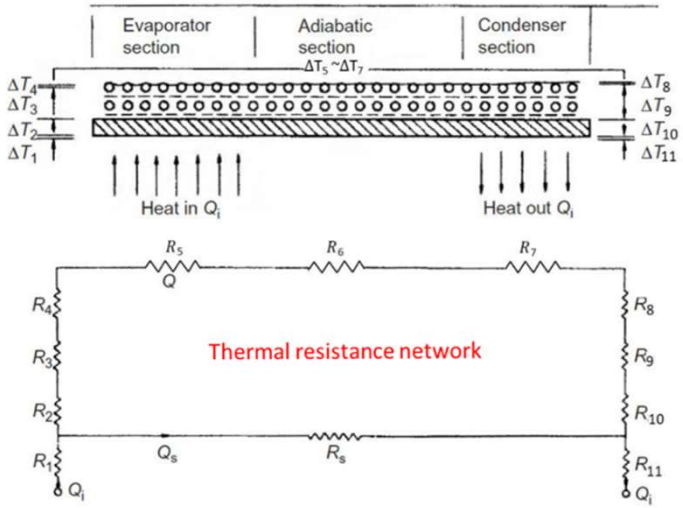


- **ANLHTP**
  - **ANLHTP is a one-dimensional heat pipe analysis code developed at ANL in the 1980s.**
  - **It simulates a sodium heat pipe based on theory, analysis, and experimental data.**
    - It assumes that the evaporator and condenser are nearly isothermal.
  - **It predicts heat pipe temperature distributions for steady-state and slow transient conditions.**

Passive Heat Transfer Mechanism of Heat Pipe

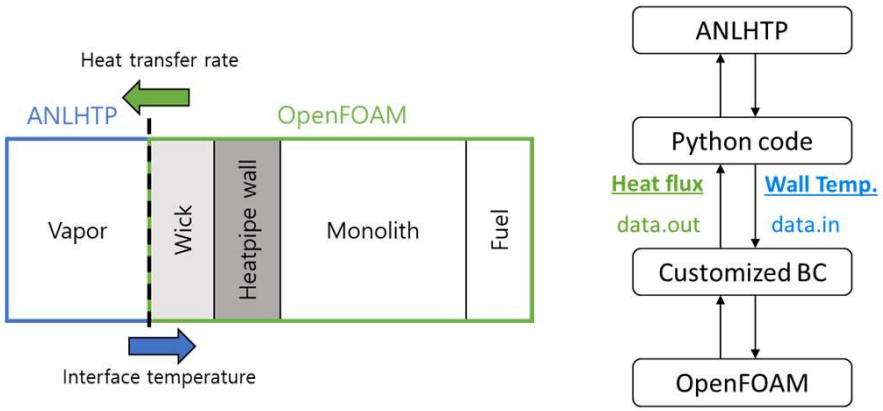


Thermal Resistance Network of ANLHTP

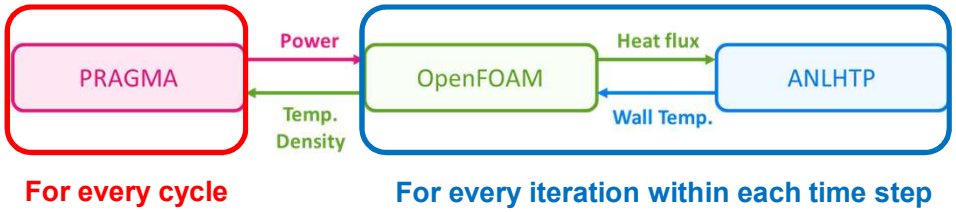


- **Coupling System of PRAGMA-OpenFOAM-ANLHTP**
  - **OpenFOAM and ANLHTP transfer heat flux and wall temperature data based on file I/O communication.**
  - **OpenFOAM-ANLHTP calculates the temperature and density of moderator based on the power calculated by PRAGMA.**
  - **Since the OpenFOAM-ANLHTP coupling system is based on a transient system, the calculation scheme should be modified to be coupled with a MC code for steady-state analysis.**
    - The time step of OpenFOAM is treated in the same way as the cycle of the Monte Carlo algorithm.
    - For a new state, OpenFOAM-ANLHTP must converge through Picard iteration within each time step.

OpenFOAM-ANLHTP Coupling System

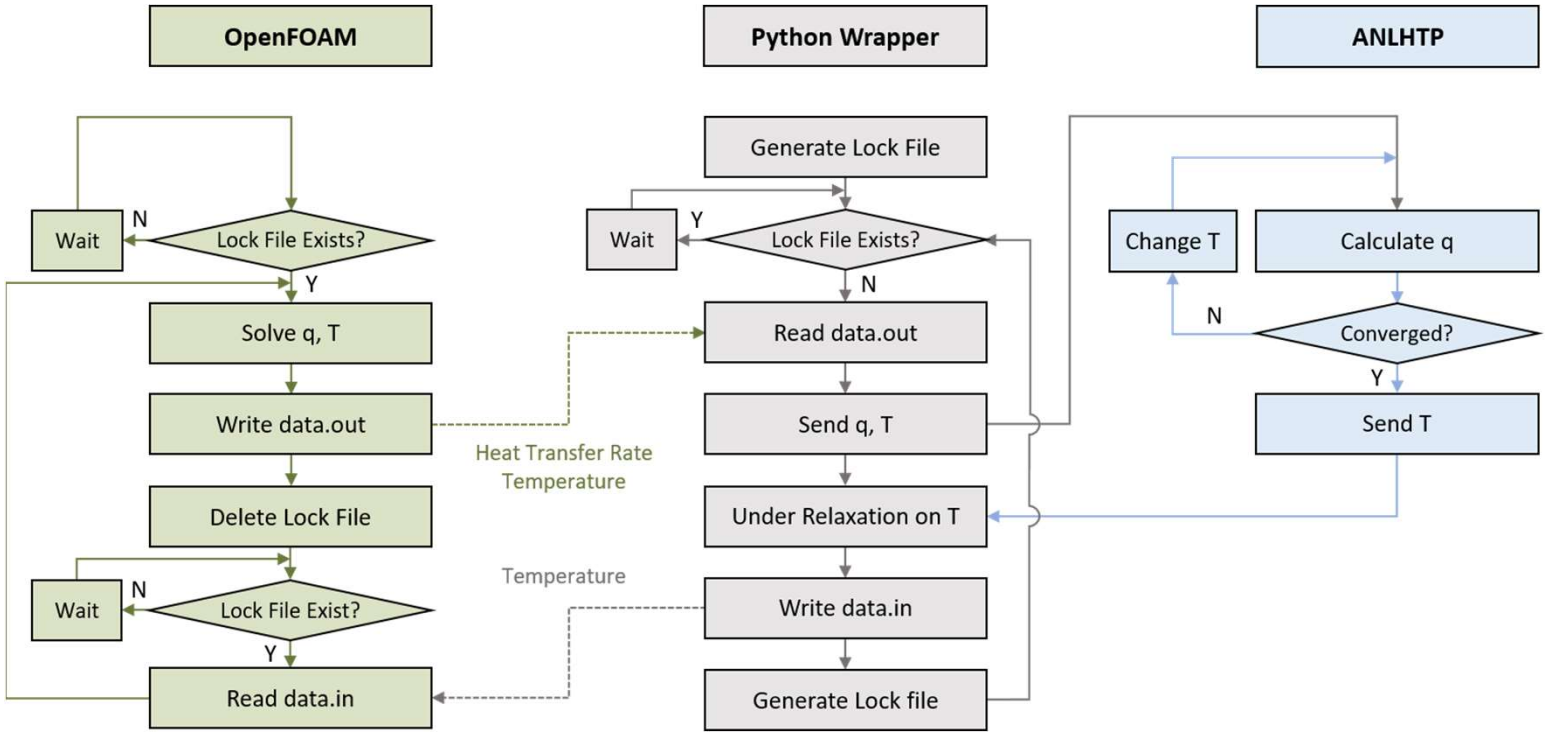


Modified OpenFOAM-ANLHTP Calculation Scheme

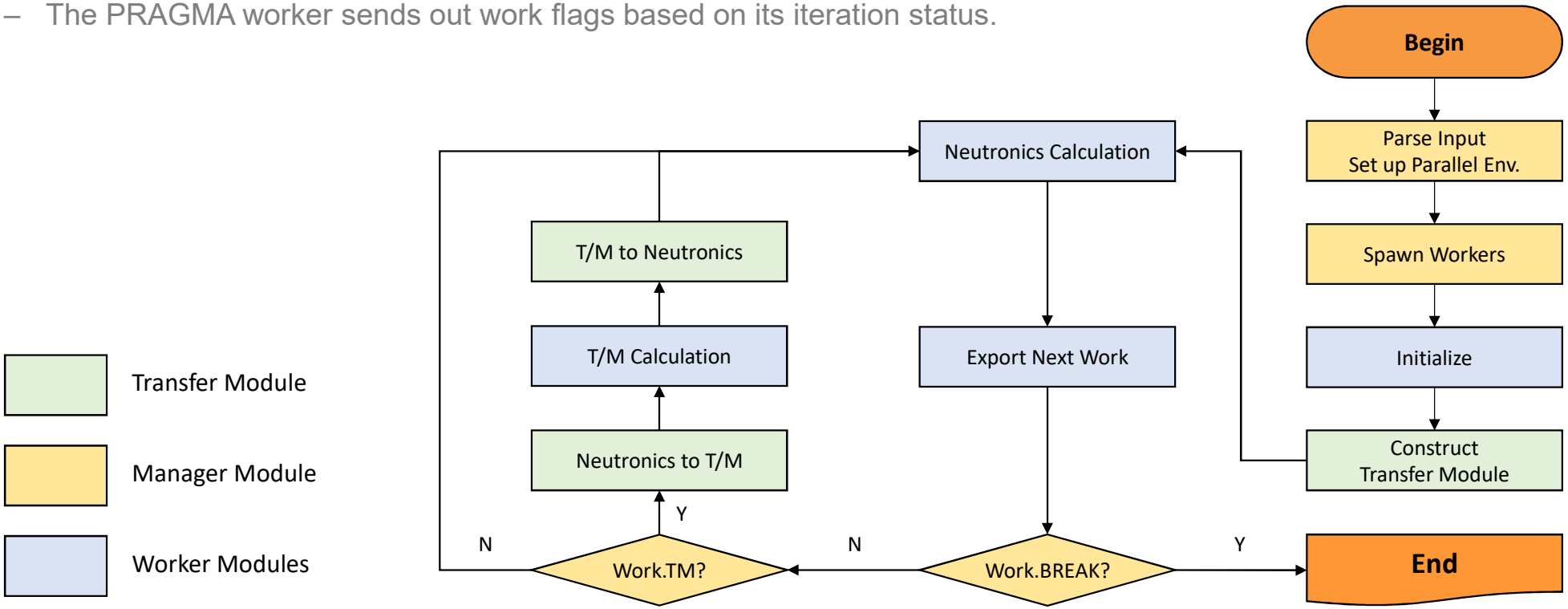


Algorithm of OpenFOAM-ANLHTP Coupling System

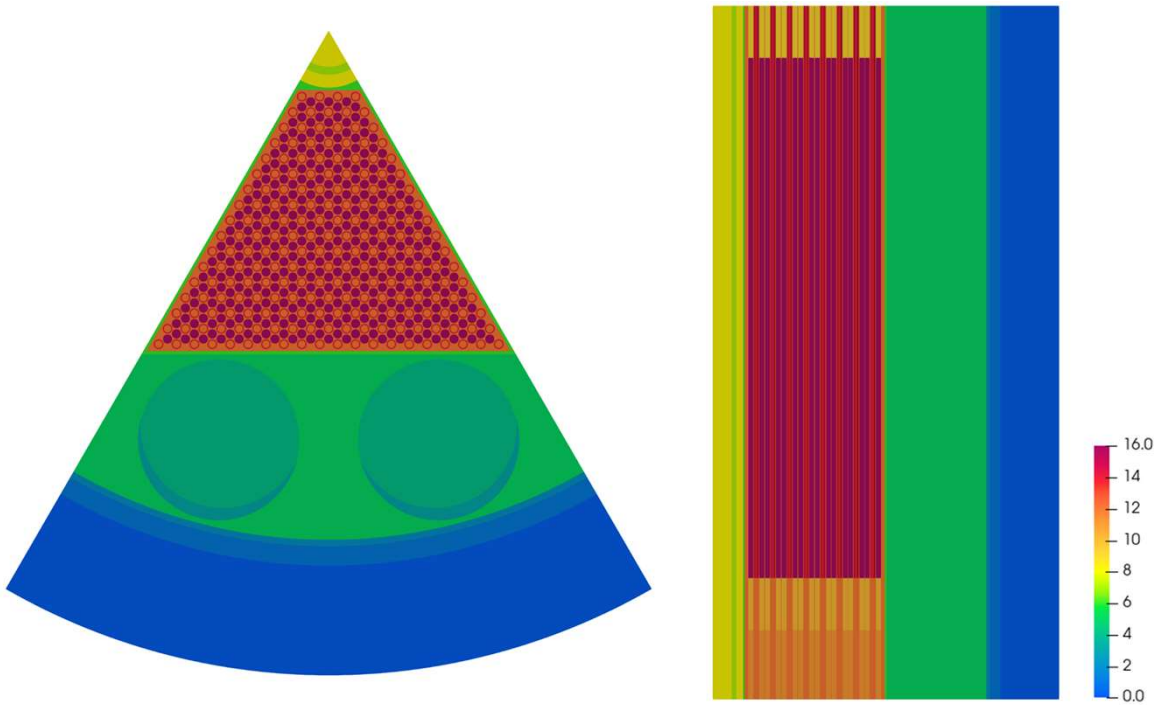
- **Simplified Flowchart of OpenFOAM-ANLHTP Coupling System**
  - The OpenFOAM-ANLHTP coupling flowchart is included in the 'T/M Calculation' block.
  - Except for the OpenFOAM-ANLHTP coupling system, all data transfer is controlled by MPI routines.



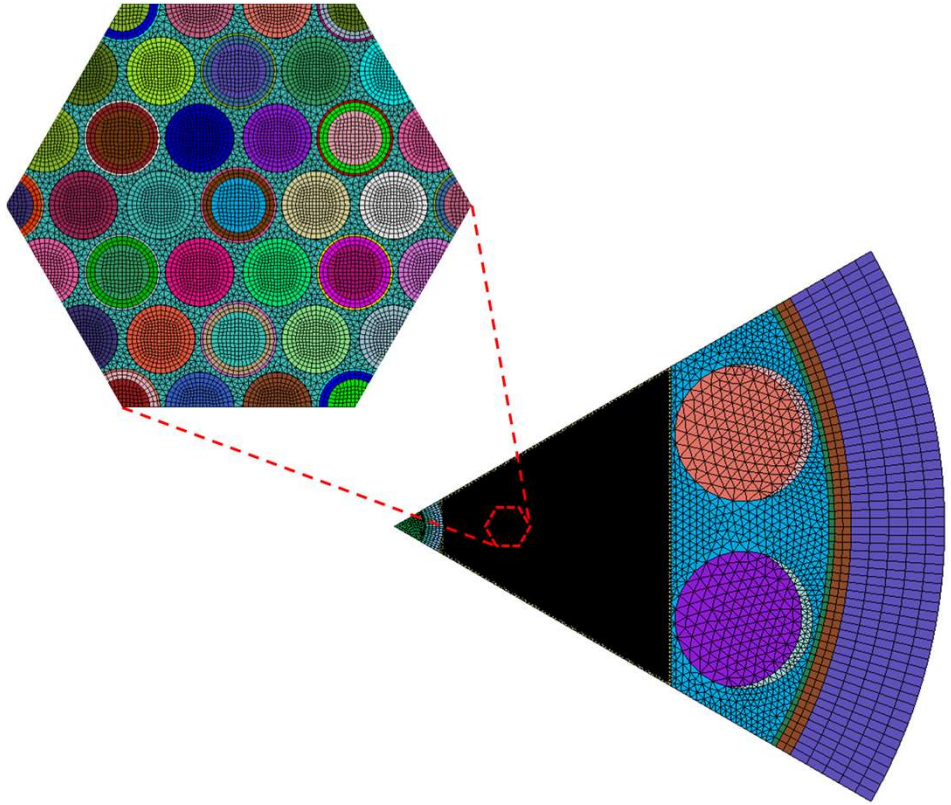
- **Algorithm of PRAGMA–OpenFOAM–ANLHTP Coupling System**
  - **The overall procedure for multiphysics coupling is controlled using the Picard iterative method and the iteration sequence is led by the PRAGMA worker.**
    - The PRAGMA worker sends out work flags based on its iteration status.



- **LANL MegaPower 3D Sector**
  - Configuration

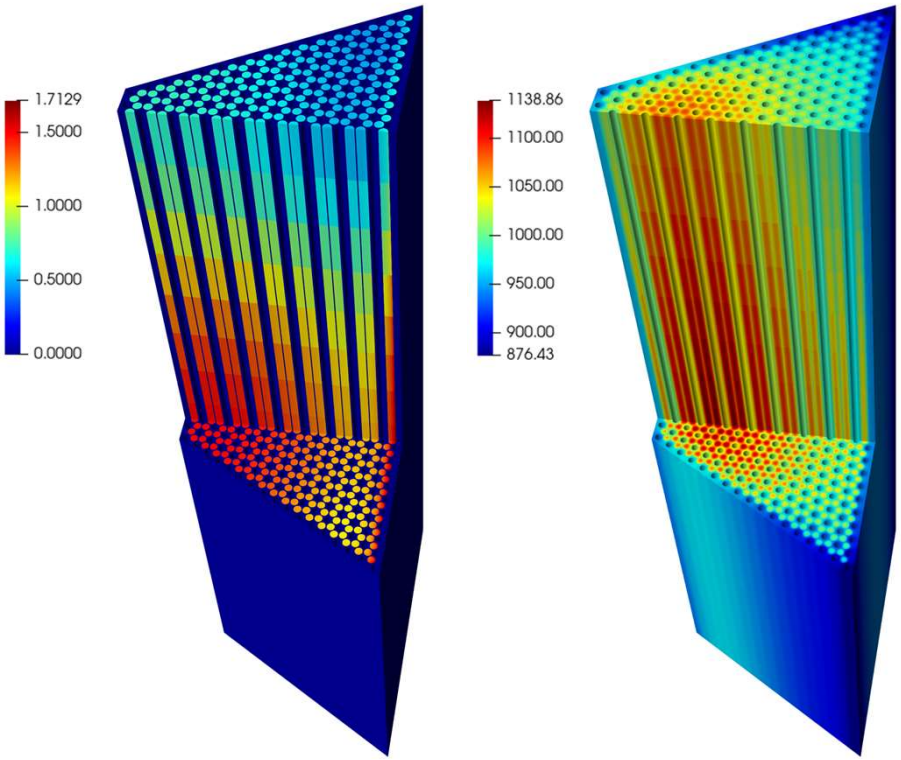


  - Mesh Granularity

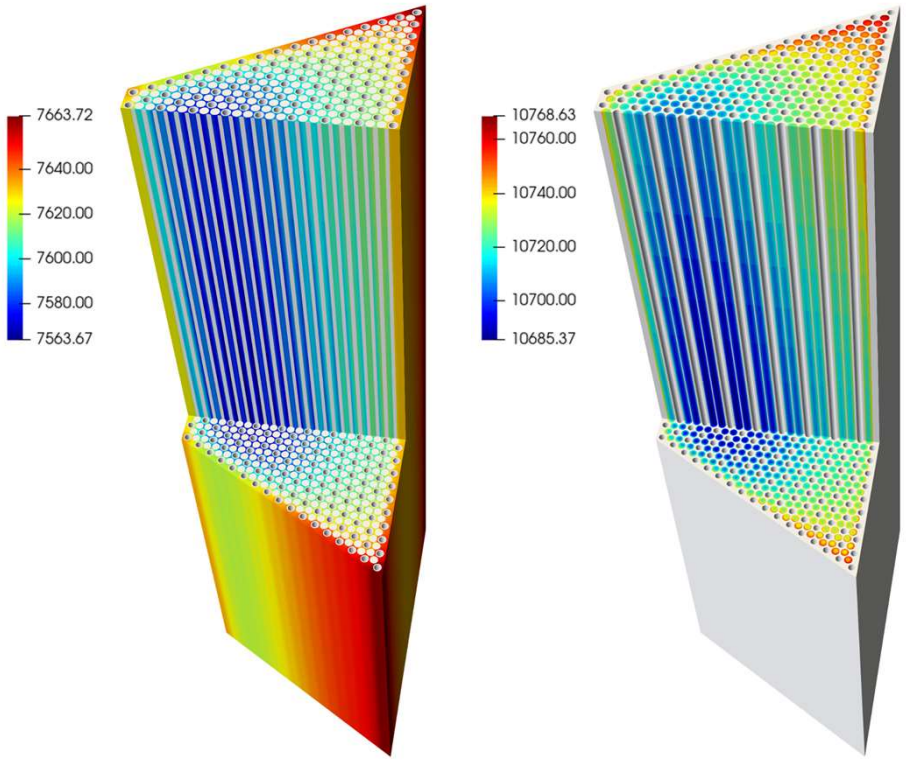


- **Coupled Calculation Results**

Normalized Power and Temperature [K]

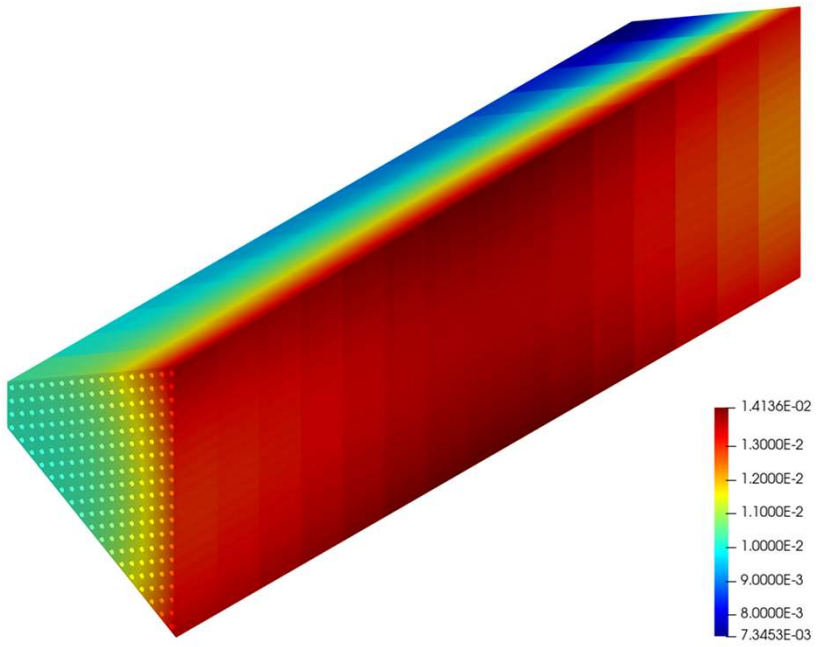


Monolith and Fuel Density [kg/m^3]

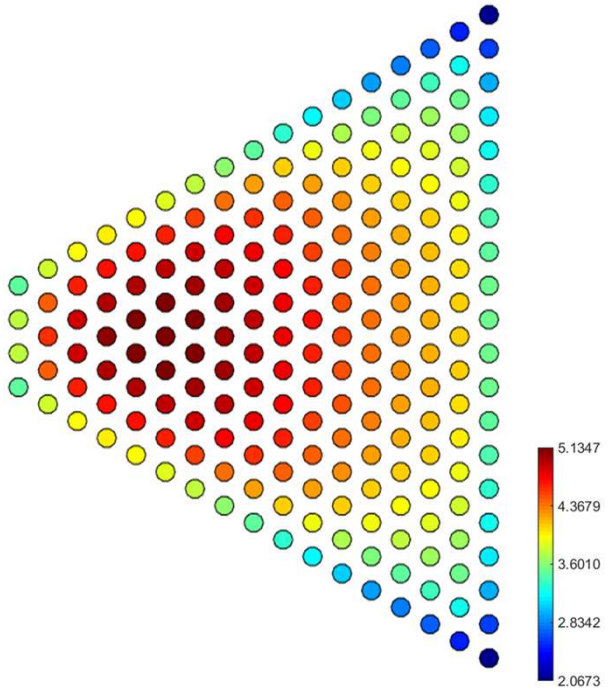


- **Coupled Calculation Results**

Total Thermal Expansion [m]



Heat Removal Rate [kW] of Heat Pipes



Conclusion & Future Works

- **Conclusion**
  - **Preliminary Development of an extensible code coupling system IRIS optimized for PWR analysis**
    - Demonstration of multiphysics simulation on the BEAVRS 2D core and a single assembly
  - **Preliminary development of a unique and efficient multiphysics coupling system for HPRs**
    - Demonstration of multiphysics simulation on LANL MegaPower 3D single sector (HPR)
    - Confirmed the soundness of multiphysics analysis capability through the fine-grain results

- **Ongoing and Future Works**
  - **Stabilization and optimization of IRIS code coupling system**
    - Demonstration of multiphysics simulation on BEAVRS 3D full core
  - **Performance optimization of thermo-mechanical and heat pipe coupled analysis**
  - **Development of mesh deformation capability to perform realistic thermo-mechanical feedback**
  - **Multi physics multi scale coupling involving VANGARD, ESCOT and MARS**
  - **SOPHIA coupling with PRAGMA for multi-physics analysis of pebble bed reactors**
  - **…**