Preliminary Verification of PRAGMA VHTR Module Enhancements for 3D Prismatic VHTR Analysis

Sung Joon Kwon, Namjae Choi, Yeon Sang Jung

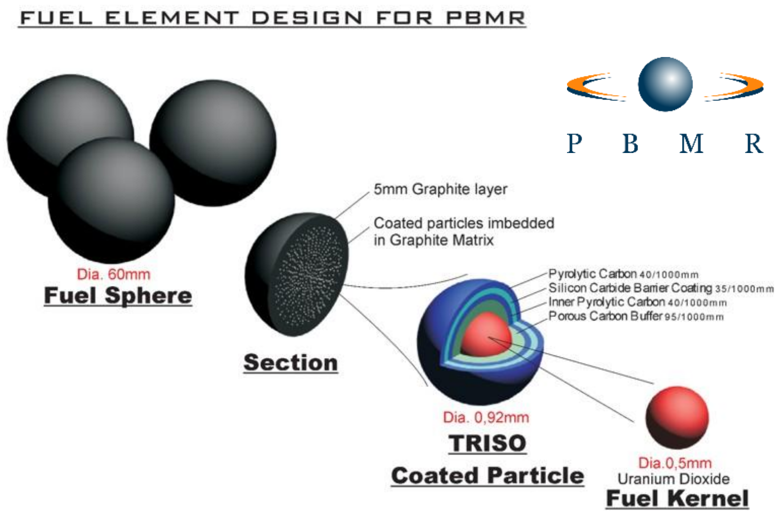
Department of Nuclear Engineering

Seoul National University

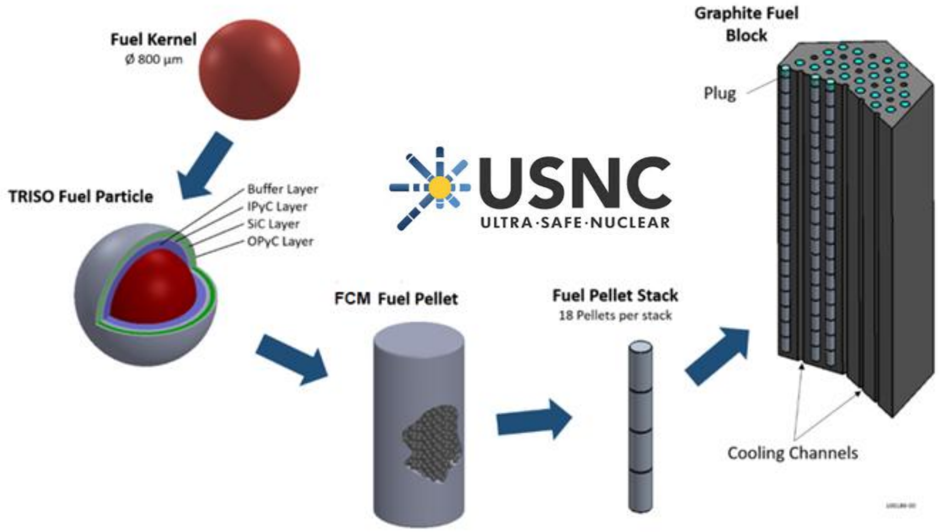
May 23rd, 2025

- **Very High Temperature Reactor (VHTR) Features**
  - **Interest in VHTRs has increased due to their enhanced safety and proliferation resistance.**
  - **The major types of VHTRs are the Pebble Bed Reactor (PBR) and the Prismatic VHTR.**
  - **The utilization of TRISO particles to provide fuel elements causes double heterogeneity in a VHTR core.**
    - Double heterogeneity makes VHTR modeling and simulations challenging.

PBR Fuel Element

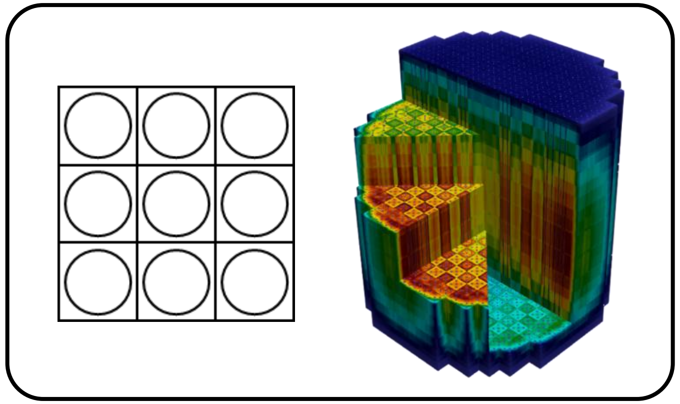


Prismatic VHTR Fuel Element

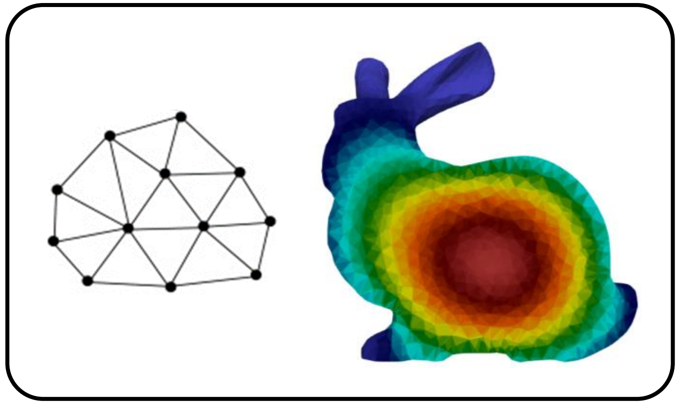


- **Power Reactor Analysis using GPU-based Monte Carlo Algorithm (PRAGMA)**
  - **Funded by KHNP through K-CLOUD project**
  - **Language: CUDA C++**
  - **Characteristics of PRAGMA**
    - Provides optimized geometry treatments and algorithms for PWR analysis
    - Enables efficient simulation within feasible time scale on a small cluster equipped with consumer-grade GPUs
    - Supports general unstructured mesh geometry treatment powered by graphics ray tracing technology
    - Can be extended to VHTR analysis with special geometry treatment and tracking algorithms for VHTRs

PWR Lattice Geometry

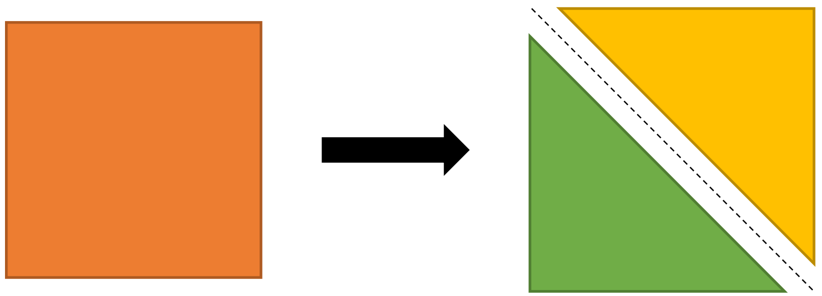


Unstructured Mesh Geometry

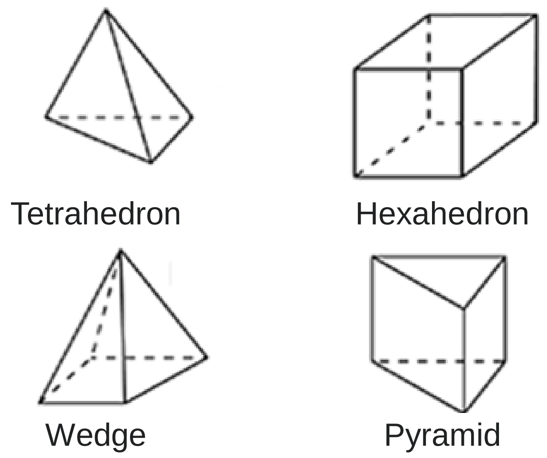


Unstructured Geometry Treatment in PRAGMA

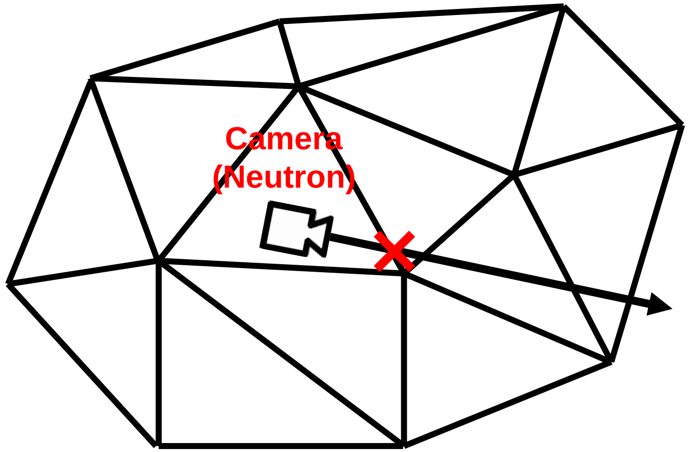
- **PRAGMA uses a CAD design model for treating an unstructured geometry.**
- **PRAGMA reconstructs an unstructured geometry based on a mesh file generated by Cubit or Fluent.**
  - The mesh generators produce meshes using four basic cells.
- **PRAGMA adopts OptiX for neutron tracking in a triangular-mesh based 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.
  - Quadrilaterals are split into triangles to exploit the built-in triangular-mesh optimized program of the ray tracing engine.



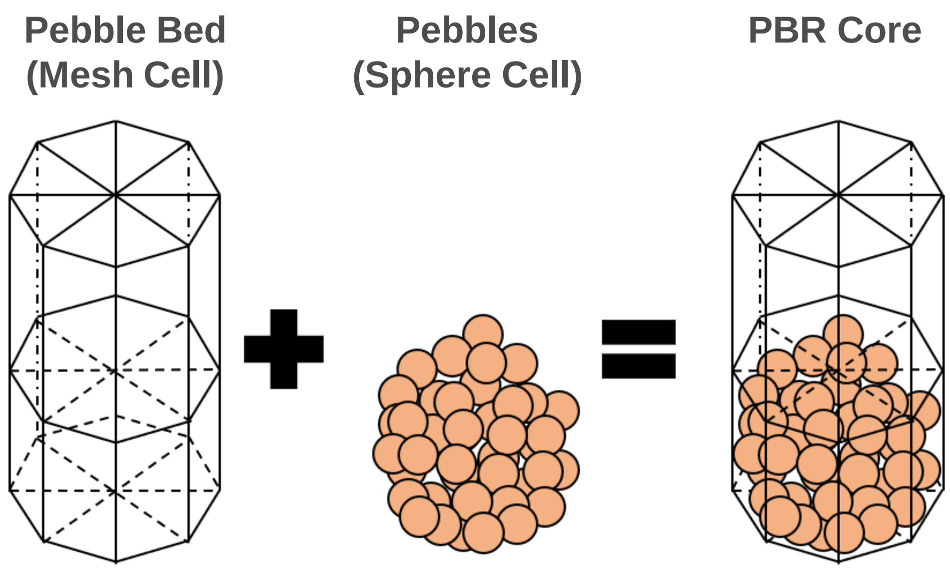
Basic Mesh Cells

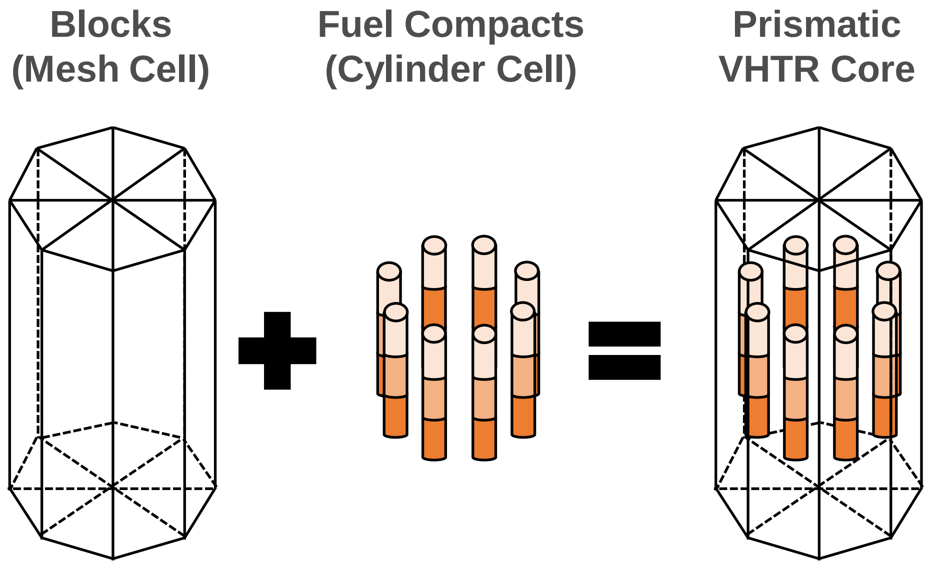


Ray Tracing for Neutron Tracking

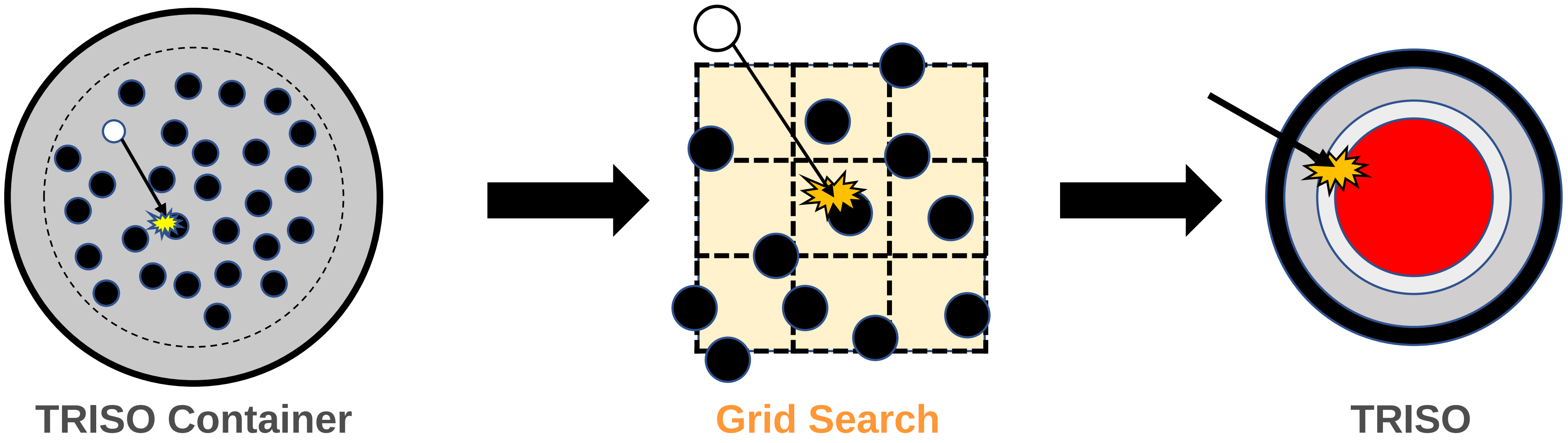


- **VHTR Modeling Strategy in PRAGMA**
  - **TRISO containers are modeled as special objects independently from the mesh-based geometry.**
    - Most structures can be modeled as volume conserved meshes, but TRISO containers should be modeled accurately due to variations in TRISO distribution.
    - It is inefficient to model the structure of a sphere and cylinder accurately using triangular meshes.
    - The special objects are superposed onto the mesh-based geometry.
  - **TRISO particles are generated explicitly in the fuel zone of a container using the Jodrey-Tory (JT) algorithm.**



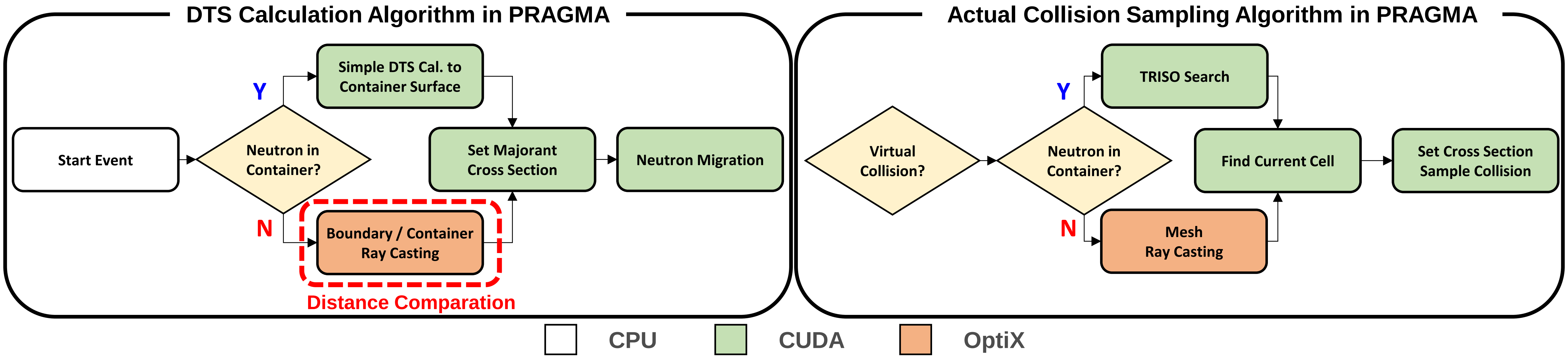


- **Double Heterogeneity Treatment of PRAGMA**
  - **The Woodcock delta-tracking scheme is adopted in a TRISO container with the container-wise majorant XS.**
  - **TRISO particles are not treated as a cell during neutron tracking such that TRISO particles are considered only when determining whether a neutron undergoes an actual collision or not.**
  - **The grid cell search strategy is adopted to find the exact neutron position in the TRISO distribution in a container.**
    - A virtual 3D grid cell with equivalent intervals is superposed onto the TRISO distribution.
    - When a neutron undergoes a virtual collision in a container, it is determined whether a neutron meets any TRISO particle in adjacent grids only.



Tracking Algorithm for VHTR Analysis in PRAGMA

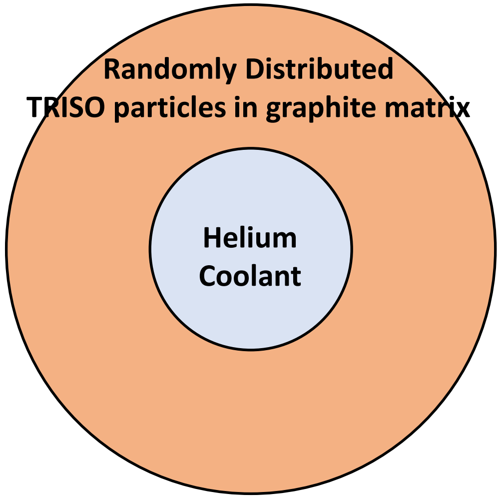
- The [1]localized delta-tracking scheme is adopted for an effective simulation.
- The container surfaces are also considered in every DTS calculation to sort neutrons based on their location.
  - For a neutron located not in a container, a DTS should be determined by comparing the distance to the nearest pebble surface and the distance to the nearest boundary surface.
  - For a neutron located in a container, a simple DTS calculation can be implemented to the container surface.



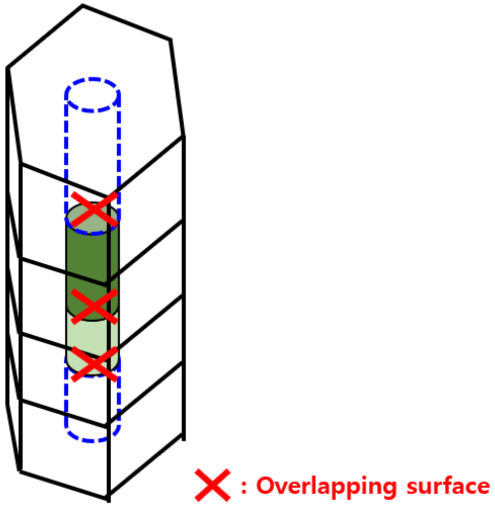
(1) N. Choi and H. G. Joo, "Analytic treatment of intra-fuel-rod temperature distributions in the GPU-based continuous energy Monte Carlo code PRAGMA," in *Transactions of the American Nuclear Society Annual Meeting*, 2020.

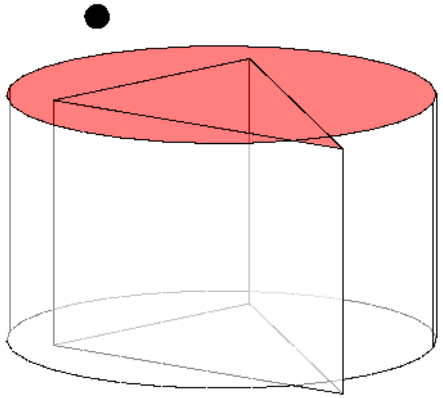
- **Limitations of PRAGMA VHTR Analysis Algorithm for 3D Prismatic VHTRs**
  - **An annular type compact can not be modeled due to the limitation of representing radially varying compositions.**
    - A container object can represent only a single fuel compact, having a single material composition and TRISO distribution.
  - **Significant degradations in the simulation performance are expected due to trapping neutrons between overlapping meshes and cylinder covers, due to truncation errors.**
    - A fuel element in a 3D prismatic VHTR core is modelled as a stack of cylindrical objects, causing overlapping surfaces.

Annular Fuel Compact in HTTR Core



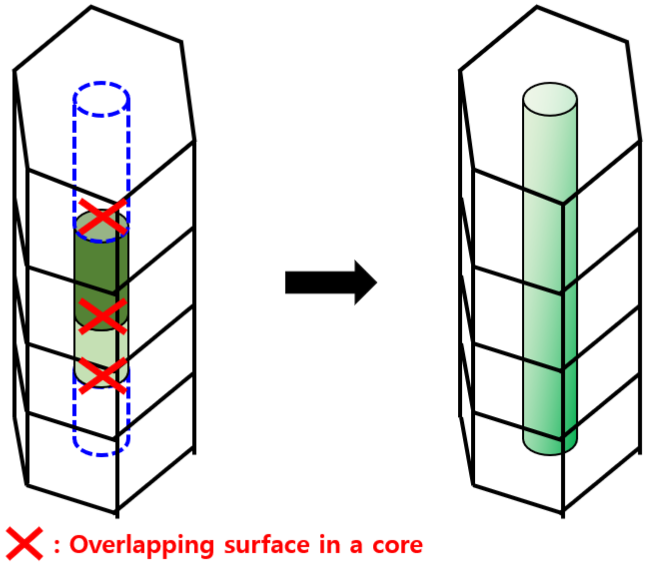
Trapped Neutron between overlapped surface



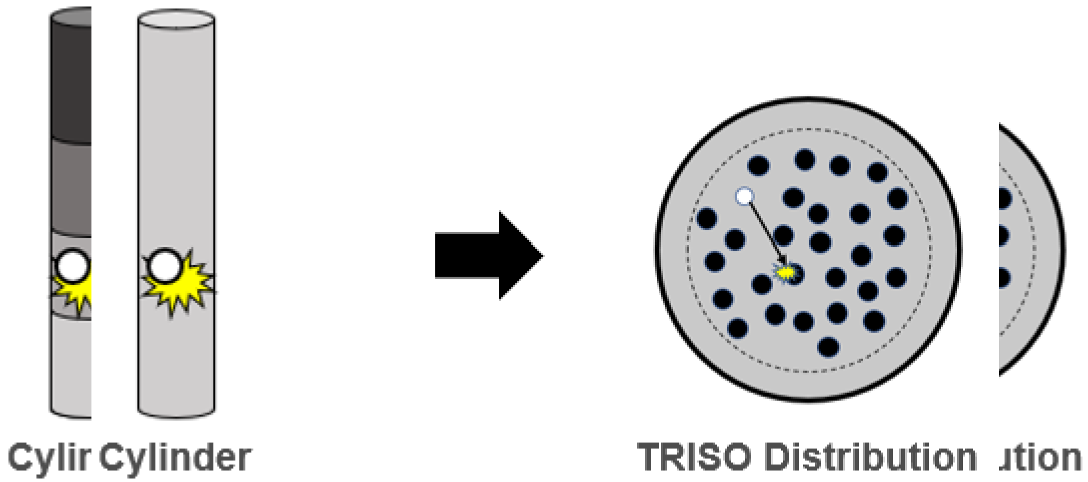


- **Refactored Geometry Modeling and Double Heterogeneity Treatment of 3D Prismatic VHTR**
  - **A cylindrical fuel element is represented as a single geometrical entity, incorporating all components, including the sleeve, helium, channel, and stacked fuel compacts.**
    - Detailed compositions within a cylinder are only considered when a neutron undergoes a virtual collision.
  - **TRISO searching process is developed according to the revised geometry modeling strategy.**

Modeling a fuel element as a single geometrical cylinder



Previous TRISO Searching Process



Verification of PRAGMA VHTR Module

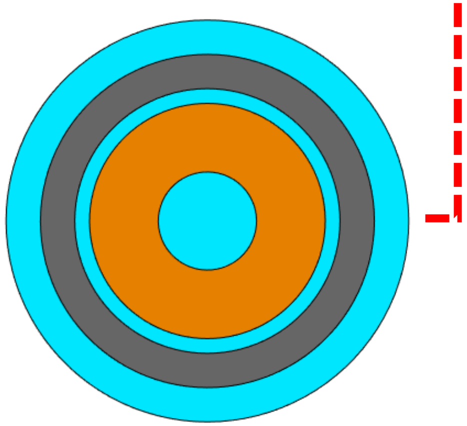
- **HTTR Benchmark Fuel Element Descriptions**
  - The High-Temperature Engineering Test Reactor (HTTR) problems are used to verify the PRAGMA VHTR analysis module.
  - In the HTTR core, there are 12 different TRISO particles having different uranium enrichments between 3.4 and 9.9 wt%.
  - With about 13,000 TRISO particles distributed in the annular fuel compact, the corresponding packing fraction is about 30%.
  - Fuel elements consist of a graphite sleeve containing 14 fuel compacts.

Fuel Element	
Number of Fuel Compacts	14
Height [cm]	58.0

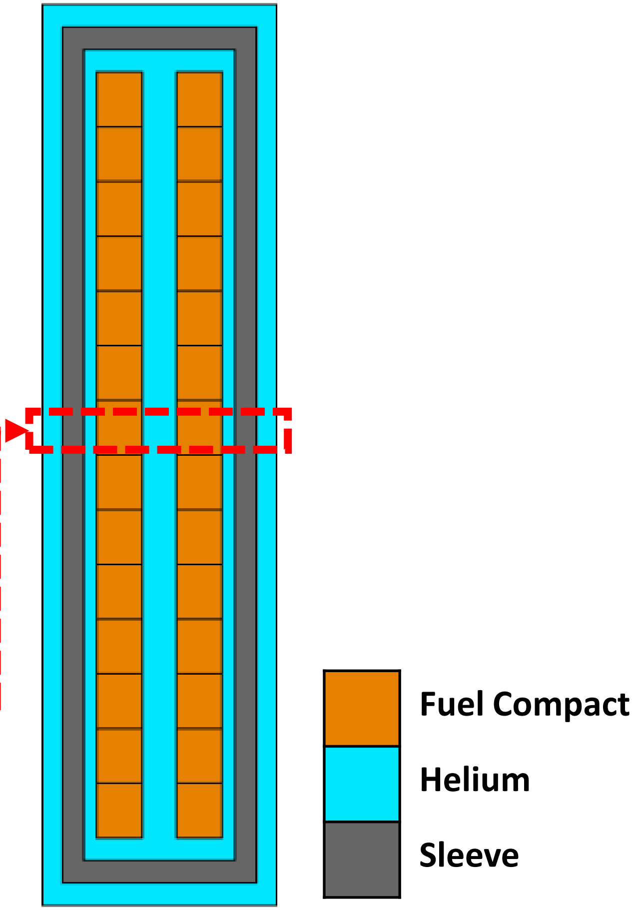
Fuel Compact	
Material	Graphite
TRISO Packing Fraction [%]	30
Height [cm]	3.9

TRISO	
Fuel Density $[g/\mathrm{cm}^3]$	10.39
Kernel Radius $[\mu m]$	300
Cooling Layer Material	PyC / PyC / SiC / PyC
Layer Density $[g/\mathrm{cm}^3]$	1.1 / 1.85 / 3.2 / 1.85
Layer Thickness $[\mu m]$	60 / 30 / 25 / 45

Horizontal Cross Section of Fuel Element



Vertical Cross Section of Fuel Element

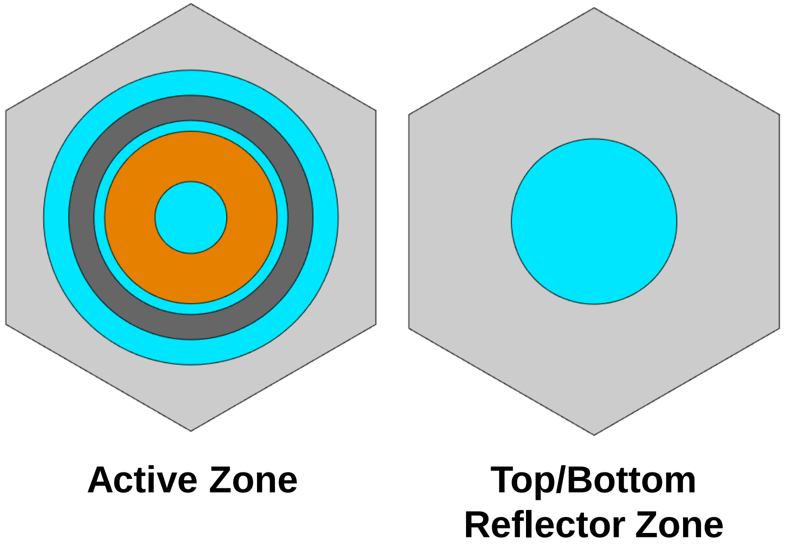


HTTR Fuel Pin Descriptions

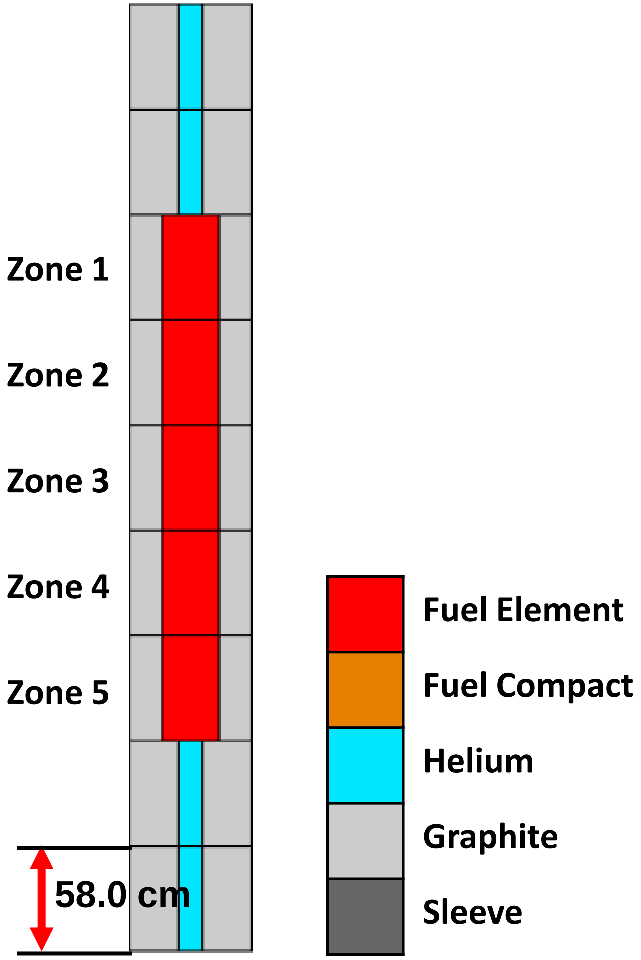
- There are **four pin types** according to **different uranium enrichments** and **natural boron contents.**
- Each fuel pin consists of five fuel elements at the axial active zone and coolant channels at top and bottom reflector zones.

Fuel Pin Description					
Pin Type		A	B	C	D
Enrichment of Uranium in TRISO particles [wt%]	Zone 1	6.7	7.9	9.4	9.9
	Zone 2	5.2	6.3	7.2	7.9
	Zone 3	4.3	5.2	5.9	6.3
	Zone 4	3.4	3.9	4.3	4.8
	Zone 5	3.4	3.9	4.3	4.8
Pin Pitch [cm]		5.15			
Height [cm]		522.0			

Horizontal Cross Section of Fuel Pin



Vertical Cross Section of Fuel Pin

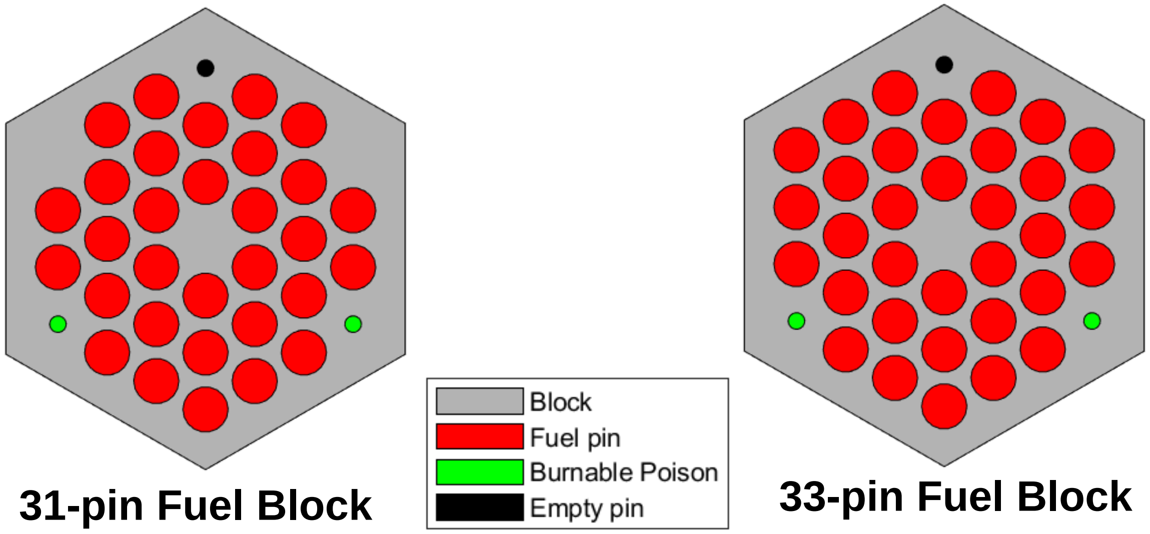


HTTR Fuel Block Descriptions

- **There are total four types of HTTR blocks according to fuel pin types and the number of fuel pins in a block.**
  - There are two types of regular hexagonal fuel blocks in the HTTR benchmark: 33-pin and 31-pin.
- **There are two burnable poisons and one empty pin at the active zone in each fuel block.**

Fuel Block Description				
Block Type	**A**	**B**	**C**	**D**
Fuel Pin	A	B	C	D
# of Fuel Pins	33		31	
Block Material	Graphite			
Block Pitch [cm]	36.0			

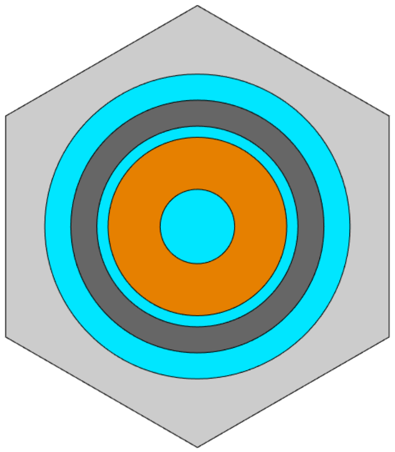
Horizontal Cross Section of Fuel Blocks



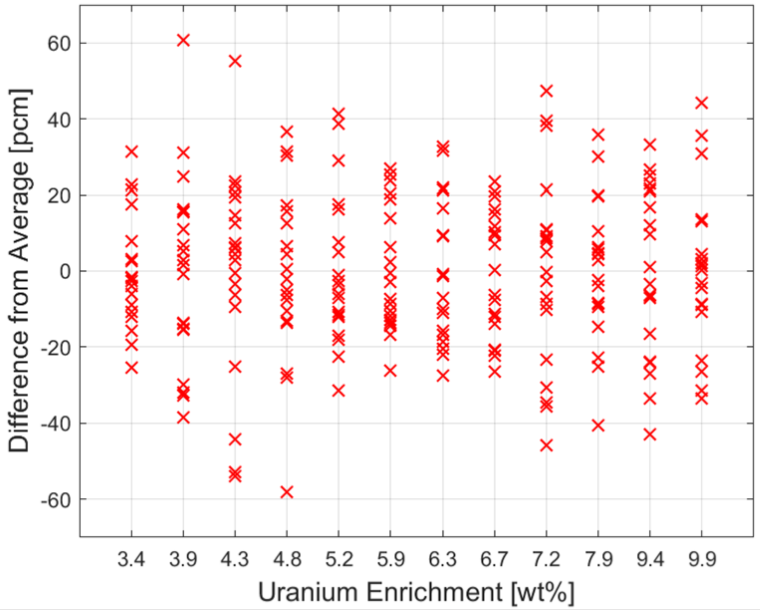
- **Random TRISO Distribution Uncertainty**
  - **Each fuel compact problem was repeated 20 times to verify the uncertainty caused by the random TRISO distribution.**
  - **It is shown that the multiplication factors are considerably affected by TRISO distribution.**
    - The real STD with the random distribution was quite large at over 16 pcm while that with the fixed distribution was around 7 pcm.

Calculation Condition	
# of Cycles	50 (Inactive) / 50 (Active)
# of Neutrons / Cycle	10,000,000
# of Repetitions	20
XS Library	ENDF/B-VII.1 (300K)
TSL Library	ENDF/B-VII.1 (296K)

Horizontal Cross Section of Fuel Compact Problem



Multiplication Factor Distribution



Verification of PRAGMA for 2D HTTR Fuel Compact Problems

- **Comparisons of 2D Fuel Compact Multiplication Factor Results by McCARD and PRAGMA**
  - **There are acceptable differences between PRAGMA and McCARD results, considering the uncertainty associated with the random TRISO distribution**
    - The maximum difference increases from 18 pcm to 87 pcm when the identical TRISO distribution is employed in every simulation.

McCARD Calculation Condition	
Number of Cycles	50 (Inactive) / 500 (Active)
# of Neutrons / Cycle	1,000,000

Multiplication Comparisons for 2D Fuel Compacts w/ Identical TRISO Distribution

Uranium Enrichment [wt%]	McCARD (M)	PRAGMA (P)	Diff. (P – M) [pcm]
3.4	1.25644 (7)	1.25657 (7)	13
3.9	1.27863 (6)	1.27861 (7)	-2
4.3	1.29303 (7)	1.29307 (5)	4
4.8	1.30789 (7)	1.30805 (7)	16
5.2	1.31806 (7)	1.31819 (7)	13
5.9	1.33283 (7)	1.33300 (7)	17
6.3	1.33990 (7)	1.34008 (8)	18
6.7	1.34622 (8)	1.34607 (7)	-15
7.2	1.35315 (7)	1.35321 (7)	6
7.9	1.36152 (7)	1.36141 (7)	-11
9.4	1.37562 (7)	1.37567 (7)	5
9.9	1.37948 (7)	1.37959 (8)	11

Multiplication Comparisons for 2D Fuel Compacts w/ Random TRISO Distribution

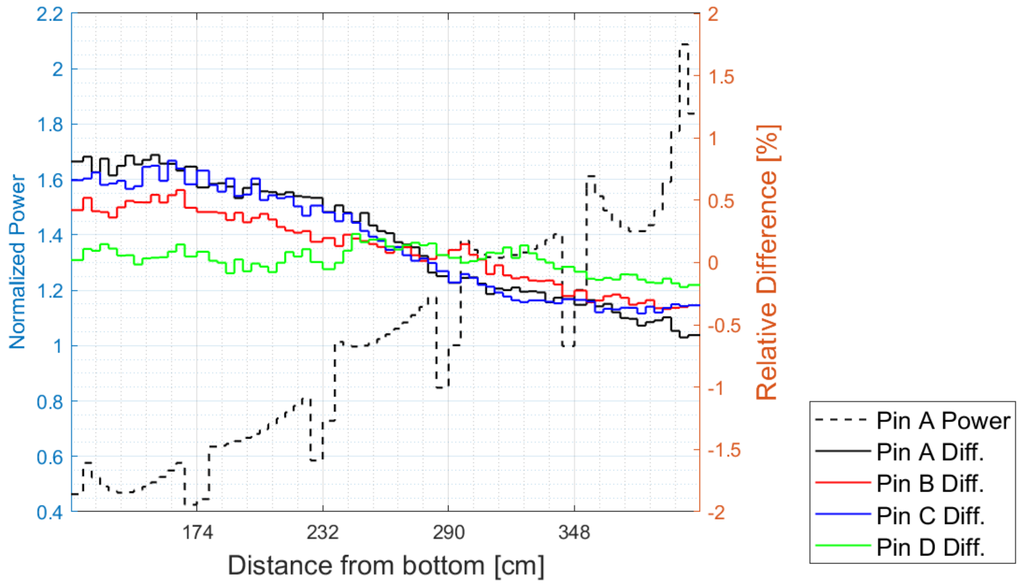
Uranium Enrichment [wt%]	McCARD (M)	PRAGMA (P)	Diff. (P – M) [pcm]
3.4	1.25574 (10)	1.25591 (6)	17
3.9	1.27810 (8)	1.27842 (7)	32
4.3	1.29214 (7)	1.29301 (7)	87
4.8	1.30785 (8)	1.30772 (7)	-13
5.2	1.31747 (8)	1.31744 (7)	-3
5.9	1.33226 (9)	1.33265 (7)	39
6.3	1.33898 (7)	1.33947 (7)	49
6.7	1.34586 (9)	1.34602 (7)	16
7.2	1.35255 (9)	1.35269 (7)	14
7.9	1.36071 (8)	1.36124 (7)	53
9.4	1.37507 (9)	1.37545 (7)	38
9.9	1.37916 (9)	1.37949 (7)	33

- **Comparisons of HTTR Fuel Pin Simulation Results by McCARD and PRAGMA**
  - **For fuel pin problems, PRAGMA results are consistent with McCARD results in view of the multiplication factor and axial power distribution.**
    - The maximum difference between multiplication factors is 38 pcm, which is acceptable considering the uncertainty from random TRISO distribution.
    - The maximum difference between axial power distributions is less than 1%.

Calculation Condition		
Code	McCARD	PRAGMA
# of Cycles	35 (Inactive) / 250 (Active)	35 (Inactive) / 50 (Active)
# of Neutrons / Cycle	1,000,000	10,000,000

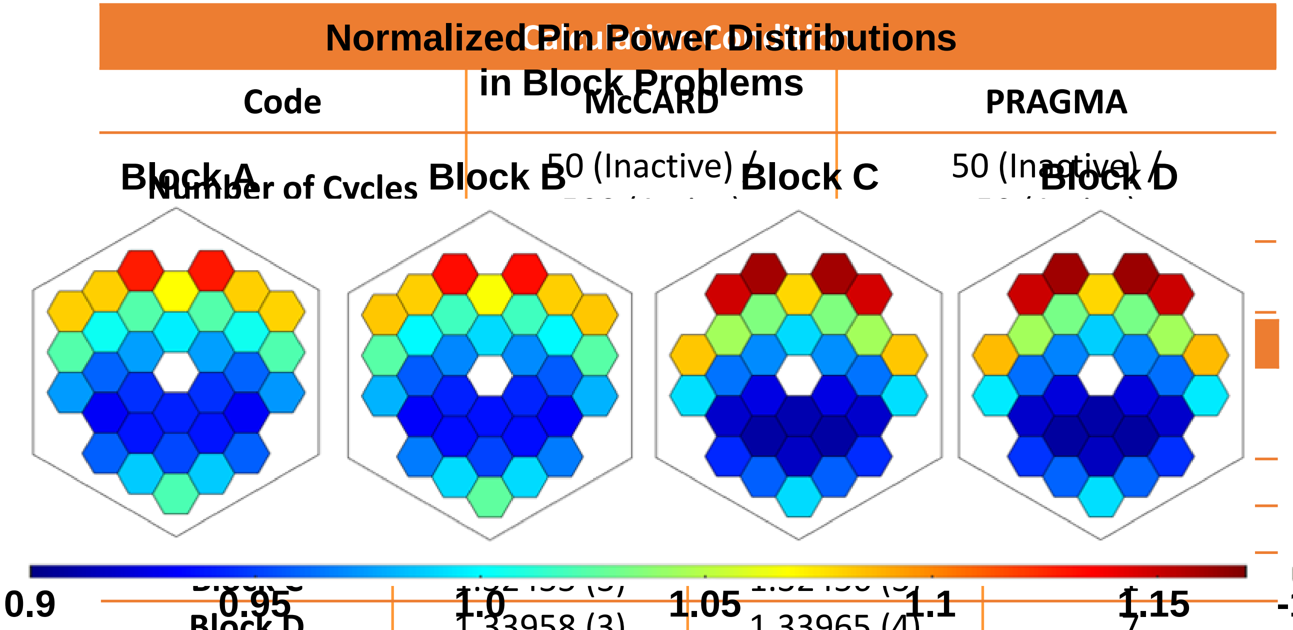
Multiplication Factor Comparisons for HTTR Fuel Pins			
Pin Case	McCARD (M)	PRAGMA (P)	Diff. (P - M) [pcm]
Pin A	1.30062 (4)	1.30077 (6)	15
Pin B	1.32296 (4)	1.32294 (7)	-2
Pin C	1.33903 (5)	1.33929 (8)	26
Pin D	1.34719 (5)	1.34757 (6)	38

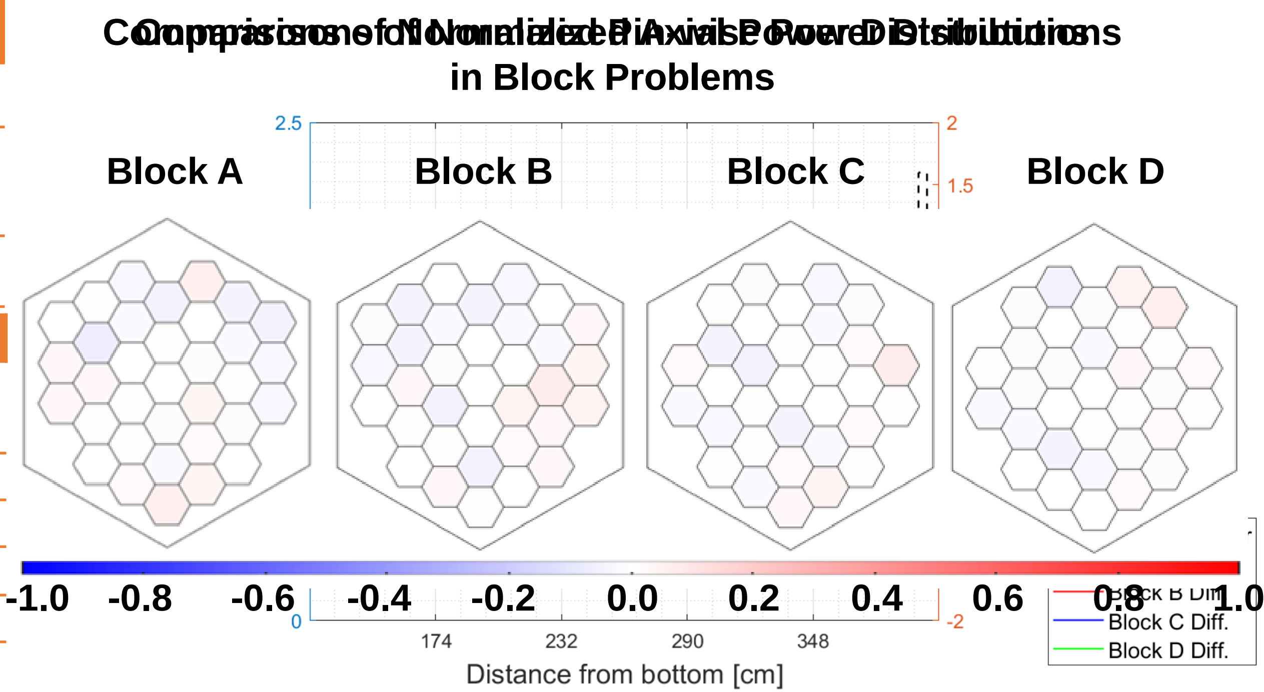
Comparisons of Normalized Axial Power Distributions in Pin Problems



Verification of PRAGMA for HTTR 3D Fuel Block Problems

- **Comparisons of HTTR 3D Fuel Block Simulation Results by McCARD and PRAGMA**
  - **For fuel block problems, PRAGMA results are consistent with McCARD results in view of the multiplication factor, axial power distribution, and pin-wise power distribution.**
    - The maximum difference of multiplication factor results is 9 pcm, which is acceptable.
    - The maximum difference between axial power distributions is less than 0.4% for all cases.
    - The maximum differences of pin power distributions calculated by McCARD and PRAGMA are less than 0.07%.



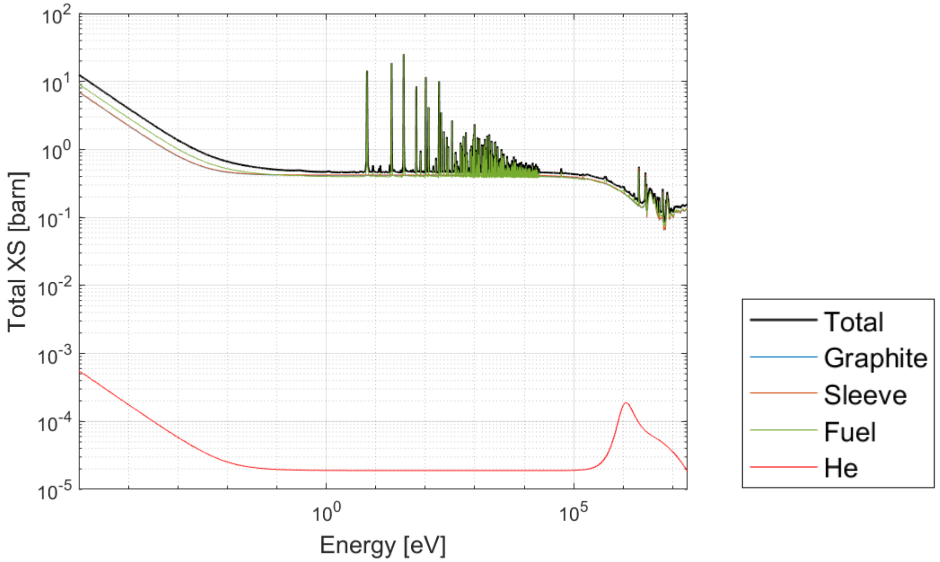


Improvements in Computational Performance of PRAGMA VHTR Module

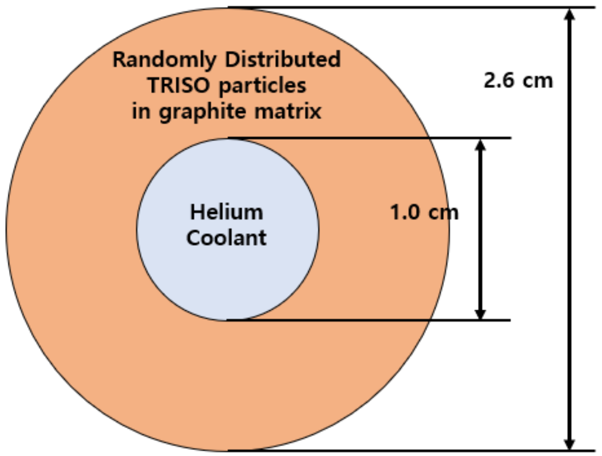
Necessity of Delta-Tracking Application in an Annular Type Fuel Compact

- **Region-wise Delta-Tracking (RDT) Development for Annular type Fuel Compact**
  - There is significant disparity between majorant cross sections of helium and other materials in a fuel compact.
  - The unnecessary virtual collisions are expected in the helium coolant region due to significantly low majorant cross sections of helium.
  - The localized delta-tracking scheme is extended to RDT, to apply the delta-tracking to each region of a fuel element having several material compositions.

Comparisons of Majorant Cross Sections in a HTTR Fuel Element



Horizontal Cross Section of HTTR Fuel Compact



- **Calculation Specifications of PRAGMA and McCARD for Computational Time Comparison**
  - **To assess the effect of RDT scheme, PRAGMA simulations are conducted both with and without RDT schemes for all cases.**
    - The effectiveness of the RDT scheme should be assessed regarding its impact on computing time, as implementing the RDT scheme in a cylinder necessitates additional distance calculations for surface of each region.
  - **McCARD and PRAGMA employ the same number of inactive cycles and the same total number of histories in active cycles.**
    - McCARD simulations are performed with 200 MPI processes and PRAGMA simulations are performed with 4 MPI processes.

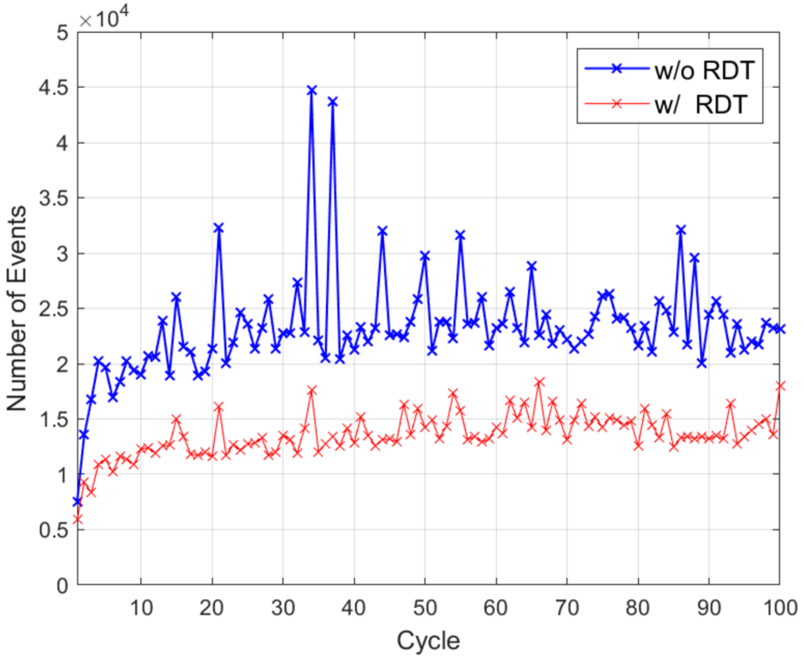
Computational Processors		
Code	**PRAGMA**	**McCARD**
# of Processes	**4**	**200**
CPU	2 x Intel Xeon E5-2630 v4 @ 2.2Hz	20 x Intel Xeon Silver 420R @ 2.4Hz
GPU	4 x NVIDIA GeForce RTX 2080 Ti	-

Calculation Condition		
Code	**McCARD**	**PRAGMA**
# of Cycles	50 (Inactive) / 500 (Active)	50 (Inactive) / 50 (Active)
# of Neutrons / Cycle	1,000,000	10,000,000

Computational Performance of PRAGMA for 3D HTTR Fuel Blocks

- **Computing Time Comparisons of PRAGMA and McCARD for 3D HTTR Fuel Blocks**
  - **The number of events per cycle significantly decreases after applying the RDT scheme in fuel elements.**
    - The average number of events per cycle decreases by almost half, employing the RDT scheme.
  - **The computing time of PRAMGA is reduced by about 30%, which exhibits the effectiveness of RDT scheme.**
  - **PRAGMA out-performs McCARD in view of the computational performance.**

Number of Events in HTTR Fuel Block 1 Simulation

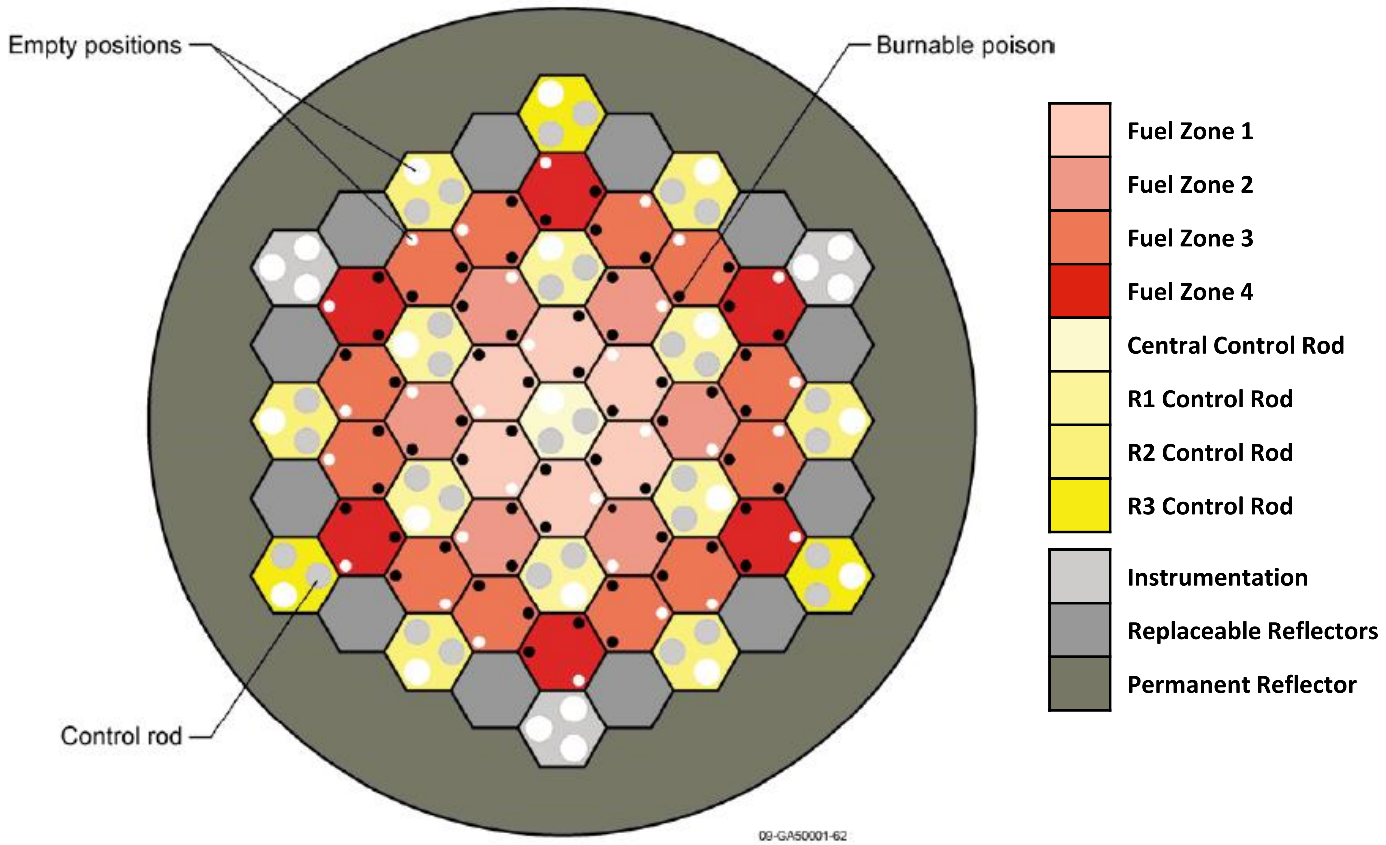


Average Number of Events per Cycle in PRAGMA Simulations			
Case	w/o RDT (A)	w/ RDT (B)	Ratio (B / A) [%]
Block 1	23266	13562	58.3
Block 2	23381	13378	57.2
Block 3	24289	12995	53.5
Block 4	24475	12935	52.8

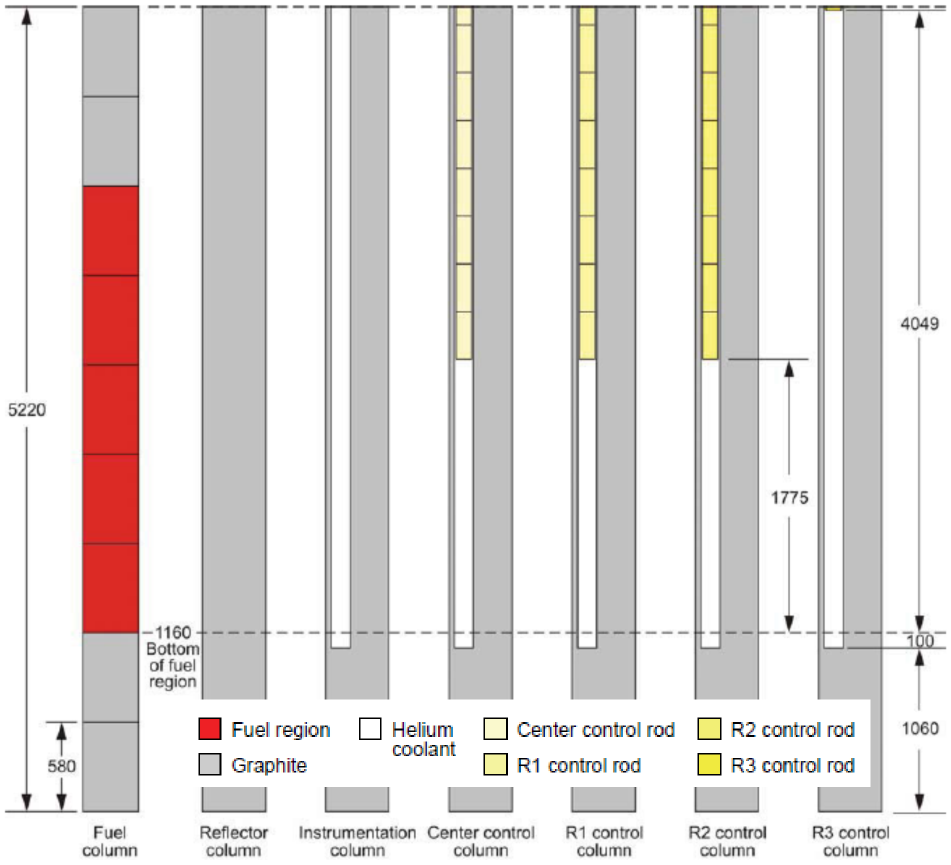
Computing Time Comparisons between McCARD and PRAGMA			
Case	McCARD (M)	PRAGMA w/o RDT (P)	Ratio (P / M) [%]
Block 1	4h 43m 28s	35m 29s	12.5
Block 2	4h 31m 59s	34m 46s	12.8
Block 3	4h 11m 27s	33m 53s	13.5
Block 4	4h 7m 14s	33m 46s	13.7

- **HTTR 3D Core Benchmark Description**

Horizontal Cross-sectional View of HTTR Core



Vertical Cross-sectional View of HTTR Core



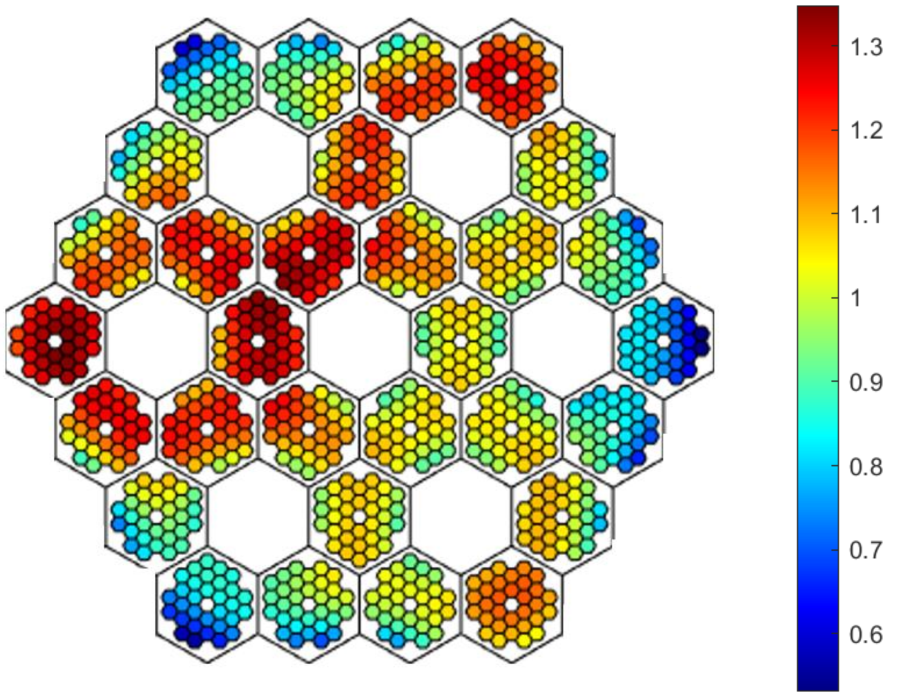
Preliminary Verification of PRAGMA for HTTR 3D Core Problem

- **HTTR 3D Core Calculation Results using PRAGMA**
  - There is an **acceptable difference between multiplication factors** by MCNP5 and PRAGMA.
  - The total computing time is almost 1 hour 30 minutes with 200 millions of neutrons per cycle.

Calculation Condition	
# of Cycles	50 (inactive)/ 50 (active)
# of Neutrons / Cycle	200,000,000
Library	ENDF/B-VII.0 (300K)
# of GPUs	24 x NVIDIA RTX A5000

Calculation Results		
Multiplication Factor	MCNP5 (M)	1.02220 (10)
	PRAGMA (P)	1.02252 (1)
	Diff. (P – M)	32 pcm
Computing Time		1h 30m 37s

Pin-wise Power Distribution of HTTR Core



- **Developed Efficient GPU-based VHTR Analysis Module for 3D Prismatic VHTRs**
  - **The geometry modeling and tracking algorithms were developed for 3D VHTR core simulations.**
  - **The Region-wise Delta-Tracking (RDT) scheme was introduced to address potential computational performance degradation with multiple material compositions.**

- **Verified Acceptable Differences of PRAGMA from McCARD for HTTR 3D Problems**
  - **The maximum multiplication factor differences of the pin problems and block problems were 38 pcm and 9 pcm, respectively.**
    - The differences are acceptable in view of the uncertainty associated with the random TRISO distribution.
  - **The axial power distribution differences of the pin problems and block problems were less than 1.0% and 0.4%.**
  - **For block problems, the maximum differences in pin power distributions was 0.07%, respectively.**

- **Verified Computational Performance of PRAGMA VHTR Analysis Module**
  - **The number of events per cycle significantly decreases after applying the RDT scheme in fuel elements**
  - **The RDT scheme reduced PRAGMA's computing time by approximately 30%.**
  - **PRAGMA performance was at least 7 times faster than McCARD performance for HTTR block problems.**
    - McCARD – 200 MPI Processes / PRAGMA – 4 MPI Processes

- **Performed Preliminary Verification for the HTTR 3D Core Problem**
  - **Acceptable agreement was observed in the multiplication factors between MCNP5 and PRAGMA.**
    - The difference in the calculated multiplication factor between PRAGMA and MCNP5 was 31 pcm.
  - **The total computing time was almost 1 hour 30 minutes with 200 millions of neutrons per cycle.**

- **Future Plan**
  - **The VHTR analysis module in PRAGMA will be further verified with 3D VHTR benchmark problems.**
    - PRAGMA will be used to simulate the HTTR and HTR 3D full cores.
  - **PRAGMA will be coupled with the SOPHIA code for a multi-physics analysis of PBRs.**
    - It is expected that the temperature calculation for pebbles will also be solved by SOPHIA.
  - **A depletion calculation scheme optimized for a PBR core will be developed in the VHTR analysis module in PRAGMA.**

Preliminary PRAGMA-SOPHIA Coupled Simulation