西安交通大學
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Nuclear Thermal-hydraulic Lab

5th Joint ICTP-IAEA Workshop

Multiphysics modelling of Gen-IV reactors Part 2 – MOOSE

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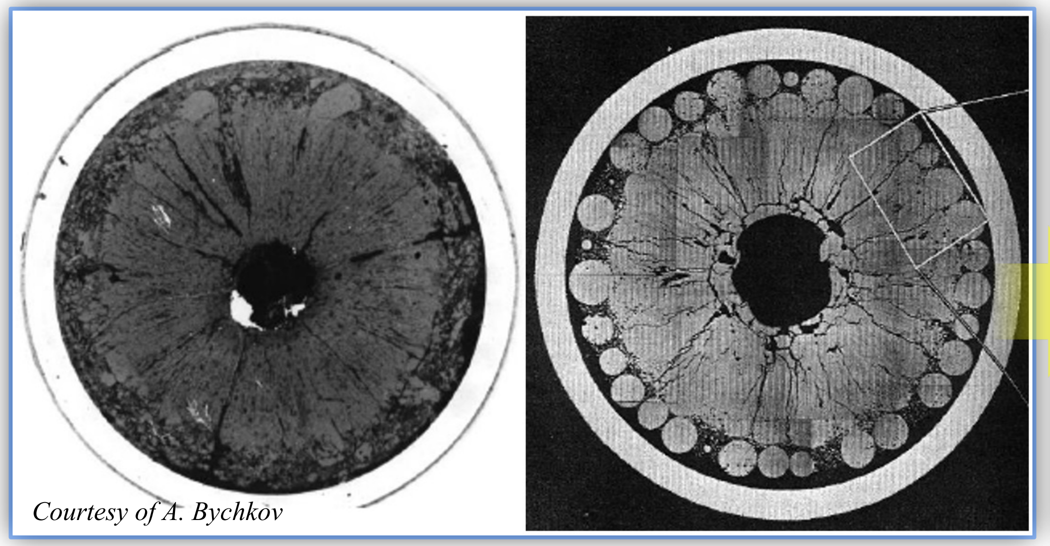
Contents

4.1 Research background

Safety and reliability of Gen-IV reactors:

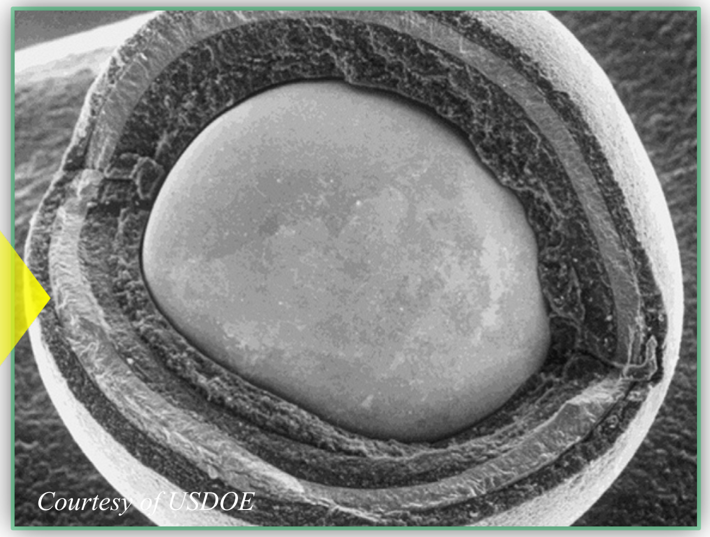
- **Nuclear fuel pin is the key component of Gen-IV reactors. Its mechanical strength and healthy will be weakened after neutron irradiation.**
- **After Fukushima accident, the fuel behavior prediction and high safety fuel are urgently required.**

After irradiation – BN600 pin & TREAT pin



2011 Fukushima accident

TRISO – "Most robust fuel on Earth"



Fuel safety is the first consideration!

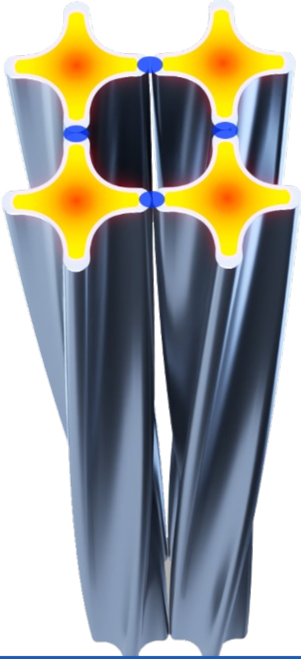
Goals of Gen-IV reactors
✓ *Sustainability* ✓ *Economics* ✓ ***Safety and reliability*** ✓ *Non-proliferation and protection*

4.1 Research background

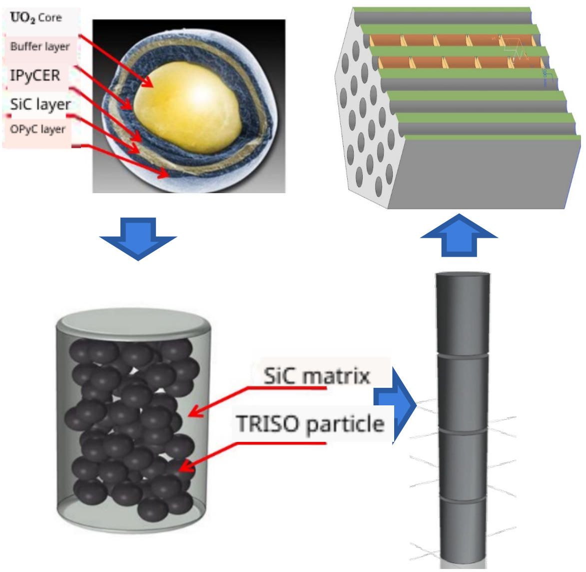
Challenges of advanced nuclear fuel in Gen-IV reactors:

- ATF, helical cruciform fuel (HCF), and TCR fuel **require high-fidelity multi-physics analysis.**
- Legacy tools (e.g., FRAPCON) lack flexibility for complex geometries/coupling.

ATF: SiC cladding



Helical cruciform fuel



Particle dispersion fuel

Traditional software like **FRAPCON**

- limited to simple structures
- limited to few physics

↓ Major demands

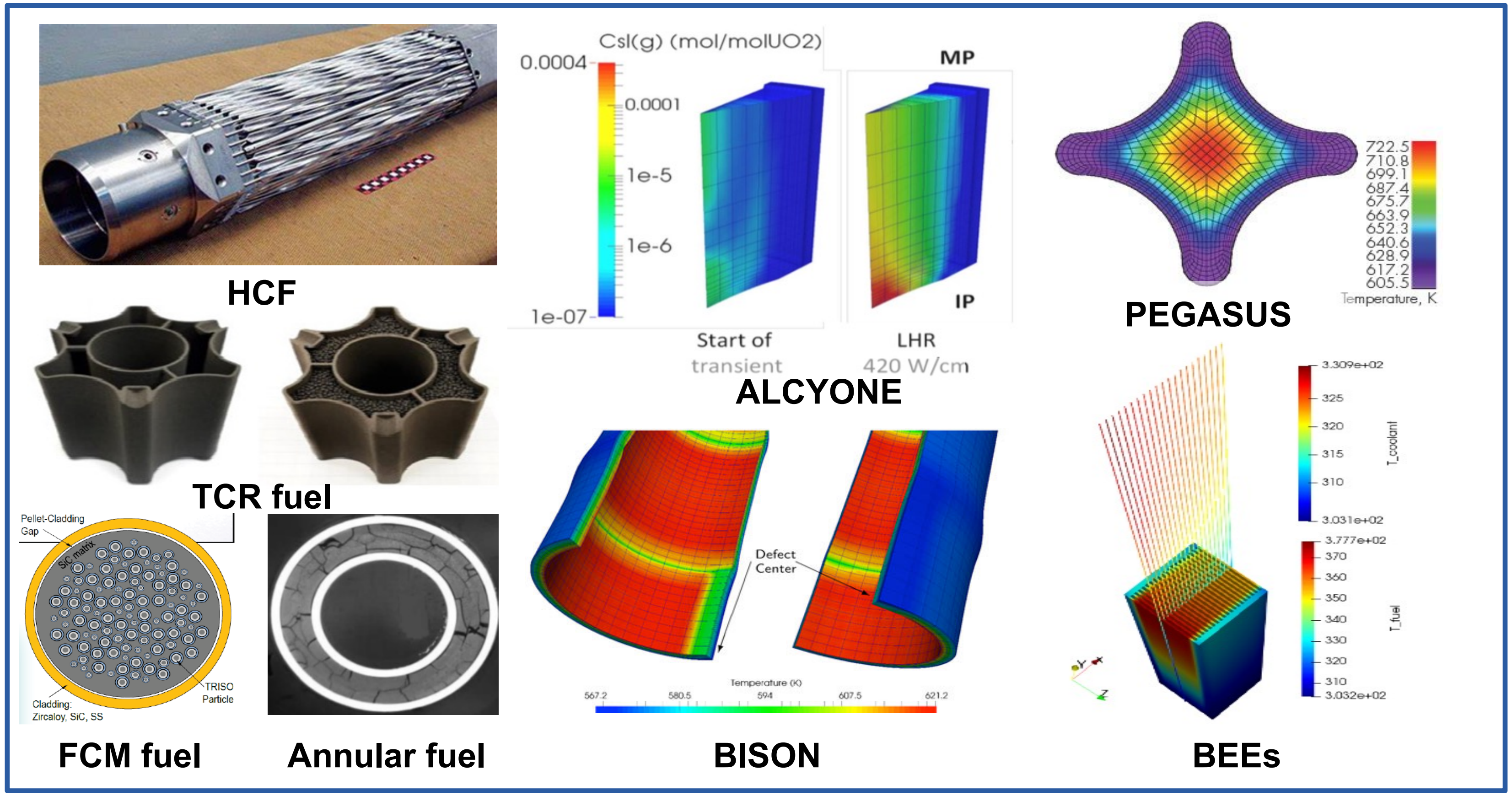
Multi-physics + high precision numerical algorithm

4.1 Research background

Why Finite Element Method (FEM)?

- **Advantages: High accuracy for solid mechanics analysis.**
- **Industry trend: FALCON(EPRI), BISON (INL), ALCYONE (CEA) all adopt FEM.**

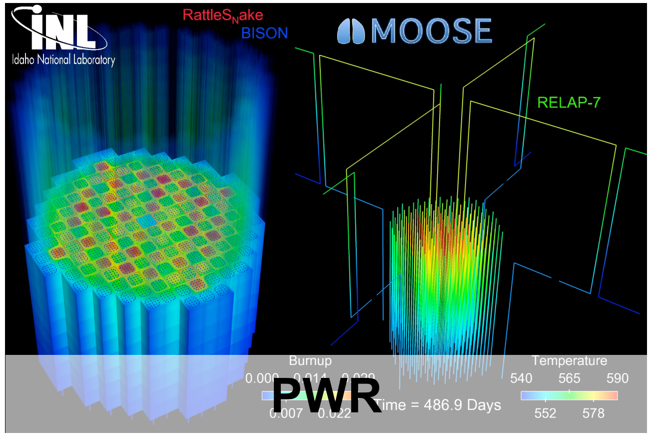
Code	Developer
COMSOL	Commercial software
ABAQUS	Commercial software
BISON	INL/USA
FALCON	EPRI/USA
PEGASUS	SI/USA
DIONISIO	CNEA/Argentina
ALCYONE	CEA, FRAMATOME, EDF/French
MERCURY	KAERI/Korean
PRIME	UNIST/Korean
BEEs	XJTU/China



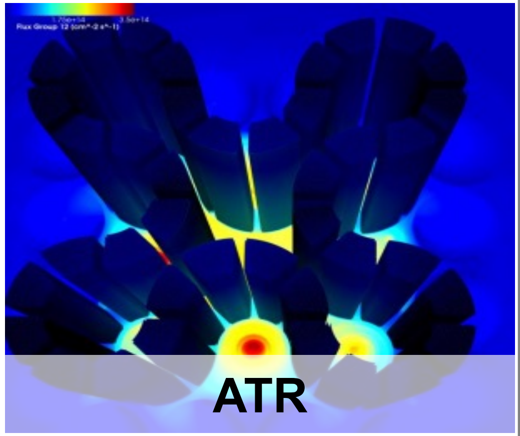
4.1 Research background

MOOSE is an open-source, FEM based computational framework for multi-physics coupling simulations. Key capabilities include:

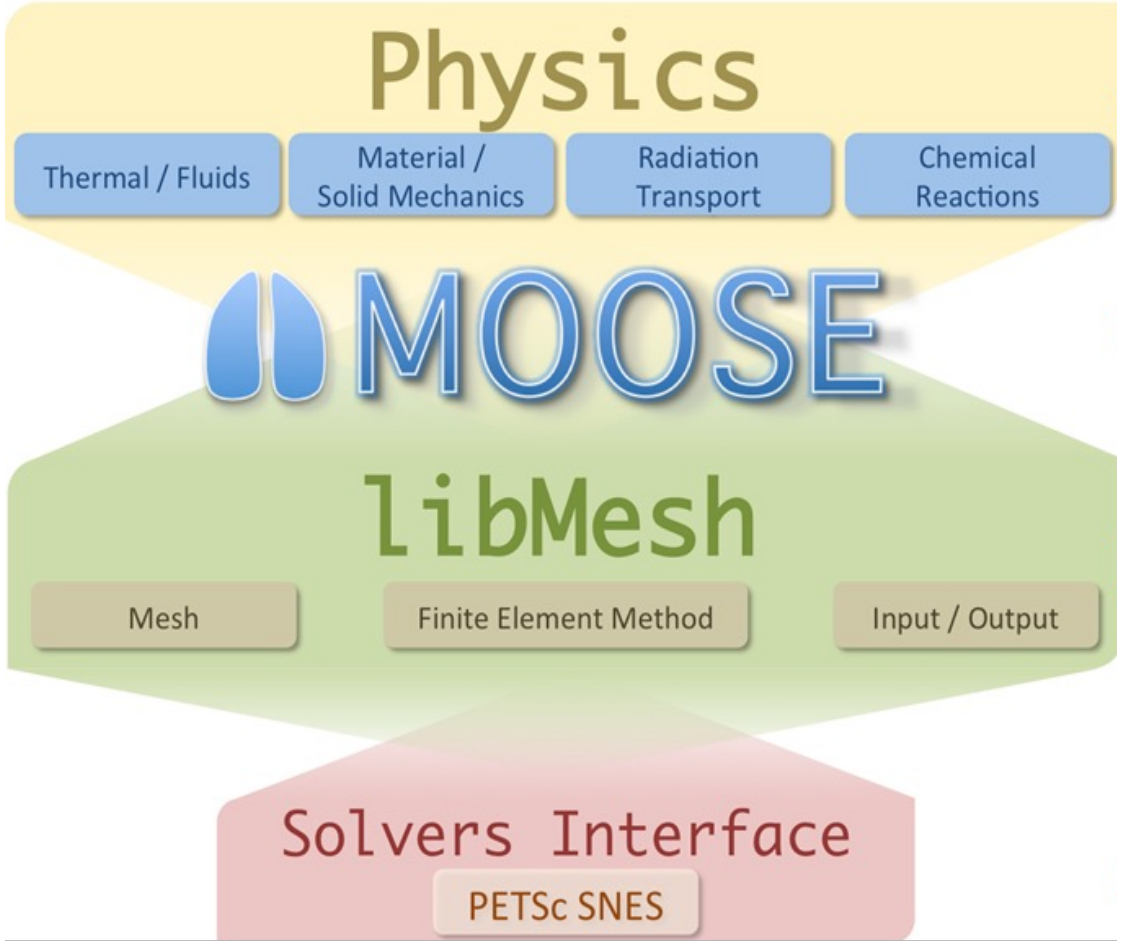
- **High-Performance Computing**
- **Advanced Numerical Methods**
- **Extensibility**
- **Modular Architecture**



PWR



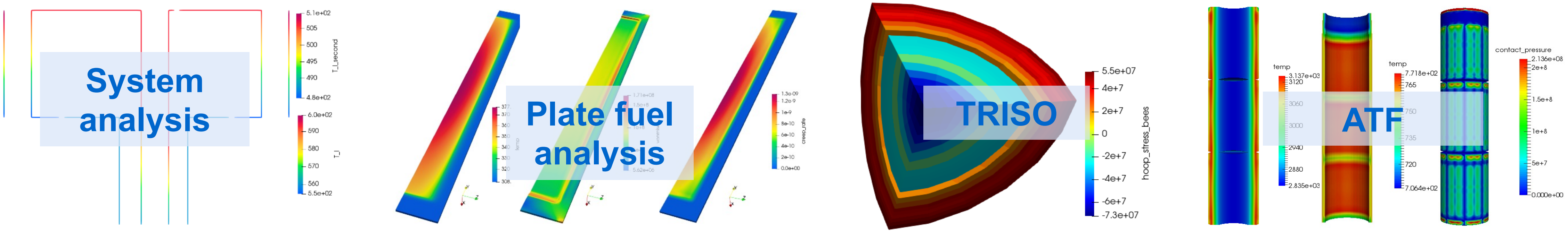
ATR

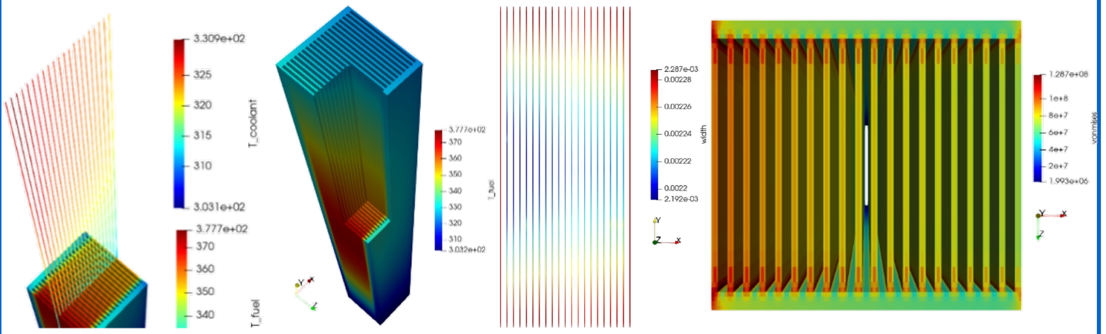


4.2 Introduction of code BEEs

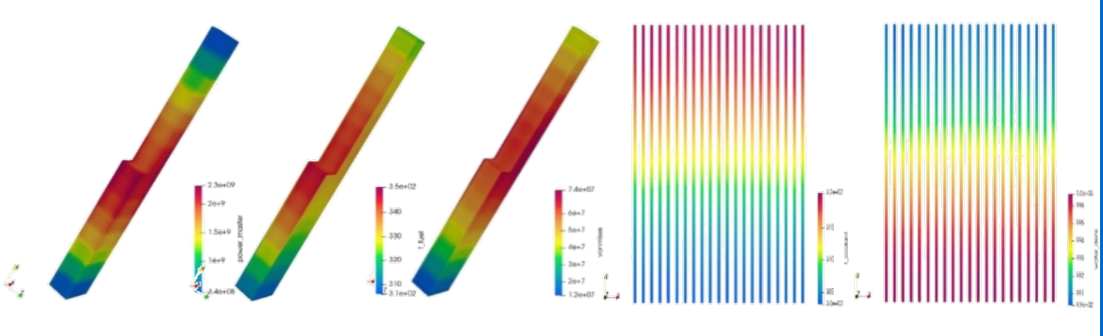
BEEs is developed by XJTU-NuTheL: Multi-Fuel Simulation Platform

- **Fuel types: Rod, annular, plate, TRISO.**
- **Physics: Irradiation-thermal-mechanical coupling + Fluid-structure interaction (FSI).**





FSI



Irradiation-Thermal-Mechanical coupling simulation

4.3 BEEs for Rod fuel

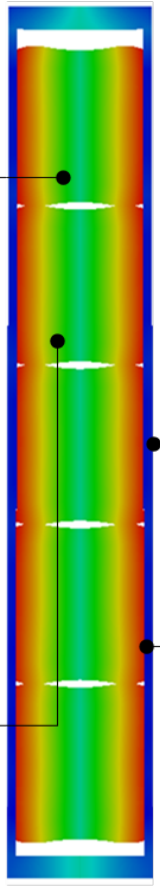
➢ **Features overview**

Pellet

- Thermodynamic properties
- Relocation (rupture)
- Densification
- Thermal expansion
- Fission product swelling
- Fission gas release
- Grain growth
- Elasto-plasticity

Auxiliary

- TUBRNP burnup model
- Cavity temperature
  - ✓ Thermal conductivity
  - ✓ Density
  - ✓ Viscosity
- Contact model
- Internal pressure
- Integrated neutron flux



Cladding

- Thermodynamic properties
- Thermal expansion
- Irradiation growth
- Oxidation
  - ✓ Normal operating conditions
  - ✓ High-temperature oxidation
- Phase transformation
- Plastic deformation
- Creep
  - ✓ Thermal creep
  - ✓ Irradiation-induced creep
  - ✓ High-temperature creep
- Hydrogen absorption
- Failure criteria
  - ✓ Critical stress
  - ✓ Critical creep rate

Gap

- Heat transfer coefficient
  - ✓ Thermal conductivity (MATPRO)
  - ✓ He-Xe-Kr gas mixture
- Gap heat transfer

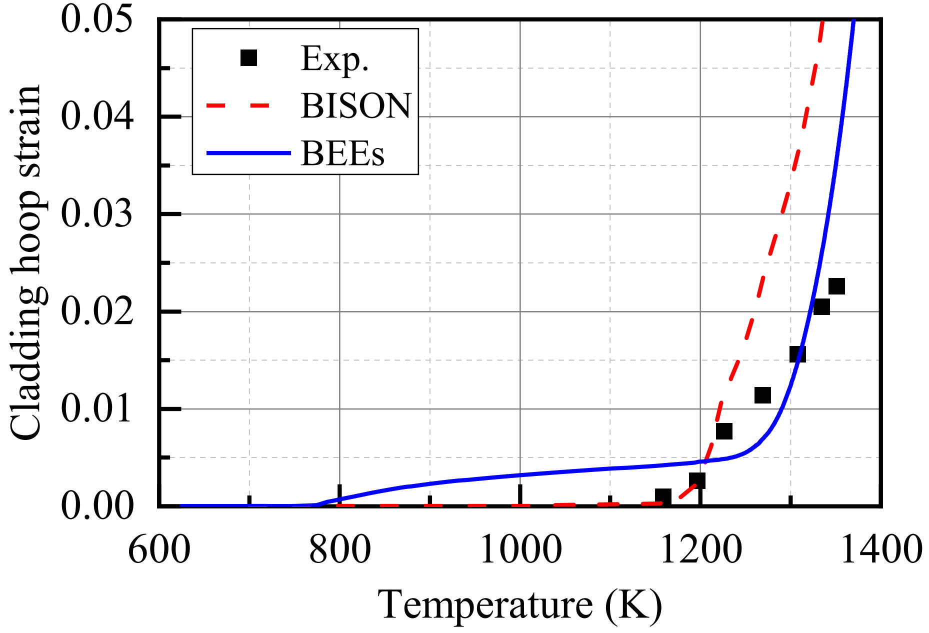
4.3 BEEs for Rod fuel

Category	Source	Validation Content
Module Validation	Hardy tube experiment	High-temperature creep
	Yoo H Y experiment	High-temperature oxidation
	George P. Sabol experiment	Cladding phase transformation
	Khan M K experiment	Failure criteria
	Geelhood experiment	Cladding elastic-plasticity
	Kammenzind experiment	Cladding corrosion & hydrogen absorption
Benchmark cases	Hypothetical fuel rod simulation	Pellet temperature, fission gas, gap
	Benchmark 15309	Pellet temperature, cladding temperature
	RISØ AN3 experiment	Pellet temperature, fission gas release
Steady-State Validation	IFA-432 experiment	Pellet temperature
	BR-3 experiment	Fission gas release
LOCA Validation	MT-4/MT-6 experiments	Cladding temperature, cavity temperature, internal pressure
RIA Validation	Na2 experiment	Pellet temperature, cladding temperature, cladding deformation

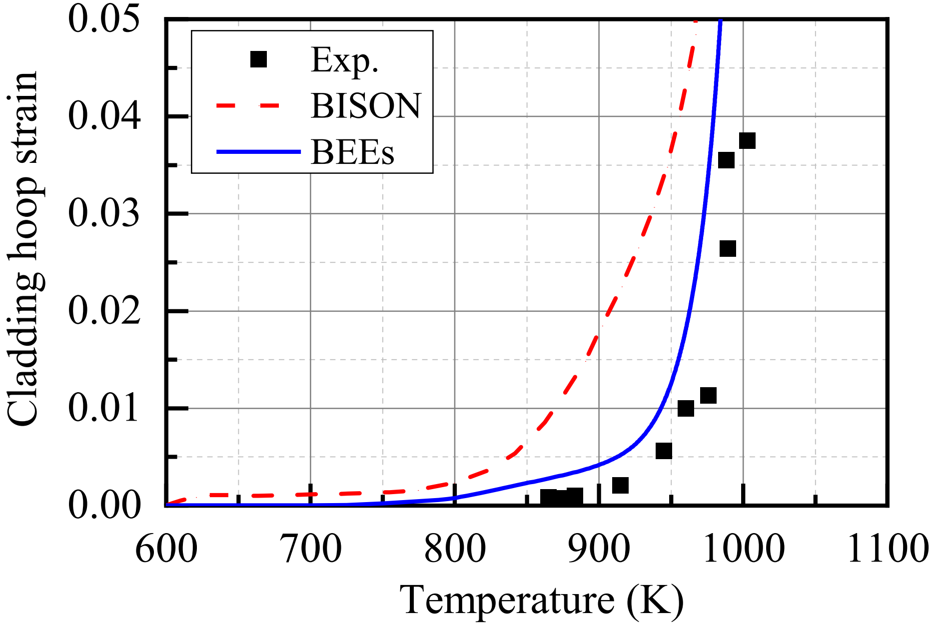
4.3 BEEs for Rod fuel

- The cladding hoop strain of rod fuel is validated with experiments under **0.3 MPa and 0.5 MPa** conditions.
- With the increase of temperature, the cladding hoop strain increases because of **thermal creep behavior**.
- BEEs show **good prediction ability for thermal creep behavior**.

Rod inner pressure 0.3 MPa

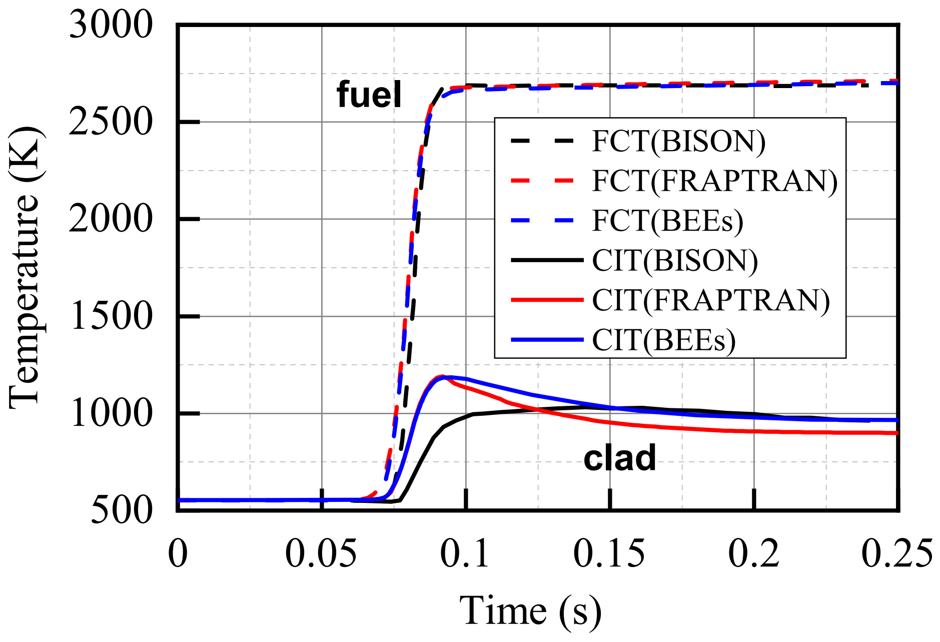


Rod inner pressure 5.5 MPa

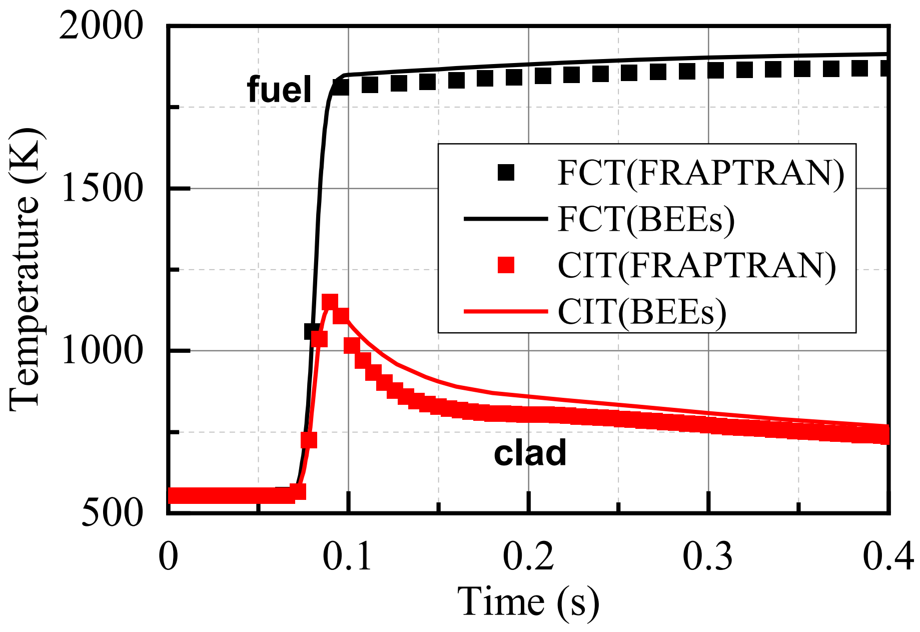


4.3 BEEs for Rod fuel

- CABRI REP-NA is a reactivity-initiated accident (RIA) experiment conducted by IRSN, which is used to evaluate the ability of BEEs for analyzing RIA.
- BEEs has similar prediction results with FRAPTRAN and BISON, showing good numerical accuracy.



RIA simulation for CABRI REP-Na2

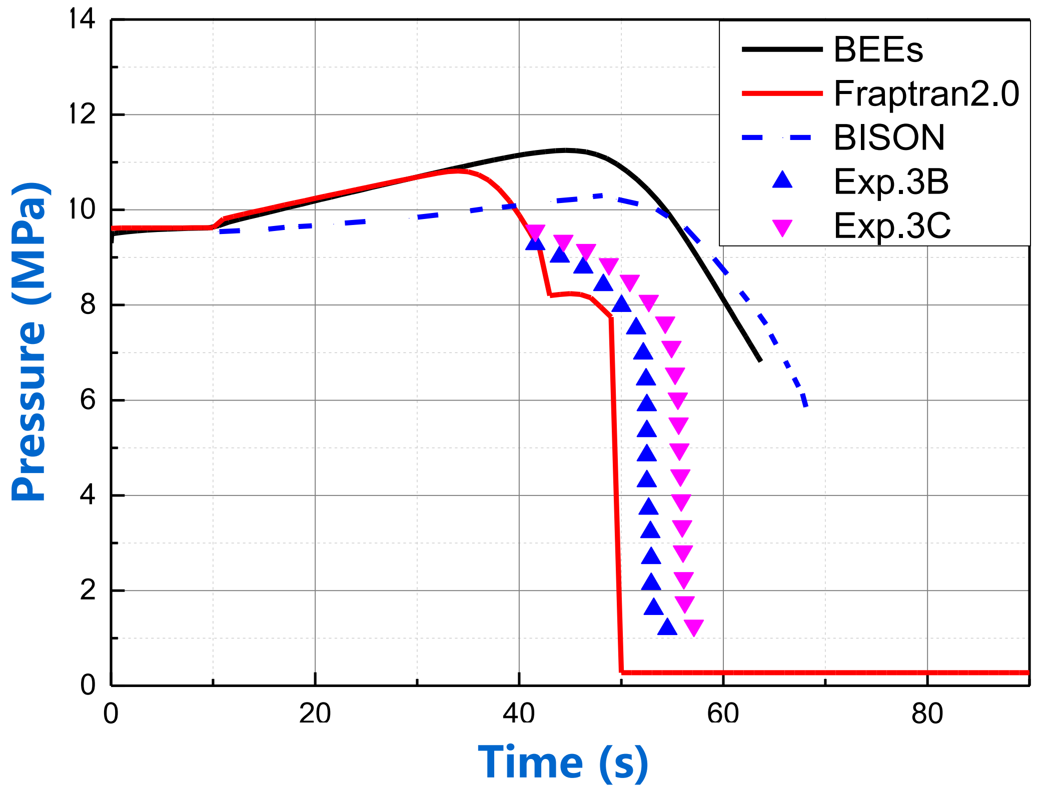


RIA simulation for CABRI REP-Na3

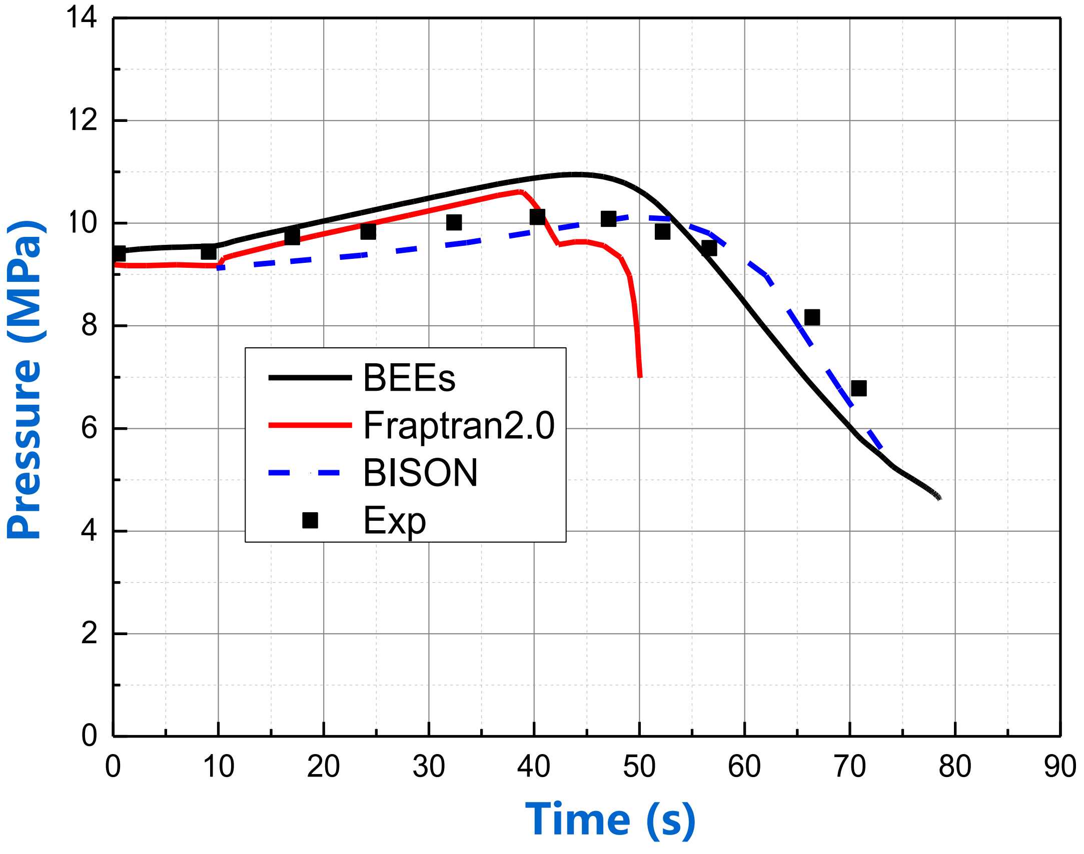
Comparison of fuel centerline temperature (FCT) and cladding inside temperature (CIT) to predicted results by FRAPTRAN (He et al., 2019b) and BISON (Perez et al., 2013)

4.3 BEEs for Rod fuel

- LOCA accidents are validated by MT-4/6 experiments, that BEEs has reasonable predictions.
- Above discussions indicate BEEs **has good prediction ability for steady, RIA, and LOCA conditions.**



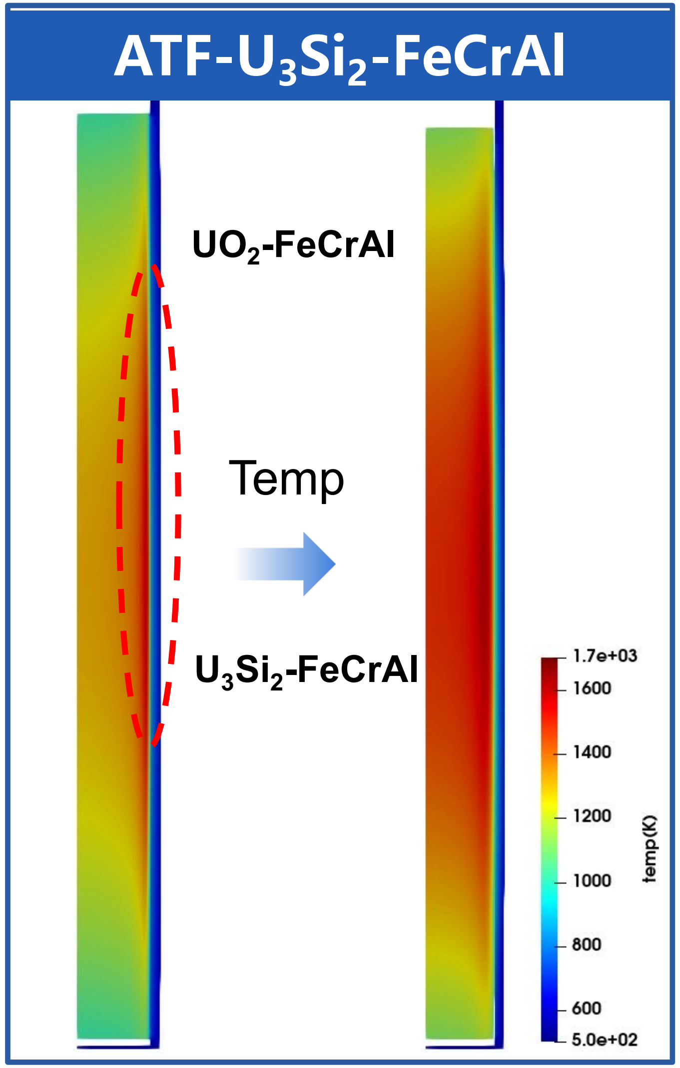
LOCA accident simulation for MT-4

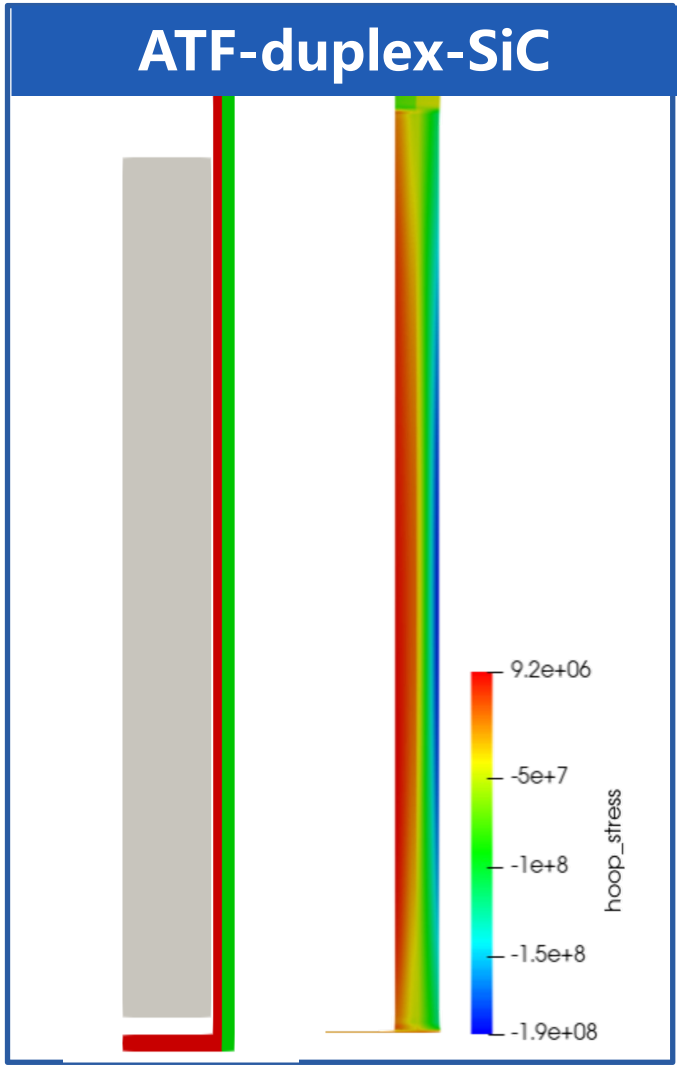


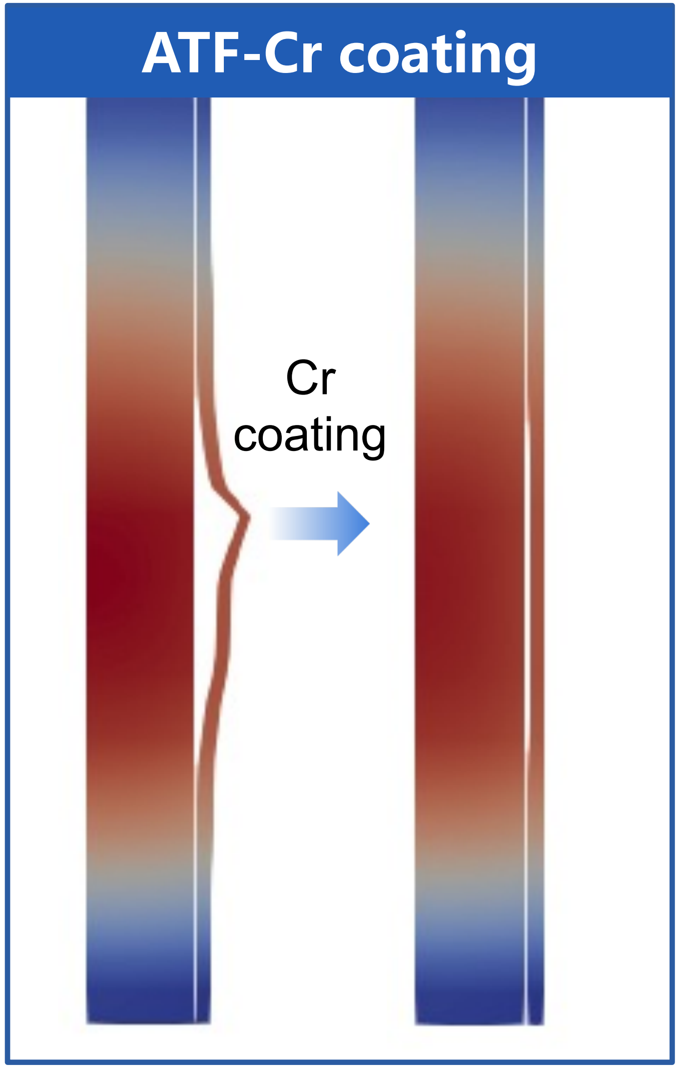
LOCA accident simulation for MT-6

4.3 BEEs for Rod fuel

- BEEs also supports simulation of different cladding types, such as SiC composites and Cr coating.



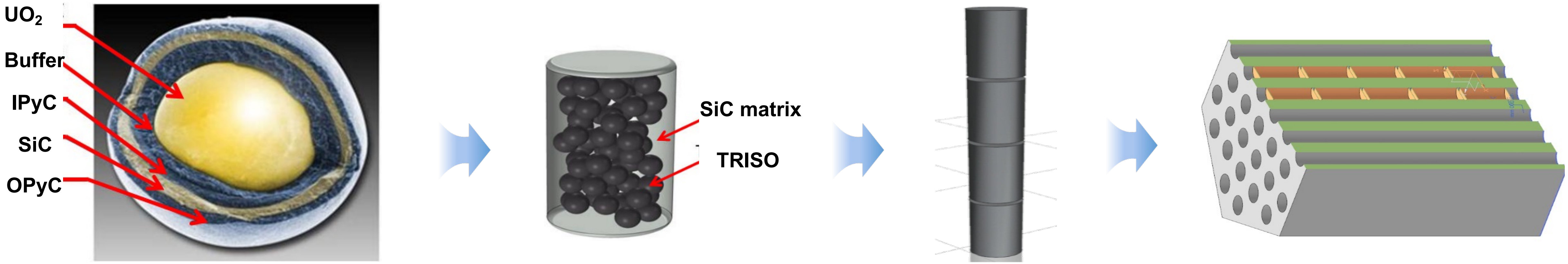




4.4 BEEs for TRISO fuel

High safety novel fuel TRISO used for Gen-IV small modular reactor (SMR)

- compact fuel consists of thousands of tri-isotropic fuel (TRISO) particles dispersed in silicon carbide (SiC) matrix.
- The SMR fuel is high volume packing fraction and horizontally placed within graphite channels



TRISO particle **Fuel pellet** **Fuel rod** **Assembly**

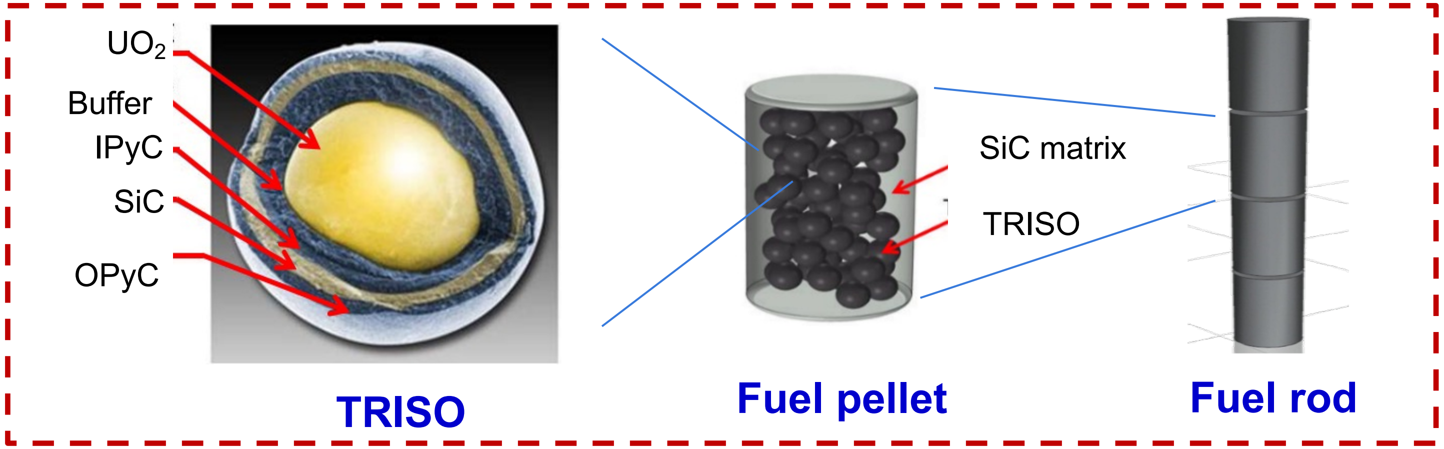
4.4 BEEs for TRISO fuel

Material properties

- Thermal conductivity
- Density
- Specific heat capacity
- Elastic properties

Irradiation behaviors

- Irradiation swelling
- Creep deformation
- Fission gas release
- Burnup model



Failure model

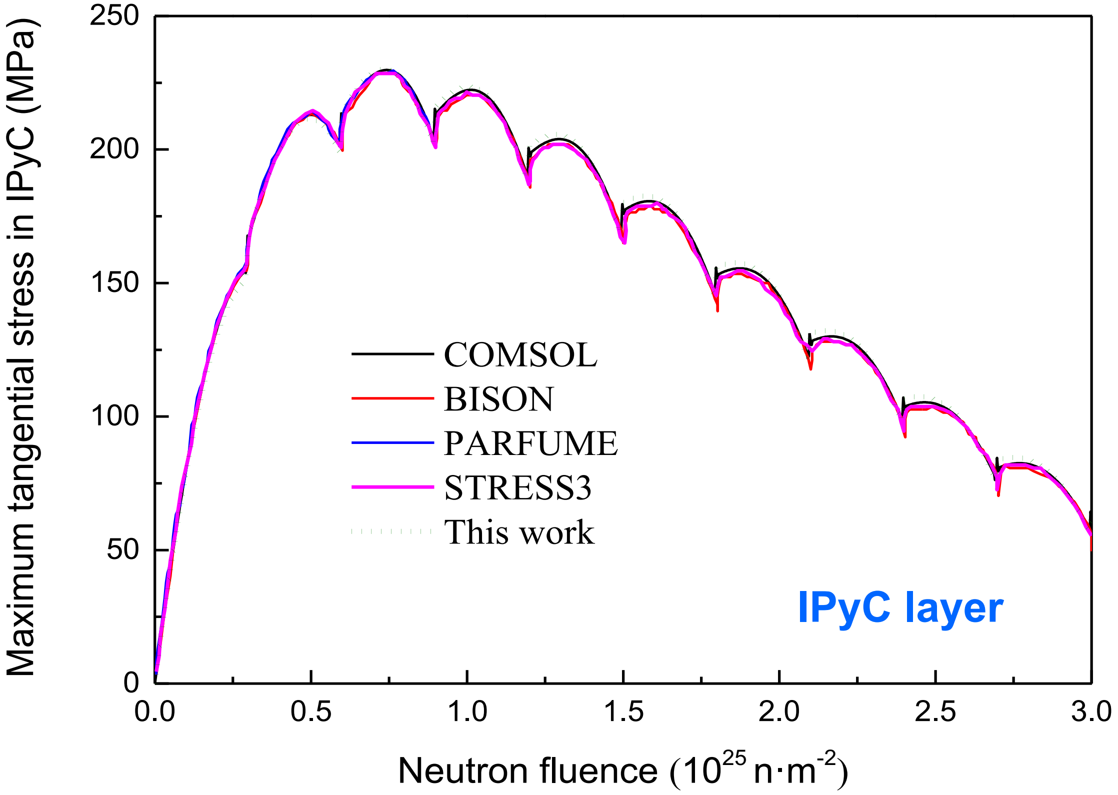
- Core migration
- Pd corrosion
- SiC failure

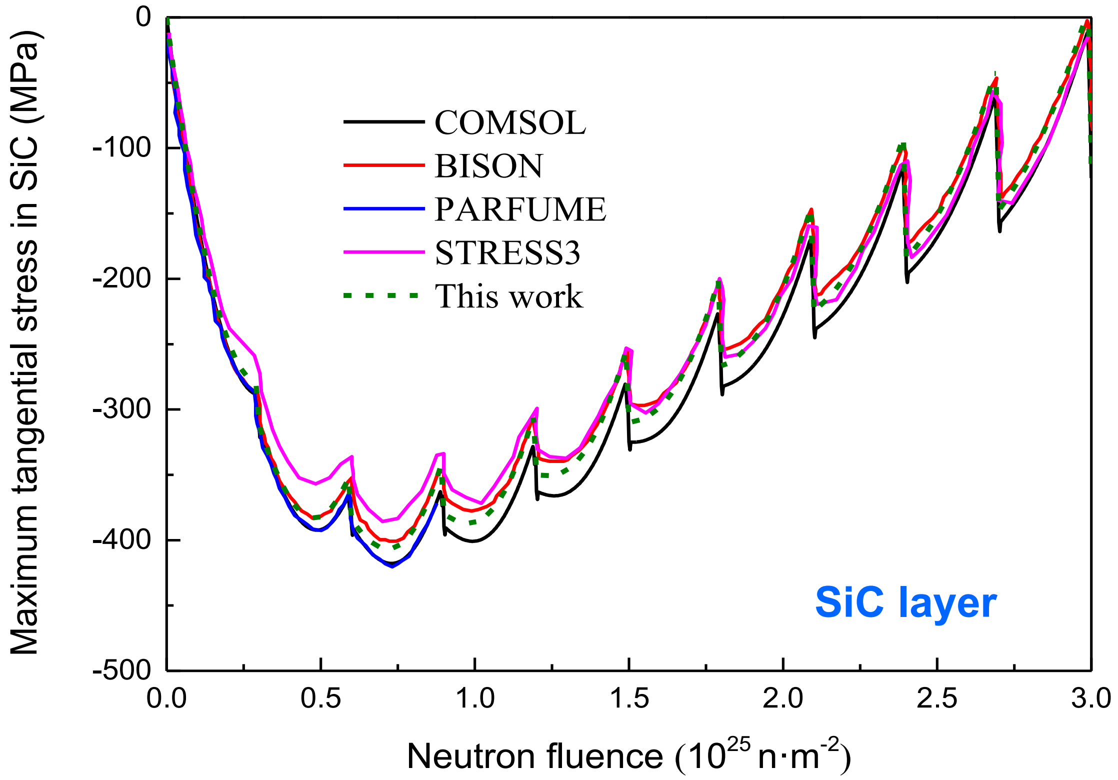
Other

- Gap heat transfer
- Gap internal pressure
- Contact model
- Cohesive zone model

4.4 BEEs for TRISO fuel

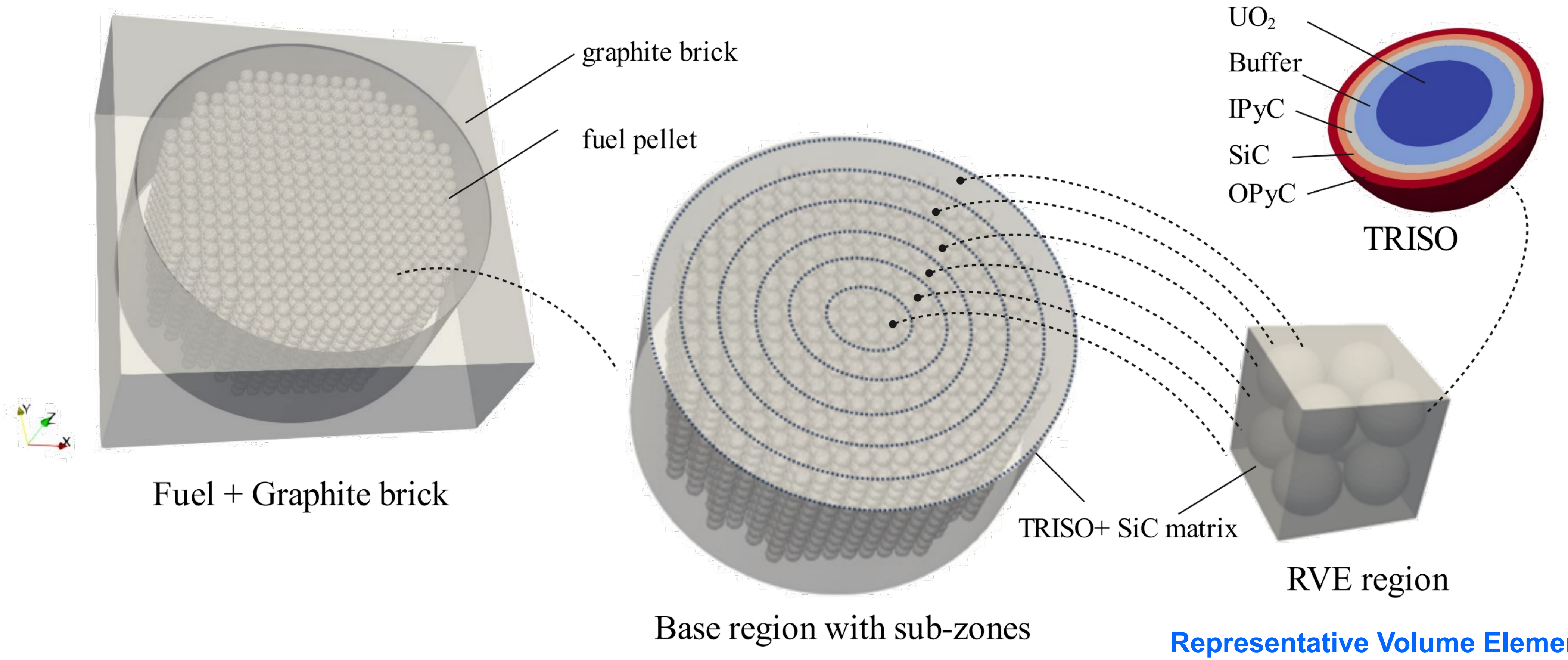
- BEEs is validated with the IAEA CRP-6 benchmark for TRISO fuel. Tangential stresses in iPyC and SiC layers during neutron irradiations are focused.
- The results of BEEs are consistent with those of COMSOL, BISON, PARFUME, and STRESS3, showing the reliable numerical predictions.





4.4 BEEs for TRISO fuel

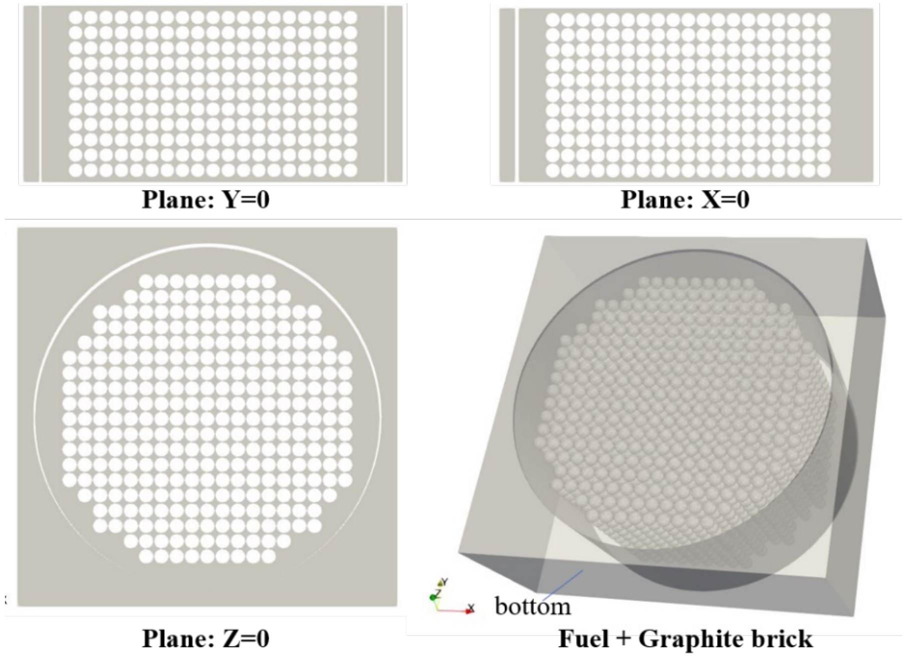
- One fuel pin contains thousands of TRISO particles, needing amount of computational workloads.
- "Base + RVE" multi-scale method is proposed for large-scale simulation. Base region is used to determine the global behavior and RVE performs the high accuracy simulation of TRISO and matrix.



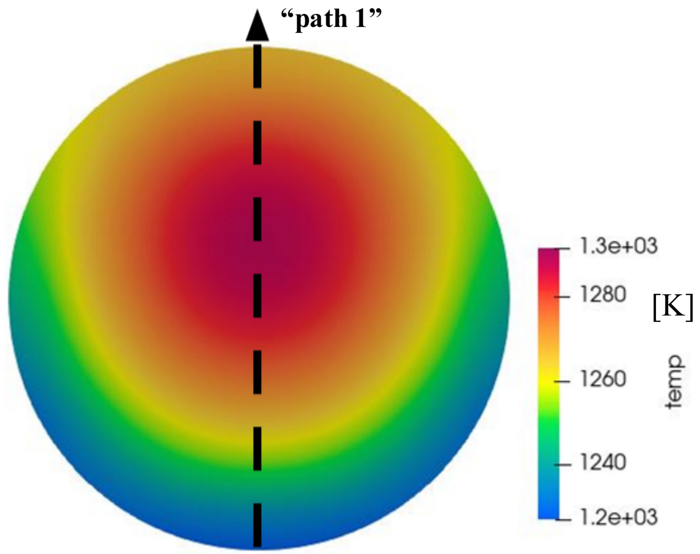
Representative Volume Element

4.4 BEEs for TRISO fuel

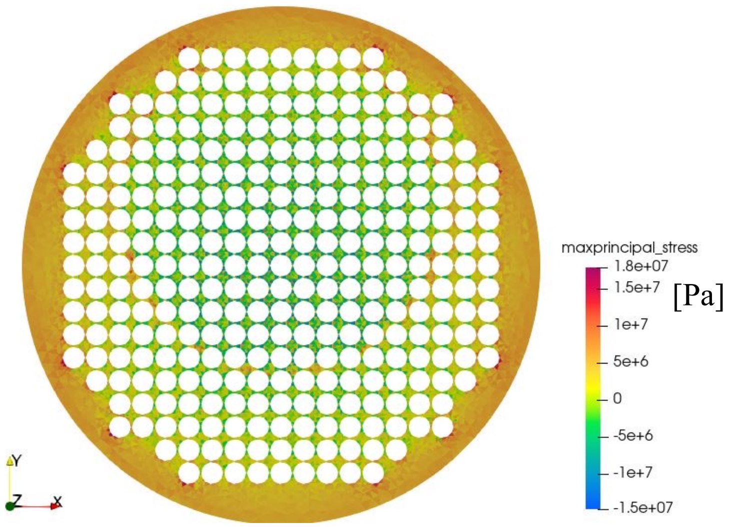
- A typical fuel pin with TRISO particles in SMR is modeled and analyzed with "Base-RVE" method.
- Base region computes the global temperature behavior, supplying the accurate boundary condition to RVE. The high resolution results is evaluated in RVE, and stress concentration is also observed.



Fuel geometry and cross-sections view



Temperature of SiC matrix at EOL



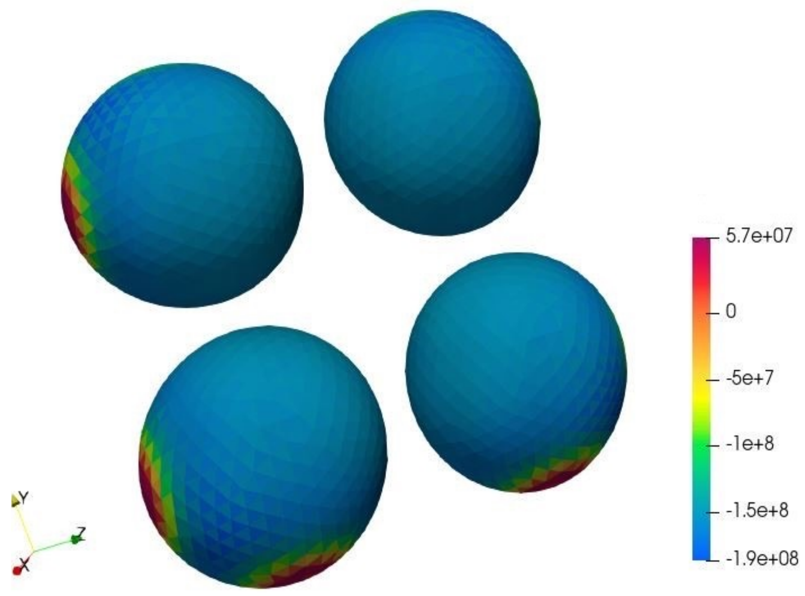
Max principal stress of SiC matrix at EOL

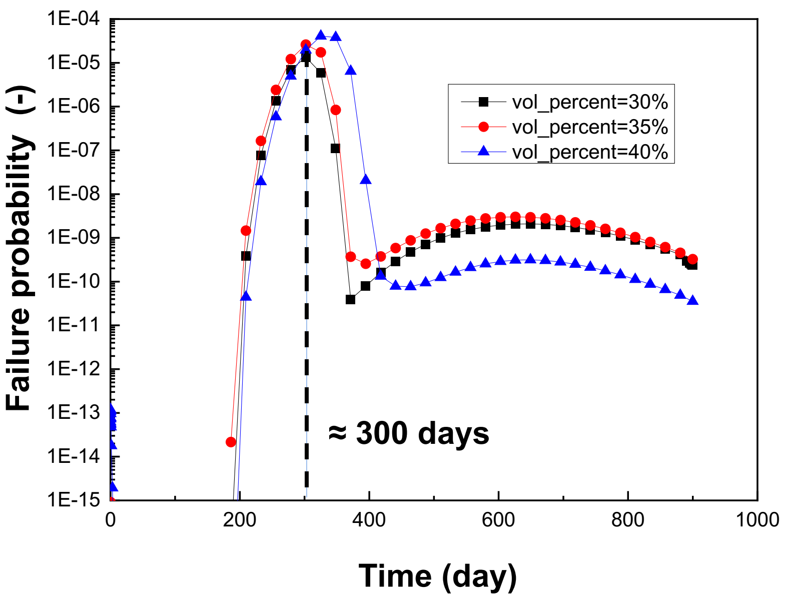
Base region

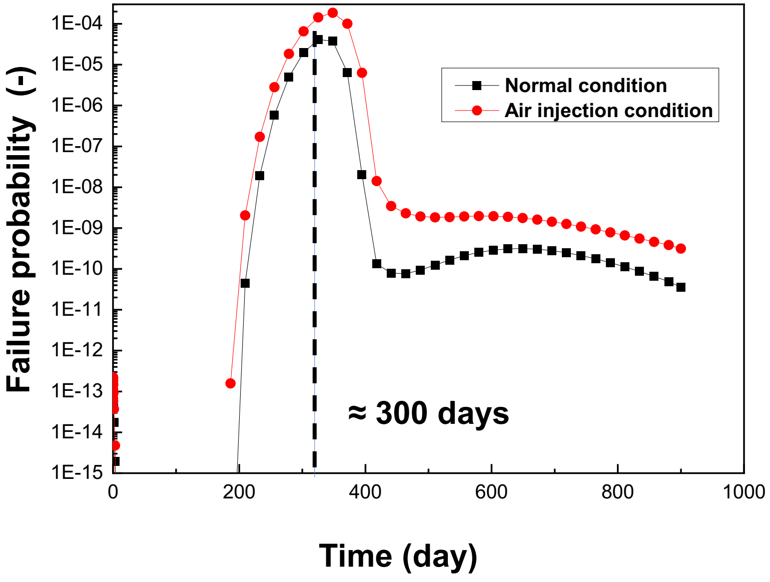
RVE region

4.4 BEEs for TRISO fuel

- **Several key factors (such as volume package fraction and operating conditions) on fuel performance of TRISO is investigated, revealing the typical patterns with failure probability prediction.**
- **CVD-SiC layer of TRISO bares the largest shear stress, which need to be concerned at 300 days.**







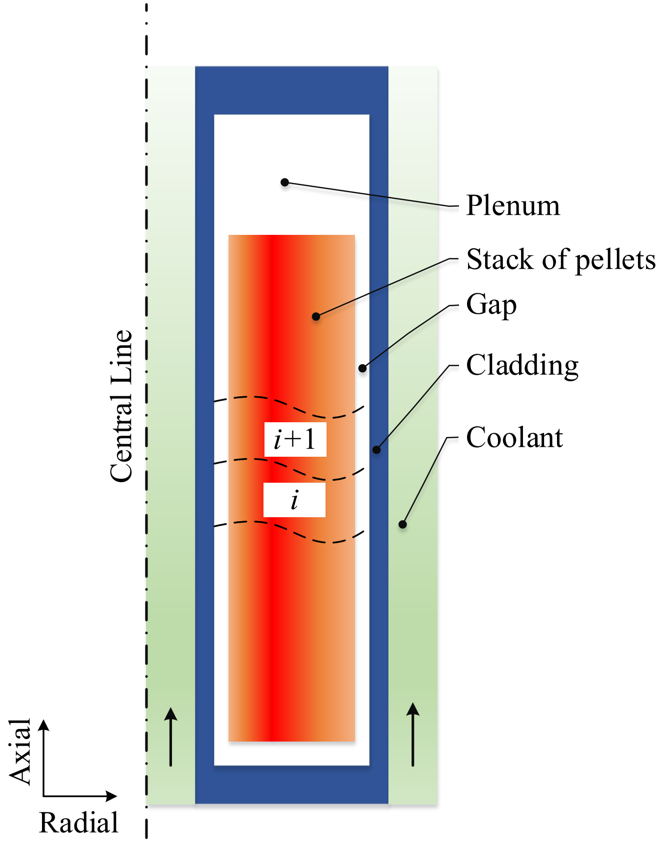
Shear stress of CVD-SiC layer

Different volume fractions

Normal and accident conditions

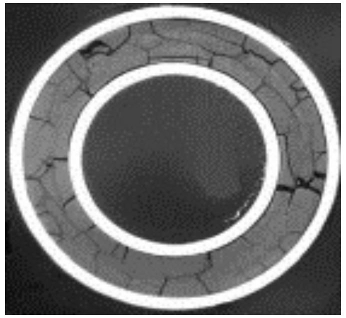
4.5 BEEs for Annular fuel

Dual-cooled annular fuel design, is one of the promising concepts to enhance fuel performance and further improve reactor economy.



Given its novel structure, there are several specific phenomena for annular fuel.

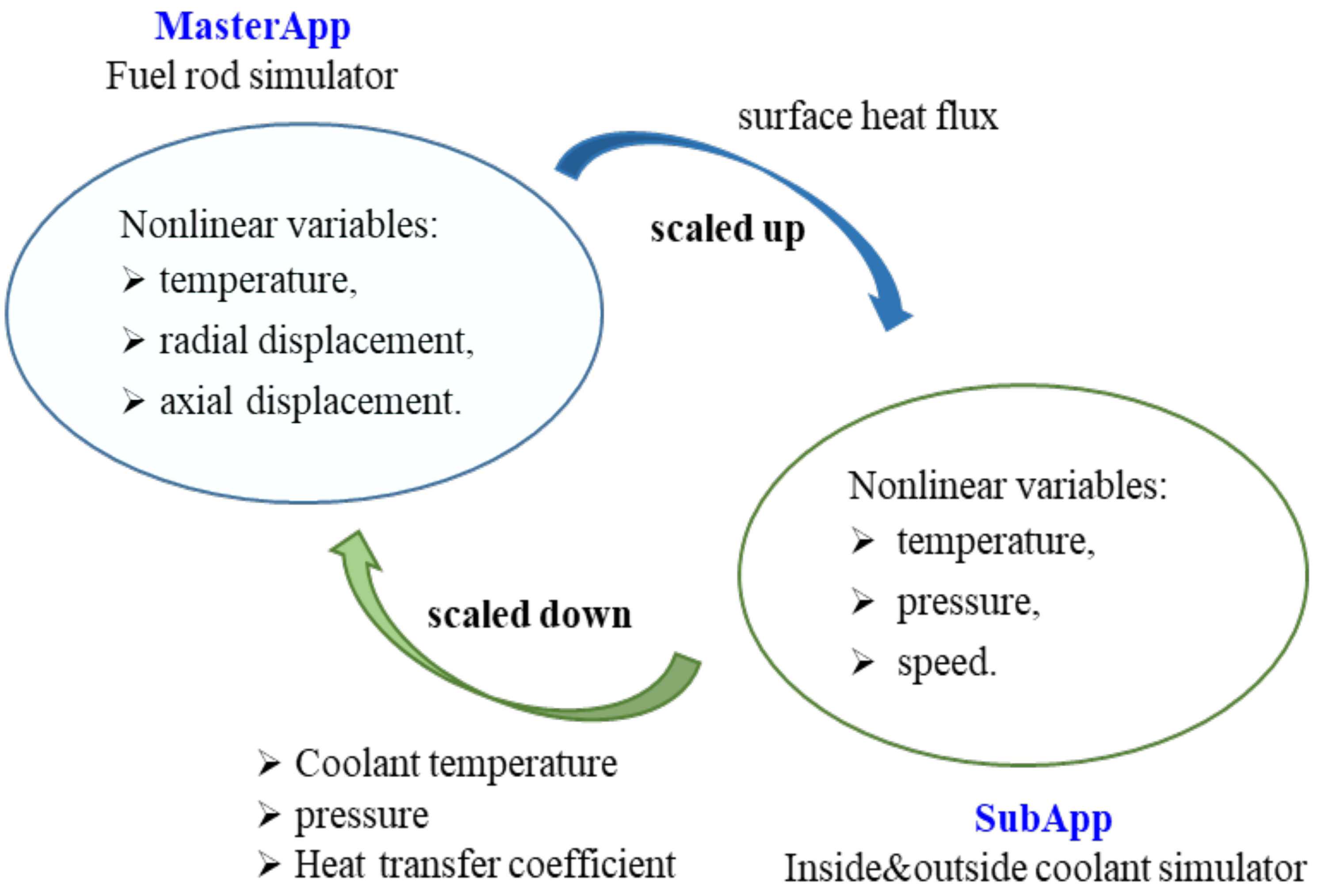
- coolant mass distribution **between internal and external (I&E)** channels
- heat split
- I&E fuel relocation
- deformation between inner and outer cladding



4.5 BEEs for Annular fuel

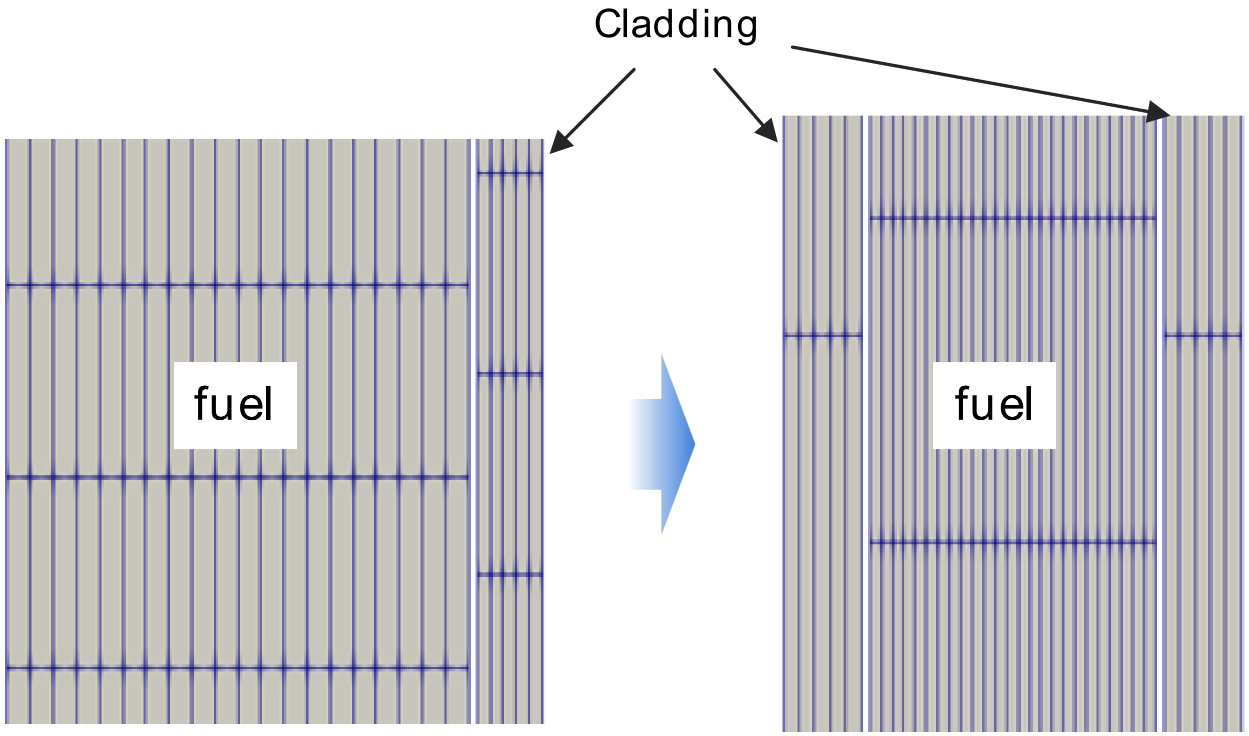
Region	Physical models
Fuel	1) Thermal conductivity, Young's modulus, and Poisson's ratio 2) Fuel expanding* 3) Densification 4) Relocation* 5) Thermal expansion 6) Rim effect* 7) Fission gas release*
Cladding	1) Thermal conductivity, Young's modulus, and Poisson's ratio 2) Irradiation growth 3) Thermal expansion 4) Irradiation-induced creep 5) Thermal creep
Plenum	1) Plenum temperature 2) Plenum pressure
Fuel-cladding gap	1) Gap conductivity 2) Thermal & mechanical contact
Coolant	Closed channel flow distribution modeling*

- Fuel rod and coolant coupling analysis method.



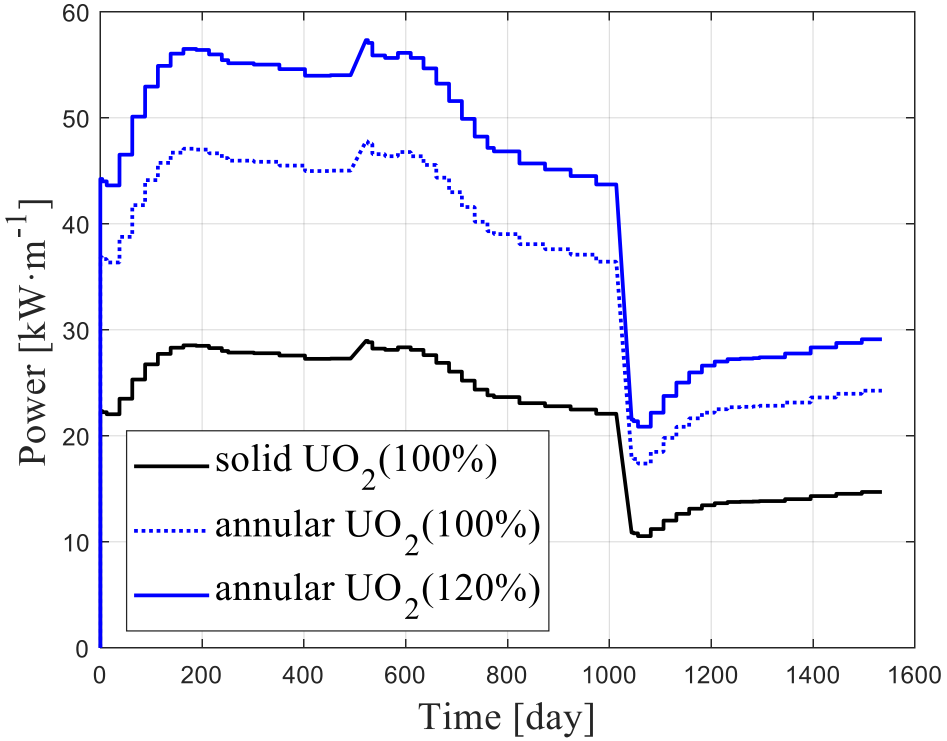
4.5 BEEs for Annular fuel

- The annular fuel can be modeled from rod fuel, in which two types fuel are similar for meshing.
- **Annular fuel could enhance the fuel pin power density**, showing good neutronics economy.



UO$_2$-Zircaloy4 rod fuel

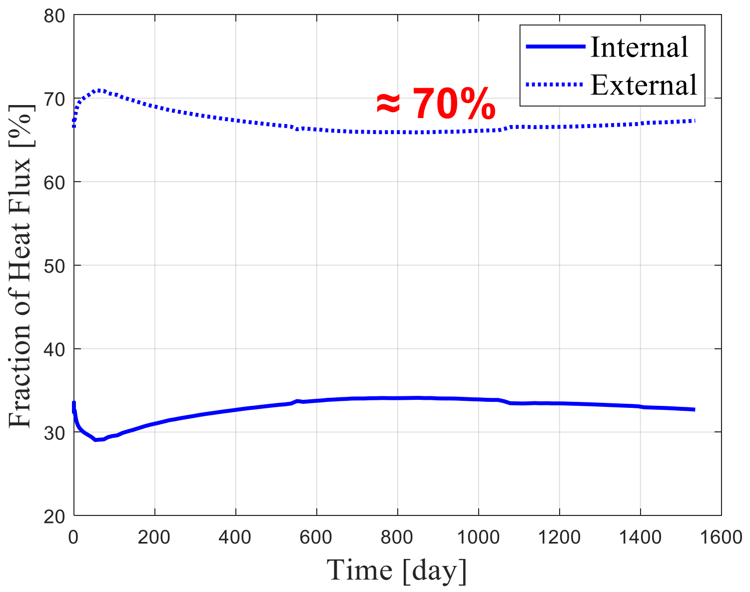
UO$_2$-Zircaloy4 annular fuel



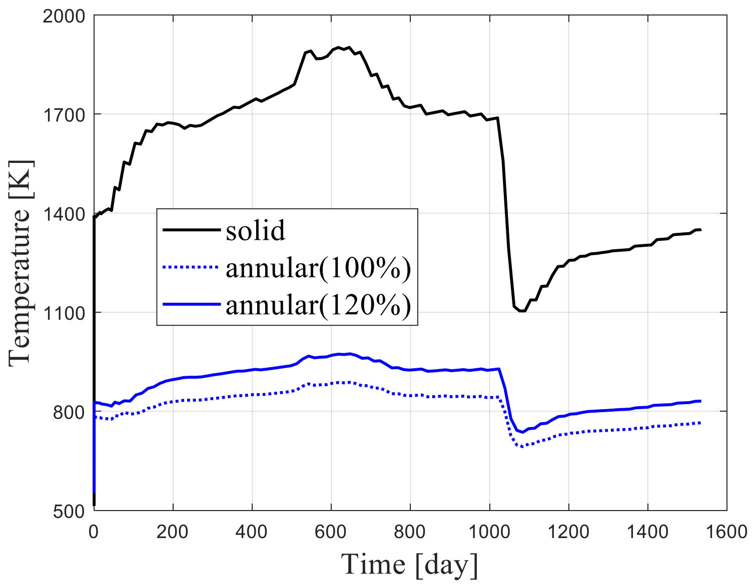
Averaged rod power for rod and annular fuels

4.5 BEEs for Annular fuel

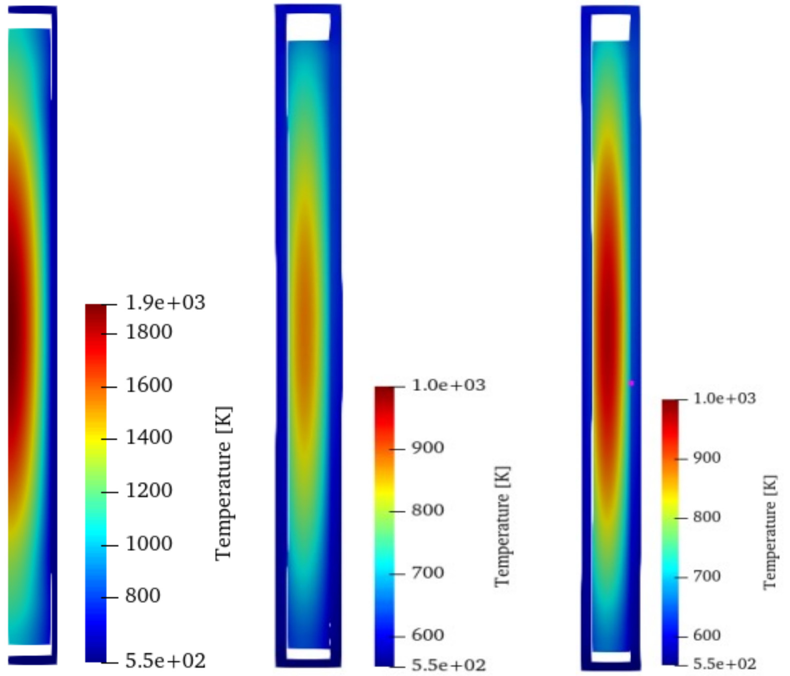
- Benefitted from the lower heat transfer resistance to the external coolant channel, **near 70% fraction of heat flux is transferred to the external coolant.**
- The max temperature of annular fuel **decreases about 900 K** when compared with rod fuel, and the fuel radial expansion also decreases, showing a large margin to fuel safety.



Heat flux



Max temperature



Rod fuel

100% power

120% power

Annular fuel

4.6 BEEs for Plate fuel

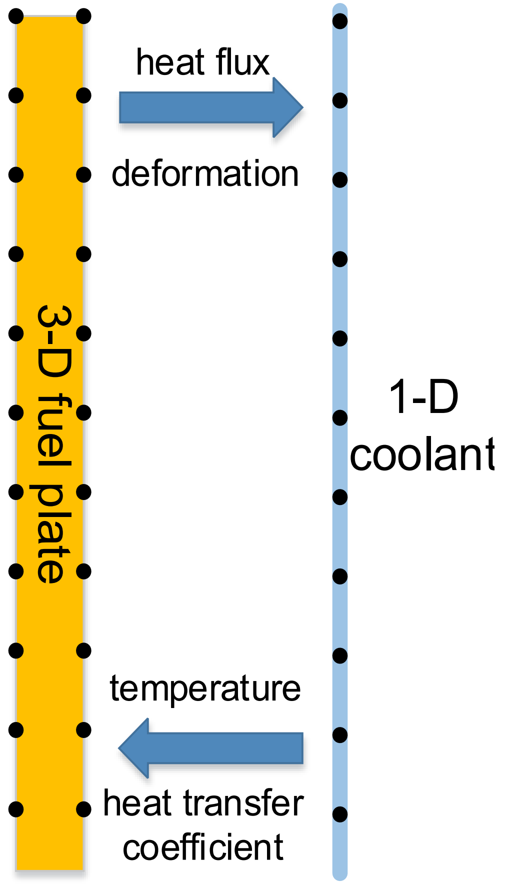
➢ **Coupling 3D solid domain with 1D fluid domain is adopted for multi-channel simulation of plate fuel assembly. Key parameters**

✓ **Coolant-BEEs-system (following section)**

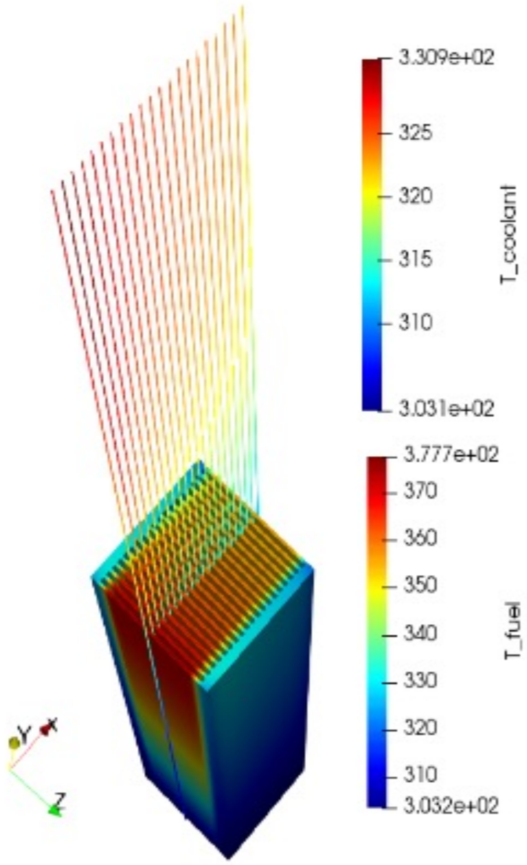
- Three major conservation equations
- Coolant properties
- Coupled heat source
- Flow distribution

✓ **Plate-type fuel**

- Equivalent properties of dispersion-type materials
- Behaviors: thermal expansion, irradiation swelling, etc.
- Coupled coolant boundary
- Nonlinear deformation: creep, plasticity



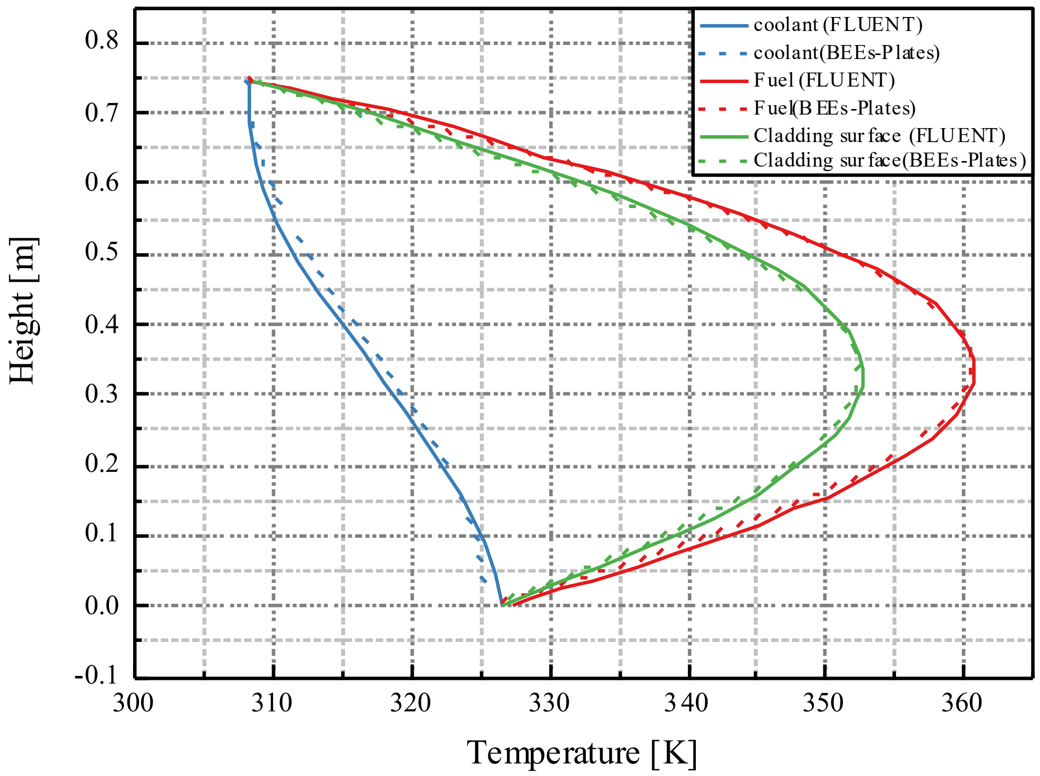
Coupling schematic



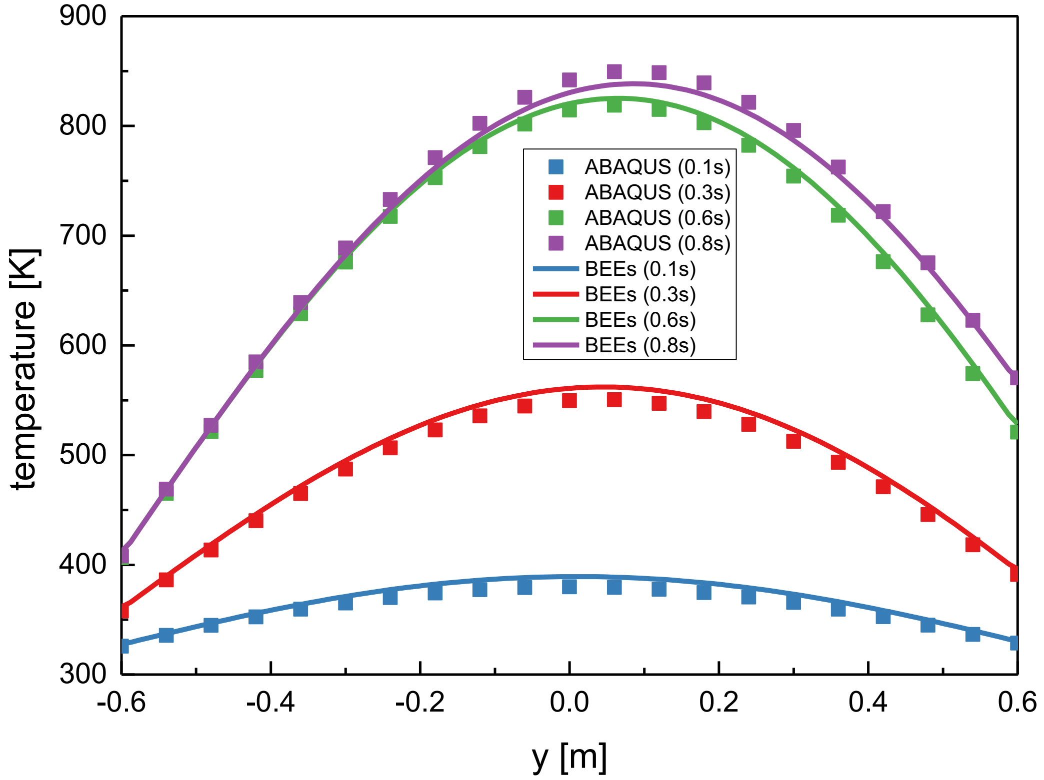
Temperature distribution

4.6 BEEs for Plate fuel

Code-to-code validation: By comparing FLUENT and ABAQUS software respectively, the correctness of the 3D-1D coupling framework established in this study is verified. The comparison results show that the BEEs accurately calculate the coolant and fuel temperatures.



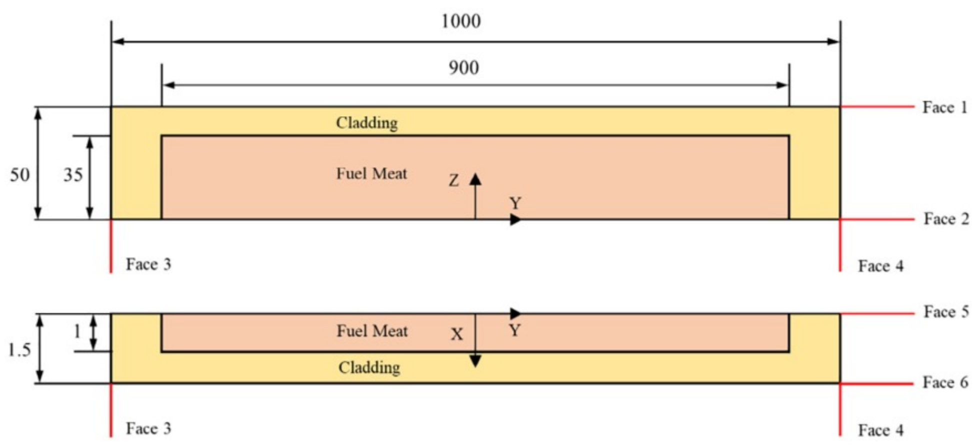
Comparison with FLUENT



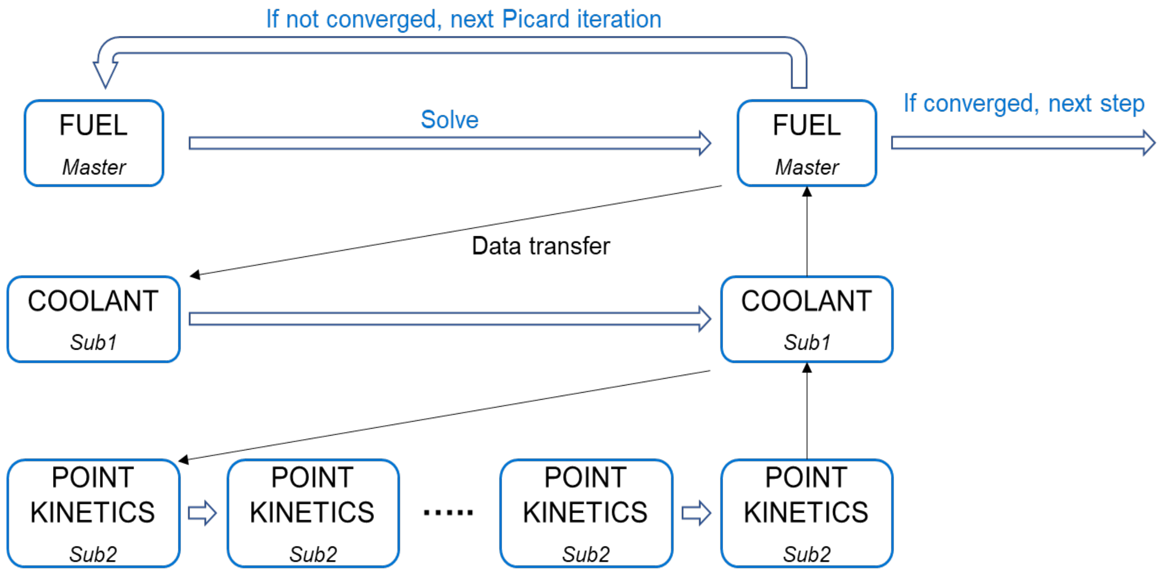
Comparison with ABAQUS

4.6 BEEs for Plate fuel

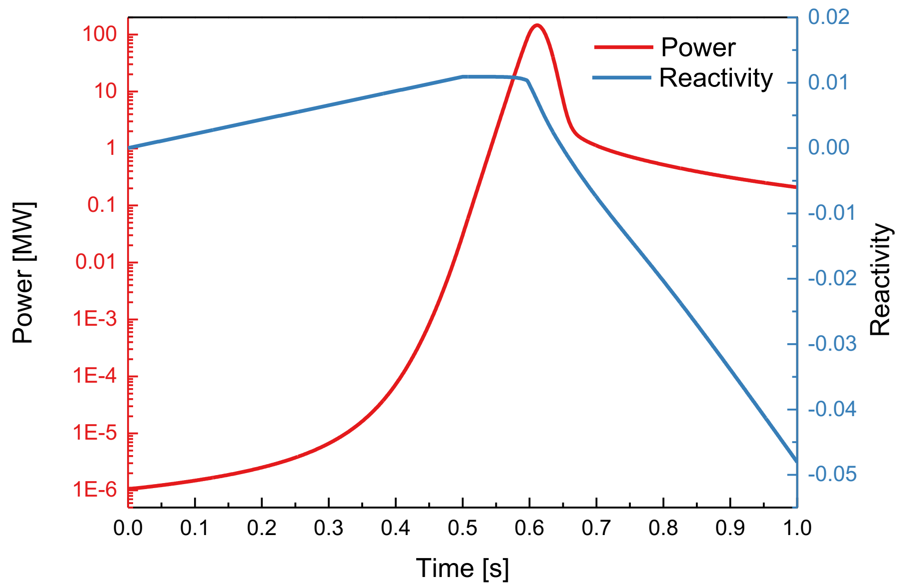
- The coupling model consists of point reactor model (0D), 1D coolant model and 3D solid plate fuel model. Each model adopts different time steps and employs sub-cycling.
- Full coupling is applied to internal variables within each model, while strong coupling Picard iteration is used between different physical fields.



Simulation object: 1/4 fuel plate



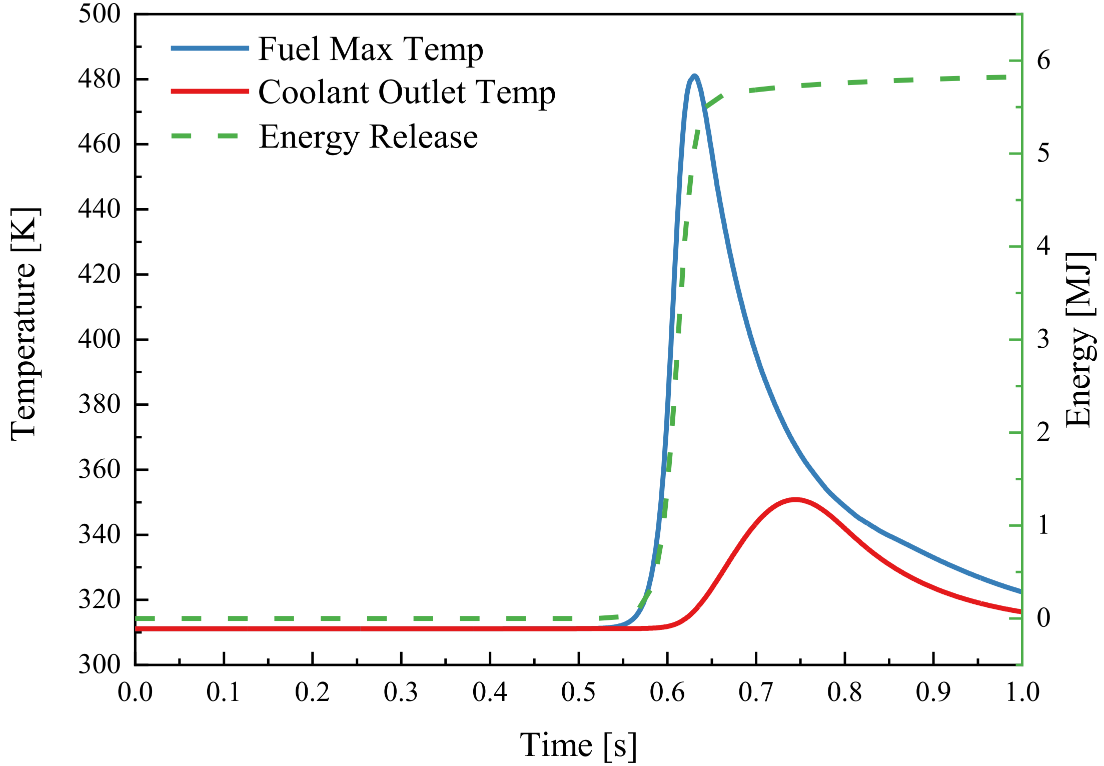
Coupling schematic



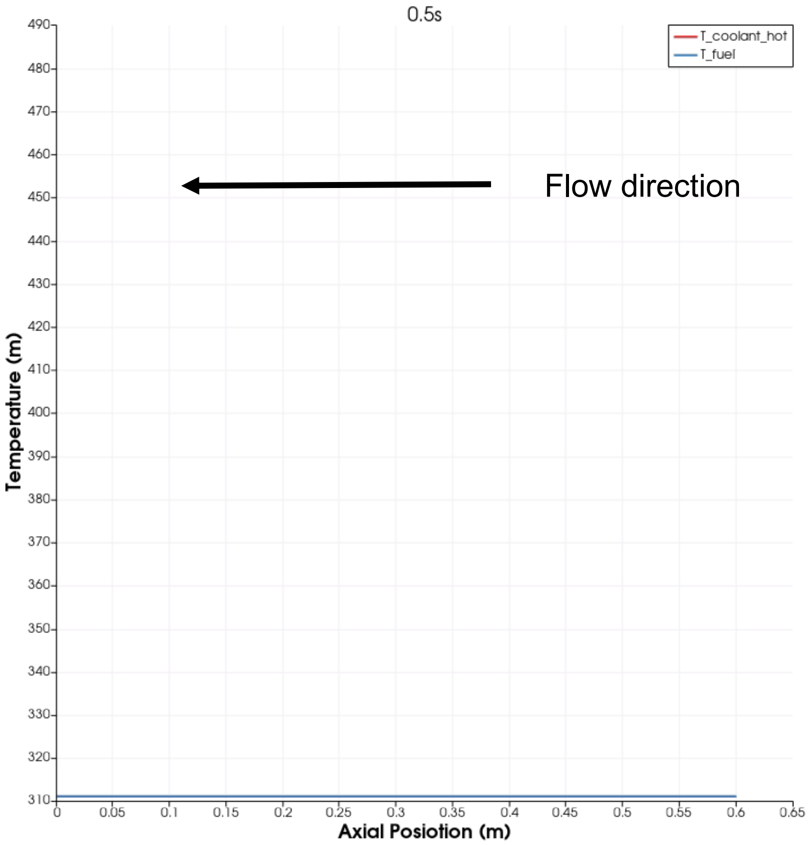
Power/Reactivity Change

4.6 BEEs for Plate fuel

The energy release during RIA firstly accumulated in the fuel elements, causing a sudden increase in temperature. Approximately 0.2 seconds later, the energy is transferred to the coolant through convection and is then discharged from the reactor core at the outlet of the channel.



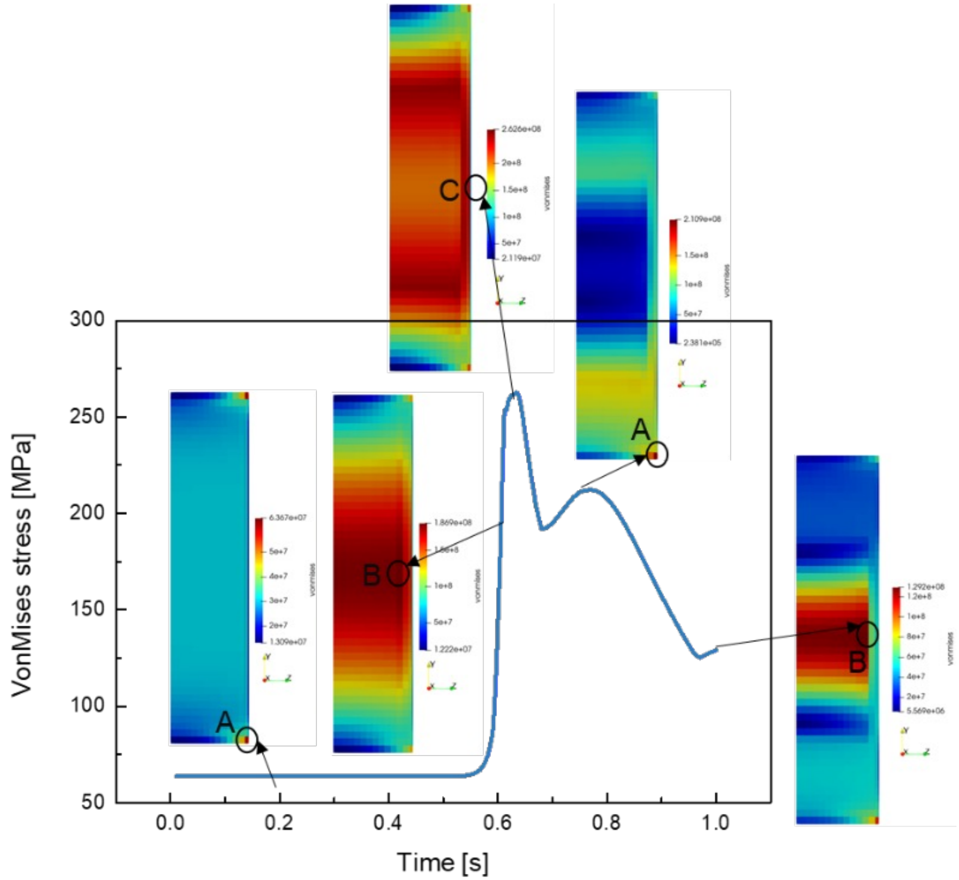
The max temperature of the fuel element and the coolant



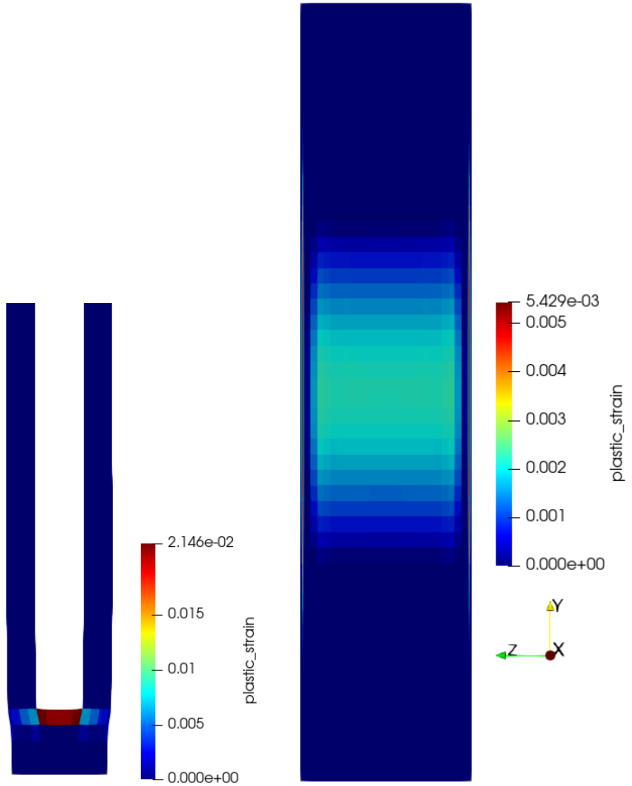
Temperature variations of fuel and coolant under RIA conditions

4.6 BEEs for Plate fuel

- The mechanical deformation and fuel stress distribution of the fuel element under RIA is simulated and analyzed, which maximum stress changes repeatedly.
- The irreversible cladding plastic deformation caused by the RIA process is captured.



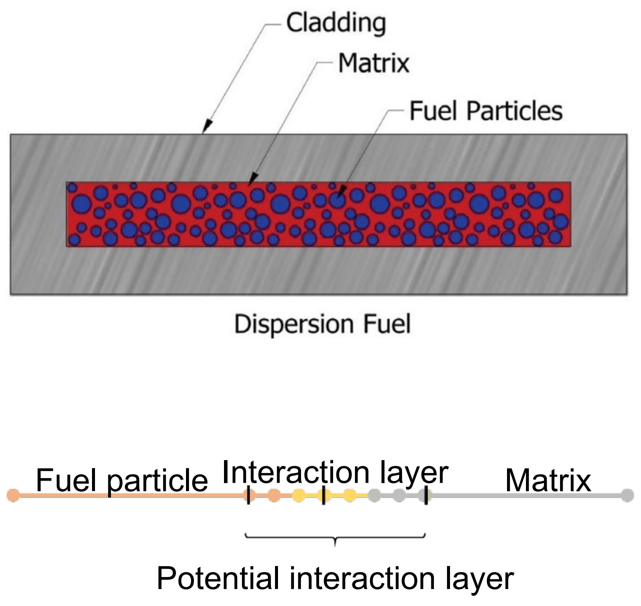
Fuel Stress Change



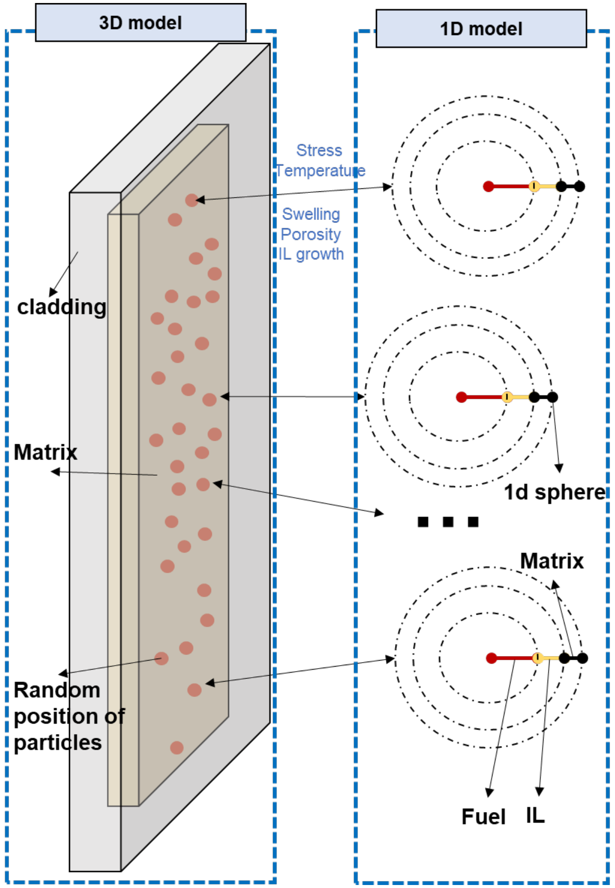
Plastic strain after RIA

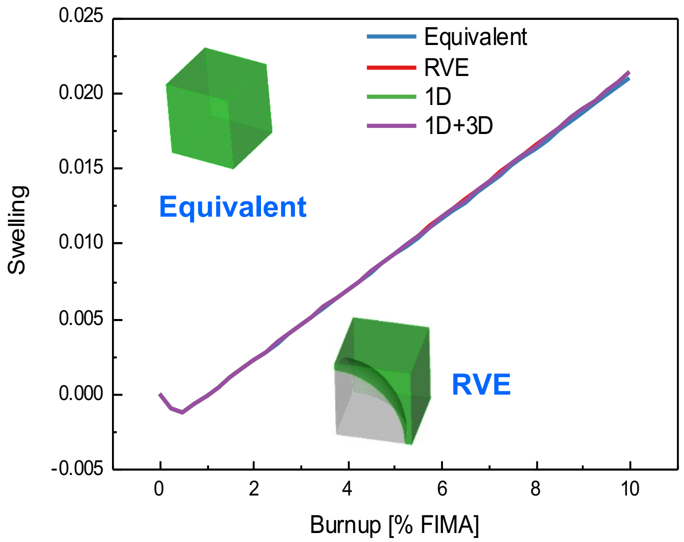
4.6 BEEs for Plate fuel

- The multi-scale coupling model for plate fuel analysis is developed.
- Employing a 3D equivalent model to calculate the overall behavior of particle-dispersed plate-type fuel while using a 1D model to calculate the behavior of micro fuel particles

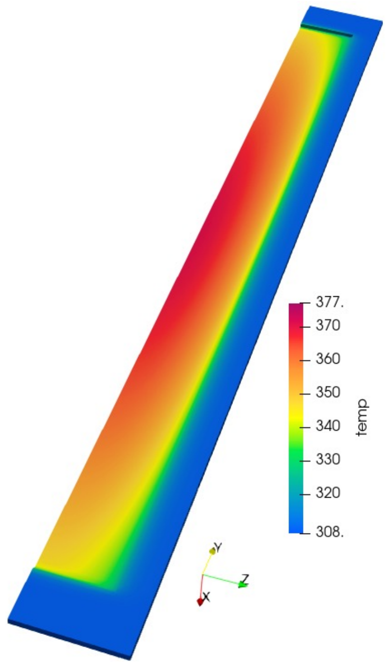


Micro fuel particles 1D model
&
Coupling strategy

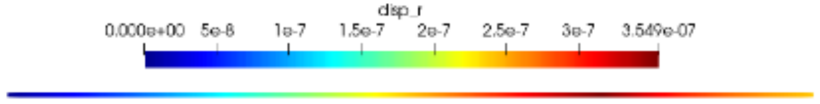




Coupling strategy validation



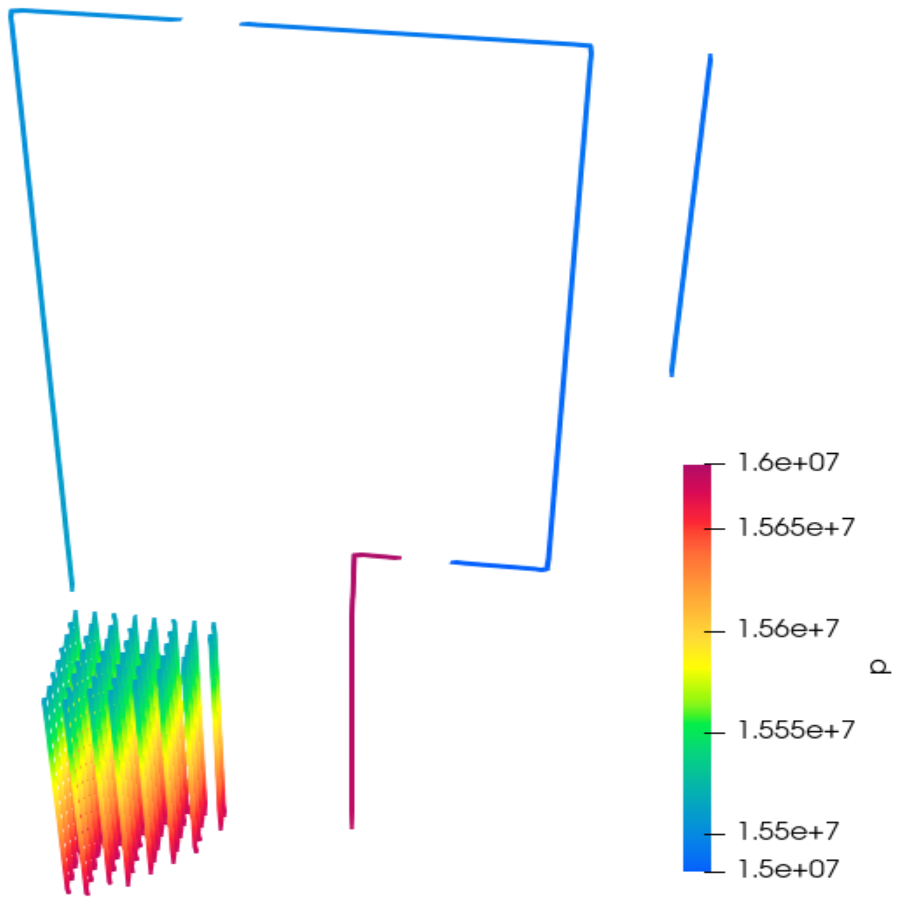
1D+3D coupling analysis



4.7 BEEs for Thermal-hydraulics

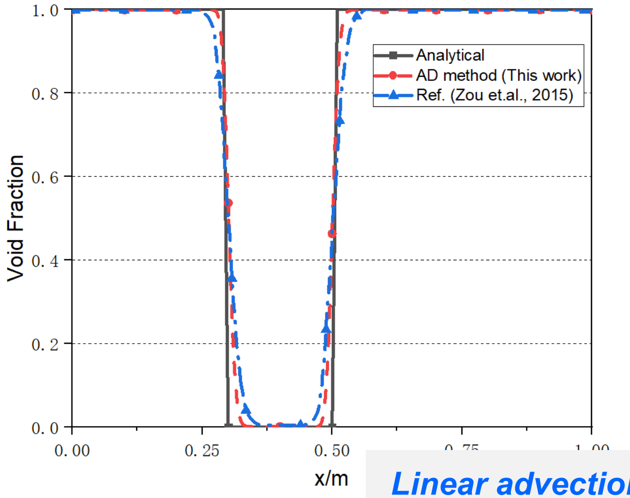
To support the future multi-physics coupled simulation, a new reactor system analysis code , BEEs-system, has been developed.

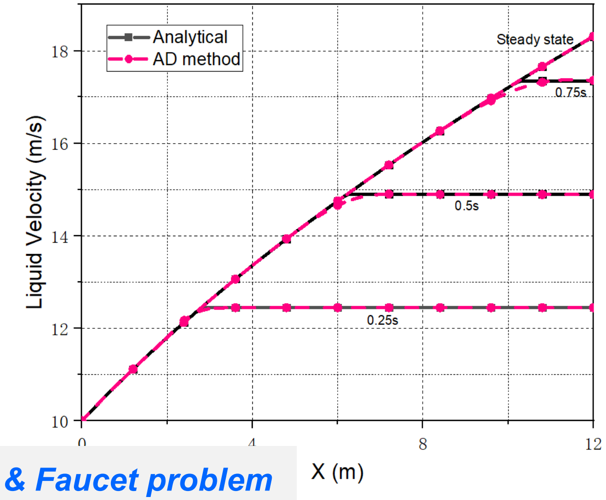
- **Two-fluid six-equation model**
- **constitutive correlations**
  - *the models of flow regimes*
  - *flow-regime-related models*
- **Automatic differentiation (AD) was employed to replace the traditional method of artificially deriving Jacobian matrix elements.**
- **verified and validated for both transients and boiling conditions simulations**

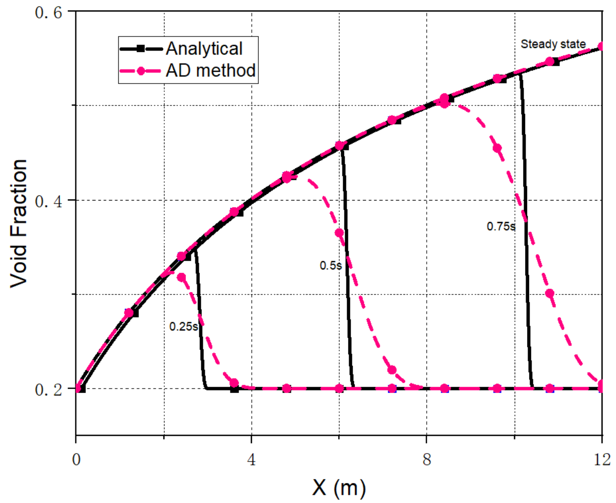


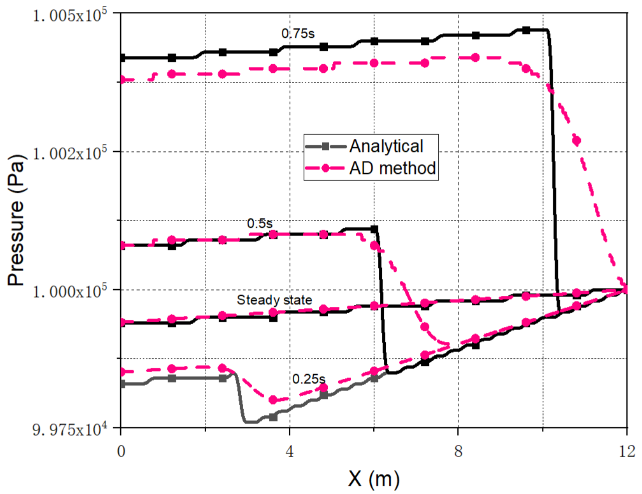
4.7 BEEs for Thermal-hydraulics

- BEEs for thermal-hydraulics is developed with **rDG** (*reconstructed discontinuous Garlerkin*) **method** in MOOSE.
- The solver is fully validated with **unit-test cases, two-phase flow experiments, and system benchmark.**

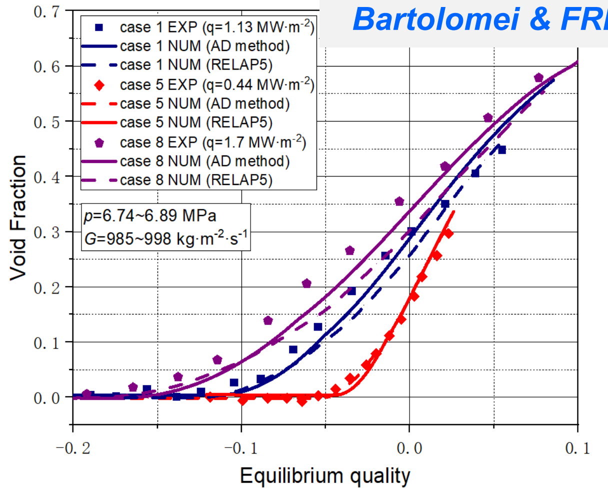


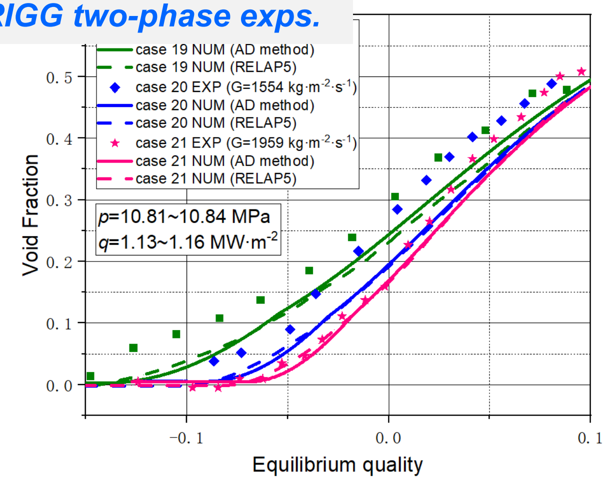




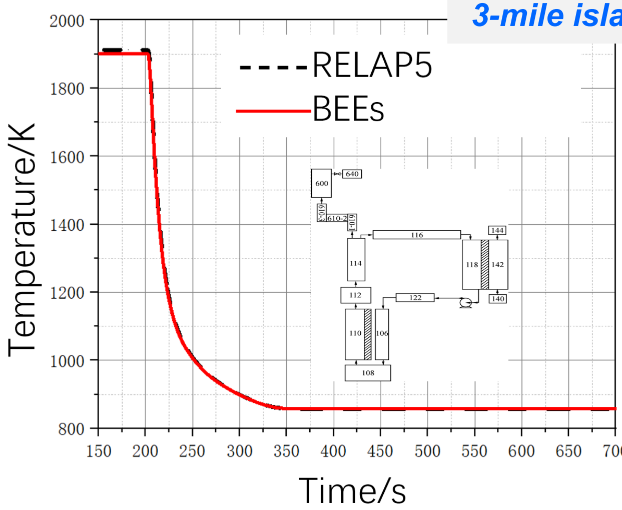


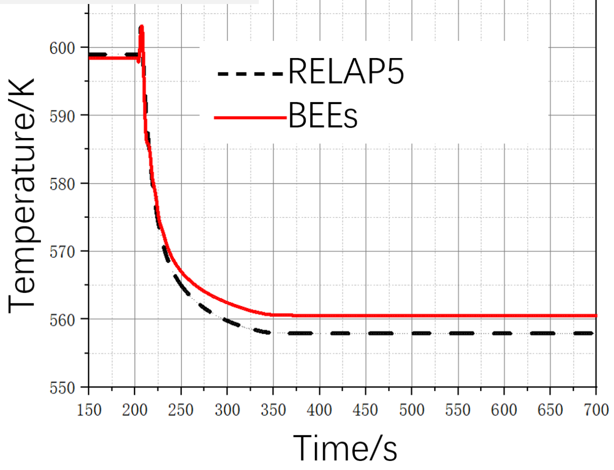
Linear advection & Faucet problem





Bartolomei & FRIGG two-phase exps.



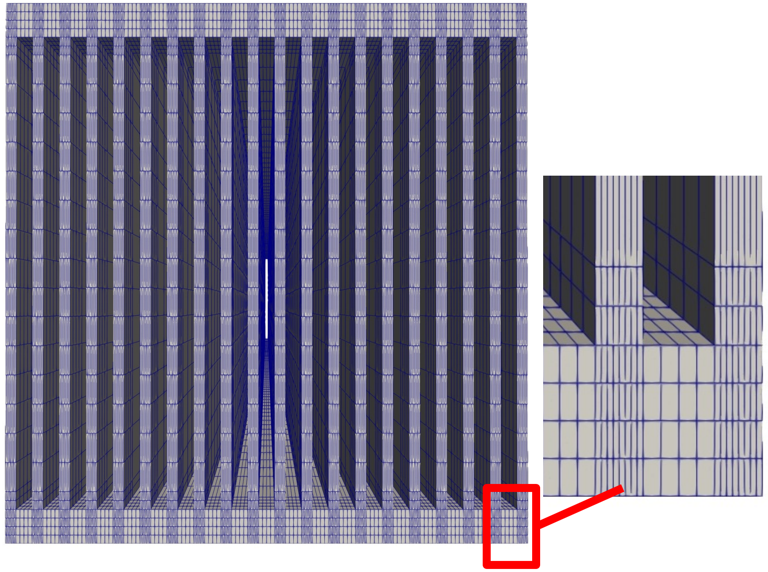


3-mile island PWR system

4.8 Multi-physics coupling

Research object and its modeling

- A 20-plates fuel assembly of Japan Research Reactor-3 (JRR-3) is selected.
- Multiphysics coupling calculation considering burnup of fuel assembly with enrichment of 19.5% is completed.



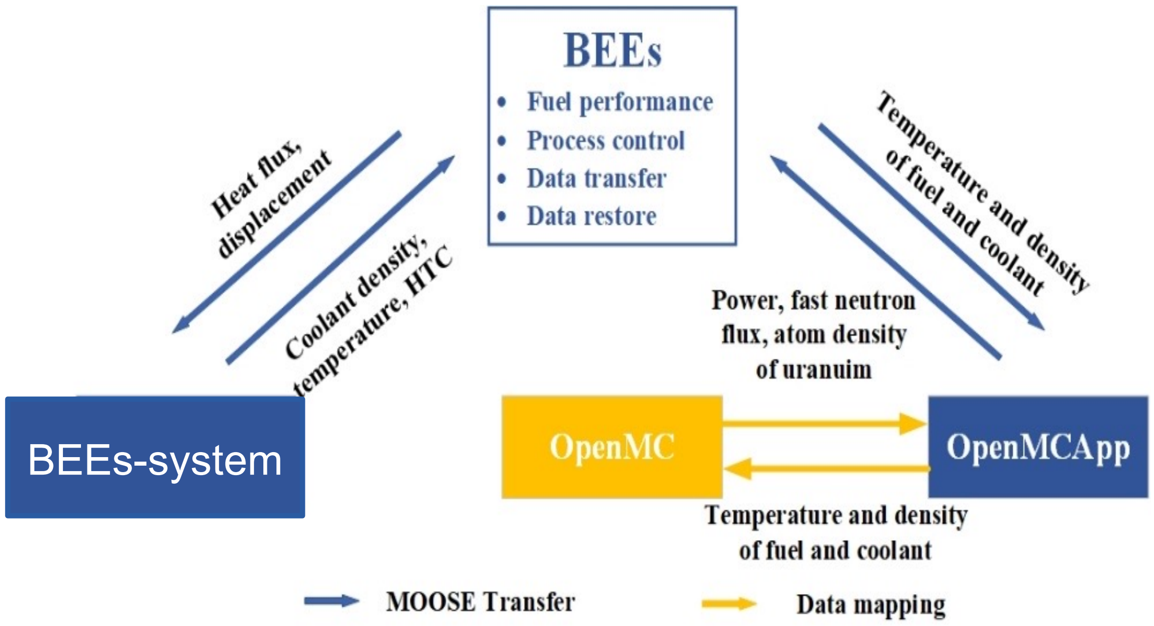
JRR-3 fuel assembly

Modeling parameters of assembly

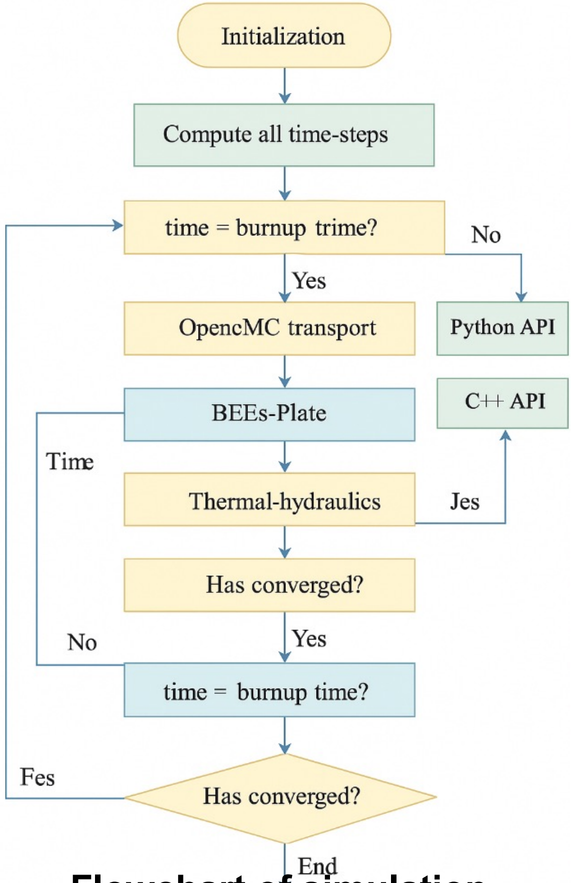
Parameters	Value	Parameters	Value
Clad	6061-Al	Total power	1.111 MW
Fuel meats	U_3Si_2-Al	Fuel density	6.975 g·cm^{-3}
Height of clad	770 mm	Height of fuel meats	750 mm
Length of clad	66.6 mm	Length of fuel meat s	61.6 mm
Width of clad	1.52 mm	Width of fuel meats	0.76 mm
Velocity of coolant	3.4 m/s	Pressure	15.5 MPa
Inlet temperature	311.15 K		

4.8 Multi-physics coupling

- Both the internal and external coupling are used to establish neutronics / thermal-hydraulics / fuel performance analysis framework.
- Real-time depletion data are used for fuel performance analysis with python API.



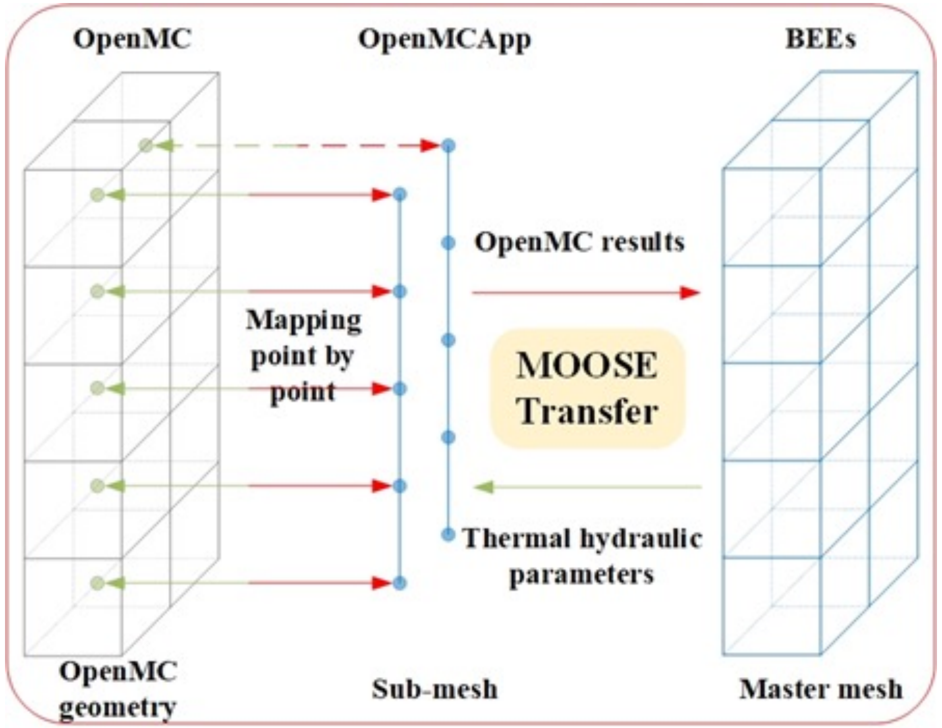
Data transfer scheme



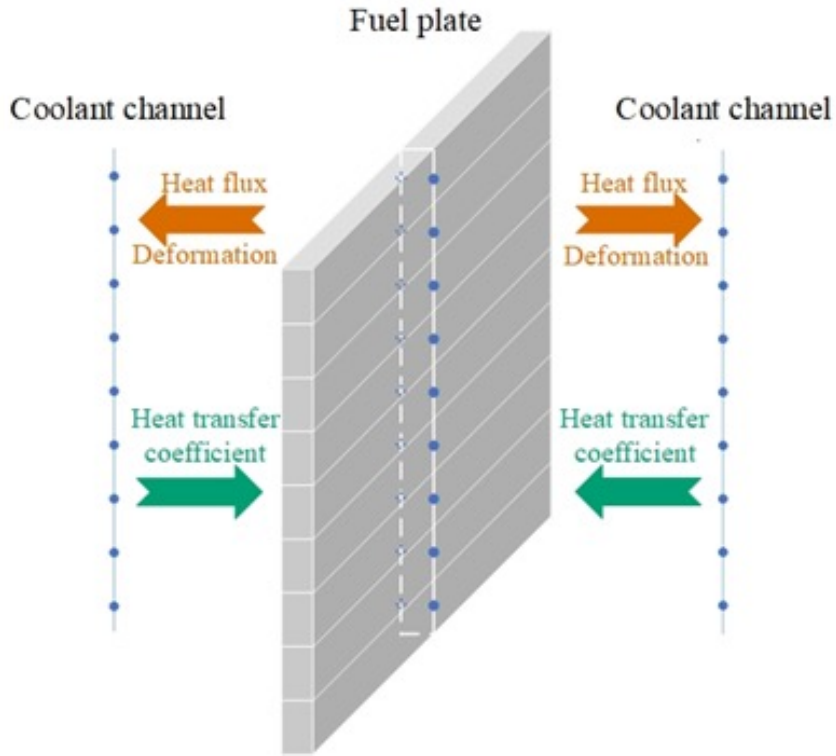
Flowchart of simulation

4.8 Multi-physics coupling

- 3D-1D data mapping scheme for OpenMC/MOOSE and BEEs-Plate/BEEs-System.
- Inverse Distance Weighted Interpolation is used to map data between OpenMCApp and BEEs.



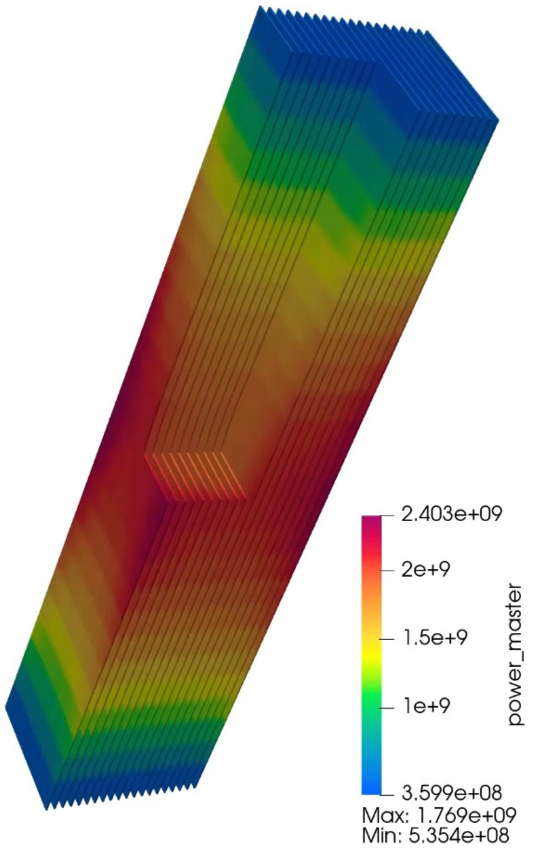
OpenMC+BEEs-plate data mapping method



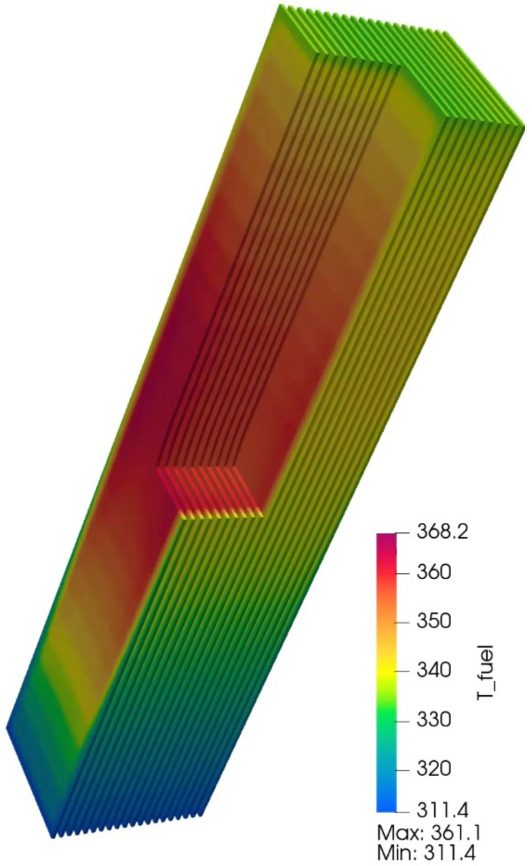
BEEs-plate+BEEs-system data mapping solution

4.8 Multi-physics coupling

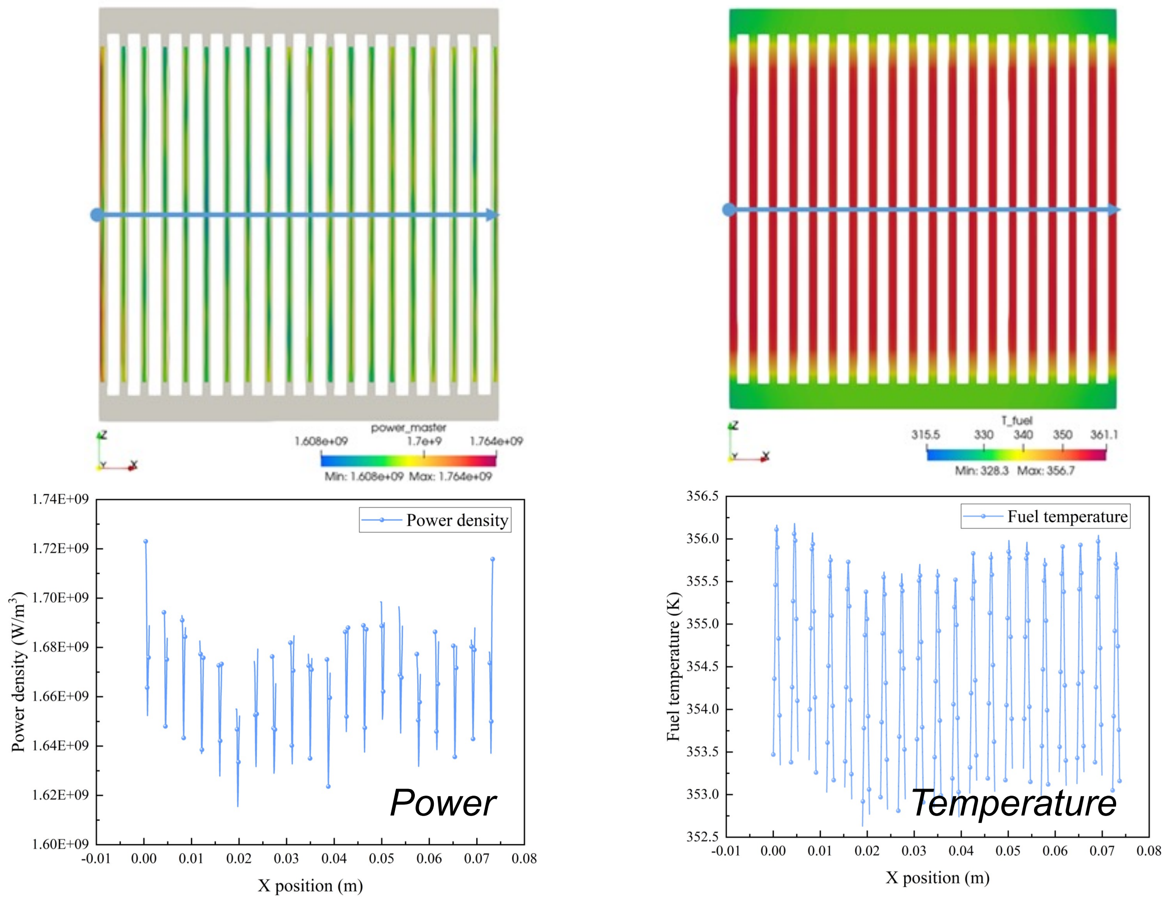
- Detailed power and temperature distributions with time of JRR-3 assembly are obtained.
- Shielding effect of power in fuel plate can be accurately captured.



Power



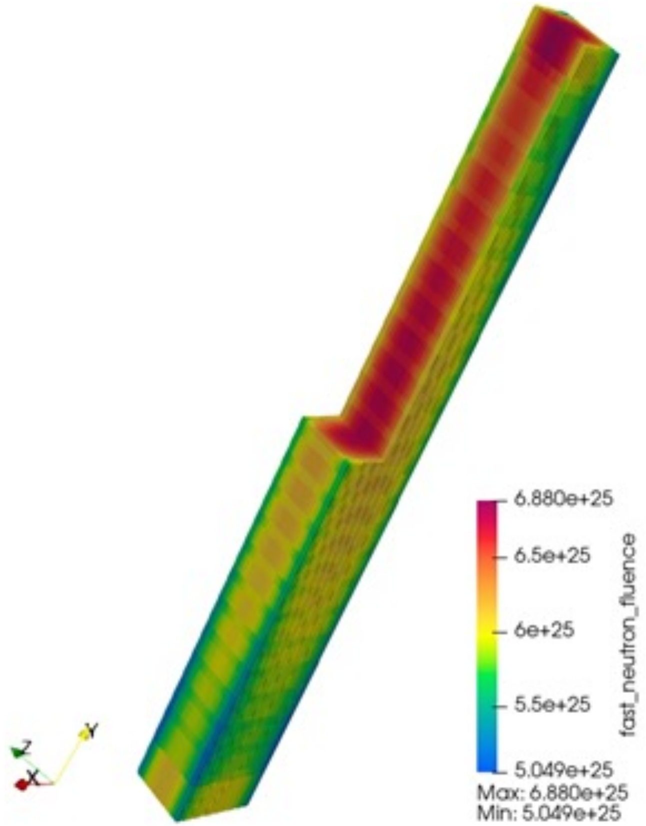
Temperature



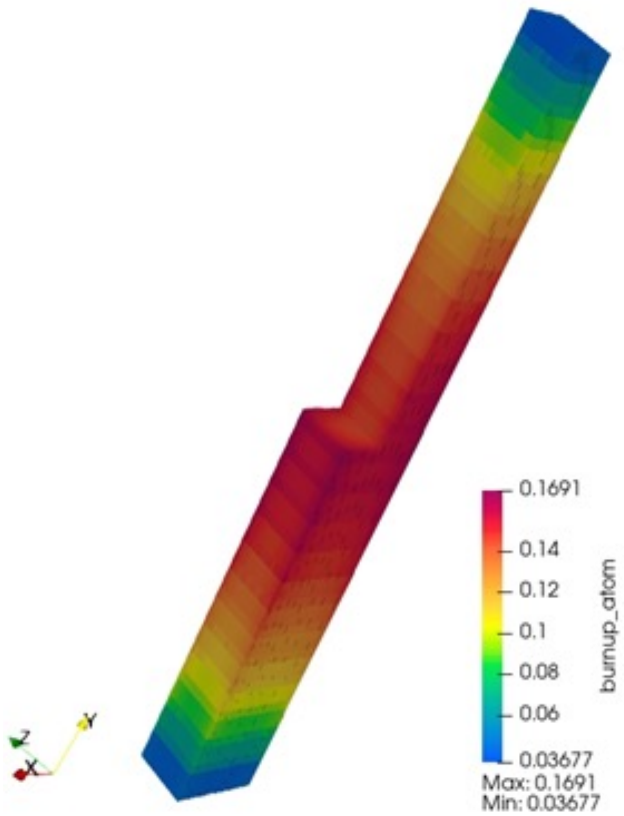
Characteristic line probes

4.8 Multi-physics coupling

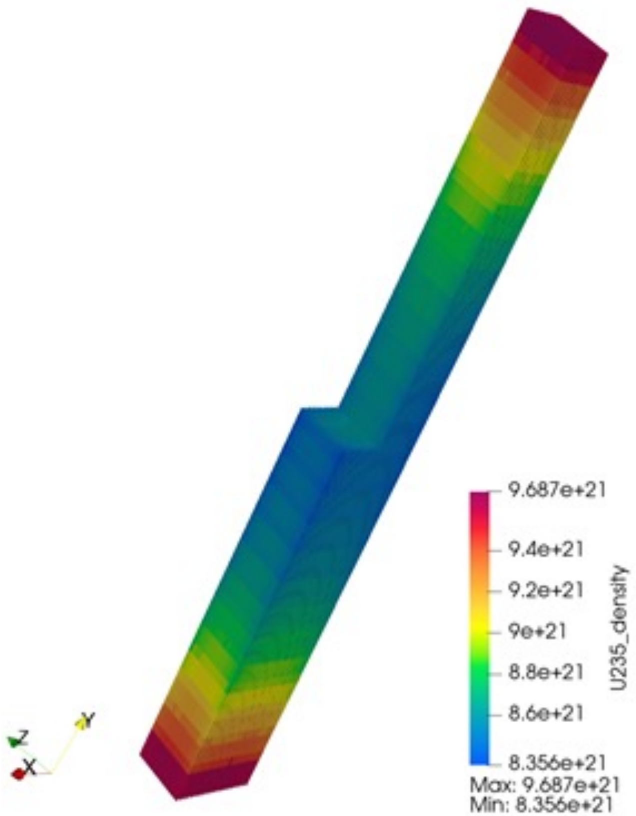
- Maximum fast neutron flux occurs in the central region
- The maximum fuel burnup reaches 16.91% FIMA after 231 days



Fast neutron fluence



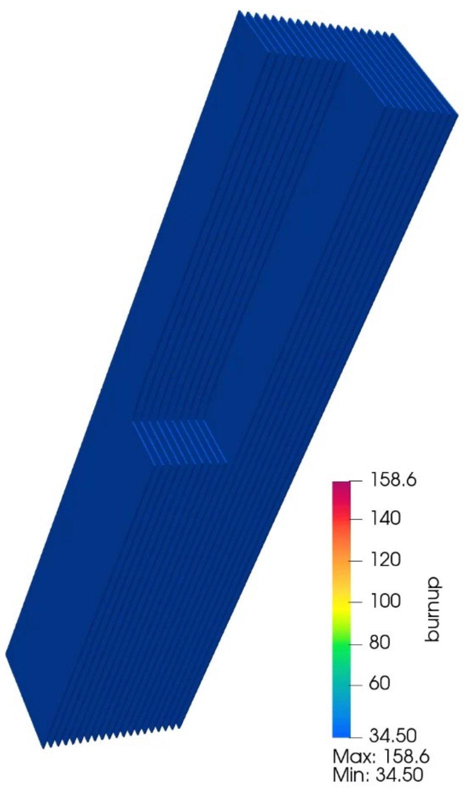
Burnup (FIMA)



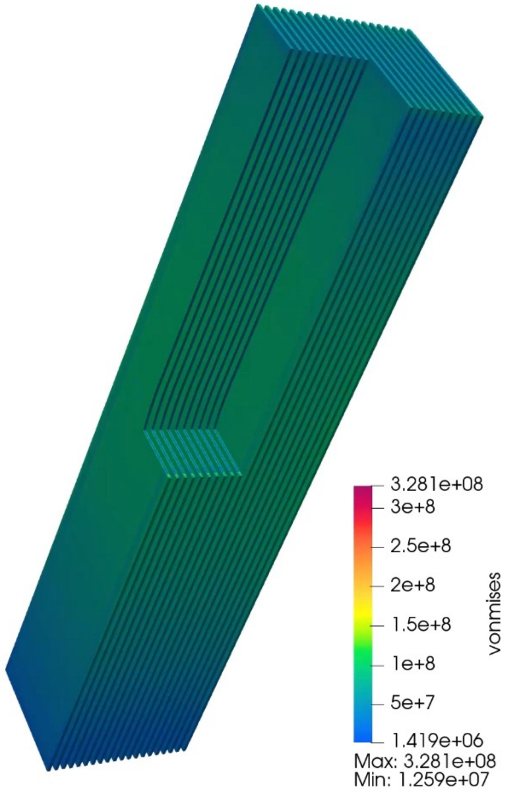
Atom density of uranium (n/cm^3)

4.8 Multi-physics coupling

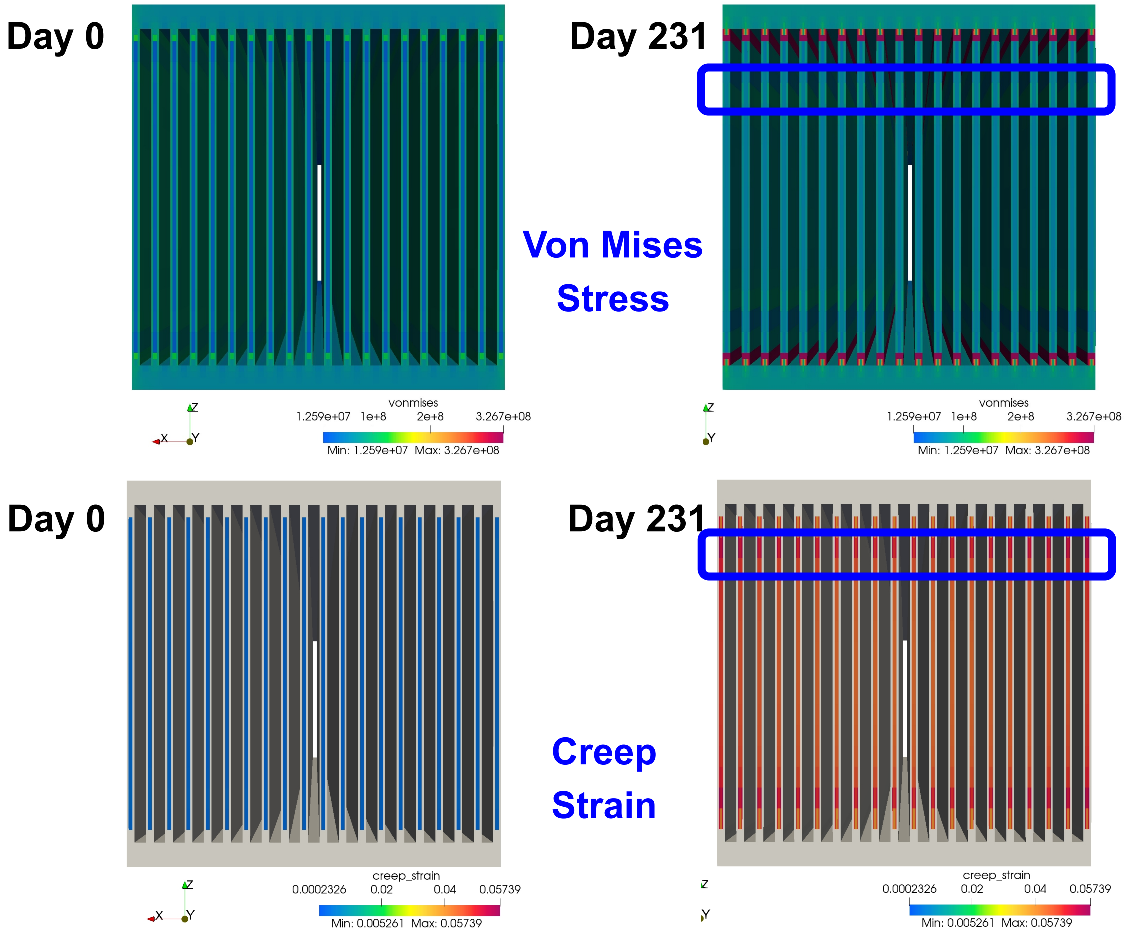
- Maximum stress occurs in the **contact area of cladding-connecting** components
- Creep of fuel reduces the stress in the fuel meat



Fuel burnup

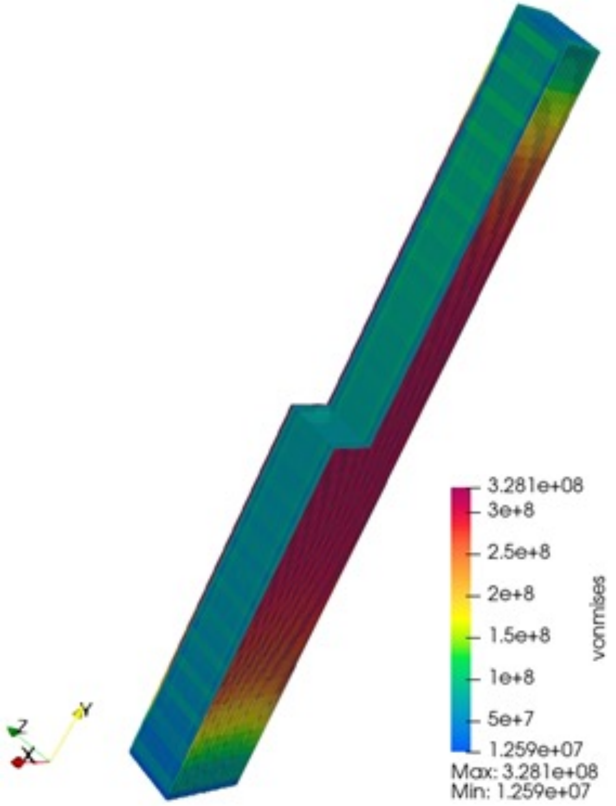


Von Mises Stress

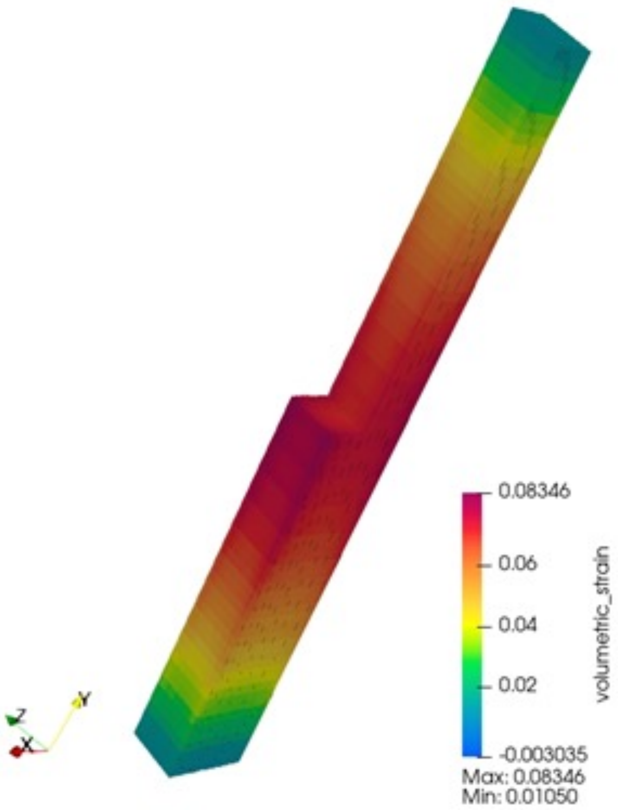


4.8 Multi-physics coupling

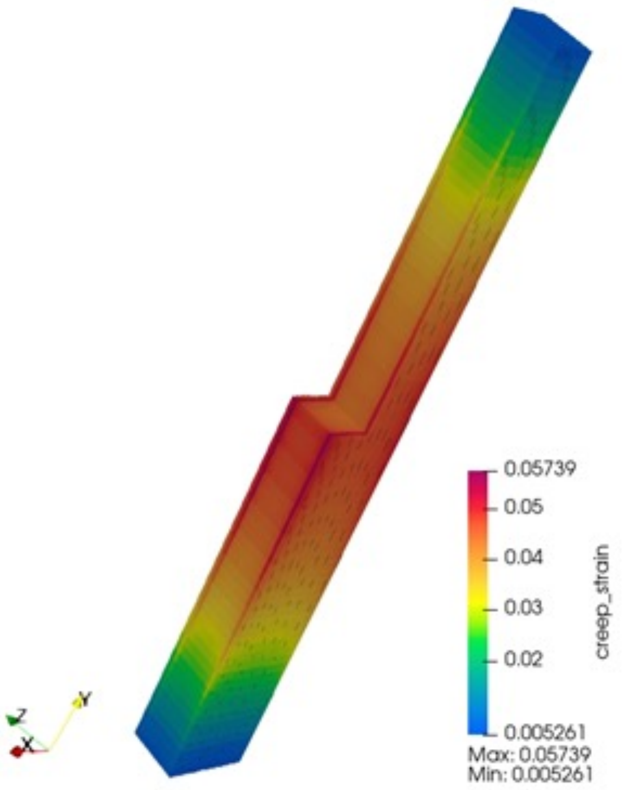
- **After 231 days, the maximum stress of fuel assembly reached 328.1MPa, which exceeds the stress limitation 276 MPa of 6061-alloy.**
- **It can be found that volumetric strain is mainly controlled by temperature distribution.**



Von Mises Stress



Volumetric strain of fuel meat

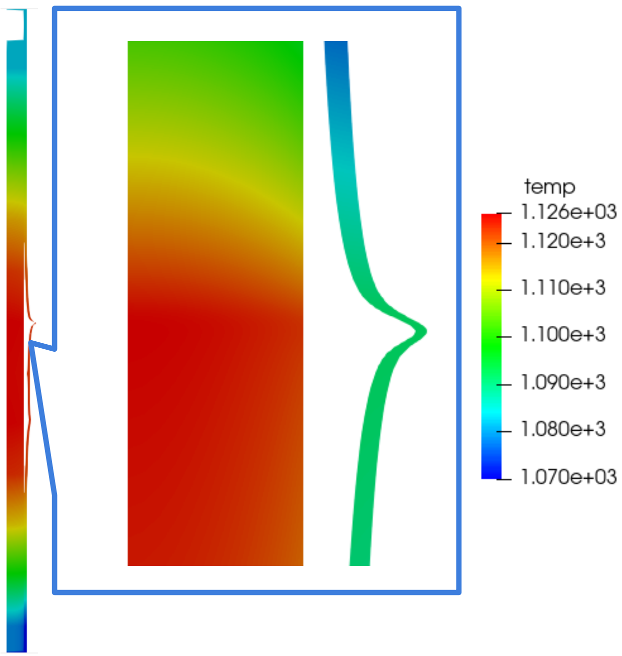


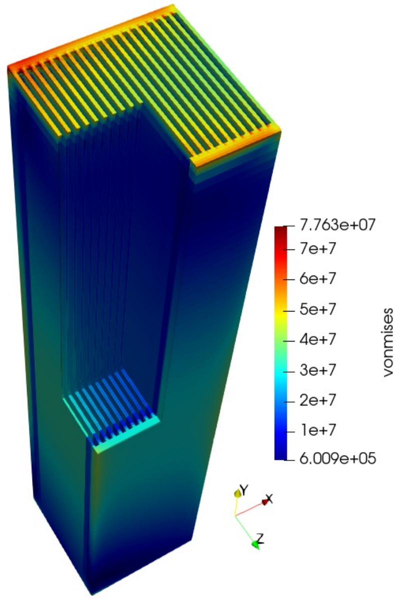
Creep strain of fuel meat

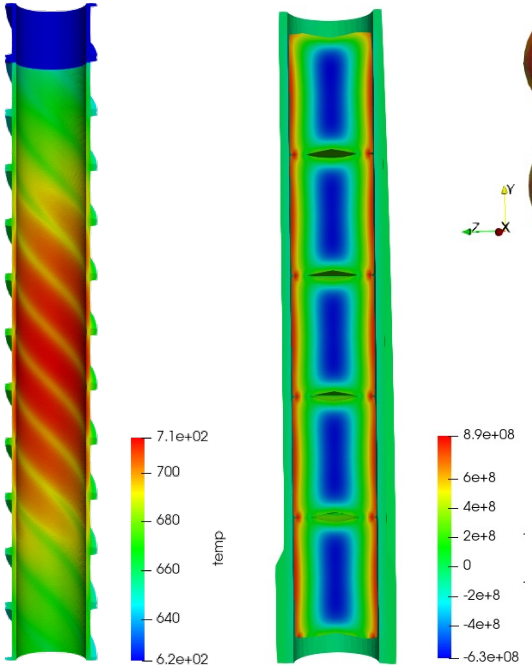
4.9 Summary

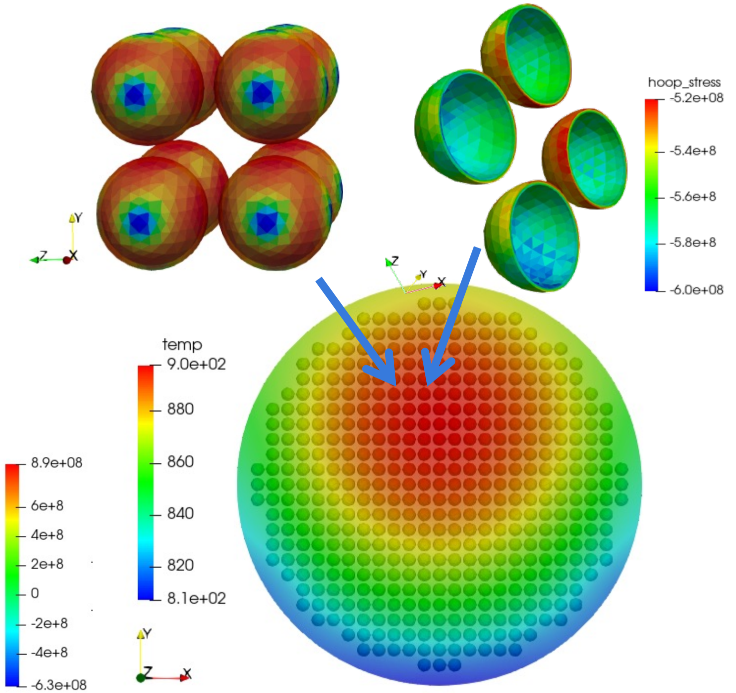
Developed by the XJTU-NuTheL group at Xi'an Jiaotong University, BEEs is an unified fuel performance simulation code.

- Supports several fuel types, including solid rod fuel, annular fuel, plate fuel, and TRISO.
- Serves as both a fuel design tool and an independent performance evaluation platform.









Thank You!