Science and Technology Facilities Council

Leveraging Large-Scale CFD to Improve Nuclear Reactor Safety and Support the Development of Engineering Modelling Tools

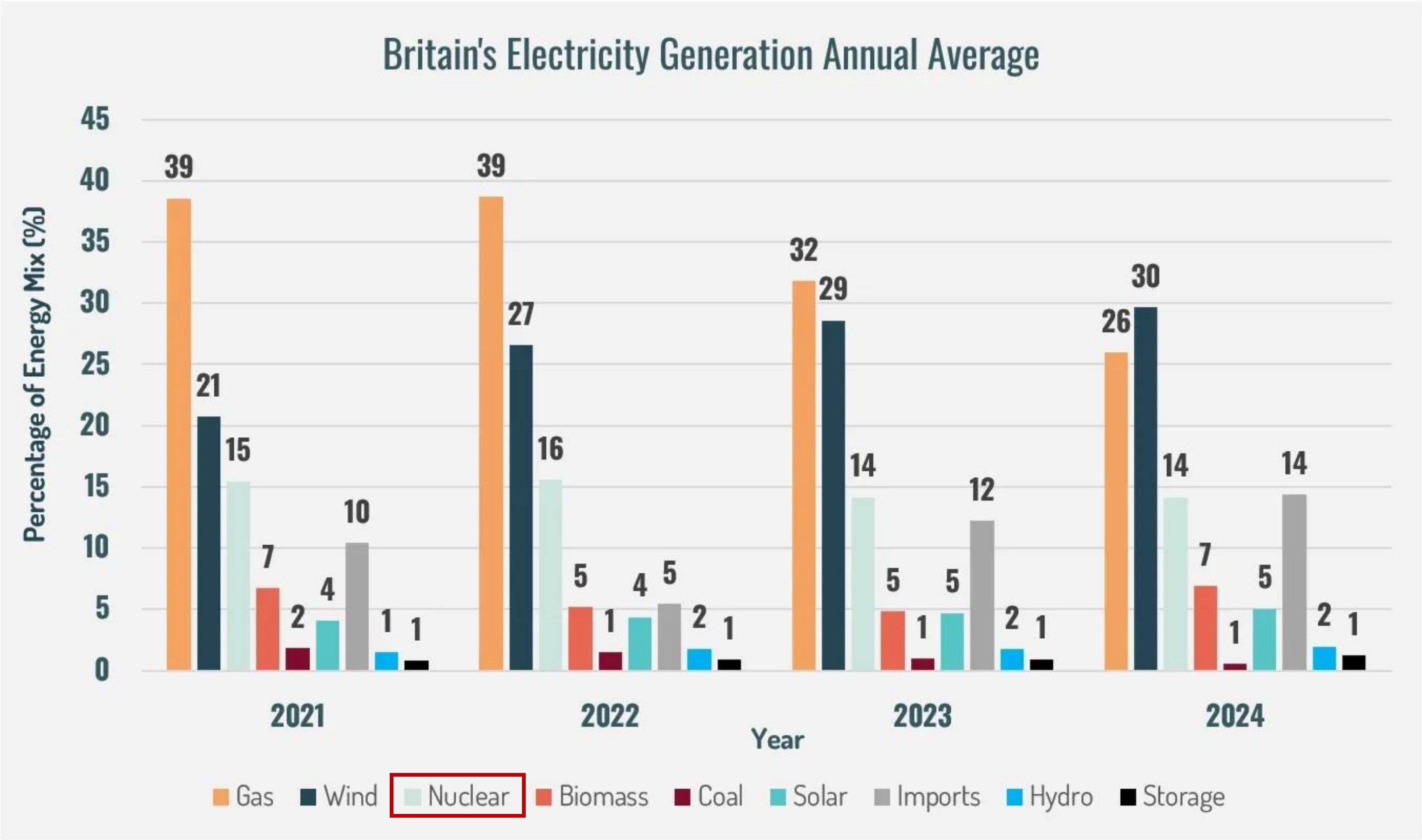
Bo Liu[1,*], Wei Wang[1], Stefano Rolfo[1], Charles Moulinec[1]

[1] Scientific Computing,
UKRI Science and Technology Facilities Council
* Correspondence: bo.liu@stfc.ac.uk

ARCHER2 Celebration of Science 2025 | Edinburgh
14th – 15th May 2025

Nuclear Energy

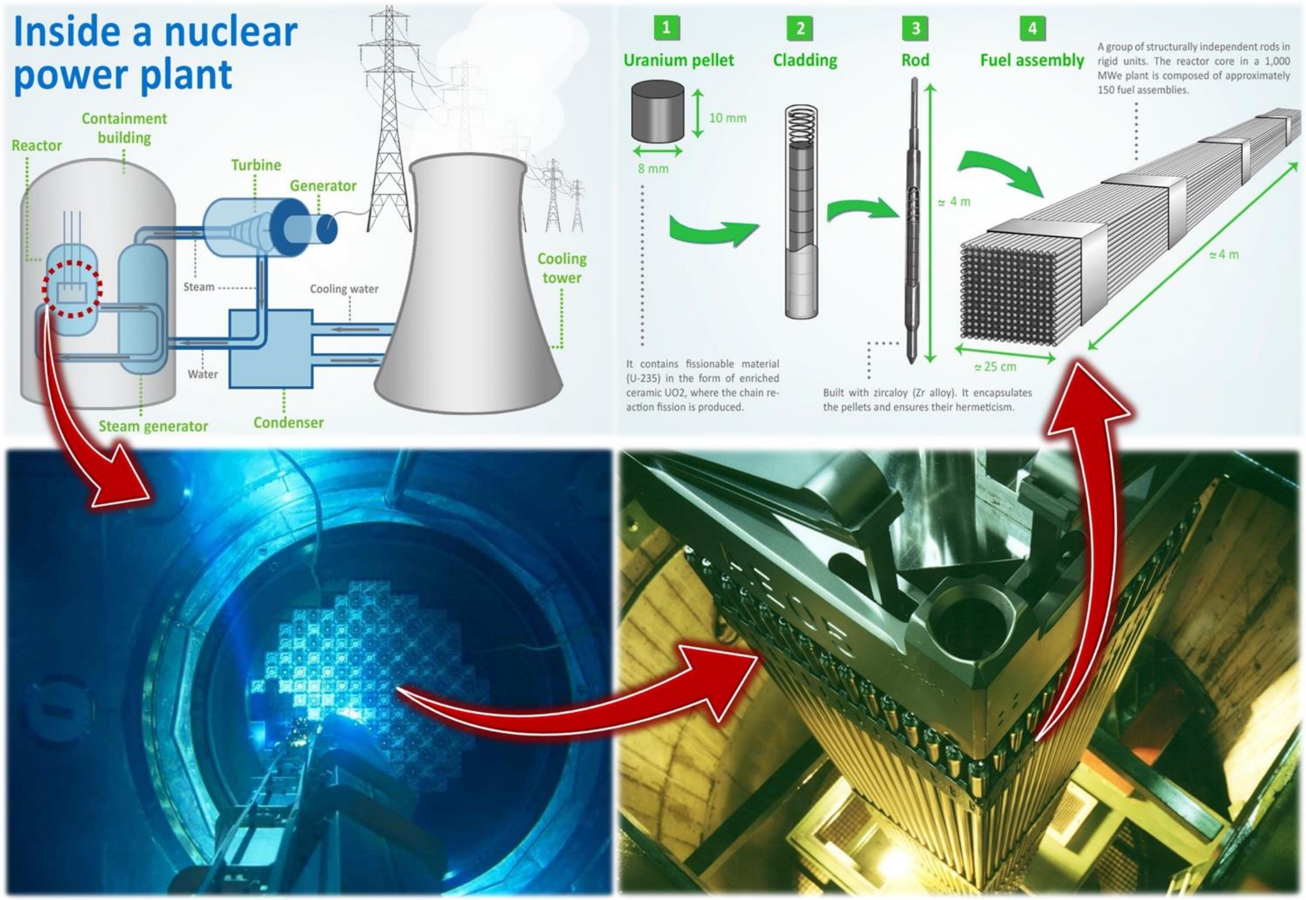
- Nuclear energy provides **clean, stable** generation of electricity
- It plays a crucial role in helping the UK achieve Net-Zero by 2050
- By 2024, nuclear generation fell to 38.2 TWh, 13.7% of the mix
- This is due to ageing plants and outages
- Declining nuclear output risks creating gaps in stable energy supply that must be addressed
- The UK has been actively pursuing advanced nuclear technologies for next generation reactors, such as AMR, HTGR



Britain's electricity generation by energy source (2021-2024)
Data Source: National Grid ESO

Thermal Hydraulics Simulations

What a nuclear reactor looks like and how it works?



- **Challenges**
  - Safety is the highest priority in nuclear reactor design and operation
  - Detailed understanding of complex thermal hydraulic behaviours within the core is essential
  - Direct experimental measurements under reactor condition is expensive or impractical
  - Numerical simulation is a critical tool to gain insights into reactor physics and behaviour
  - Huge number of coolant channels and broad range of physical scales pose significant challenges to numerical simulations
  - HPC serves as an powerful tool for addressing these challenges through advanced, large-scale modelling

Outline

Case study 1

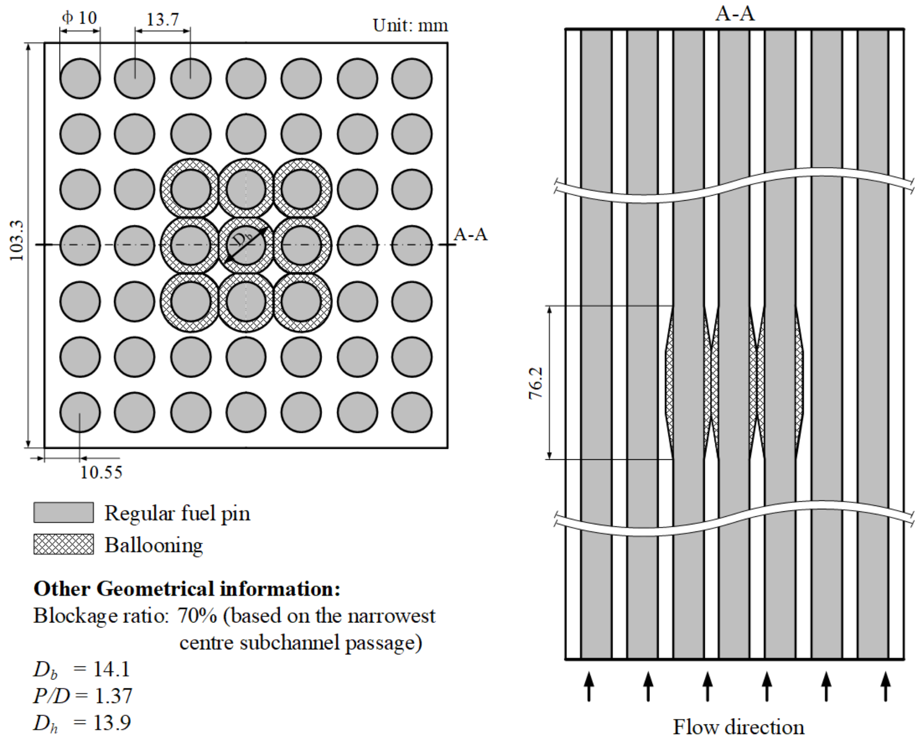
- ***High-Fidelity Simulations to Improve Performance and Safety of Pressurised Water Reactors***
  ARCHER2 Pioneer Project (2021 – 2022)
  by Charles Moulinec, Wei Wang, Bo Liu, Shuisheng He and Juan Uribe

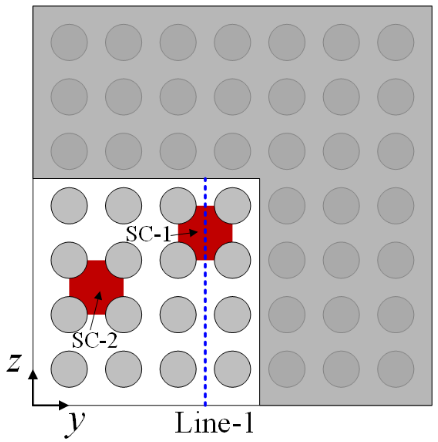
Case study 2

- ***Assessment of the Performance and Passive Cooling Capabilities of High Temperature Gas-cooled Reactors using High-Fidelity Simulations***
  ARCHER2 Pioneer Project (2023 – 2025)
  by Bo Liu, Charles Moulinec, Wei Wang
- ***Development of a cost-effective simulation tool for transient processes in High Temperature Gas-cooled Reactors***
  Industry Impact Fund (I2F) Project (2024)
  by Bo Liu, Charles Moulinec, Wei Wang, Stefano Rolfo

Case Study 1

- **Modelling of a PWR rod bundle with clad ballooning**
- Over-heating of fuel rods - a common scenario in design-based nuclear reactor accidents
- Leading to localised fuel cladding "swelling" or "ballooning
- Potentially result in blockage of fuel channels, altering reactor’s thermal hydraulic behaviour





Mean and RMS velocities were measured along horizontal lines (Line-1) of various axial locations [1]

[1] Creer, J., Bates, J. and Sutey, A., “Turbulent flow in a model nuclear fuel rod bundle containing partial flow blockages”, Nuclear Engineering and Design, 52(1), pp. 15–33 (1979).

CFD modelling

▪ Cases simulated

- Two cases are simulated, including an isothermal case and a non-isothermal case
- Both URANS and LES methods were employed, using the k-ω SST turbulence model for URANS and the Wall-Adapting Local Eddy-viscosity (WALE) model for LES

Table 1 Flow and thermal conditions of the cases investigated

Case	U_0 [m/s]	T_0 [°C]	q [kW/(m²•s)]	p [bar]	Re_0
1	1.737	29.4	0	1.2	2.98×10^4
2	0.7	282	60	156	7.73×10^4

Table 2 Mesh sizes used in the simulations

Mesh size [No. cells]	Case 1	Case 2
URANS	598,845,312	615,906,432
LES	701,212,032	1,160,539,440

CFD modelling

▪ The CFD software used

code_saturne EDF

- https://www.code-saturne.org/cms/web/
- https://github.com/code-saturne/code_saturne

- Open-source multi-purpose CFD software by EDF
- Finite volume method with unstructured mesh
- User-friendly GUI and well-designed user functions
- New version (v9) to come in summer 2025 (with GPU acceleration as well as some other new features)

▪ Scalability on ARCHER2

- Scalability tested for a lid-driven cavity flow
- Code_Saturne shows excellent parallel scalability on ARCHER2
  - 889M cell mesh

Threads / Nodes	Runtime / s	Speedup	Efficiency
4,096 / 32	14.953	1	100%
8,192 / 64	7.245	2.064	103%
16,384 / 128	3.528	4.238	106%
32,768 / 256	1.908	7.839	98%
65,536 / 512	1.245	12.014	75%

  - 7B cell mesh

Threads / Nodes	Time in solver	Speedup	Efficiency
32,768 / 256	19.826	1	100%
65,536 / 512	10.843	1.829	91%
131,072 / 1,024	5.301	3.740	94%

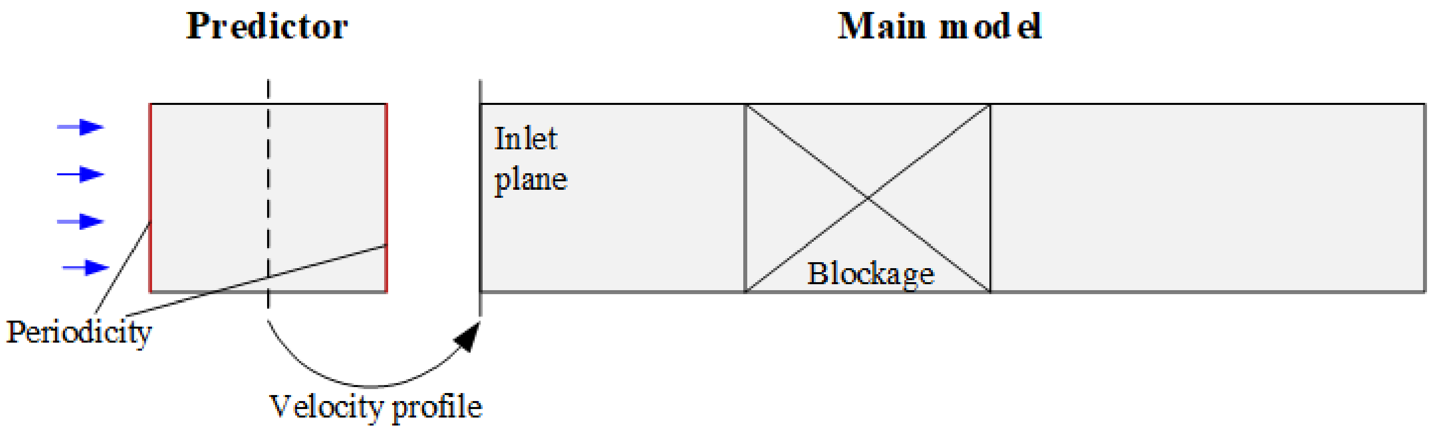
CFD modelling

- **Simulation strategies**

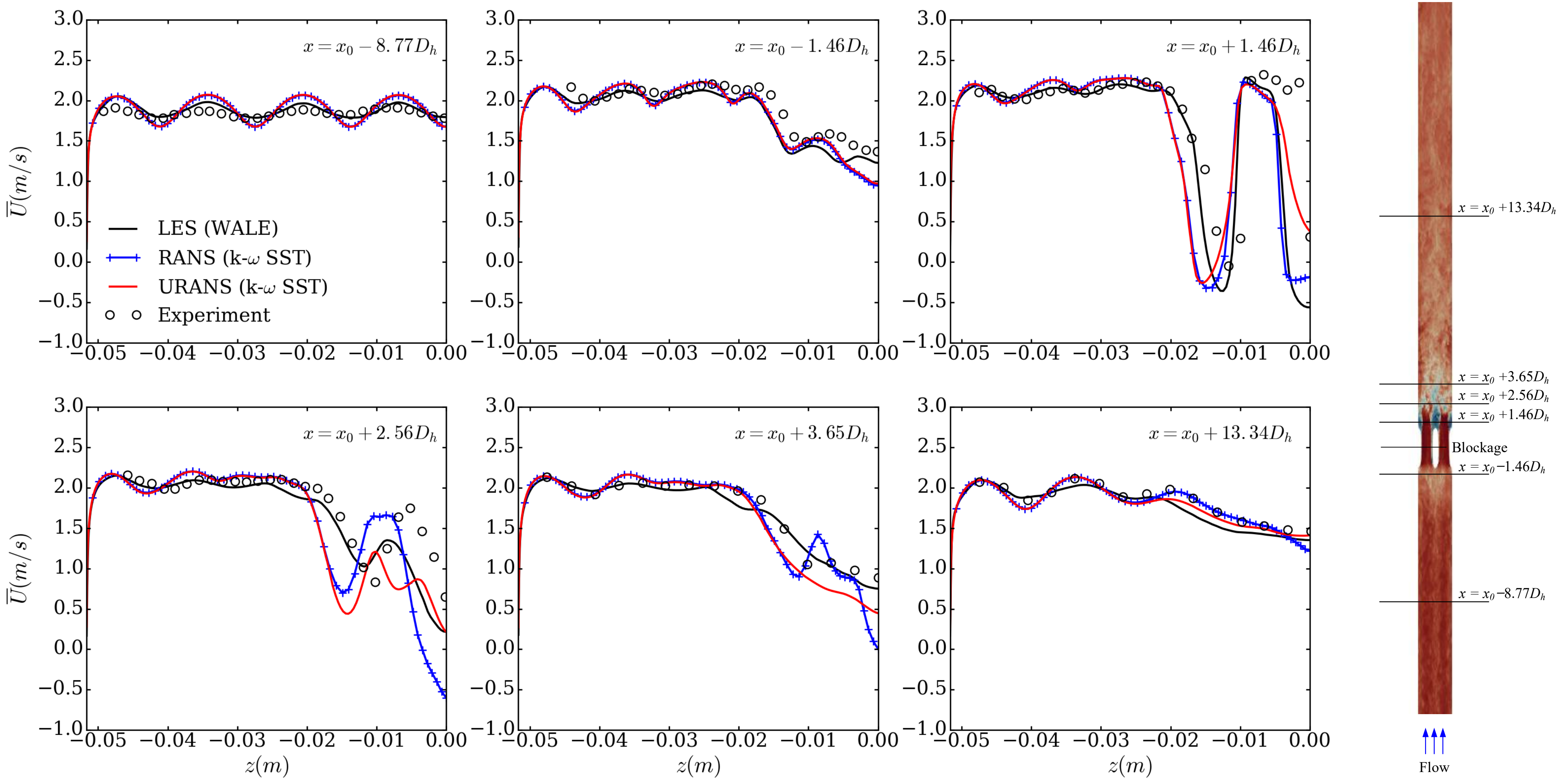
- Based on the mesh size and the scalability test, a maximum of **512 nodes** (65,536 CPU cores) is used

Mesh size [No. cells]	Case 1	Case 2
RANS	48,197,664	N/A
URANS	598,845,312	615,906,432
LES	701,212,032	1,160,539,440
LES: *predictor*	102,366,720	192,383,760
LES: *main geometry*	598,845,312	968,155,680

- Inlet boundary condition for the LES model
  - a precursor turbulence predictor is run alongside the main model
  - The predictor domain features periodicity in the flow direction to generate fully developed velocity profiles
  - The profiles are transferred to the inlet plane of the main model at each time step

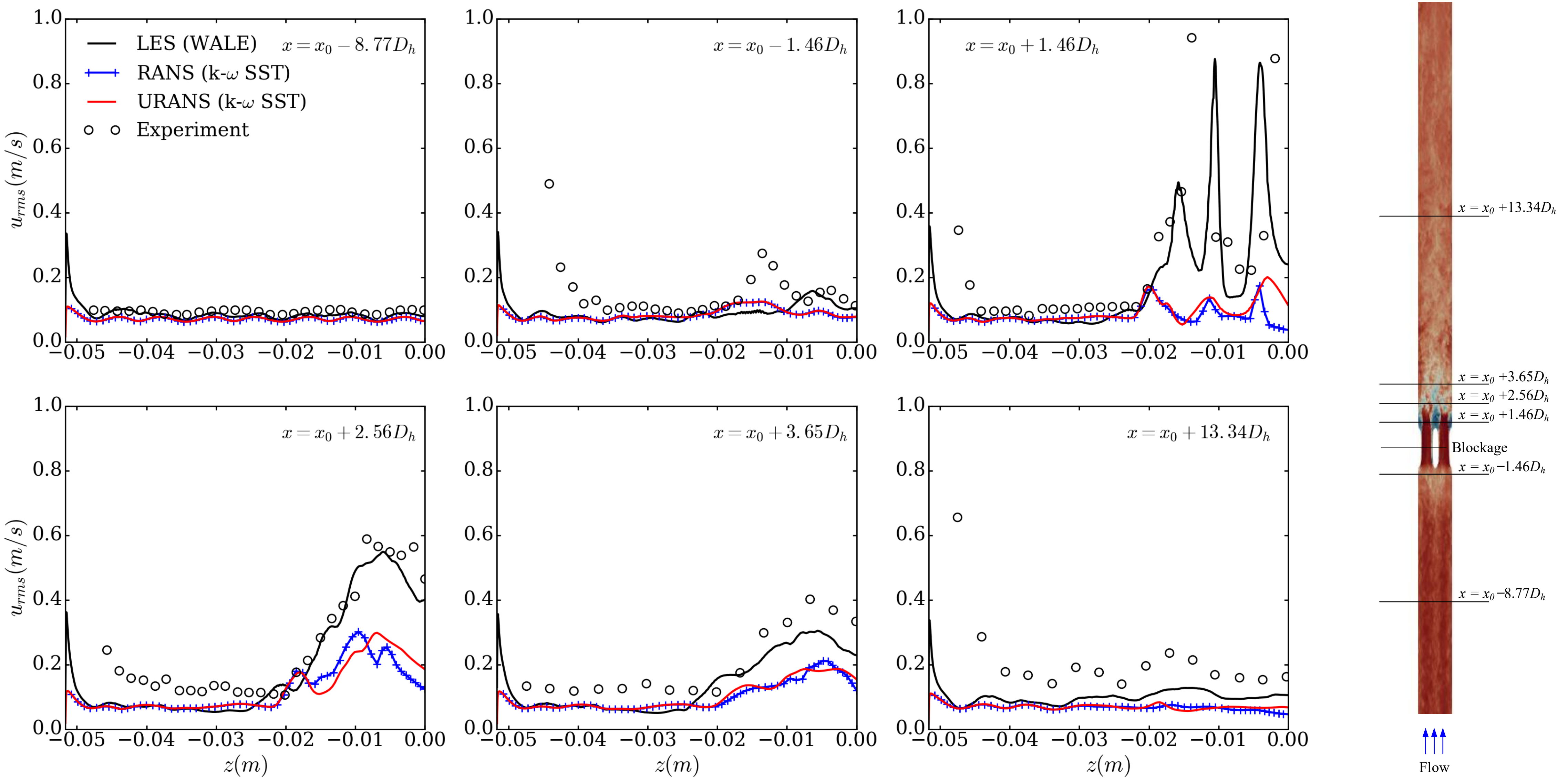


Some results



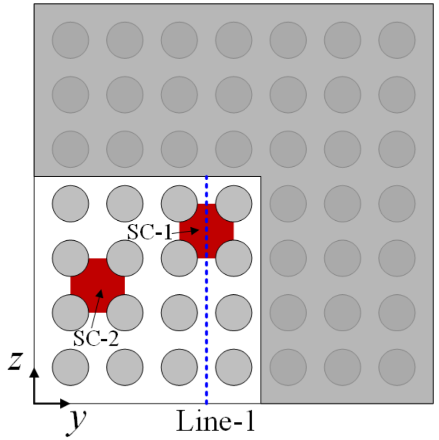
Some results

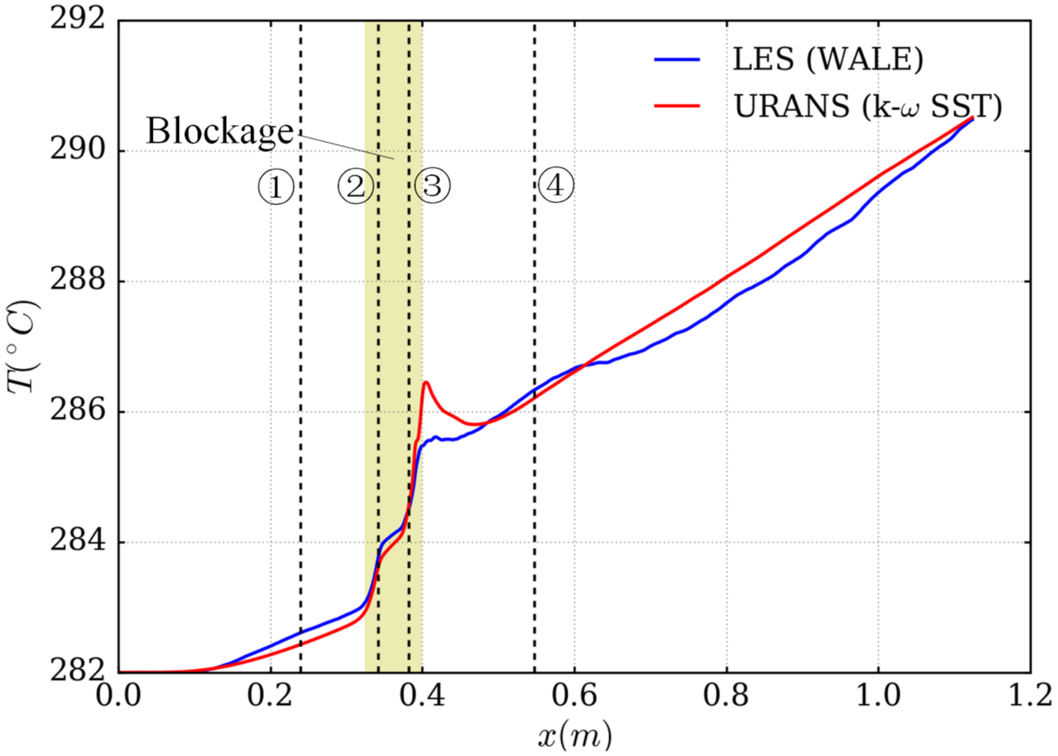
$$u_{rms,LES} = \sqrt{\overline{UU} - \overline{U} \cdot \overline{U}} \qquad u_{rms,RANS} = \sqrt{2/3 \cdot k}$$

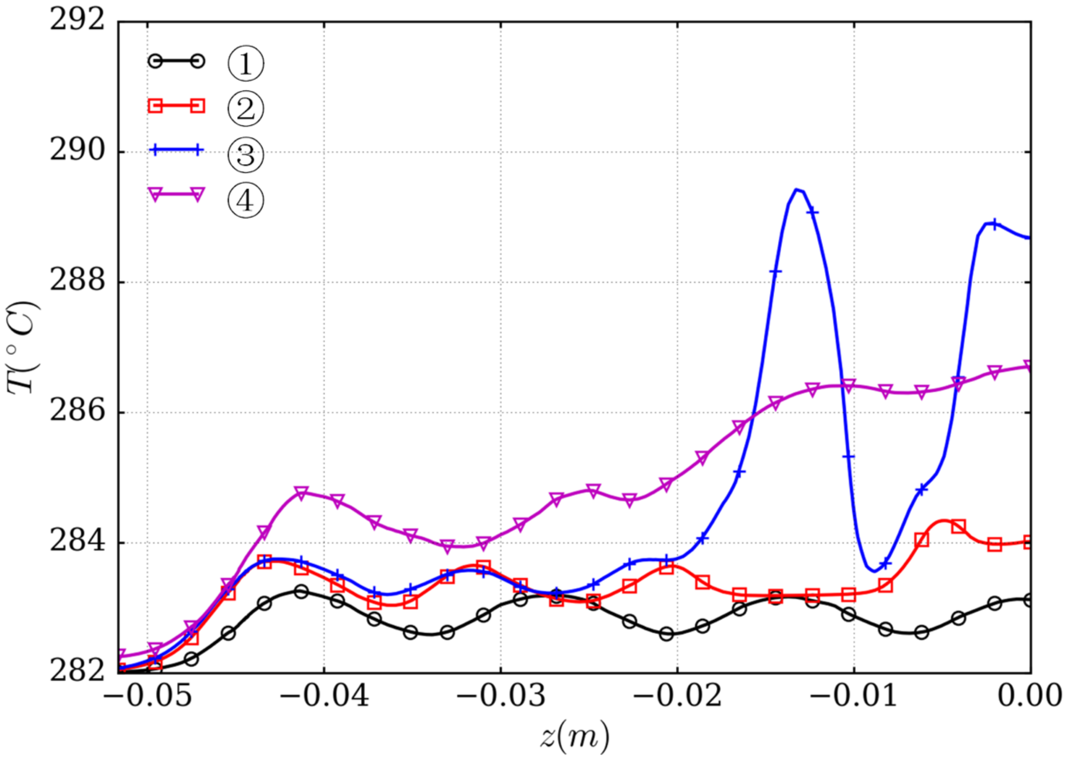


Some results

- **Temperature distributions in case 2**
  - Mean temperature along the centre line of subchannel No. 1 (URANS, LES)
  - Mean temperature profiles over Line-1 at several axial locations (LES)

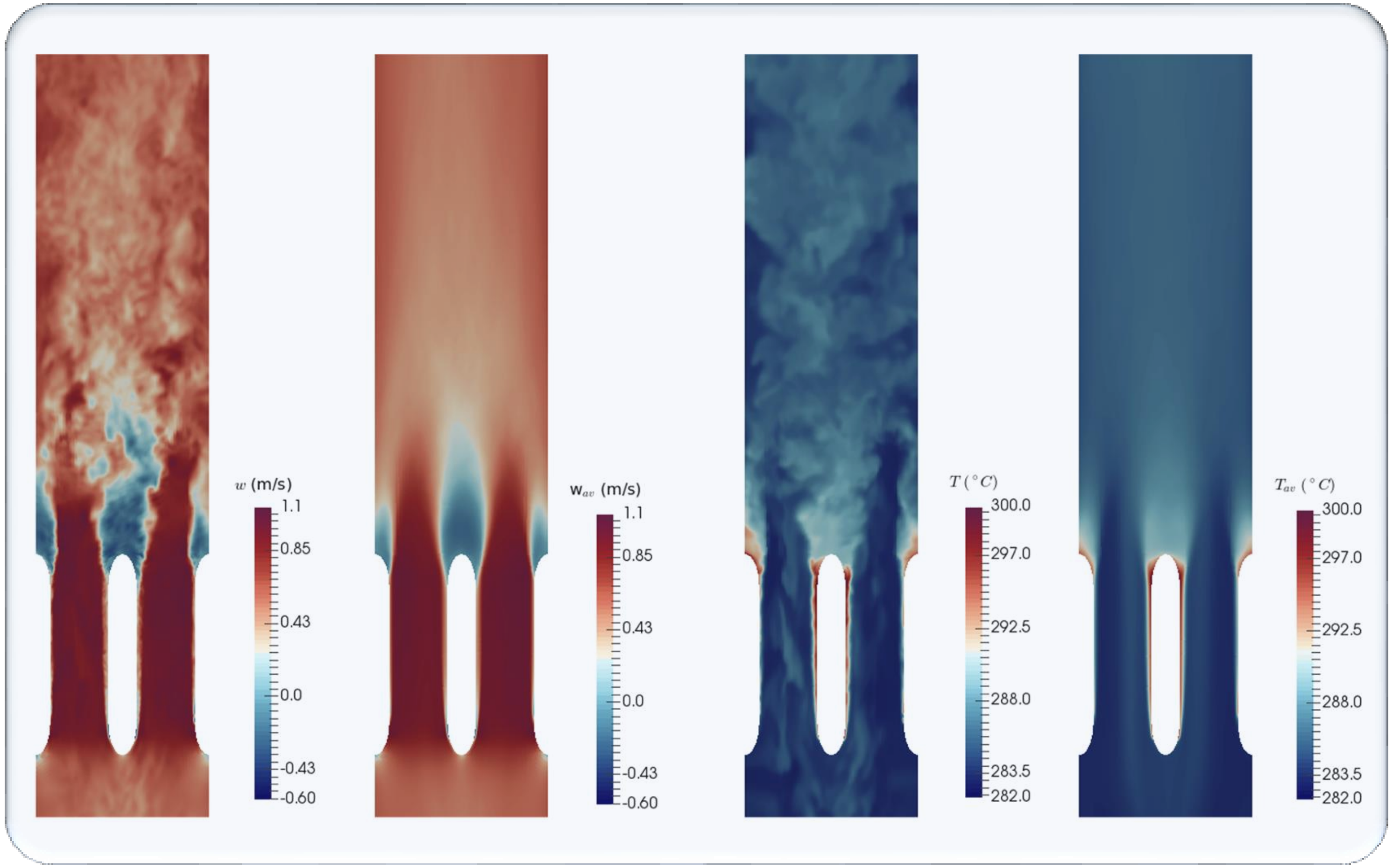






Summary

- Both URANS and LES can well predict the flow redistribution near the ballooning, where LES gives slightly better predictions.
- LES predicts the RMS fluctuating velocity very well, especially in the near downstream of the ballooning, while URANS severely under-predicts it.
- In the non-isothermal case, local hot spots is predicted to form in the narrow gaps, and they are more likely to appear at the downstream side of the ballooning.



Case study 2

- **Modelling of Loss of Flow Accident (LOFA) in an HTGR core**

- Why **HTGR** is interested?

- HTGRs have been prioritised by the UK government as candidates for next-generation nuclear power systems

- What is **LOFA**?

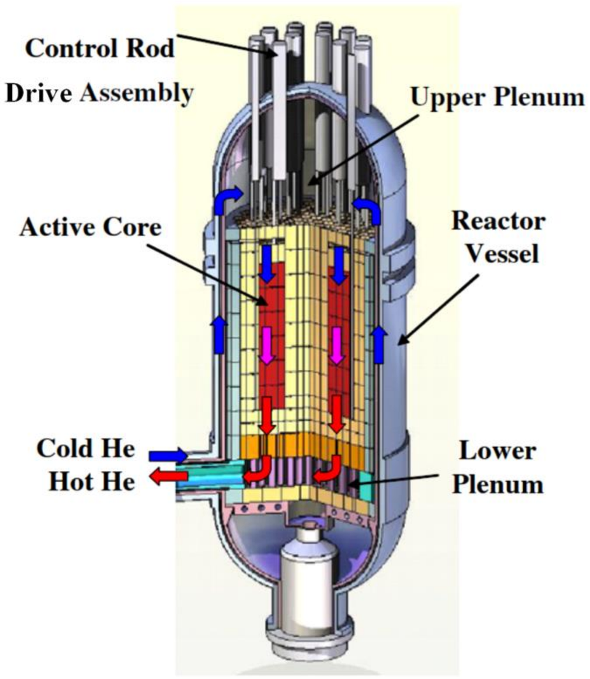
- LOFA (Loss of Flow Accident) is a key accident scenario that poses challenges to safe operation of the reactor
- Understanding reactor behaviour under LOFA conditions is essential for ensuring safety
- During LOFA, decay heat removal involves complex physics, including 3D thermal conduction, radiation, and natural convection

- **Challenges & solutions**

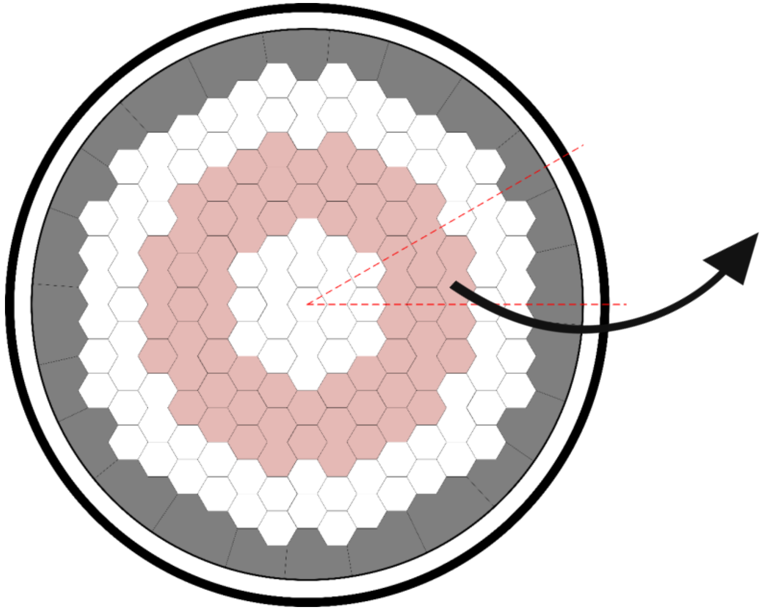
- The long transient adds additional challenge to numerical modelling, even with HPC resources
- High-quality CFD simulations generate valuable data to support the development of engineering tools, such as SubChanCFD, a cost-effective coarse-grid method developed by our team.

HTGR core configuration

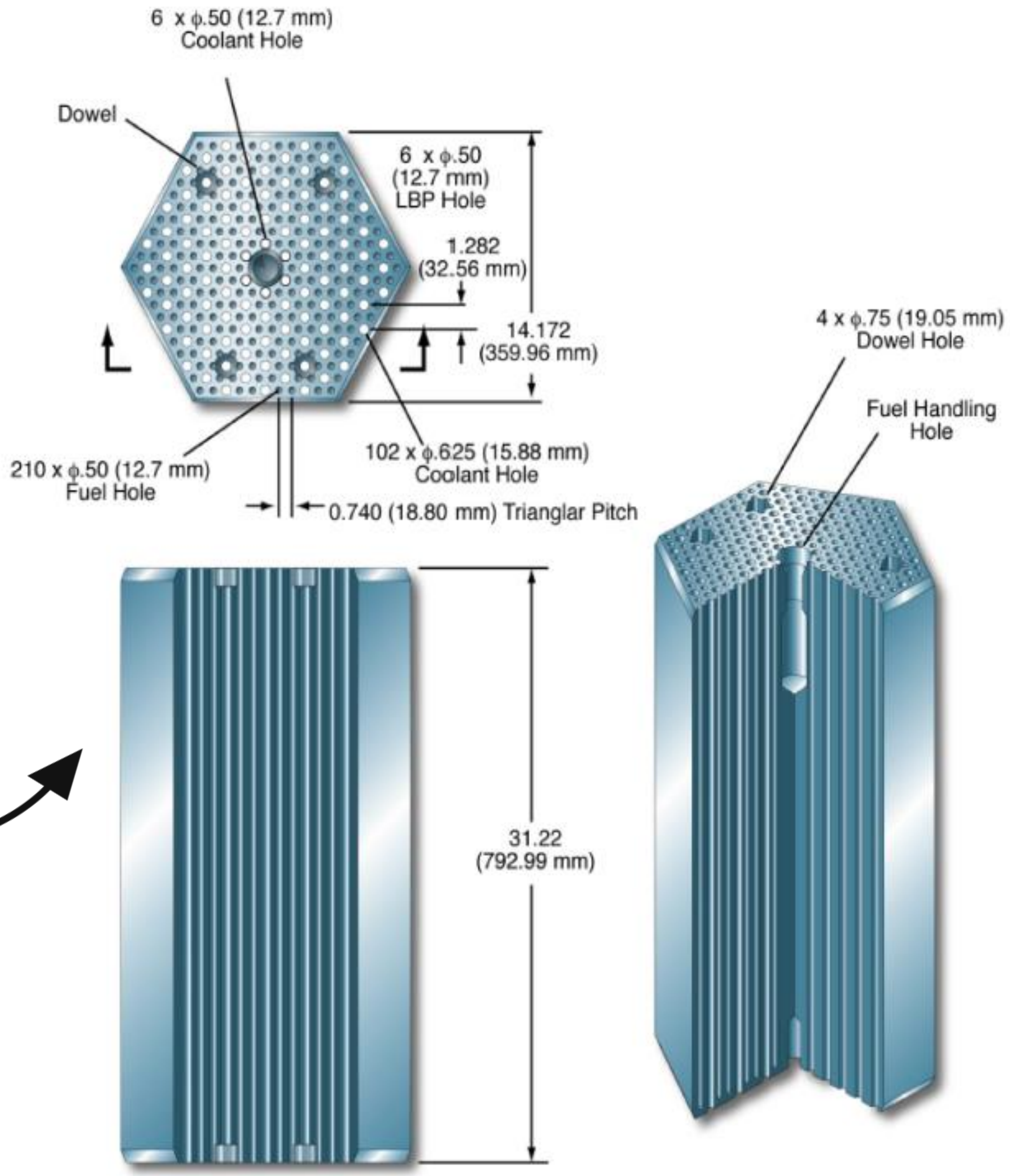
- **Prismatic reactor design** featuring hexagonal fuel assemblies and graphite reflectors
- **Helium** used as coolant removes heat through cylindrical coolant channels



Reactor core



Cross-sectional core structure

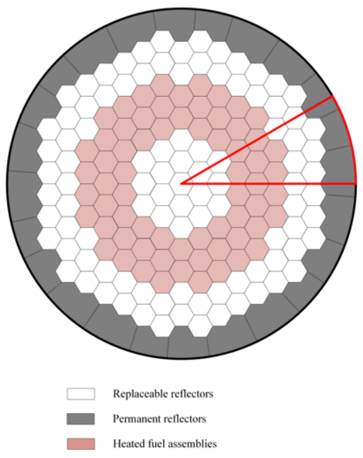


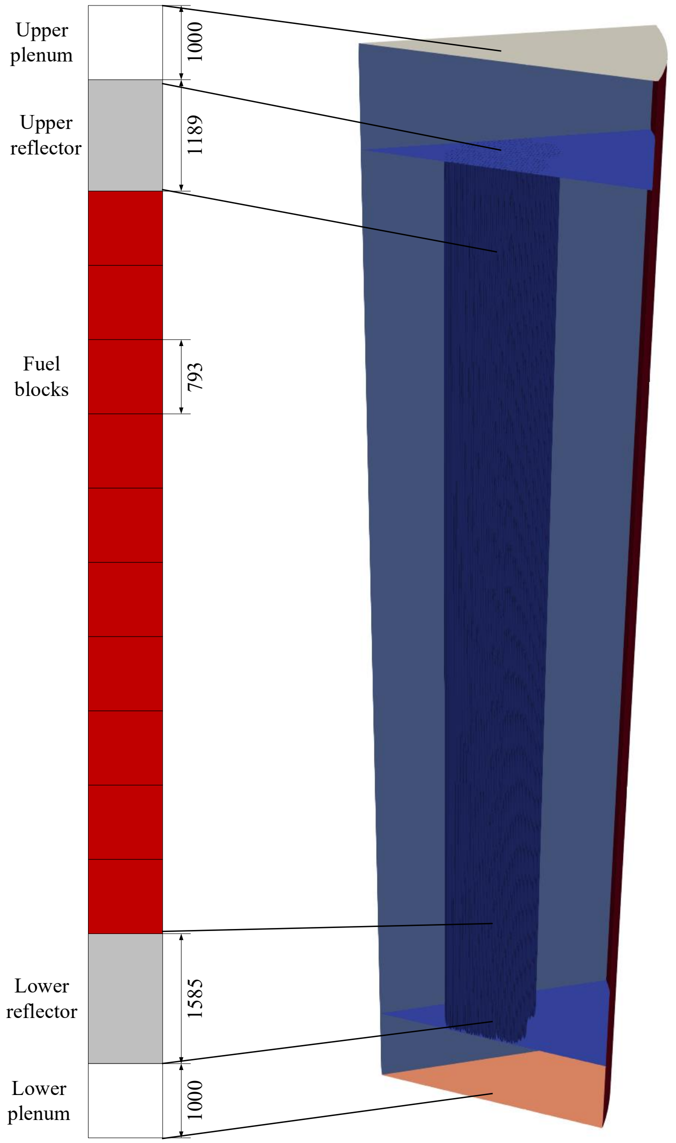
Standard fuel bock
(J W Sterbentz, 2016)

CFD modelling

- **Computational domain**

- The computational domain is based on a **1/12th** sector
- Each fuel assembly consists of 10 standard fuel blocks stacking axially
- Graphite reflectors are added to the top and bottom of the heated fuel section:
  - Upper reflector: 1.189 m
  - Lower reflector: 1.585 m
- Upper and lower plena are considered to provide flow path for natural circulation of the coolant
- The plena are represented using simplified box-like geometries
- Bypass and cross-flow gaps are not considered

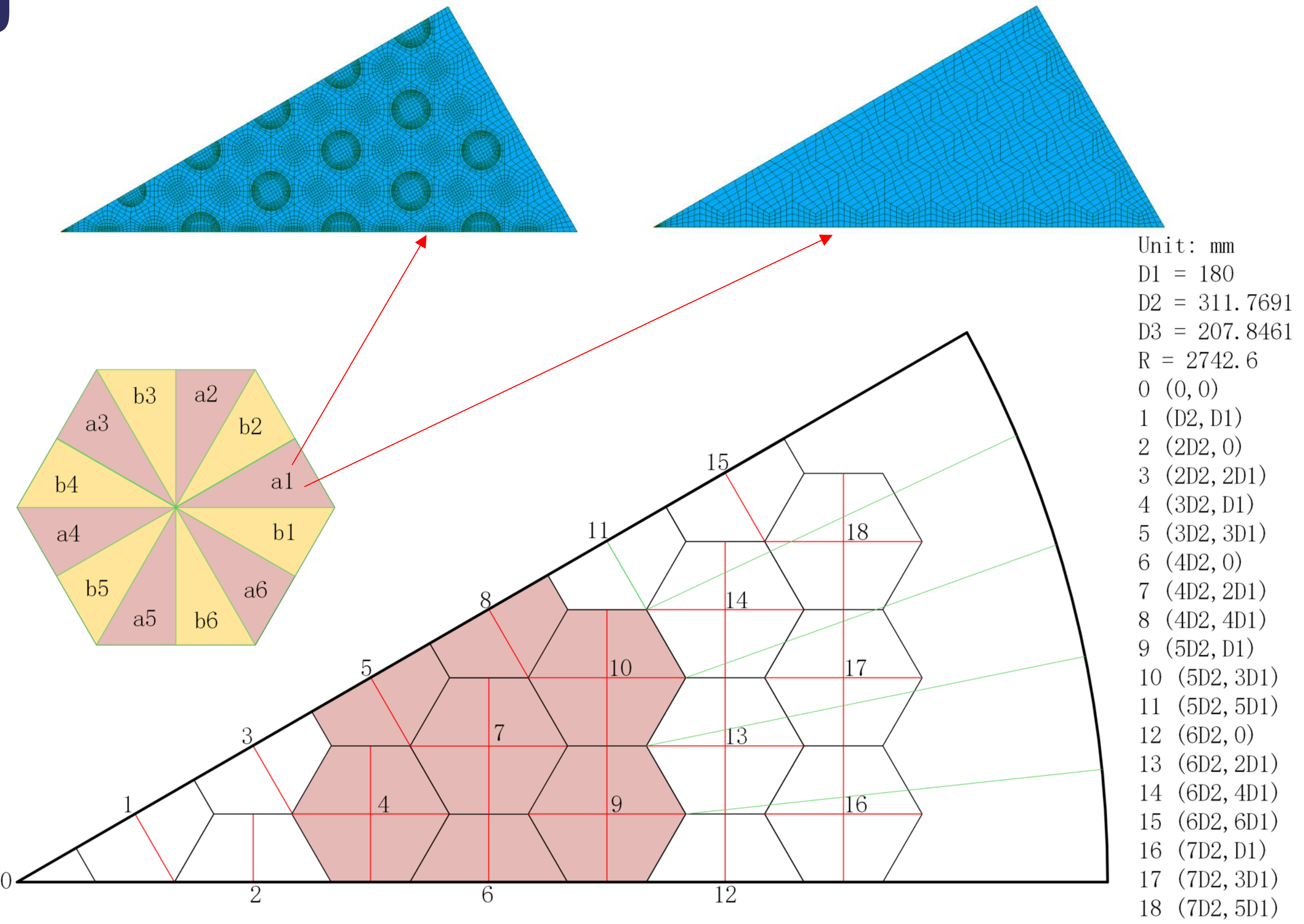




CFD modelling

- **Meshing**

- **Sub-meshes** are first generated for the 1/12th sector of single fuel blocks and graphite reflectors
- The final mesh is created by combining the 93 individual sub-meshes
- The total mesh size is of around **900 million** cells

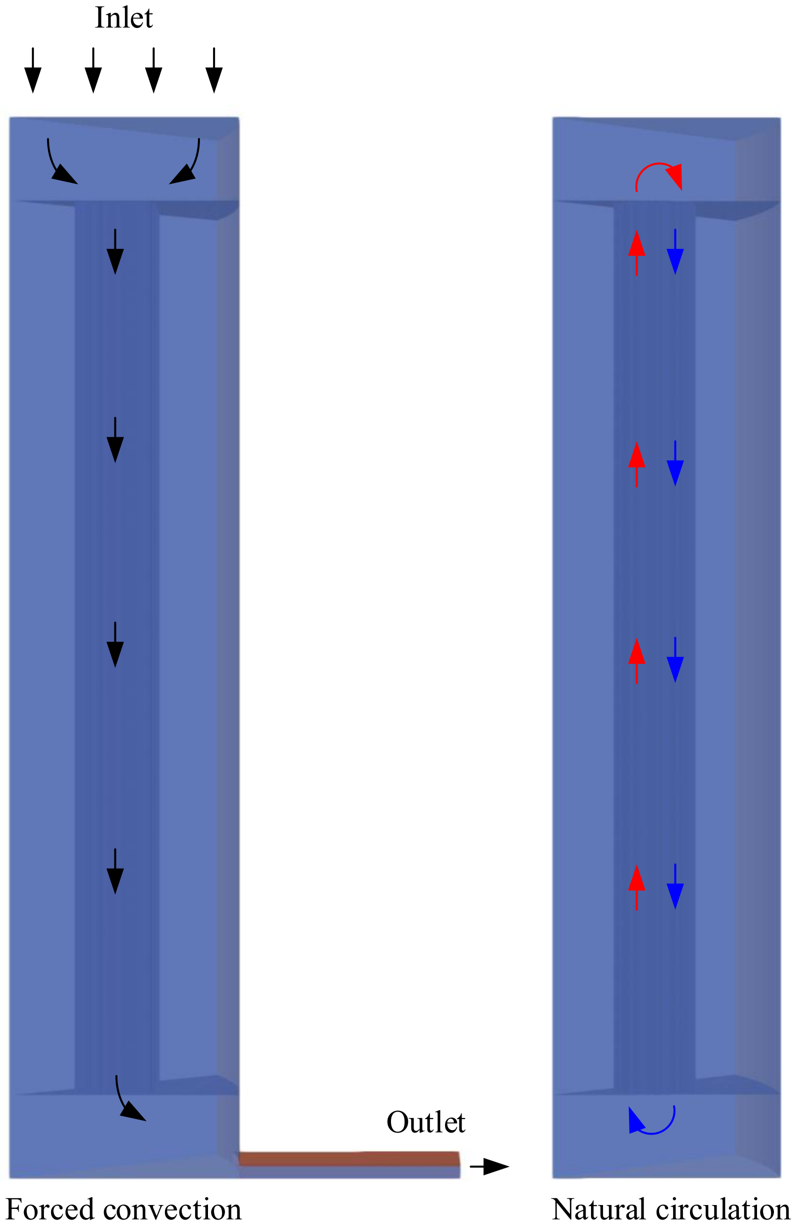


Science and Technology Facilities Council

CFD modelling

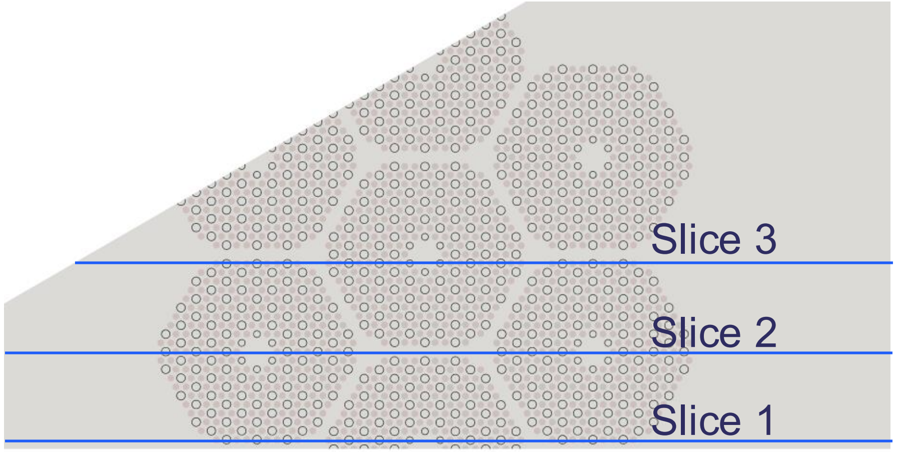
- **Initial and boundary conditions**
  (based on GA's PMR-600)
- Coolant mass flow rate: 14.3484 kg/s
- Fuel power density: 31.6 MW/m3
- Coolant inlet temperature: 490 °C
- Coolant outlet temperature: ~ 950 °C
- Core outer surface: constant temperature at 490 °C

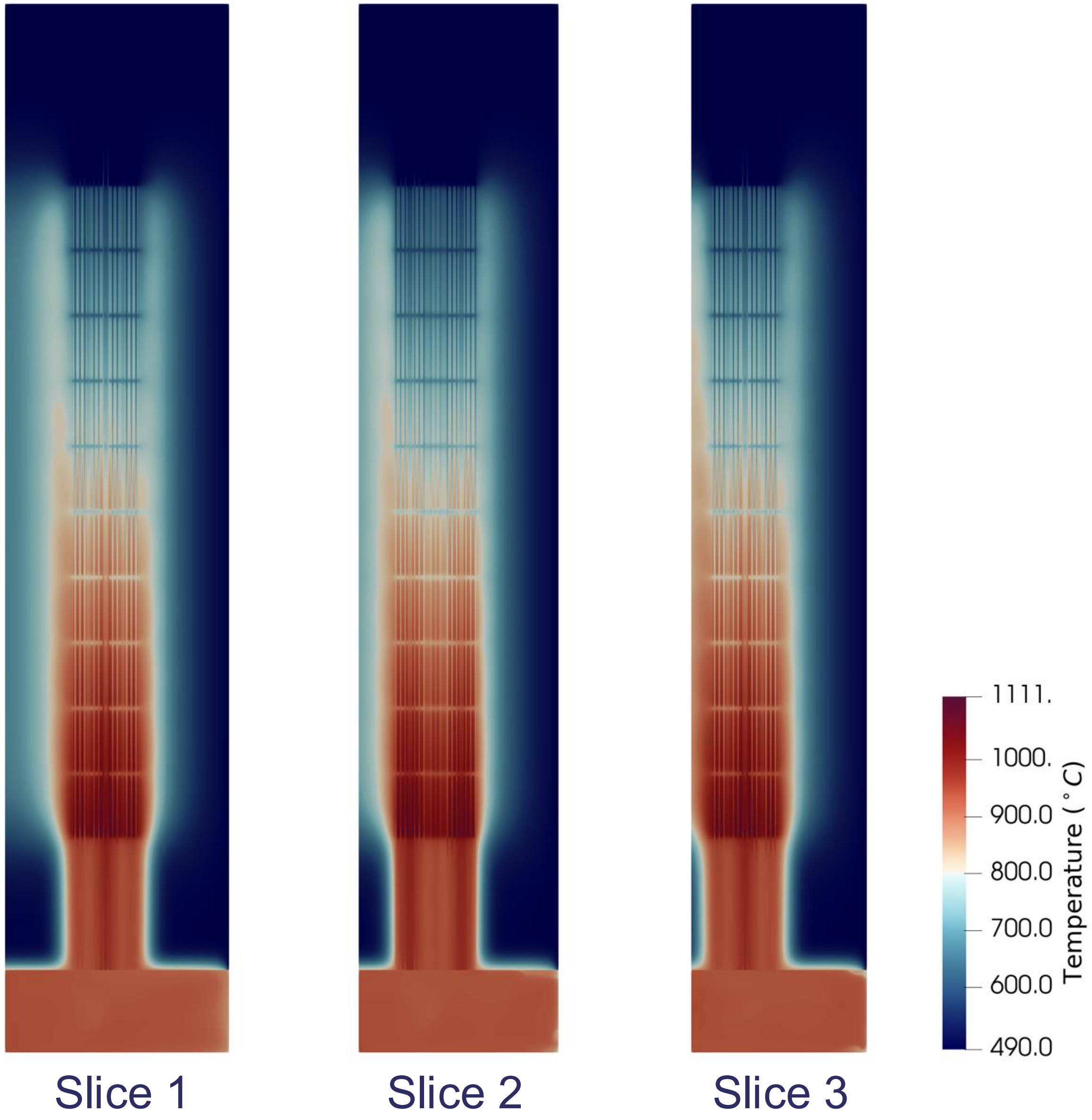
- **LOFA simulation**
- At LOFA onset, all inlets and outlets are replaced with wall boundaries to simulate a sudden pump trip
- Heating power is reduced to ~10% of the steady-state operation to represent decay heat
- Natural circulation is expected to arise, driven by temperature gradients and density differences



Sample results

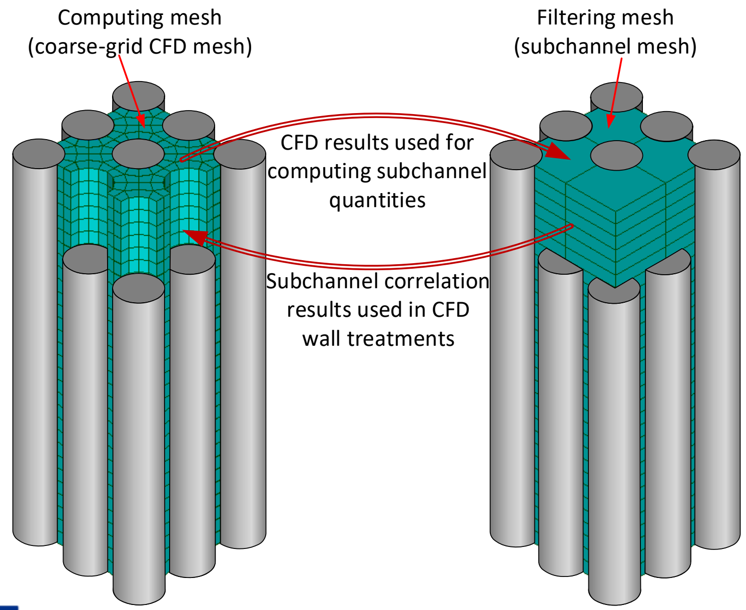
- **Core temperature distribution**
  - CFD simulation provides detailed, 3-D flow and temperature distributions

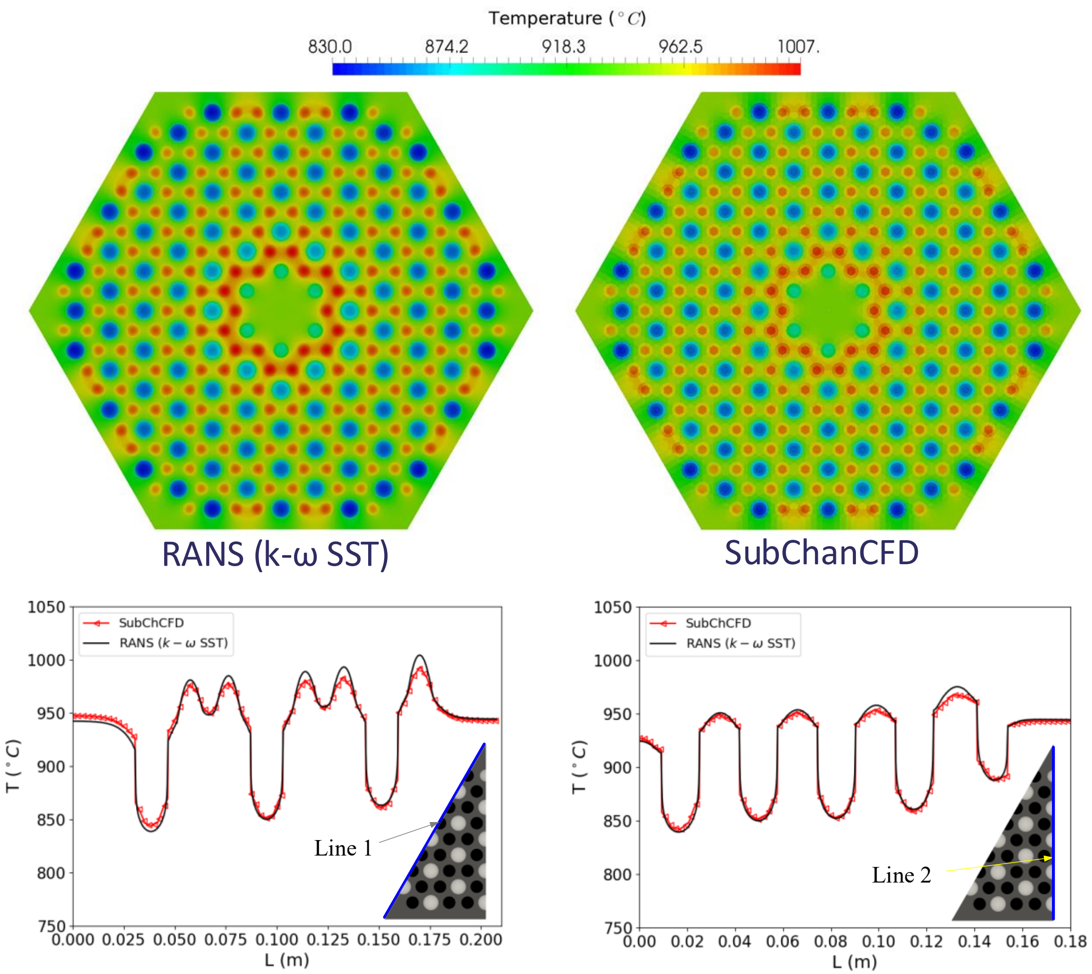




Engineering tool development

- **SubChanCFD [2]**
- 3-D coarse CFD approach developed for simulation of various types of nuclear reactors
- Using well-validated empirical correlations for closure modelling
- Reduces computational cost by 2 - 3 orders of magnitude compared to conventional CFD



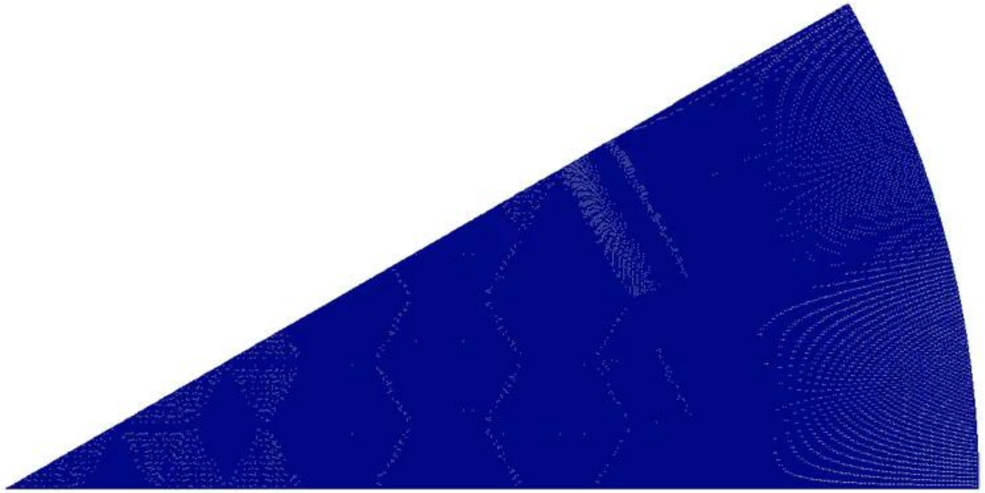


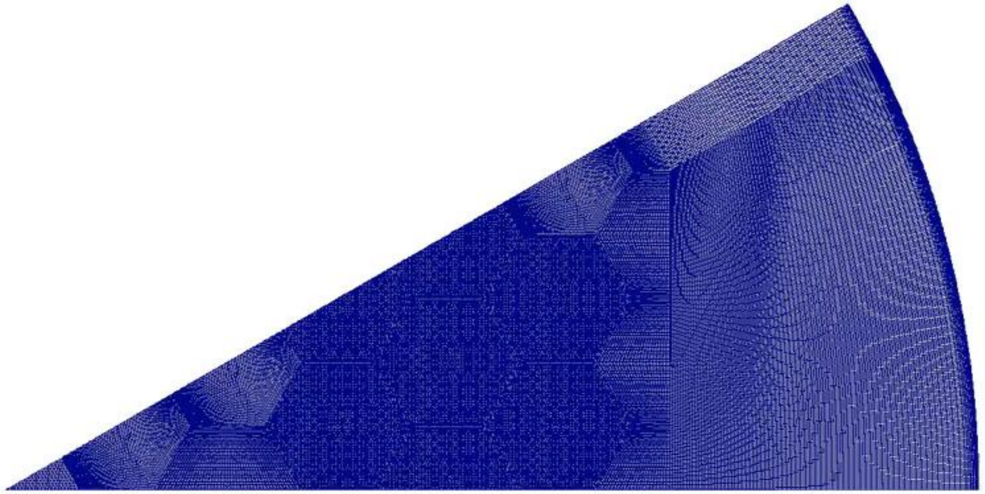
Recently extended for HTGRs

[2] Liu B, He S, Moulinec C, et al. Sub-channel CFD for nuclear fuel bundles[J]. Nuclear Engineering and Design, 2019, 355: 110318.

Computational cost

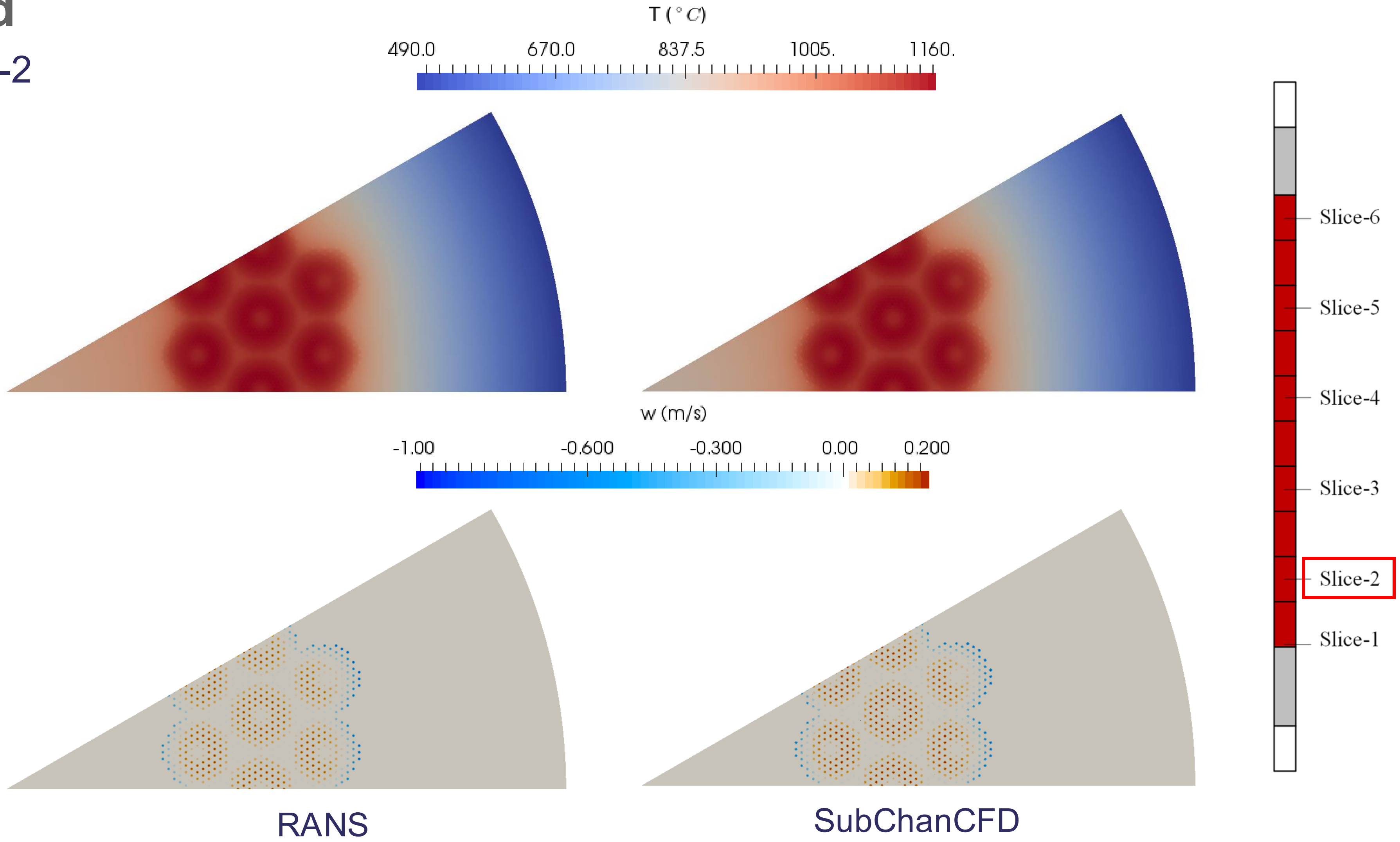
- **Meshes**
  - For both approaches, sub-meshes were initially generated to capture periodic patterns
  - These sub-meshes were then combined to form the final mesh
  - Final mesh sizes:
    - **SubChanCFD:** ∼60 million cells
    - **RANS CFD (k-ω SST):** ∼900 million cells
- **Simulation on ARCHER2**
  - Estimated computational cost for 1,000 seconds:
    - **SubChanCFD (32 nodes):** ∼3,000 CUs
    - **RANS CFD (256 nodes):** ∼120,000 CUs





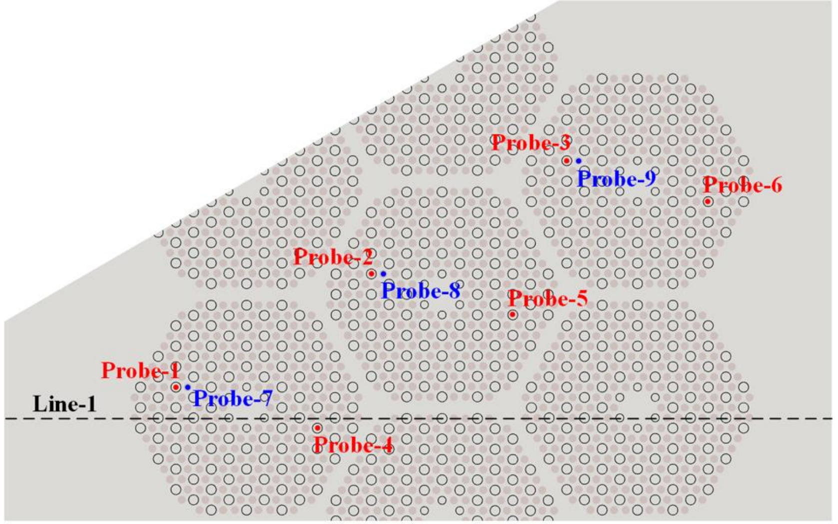
Model validation

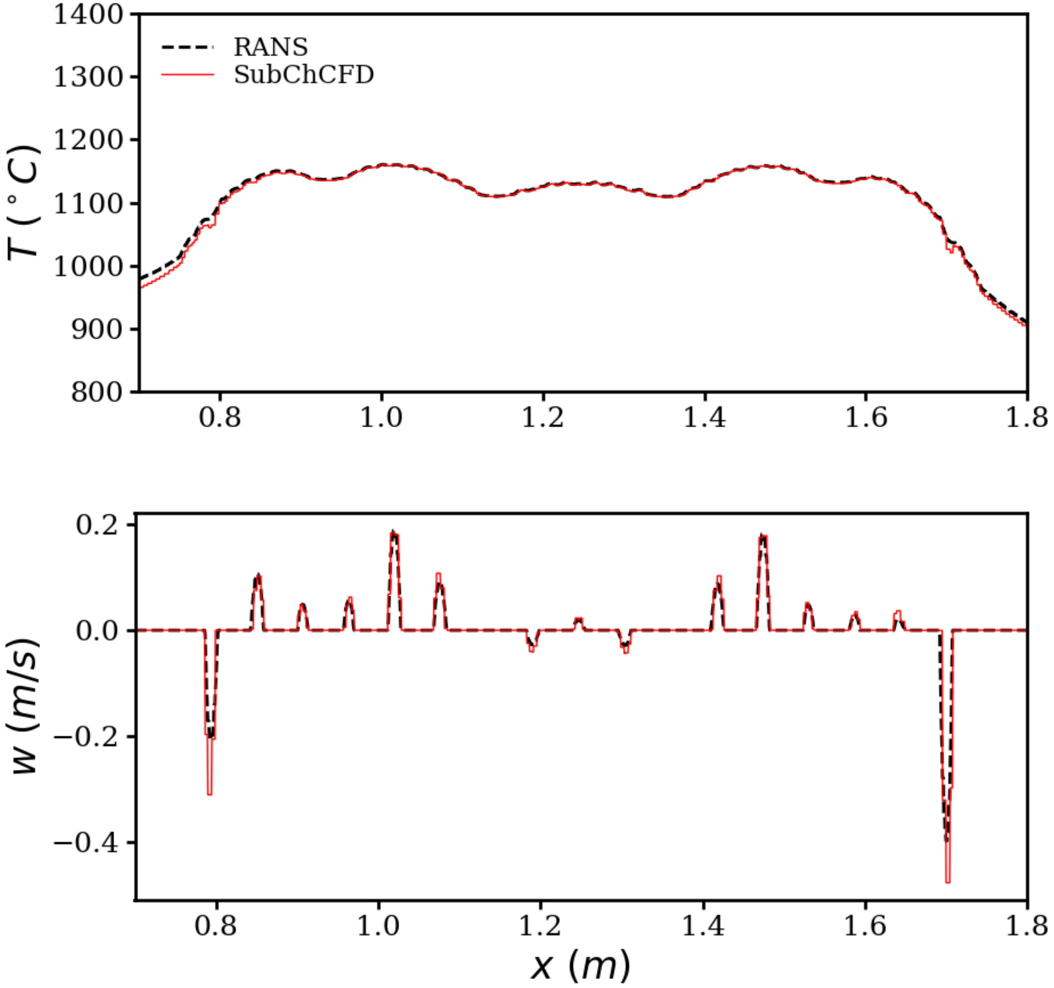
- **Temperature field**
  - t = 503 seconds at Slice-2
  - The overall temperature and vertical velocity distribution patterns are in very good agreements between SubChanCFD and RANS

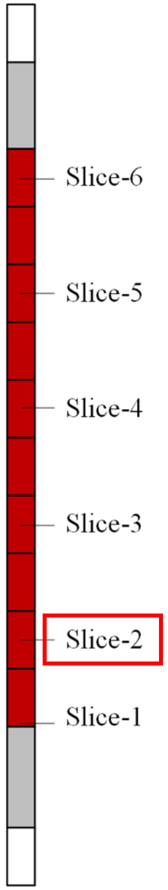


Model validation

- **Line plots**
  - Line-1 at location of Slice-2 is used
  - Temperature and coolant velocity predictions by the two approaches are in excellent agreement

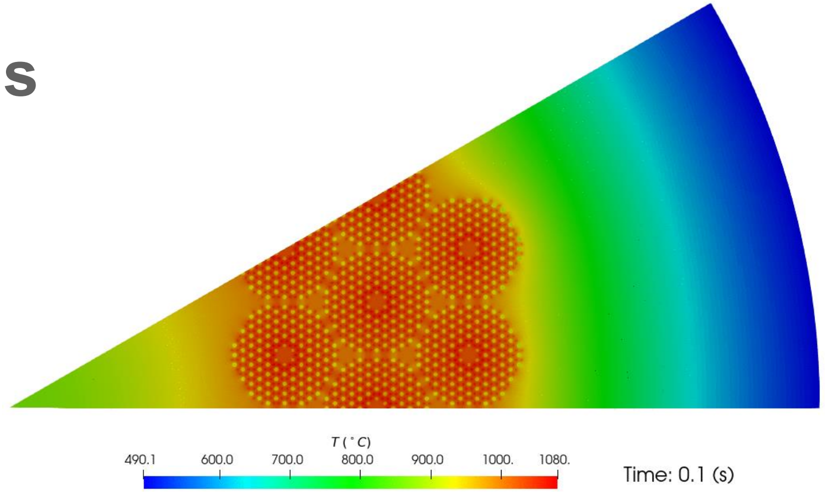


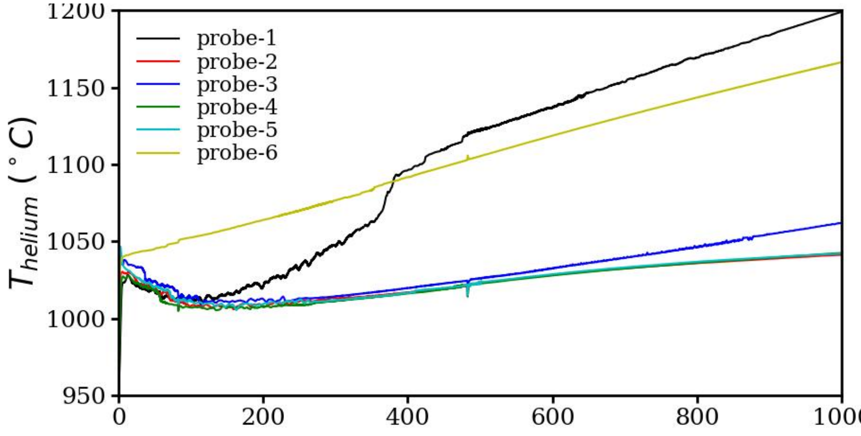


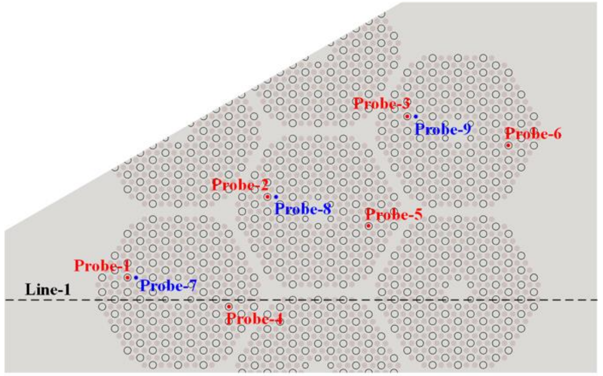


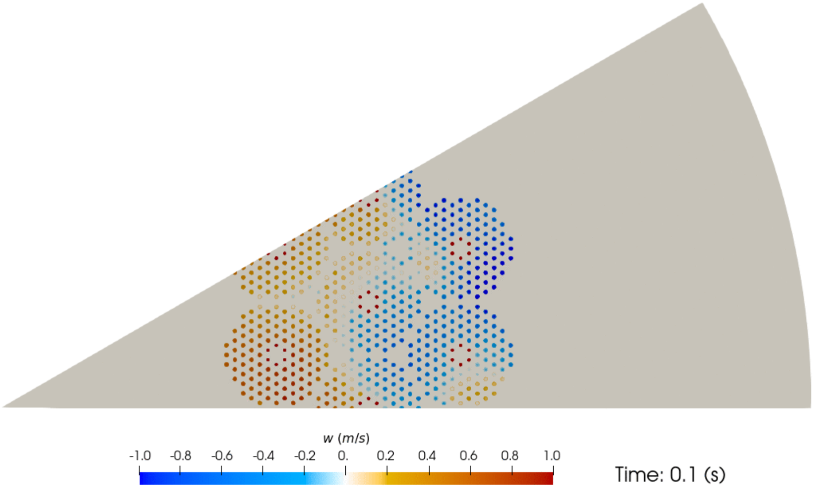
SubChanCFD simulation

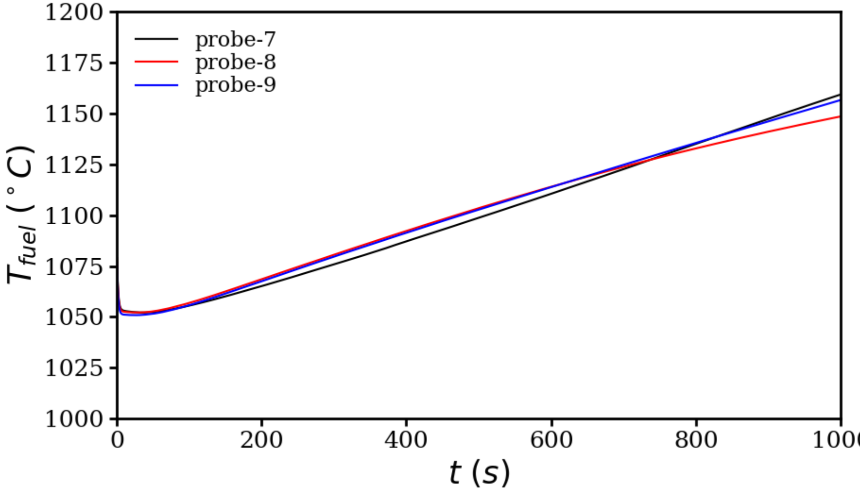
- **Time history of 1000 s**
  - 3-stage evolution
    - Rapid show-down (~5s)
    - Redistribution (~5 - 100s)
    - Re-development (> 100s)











Summary

- CFD simulation of a LOFA transient in an HTGR is highly computationally intensive due to the large reactor core and the long duration of the transient.
- Thanks to the extensive computational resources provided by the ARCHER2 Pioneer Project, we conducted full core-scale simulations of the initial stage of the LOFA transient.
- The resulting high-quality CFD data not only enhances our understanding of the underlying physics but also serves as valuable benchmarking data for the development of engineering tools.
- This data was used to validate SubChanCFD, a cost-effective coarse-grid approach developed by our team.
- With this validated approach, LOFA simulations using SubChanCFD can extend beyond 1,000 seconds with significantly reduced computational cost.

Questions?