Simulation of liquid metal flows - the role of open-source tools from physical understanding to industrial applications

Lilla Koloszar - von Karman Institute, BE

Understanding the physics of liquid metals

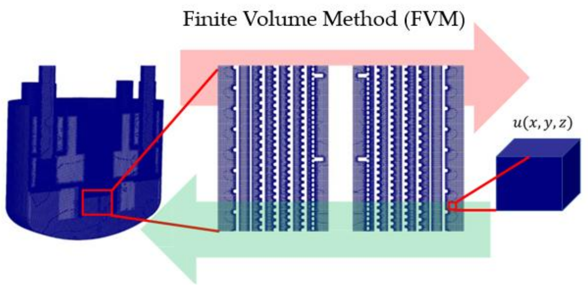
The special case of liquid metals

	
Opaque	Transparent
Usually hot	Usually ‘normal’ temperatures
High thermal conductivity	Low thermal conductivity
Very low Prandtl number	**High Prandtl number**
Very low kinematic viscosity	**Low kinematic viscosity**
Large surface tension	**Small surface tension**

Liquid metals: consequence in CFD simulations

Two fundamental ingredients:

- Turbulent flows
- Low Prandtl numbers



Reynolds Aveaged Navier-Stokes (RANS)

$$\frac{\partial U_i}{\partial t} + \frac{\partial (U_i U_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\upsilon \frac{\partial U_i}{\partial x_j} - \overline{u_i u_j}\right)$$

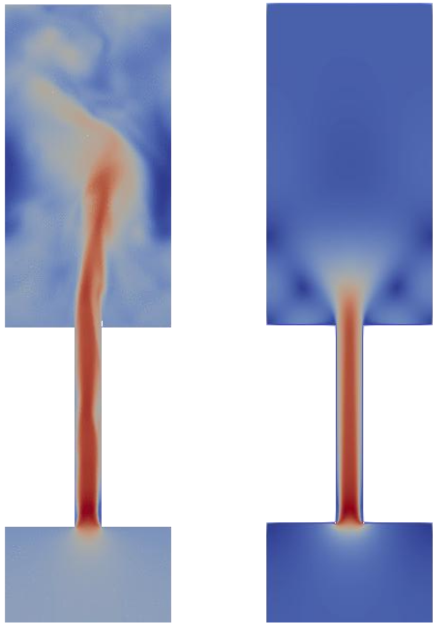
$$\frac{\partial T}{\partial t} + \frac{\partial (U_i T)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\alpha \frac{\partial T}{\partial x_i} - \overline{u_i \theta}\right)$$

Large Eddy Simulation LES

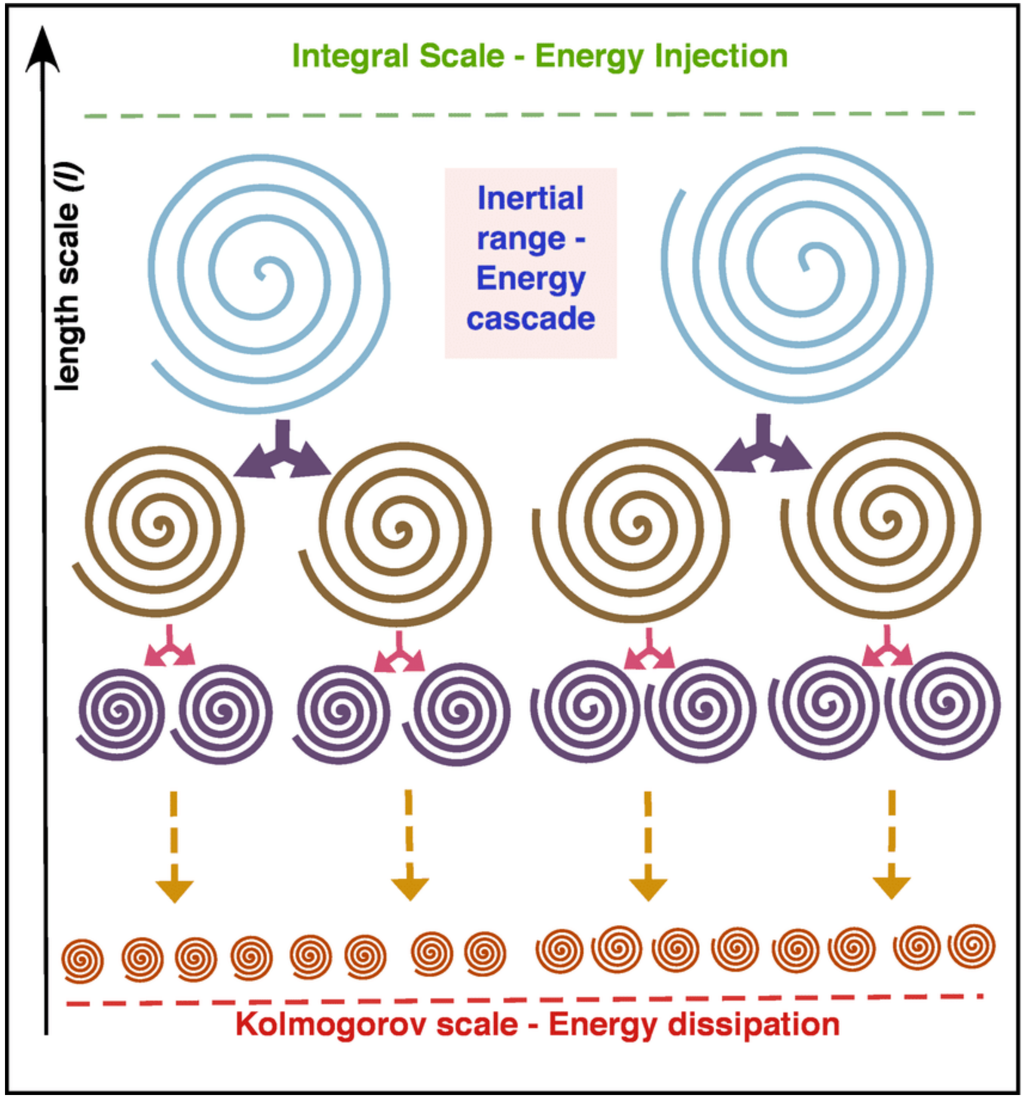
$$\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial \tilde{u}_i}{\partial x_j} + \tau_{ij}\right)$$

$$\frac{\partial \tilde{T}}{\partial t} + \tilde{u}_j \frac{\partial \tilde{T}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\alpha \frac{\partial \tilde{T}}{\partial x_j} + q_j\right)$$

$$\tau_{ij} = \tilde{u}_i \tilde{u}_j - \widetilde{u_i u_j} \qquad q_j = \tilde{T}\tilde{u}_j - \widetilde{T u_j}$$



Energy cascade



Liquid metals: consequence in CFD simulations

Two fundamental ingredients:

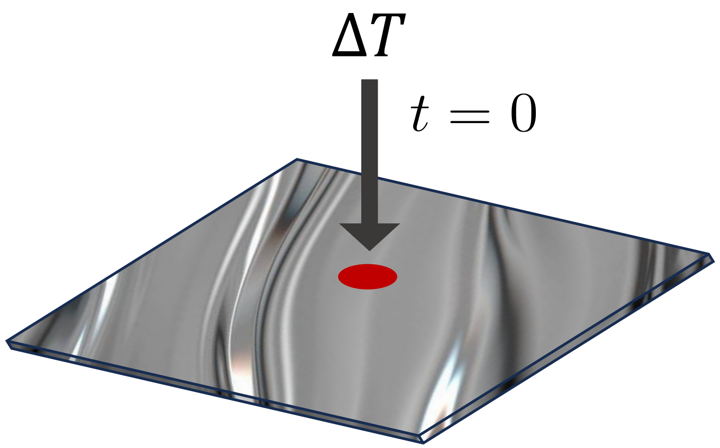
- Turbulent flows
- Low Prandtl numbers

$$Pr = \frac{\nu}{\alpha}$$

$$\frac{\partial U_i}{\partial t} + \frac{\partial (U_i U_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial U_i}{\partial x_j} - \overline{u_i u_j}\right)$$

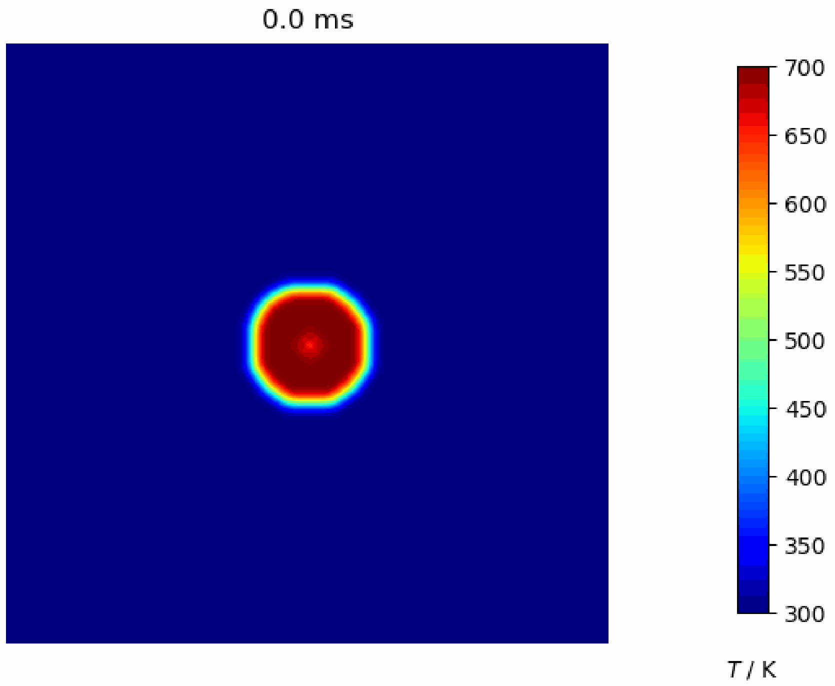
$$\frac{\partial T}{\partial t} + \frac{\partial (U_i T)}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\alpha \frac{\partial T}{\partial x_i} - \overline{u_i \theta}\right)$$

In liquid metals, compared to common fluids (e.g. air), a **thermal perturbation propagates further and faster**

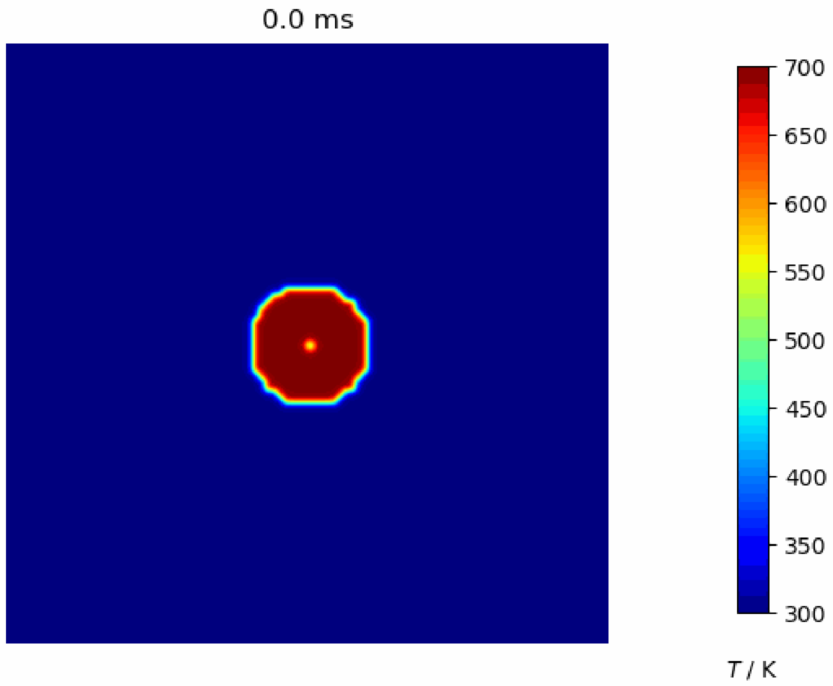


Evolution of the thermal perturbation in time

Low Prandtl $\alpha >> \nu$

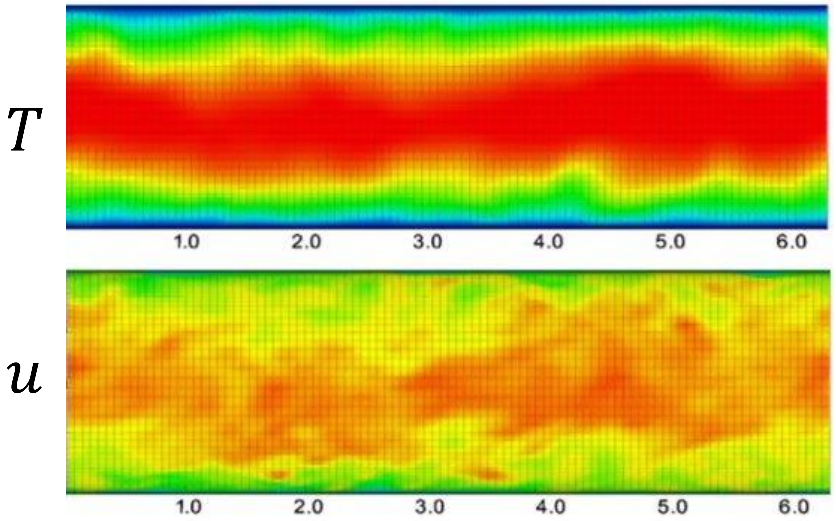


Near unity Prandtl $\alpha \simeq \nu$



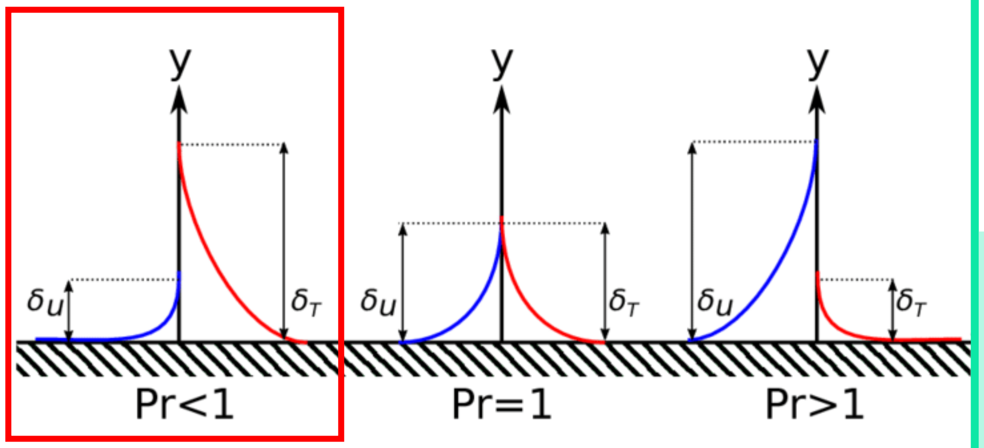
Low Prandtl fluids: main consequences on $\overline{\mathbf{u}\theta}$

Breakup of **thermal/momentum similarity**

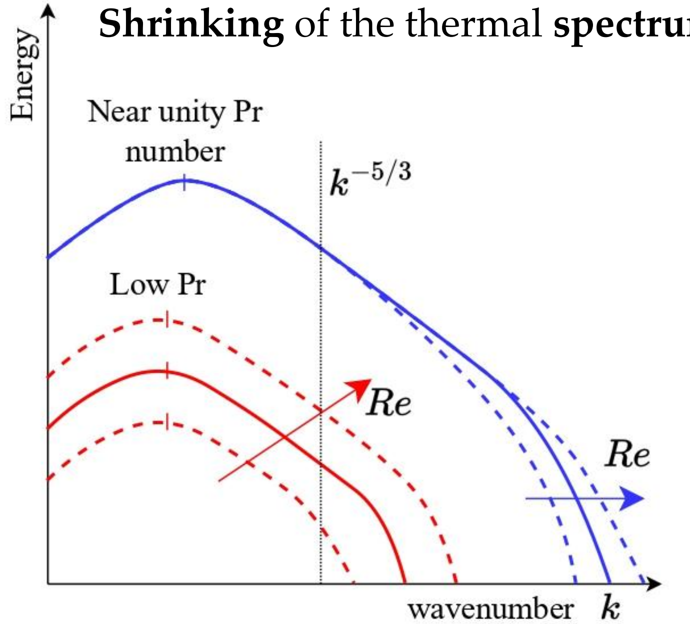


Extension of **thermal boundary layer**

Liquid Metals



Shrinking of the thermal **spectrum**



Breakup of **scale separation**

Non-local effects

$$\overline{u_i\theta}(\mathbf{x},t) = \frac{l_\theta}{\tau_\theta}\Delta\theta\mathcal{F}_i\left[T^*(\mathbf{y},s) - T^*(\mathbf{x},s)\right]$$

$$T^*(\mathbf{y},s) - T^*(\mathbf{x},s) =$$

$$\left[\frac{(y_i - x_i)}{l_\theta}\frac{\partial T}{\partial x_i}\frac{l_\theta}{\Delta\theta} + \frac{(s-t)}{\tau_\theta}\frac{(y_i - x_i)}{l_\theta}\frac{\partial^2 T}{\partial t\partial x_i}\dots\right]$$

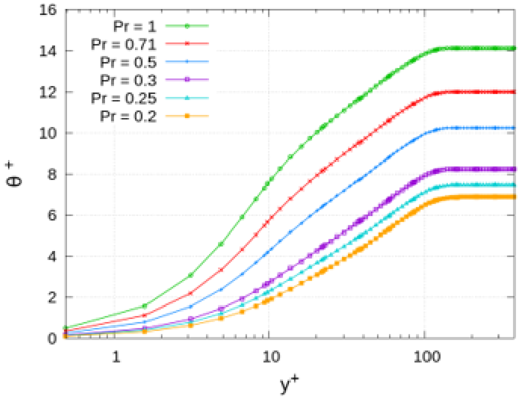
Reynolds'analogy

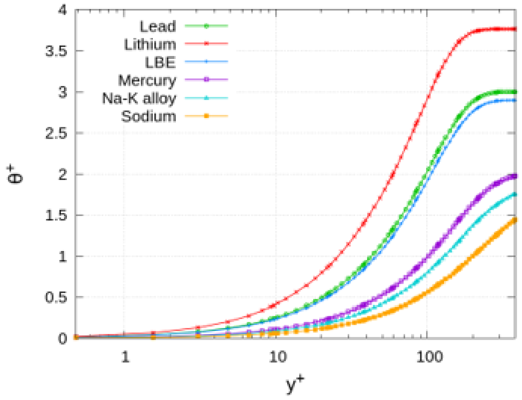
$$\overline{\mathbf{u}\theta} = -\frac{\nu_t}{Pr_t}\nabla T$$

Eddy viscosity

$$\nu_t \simeq C_\mu\frac{k^2}{\epsilon}$$

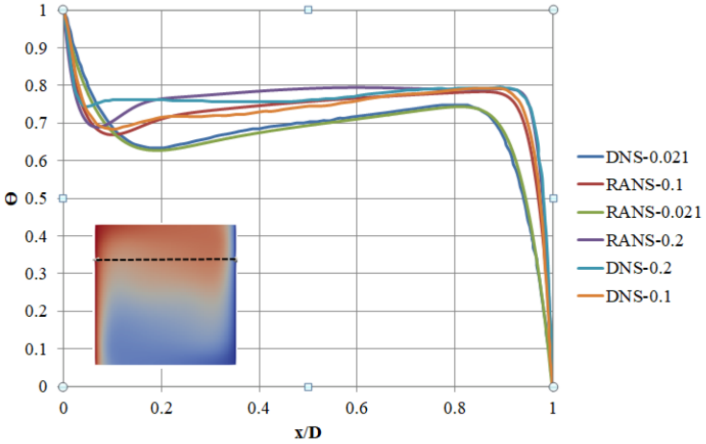
Direct Numerical Simulations for better understanding – Nek5000/NekRS

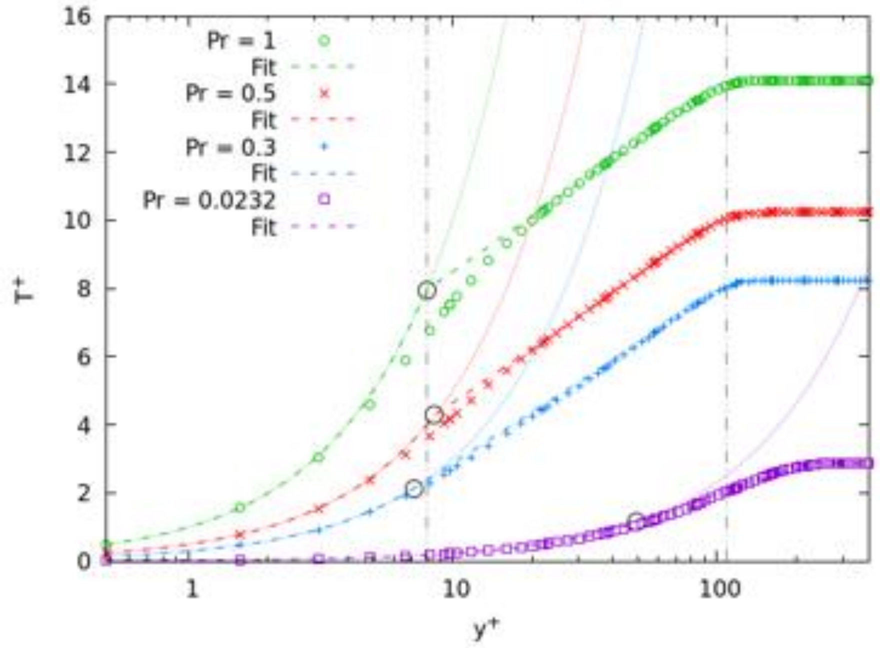




DNS of turbulent convection in a differentially heated cavity with $Pr = 0.021$ and $Gr = 1.8 \times 10^8$

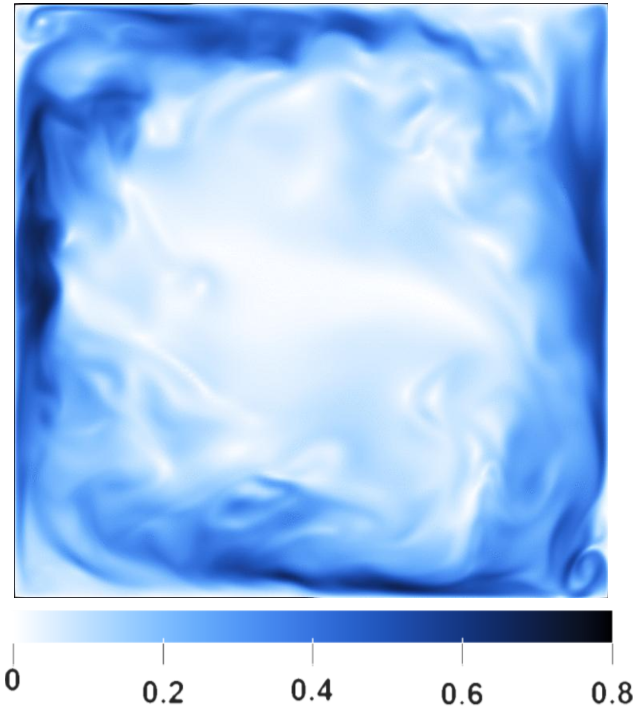
Validation of thermal models with OpenFOAM 9



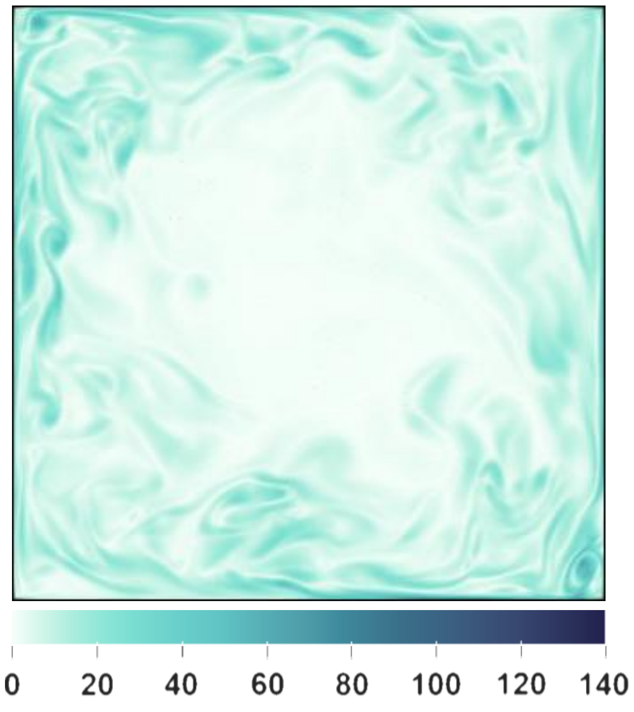


Is it possible to generalize the near wall thermal behavior (wall function) for different Prandtl numbers?

Velocity magnitude



Vorticity

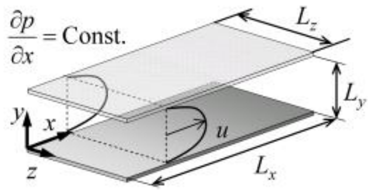


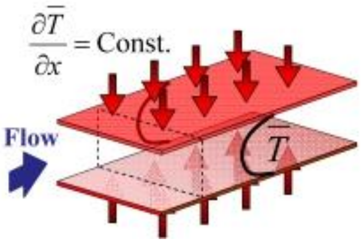
Translating the academic physics to real life applications

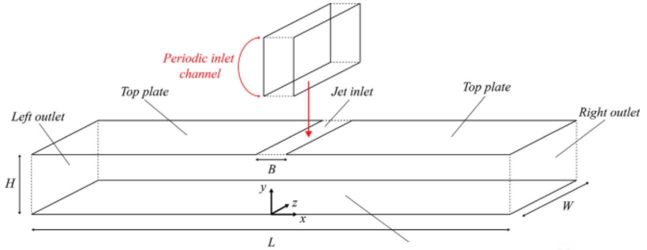
Validation of thermal turbulence models

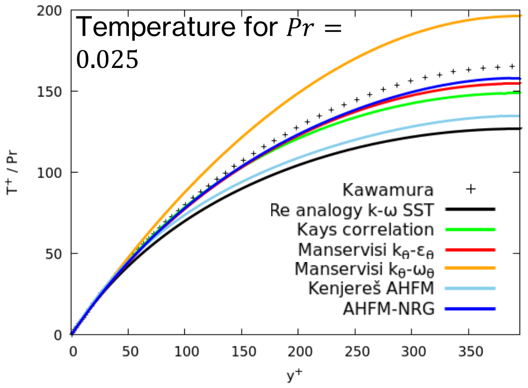
Kawamura, Ohsaka, Abe, Zamamoto
DNS of turbulent heat transfer in channel flow with low to medium-high Prandtl number fluid
International Journal of Heat and Fluid Flow 19 (1998) 482-491.
(https://www.rs.tus.ac.jp/t2lab/db/poi/poi.html)

M. Duponcheel, Y. Bartosiewicz
Direct Numerical Simulation of Turbulent Heat Transfer at Low Prandtl Numbers in Planar Impinging Jets
(https://doi.org/10.1016/j.ijheatmasstransfer.2021.121179)

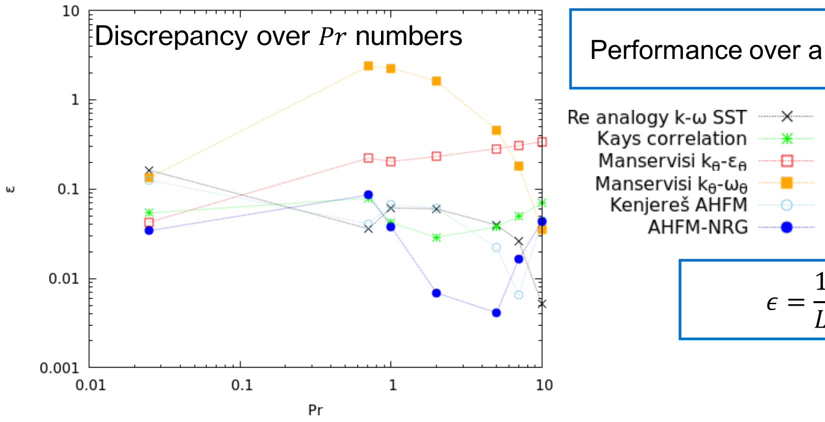








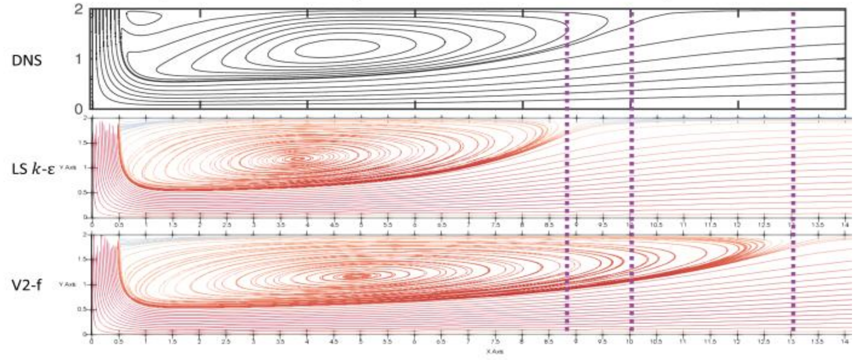
Different thermal turbulence models with k-ω SST momentum turbulence model in a channel at $Re_\tau = 395$

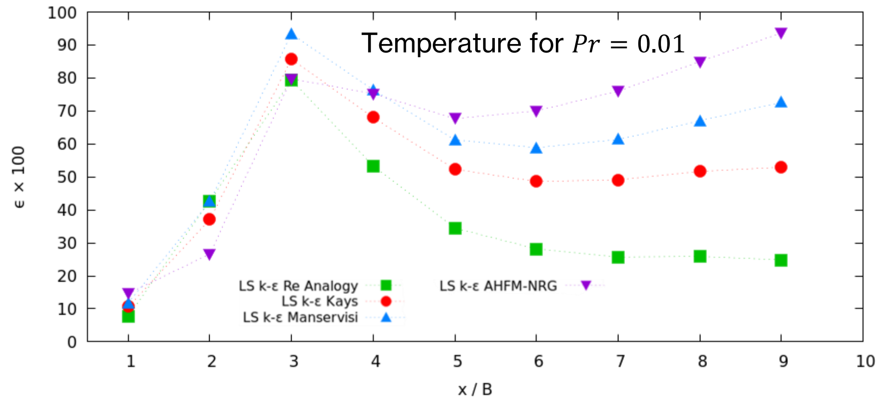


Performance over a range of Prandtl numbers

$$\epsilon = \frac{1}{L}\int_0^L \left| \frac{\phi - \phi_{DNS}}{\phi_{DNS}} \right| \mathrm{d}y$$

- Quite large difference in the prediction of the reattachment point





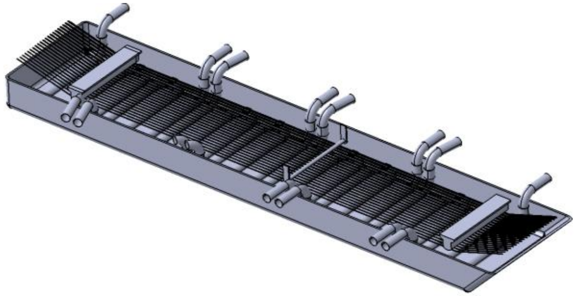
Metallurgy - Moving wires in molten metal bath

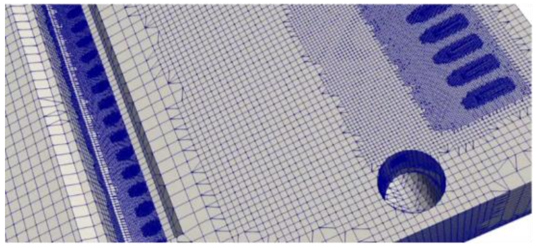
- Development of a numerical model for a CHT system, to consider the interaction between solid and fluid verified on a simplified system in steady state condition

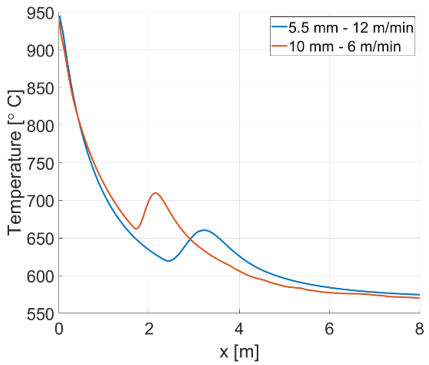
- The energy equation for the solid has been modified to consider the translational velocity and to introduce the heat source due to the phase transformation

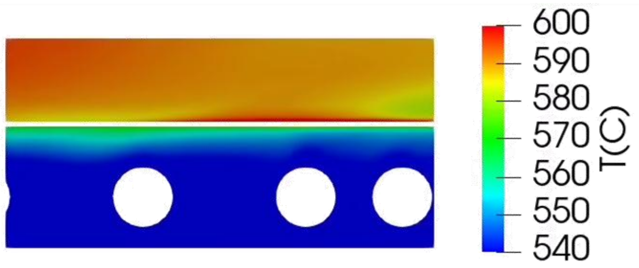
- Continuity problem in the solver due to the sudden change of direction of the wire
- Coded boundary conditions are used to define the direction of the velocity along the wires to avoid the presence of normal components on the walls

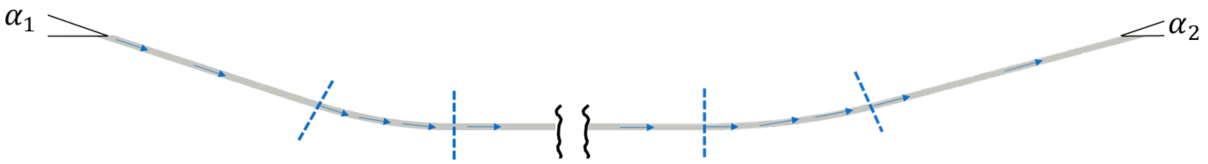
- Temperature probes have been defined to control the amount of cooling power (CP) and heating power (HF) in the system

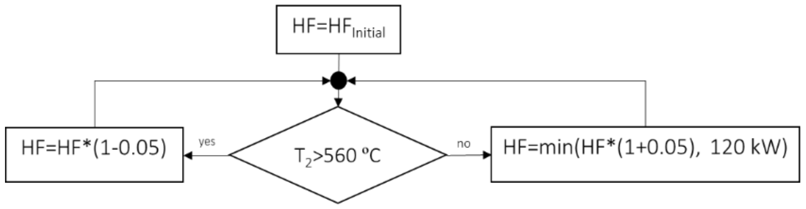




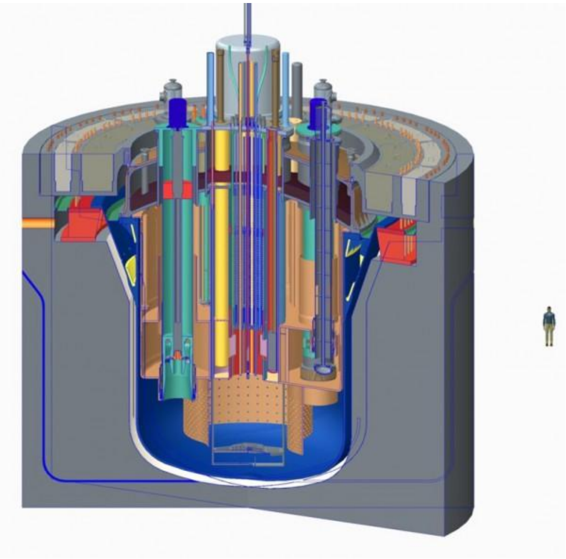






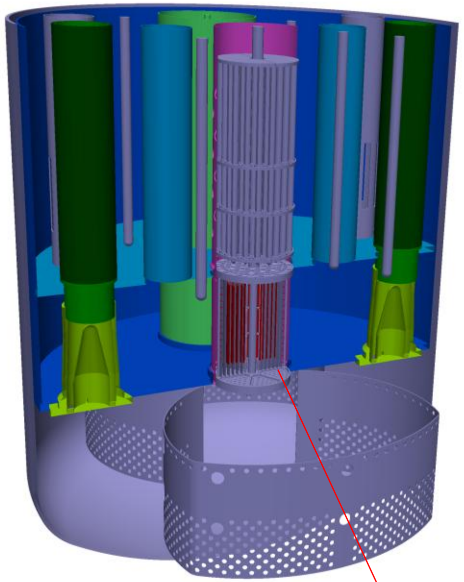


Multi-purpose HYbrid Research Reactor for High-tech Applications



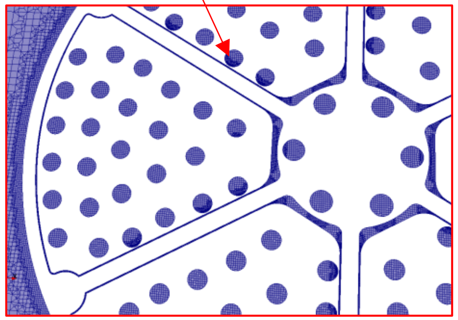
Transmutation: the final volume of residual nuclear waste is reduced by a factor 100 and the natural radiation level is already reached after 300 years.

With MYRRHA, also focuses on the development of new **therapeutic radio-isotopes** that can fight cancer cells in a more targeted way and thereby significantly reduce the side effects for patients.



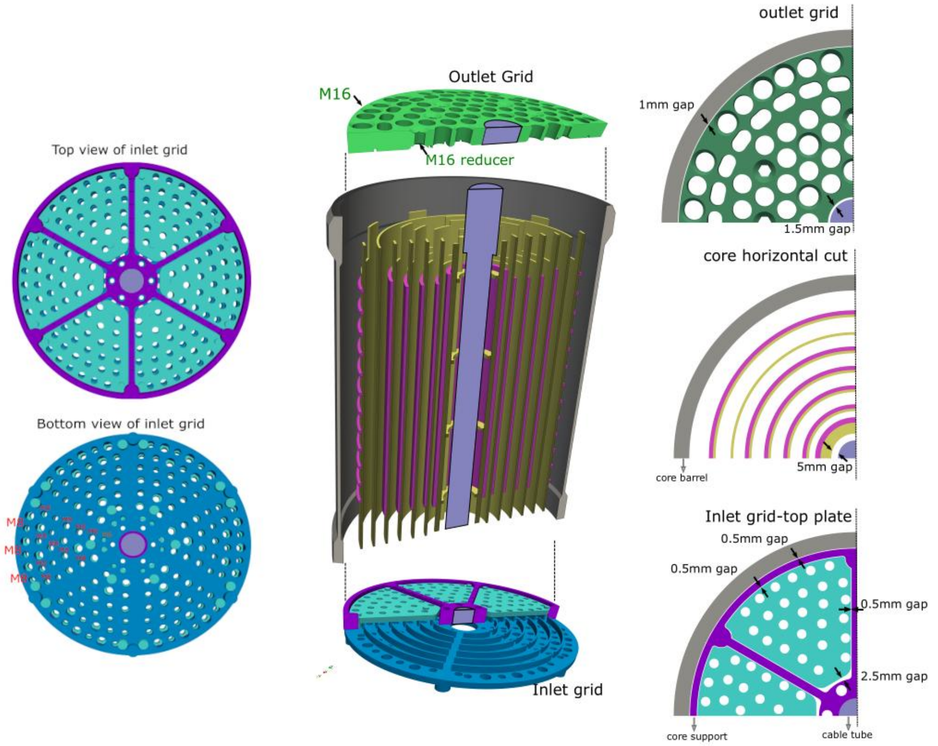
MYRRHA – thanks to its fast neutrons – will reach **irradiation conditions** that are closer to that of a fusion reactor

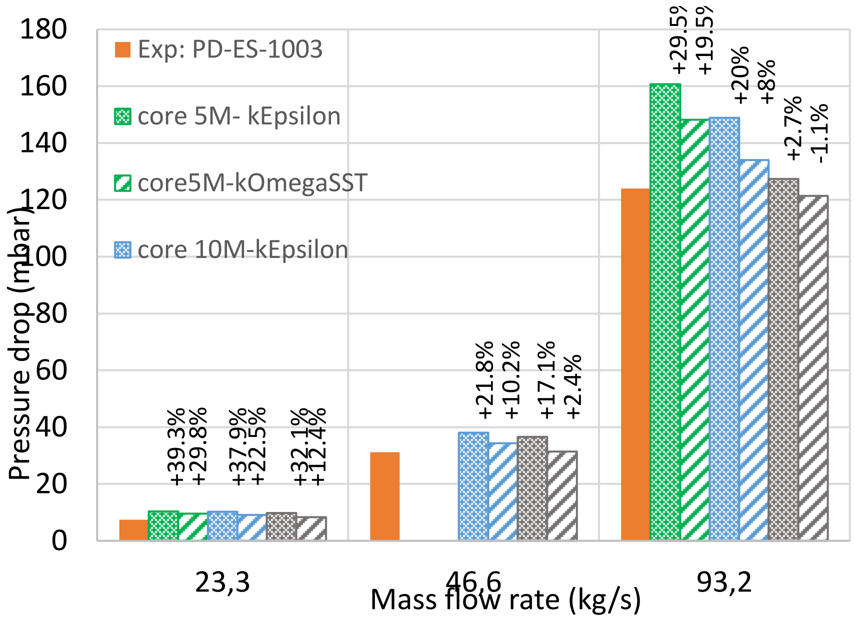
The E-SCAPE (**European SCAled Pool Experiment**) facility is a thermal hydraulic 1/6-scale model of the primary system of the MYRRHA reactor pool, with a 100 kW electrical core simulator, cooled by LBE.

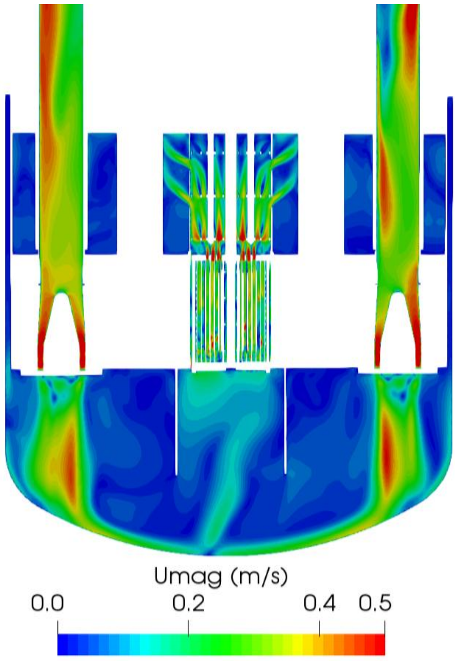


Mesh resolution – HPC system – Time scales

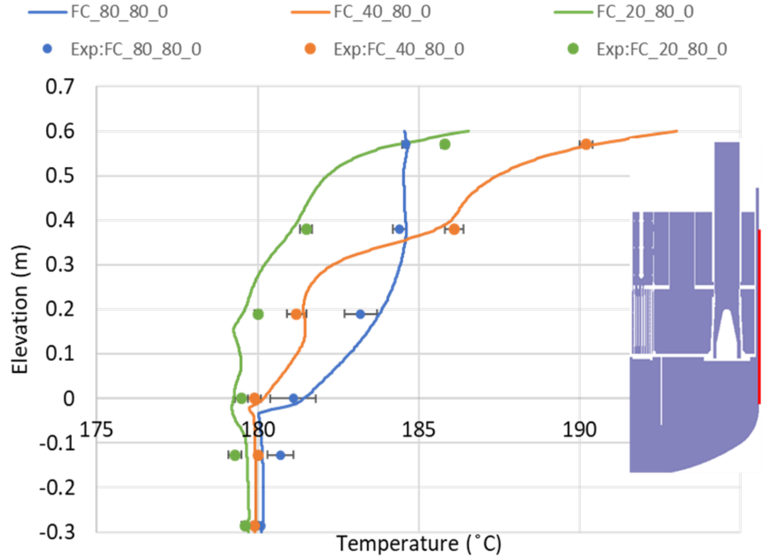
Several quasi-steady state cases have been simulated in order to validate the proposed CFD approach for **forced and mixed convection**.



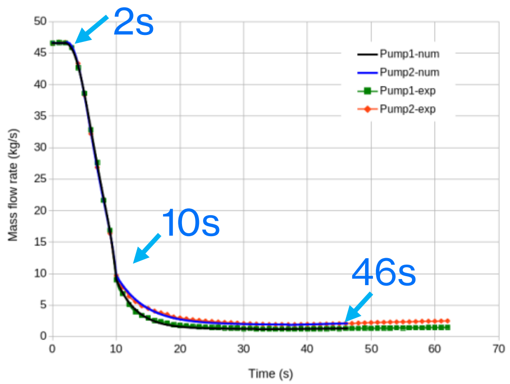




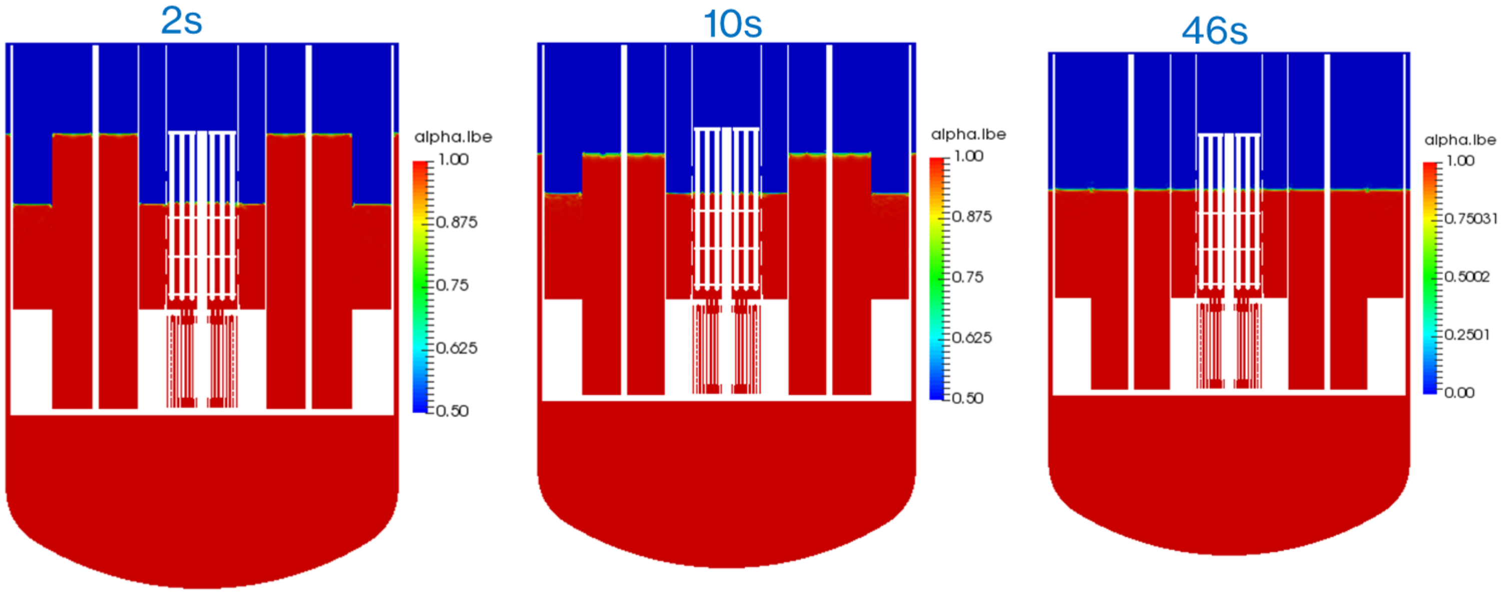
Corresponding Case	Total cell number	CHT included	Piping included
FC Iso-Mesh1	150 Millions	No	Partially
FC Iso-Mesh2	280 Millions	No	Partially
FC Iso-Mesh3	322 Millions	No	Partially
FC Heated	180 Millions	Yes	Partially
NC Heated	317 Millions	Yes	Fully



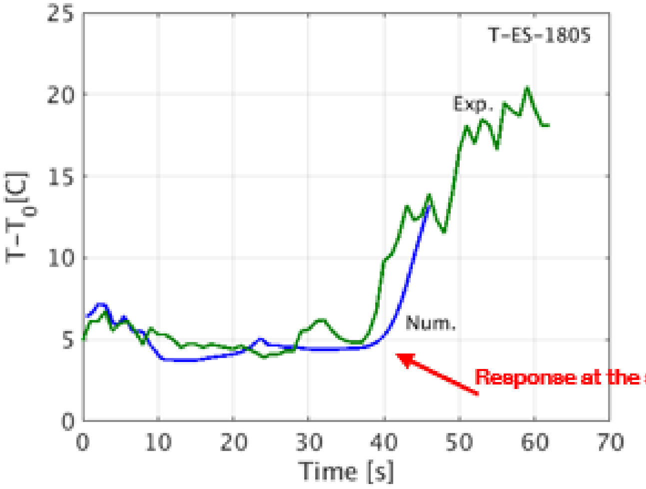
Accidental scenarios: transient loss of flow

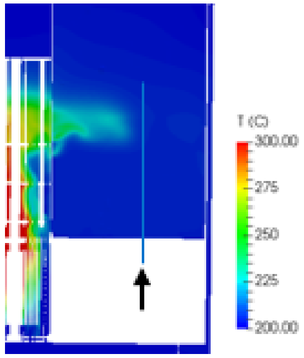


Evolution of the LBE level during the LOF



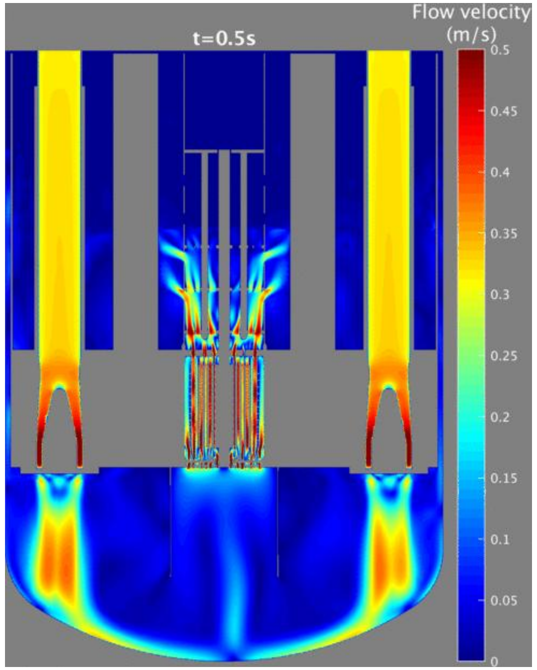
Demonstration of Heavy Liquid Metal Fast Reactor’s passive safety feature.

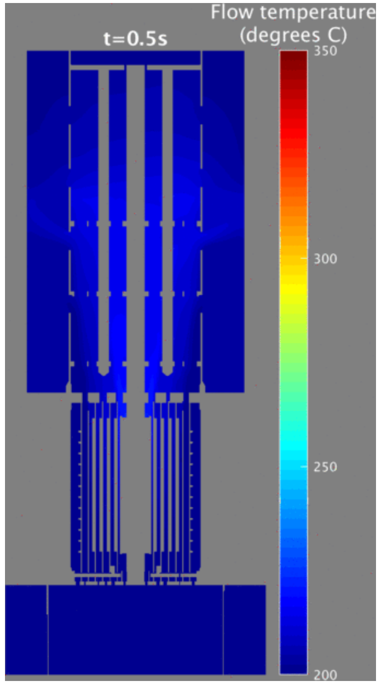




Plane 45-225 (TC instrumentation bar)

Time-response of the system is well captured!





Large data (?) models for liquid metal flows

AI for turbulence modeling

General closure problem

$$\overline{\mathbf{u}\theta} = -\mathbf{D}\nabla T$$

$$\mathbf{D} = \mathcal{F}\left(\mathbf{b}, \mathbf{S}, \boldsymbol{\Omega}, \nabla T, k, \epsilon, k_\theta, \epsilon_\theta, \alpha, \nu\right)$$

Rotational invariance
(Tensor Representation Theory)

$$\mathbf{QDQ}^T = \sum_{i=1}^{n} c_i \mathbf{QT}^i\mathbf{Q}^T$$

$$c_i = f_i(\pi_j, Re_t, Pr)$$

The modeling reduces to a set of scalar coefficients

Consistency with the **second law of thermodynamics**

Realizability

$$\mathbf{D} = \left[(\mathbf{A}+\mathbf{A}^T)(\mathbf{A}^T+\mathbf{A}) + \frac{k}{\epsilon^{0.5}}(\mathbf{W}-\mathbf{W}^T)\right]$$

$$\mathbf{A} = \sum_{i=1}^{n} a_i \mathbf{T}^i, \quad \mathbf{W} = \sum_{i=1}^{n} w_i \mathbf{T}^i$$

$$w_i = f_i(\pi_j, Re_t, Pr)$$

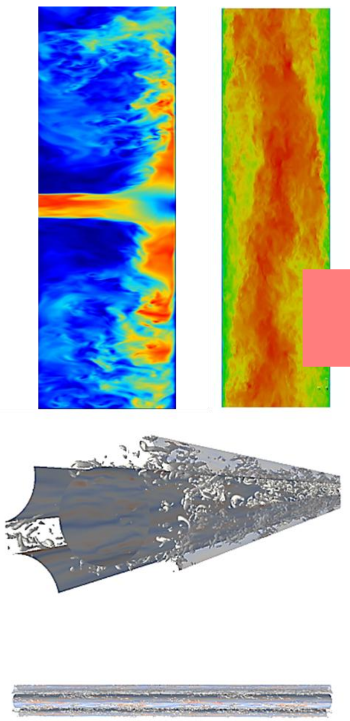
$$a_i = f_i(\pi_j, Re_t, Pr)$$

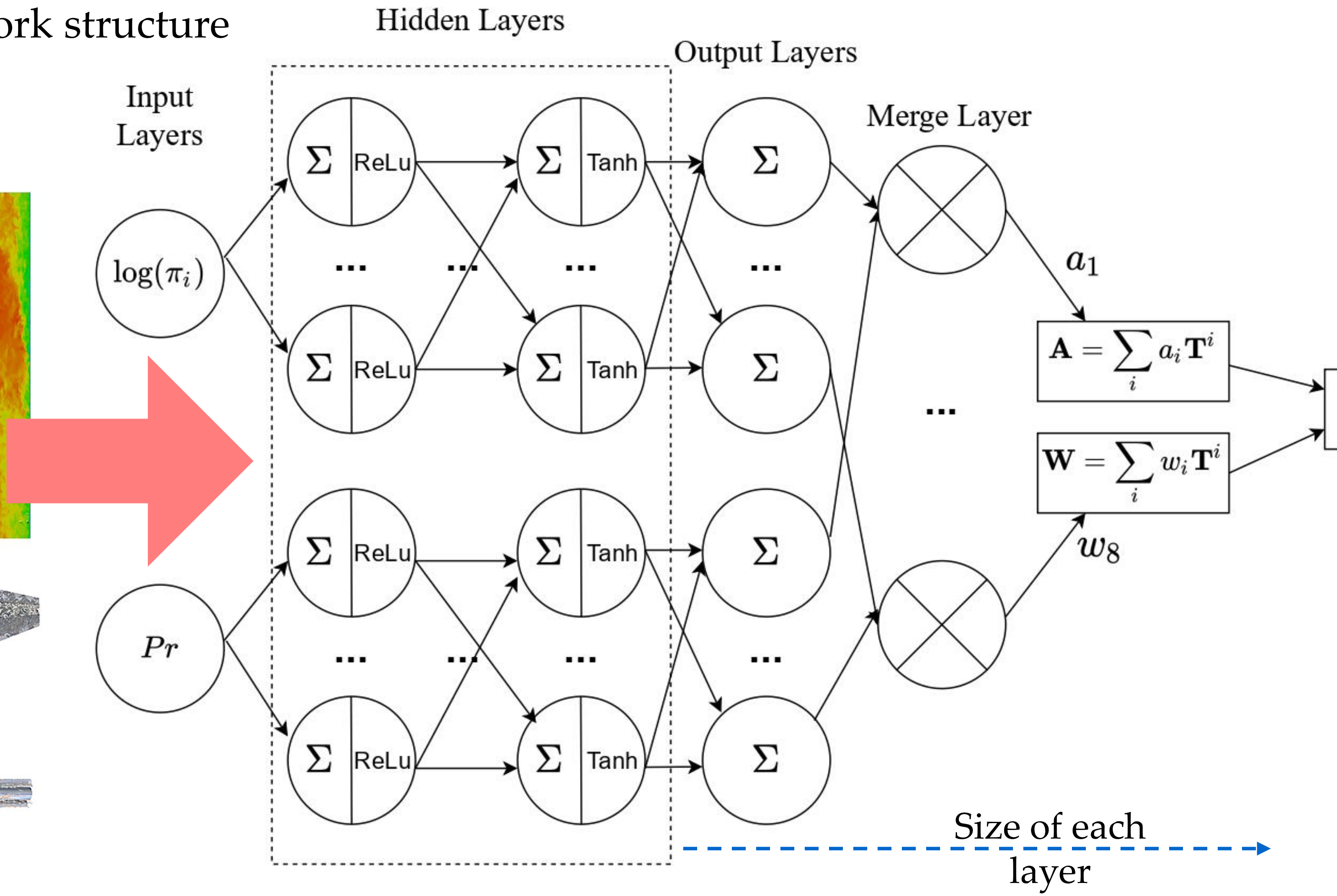
16 variable closure coefficients, very **high-dimensional problem**

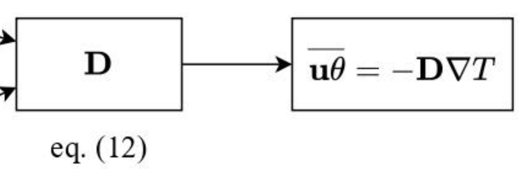
Invariant Basis	Tensor Basis
$\pi_1 = \frac{k^2}{\epsilon^2}\{\mathbf{S}^2\}$, $\pi_2 = \frac{k^2}{\epsilon^2}\{\boldsymbol{\Omega}^2\}$, $\pi_3 = \{\mathbf{b}^2\}$, $\pi_4 = \frac{k}{\epsilon}\{\mathbf{bS}\}$, $\pi_5 = \{\mathbf{b}_2\}$, $\pi_6 = \{\mathbf{bS\Omega}\}\frac{k^2}{\epsilon^2}$, $\pi_7 = \frac{\lVert\nabla T\rVert}{\sqrt{k_\theta}}\frac{k^{3/2}}{\epsilon}$, $\pi_8 = R = \frac{k_\theta \epsilon}{k \epsilon_\theta}$, $Re_t = \frac{k^2}{\epsilon\nu}$, $Pr = \frac{\nu}{\alpha}$	$\mathbf{T_1} = \frac{k}{\epsilon^{1/2}}\mathbf{I}$, $\mathbf{T_2} = \frac{k}{\epsilon^{1/2}}\mathbf{b}$, $\mathbf{T_3} = \frac{k^2}{\epsilon^{3/2}}\mathbf{S}$, $\mathbf{T_4} = \frac{k^2}{\epsilon^{3/2}}\boldsymbol{\Omega}$, $\mathbf{T_5} = \frac{k^2}{\epsilon^{3/2}}\mathbf{bS}$, $\mathbf{T_6} = \frac{k^2}{\epsilon^{3/2}}\mathbf{b\Omega}$, $\mathbf{T_7} = \frac{k^3}{\epsilon^{5/2}}\mathbf{S\Omega}$, $\mathbf{T_8} = \frac{k^3}{\epsilon^{5/2}}\mathbf{bS\Omega}$

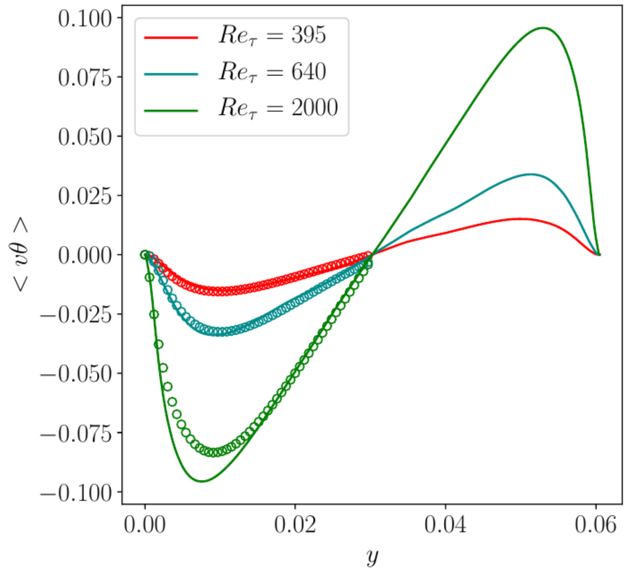
Data-driven Algebraic Heat-Flux Model

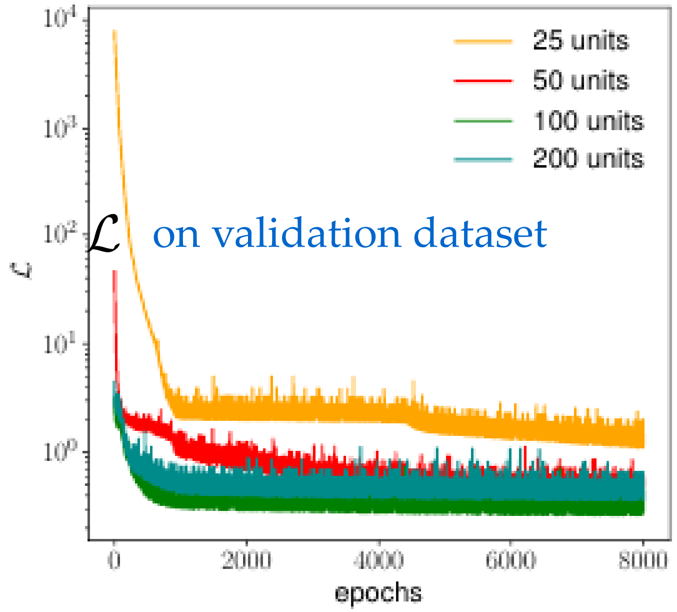
Neural network structure











PYTORCH → OpenFOAM

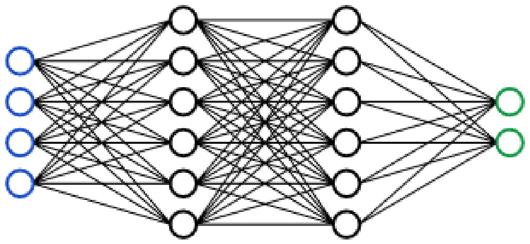
$$\mathbf{D} = \left[(\mathbf{A}+\mathbf{A}^T)(\mathbf{A}^T+\mathbf{A}) + \frac{k}{\epsilon^{0.5}}(\mathbf{W}-\mathbf{W}^T)\right]$$

As good as the input data, as good as the training data

RANS velocity field is usually not so accurate compared to the DNs data used for training

DNS input data

RANS input data

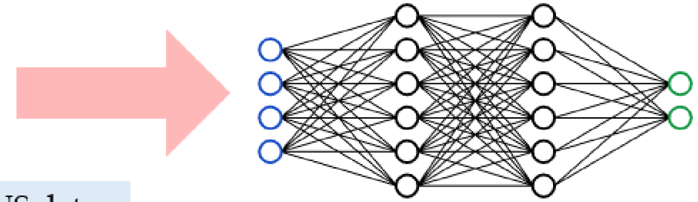


Loss function

$$\mathcal{L} = \mathcal{L}_{DNS} + \alpha \mathcal{L}_{RANS}$$

$$\mathbf{D} = \mathcal{F}\left(\mathbf{b}, \mathbf{S}, \boldsymbol{\Omega}, \nabla T, k, \epsilon, k_\theta, \epsilon_\theta, \alpha, \nu\right)$$

$\overline{u_i u_j}$

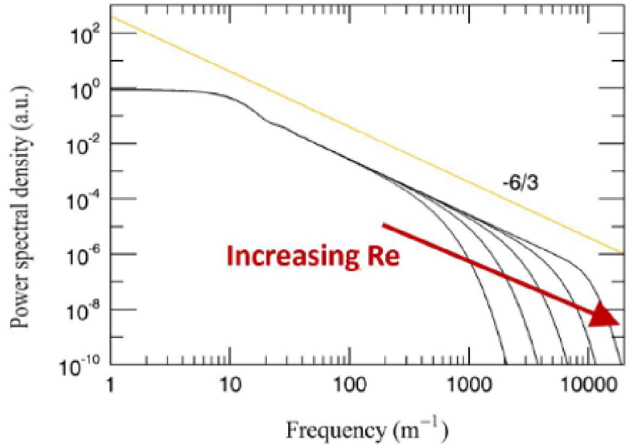


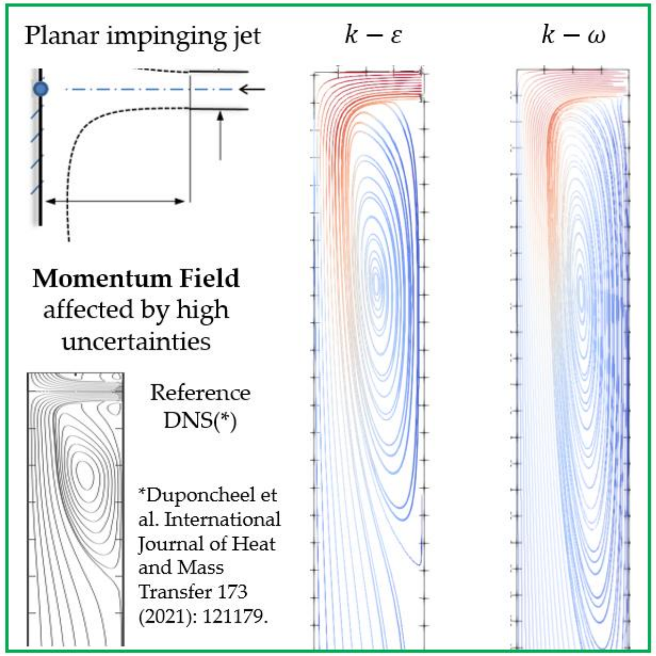
$\overline{u_i \theta}$

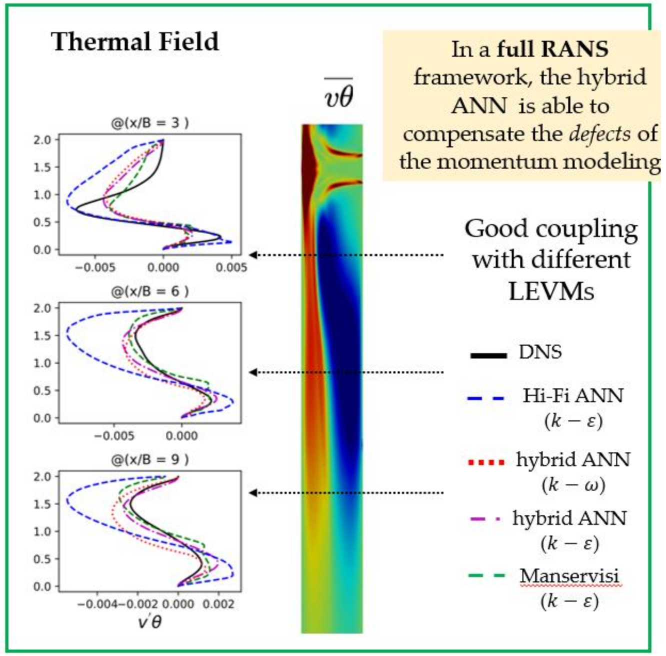
Typically, DNS data are available at moderate/low Re and canonical flows

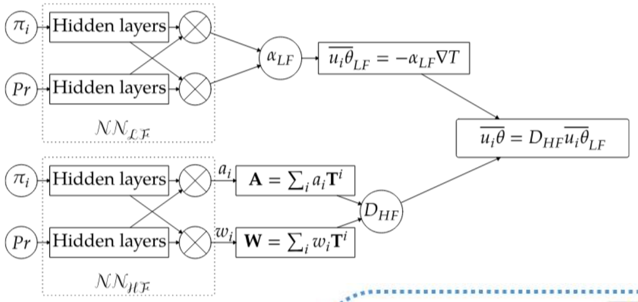
Then, **how to predict** at:

- High Re?
- Complex flow configurations?



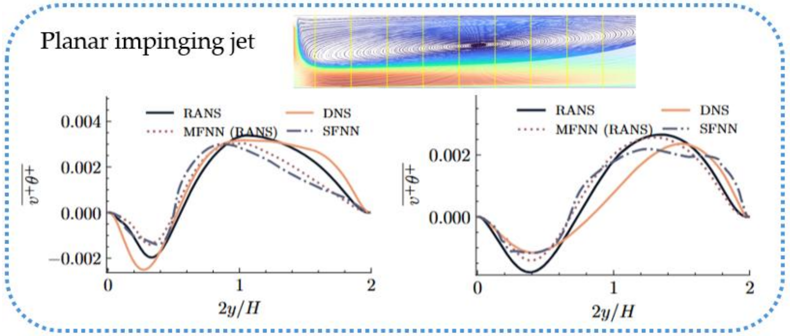






Can be considered in training…

… cannot be guaranteed in application.

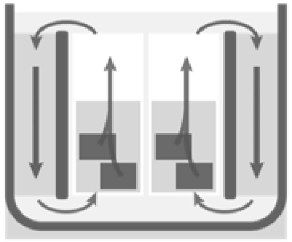


AI, the historically open-source environment

AI for uncertainty quantification

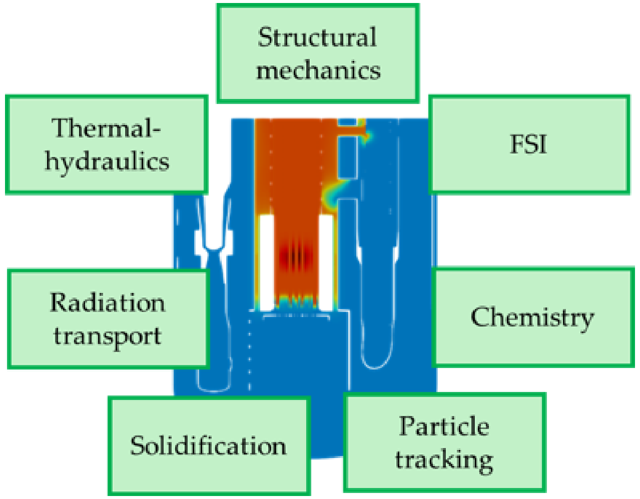
Why UQ?

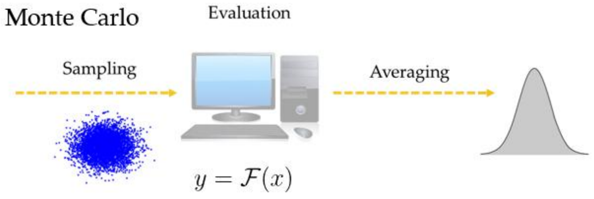
Critical **sensitivity** to perturbations

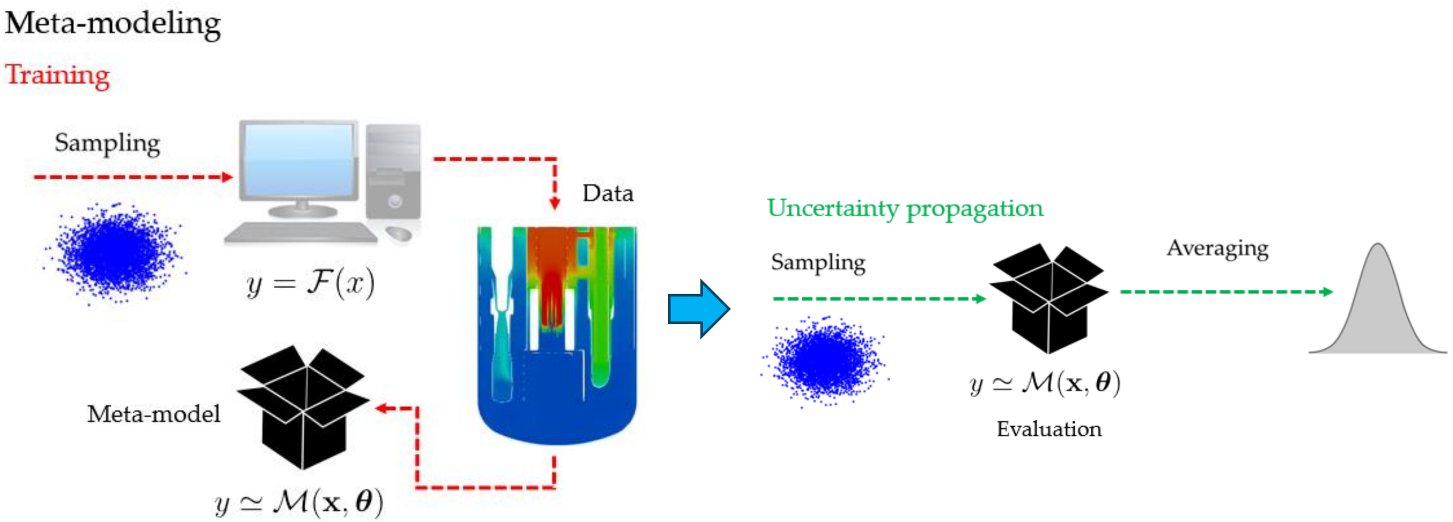


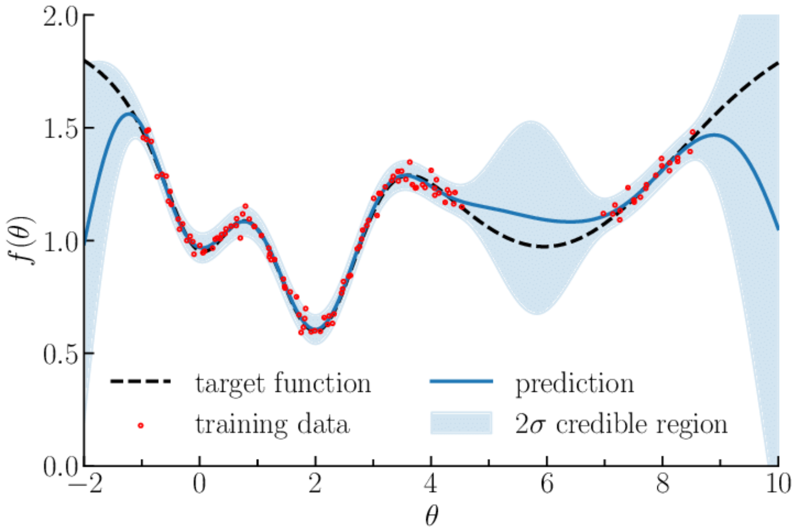
Natural convection: the small engaged driving forces lead to significant uncertainties in temperature field and flow patterns

Multi-scale and **multi-physics** environment





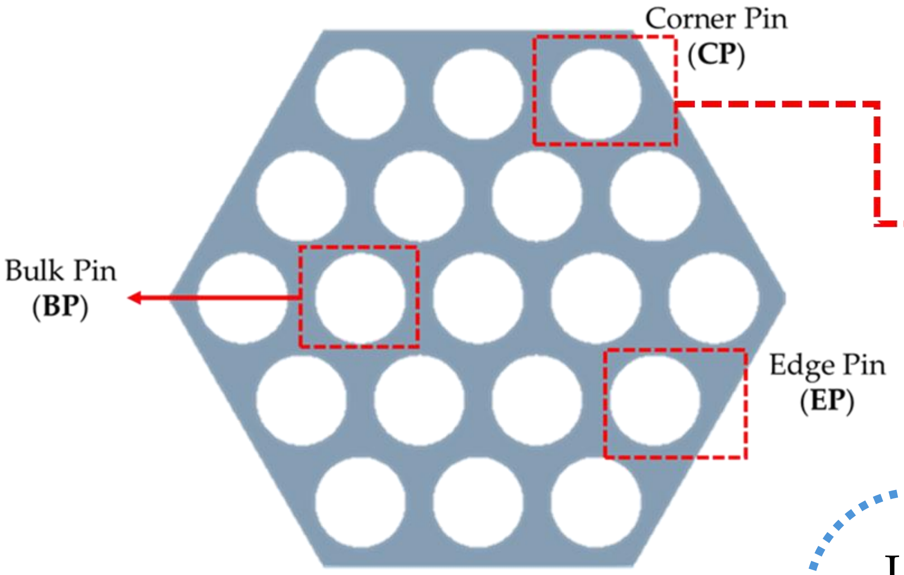


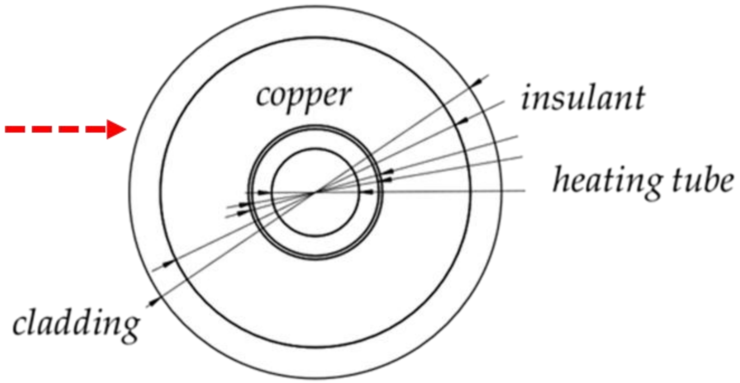


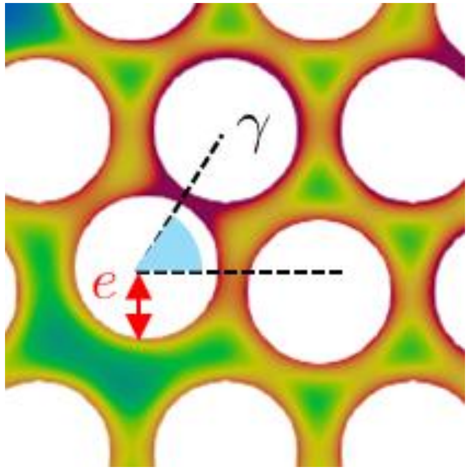
- **Types of meta-models**
  - Gaussian Processes (GPs)
  - Polynomial Chaos Expansion
  - Polynomial Chaos Kriging
  - Artificial Neural Networks

Quantifying uncertainties due to deformations

ANSELMUS benchmark







Surrogate model:
multi-fidelity **Gaussian Process**

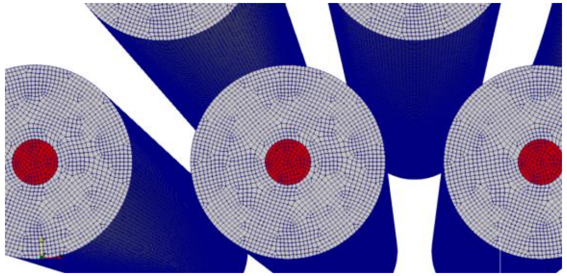
$$y_t(x), t = 1, ..., s$$

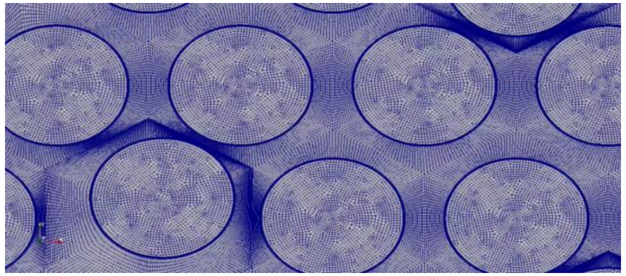
$$y_t(x) = \rho_{t-1}(x) y_{t-1}(x) + \boxed{\delta_t(x)} \rightarrow \text{GP}$$

$$\rho_{t-1}(x) = g_{t-1}(x) \beta_{\rho_{t-1}}$$

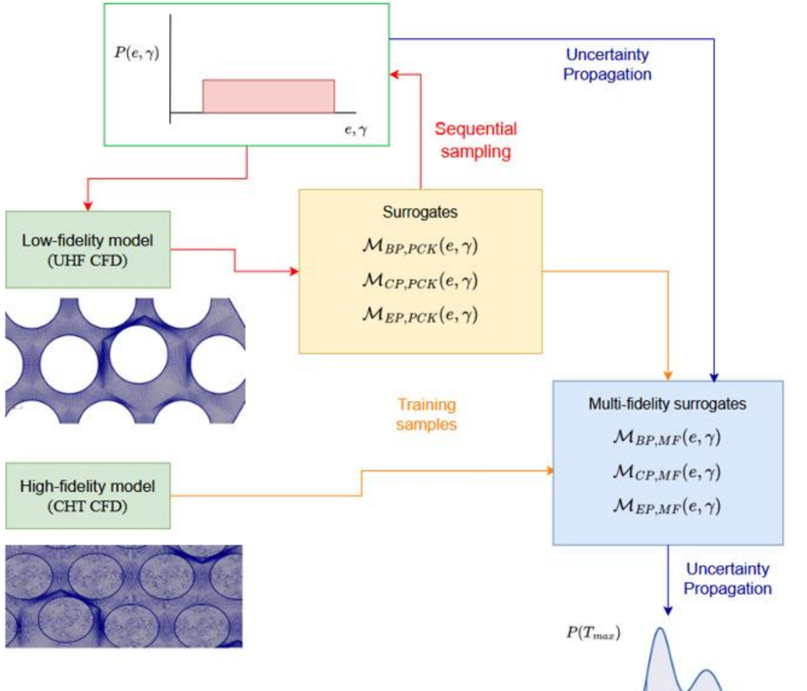
Leveraging **multi-fidelity** data sources

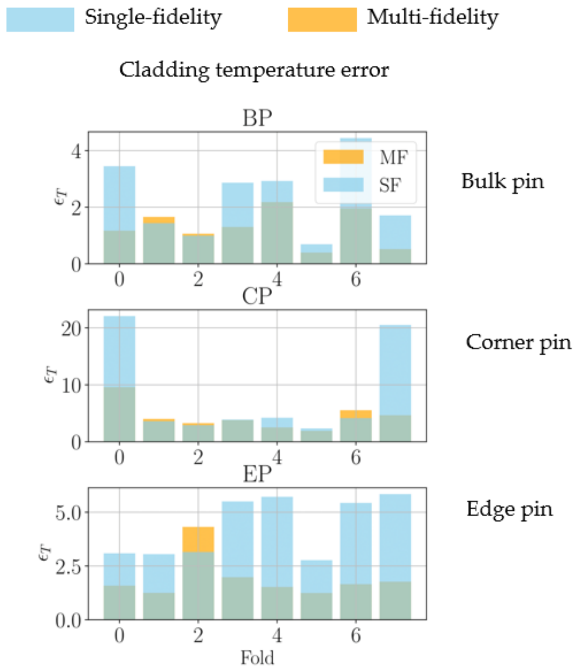
- Uniform Heat Flux (UHT) simulation (fluid only): *low fidelity*
- **CHT simulation**: *high fidelity (solid + fluid)*

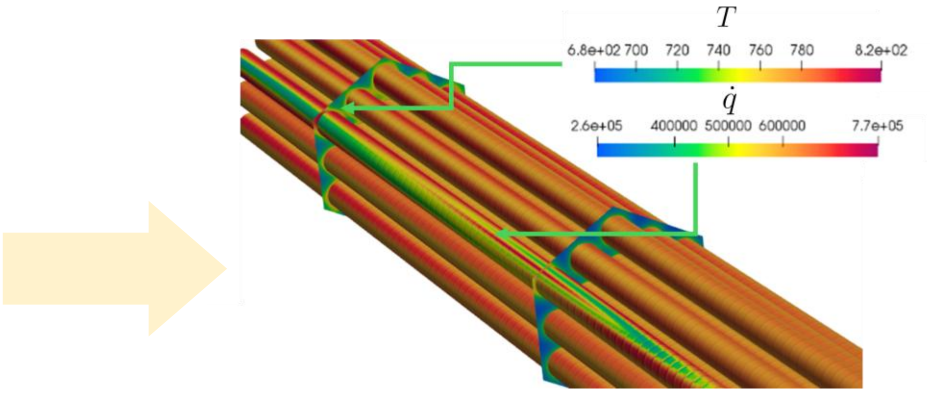


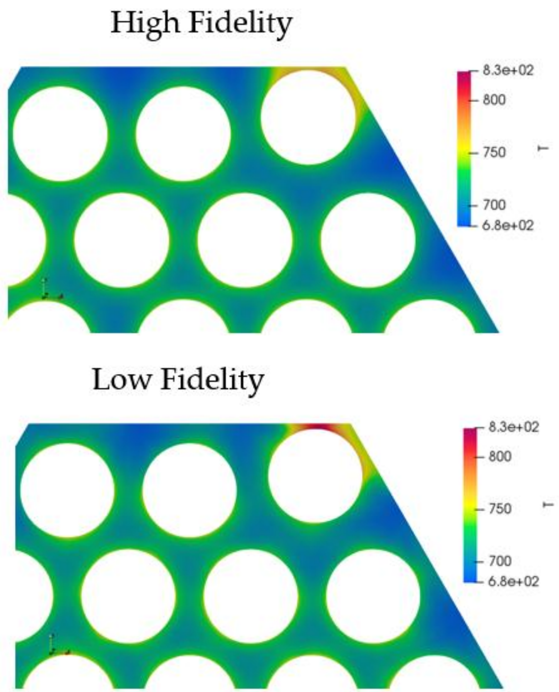


Quantifying uncertainties due to deformations

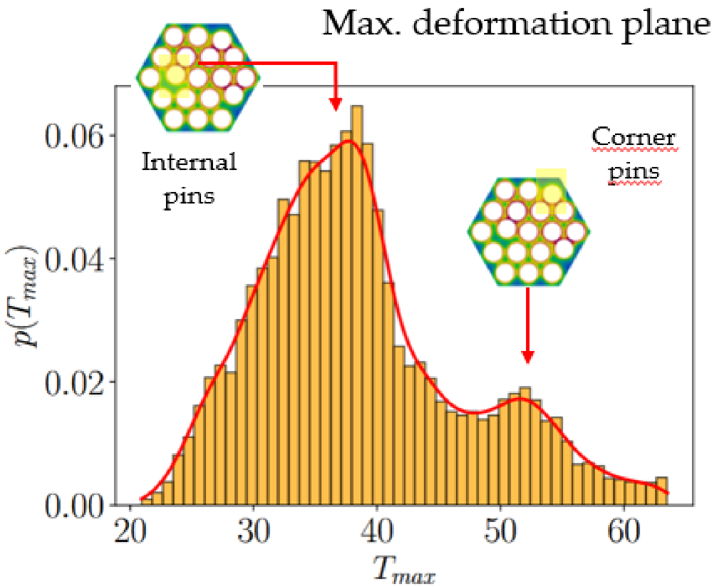


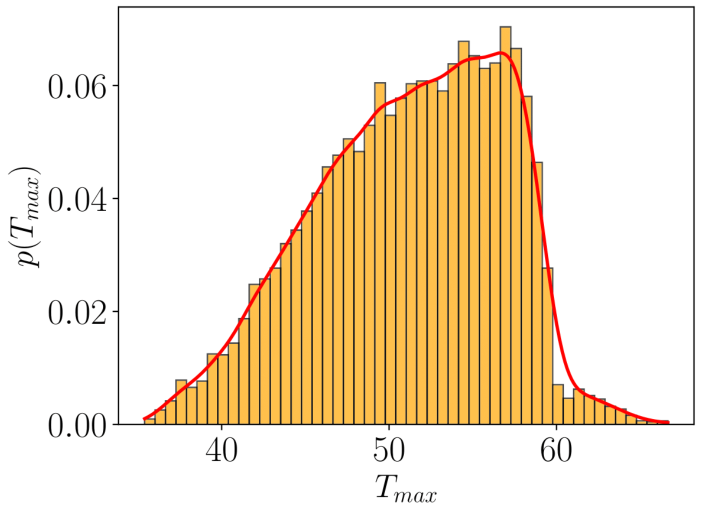






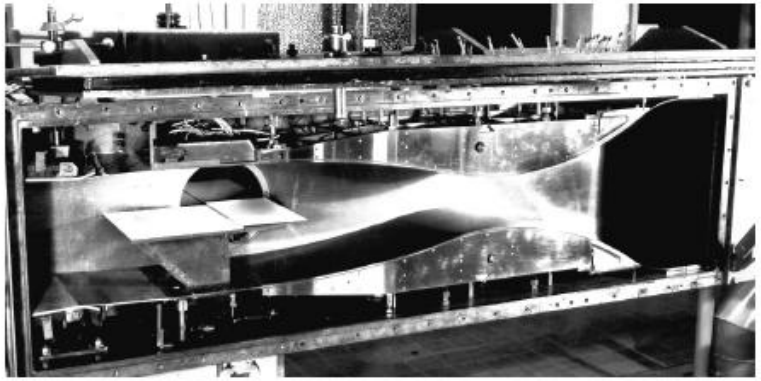
Redistribution of the heat flux at the cladding surface mitigates temperature peaks





The von Karman Institute

THE HORIZONTAL CLOSED TEST SECTION OF THE SUBSONIC WIND TUNNEL



THE NEW SUPERSONIC NOZZLE

"Training in Research through Research"

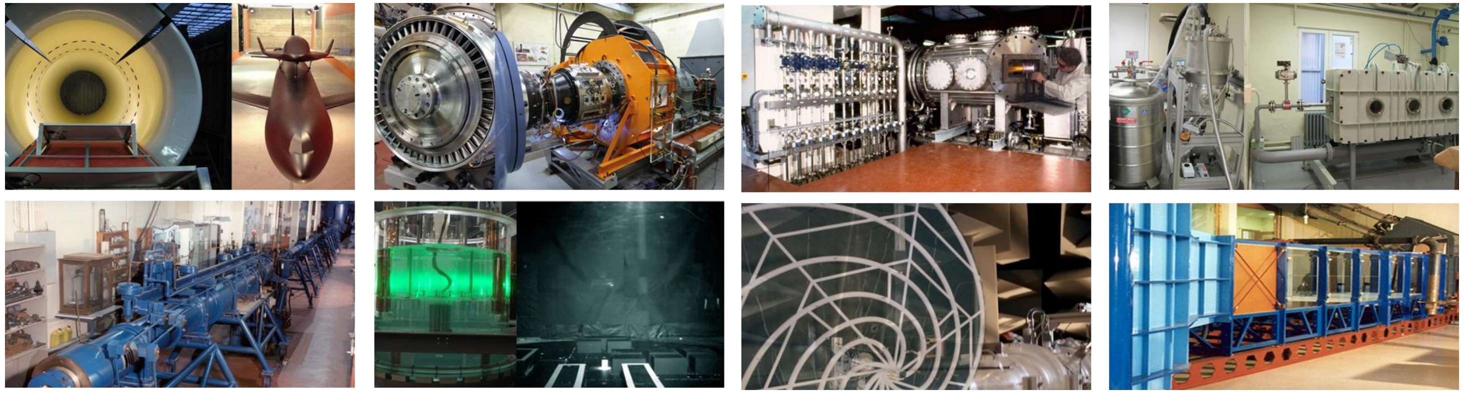
- Founded in 1956
- as Belgian-American Training Center for Experimental Aerodynamics (TCEA)
- renamed von Karman Institute in 1963

THEODORE VON KÁRMÁN RECEIVING THE NATIONAL MEDAL OF SCIENCE FROM PRESIDENT KENNEDY IN 1963

The von Karman Institute in numbers

140

140 staff members, agile organization



48

- 48 experimental facilities
- 3 unique in the world

22

- 22 nations on-the-spot
- A melting pot for research & education

242

- 242 students
- Research Master: 39
- Short Training program + Belgian Master Thesis: 95
- PhD: 84
- Postdoc: 24

1900

- 1900 alumni
- Dedicated network for international development

70th academic year 2025-2026

Education

Belgium
Bulgaria
Czech Republic
France
Germany
Greece
Hungary
Iceland
Italy
Luxembourg
Netherlands
Norway
Portugal
Romania
Turkey
United States

- Research Master Program
- Doctoral Program
- Short Training Program

Lecture Series

- courses on special topics
- For industry, academics, military participation
- Invited international lectures

Research activities

- Aerospace
- Turbomachinery
- Industrial Processes
- Environmental Flows
- Fluid Engineering & Measurements

Profesional trainings

Education

Title	Type	Date
Introduction to Measurement Techniques	LS classic	06-10 October 2025
Workshop on Heat pump Noise Day	Workshop	14 Nov 2025
Physics of Atmosphere	LS classic	19-21 Nov 2025
Introduction to Ground Testing Facilities	VKI Course	19-21 January 2026
Introduction to CFD	LS classic	26-30 January 2026
Hands on Machine Learning for Fluid Dynamics	VKI Course	02-06 February 2026
Radial Compressor Design (pro. usual)	VKI Course	09-13 February 2026
Introduction to Aeroelasticity	VKI Course	16-20 February 2026
Flow Control	LS classic	23-27 February 2026
OpenFoam Courses	VKI Course	24-26 March 2026
Icing Physics and Ice Accretion Simulation	VKI Course	30/03-03/04/2026 or 06-10/04/2026
Turbomachinery Aeroelasticity LS	LS classic	13-17 April 2026
Assessment of heavy-liquid-metal systems	LS classic	20-24 April 2026
Multiphase flows	LS classic	05-08 May 2026
AIAA Aeroacoustics Conference	Conference	26-29 May 2026
LES and related techniques	LS classic	08-12 June 2026
Quantum CFD	LS classic	06-10 July 2026
Open Engine Technology (Rise Engine)	LS classic	13-17 July 2026

Lecture Series

- courses on special topics
- For industry, academics, military participation
- Invited international lectures

Research activities

- Aerospace
- Turbomachinery
- Industrial Processes
- Environmental Flows
- Fluid Engineering & Measurements

Thank you for your attention!