

Quantum Computing: a Grand Era for Simulating Fluid?

ACAT 2022 (by CERN - European Organization for Nuclear Research -)

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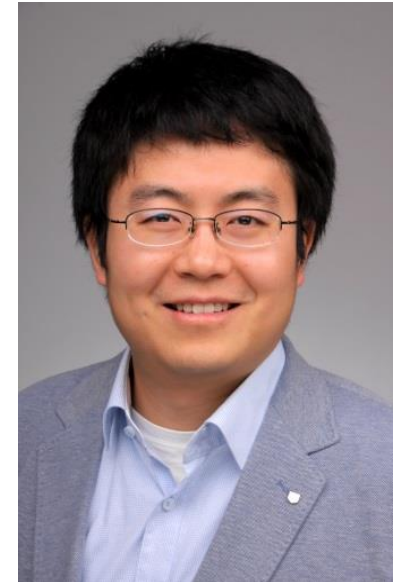
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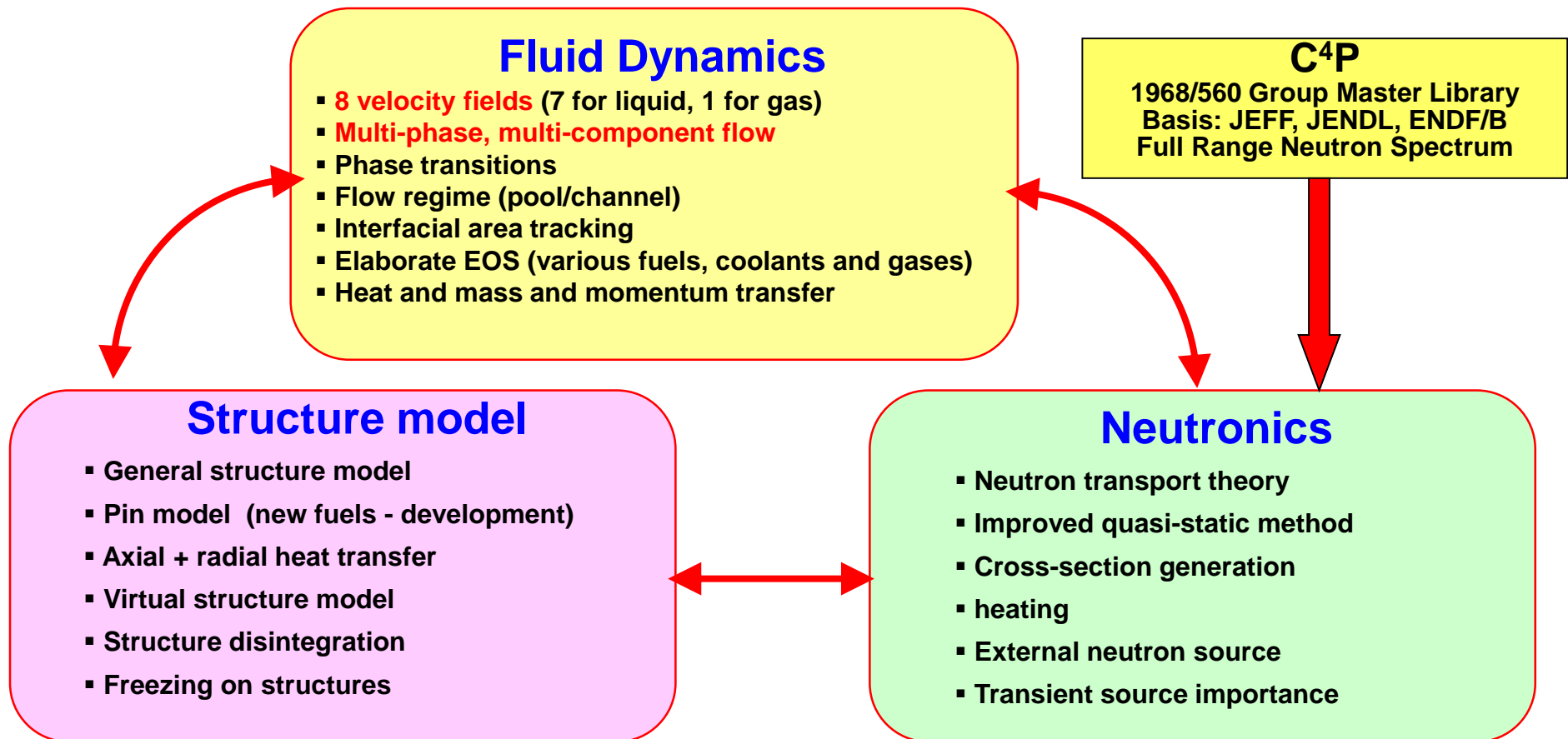
Prof. Dr. Rui Li

- 2018 ~ now: Professor, Deggendorf Institute of Technology, Germany
- 2012 ~ 2018: Researcher, Karlsruhe Institute of Technology, Germany
 - Nuclear Safety (Transmutation) Simulation: <https://www.inr.kit.edu/975.php>
 - Steinbuch Centre for Computing: InstitutsCluster II (IC2), bwUniCluster 2.0+GFB-HPC
- 2008 ~ 2012: Ph.D. in Nuclear Engineering, Tokyo Institute of Technology, Japan
 - Dissertation: Computational fluid dynamics study on liquid droplet impingement erosion
 - Tsubame Supercomputer

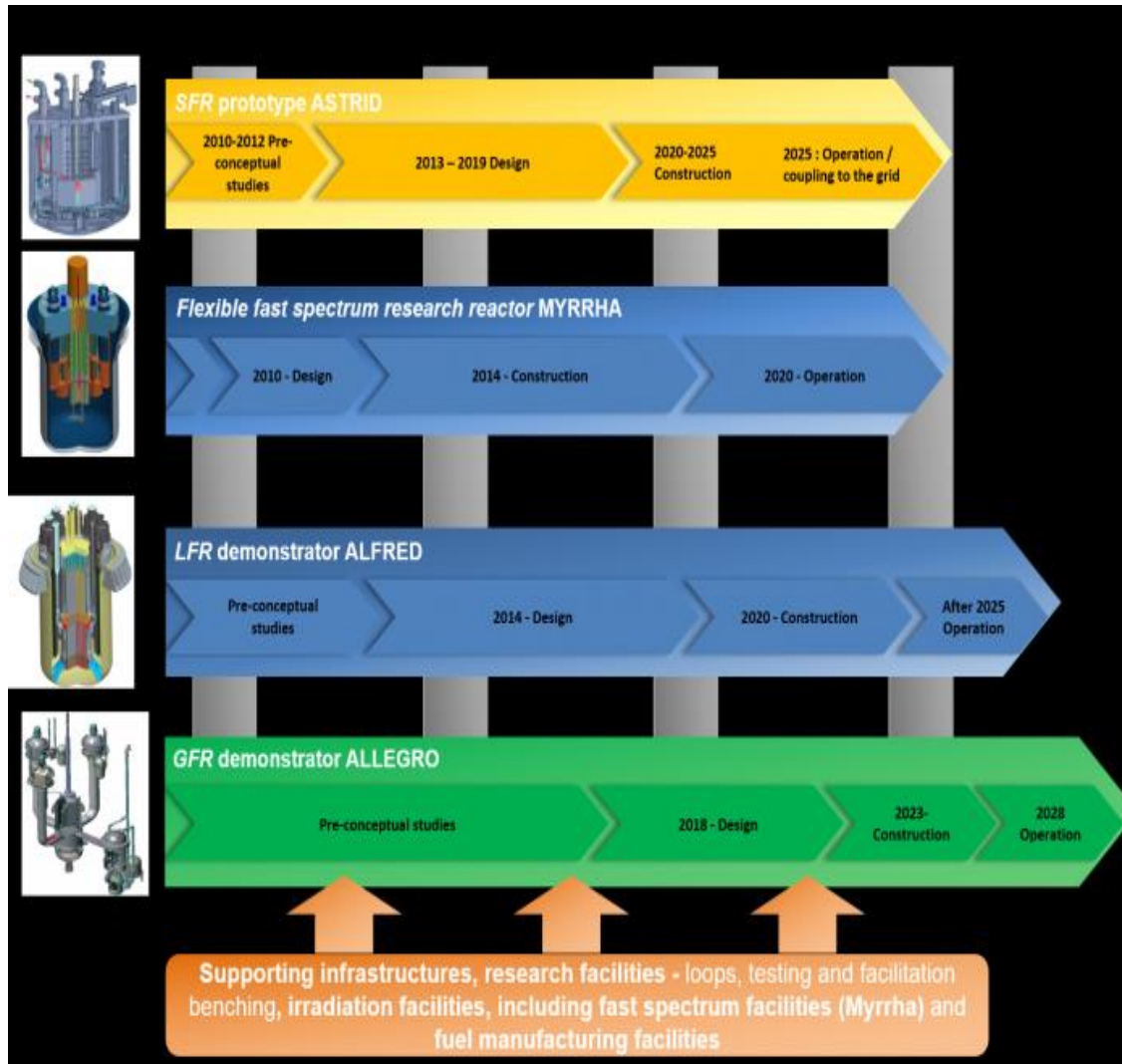


Multi-physics Code simulating Transport Phenomena

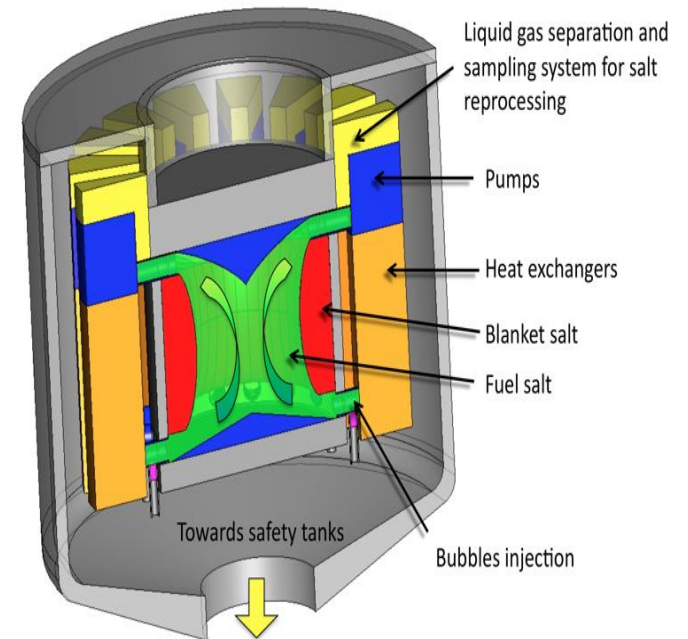
2D and 3D fluid dynamics code coupled with a **structure model** and a space-, time- and energy-dependent **neutron dynamics model**



European Sustainable Nuclear Industrial Initiative (ESNII) systems and MSFR

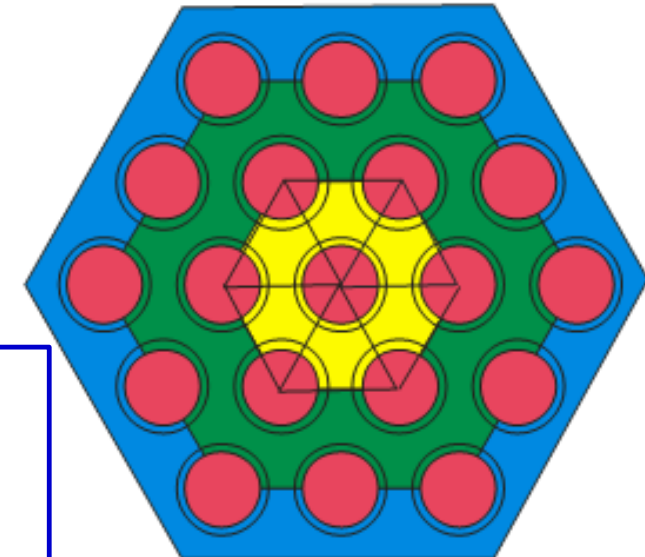
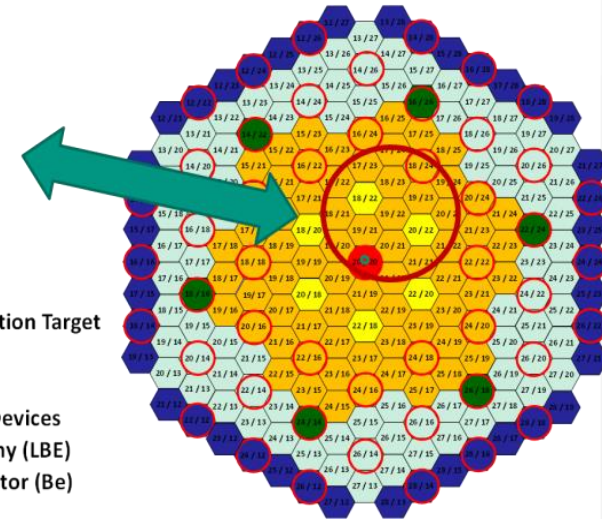
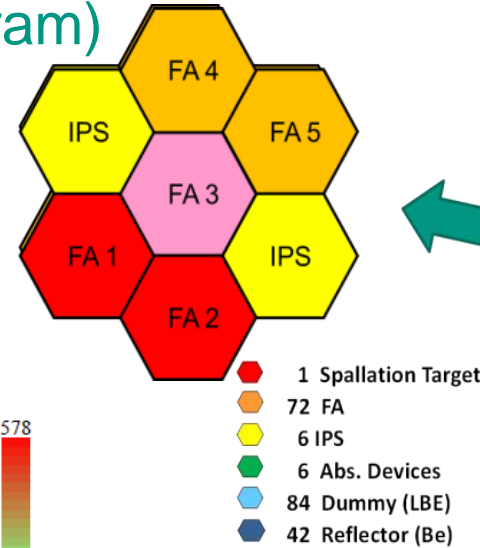
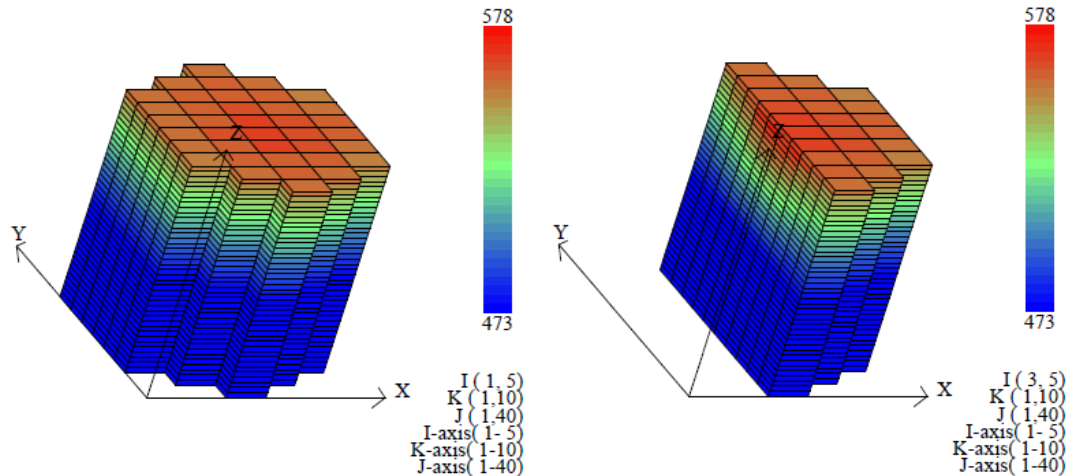


- **SFR, ADS/LFR, GFR: near term**
- **MSFR: long term**



Safety Analysis for Advanced Energy Systems (EU Commission, FP-7 Research Program)

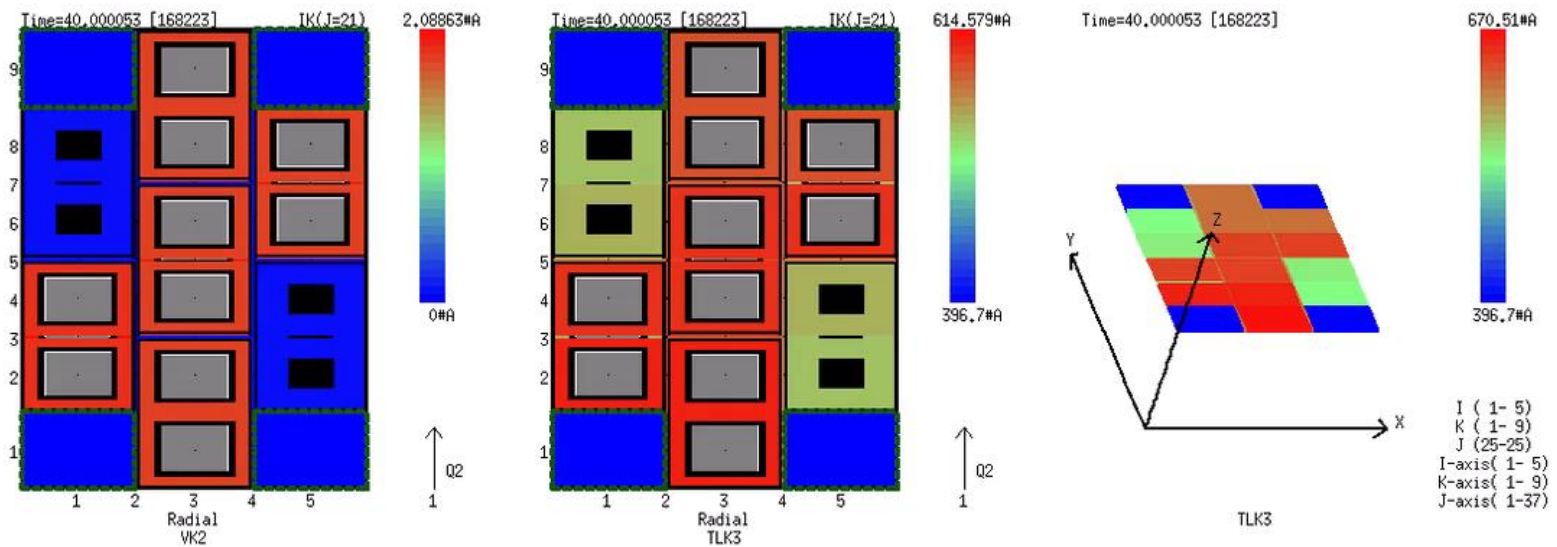
- Lead-bismuth eutectic (LBE) as coolant
- MYRRHA Reactor, SCK CEN, Begium
- Applied to 2D/3D Fuel Assembly Blockage
- Inter-wrapper Gap Model
- Macroscopic Continuum Differential Model



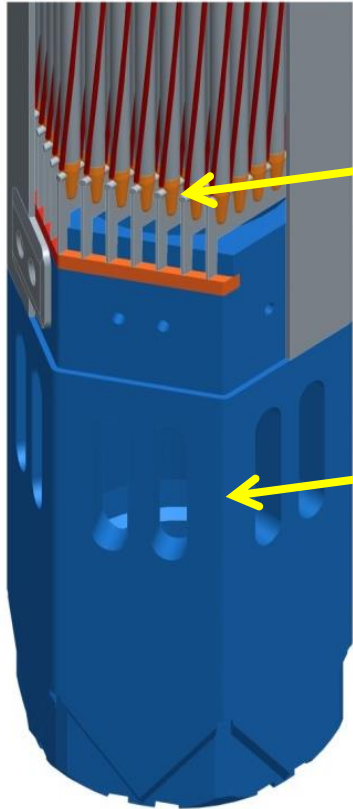
#Please refer:

- ① R. Li et al. 3D Numerical Study of LBE-cooled fuel assembly in MYRRHA using SIMMER-IV code, Annals of Nuclear Energy, 2017, (104C): 42-52.
- ② R. Li et al. Studies of Fuel Dispersion after Pin Failure: Analysis of Assumed Blockage Accidents for the MYRRHA-FASTEF Critical Core, Annals of Nuclear Energy, 2015, (79): 31-42.
- ③ R. Li et al. Study on Severe Accident Scenarios: Pin Failure Possibility of MYRRHA-FASTEF Critical Core, Energy Procedia, 2015, (71): 14-21.

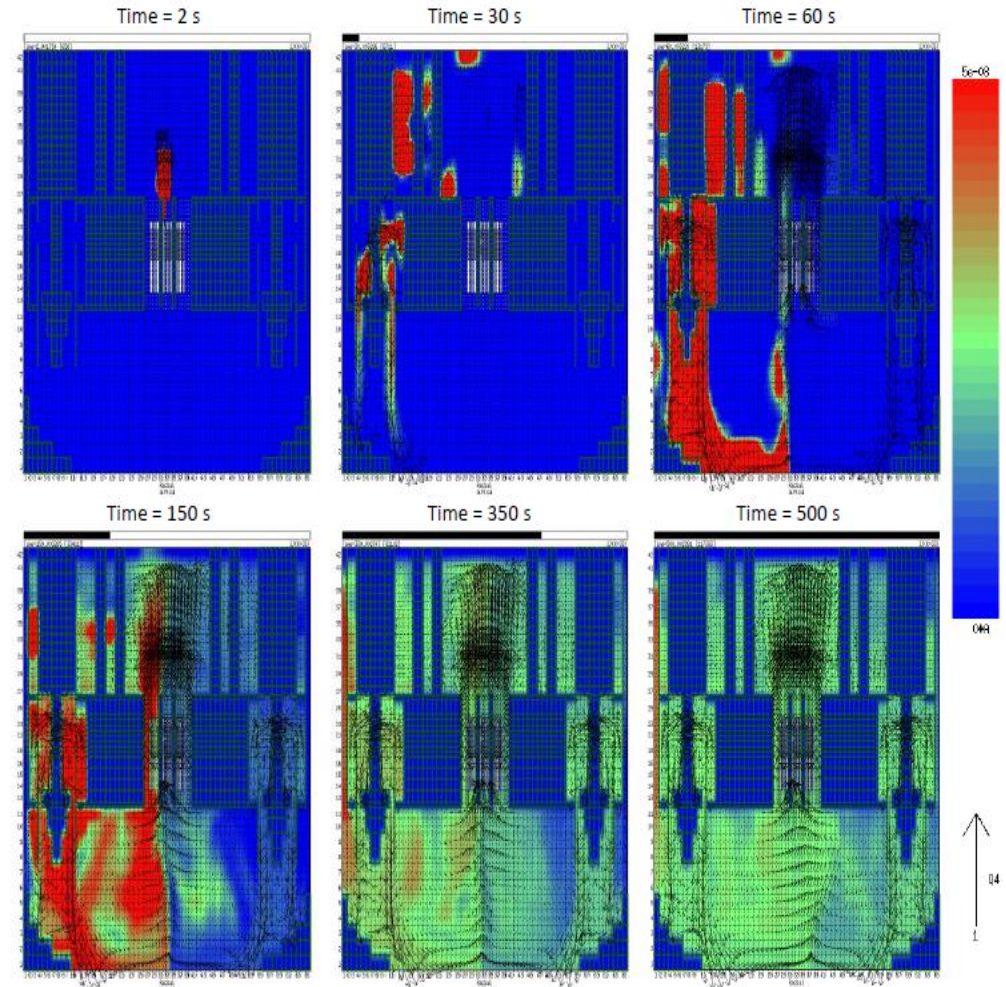
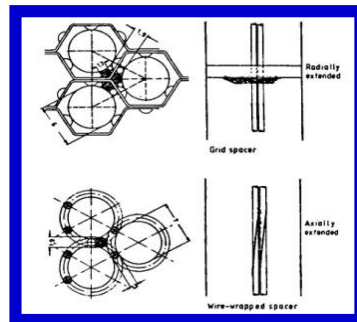
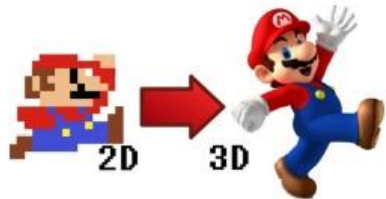
TECHNISCHE
HOCHSCHULE
DEGGENDORF



2D Simulation: fuel dispersion after blockage in the core

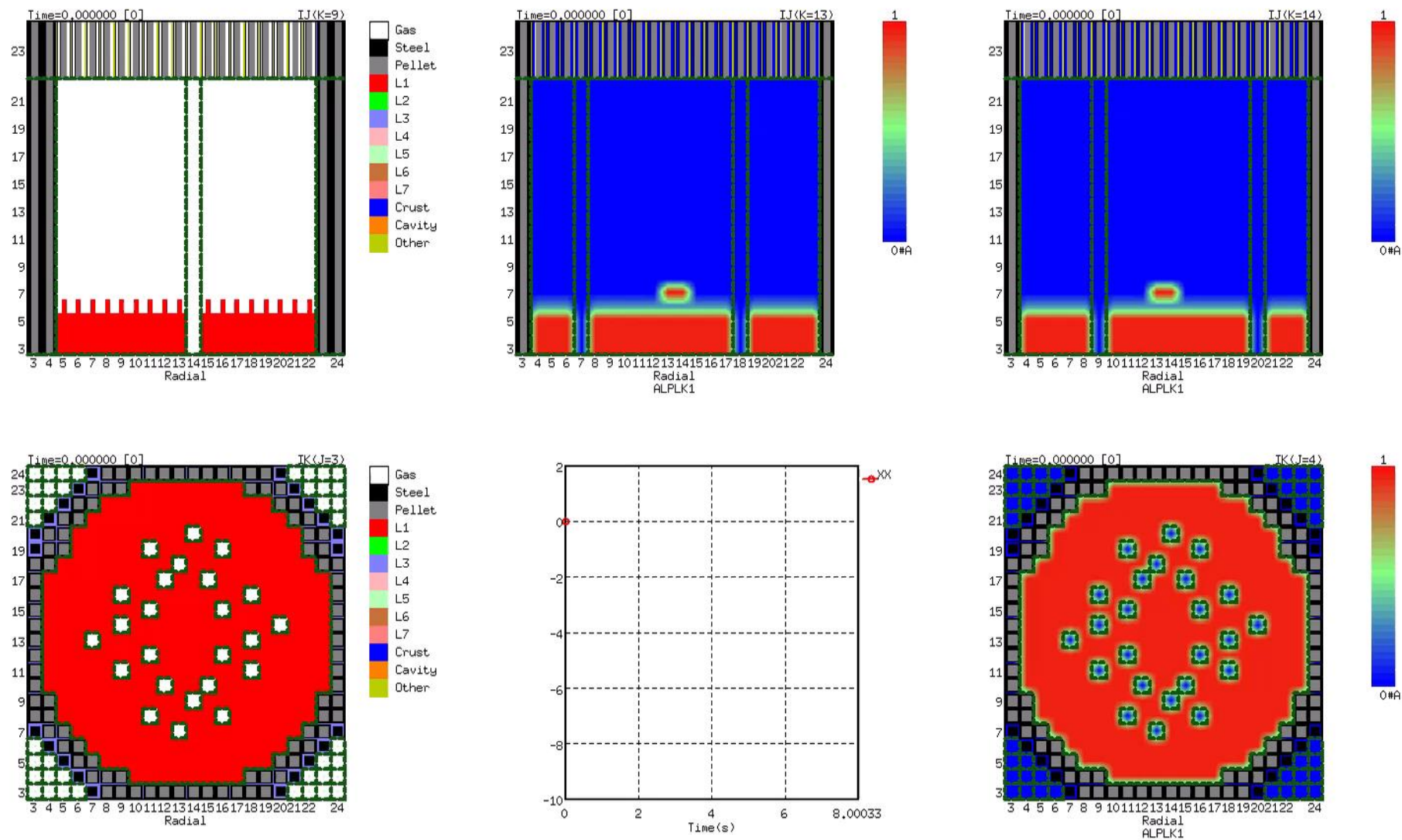


- **Internal Blockage** : Internal blockage inside fuel SA by debris accumulation or swelling (simulated by thin plate)
- **External Blockage** : Central hole in SA foot part is blocked, coolant enters only through the side openings
- **Background of blockage problem** : FERMI, SPX, Russian Alpha Class Sub



Fuel dispersion in LBE after failure of pins due to blockage formation in the core

3D Simulation: Investigation on Upper Bounds of Recriticality Energetics of Hypothetical Core Disruptive Accidents in Sodium Cooled Fast Reactors



Continuity: $\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$ Ideal gas law: $P = \rho RT$

x-momentum: $\rho \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) = \rho g_x - \frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left(2\mu \frac{\partial u}{\partial x} + \lambda \vec{\nabla} \cdot \vec{V} \right) + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right]$

y-momentum: $\rho \left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) = \rho g_y - \frac{\partial P}{\partial y} + \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right] + \frac{\partial}{\partial y} \left(2\mu \frac{\partial v}{\partial y} + \lambda \vec{\nabla} \cdot \vec{V} \right) + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right]$

z-momentum: $\rho \left(u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) = \rho g_z - \frac{\partial P}{\partial z} + \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left(2\mu \frac{\partial w}{\partial z} + \lambda \vec{\nabla} \cdot \vec{V} \right)$

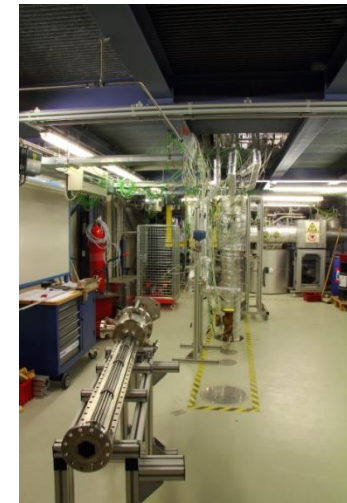
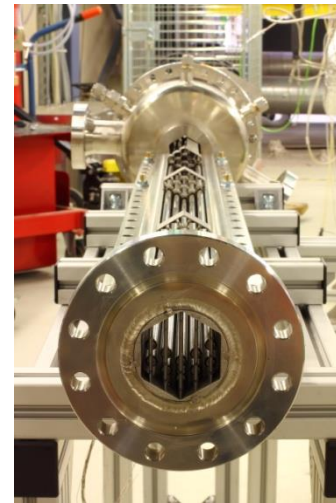
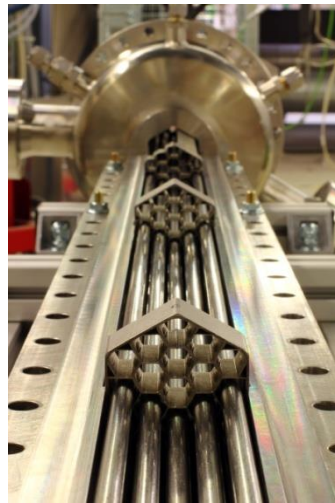
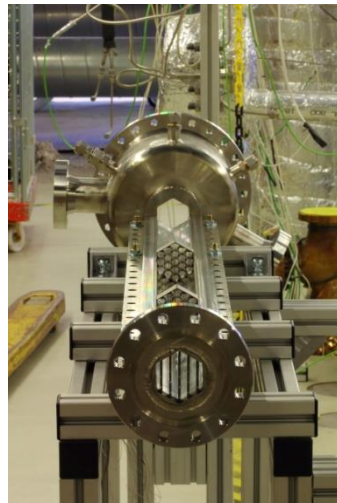
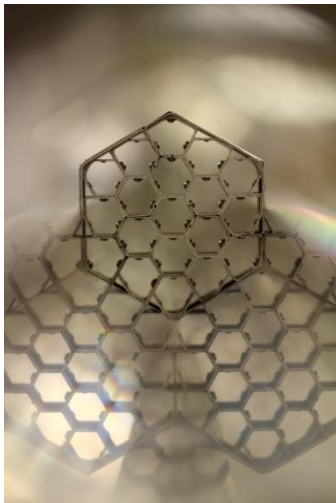
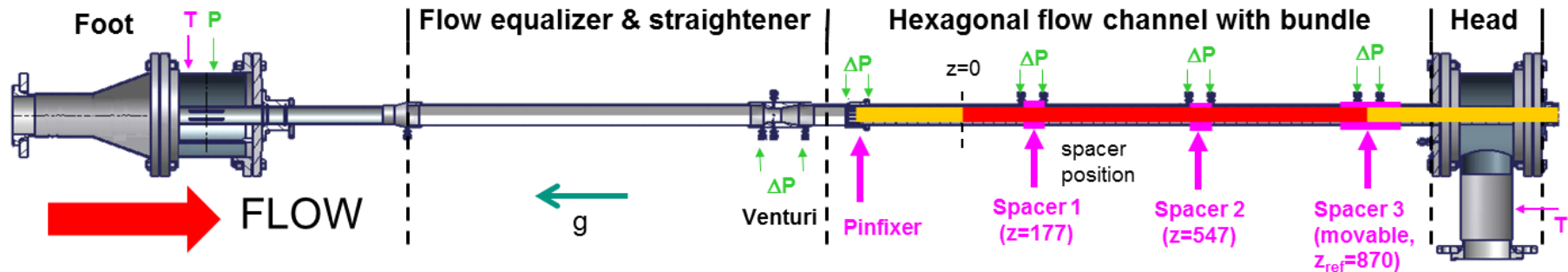
Energy: $\rho c_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} \right) = \beta T \left(u \frac{\partial P}{\partial x} + v \frac{\partial P}{\partial y} + w \frac{\partial P}{\partial z} \right) + \vec{\nabla} \cdot (k \vec{\nabla} T) + \Phi$

**Any fluid dynamics theoretical model or numerical approach is temporary,
physical understanding of flow is forever.**

-----Dietrich Küchemann

An Example: Heat Transfer in Subchannels

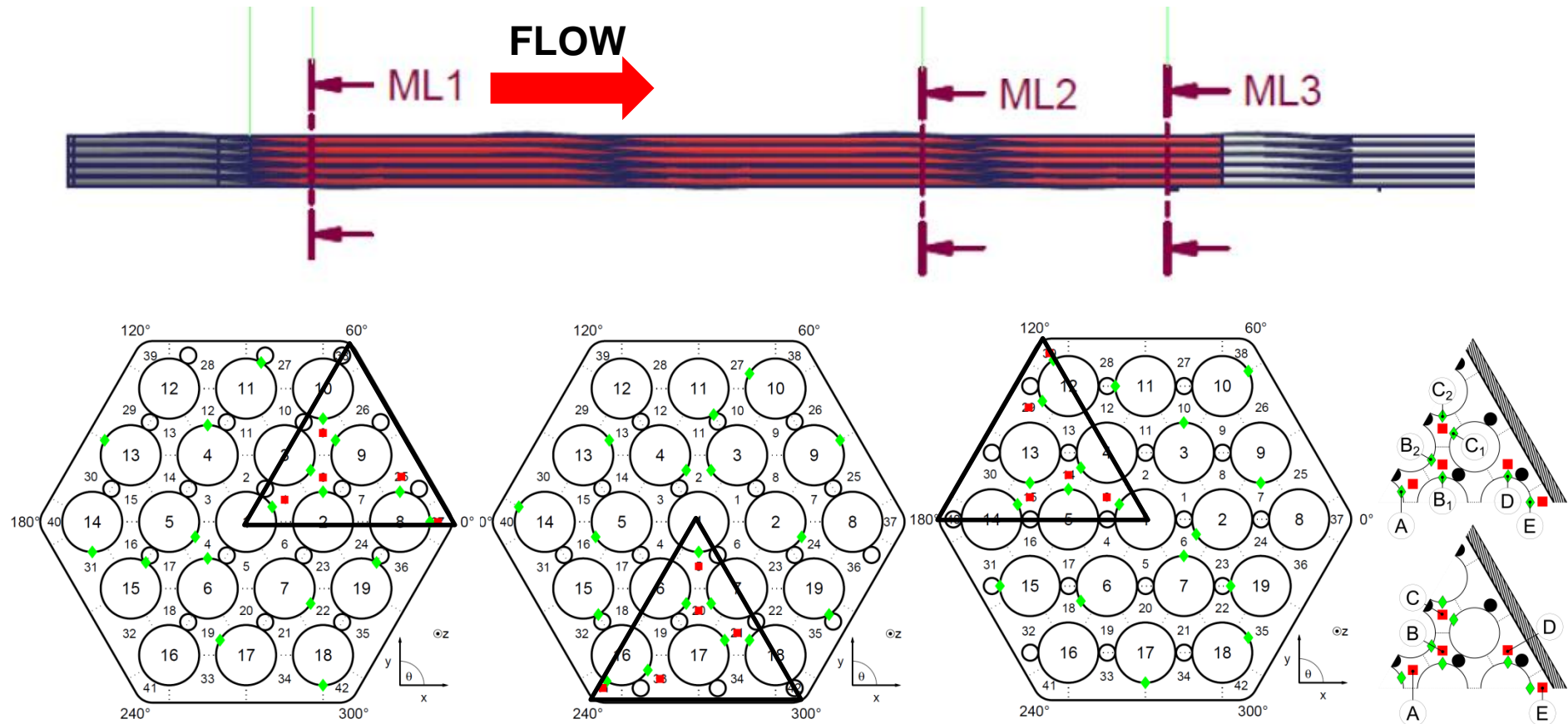
Experiment at KALLA, Karlsruhe: Hexagonal 19-rod bundle with grid spacers



■ 19 pins ■ $D=8.2 \text{ mm}$ ■ $P/D = 1.4$ ■ $L = 870 \text{ mm}$ ■ $A = 1260 \text{ mm}^2$

#Please refer: J. Pacio et al. Experimental study of heavy-liquid metal (LBE) flow and heattransfer along a hexagonal 19-rod bundle with wire spacers, Nuclear Engineering and Design 301, pp 111–127 (2016)

Experiment at KALLA: 3 measuring levels on LBE Temperature



- 3 measuring levels
- Identical sectors

- 3x18 Twall (0.5 mm)
- 3x5 Tsch (0.25 mm)

- #11, #15 and #19 are behind the wire

- For the **macroscopic pin models** in the SIMMER code, the heat mixing between subchannels flow has to be considered, therefore, the **inter-cell heat conduction term** has been adjusted in a way that in all directions the coolant heat conduction between the cells is calculated.
- We introduced an empirical “**heat mixing factor**” in front of the heat conduction term in the energy conservation equation. This “heat mixing factor” plays the same role as “**mixing parameter**” in the classical subchannels analysis**.
- Such effort can compensate the underestimation of the heat transfer due to the coarse mesh which cannot fully represent the temperature gradient.
- The energy conservation equation with heat mixing factor is written as:

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\vec{v} \rho e) = Q + \nabla \cdot q, \text{ where } q = -C_{\text{mixing}} (k_c + k_T) \cdot \nabla T$$

- q is the heat flux at the cell interface, C_{mixing} is newly introduced.
- k_c Microscopic thermal conductivity, k_T Turbulent thermal conductivity.
- Implemented in the subroutine **heat mixing factor C_{mixing}**

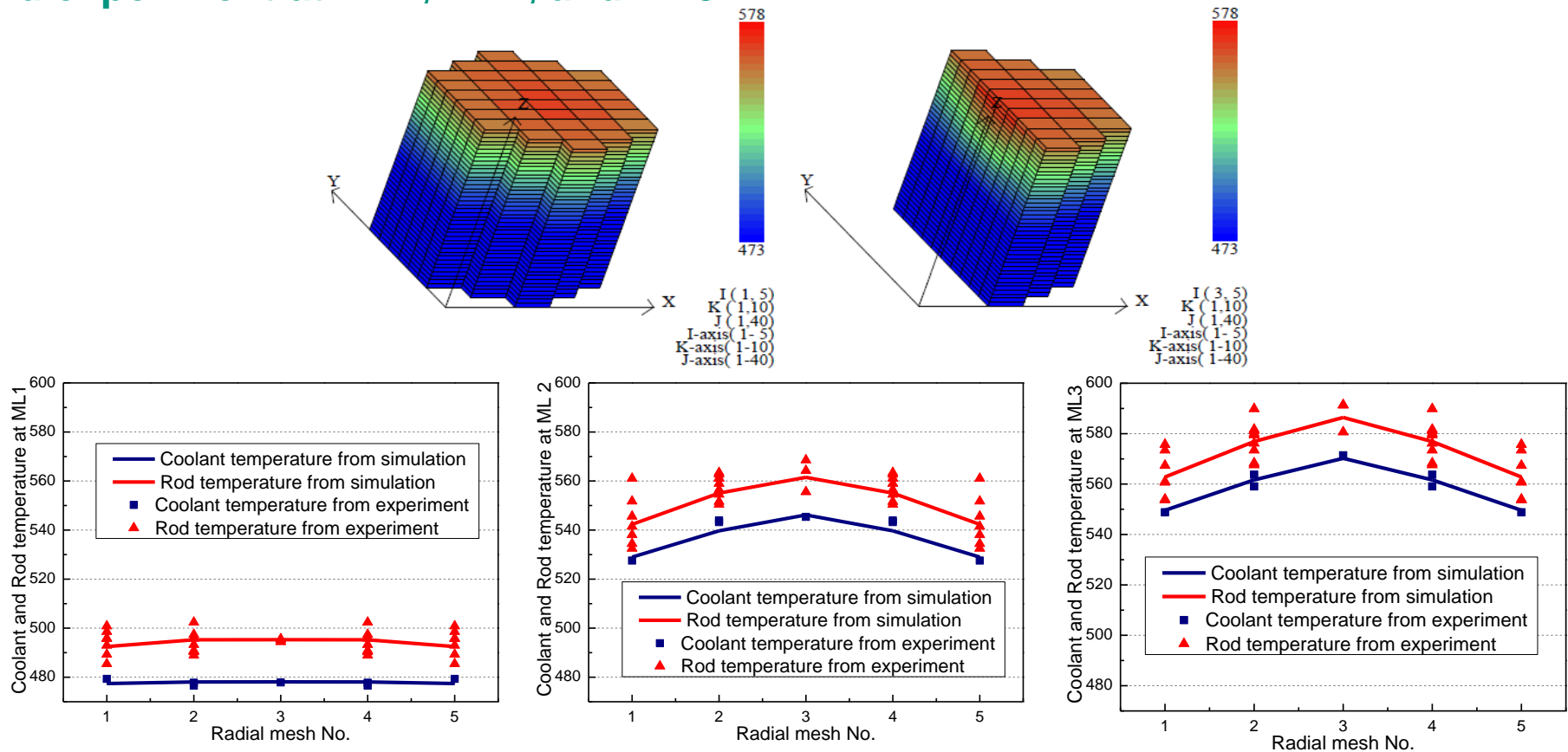
#Please refer:

**H Ninokata et al. Distributed resistance modeling of wire-wrapped rod bundles. Nuclear Engineering and Design, 104:93–102 (1987)

**S.K. Cheng, et al, Hydrodynamic models and correlations for rod bundles, Bundle friction factors, subchannel friction factors and mixing parameters, Nuclear Engineering and Design. 92: 227-251 (1986)

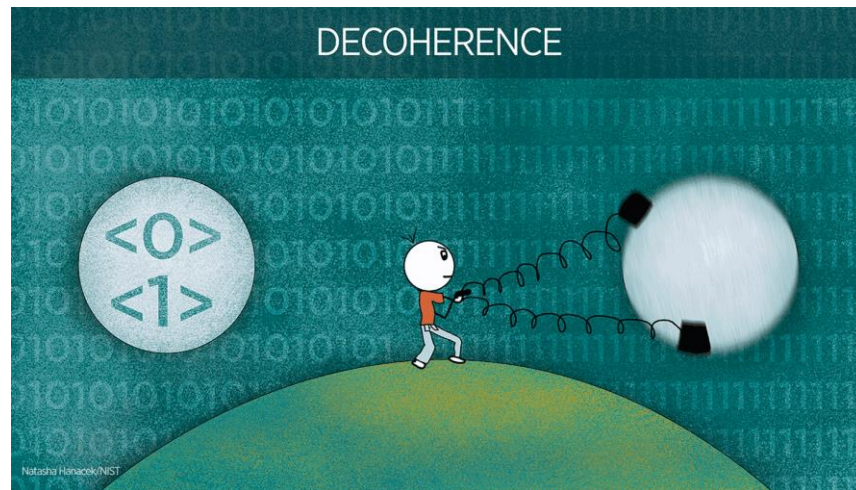
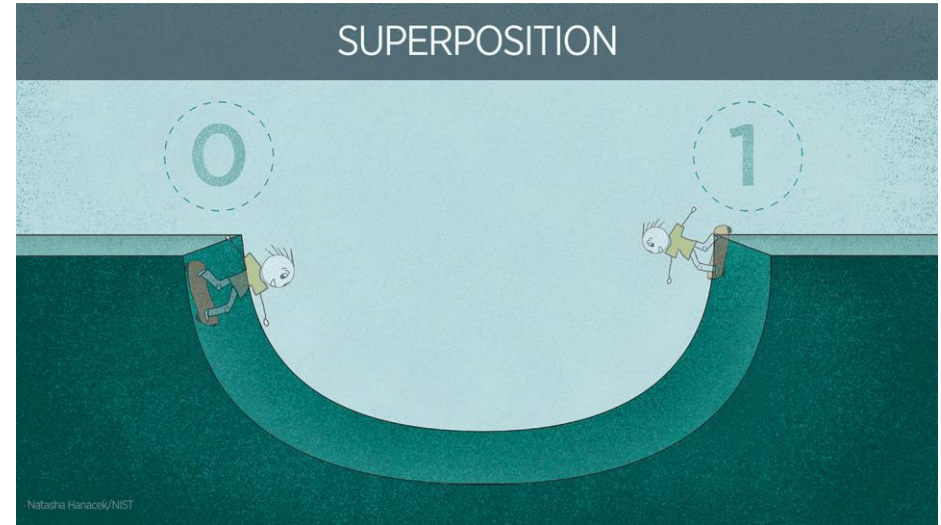
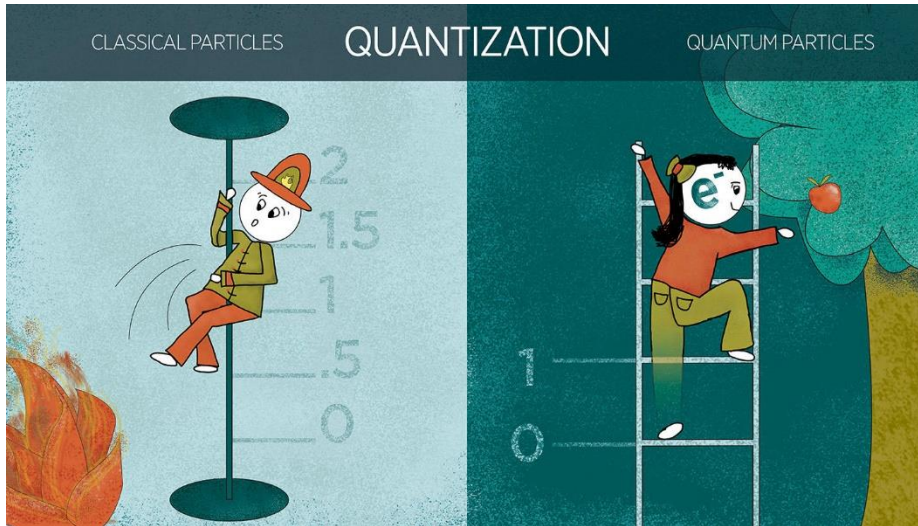
Because of the computational limitations, the physicists need to make reasonable modellings and assumptions.

Comparison of the coolant and rod temperature from simulation and experiment at ML1, ML2, and ML3.



- The comparison shows that the simulation results agree well with the experiment, to some extents, it **confirms that the macroscopic pin bundle model developed** is good for the global value as it uses the correct correlation.

#Please refer: R. Li et al. 3D Numerical Study of LBE-cooled fuel assembly in MYRRHA using SIMMER-IV code, Annals of Nuclear Energy, 2017, (104C): 42-52.



#Please refer: <https://www.nist.gov/physics/introduction-new-quantum-revolution/strange-world-quantum-physics>.

Quantum Gates, Circuits and Algorithms

Gates and rotations in Bloch sphere	Circuit representation	Matrix representation	Truth table	
<i>I</i> gate: no rotation is performed.		$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	Input	Output
			$ 0\rangle$	$ 0\rangle$
			$ 1\rangle$	$ 1\rangle$
<i>X</i> gate: rotates the qubit state by π about the x-axis.		$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	Input	Output
			$ 0\rangle$	$ 1\rangle$
			$ 1\rangle$	$ 0\rangle$
<i>Y</i> gate: rotates the qubit state by π about the y-axis.		$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	Input	Output
			$ 0\rangle$	$i 1\rangle$
			$ 1\rangle$	$-i 0\rangle$
<i>Z</i> gate: rotates the qubit state by π about the z-axis.		$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	Input	Output
			$ 0\rangle$	$ 0\rangle$
			$ 0\rangle$	$- 1\rangle$
<i>S</i> gate: rotates the qubit state by $\pi/2$ about the z-axis.		$S = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/2} \end{pmatrix}$	Input	Output
			$ 0\rangle$	$ 0\rangle$
			$ 1\rangle$	$e^{i\pi/2} 1\rangle$

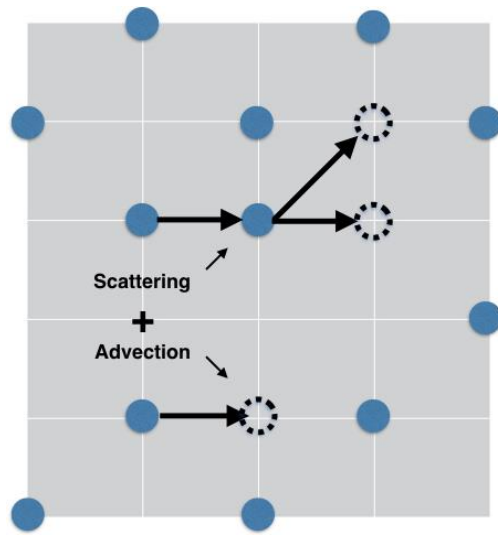
Gates and rotations in Bloch sphere	Circuit representation	Matrix representation	Truth table	
<i>T</i> gate: rotates the qubit state by $\pi/4$ about the z-axis.		$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$	Input	Output
			$ 0\rangle$	$ 0\rangle$
			$ 1\rangle$	$e^{i\pi/4} 1\rangle$
<i>H</i> gate: rotates the qubit state by π about an axis diagonal in the x-z plane. This is equivalent to an X-gate followed by a $\frac{\pi}{2}$ rotation about the y-axis.		$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$	Input	Output
			$ 0\rangle$	$\frac{ 0\rangle + 1\rangle}{\sqrt{2}}$
			$ 1\rangle$	$\frac{ 0\rangle - 1\rangle}{\sqrt{2}}$
CNOT gate: applies an X-gate to the target qubit if the control qubit is in state $ 1\rangle$.		$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	Input	Output
			$ 00\rangle$	$ 00\rangle$
			$ 01\rangle$	$ 01\rangle$
			$ 10\rangle$	$ 11\rangle$
			$ 11\rangle$	$ 10\rangle$
CPHASE gate: apply a Z-gate to the target qubit if the control qubit is in state $ 1\rangle$.		$CPHASE = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$	Input	Output
			$ 00\rangle$	$ 00\rangle$
			$ 01\rangle$	$ 01\rangle$
			$ 10\rangle$	$ 10\rangle$
			$ 11\rangle$	$- 11\rangle$

#Please refer: Michael A. Nielsen, Quantum Computation and Quantum Information.

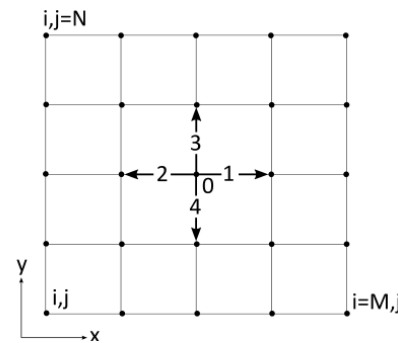
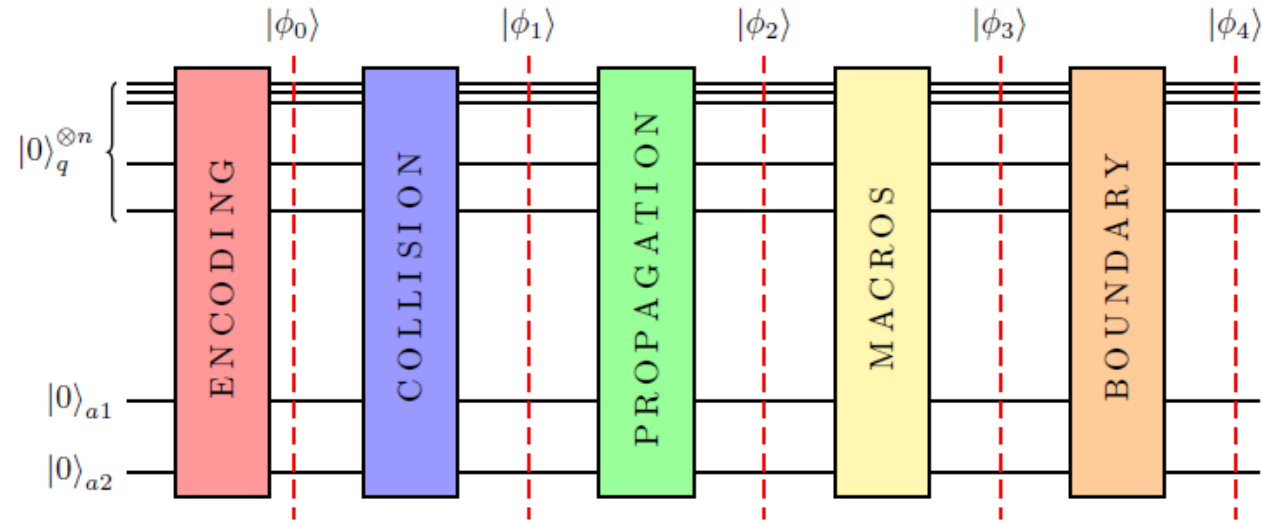
Flow Problem	Numerical method	Quantum Computing Approach
2D cavity flow	Lattice Boltzmann method (LBM)	stream function–vorticity form of the flow equations is solved using a D2Q5 (two dimensions, five speeds) configuration of LBM represented with quantum circuits
Fluid density on a 2D lattice	Lattice Boltzmann method (LBM)	Based on analogies between Dirac and LBM equations, a full quantum mapping of transport equations in fluid flows.
Time evolution of the Burgers equation	finite difference	quantum-classical hybrid approach, evaluating the cost function with a gate-based quantum computer and optimizing variational parameters on a classical computer
steady-state inviscid, compressible flow through a nozzle	finite difference	spatial discretization: partial differential equations the nonlinear ordinary differential equation based on the quantum amplitude estimation algorithm
Poisson equation	finite difference	Algorithm and circuit solving the Poisson equation. Hamiltonian simulation techniques can be combined.

#Please refer:

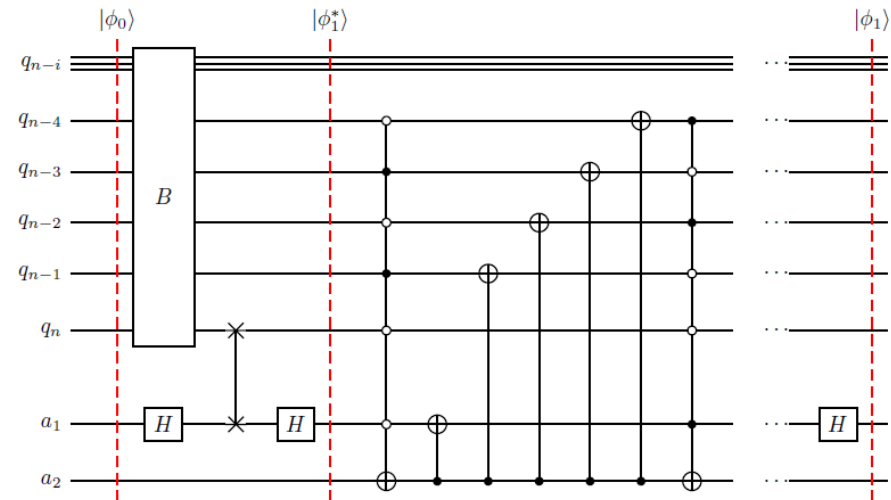
- ① L. Budinski, Quantum algorithm for the Navier Stokes equations by using the stream function vorticity formulation and the lattice Boltzmann method, Int.J.Quant.Inf. 20,2150039 (2022)
- ② A. Mezzacapo, et al. Quantum Simulator for Transport Phenomena in Fluid Flows. Sci Rep 5, 13153 (2015).
- ③ M. Lubasch et al. Variational quantum algorithms for nonlinear problems. Phys. Rev. A, , 101, 010301. (2020)
- ④ F. Gaitan, Finding Solutions of the Navier-Stokes Equations through Quantum Computing, Recent Progress, a Generalization, and Next Steps Forward. Advanced Quantum Technologies, 4, 2100055. (2021)
- ⑤ Y. Cao et al. Quantum algorithm and circuit design solving the Poisson equation, New J. Phys. 15 013021. (2013)



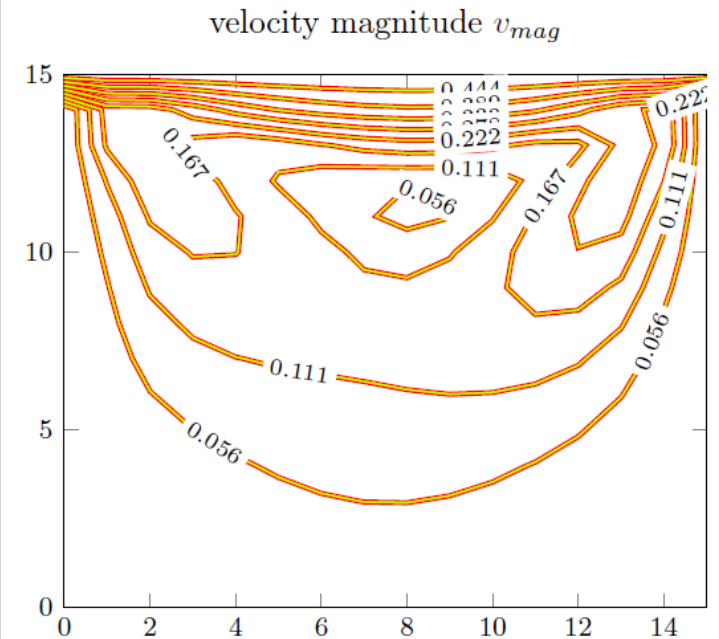
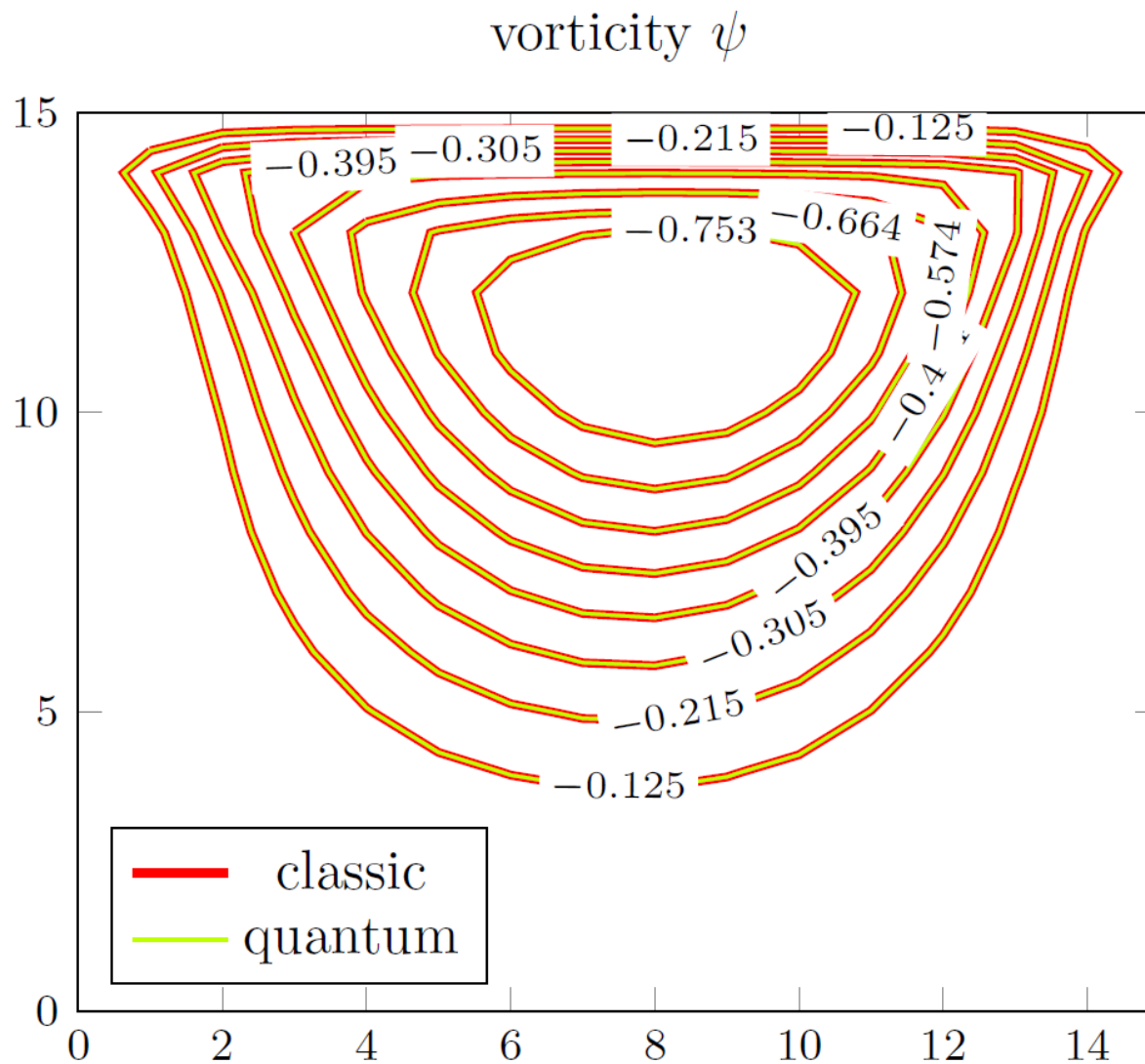
Schematic of an LBM simulation



#Please refer: L. Budinski, Quantum algorithm for the Navier Stokes equations by using the stream function vorticity formulation and the lattice Boltzmann method, Int.J.Quant.Inf. 20,02, 2150039 (2022)



Quantum circuit for implementing the collision step.



Comparison:
quantum algorithm using the
classical FORTRAN, for **cavity**
flow simulated by the D2Q5
LBM.

#Please refer: L. Budinski, Quantum algorithm for the Navier Stokes equations by using the stream function vorticity formulation and the lattice Boltzmann method, Int.J.Quant.Inf. 20,02, 2150039 (2022)

Preliminary Lattice Boltzmann Method Simulation using Intel® Quantum SDK

T. Shinde, H. Liebelt, R. Li, **Thursday 17:40**

Track 3: Computations in Theoretical Physics: Techniques and Methods

Beitrag ID: 206

Typ: Oral

Preliminary Lattice Boltzmann Method Simulation using Intel® Quantum SDK

Donnerstag, 27. Oktober 2022 17:40 (20 Minuten)

The present work is based on the research within the framework of cooperation between Intel Labs and Deggendorf Institute of Technology, since the Intel® Quantum SDK (Software Development Kit) has recently released. Transport phenomena e.g. heat transfer and mass transfer are nowadays the most challenging unsolved problems in computational physics due to the inherent nature of fluid complexity. As the revolutionary technology, quantum computing opens a grand new perspective for numerical simulation including the computational fluid dynamics (CFD). It is true that the current CFD algorithms based on the different scales (e.g. macroscopic or microscopic) need to be translated into quantum system. In the current work the quantum algorithms have been preliminarily implemented for fluid dynamics using the Intel Quantum SDK, one mesoscopic approach has been applied i.e. to solve the lattice Boltzmann equation. Taking the simplest transport phenomena as a starting point, the preliminary quantum simulation results have been validated with the analytical solution and the classical numerical simulation. The potential of quantum in simulating fluid will be discussed.

Quantum Computing for Navier-Stokes Equations

Continuity: $\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$ Ideal gas law: $P = \rho RT$

x-momentum: $\rho \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} \right) = \rho g_x - \frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left(2\mu \frac{\partial u}{\partial x} + \lambda \vec{\nabla} \cdot \vec{V} \right) + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right]$

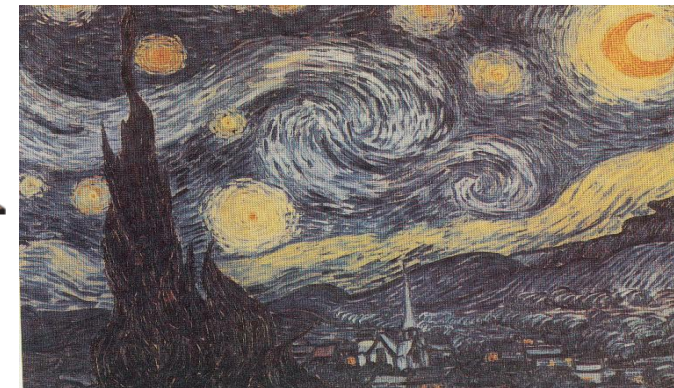
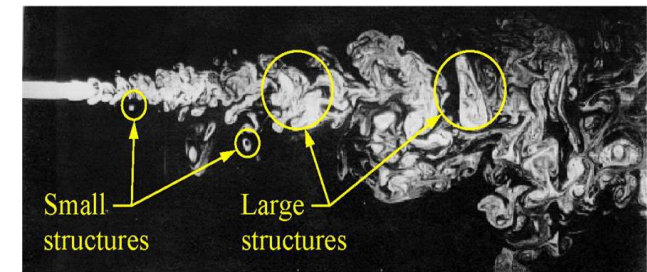
y-momentum: $\rho \left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} \right) = \rho g_y - \frac{\partial P}{\partial y} + \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) \right] + \frac{\partial}{\partial y} \left(2\mu \frac{\partial v}{\partial y} + \lambda \vec{\nabla} \cdot \vec{V} \right) + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right]$

z-momentum: $\rho \left(u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} \right) = \rho g_z - \frac{\partial P}{\partial z} + \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \right] + \frac{\partial}{\partial z} \left(2\mu \frac{\partial w}{\partial z} + \lambda \vec{\nabla} \cdot \vec{V} \right)$

Energy: $\rho c_p \left(u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} + w \frac{\partial T}{\partial z} \right) = \beta T \left(u \frac{\partial P}{\partial x} + v \frac{\partial P}{\partial y} + w \frac{\partial P}{\partial z} \right) + \vec{\nabla} \cdot (k \vec{\nabla} T) + \Phi$

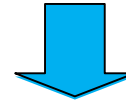
Partial Differential Equations

Turbulent Flow Structures

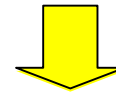


Van Gogh's 'Starry Night'

start



discretizing the spatial domain
reduces the system of Partial Differential Equations (PDEs) to a
system of Ordinary Differential Equations (ODEs)



a quantum nonlinear ordinary differential Equations ODE algorithm



store and return

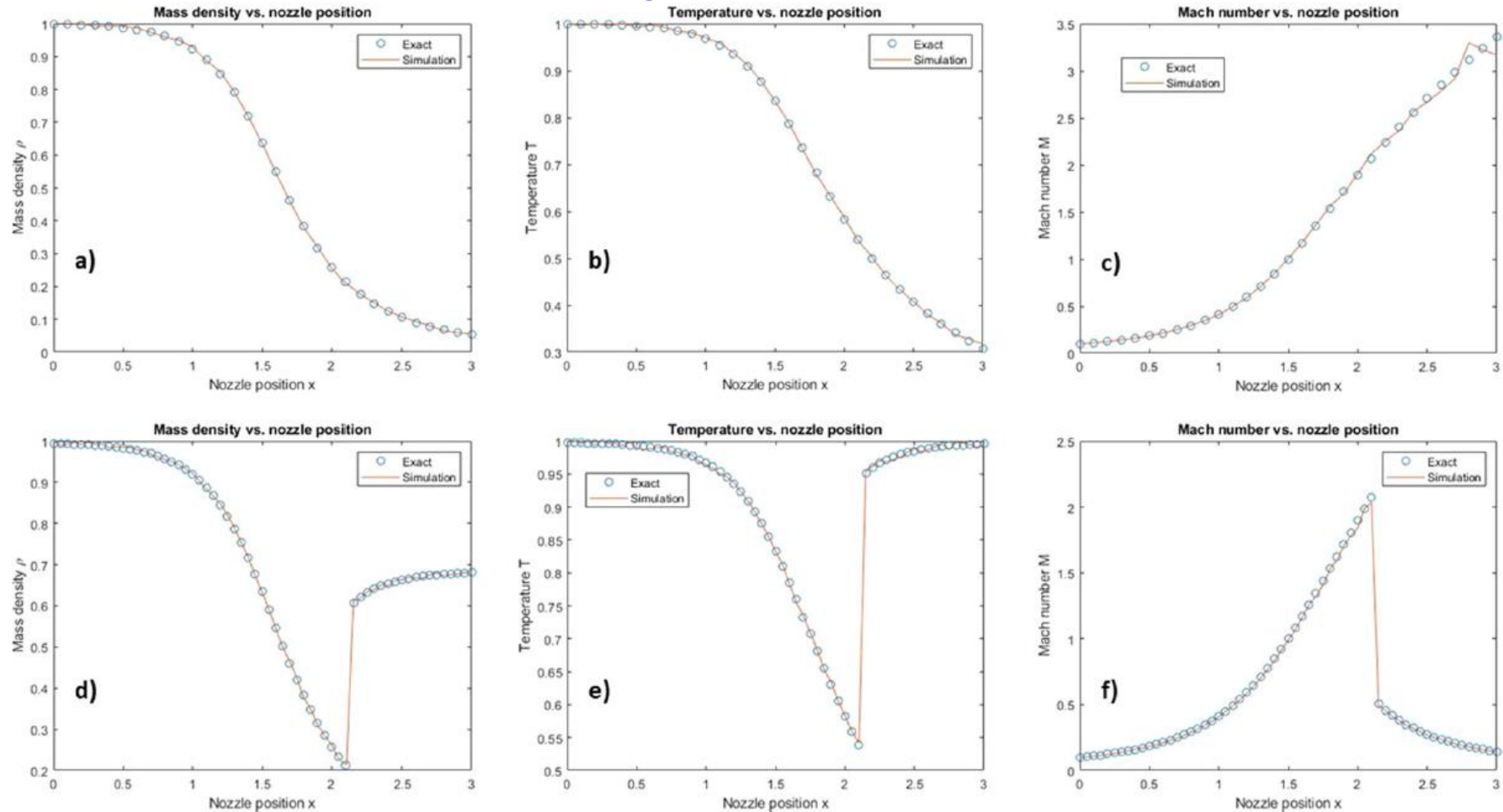


Kacewicz' quantum nonlinear ODE algorithm

#Please refer: ① F. Gaitan, Finding Solutions of the Navier-Stokes Equations through Quantum Computing, Recent Progress, a Generalization, and Next Steps Forward. Advanced Quantum Technologies, 4, 2100055. (2021)

②B. Kacewicz, Almost optimal solution of initial-value problems by randomized and quantum algorithms J. Complex. 22, 676. (2006)

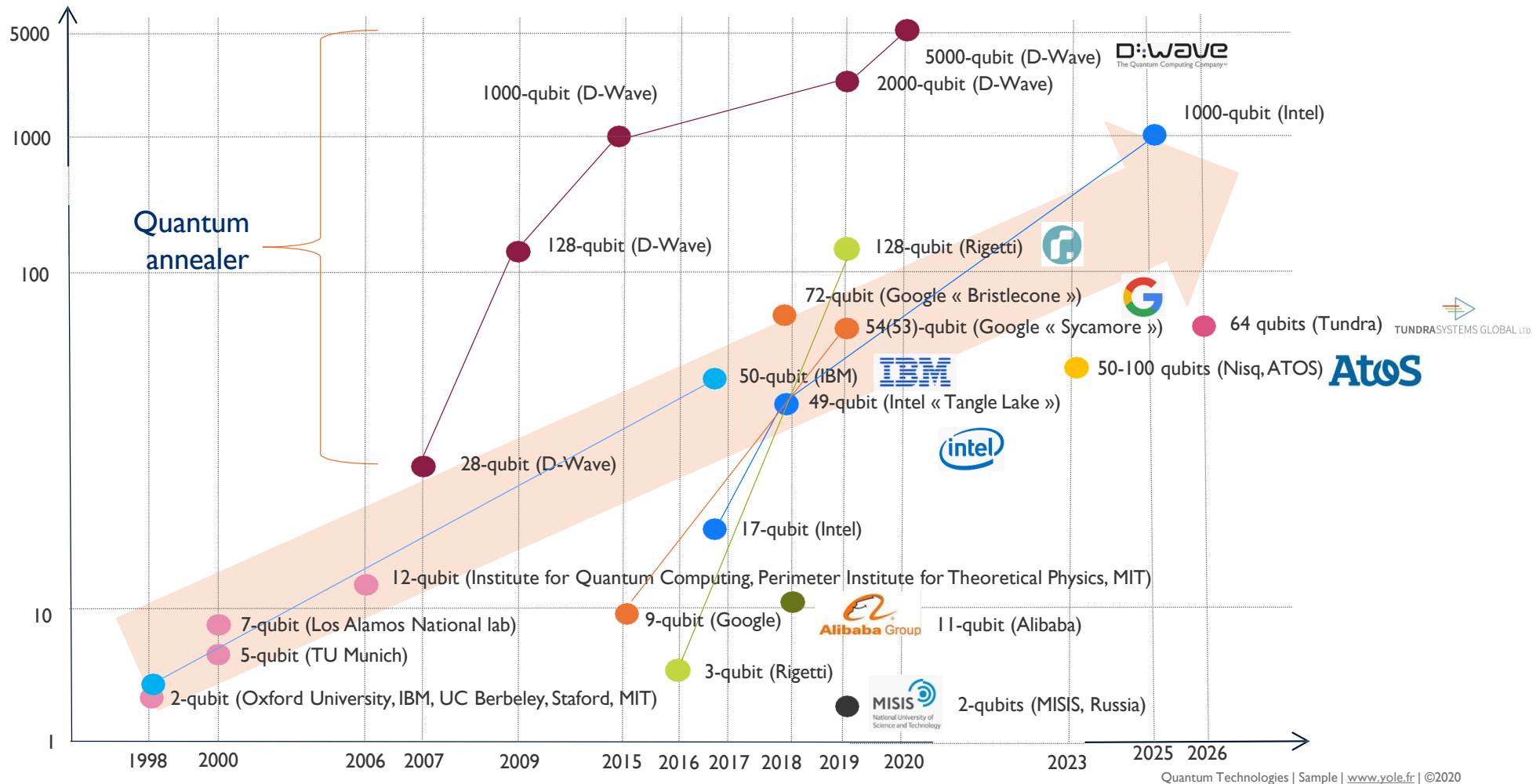
Comparison: quantum Navier-Stokes simulation results and analysis solution for steady-state, inviscid, compressible flow through a **de Laval nozzle**.



#Please refer: F. Gaitan, Finding flows of a Navier–Stokes fluid through quantum computing. npj Quantum Inf. 6, 61 (2020).

Quantum Simulator v.s. Roadmap for Quantum Computer

Graph below shows physical qubits roadmap (to be remembered: for a quantum computer, 50 logic qubits minimum are required → it means 5000 physical qubits)



#Please refer: www.yole.fr

Please see more details with Prof. Dr. Liebelt (next talk)

Quantum Computing in Data Center

Future: Combination of High-Performance Computing and Quantum Computing



Deggendorf Institute of Technology: a teaching data center of such concept is being developed with involvement of students.

Please see more details with Prof. Dr. Liebelt (next talk)

Concluding Remarks

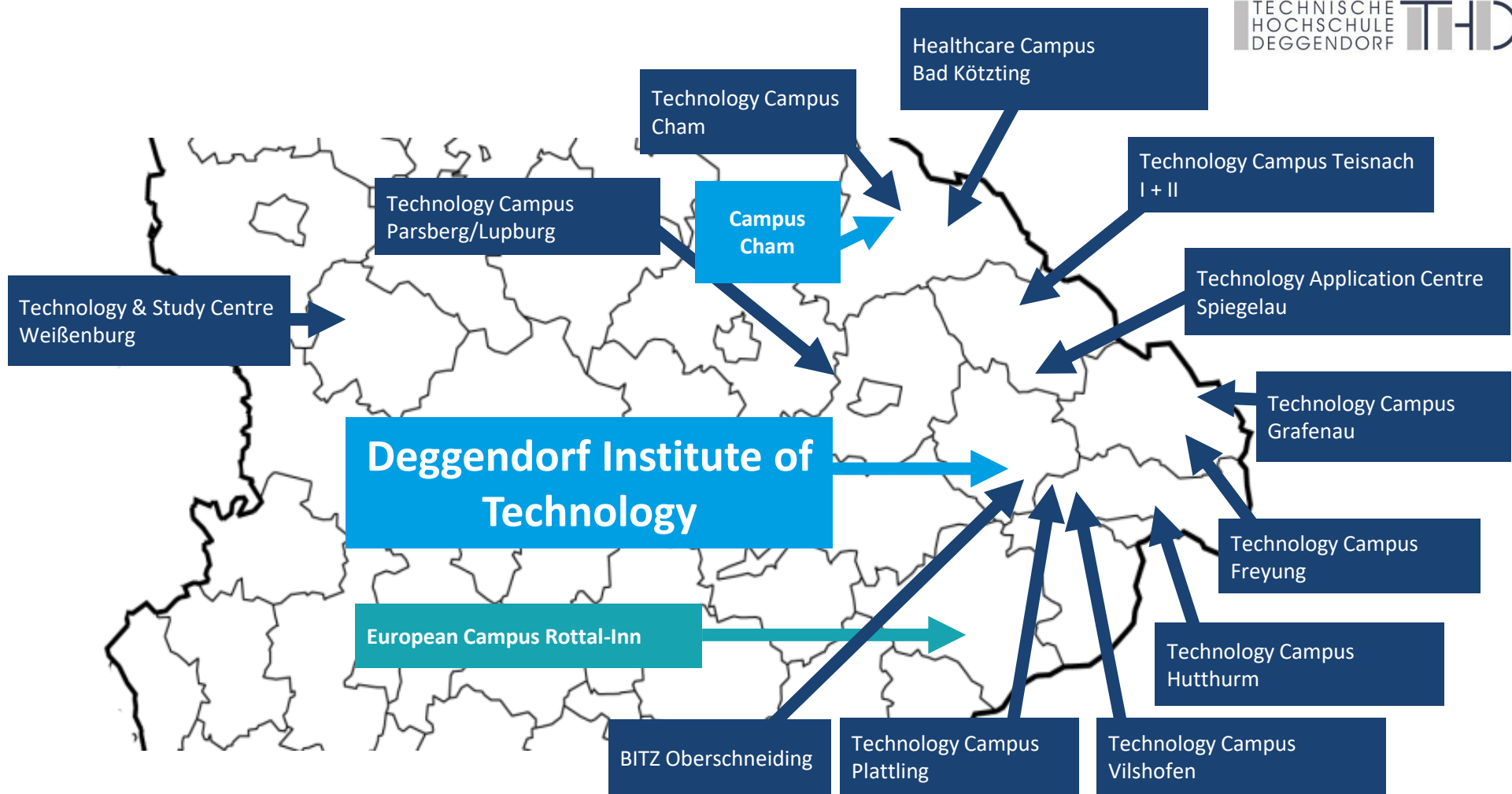
Transport phenomena remains nowadays still the most challenging unsolved problem in computational physics, though the high-performance computing has been applied.

Using classical simulations of accident scenarios in advanced reactors as example, the advantage and disadvantage of **current multi-physics code systems** coupling reactor kinetics and fluid dynamics are shortly presented.

As the tomorrow' technology, **quantum computing** opens however a grand new perspective for numerical simulations for transport phenomena. **Two concrete examples** are briefly presented with details namely: first one based on lattice Boltzmann method, the second one based on quantum Navier-Stokes algorithm.

Quantum computer in data center is hopefully the future.

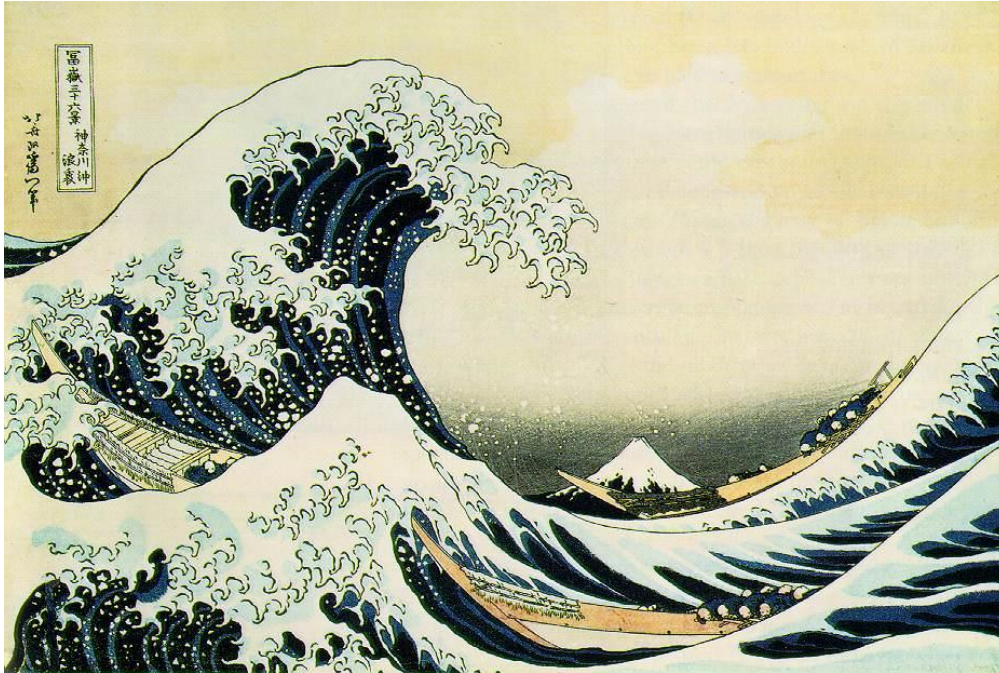
Acknowledgement: Intel Mindshare Curriculum Program



Questions?

**Thank you for
your attention**

Backup Slides



The Great Wave Off Kanagawa



Van Gogh's `Starry Night'

