Karlsruhe Institute of Technology

OECD/NEA Second Multi-Physics Model Validation Workshop (MPMV-2)
June 26-27, 2019. GRS, Germany.

KIT Multi-Physics Developments for Reactor Analysis

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Institute for Neutron Physics and Reactor Technology (INR)

Content

- Motivation
- KIT strategy
- Current R&D topics
- Multi-physics advanced codes based on transport and subchannel solvers
- How to validate pin-by-pin deterministic solutions?
- High-fidelity multi-physics codes based on Monte Carlo
- Validation of high fidelity codes
- Summary and Outlook

Motivation

Complex Physics:

- Increasing complexity of core loading
- High burn-up
- Quite different core designs PWR, BWR, SMR, Gen-IV, research reactors

Huge and cheap HPC-Capability

- European HPCs: PRACE (Partnership for Advanced Computing in Europe)
- HPC-clusters in the Federal State Baden Württemberg (BW)
  - FIVE HPC centers
  - **One at KIT for Energy**

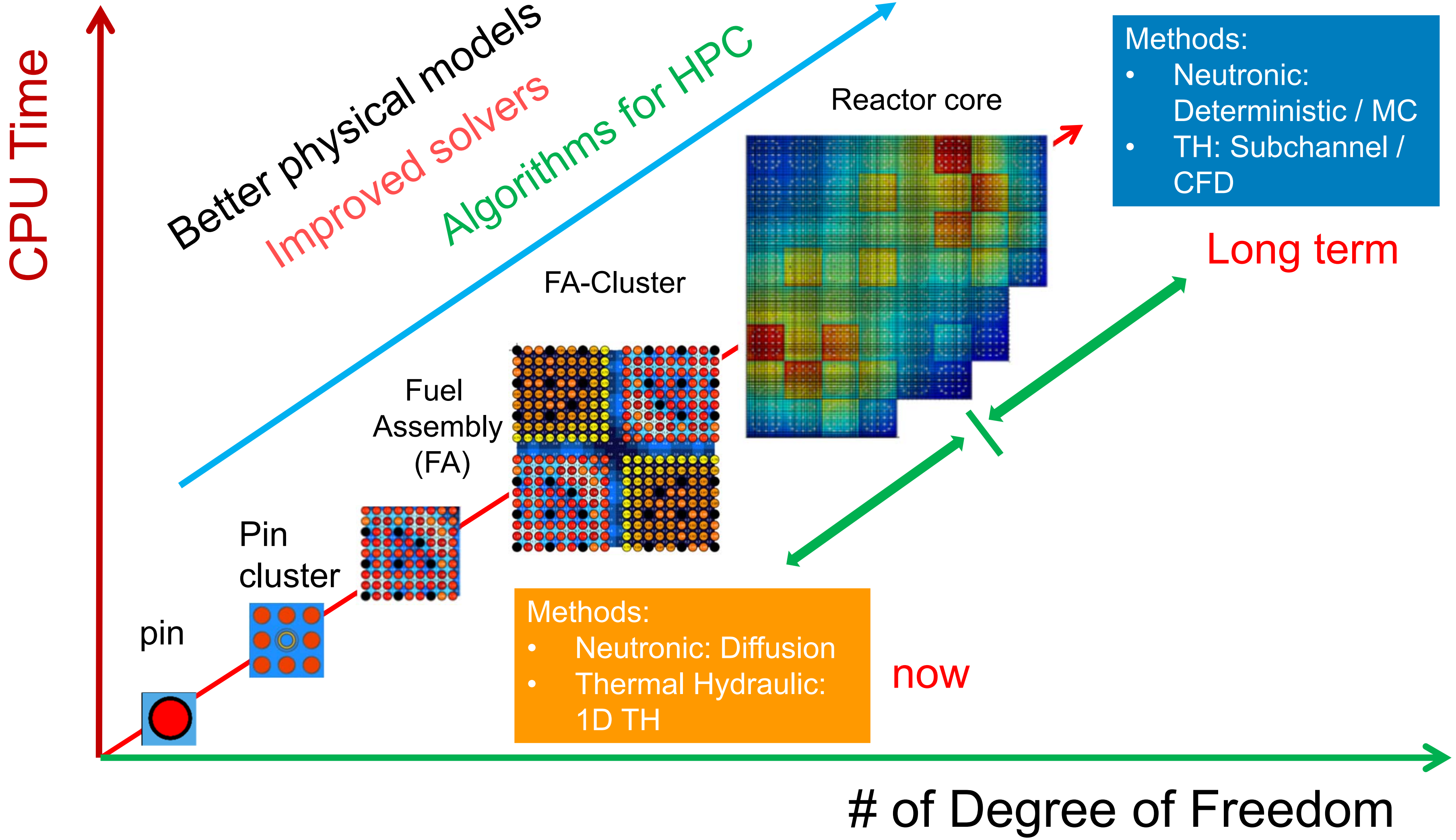
HPC Infrastructure at Baden Württemberg

- bwForCLuster MLS/WISO: Economics /social sciences (Mannheim/Heidelberg)
- bwForCLuster JUSTUS: Chemistry (Ulm)
- bwForCLuster NEMO: Neuro sciences. Microsystems, elementary particle physics (Freiburg)
- bwForCLuster BinAC: Bio informatics and Astrophysics
- **Research High Performance Computer ForHLR I and II at KIT for energy research**
  - Phase I: applications with many thousands processors
  - Phase II: applications with many hundred thousands

KIT SCC ForHLR I

KIT SCC ForHLR II

Motivation: Challenges for core Physics



CPU Time

Better physical models

Improved solvers

Algorithms for HPC

Reactor core

FA-Cluster

Fuel Assembly (FA)

Pin cluster

pin

Methods:
- Neutronic: Deterministic / MC
- TH: Subchannel / CFD

Long term

Methods:
- Neutronic: Diffusion
- Thermal Hydraulic: 1D TH

now

# of Degree of Freedom

KIT
Strategy for the Development of Safety Analysis Codes

Selection of Key Safety Topics combining innovative Research with E&T

- Reflecting needs of German situation
- Following international trends

Integration of RPD activities in national / international activities and programs

- EU projects
- National programs and projects of BMBF, BMWi, etc.

Combination

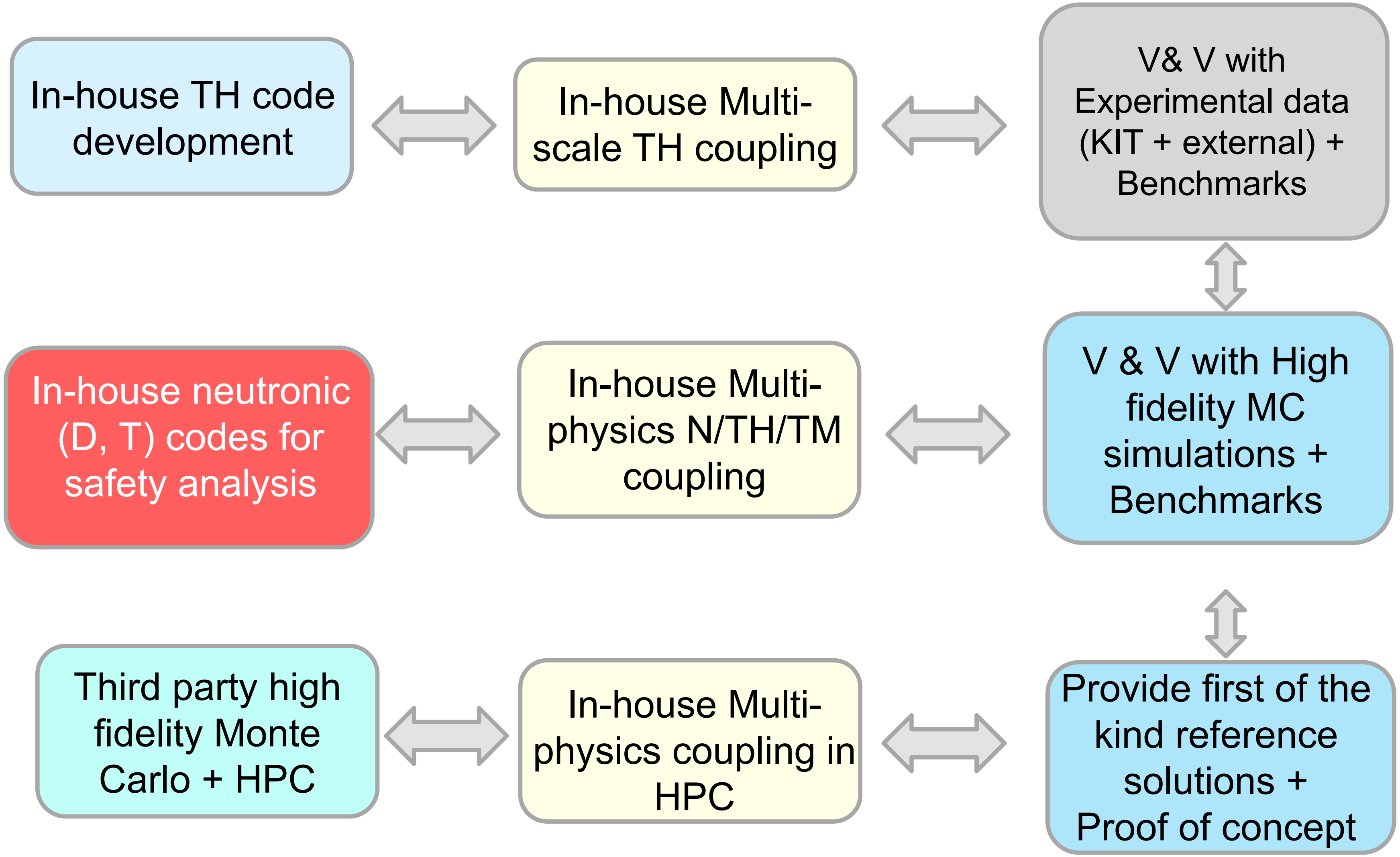
In-house HGF* (KIT, HZDR) code development and use of international codes

Make use of HPC and new algorithms and methods

*** HGF: Helmholtz Association of Research Centres**

Current R&D Topics

HGF Reactor Safety Research Topics



In-house TH code development

In-house Multi-scale TH coupling

V& V with Experimental data (KIT + external) + Benchmarks

In-house neutronic (D, T) codes for safety analysis

In-house Multi-physics N/TH/TM coupling

V & V with High fidelity MC simulations + Benchmarks

Third party high fidelity Monte Carlo + HPC

In-house Multi-physics coupling in HPC

Provide first of the kind reference solutions + Proof of concept

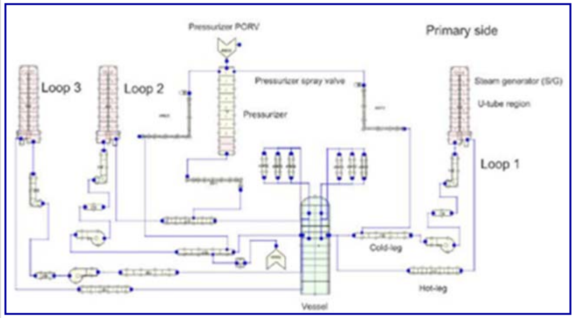
HGF: Helmholtz Association of Research Centres

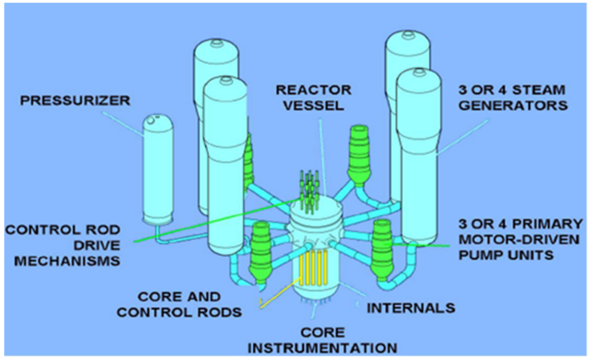
KIT Multi-Scale Thermal Hydraulic Coupling

Goal: Improve the description of TH phenomena inside the RPV, Core and Loops

System TH Code: TRACE, RELAP5: whole NPP simulation at macro scale

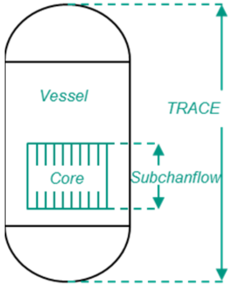
- 1D or 3D coarse mesh TH
- Empirical correlations
- Fast running

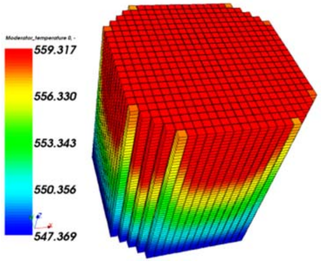




Subchannel TH Code: SUBCHANFLOW, CTF: simulation of the **reactor core** TH at **component scale**.

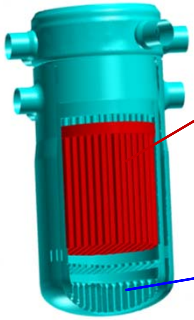
- Detailed description of cross flow physics between Sub-channels or fuel assemblies





CFD Codes:

- 3D simulation at different details (mm to m)
- Less empirical models
- Almost exact geometry
- Porous media approach to reduce CPU and make it practicable

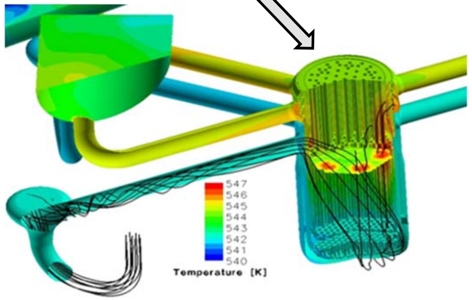


Core N and TH:

- **TRACE/PARCS**
- **SCF/PARCS**

Blue:
CFD: DWC, LPLN, UPLN

PhD K. Zhang



LOOPS:

- **TRACE, RELAP5**

RPV except Core:

- **CFD**

Core:

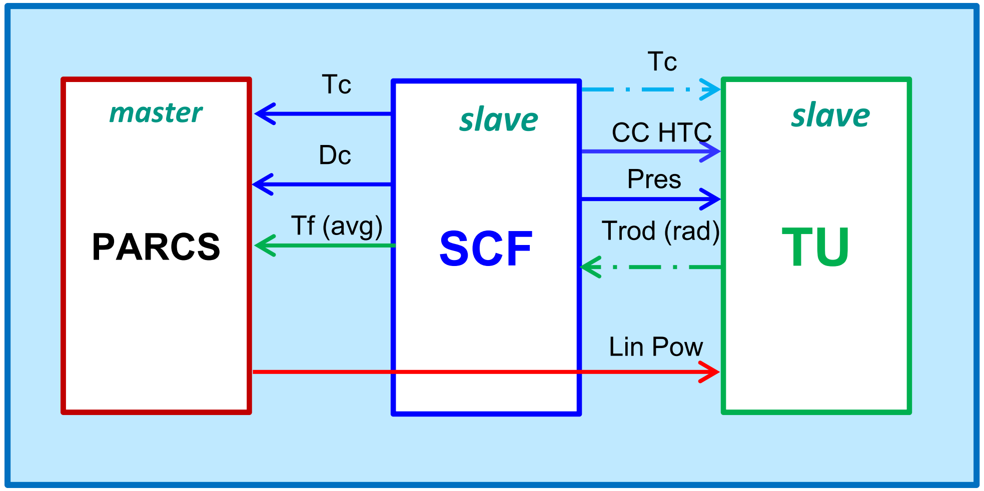
- **TRACE/PARCS**
- **SCF/PARCS**

Coupling of Neutronic/Subchannel-TH/Pin Mechanics Solvers (e.g. PARCS/SCF/TRANSURANUS)

Goals:

- **Improve description of core behaviour under irradiated conditions during life time**

- **Coupling approach:**



Transferred variables

Tc	*Coolant temperature*
Dc	*Coolant Density*
Tf	*Fuel Temperature*
Trod	*Rod radial temperature*
Lin Pow	*Linear Power*
Pres	*Pressure*
CC HTC	*Clad-Coolant heat transfer coefficient*

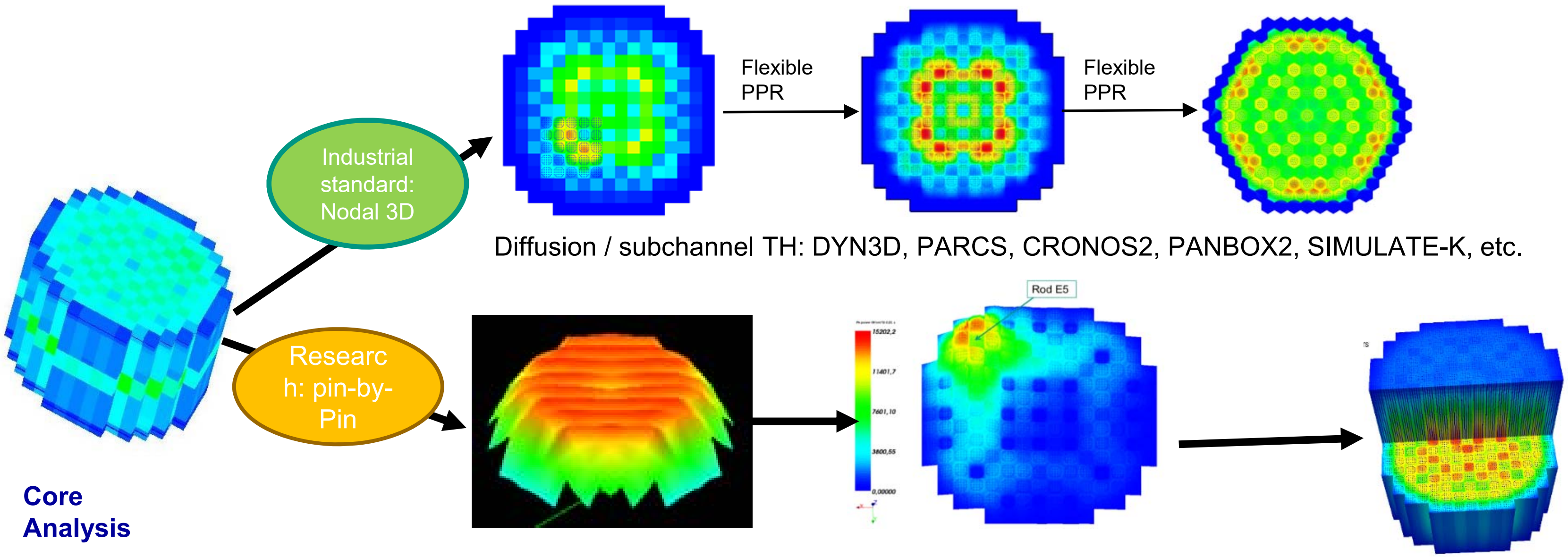
MPI-based Approach

PhD J. Basualdo

Multi-physics advanced codes based on transport solvers and subchannel codes

From
Industry standards to Pin/subchannel-based Core Analysis

- Best-estimate codes: based on nodal diffusion and coarse TH (1D, 3D)
  - TRACE/PARCS, ATHLET/DYN3D, CATHARE/CRONOS2, RELAP5/PANBOX/COBRA, CASCADE-3D, PARCS/SCF, PARCS/CTF, etc. combined with Pin Power Reconstruction



Industrial standard: Nodal 3D

Flexible PPR

Flexible PPR

Diffusion / subchannel TH: DYN3D, PARCS, CRONOS2, PANBOX2, SIMULATE-K, etc.

Research: pin-by-Pin

Core Analysis

Diffusion /subchannel TH
COBAYA4-CTF

Transport (SP3, MOC) /subchnel TH
DUNSUB5.0, MPACT/CTF

Monte Carlo /Subchannel TH
SERPENT/SCF, MC21/CTF

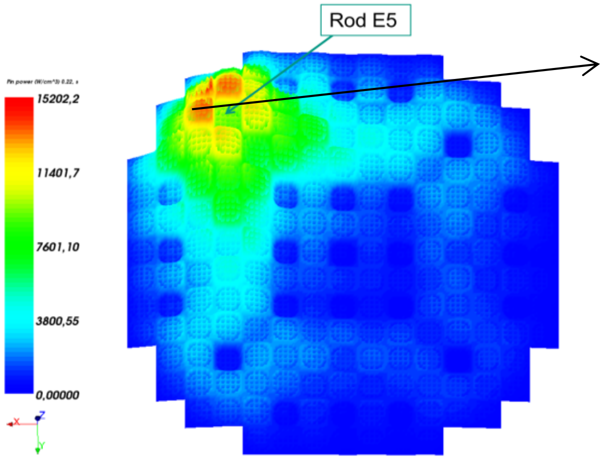
KIT: Advanced Neutronic /thermal hydraulic coupling at pin level:

- Replace nodal diffusion by transport solvers (SP3) and system TH by SCF: DYNSUB5
- Under development: PARCS-SP3 / SUBCHANFLOW Coupling based on ICoCo method

Example: Pin-by-pin full core analysis DYNSUB5 Analysis of the PWR MOX REA

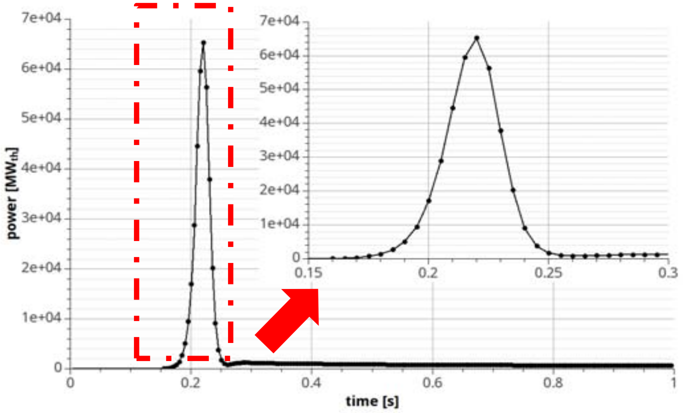
DYNSUB5 Analysis of PWR REA

- Simulation: Transient HZP (3.565kW), TC=560 K
- Ejected rod: E5 within 0.1 s
- Time step: 5 ms



Highest power in fresh UOX

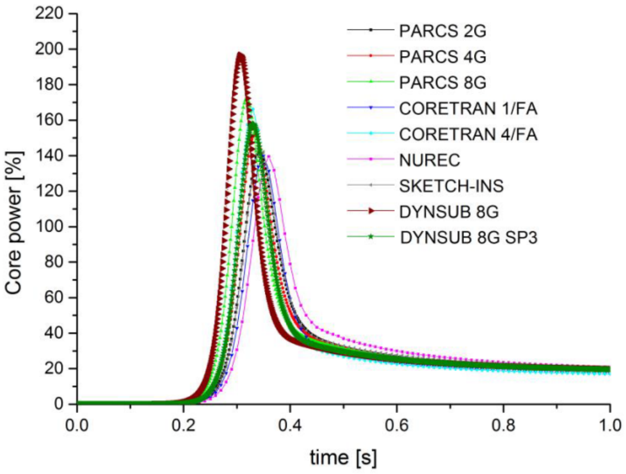
HZP rod ejection accident (REA): axially cumulated power density distribution [W/cm³] at 0.22s



Evolution of thermal power during HZP rod ejection accident (REA)

Validation needed!

- experimental data or
- High fidelity MC-solutions



Code-to-code comparison: Nodal and SP3 Solutions

PhD: M. Däubler

Run statistics:

- Platform: Xeon E5620
- 4 CPUs
- Run time: 14 days and 7 h

- Re-factoring of serial solvers!
- New parallel solvers needed!

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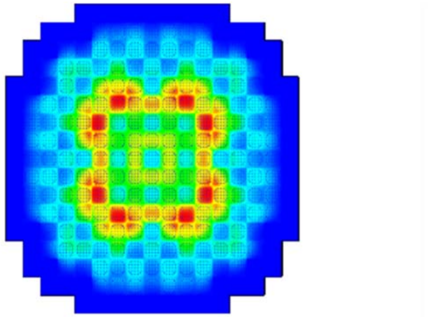
How to Validate the Pin-by-Pin Deterministic Solutions?

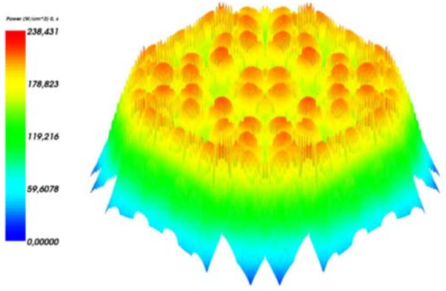
Motivation:
Validation of Numerical codes used in Industry and Licensing

- Diffusion + Pin Power Re-construction (PPR)



DYN3D-PPR: **NURISP PWR Boron Dilution Benchmark**

- SP3 Transport /Subchannel



DYNSUB5: **3D Pin Power Density [W/cm³]**

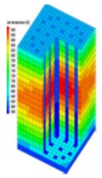
Advanced Deterministic Methods

Experimental Data

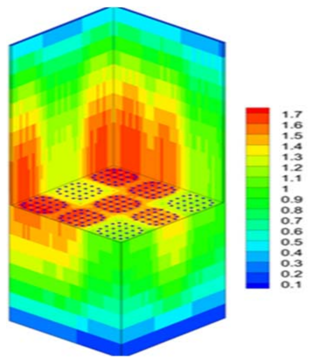
OR

Monte Carlo with TH feedback provide reference solutions

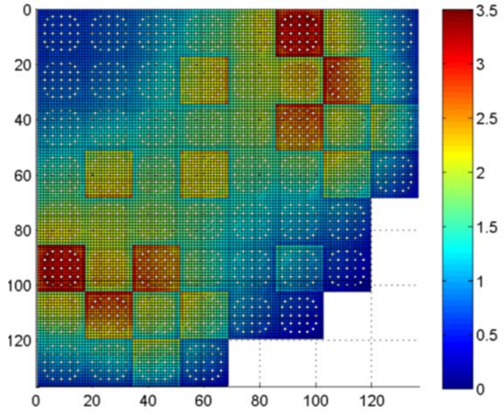
Code-to-code benchmarking



PWR FA



PWR 3x3 FA Cluster



PWR ¼ Core (56 FAs)

MCNP5/SUBCHANFLOW:
High Fidelity Simulations at pin level

KIT High-Fidelity Coupled codes based on MC-solvers for pin-level solution of full PWR cores:

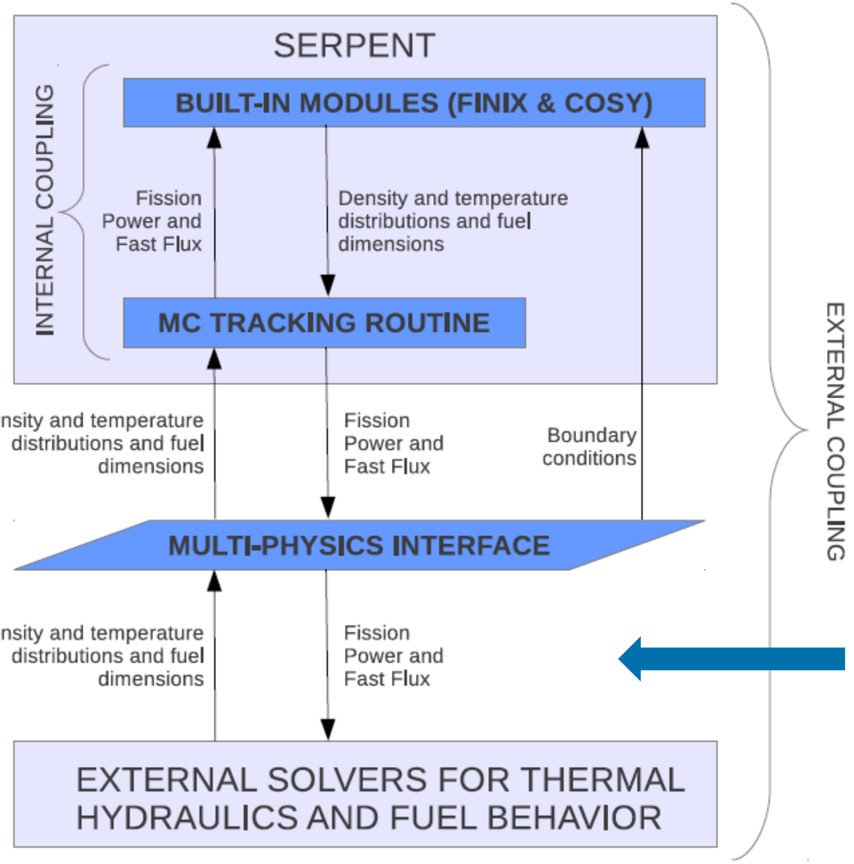
- **Internal coupling of MCNP5/SUBCHANLOW**

- Internal coupling of SERPENT2/SUBCHANFLOW

Internal Serpent2/SUBCHANFLOW coupling

Data exchange via memory

SUBCHANFLOW



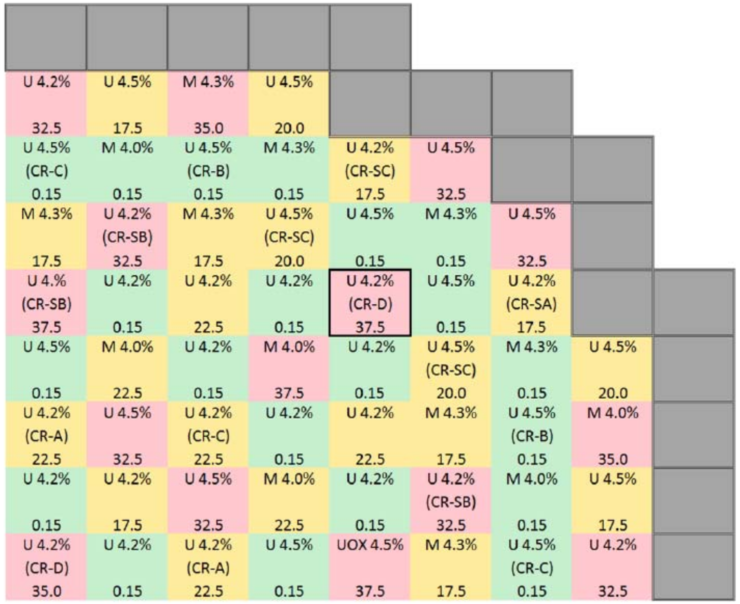
ASCII file I/O

M. Daeubler, B. L. Sjenitzer, A. Ivanov, V. Sanchez, R. Stieglitz und R. Macian-Juan, „High-fidelity coupled Monte Carlo neutron transport and thermal-hydraulic simulations using Serpent 2/SUBCHANFLOW," *Annals of Nuclear Energy*, pp. 352-375, 2015.

PhD: M. Däubler

Serpent2/SCF:
High fidelity Simulation of the HFP PWR MOX/UOX Core (1/2)

Channel and sub-channel TH model of OECD NEA and U.S. NRC PWR MOX/UO2 core transient benchmark



U 4.2% 32.5	U 4.5% 17.5	M 4.3% 35.0	U 4.5% 20.0					
U 4.5% (CR-C) 0.15	M 4.0% 0.15	U 4.5% (CR-B) 0.15	M 4.3% 0.15	U 4.2% (CR-SC) 17.5	U 4.5% 32.5			
M 4.3% 17.5	U 4.2% (CR-SB) 32.5	M 4.3% 17.5	U 4.5% (CR-SC) 20.0	U 4.5% 0.15	M 4.3% 0.15	U 4.5% 32.5		
U 4.% (CR-SB) 37.5	U 4.2% 0.15	U 4.2% 22.5	U 4.2% 0.15	U 4.2% (CR-D) 37.5	U 4.5% 0.15	U 4.2% (CR-SA) 17.5		
U 4.5% 0.15	M 4.0% 22.5	U 4.2% 0.15	M 4.0% 37.5	U 4.2% 0.15	U 4.5% (CR-SC) 20.0	M 4.3% 0.15	U 4.5% 20.0	
U 4.2% (CR-A) 22.5	U 4.5% 32.5	U 4.2% (CR-C) 22.5	U 4.2% 0.15	U 4.2% 22.5	M 4.3% 17.5	U 4.5% (CR-B) 0.15	M 4.0% 35.0	
U 4.2% 0.15	U 4.2% 17.5	U 4.5% 32.5	M 4.0% 22.5	U 4.2% 0.15	U 4.2% (CR-SB) 32.5	M 4.0% 0.15	U 4.5% 17.5	
U 4.2% (CR-D) 35.0	U 4.2% 0.15	U 4.2% (CR-A) 22.5	U 4.5% 0.15	UOX 4.5% 37.5	M 4.3% 17.5	U 4.5% (CR-C) 0.15	U 4.2% 32.5	

Quantity	Value
Power	3565 MW
Core mass flow rate	15849.4 kg/s
Inlet pressure	15.5 MPa
Coolant inlet temperature	560 K

Core Thermal hydraulics:

- 193 subchannels
- 20 axial levels

Core model at subchannel level:

- Neutronics nodes: 55777 pins and guide tubes
- Thermal hydraulics: 35 axial levels, 62532 sub channels
  Fluid: 2.2 M cells, Solid: 23.4 M
- Solution approach: Pin-by-pin solution

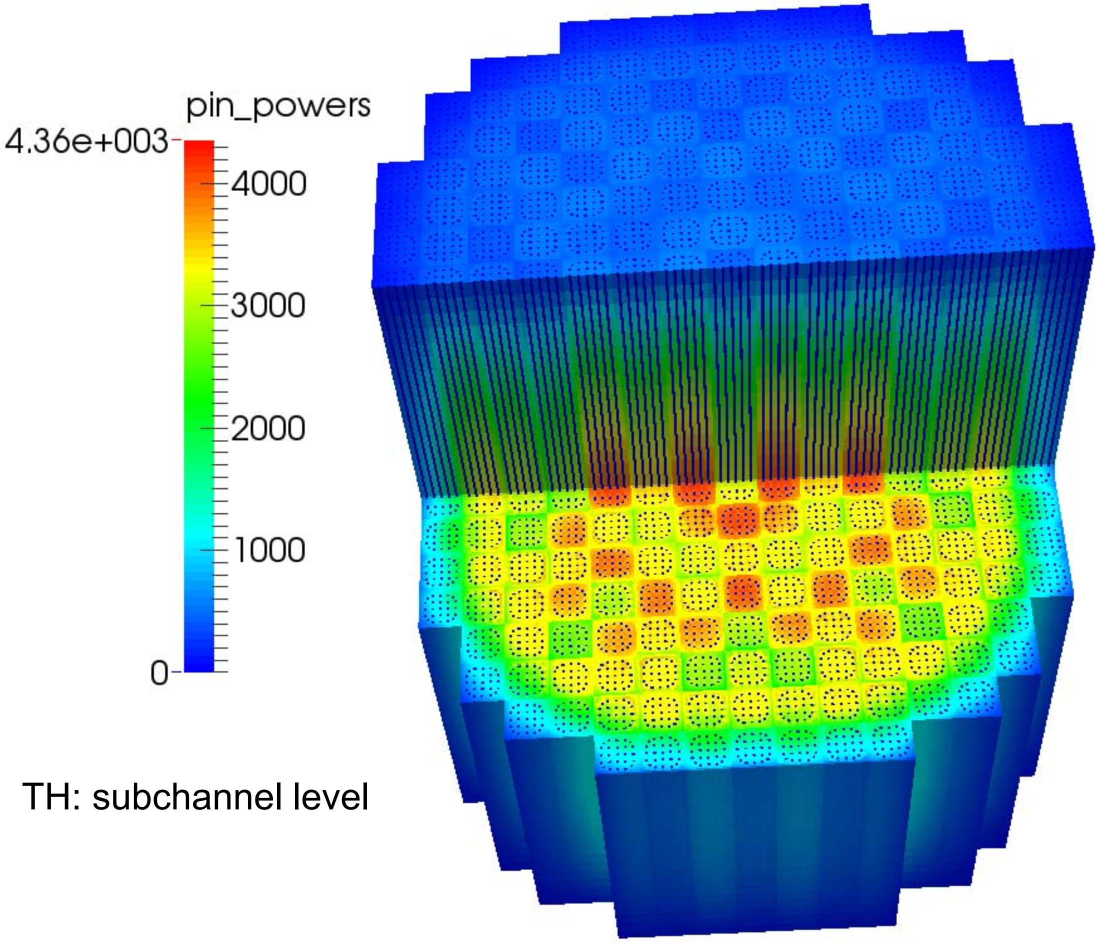
Per iteration step:

- 4 E6 neutrons per cycle
- 650/2500 inactive/active cycles

Convergence criteria:

- T-Doppler and M-density= < 0.5 %

Serpent2/SCF:
High fidelity Simulation of the HFP PWR MOX/UOX Core (2/2)



TH: subchannel level

SSS2/SCF: 3D Power Distribution

5M neutrons per cycle, 2000 active cycles per iteration

- **SSS2/SCF Subchannel level: 5.8 CPU years at KIT IC2 HPC Cluster:**
  - **Intel Xeon E5-2670, InfiniBand**

- **KIT IC2 HPC: 16 to 2048 cores (1 to 128 nodes)**
- **5.8 CPU-Y= 5.8 x 365 d / 2048 = 1.03 days**

KIT IC2: one node of 16 cores: 64 GB memory

PhD: M. Däubler

Validation of high-fidelity solvers

Serpent2/SCF Validation

Code-to-code comparison

- OECD NEA/ US NRC PWR MOX/UOX REA Core Transient Benchmark (ss conditions)

Code-to-data comparison

- Experiments like VENUS 1 and 2 critical experiments

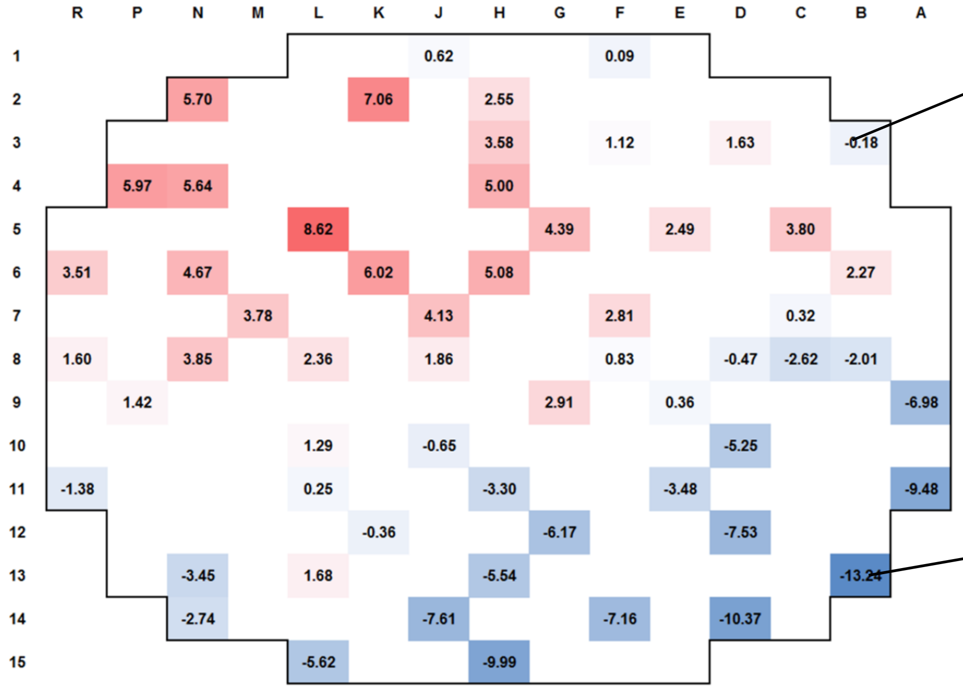
- MIT BEAVRS benchmark
  - HZP physics test
  - HP measurements at 18 days (693 MWth) after BOL

- SPERT III E steady state conditions

SERPENT2/SCF Validation

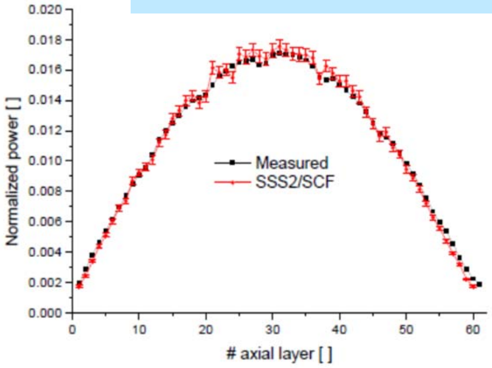
MIT BEAVRS benchmark

- HZP physics test
- HP measurements at 18 days (693 MWth) after BOL

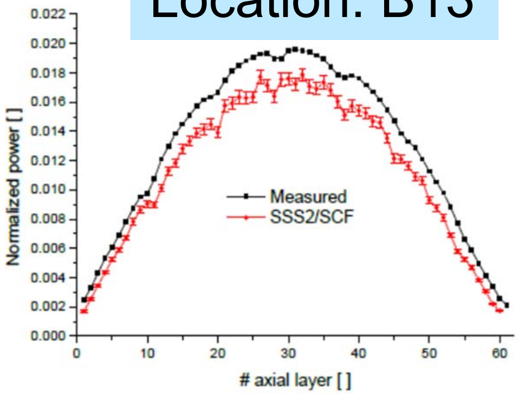


	R	P	N	M	L	K	J	H	G	F	E	D	C	B	A
1							0.62			0.09					
2			5.70			7.06		2.55							
3								3.58		1.12		1.63		-0.18	
4		5.97	5.64					5.00							
5					8.62				4.39		2.49		3.80		
6	3.51		4.67			6.02		5.08						2.27	
7				3.78			4.13			2.81			0.32		
8	1.60		3.85		2.36		1.86			0.83		-0.47	-2.62	-2.01	
9		1.42							2.91		0.36				-6.98
10					1.29		-0.65					-5.25			
11	-1.38				0.25			-3.30			-3.48				-9.48
12						-0.36			-6.17			-7.53			
13			-3.45		1.68			-5.54						-13.24	
14			-2.74				-7.61			-7.16		-10.37			
15					-5.62			-9.99							

Location: B03



Location: B13



PhD: M. Däubler

M. Daeubler, L. Mercatali, V. Sanchez, R. Stieglitz und R. Macian-Juan, „Validation of the Serpent 2-DYNSUB code sequence using the Special Power Excursion Reactor Test III (SPERT III),“ p. Submittet to ANE for publication, 2015.

Final Conclusions and Outlook

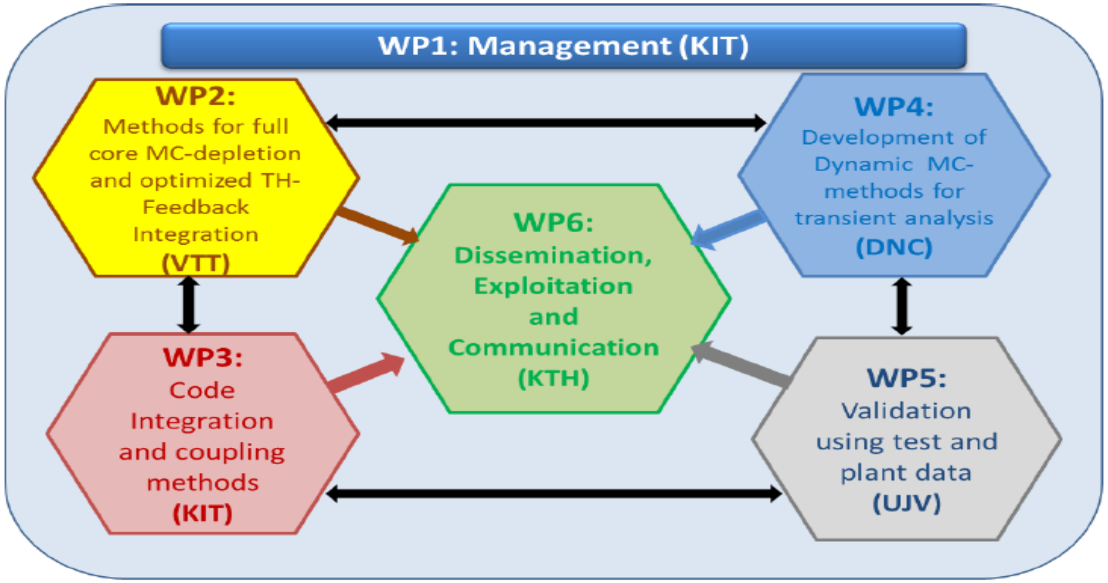
Conclusions:

- Numerical simulation tools for safety evaluations undergo continuous developments and must correspond to the state-of-the-art
- Need to move towards the increase of the spatial and energy resolution is recognized
- Advances in computer power paves the ways for high fidelity simulations and full use of big HPC-clusters now available

Outlook:

- New powerful full transport solvers based on PN, SN and MOC are under development e.g. SCOPE2, nTRACER, MPACT
- Development of dynamic Monte Carlo codes (prompt and delayed neutrons, control rod movements) strong competitors of classical deterministic codes safety-related applications (long term)
  - **EU H2020 McSAFE Project (KIT Coordinator): 2017- 2020**

McSAFE:
High Performance Monte Carlo Methods for SAFEty Demonstration



WP1: Management (KIT)

WP2: Methods for full core MC-depletion and optimized TH-Feedback Integration **(VTT)**

WP3: Code Integration and coupling methods **(KIT)**

WP4: Development of Dynamic MC-methods for transient analysis **(DNC)**

WP5: Validation using test and plant data **(UJV)**

WP6: Dissemination, Exploitation and Communication **(KTH)**

EU H2020 McSAFE (2017- 2020): coordinated by V. Sanchez (KIT)

More details in:
www.mcsafe-h2020.eu