Karlsruhe Institute of Technology

Reactor Physics and Dynamic Group (RPD)

KIT Multi-Physics Developments for Reactor Analysis

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Institute for Neutron Physics and Reactor Technology (INR)

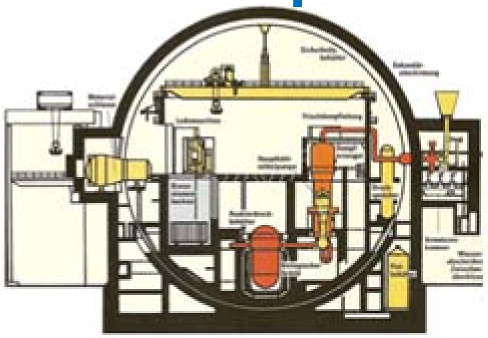
Content

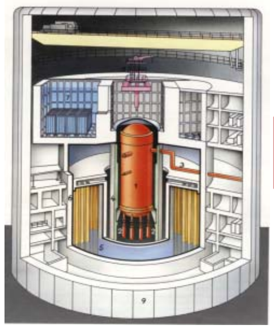
- Motivation
- KIT strategy for R&D
- Coupling of transport solvers with subchannel codes
- How to validate pin-by-pin deterministic solutions?
- Coupling of Monte Carlo with subchannel codes
- Validation of high fidelity codes
- Summary and Outlook

Motivation- Development of Reactor Technology

Gen- II LWR:

PWR Konvoi

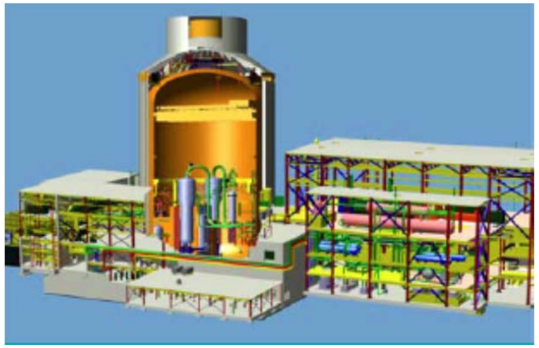




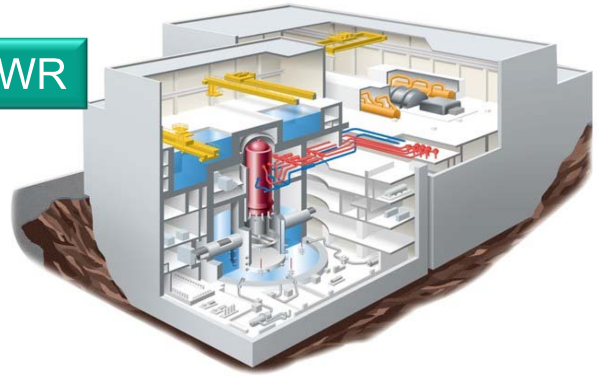
BWR Type-72

Gen- III LWR:

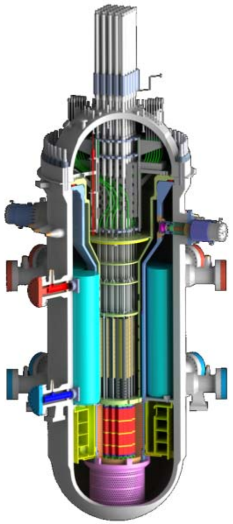
AP-1000



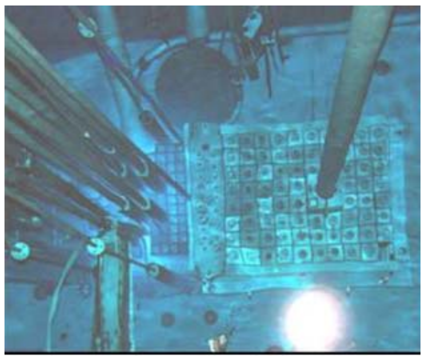
ABWR



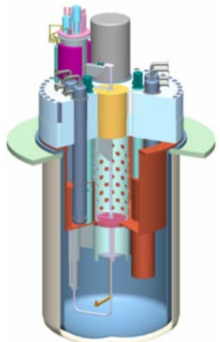
Gen-IV:



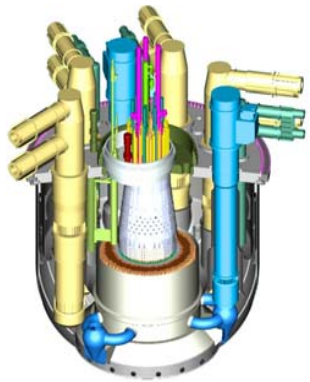
SMR SMART



MTR
Research Reactors



LFR (ADS)

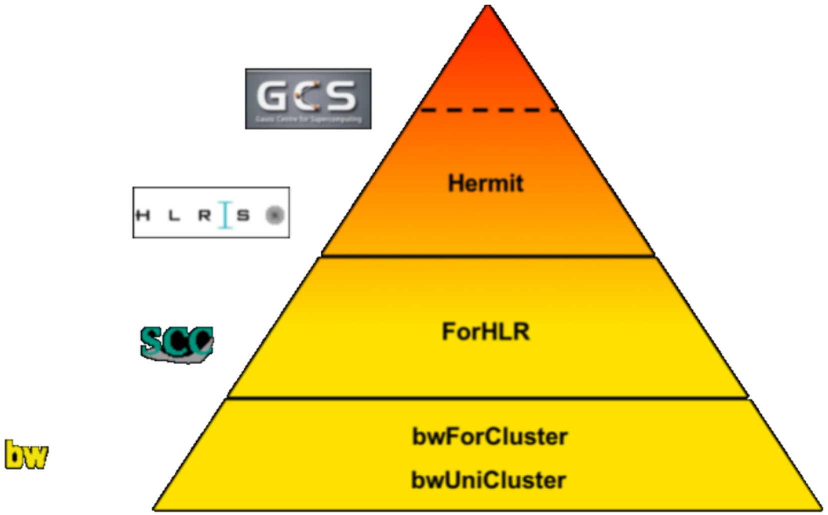


SFR

Motivation-
Increasing Cheap and Powerful Computer Clusters

Karlsruhe Institute of Technology

- **PRACE: Partnership for Advanced Computing in Europe**
  - Barcelona Supercomputing Center (Spain),
  - CINECA – Consorzio Interuniversitario (Italy)
  - EPCC at the University of Edinburgh (UK),
  - GCS Gauss Centre for Supercomputing (Germany)
  - Maison de la Simulation (France)
- **HPC computer Centers in state Baden Württemberg**



KIT HPC Infrastructure

bwUniCluster (bwHPC concept, Tier 3, BW Unis)

- 872 SMP-parallel nodes, 86 TB main memory, 444 TFLOPS peak power and Job with small number of processors

bwForCluster (4 Research HPC Clusters in BW)

- 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 astro physics

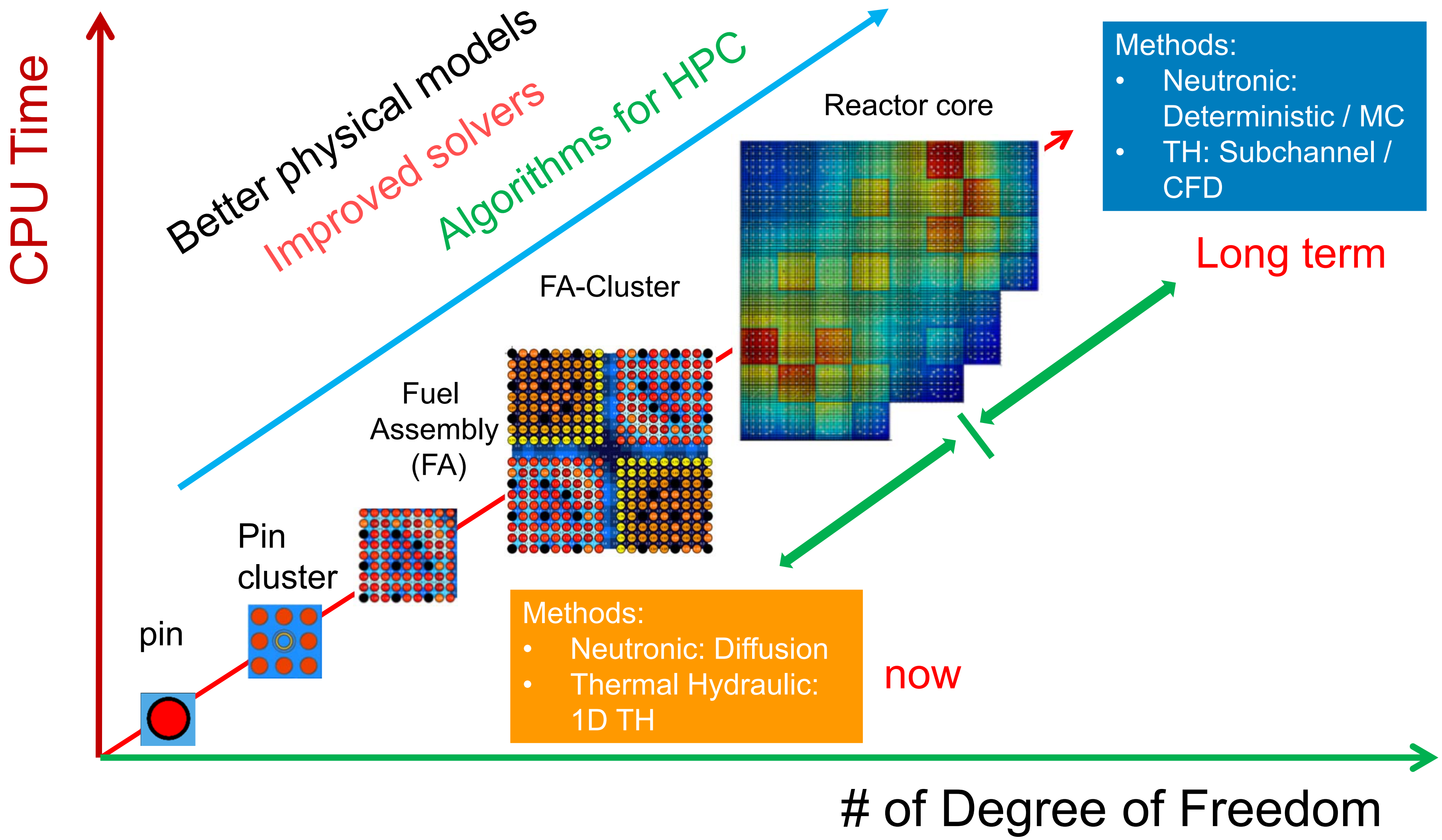
Research High Performance Computer ForHLR I and II (Trier 2)

- Phase I: applications with many thousands processors
- Phase II: applications with many hundred thousands processors (
  - Intel Xeon-processors, 1.2 PFLOPS power, 24 000 cores
  - KIT/INR: McSAFE Project: 100 000 CPUs

KIT SCC ForHLR I

KIT SCC ForHLR II

Motivation: Challenges for core Physics



KIT/INR
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.

Strategic Partnership with Key Players

- Industry partnership based on innovative research
- Regulators and TSO
- Research centers and universities (national, international)

Combination of In-house code development and use of external numerical tools

Make use of HPC and development of algorithms

KIT/INR Research Topics (Examples)

Selected research directions:

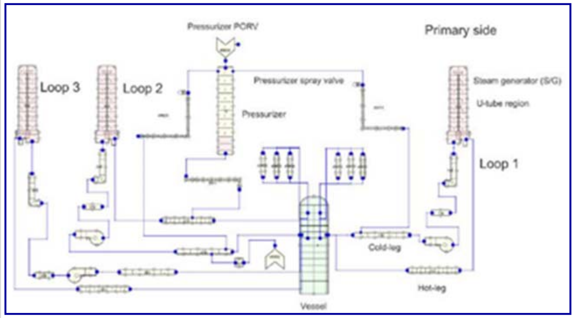
- Code development /extensions for improved core analysis including neutronics, thermal hydraulics, thermo-mechanics, chemo-physical phenomena important for DBA and SEVERE ACCIDENTS
- Extend and improve prediction capability by multi-physics and multi-scale approaches for DBA analysis
- Development and validation of SEVERE ACCIDENT codes
  - SAM-optimization for BWR and PWR
- Uncertainty quantification of numerical safety analysis tools
- Verification, validation and application to different reactor types

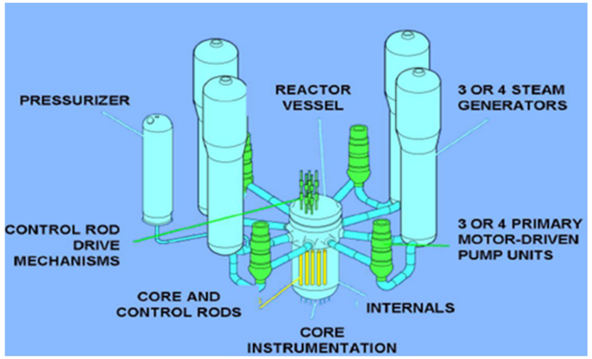
KIT Multi-Scale Thermal Hydraulic Coupling

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

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

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



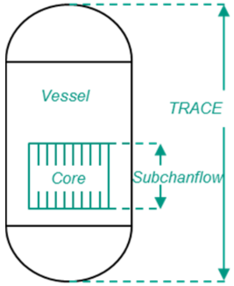


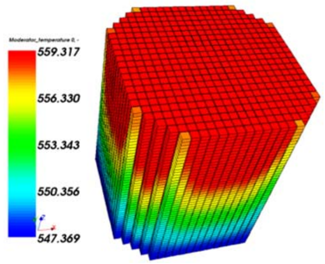
CFD Codes:

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

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

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

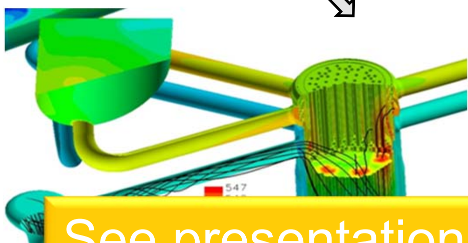




LOOPS:
- **TRACE, RELAP5**

Core N and TH:
- **TRACE/PARCS**
- **SCF/PARCS**

Blue:
CFD: DWC, LPLN, UPLN



See presentation of PhD K. Zhang

RPV except Core:
- **CFD**

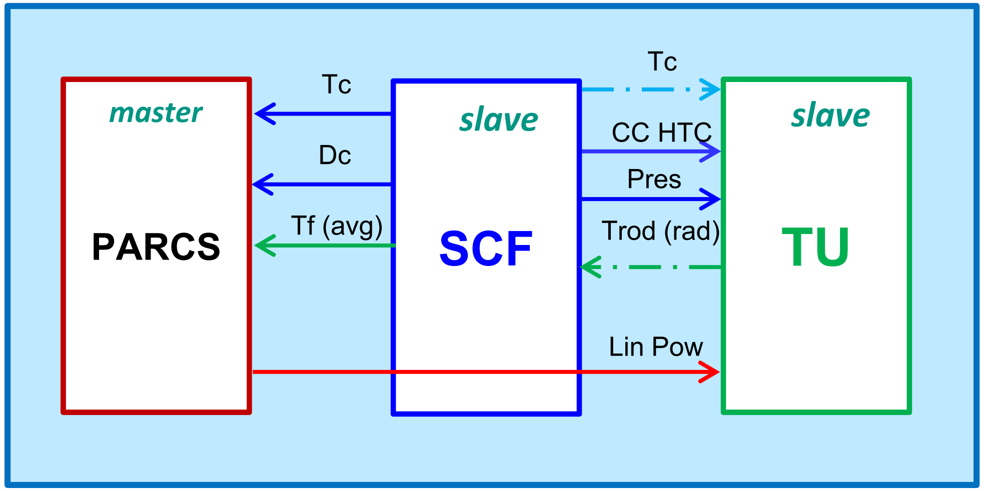
Core:
- **TRACE/PARCS**
- **SCF/PARCS**

Coupling of Neutronics-Thermal Hydraulics and Thermo- Mechanics

MPI-based
Coupling of 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

See presentation of PhD J. Basualdo

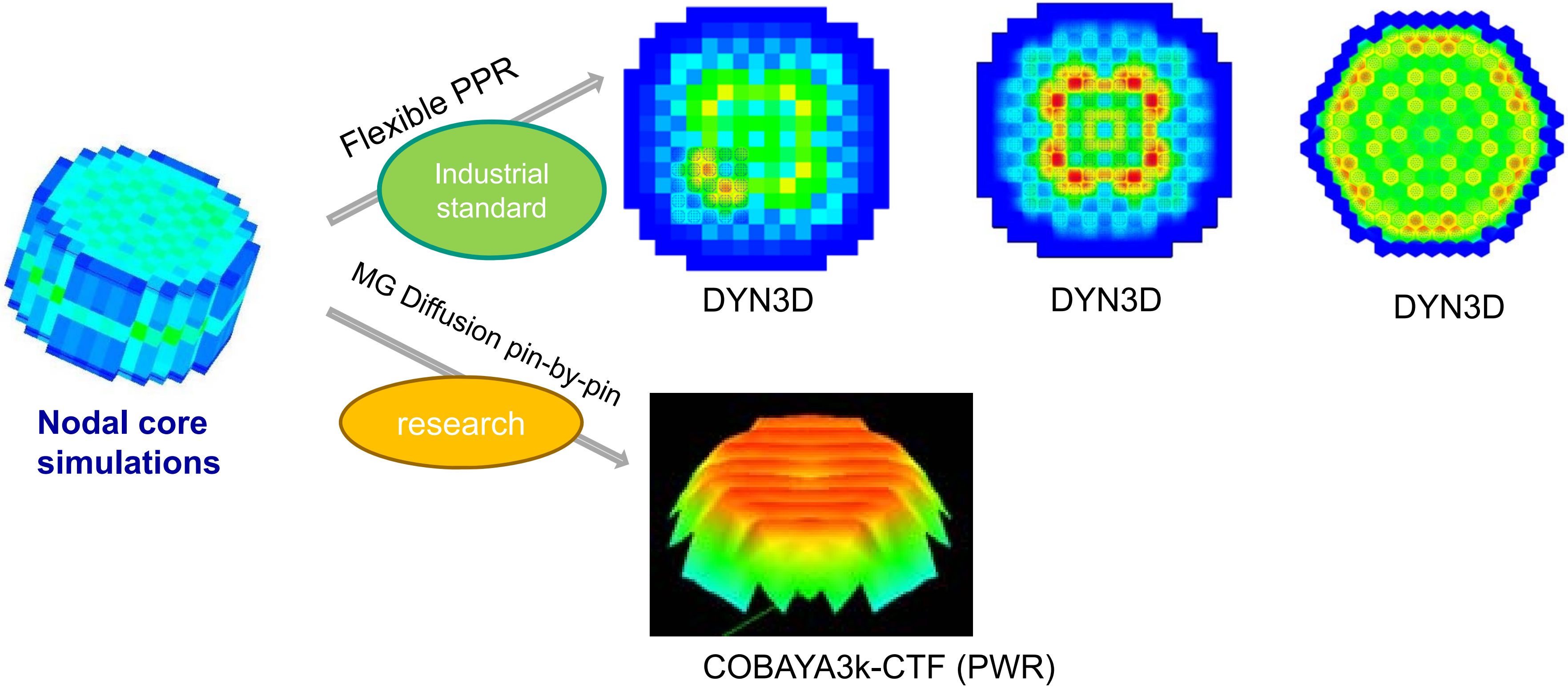
Coupling of Transport Solvers with subchannel codes

(DYNSUB5)

Motivation:
From industry standard to advanced N/TH core simulations

Best-estimate codes: based on nodal diffusion and coarse TH (1D, 3D)

- TRACE/PARCS, ATHLET/DYN3D, CATHARE/CRONOS2, etc.



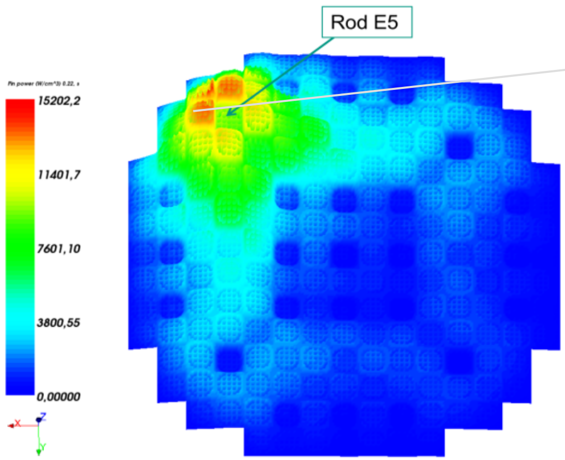
Next step: Advanced Neutronic /thermal hydraulic coupling:

- Replace nodal diffusion by **transport solvers (SP3)** and system TH by **SCF**: DYNSUB5

Pin-by-pin
DYNSUB5 Transient Analysis of the PWR MOX REA

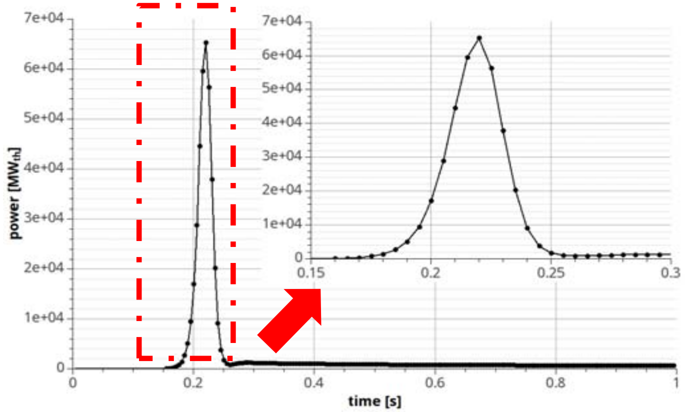
DYNSUB5 Analysis of PWR REA

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



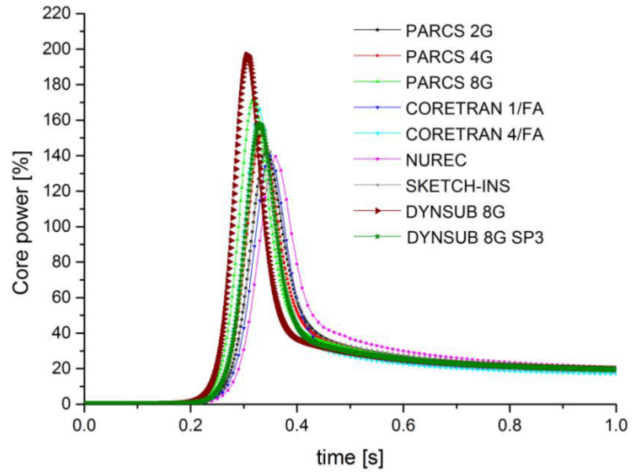
Highest power in fresh UOX

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 with experimental data needed



Code-to-code comparison: Nodal and SP3 Solutions

PhD: M. Däubler

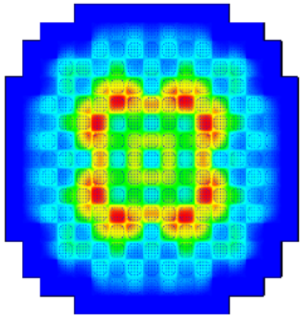
Run statistics:

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

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

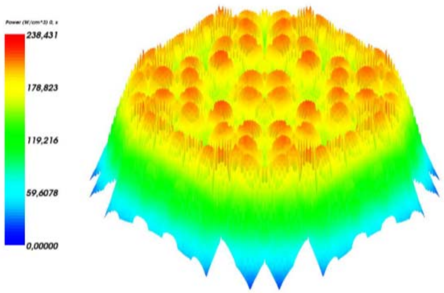
Motivation:
Validation of Numerical codes used in Industry and Licensing

- Diffusion + Pin Power Re-construction (PPR)



DYN3D-PPR: NURISP PWR Boron Dilution Benchmark

- SP3 Transport /Subchannel



DYNSUB5: 3D Pin Power Density [W/cm³]

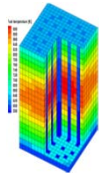
Advanced Deterministic Methods

Experimental Data

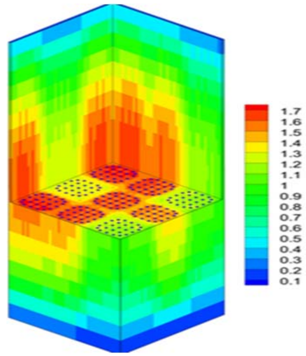
OR

Monte Carlo with TH feedback provide reference solutions

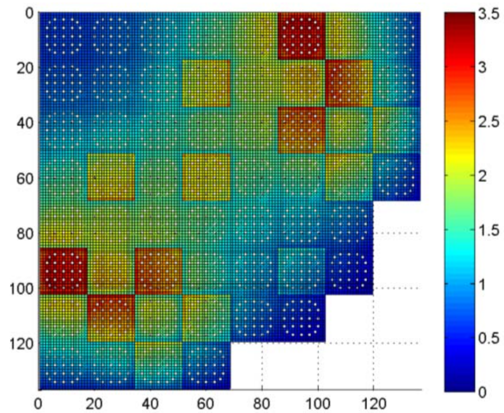
Code-to-code benchmarking



PWR FA



PWR 3x3 FA Cluster

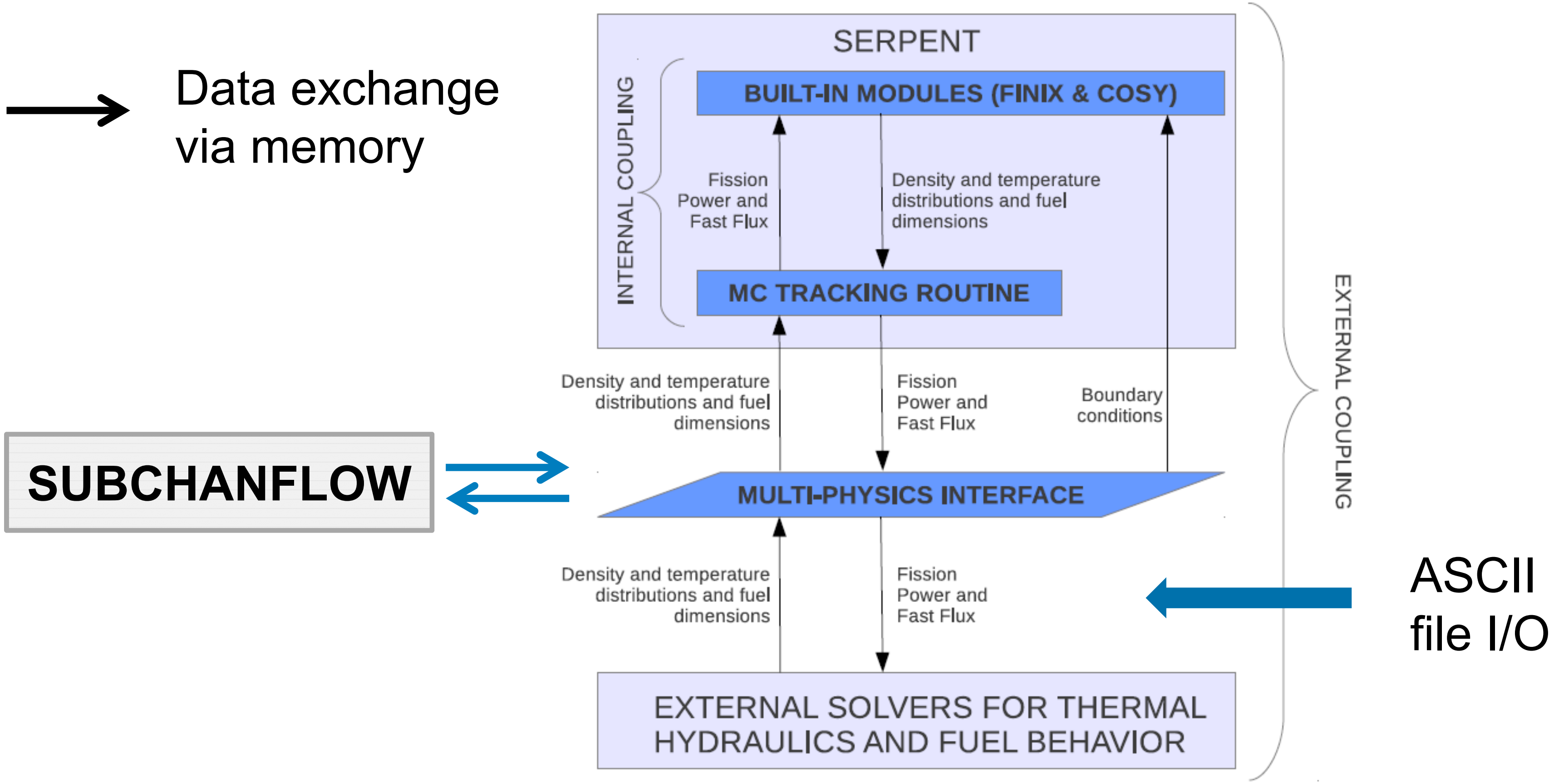


PWR ¼ Core (56 FAs)

MCNP5/SUBCHANFLOW: High Fidelity Simulations at pin level

- Internal coupling of MCNP5/SUBCHANLOW
- Internal coupling of SERPENT2/SUBCHANFLOW

Internal Serpent2/SUBCHANFLOW coupling



PhD: M. Däubler

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.

SERPENT2/SCF Coupling: Main Features

Feedback treatment: same as original SERPENT

Fuel temperature:

- Predicted by SUBCHANFLOW (Cartesian mesh-based)
- TMS is not applicable to thermal bound scattering (S(α,β) thermal scattering data) and unresolved resonances probability table sampling
  - New approach to treat thermal bound scattering: Automatically fall back of SERPENT to stochastic mixing where TMS is not applicable

Moderator density:

- Predicted by SUBCHANFLOW and passed to MC tracking routine via multi-physics interface
- Methods to pass density to MC tracking routine: Cartesian mesh-based, point-wise and user-defined functional distribution

Internal coupling

- Automatic generation of geometry tables for TH solver (SCF) assuring appropriate mapping between N and TH
- Relaxation scheme based on Stochastic Implicit Euler method (J. Dufek)
- Convergence criteria based on l^2-norm (Euclidean Norm) for feedbacks (Doppler or moderator density)

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

Karlsruhe Institute of Technology

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:

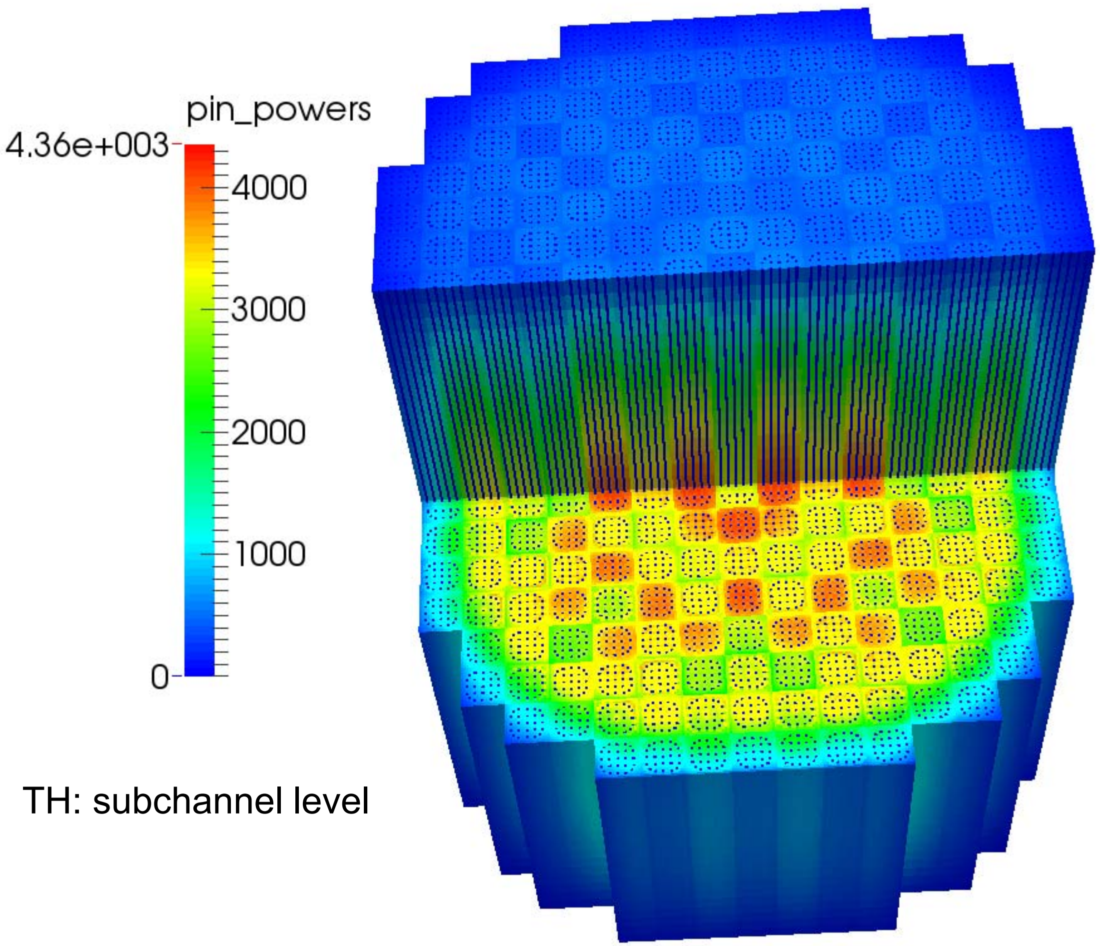
- 4 E6 neutrons per cycle
- 650/2500 inactive/active cycles

Convergence criteria:

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

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

5M neutrons per cycle, 2000 active cycles per iteration



TH: subchannel level

SSS2/SCF: 3D Power Distribution

- **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

How to make sure that MC/TH solutions are accurate?

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

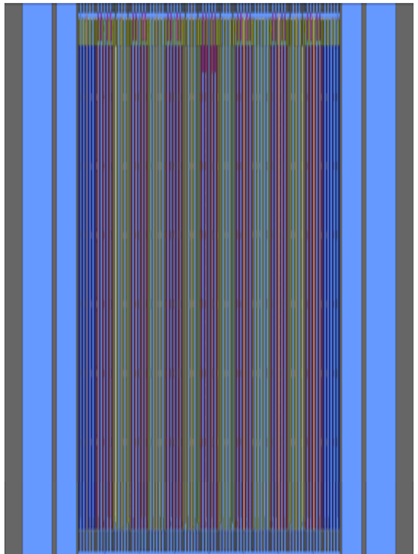
- MIT BEAVRS benchmark
  - HZP physics test
  - HP measurements at 18 days (693 MWth) after BOL

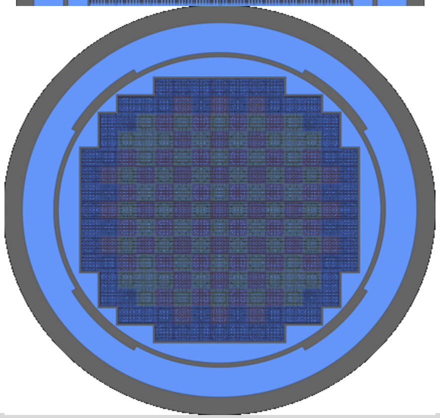
- SPERT III E steady state conditions

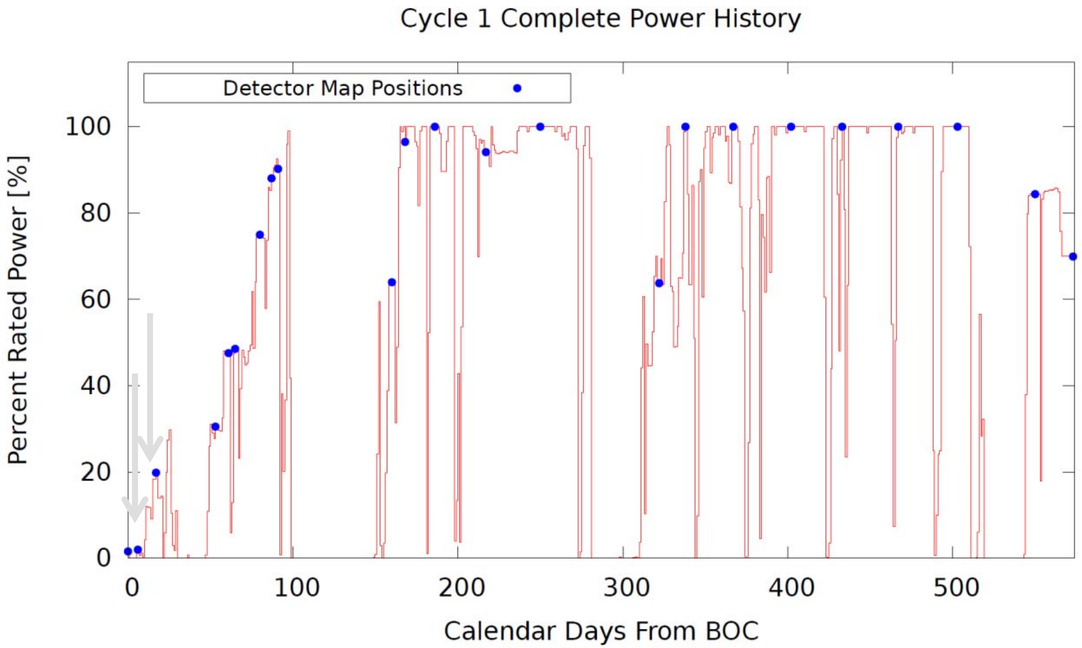
PWR BEAVRS Cycle 1

HZP physics tests (25 MWth)

HP measurements at 18 calendar days (692.7 MWth) after BOL







BEAVRS Cycle 1: power history

SERPENT2/SCF Validation

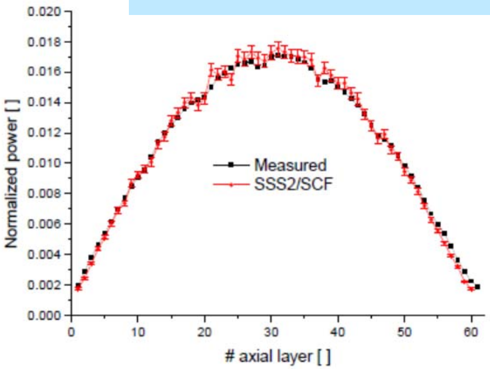
Karlsruhe Institute of Technology

MIT BEAVRS benchmark

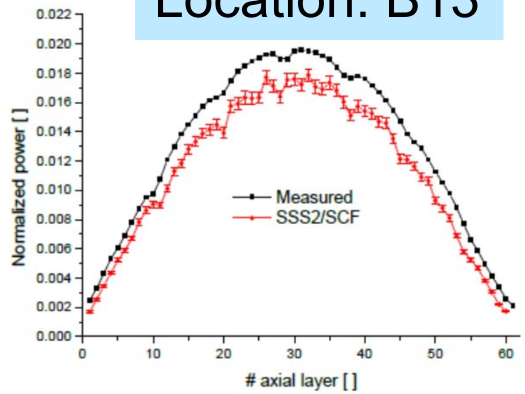
- HZP physics test
- HP measurements at 18 days (693 MWth) after BOL

	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:

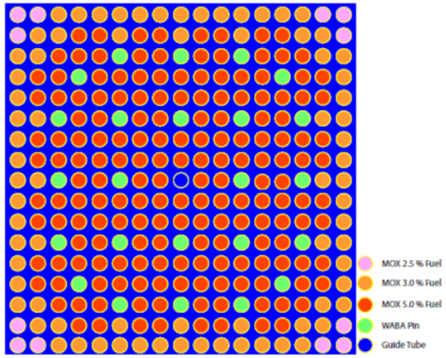
- Numerical simulation tools for safety evaluations undergo continuous developments and must correspond to the state-of-the-art
- Need to move towards the increase of the spatial and energy resolution is recognized
- Advances in computer power paves the ways for high fidelity simulations and full use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

Outlook:

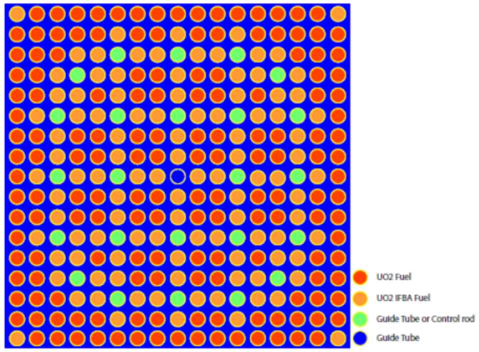
- New powerful full transport solvers based on PN, SN and MOC are under development e.g. SCOPE2, nTRACER, MPACT
- Development of dynamic Monte Carlo codes (prompt and delayed neutrons, control rod movements) strong competitors of classical deterministic codes safety-related applications (long term)
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

Outlook: Dynamic MC/TH: REA Analysis (PWR 3x3 Minicore)

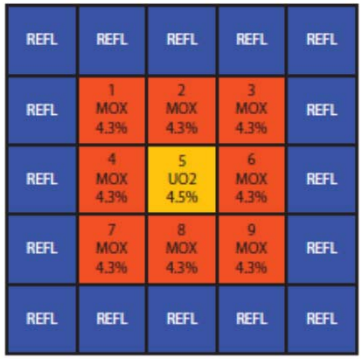
Boundary conditions HFP	
Core Power	100MW
Mass flow rate (core)	739.08 kg/s
Mass flow rate (FA)	82.12 kg/s
Core Outlet pressure	15.40 Mpa
Coolant inlet temperature	560 K
Boron concentration	200 ppm (nuclide density)
Insertion depth control rods	0.0 cm
Boundary conditions HZP	
Core Power	1 W
Mass flow rate (core)	739.08 kg/s
Mass flow rate (FA)	82.12 kg/s
Core Outlet pressure	15.40 Mpa
Coolant inlet temperature	560 K
k_{eff} $(t = 0\ s)$	1.0000
Insertion depth control rods	232.433 cm
Scenario	CR ejection, linear speed fully out at 0.1 s



MOX FA



UOX FA

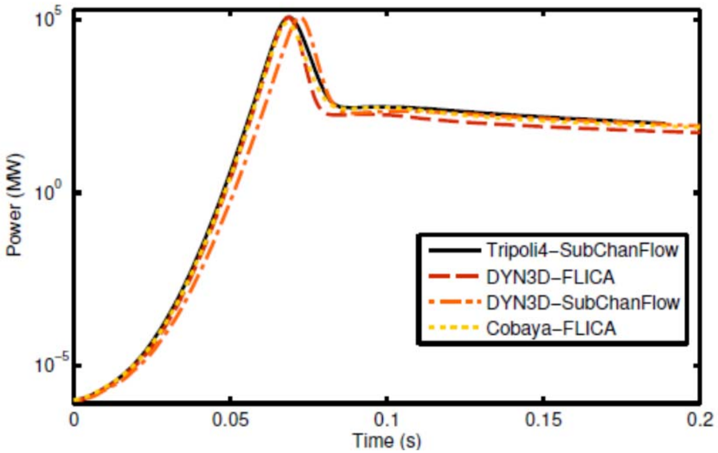


Minicore: 3x3 FA (UOX/MOX)

REA Scenario:

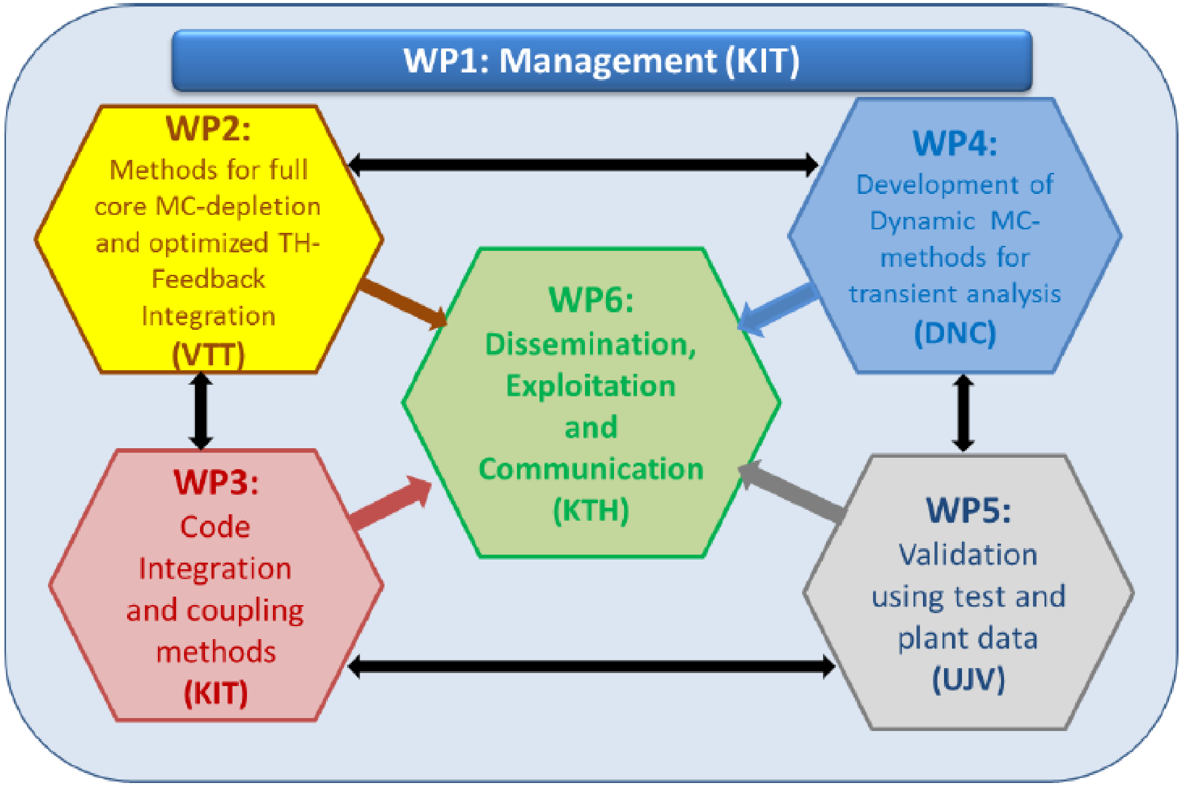
HZP Ejection of CR within 0.1 s

Bart L. Sjenitzer, J. Eduard Hoogenboom , Javier Jiménez Escalante , Victor Sanchez Espinoza; Coupling of dynamic Monte Carlo with thermal-hydraulic feedback. ANE 76 (2015)27-39.



Power evolution: comparison of MC/TH and NodalDiffusion/TH Codes

McSAFE:
High Performance Monte Carlo Methods for SAFEty Demonstration



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