OECD Multi-Physics Model Validation Workshop (MPMV-2)
GRS (Garching - GERMANY)
June 26-28, 2019

Advanced multi-physics modelling activities within the EU McSAFE Project

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Content

- ❑ Project motivation & goals
- ❑ Coupling approaches
- ❑ Results
- ❑ Summary

This project is funded by the Horizon 2020- Research and Innovation Framework Programme under the GA Nr.755097

Introduction and project motivation

- **Core analysis relies mainly on deterministic neutronic codes (daily work)**
  - Current approach include multiple approximations (homogenization, cross section data preparation, diffusion approximation)
  - Pin power approximately reconstructed from 2D lattice calculations
  - Pinwise SP_3 and S_N solvers are still under development (full parallel).
    - Serial solvers very time and memory expensive
    - Parallel versions under development

- **Experimental data at pin level is scarce and not easy to be measured (pin power)**
  - Insufficient data for code validation, evaluation of uncertainties

- **Alternative / supplementary option:**
  - Use of MC codes capable of simulating the neutron transport without approximations
  - Obtain reliable data for any core state at fuel pin level
  - Potential use taking advantage of HPC and parallelization

Innovative solutions needed to pave the way for industry-like applications

McSAFE – High Performance Monte Carlo Methods for Safety Demonstration

- **<u>McSAFE</u>** is based on innovative ideas developed within the EU 7th FP HPMC Project (High Performance Monte Carlo Core Analysis: 2011-2014)

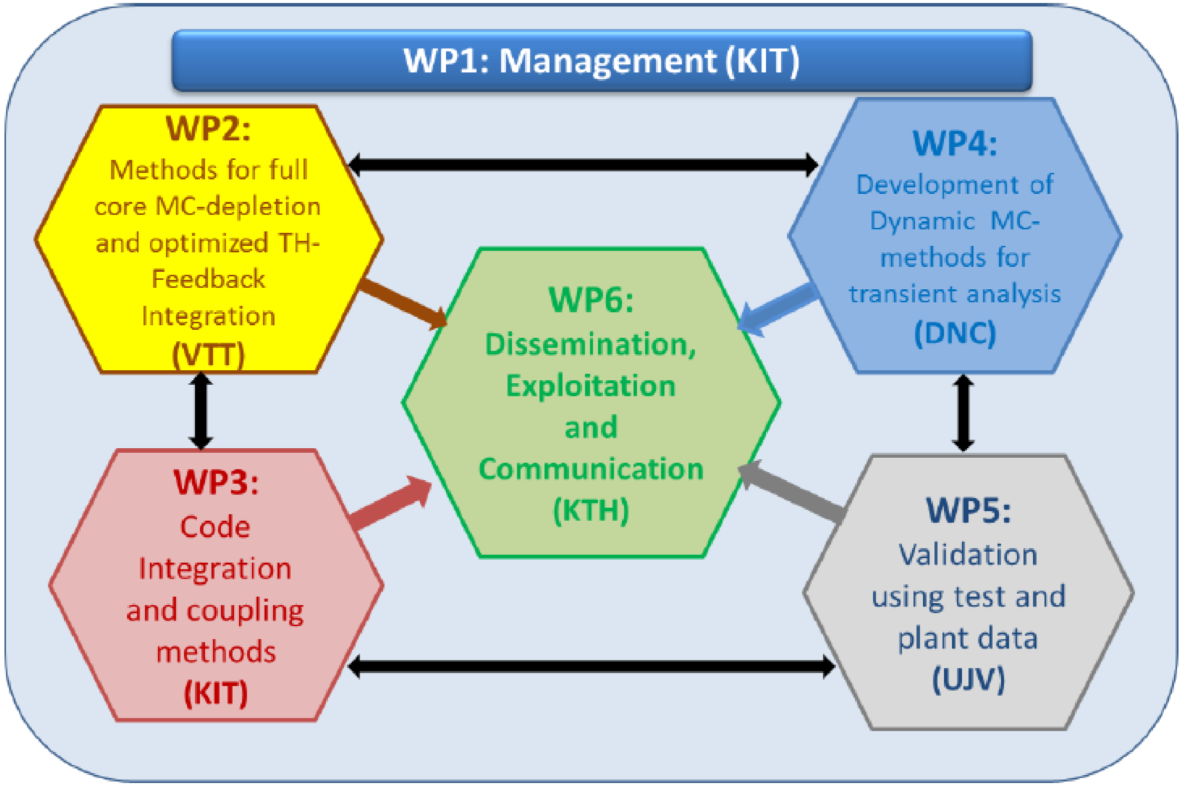
(Proof of concept)

- **<u>Goal</u>: move MC methods towards industrial applications**
  - **Generalize N/TH/TM coupling**
  - **Optimize depletion simulations (stability, CPU, memory requirements)**
  - **Enable analysis of transients such as RIA and others (Safety)**
  - **Validate MC tools using experimental data**
  - **Solve whole cores making use of HPC – provide reference solutions**

(Industry-like applications➔ McSAFE)

- **<u>Final scope</u>**: Move towards high fidelity multi-physics calculations using advanced codes and methodologies in order to perform NPP core level calculations including depletion and TH-feedback in a full scope approach (i.e. pin level)

McSAFE structure



McSAFE numerical tools and coupling approaches

- Focus on the further development of European MC, TH and TM codes on the coupled systems already developed during the HPMC project

Methods	Monte Carlo (MC)	Thermal-Hydraulic (TH)	Termo-Mechanics (TM)
Static MC (External coupling using NURESIM)	TRIPOLI SERPENT MONK	SCF SCF SCF	TRANSURANUS
Static MC (Internal Coupling)	SERPENT	SCF	TRANSURANUS
Dynamic MC-TH	DynTRIPOLI DynSERPENT DynMCNP	SCF SCF SCF	
Dynamic MC-TH-TM	DynTRIPOLI DynSERPENT	SCF, TRUST SCF	TRANSURANUS TRANSURANUS

Full-core MC-depletion and optimised thermal-hydraulic feedback integration

- **Topics:**
  - Improved algorithms for equilibrium Xe-135 calculation and stability of MC-Depletion codes
  - Methods for optimised cross-section look-up and memory utilisation in MC-codes
  - Further development of MC and MC-TH criticality calculations (e.g. variance reduction, acceleration of fission-source convergence, etc.)
  - Optimisation of internally coupled MC-TH codes to solve full-core problems.
  - Implementation of Cartesian/HEX-mesh of TH-parameter interpolation for pin-wise depletion
  - Testing the methods for PWR mini-core 3x3 FA and Small Modular Reactor (SMR) cores in a Monte Carlo performance benchmark

- **Tools:** MC-codes (mainly SERPENT) coupled with SCF
- **Testing and demonstration:** VVER mini-cores, PWR mini-cores, full cores

Full-core MC-depletion: screening of capabilities and limitations (1)

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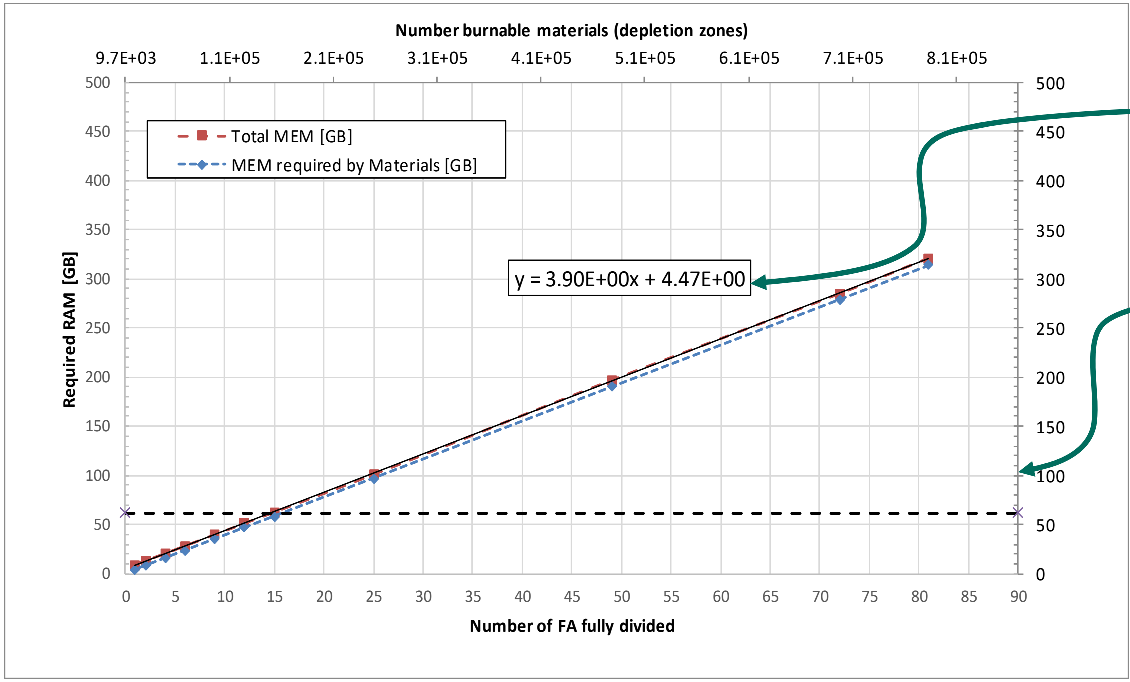
- These case was run in an ad-hoc node with up to 356GB RAM



~4GB for data and etc

Available RAM per node in FH2 HPC cluster ~64GB

→ RAM requirement increase linear with depletion zone → **~400kB per burn material**

→ **Maximum foreseen case in available HPC → 12FA**

→ **Big HPC have ~10GB per node !!!**

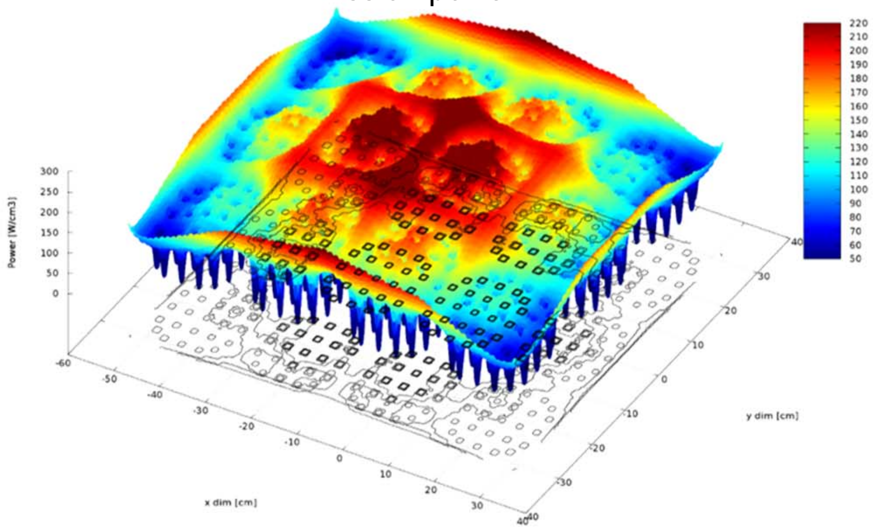
→ **Pin by pin full-core burnup leads to ~1TB** → not feasible or foreseen for a HPC in McSAFE

D. Ferraro et al.; "*Foreseen Capabilities, Bottlenecks Identification and Potential Limitations of SERPENT MC Transport Code in Large-Scale Full 3-d Burnup Calculation*", Proceedings of the ICONE-26 Conference (London, July 2018).

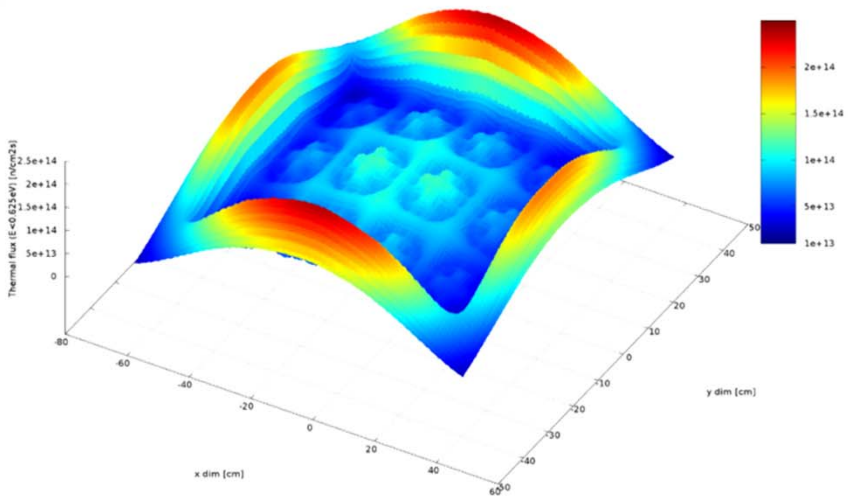
Full-core MC-depletion: screening of capabilities and limitations (2)

- Most demanding problem for FH2: 12 FAs array fully divided (~1e5 burnable zones)

Fission power



Thermal flux [E<0.625eV]



Parameter	Value	Comment
RAM memory (Total)	50.456 GB	Includes all. The node limit is 64GB. Additional memory is to be used by other codes in coupling
RAM memory (materials)	46.063 GB	Includes all
Running time @ 2.6 GHz CPU	~80e3 mins [1]	Per Iterator or corrector step
Running time @ 2.6 GHz CPU w/o IFC	~50e3 mins[1]	Per Iterator or corrector step
Calculation time overhead due to IFC	~60%	
Total active histories	2e9	2000 active cycles of 1e6 histories each

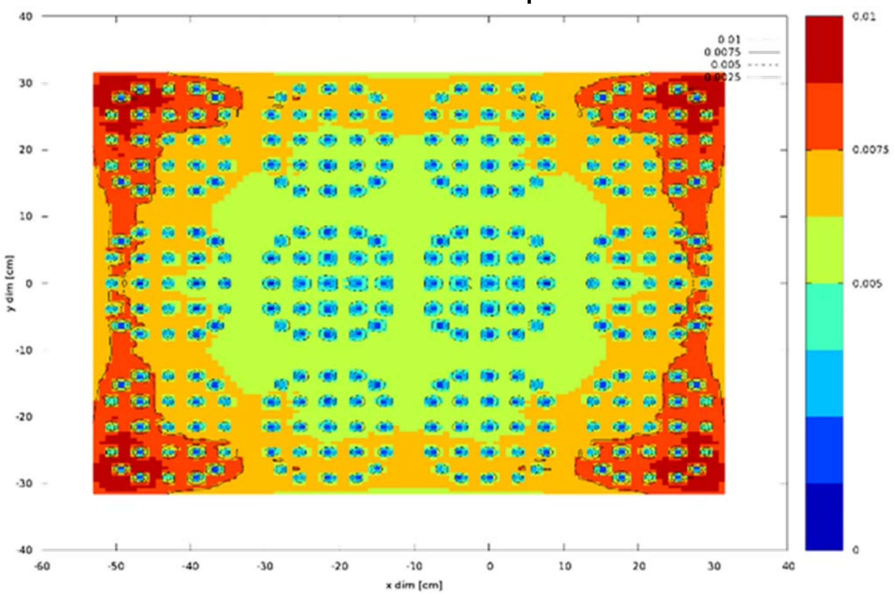
[1] 43200 mins ~1 month CPU

D. Ferraro et al.; "*Foreseen Capabilities, Bottlenecks Identification and Potential Limitations of SERPENT MC Transport Code in Large-Scale Full 3-d Burnup Calculation*", Proceedings of the ICONE-26 Conference (London, July 2018).

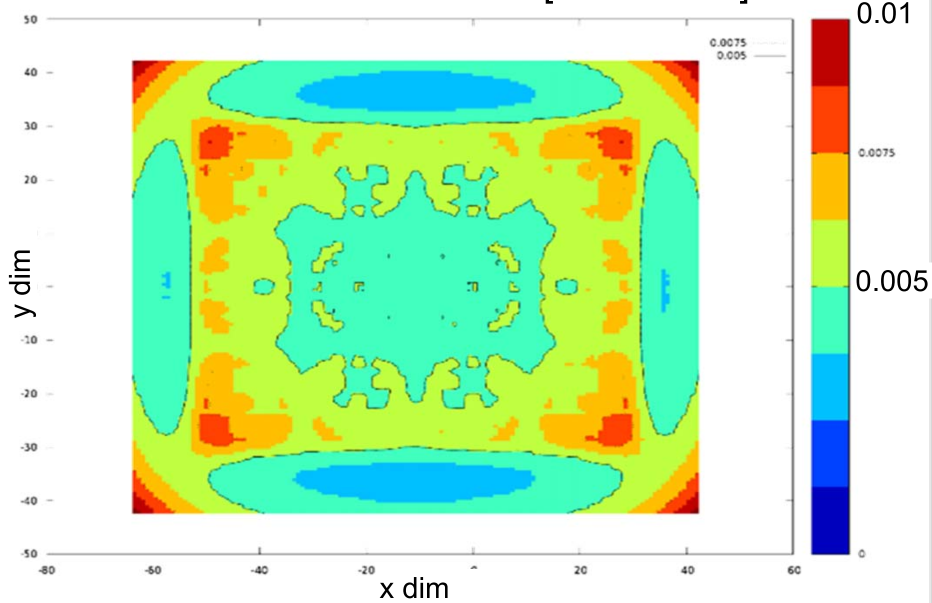
Full-core MC-depletion: screening of capabilities and limitations (3)

- Statistical convergence

Relative error Fission power



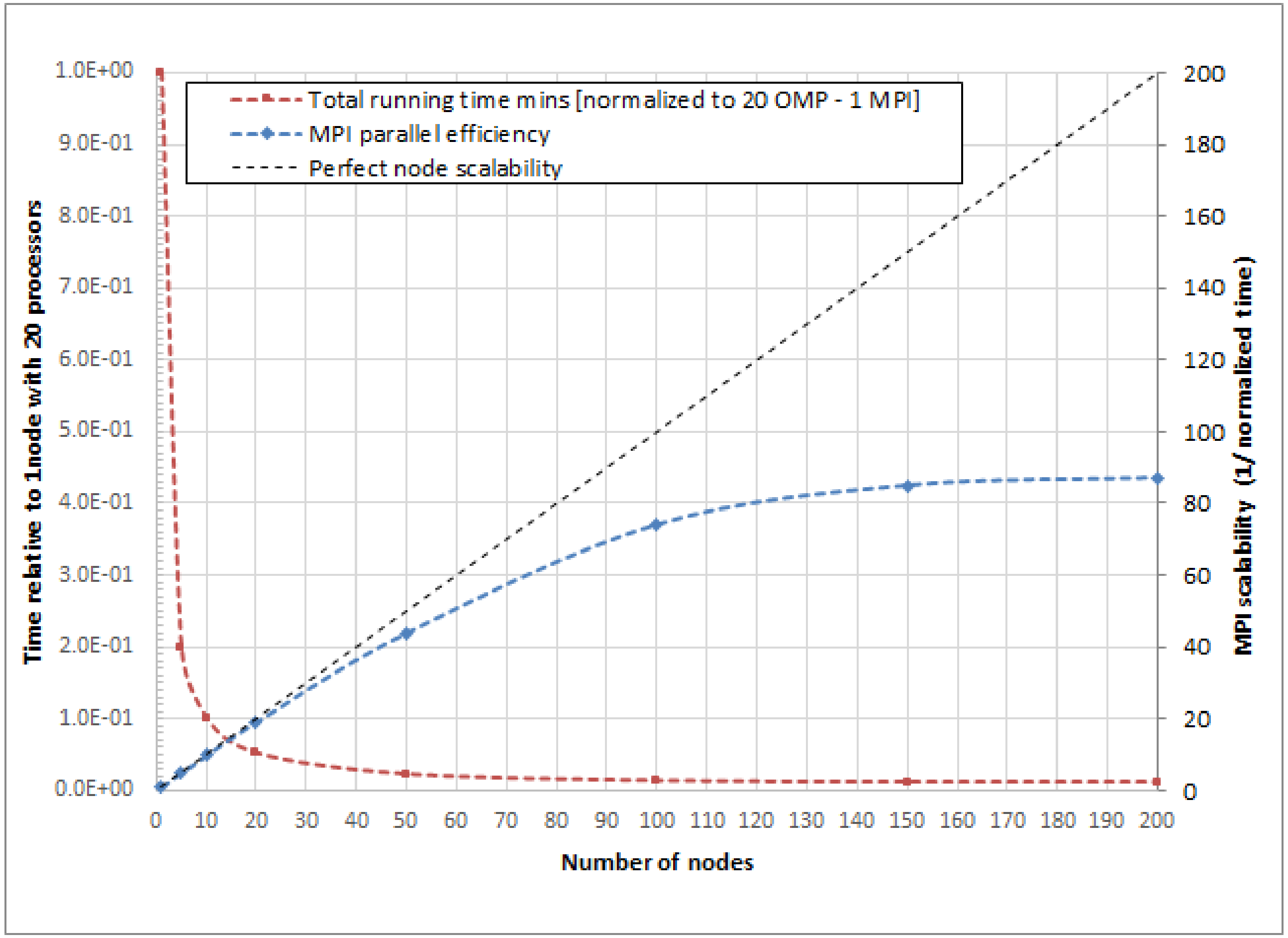
Relative error Thermal flux [E<0.625eV]



Parameter	Value			
	Max	Min	Average	Stdev
Effective multiplication factor statistical convergence	-	-	-	2.9e-5
Thermal flux detector (tally) statistical convergence	0.0723	0.0032	**0.0071**	0.0040
power flux detector (tally) statistical convergence	0.0260	0.0000	**0.0075**	0.0035

D. Ferraro et al.; “*Foreseen Capabilities, Bottlenecks Identification and Potential Limitations of SERPENT MC Transport Code in Large-Scale Full 3-d Burnup Calculation*”, Proceedings of the ICONE-26 Conference (London, July 2018).

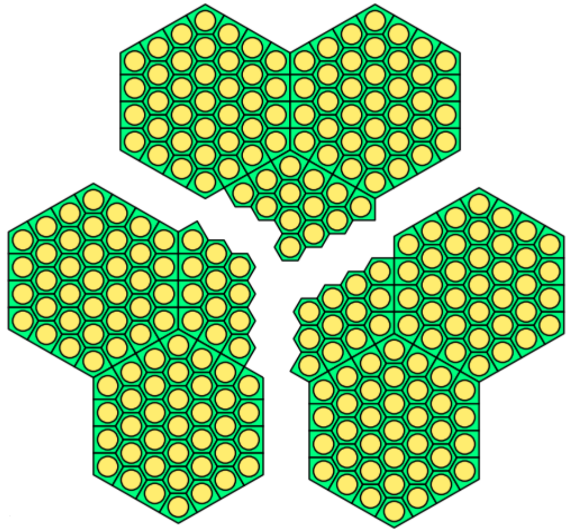
Full-core MC-depletion: scalability

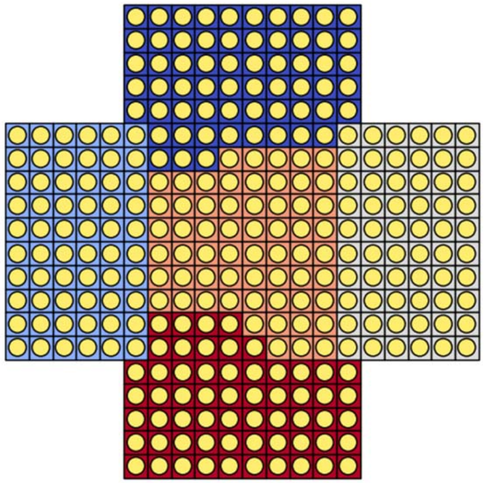


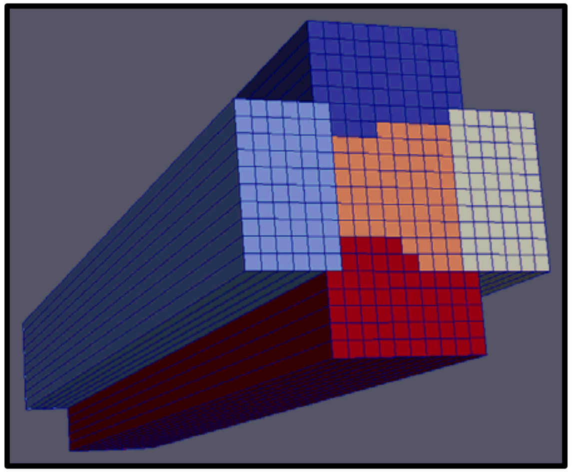
D. Ferraro et al.; "*Foreseen Capabilities, Bottlenecks Identification and Potential Limitations of SERPENT MC Transport Code in Large-Scale Full 3-d Burnup Calculation*", Proceedings of the ICONE-26 Conference (London, July 2018).

Spatial Domain Decomposition (SDD)

- **Distribution of the geometry across processes/nodes**
- **Memory scalability**
  - Tally data
  - Material data
- **Parallel execution**
  - Particles need to be communicated between domains
  - Material data
  - Burnup calculation automatically distributed







M. Garcia et al.; "*Development of a Spatial Domain Decomposition Scheme for Monte Carlo Neutron Transport*", Proceedings of the ICONE-26 Conference (London, July 2018).

Code integration and coupling methods

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- **Objectives:**
  - Support of codes integration in the NURESIM platform
  - Integration of TRIPOLI and MONK in SALOME and coupling with TH codes
    - standardised coupling based on ICoCo (MEDCoupling Library for domain mapping)
  - Integration of TRANSURANUS and coupling with coupled SERPENT-SCF code (MC-TH-TM)
    - standardised coupling based on ICoCo (MEDCoupling Library for domain mapping)
  - Adaptation of SERPENT/SCF coupling for PWR with HEX fuel assemblies including a SCF-pre-processor for HEX-mesh
  - Demonstration of the code capability using a benchmark problem or simplified test case e.g. SMR-cores, VVER-1000 Kalinin Benchmark (SS simulation)

- **Tools:** TRIPOLI/SCF, SERPENT/SCF/TU, MONK/SCF

- **Testing and demonstration:** VVER mini-cores, PWR mini-core, full cores

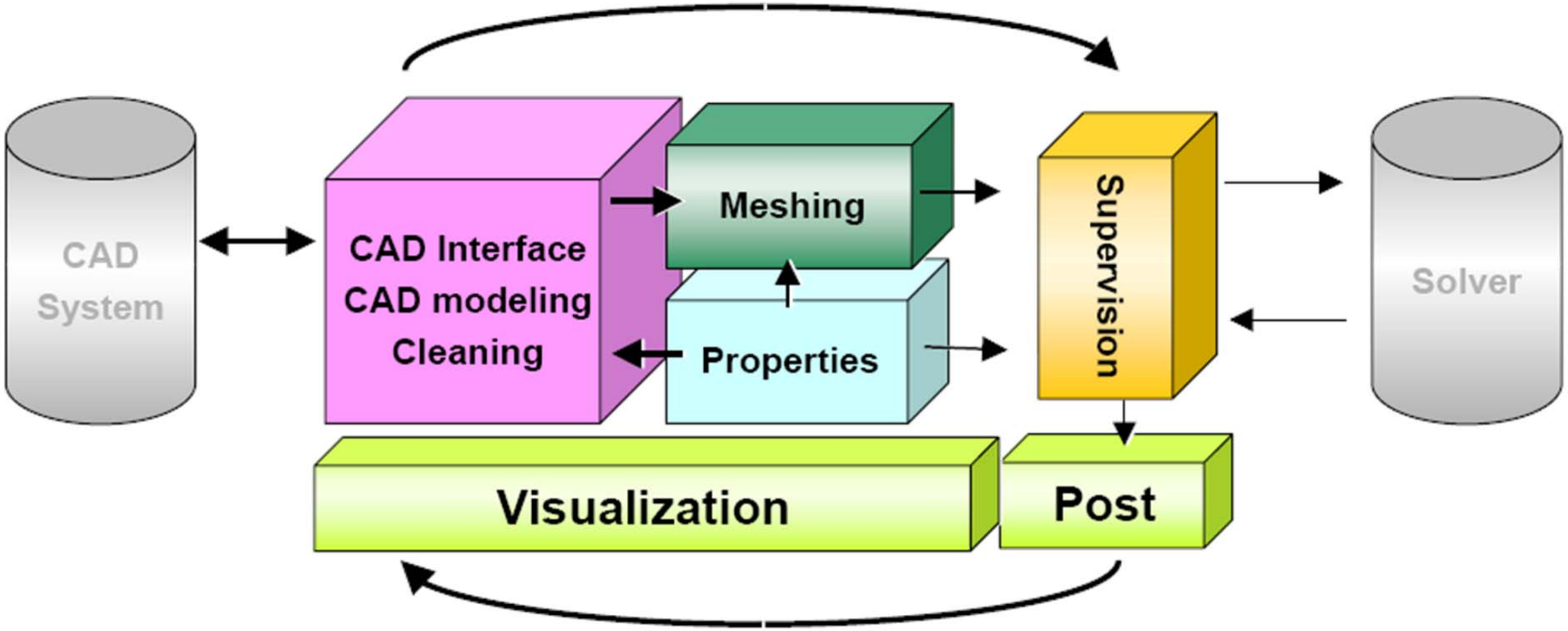
M. García et al. "Development of an Object-oriented Serpent2-SUBCHANFLOW Coupling and Verification with Problem 6 of the VERA Core Physics Benchmark" – M&C 2019

European NURESIM simulation platform

SALOME
The Open Source Integration Platform for Numerical Simulation

(v. 7.8.0)

Open Source Platform for multi-physics and multi-scale nuclear reactor simulations



New SERPENT/SCF internal coupling

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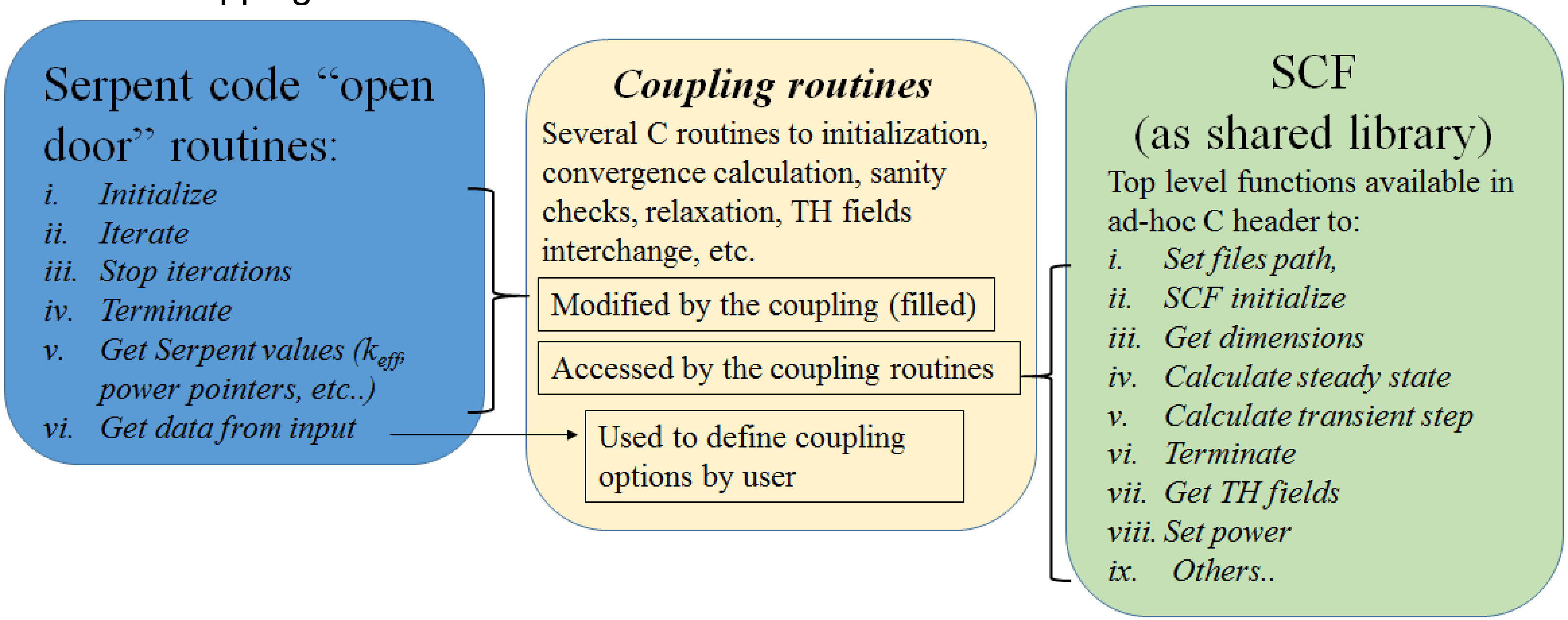
- The basics new implementation approach consists of:
  - SERPENT: several “open doors” functions
  - SCF: compilation as library (use of high level C interfaces)
  - Models of SCF are to be developed externally (with new SCF pre-processor)
  - All mapping with ad-hoc files



D. Ferraro et al.; “*Serpent/SUBCHANFLOW pin-by-pin coupled transient calculations for a PWR minicore*”, submitted for publication to ANE

Extension of the SSS2/SCF internal coupling to hexagonal geometries (1)

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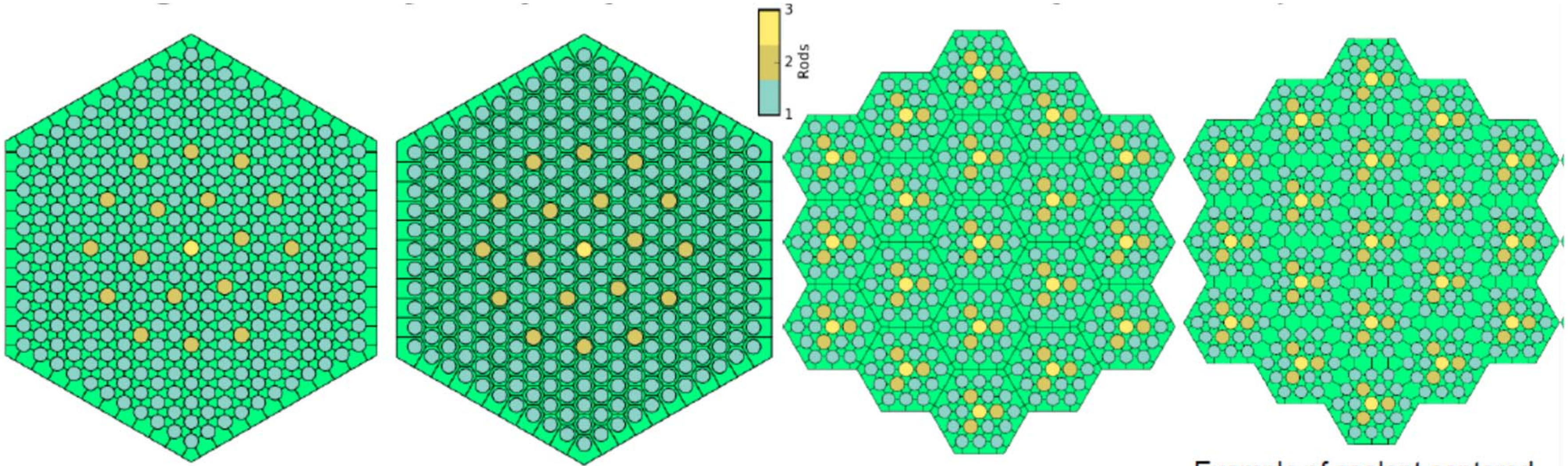
- No limitation is imposed in the coupling
- Nested IFC files can be used
- New SCF pre-processor allows coolant-centered and fuel-centered hexagonal geometries generation
- Coupling done through mapping files



Example of coolant-centered hexagonal lattice at FA level

Example of fuel-centered hexagonal lattice at FA level

Example of coolant-centered hexagonal lattice at core level

Example of coolant-centered hexagonal lattice at core level (subchannel merging)

D. Ferraro et al. *"Extension of Serpent-SCF coupling to VVER"* McSAFE project deliverable (restricted to McSAFE partners)

Extension of the SSS2/SCF internal coupling to hexagonal geometries (2)

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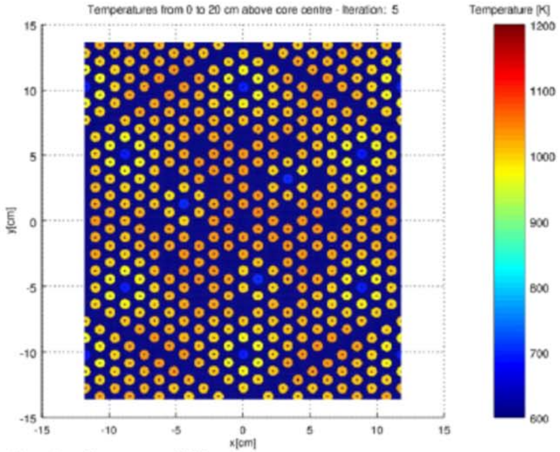
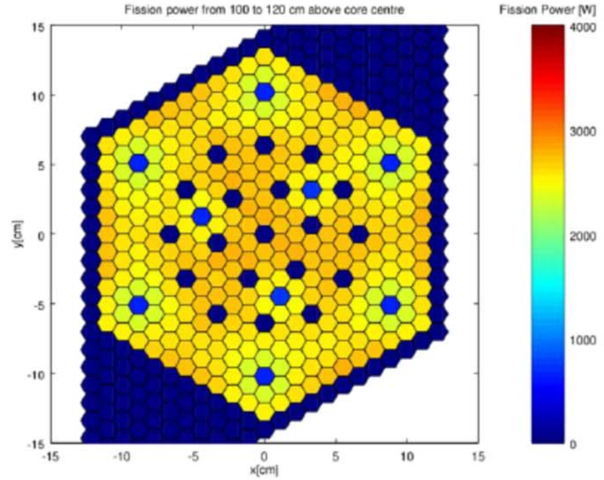
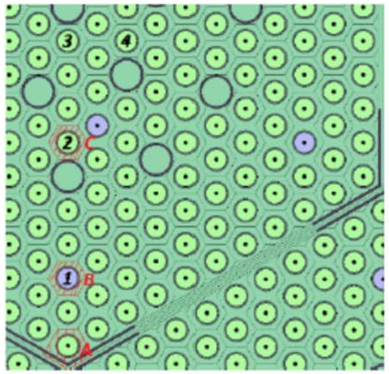
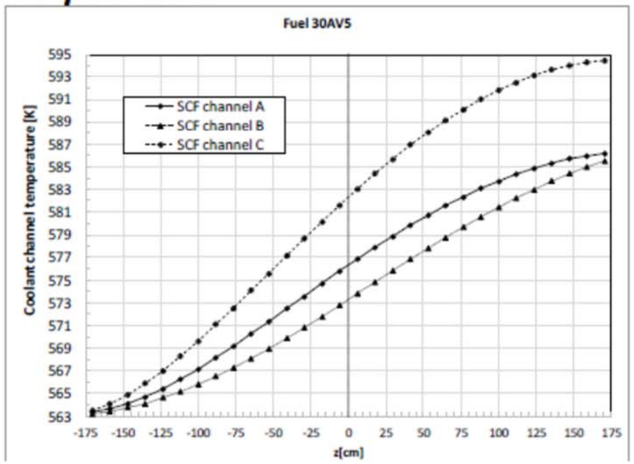
Final iteration:

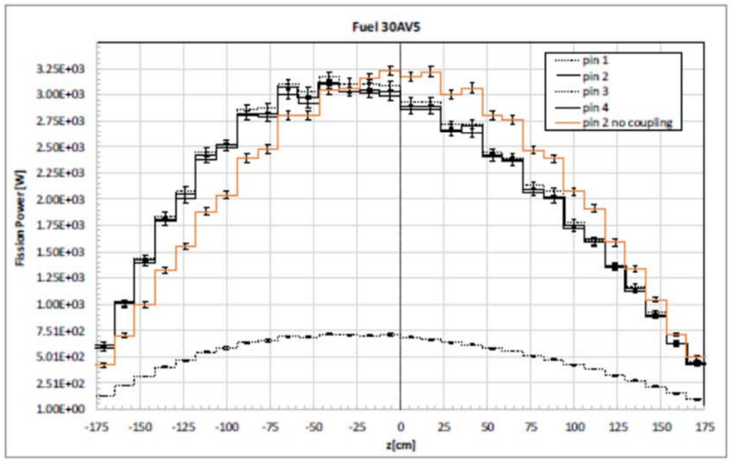






Axial profiles:





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Pin-by-pin SSS2/SCF/TU coupling results (Object Oriented approach)

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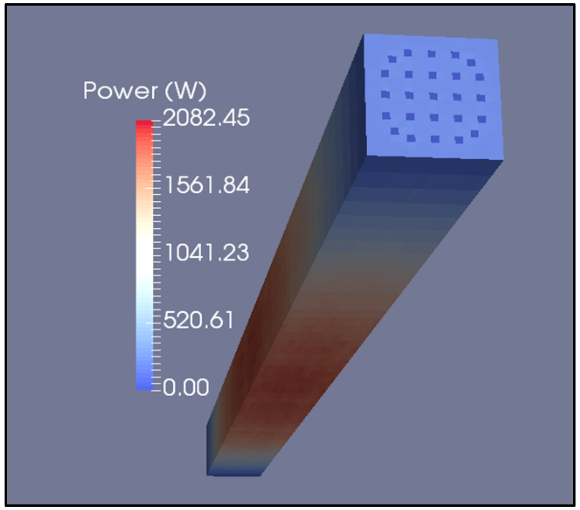
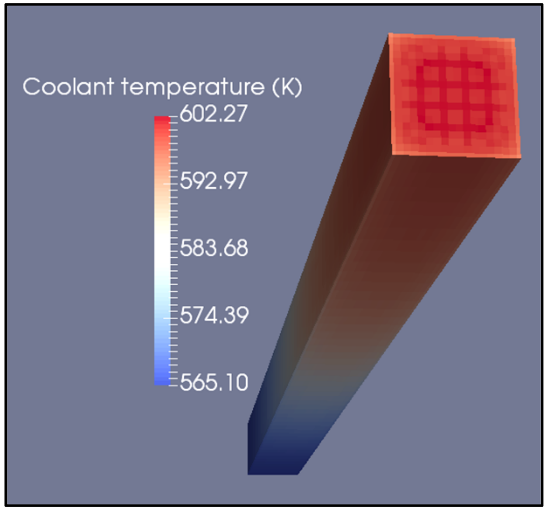
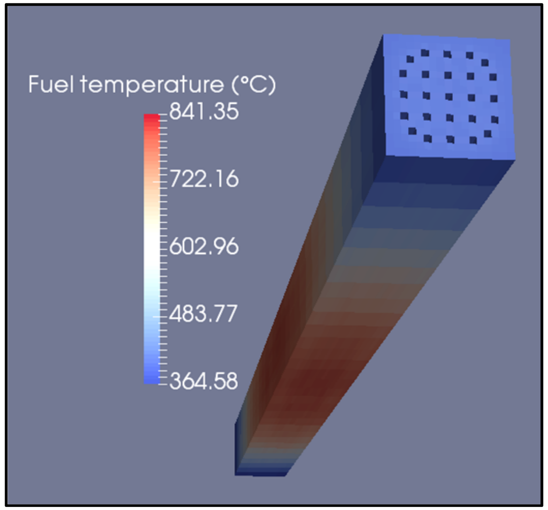
- PWR: VERA Benchmark Problem 6

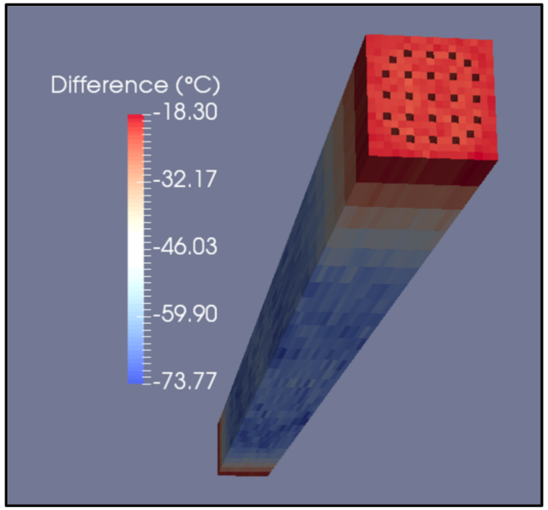






Difference: [Serpent-SCF-TU] – [Serpent-SCF]

Field	Maximum difference	Average difference
Power (W)	109.39 (10.63%)	21.62 (1.83%)
Coolant density (kg/m³)	6.00 (0.88%)	1.07 (0.16%)
Coolant temperature (°C)	2.28 (0.39%)	0.43 (0.07%)
Fuel temperature (°C)	73.77 (10.63%)	54.20 (8.15%)



M. García et al.; *"Serpent2-SUBCHANFLOW-TRANSURANUS pin-by-pin depletion calculations for a PWR fuel assembly"*, submitted to PHYSOR 2020

Pin-by-pin SSS2/SCF/TU coupling results (Object Oriented approach)

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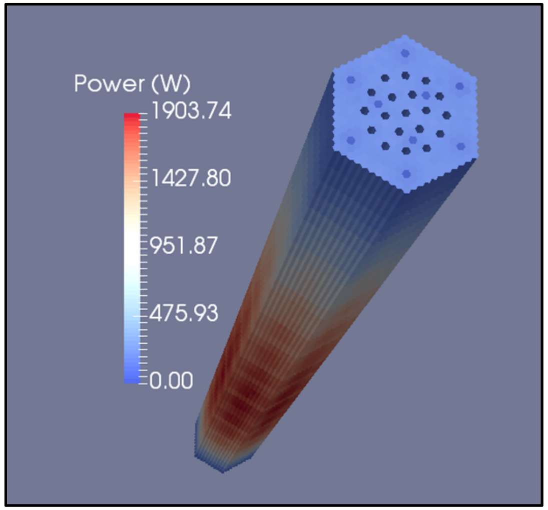
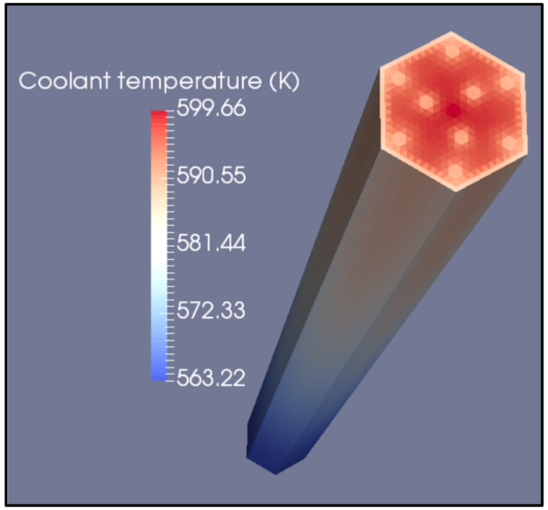
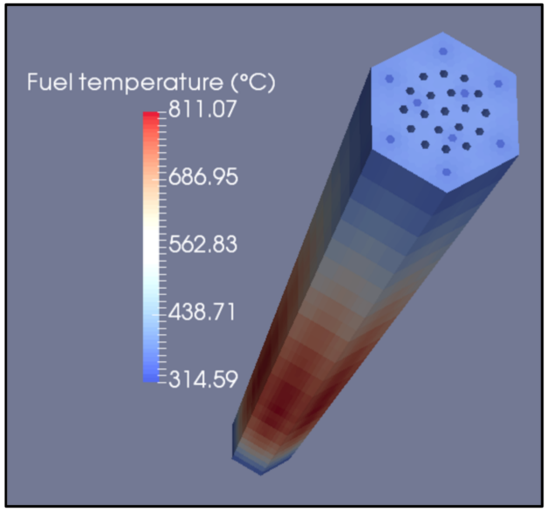
- VVER: 30AV5 VVER-1000 FA type

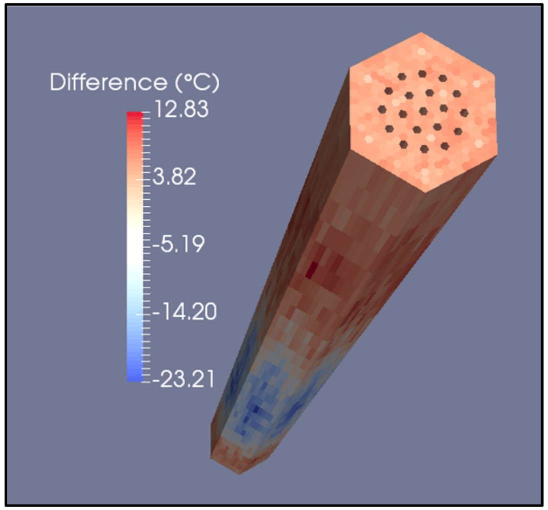






Difference: [Serpent-SCF-TU] – [Serpent-SCF]

Field	Maximum difference	Average difference
Power (W)	110.19 (15.70%)	18.51 (1.83%)
Coolant density (kg/m³)	0.43 (0.06%)	0.09 (0.01%)
Coolant temperature (°C)	0.17 (0.03%)	0.04 (0.01%)
Fuel temperature (°C)	23.21 (2.88%)	5.84 (0.91%)



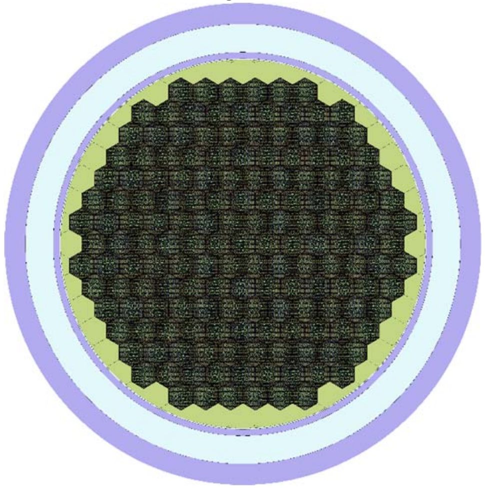
M. García et al. "*Serpent2-SUBCHANFLOW-TRANSURANUS coupling for pin-by-pin depletion calculations in PWR and VVER reactors*" (in preparation for ANE submittal)

KIT SSS2/SCF solution for a full VVER core (1)

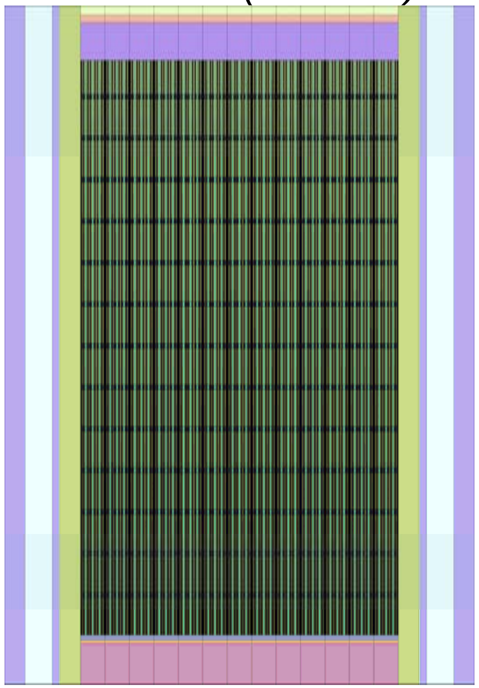
- Modeling of a full 3D coupled (by pin) VVER-1000 benchmark [1]

Serpent model

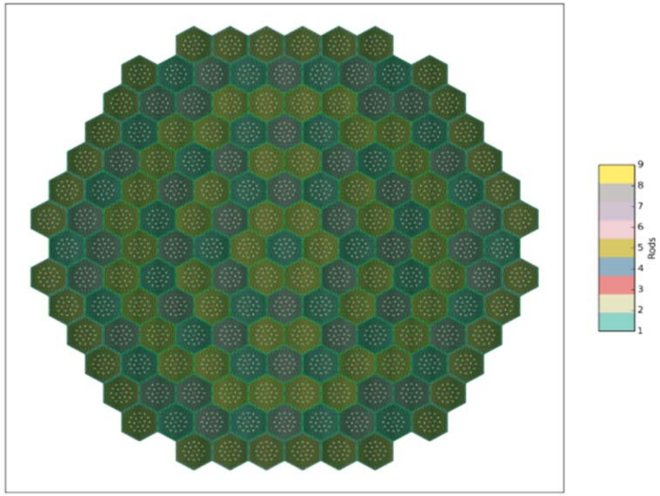
x-y cut



x-z cut (not scale)



SCF model (fuel-centered)



- ✓ Pin by pin coupling
- ✓ Simplified Xenon treatment
- ✓ Run in FH2 HPC
- ✓ Compared with reported (critical) results

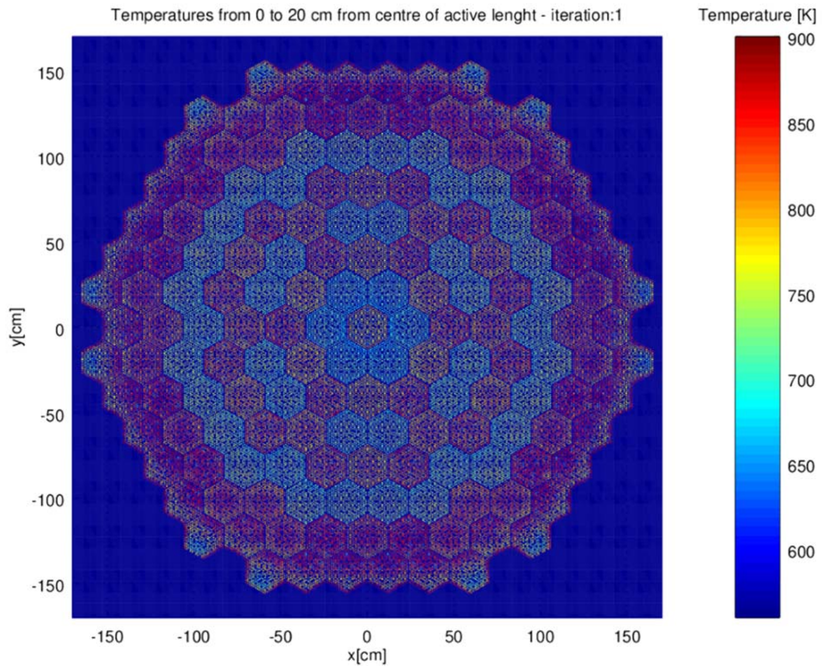
[1] Loetsch, T. et al "Corrections and additions to the proposal of a benchmark for core burnup calculations for a WWER-1000 reactor" Proceedings of the twentieth symposium of atomic energy research, (p. 790). Hungary: Kiadja and KFKI Atomenergia Kutatointezet (2010).

D. Ferraro et al. "*Serpent/SUBCHANFLOW coupled calculations for a VVER core at hot full power*" submitted to PHYSOR 2020

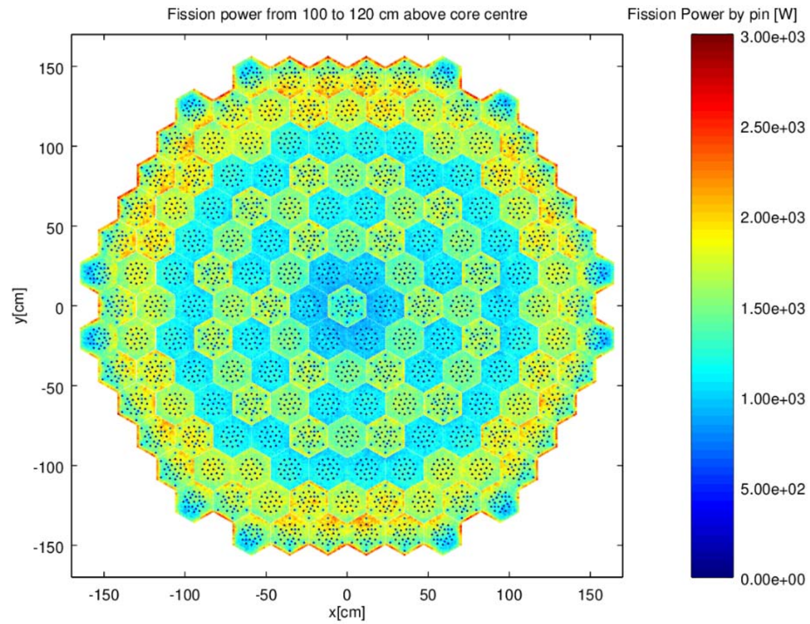
KIT SSS2/SCF solution for a full VVER core (2)

- Obtained K_{eff} = 1.00149 ± 8e-5 → Agreement ~ 150 pcm
- *Available results by pin ("high fidelity" goal):*

Converged temperature



Converged power



Further step: burnup the whole cycle (Domain decomposition becomes mandatory).

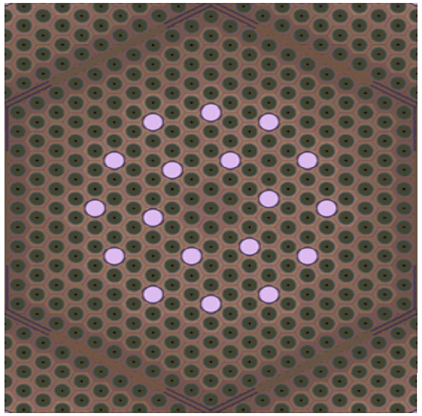
D. Ferraro et al. "*Serpent/SUBCHANFLOW coupled calculations for a VVER core at hot full power*" submitted to PHYSOR 2020

KIT SSS2/SCF solution of a VVER FA with burnup (1)

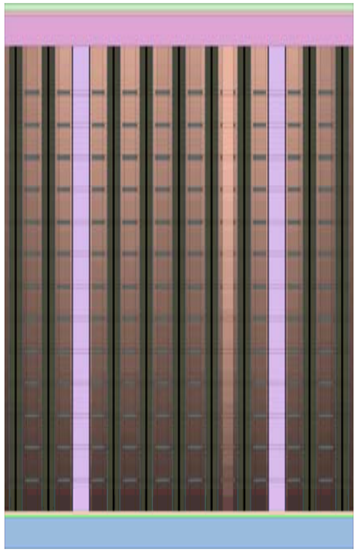
- Modeling of a full 3D coupled (by pin) VVER-1000 FA benchmark and comparison with other high fidelity projects [1].

Serpent model

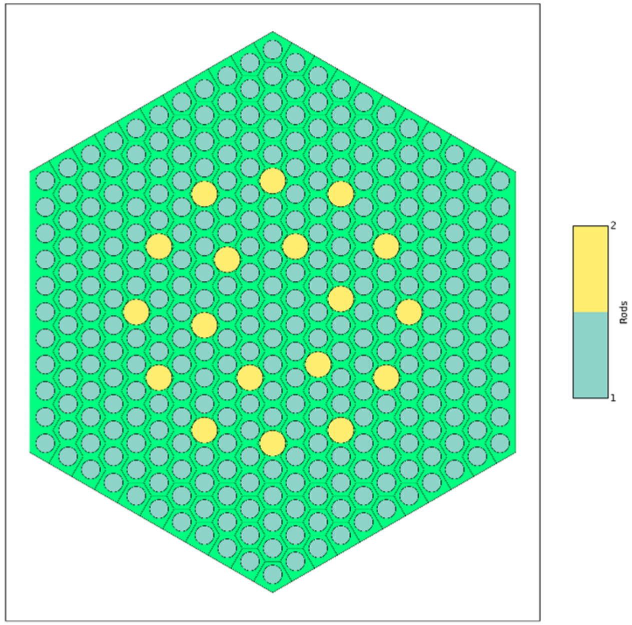
x-y cut



x-z cut (not scale)



SCF model (fuel-centered)



- ✓ Pin by pin coupling for two types of FA: w/ and w/o Burnable Poisons (Er)
- ✓ Full burnup by pin (16000 burnable zones for case w/ Burnable Poisons)
- ✓ Compared with reported results from MCU (also "high fidelity")
- ✓ Predictor Corrector burnup with TH feedback on each step

[1] Bikeev, Artem et al. "MCU Code Precision Calculation of a Full-Scale VVER-1000 Model Considering Feedbacks" Proceedings of M&C 2017.

D. Ferraro et al. "*Serpent/SUBCHANFLOW coupled calculations for a VVER fuel assemblies*" submitted to PHYSOR 2020

KIT SSS2/SCF solution of a VVER FA with burnup (2)

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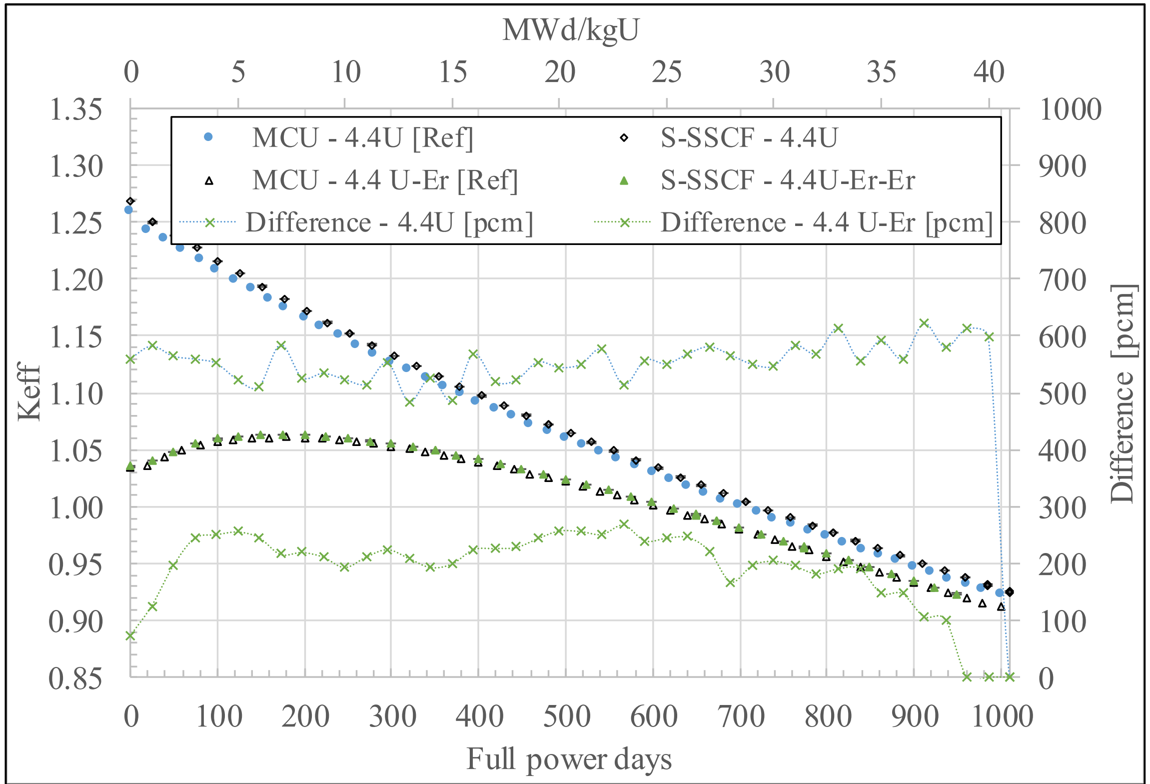
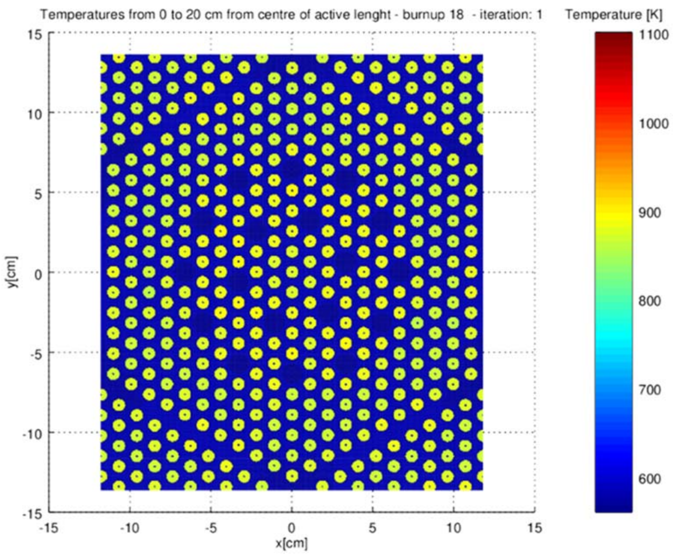
Converged reactivity comparison for both FA



Converged temperature Example (case w/o Burnable Poisons)



- ✓ Good agreement for both FA with other "high fidelity" projects
- ✓ Consistent behavior with burnup
- ✓ Results available at pin level (highly detailed)

D. Ferraro et al. "*Serpent/SUBCHANFLOW coupled calculations for a VVER fuel assemblies*" submitted to PHYSOR 2020

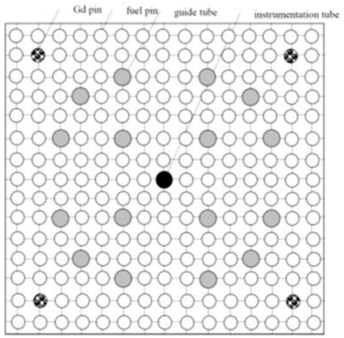
Dynamic MC for transients analysis

- **Objectives:**
  - Development of time-dependent dynSERPENT-SCF e.g. implementation of methods to account for the prompt neutron and gamma heat deposition in the coolant.
  - Development of time-dependent dynTRIPOLI-SCF.
  - Development of time-dependent dynMCNP-SCF.
  - Variance reduction for MC-codes with dynamic capability to improve the efficiency of time-dependent MC solutions e.g. Uniform Fission Sites (UFS).
  - Methods for optimal parallel scalability of MC-TH codes for dynamic simulations to take profit of massively parallel environments in the frame of industry-like applications.
  - Verification of developed tools on 3x3 pin cluster or PWR mini-core (3x3 FA)
- **Tools:** TRIPOLI/SCF, SERPENT/SCF, MCNP/SCF
- **Testing and demonstration:** PWR mini-core (3x3 FAs), SMR core (e.g. SMART core)

Serpent/SCF: REA Analysis (1)

- UAM 3-D 15x15 FA PWR minicore is used ***as basis for coupled transients***:

Fuel assembly



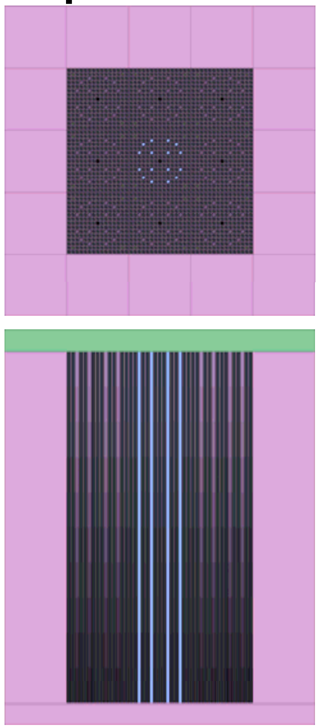
FR pitch ~1.44 cm

Minicore

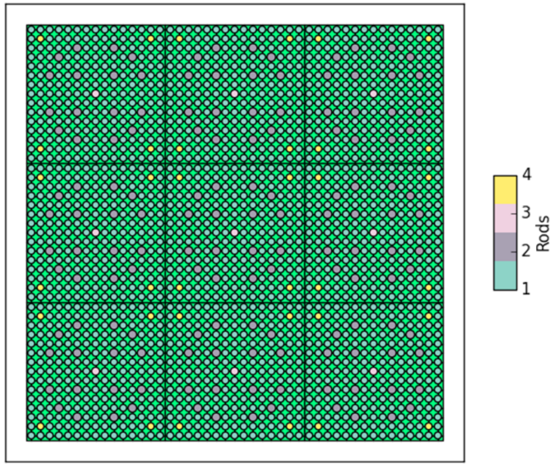
Reflector	Reflector	Reflector	Reflector	Reflector
Reflector	U	U	U	Reflector
Reflector	U	R	U	Reflector
Reflector	U	U	U	Reflector
Reflector	Reflector	Reflector	Reflector	Reflector

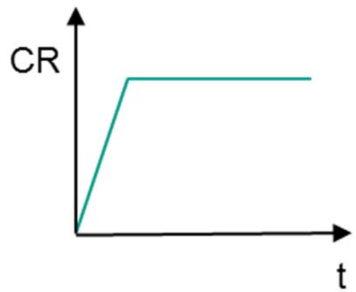
U= Unrodded
R= Rodded

Serpent model



SCF model (coolant-centered)



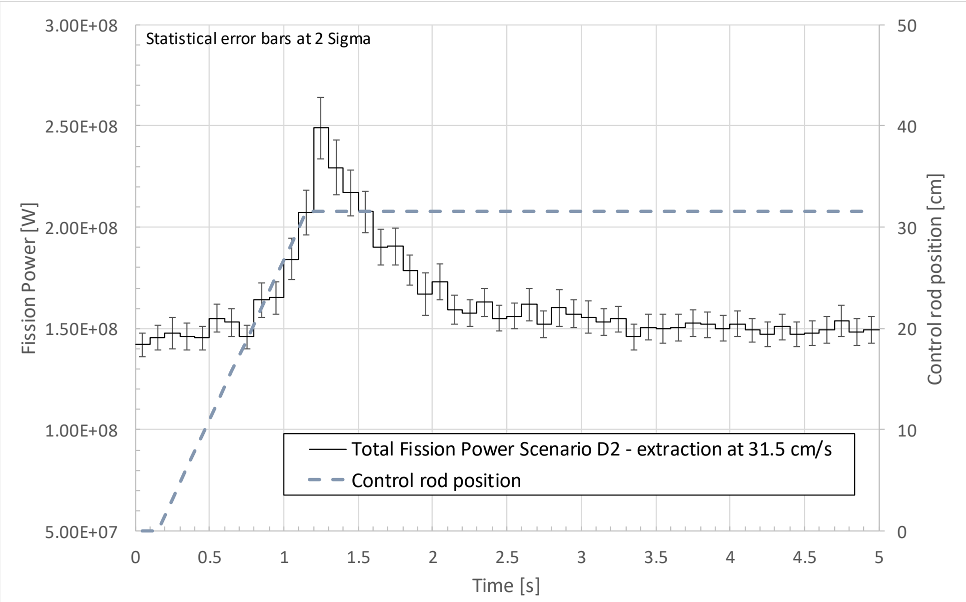


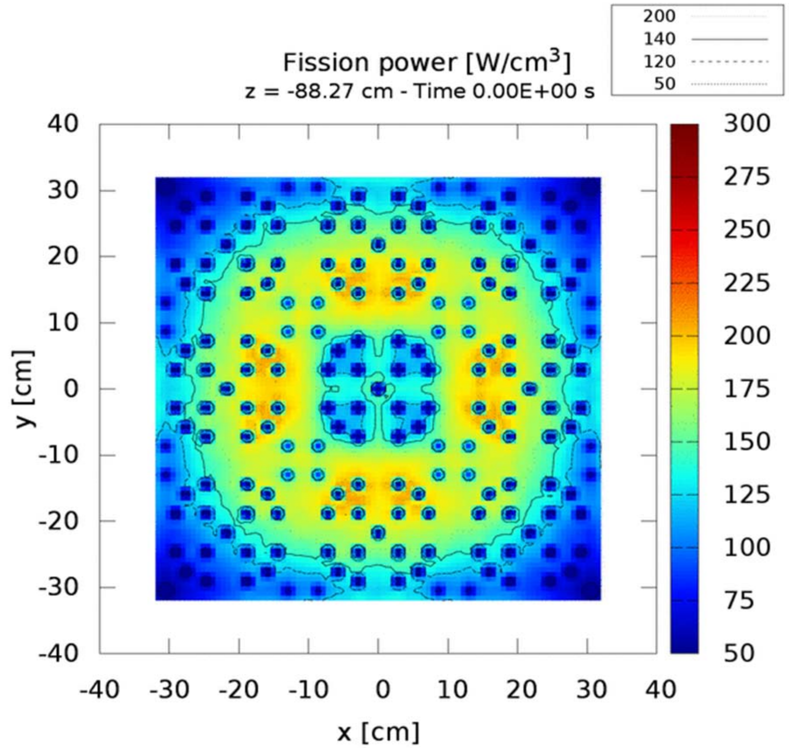
✓ RIA-kind scenarios are considered, driven by Control Rod extraction.
✓ Pin by pin coupling with SUBCHANFLOW for the transient

D. Ferraro et al.; “*Serpent/SUBCHANFLOW pin-by-pin coupled transient calculations for a PWR minicore*”, submitted for publication to ANE

Serpent/SCF: REA Analysis (2)

Power vs CR position:





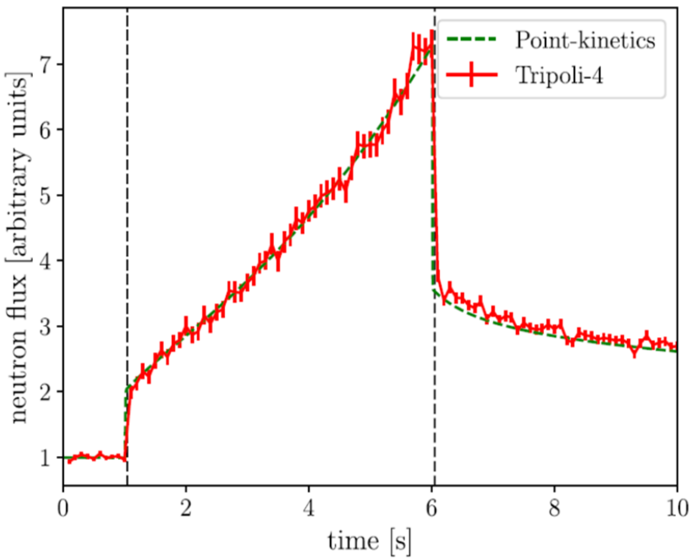
REA: ~420 pcm insertion in 1 sec

- ✓ Results obtained by pin
- ✓ Fuel temperature + density change provides the negative feedback
- ✓ Results behave as expected

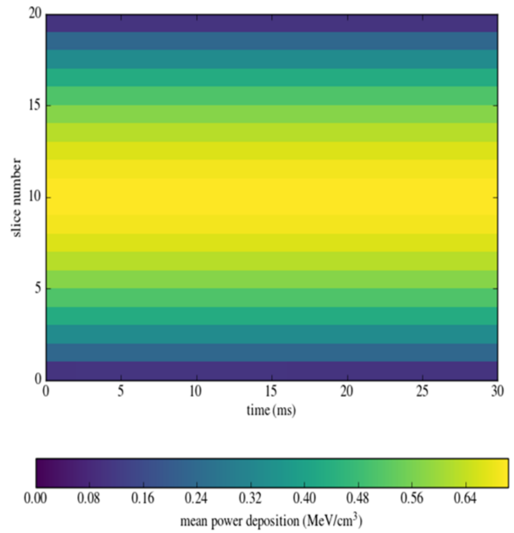
D. Ferraro et al.; "*Serpent/SUBCHANFLOW pin-by-pin coupled transient calculations for a PWR minicore*", submitted for publication to ANE

Dynamic development of TRIPOLI-4

- The TRIPOLI-4 code was extended
  - with several algorithms for the efficient solution of the coupled neutron-precursor transport equation
  - with the capability to handle moving geometry
- TRIPOLI-4 multi-physics interface has been developed to be compliant with the ICoCo specification of an API



Time evolution of the total netron flux in the SPERT-III core (Reactivity insertion at t=1s with a 0.8 cm withdrawal of the CR. The system returns to critical state at t=6 s when the CR go back to initial position)



Mean value of the neutron power deposited in each of the axial rod slices vs. time (fuel rod in a critical position)

M. Faucher et al.; "*New kinetic simulation capabilities for Tripoli-4®: Methods and applications*", Annals of Nuclear Energy 120:74-88 October 2018

Validation

- **Validation of MC-based simulations using plant data for depletion, static and dynamic core analysis using the implemented coupled approaches (UJV)**

Plant Data	Static MC-TH Problem	Static MC-TH-TM Depletion Problem	Dynamic Problem
VVER-1000	TRIPOLI SERPENT/SCF	SERPENT/SCF/TU	
PWR Konvoi	TRIPOLI/SCF SERPENT/SCF MONK	SERPENT/SCF/TU	
SPERT III E REA			DynTRIPOLI/SCF DynSERPENT/SCF DynMCNP/SCF

- International benchmarks (OECD/NEA UAM, etc.)

Dissemination and communication

- Project website: www.mcsafe-h2020.eu
  - Synthesis reports of the main project results
  - Project newsletters (subscription through website)
- McSAFE Training Course to be held at KIT in March 25-27, 2020
- **McSAFE User Group**
  - **Goal**: assessment of the McSAFE results from the user's point of view
  - **Members**: Organisations (utilities, regulatory bodies, TSO, research labs, universities) from Europe, Asia and America
- UG members contribution:
  - Feedback on methods, codes and results
  - Suggestions for further developments
  - Production pf benchmark results
  - Sharing the data for validation

Do you like to join? ➔ Send an e-mail to the coordinator: victor.sanchez@kit.edu

Summary

- Increasing demand from designers, operators, regulators and other stakeholders for advanced tools and methods in reactor analysis
- Several project around the world are oriented to tackle this demand
- The McSAFE project (EU Horizon 2020) started in 2017 and is delivering
- **improved** and **validated high-fidelity numerical simulation tools** that can be used by different end-users (industry, regulators, research centres, etc.) to provide **reference solutions to deterministic codes for safety demonstration**
- The objective is to develop tools and coupling approaches that will allow to calculate full NPP cores with depletion at the pin level
- The **McSAFE tools** can contribute **to design reactor systems with improved safety features keeping sufficient safety margins**
- Applicability of **McSAFE tools to any reactor type including SMR, research reactors and Gen-IV** and **usability for verification** of design calculation methods for innovative systems for which data are not available