H2020

McSAFE

High Performance Monte Carlo for Safety

High-fidelity multiphysics simulations for Light Water Reactors in the McSAFE H2020 project

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- The McSAFE H2020 project
- High-fidelity multiphysics
- Coupling approaches
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- Conclusions

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

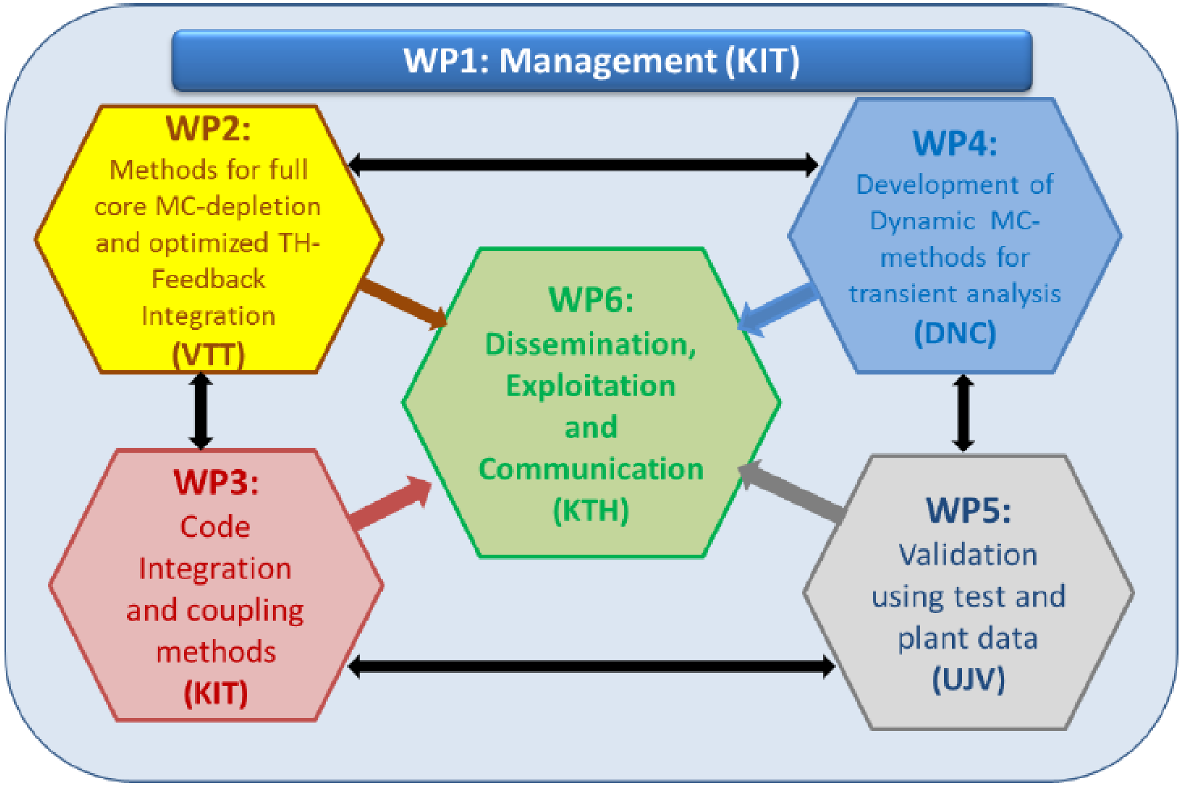
Introduction

- **Predictive simulations** = backbone of nuclear reactor safety
- Most of the tools developed when **computing** resources and capabilities were **limited**
- Shift **towards high-fidelity methods** taking advantage of progress in computing (hardware/software)
- Reactor operating closer to their safety limits due to less conservative safety evaluations
- Core analysis relies mainly on deterministic neutronic codes (daily work)
- Alternative/supplementary option:
  - Use **MC codes** capable of simulating the neutron transport without approximations
  - Obtain **reliable data** for any core state **at fuel pin level** (experimental data at pin level is scarace and not easy to be measured)
  - Potential use taking advantage of **HPC** and **parallelization**

The McSAFE H2020 project

- Three-year project (09.2017 - 08.2020)
- Participants:
  - 9 research institutions: KIT, VTT, HZDR, JRC, CEA, NRI, KTH, DNC, Wood
  - 3 industry partners: EKK, CEZ, EdF
- High-fidelity multiphysics for safety analysis of LWRs:
  - Monte Carlo neutron transport: **Serpent2, Tripoli4, MCNP, MONK**
  - Subchannel thermalhydraulics: **SUBCHANFLOW (SCF)**
  - Fuel-performance analysis: **TRANSURANUS (TU)**
- Main developments
  - Serpent2-SCF(-TU) coupling for steady-state, burnup and transient problems
  - Optimization of steady-state and transient capabilities for HPC
  - Optimization for massive (full-core pin-by-pin) depletion problems
- Validation with plant data
  - PWR-Konvoi
  - VVER-1000

McSAFE project structure



High-fidelity multiphysics

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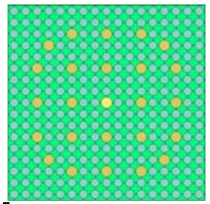
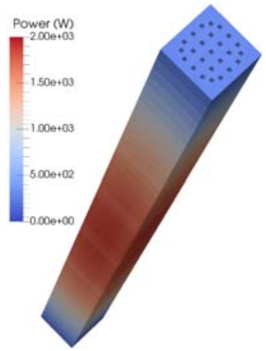
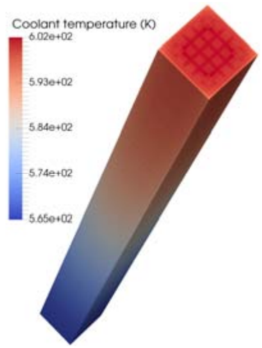
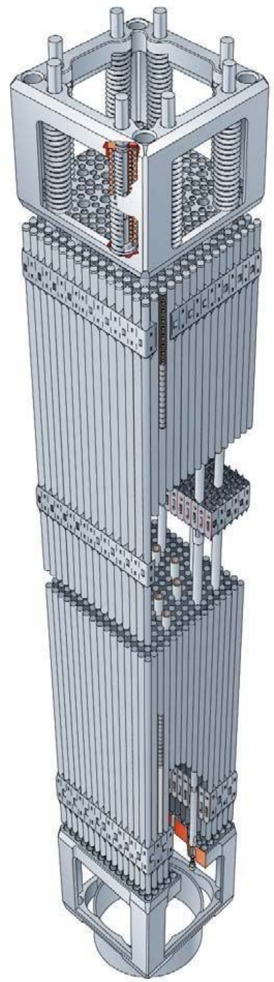
- Main objectives:
  - **Avoid approximations** (multi-scale approach) in neutronics
  - **Calculate local safety parameters directly**:
    - Burnup cycle.
    - Transient scenarios.
  - Provide **reference solutions for lower order methods**
- **Neutronics:**
  - Continuous-energy Monte Carlo neutron transport
  - Pin-by-pin power tallying and burnup calculation
- **Thermal-hydraulics:**
  - Pin-level subchannel thermal-hydraulics
  - Coolant and fuel safety parameters
- **Fuel performance:**
  - Pin-level thermomechanical analysis
  - Fuel safety parameters



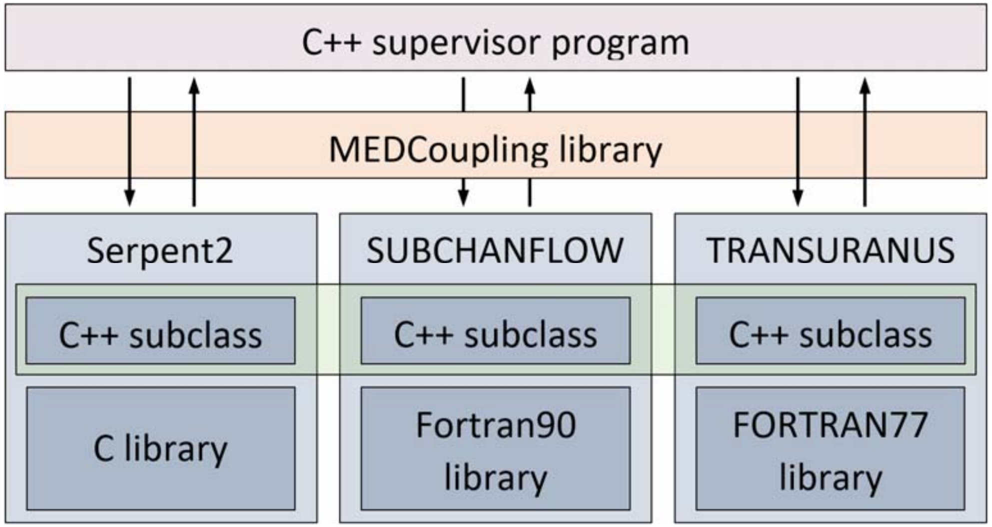






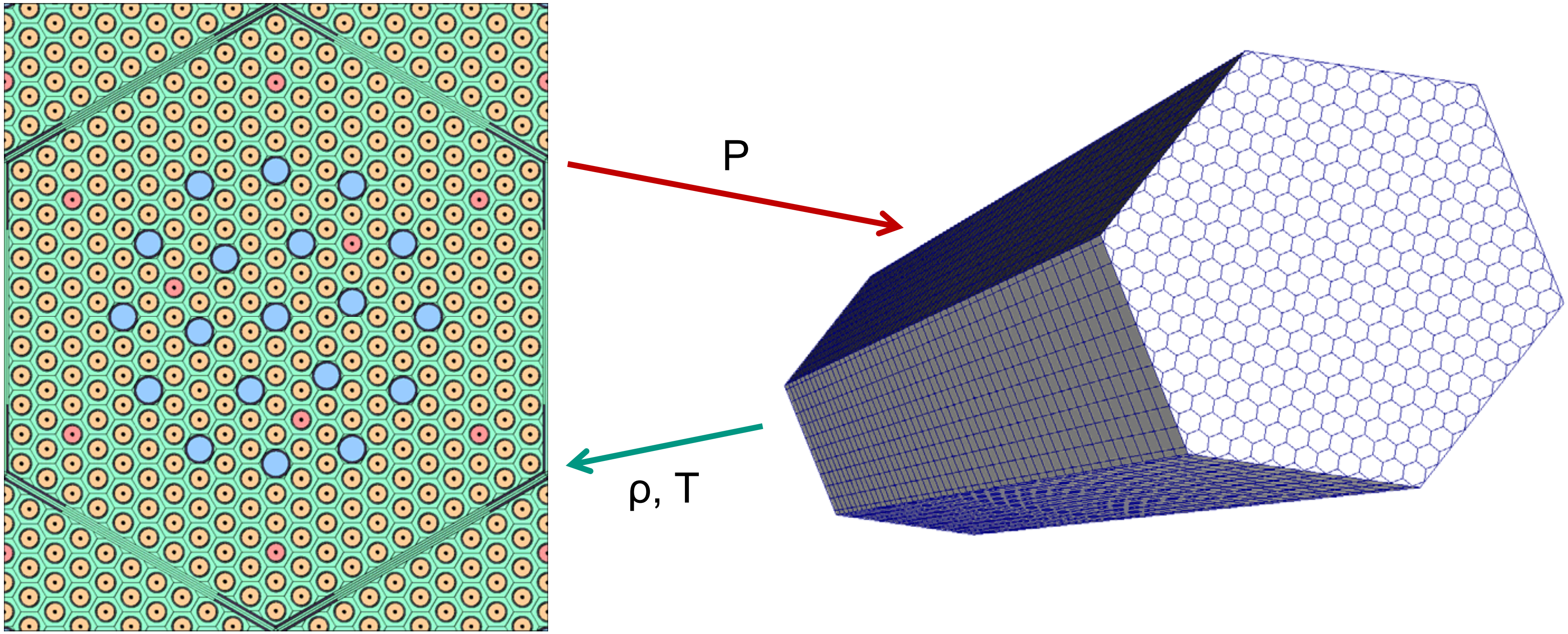
Software design

- **Master-slave internal coupling:**
  - SCF and TU (slaves) modularized and embedded in Serpent2 (master).
  - Traditional approach, reference for performance.
- **Object-oriented coupling:**
  - Serpent2, SCF and TU modularized and coupling scheme implemented in a separate supervisor program.
  - More innovative approach, potential benefits from the object-oriented design.
  - Main features:
    - Inheritance-based APIs.
    - Object-oriented supervisor.
    - Mesh-based feedback.
- Numerical method:
  - Operator splitting.
  - Picard iterations.
  - Pin-by-pin feedback.



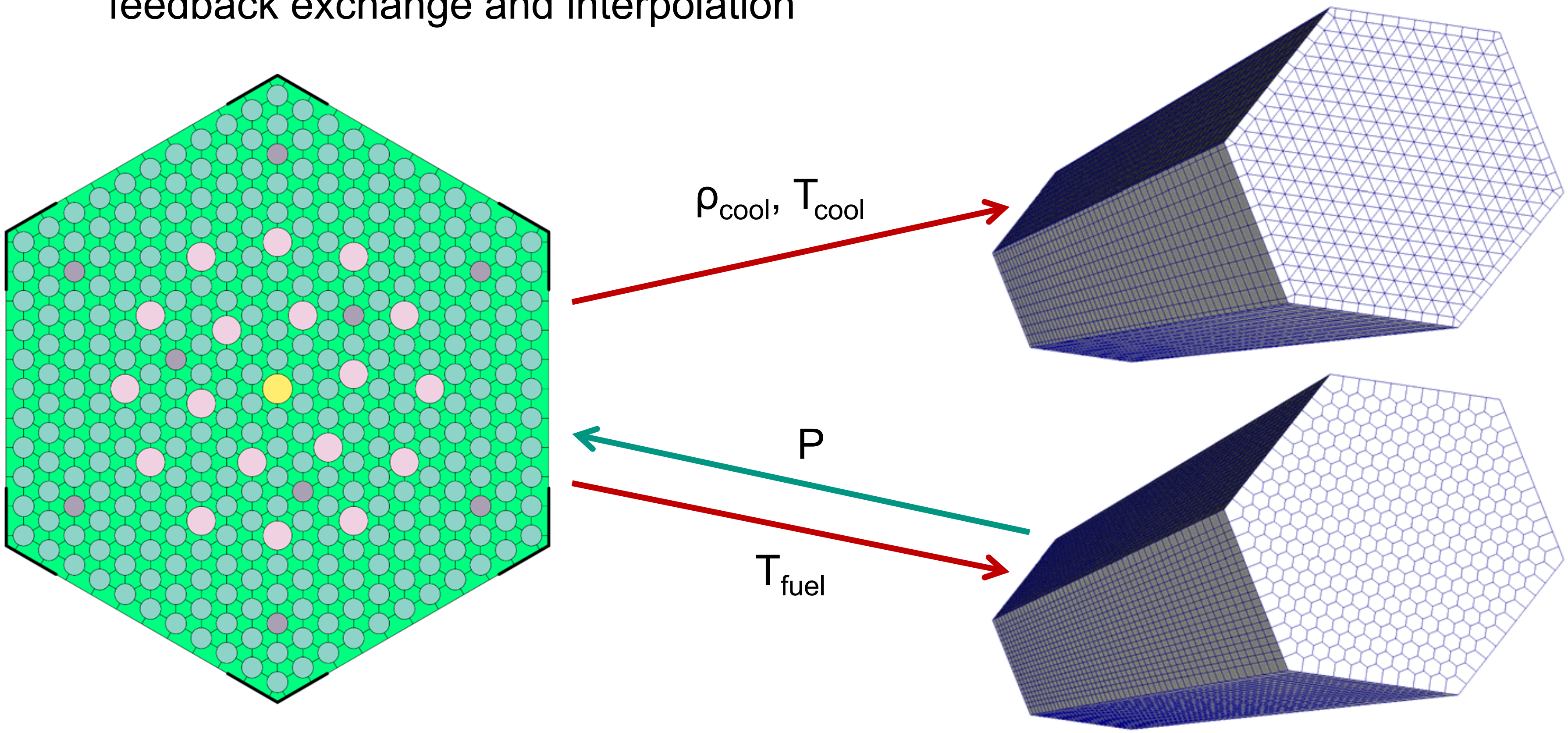
Mesh-based field exchange

- **Serpent2:**
  - Multiphysics interfaces based on superimposing meshes on the tracking geometry to set densities and temperatures and get power
  - Internal meshes represented as unstructured meshes for feedback exchange



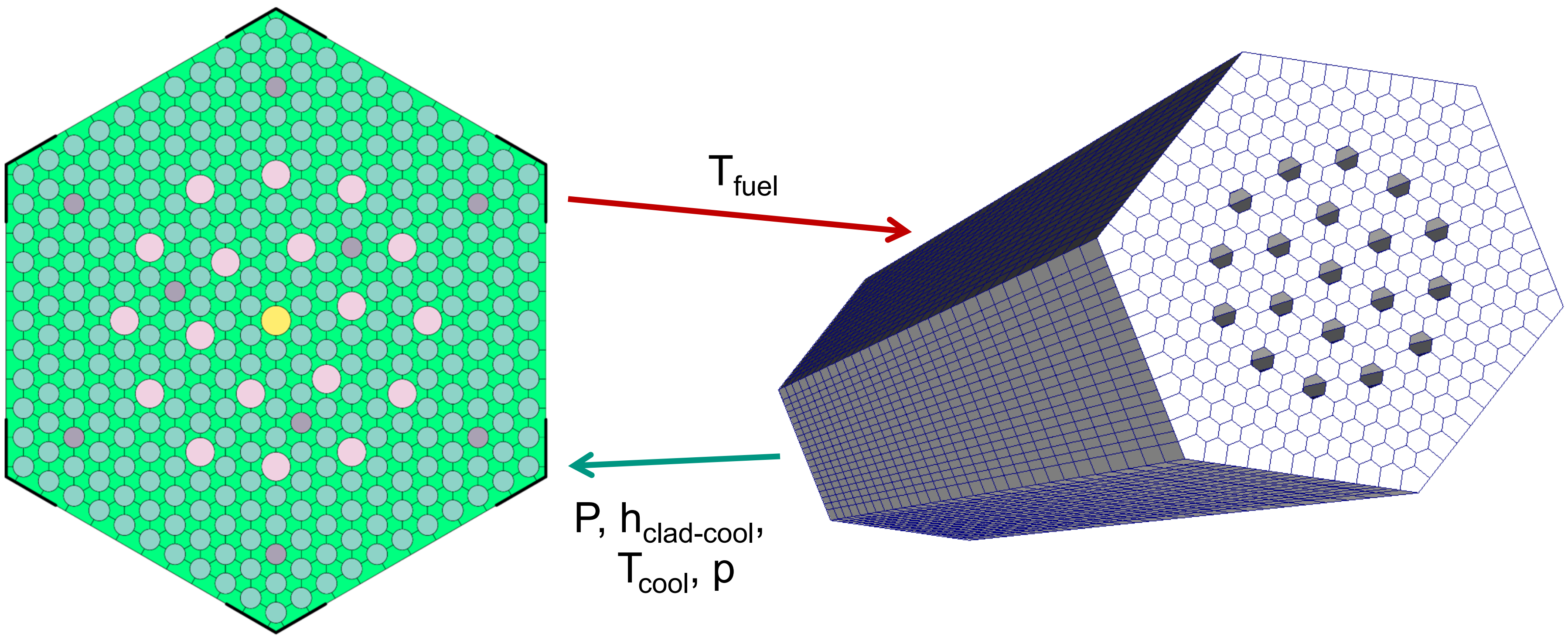
Mesh-based field exchange

- **SUBCHANFLOW:**
  - Subchannel model defined by hydraulic parameters and connectivity
  - Channel and rod geometry given by coolant and fuel unstructured meshes for feedback exchange and interpolation

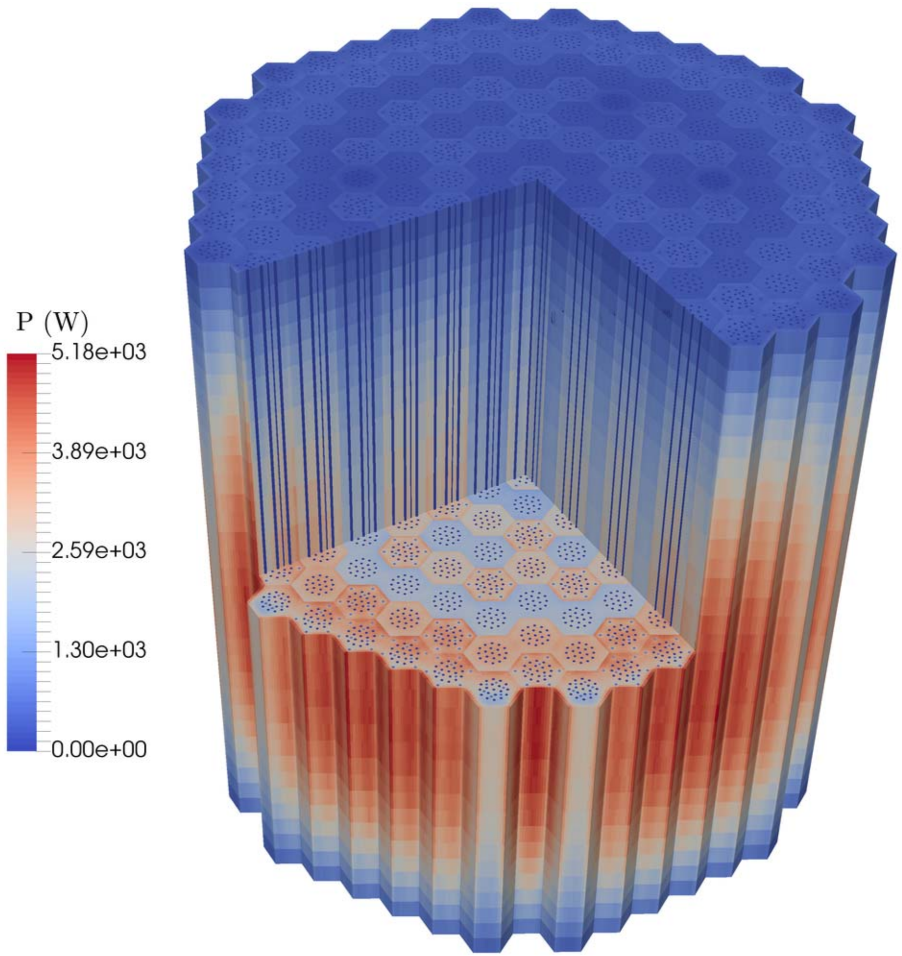


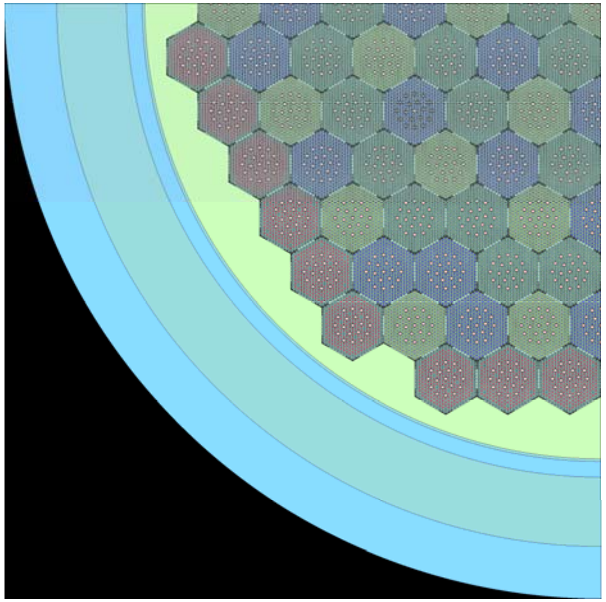
Mesh-based field exchange

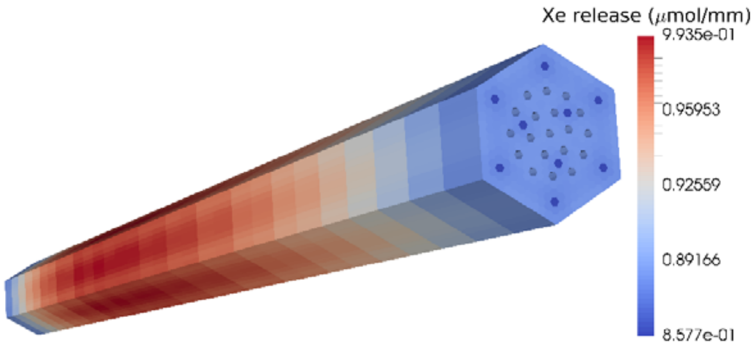
- **TRANSURANUS**:
  - Solution scheme independent for each rod
  - Rod mesh to manage input and output between the multiphysics interface and each solver instance



Depletion calculations

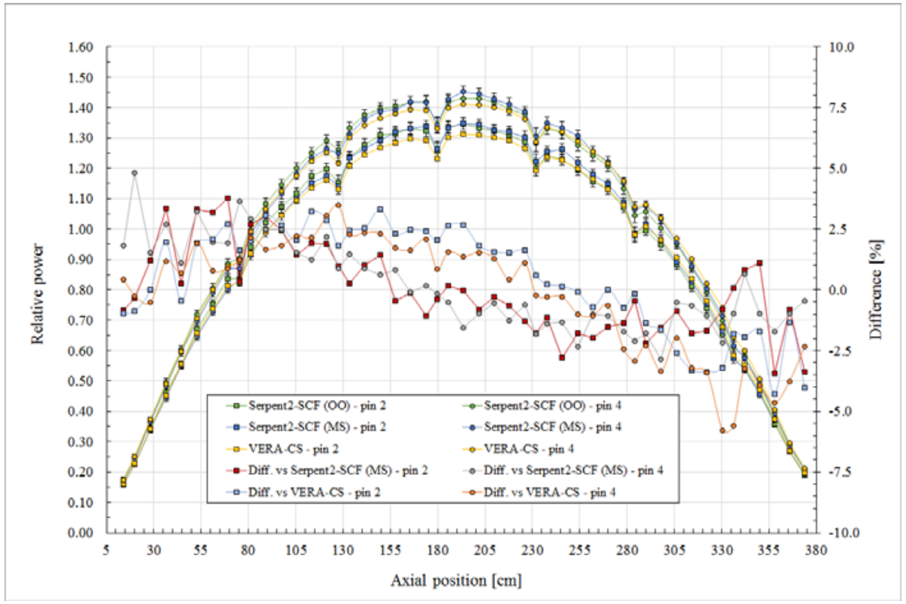




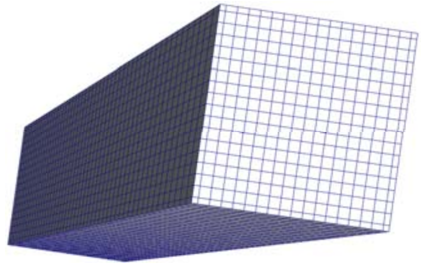


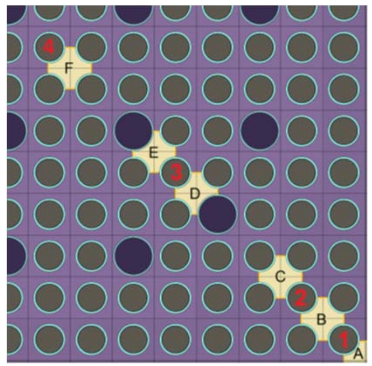
Serpent2-SCF: steady-state calculation

- Standard steady-state neutronic-thermalhydraulic coupling:
  - Power calculated by Serpent2 and used in SCF as heat source
  - Cooling conditions calculated by SCF and ρ_{cool}, T_{cool} and T_{fuel} used in Serpent2
  - Iterative scheme with pin-by-pin feedback
- Verification with the VERA Core Physics Benchmark (PWR) [1]



Result	Keff	ΔKeff (pcm)
VERA-CS	1.16361	-
RMC-CTF	1.16239±0.00010	-90
MC21-CTF	1.16424±0.00003	47
MCNP6-CTF	1.16500±0.00006	103
Serpent2-SCF (OO)	1.16552±0.00003	141
Serpent2-SCF (MS)	1.16560±0.00003	147

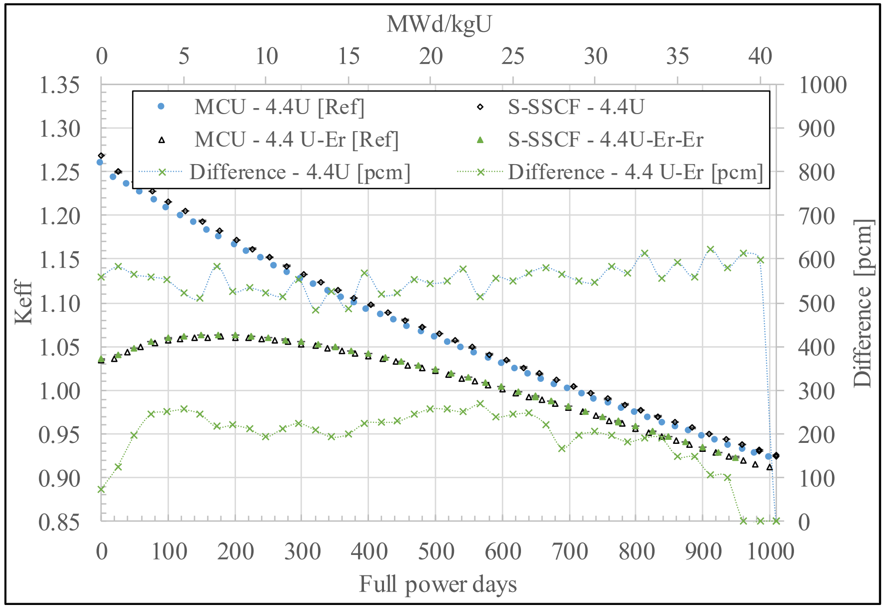


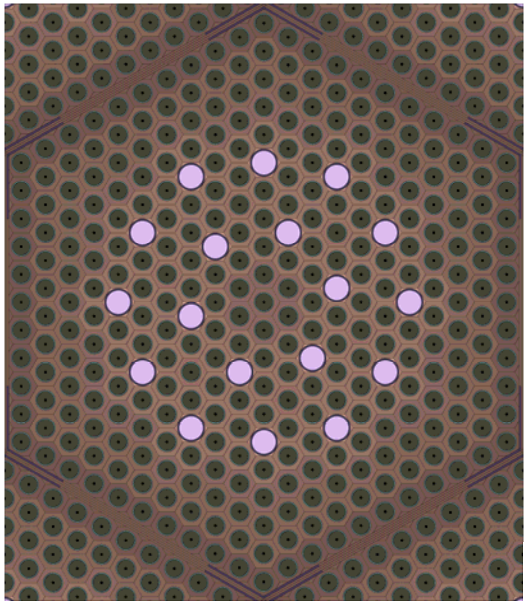


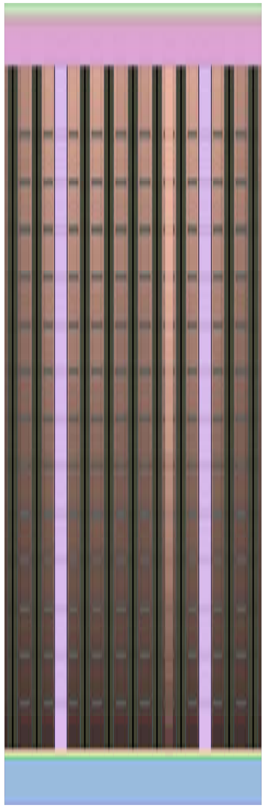
[1] "Development of an object-oriented Serpent2-SUBCHANFLOW coupling and verification with Problem 6 of the VERA Core Physics Benchmark", M. García, D. Ferraro, et al., M&C2019.

Serpent2-SCF: burnup scheme

- Monte Carlo depletion scheme with thermalhydraulic feedback:
  - Burnup calculation integrated in Serpent2
  - Predictor-corrector and Stochastic Implicit Euler (SIE) methods
  - Iterative quasi-stationary scheme with pin-by-pin feedback
- Verification with TVSA-type fuel assemblies (VVER-1000) [2]



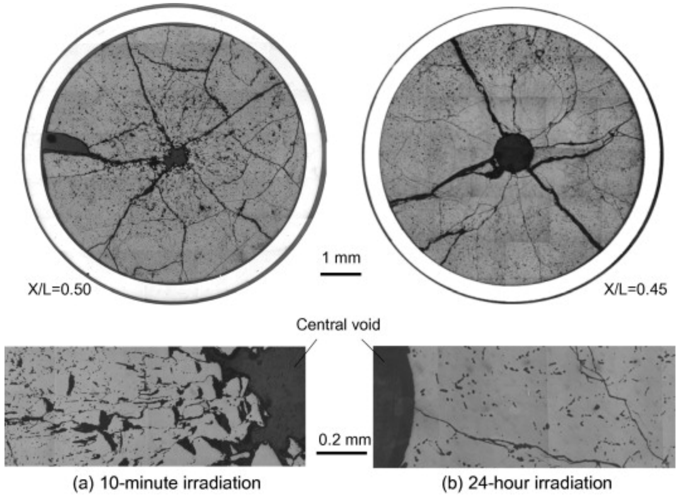


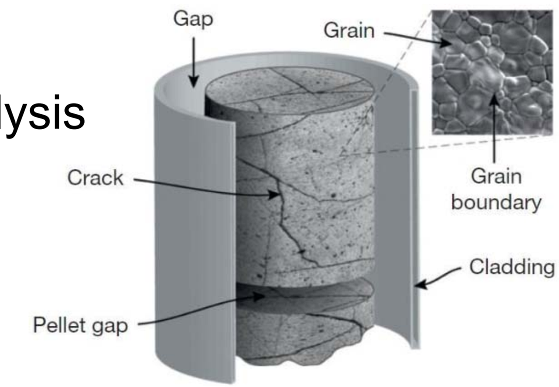


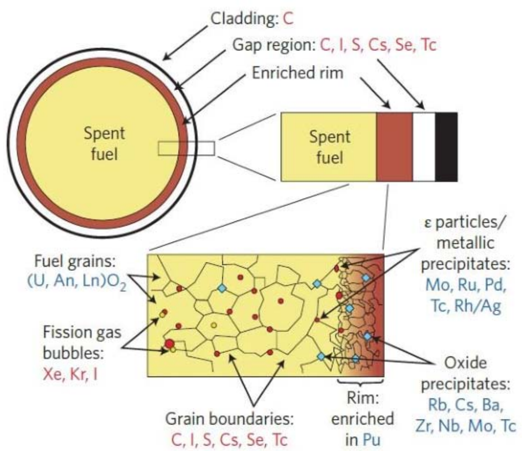
[2] "Serpent/SUBCHANFLOW coupled burnup calculations for VVER fuel assemblies", D. Ferraro, M. García, et al., PHYSOR2020 (submitted).

Serpent2-SCF-TU: motivation

- Fuel behavior during burnup:
  - Extremely complex multi-physics problem
  - Important for safety assessment
  - Potential impact on the Doppler feedback
- SCF approach:
  - Thermal properties: $c_P(T)$, $k(T)$, $\alpha_T(T)$
  - Gap width: thermal expansion, cracking and swelling dependent on burnup
  - Gap conductance: radiation and conduction
- TU approach:
  - Full thermomechanic analysis
  - Main relevant physics
  - Validated extensively
  - Reference solution

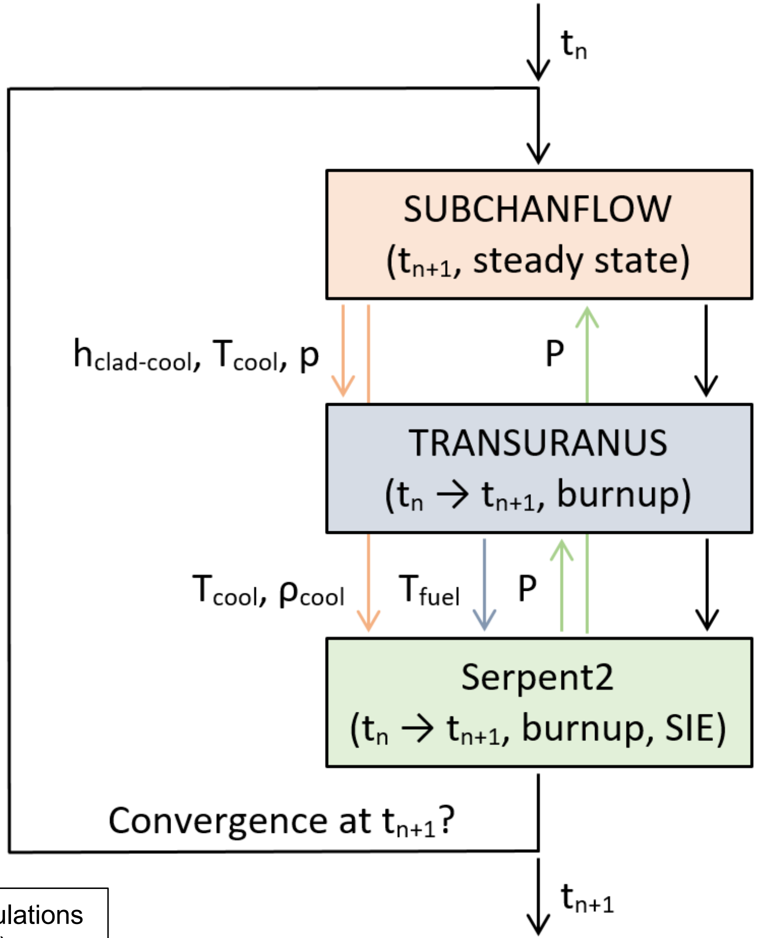






Serpent2-SCF-TU: burnup scheme

- Main features [3]:
  - Semi-implicit burnup scheme
  - Fully coupled neutronics, depletion, thermalhydraulics and thermomechanics
  - Independent depletion in Serpent2 (detailed) and TU (simplified)
  - SCF simple fuel-rod solver replaced by TU thermomechanical analysis
- Verification [4]:
  - PWR depletion problem based on the VERA Benchmark
  - Comparison with Serpent2-SCF (w/o TU)

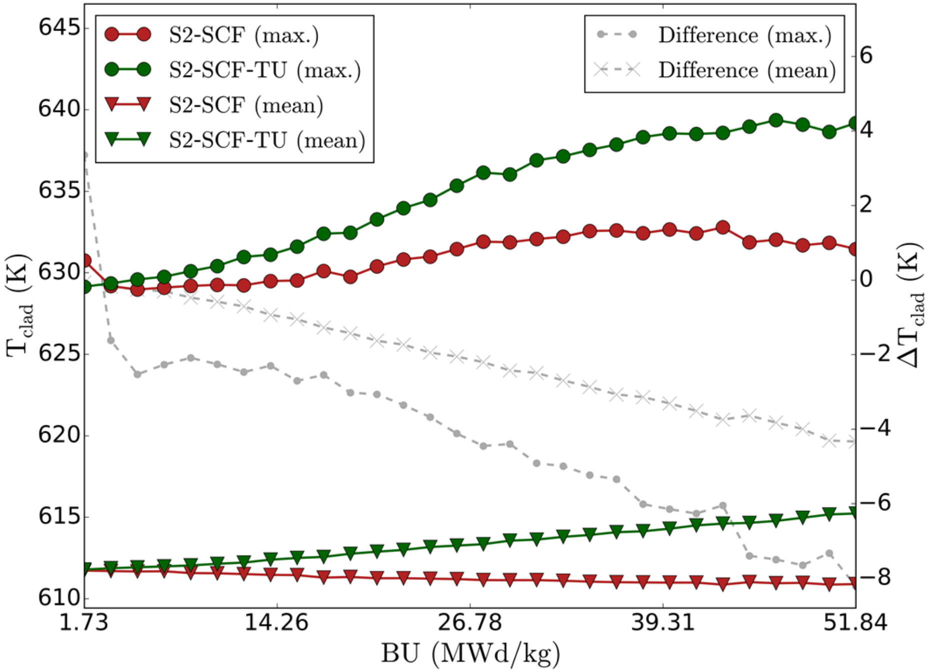


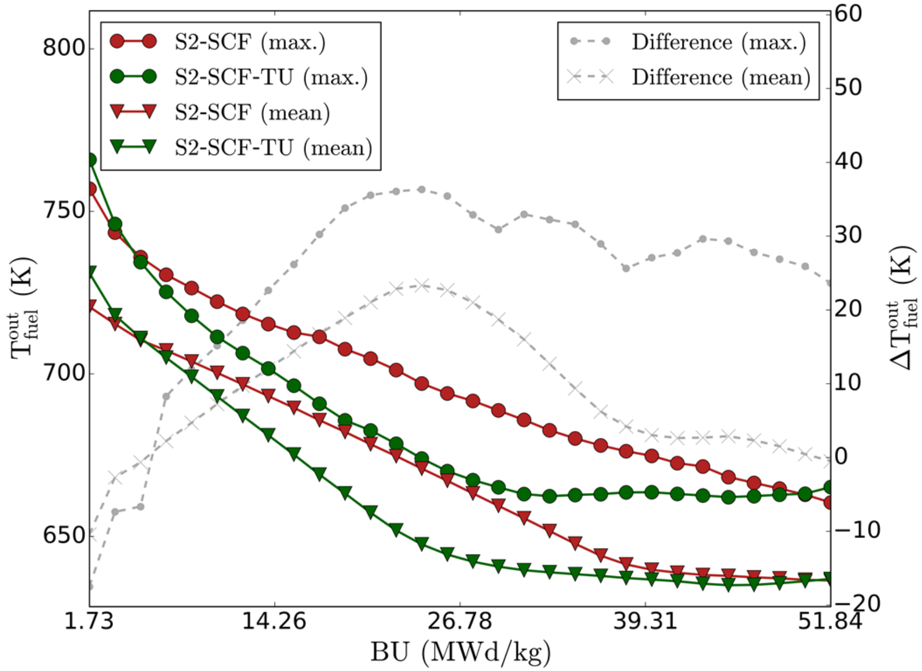
[3] "A Serpent2-SUBCHANFLOW-TRANSURANUS coupling for pin-by-pin depletion calculations in Light Water Reactors", M. García, D. Ferraro, et al., Annals of Nuclear Energy (in press).

[4] "Serpent2-SUBCHANFLOW-TRANSURANUS pin-by-pin depletion calculations for a PWR fuel assembly", M. García, D. Ferraro, et al., PHYSOR2020 (submitted).

Serpent2-SCF-TU: depletion analysis

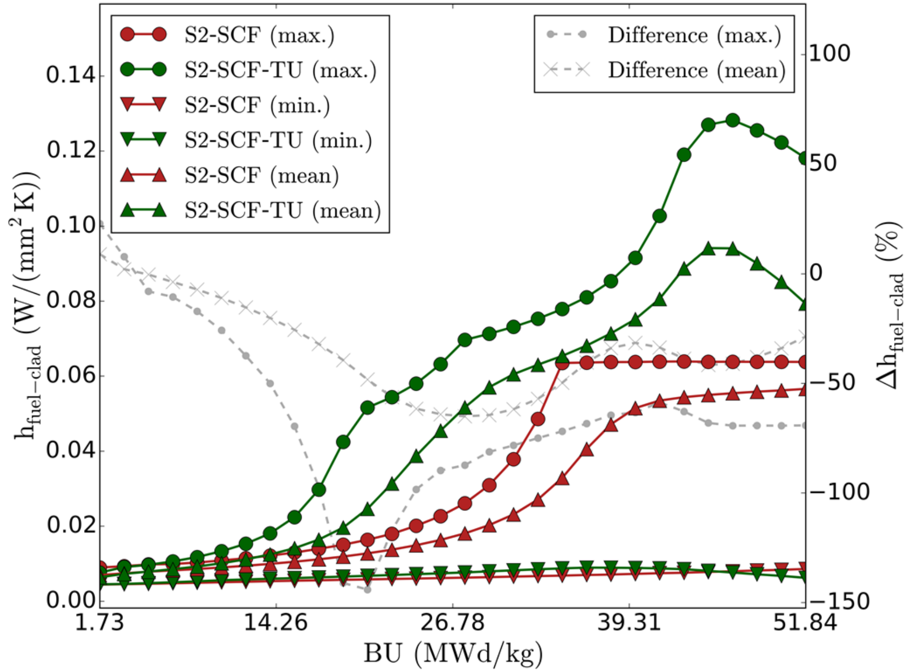
- Gap temperatures:
  - Minor differences in cladding temperatures due to material properties
  - Significant differences in fuel outer temperatures relative to the temperature step in the gap

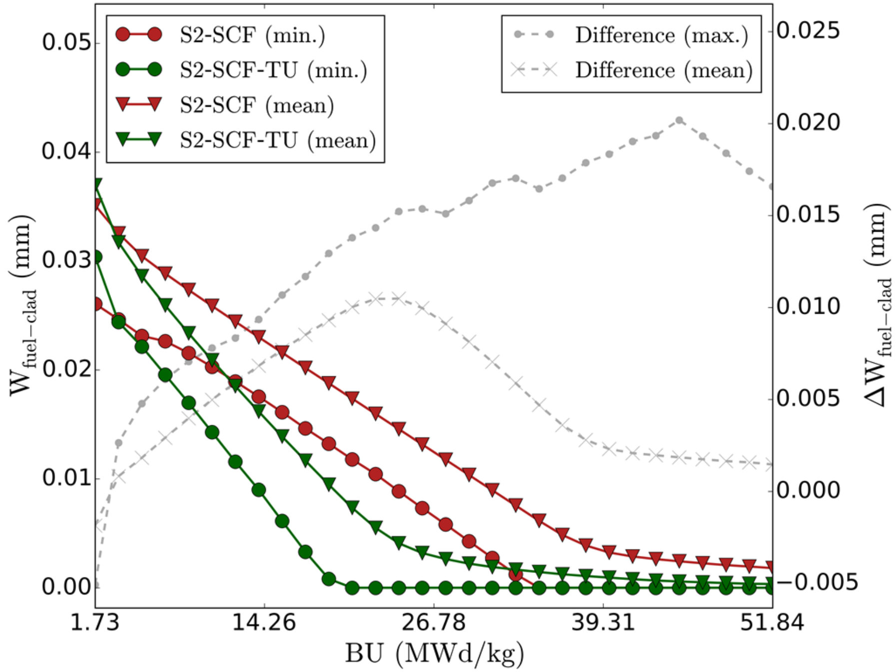




Serpent2-SCF-TU: depletion analysis

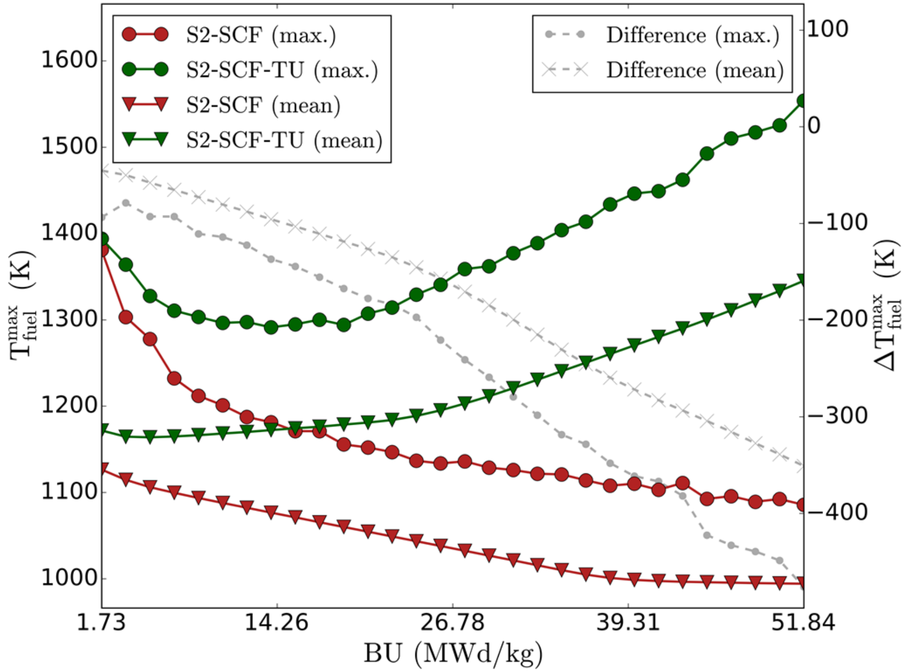
- Gap properties:
  - Heat transfer coefficient underpredicted by SCF (~50% on average)
  - Gap width over predicted by SCF (~0.005mm)
  - Larger gap temperature increase for SCF

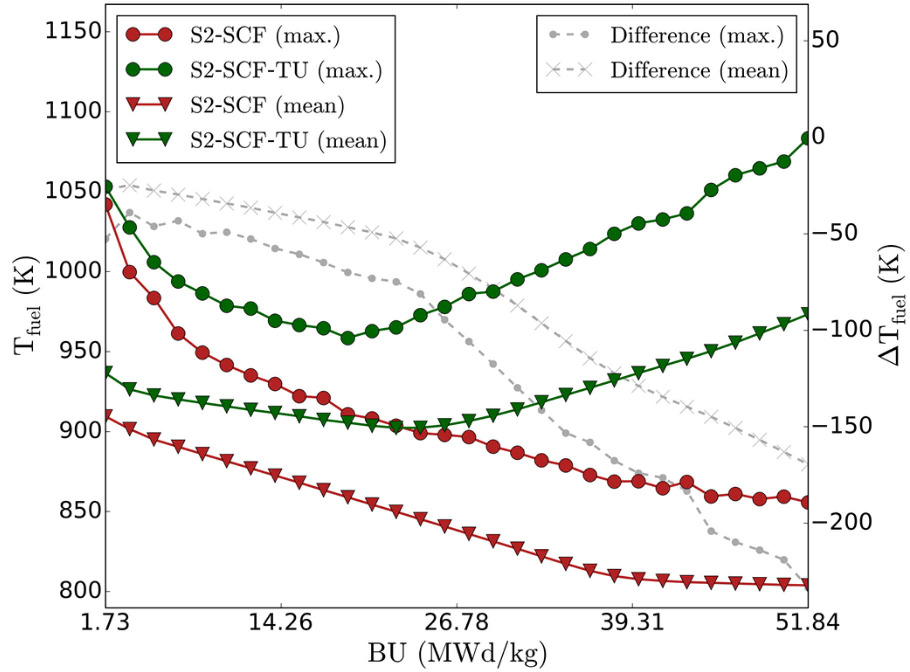




Serpent2-SCF-TU: depletion analysis

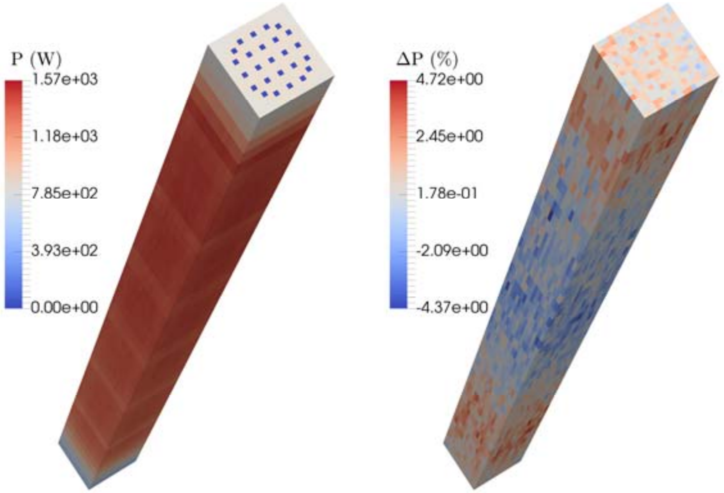
- Fuel temperatures:
  - Significant underprediction by SCF
  - Differences mostly due to conductivity degradation with burnup

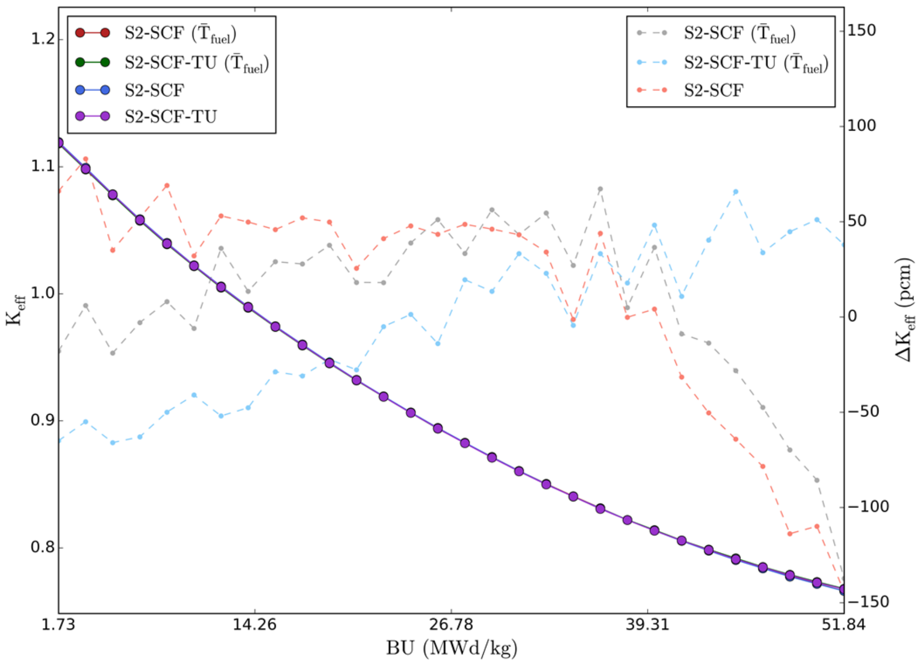


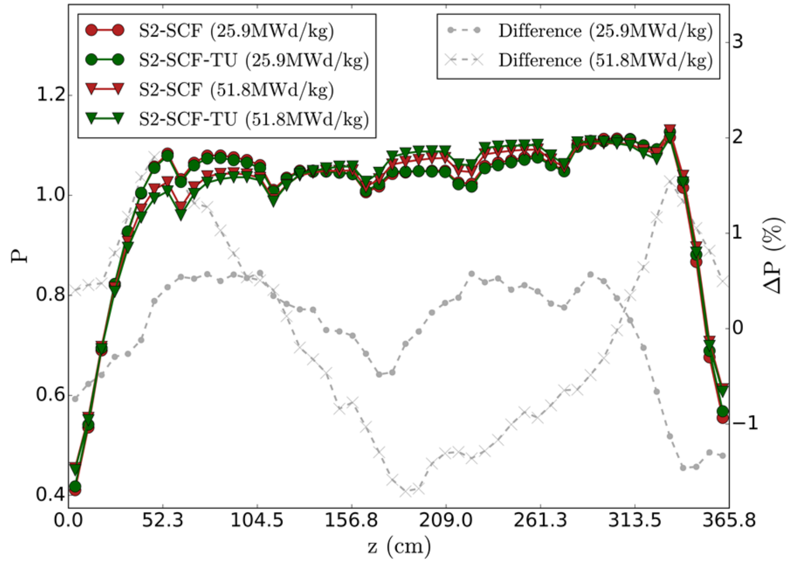


Serpent2-SCF-TU: depletion analysis

- Neutronic solution:
  - Very small impact on multiplication factor
  - No improvement using radial temperatures
  - Power dominated by statistical uncertainty

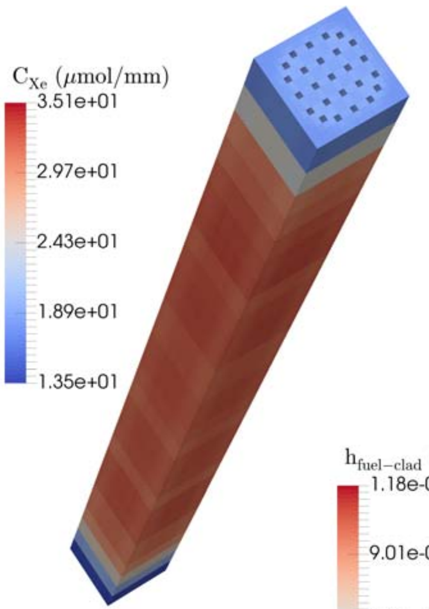




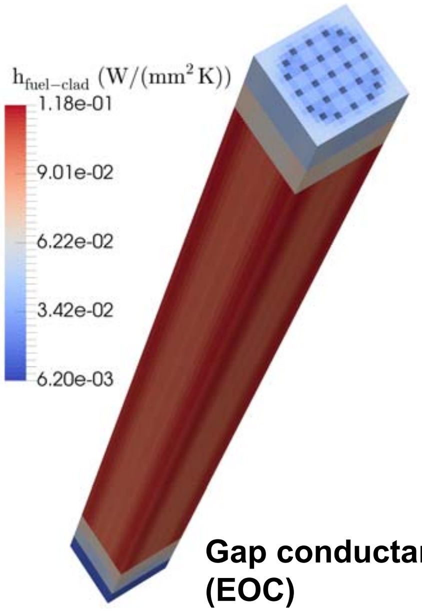


Serpent2-SCF-TU: depletion analysis

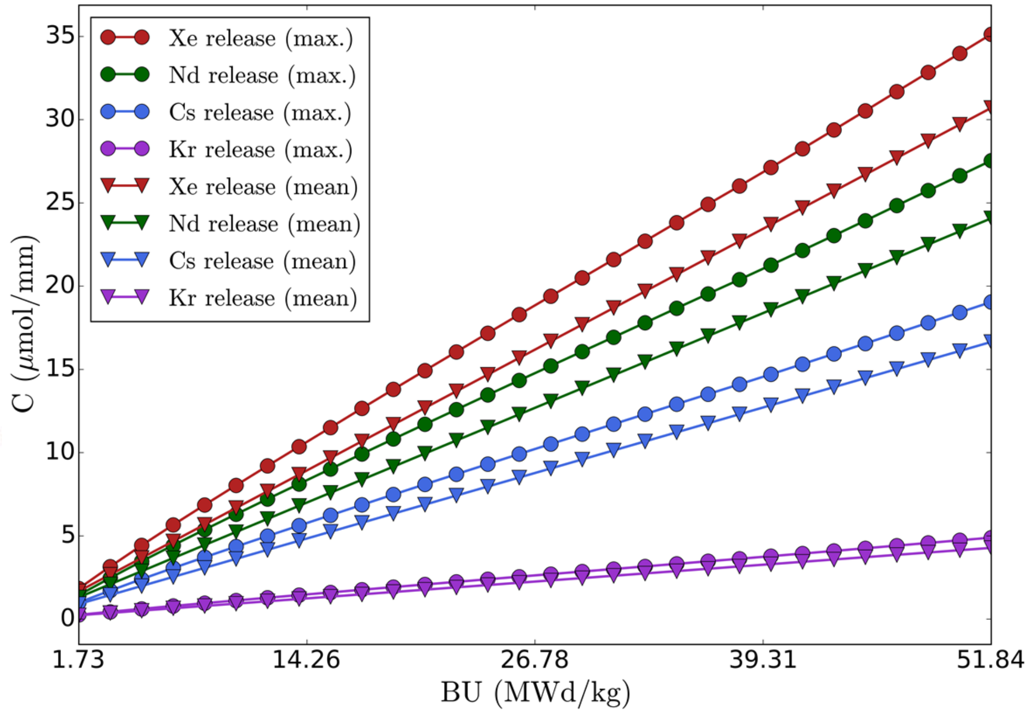
- Fuel-performance results:



Xe release



Gap conductance (EOC)



Takeaways from fully coupled burnup

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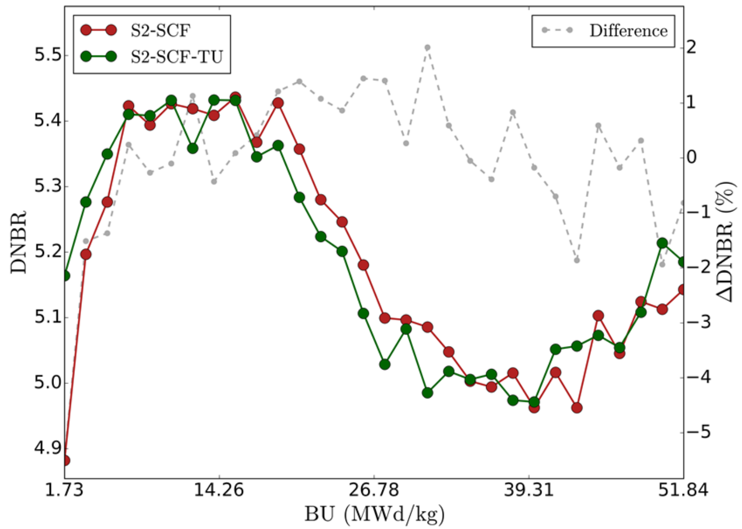
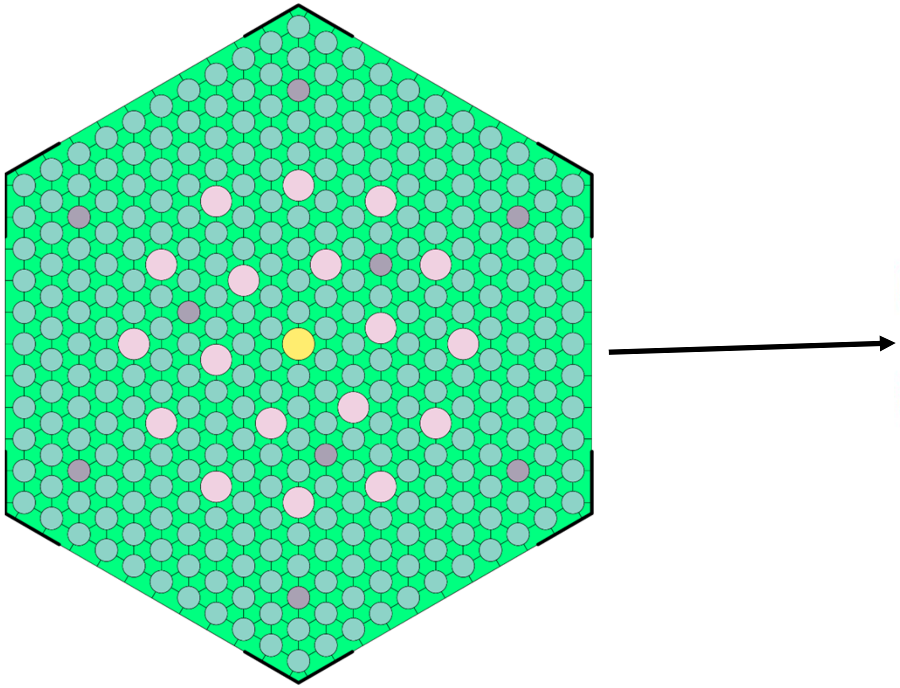
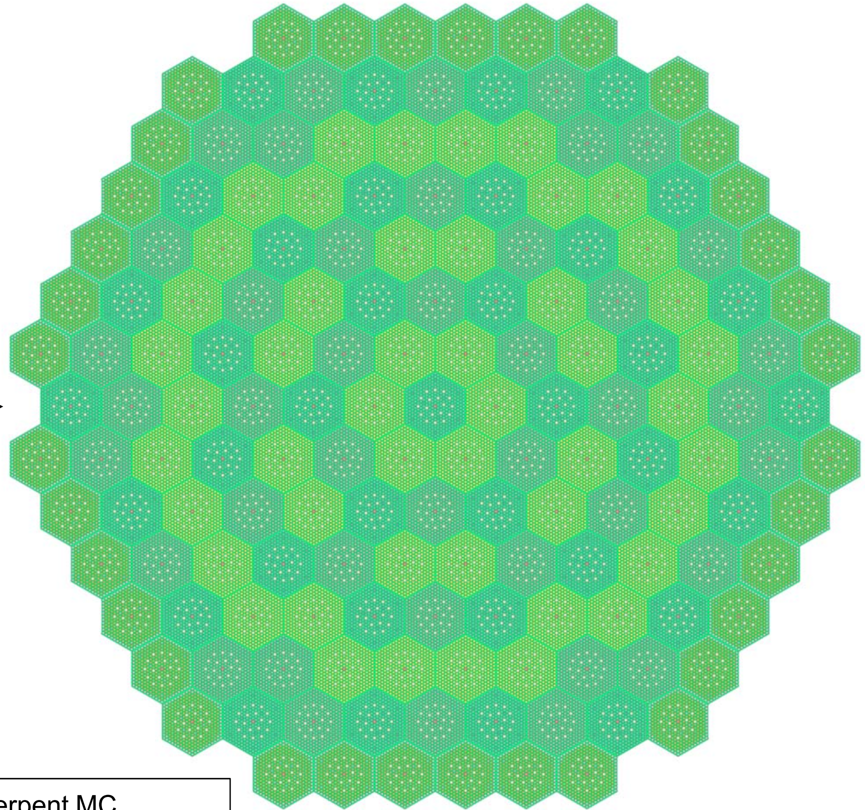
- Gap behavior:
  - Significant improvement in the conductivity and width using TU.
  - Reference solution for SCF to improve correlations
- Fuel temperatures:
  - Underprediction in SCF up to ~350K (centerline) and ~175K (average)
  - Reference solution for SCF to improve material properties
- Neutronics:
  - Minor impact in local and global results
- Safety parameters:
  - No significant impact on neutronics
  - No impact on DNBR calculation
  - Large improvement in fuel temperatures
  - Pin-by-pin fission gas release
  - Pellet-cladding interaction modelled



Towards full-core pin-by-pin depletion

- Massive computational requirements [5]:
  - ~10^9 neutrons per transport cycle
  - ~1-5TB of memory, mainly for burnable materials

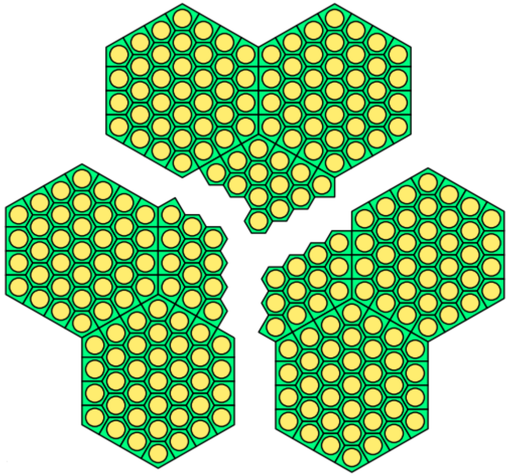


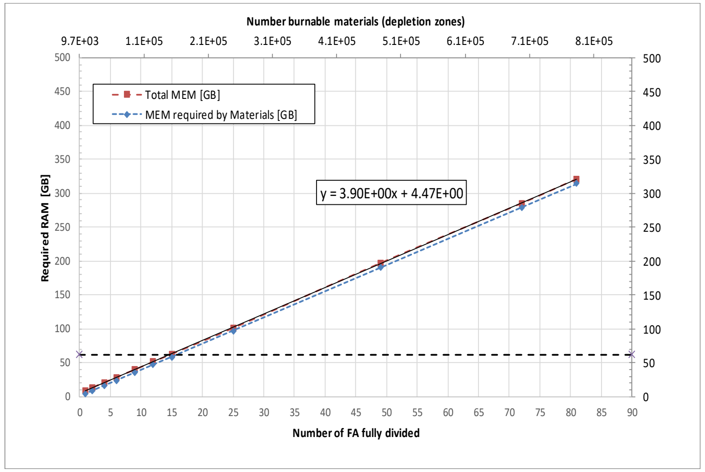


[5] "Foreseen capabilities, bottlenecks identification and potential limitations of Serpent MC transport code in large-scale full 3-D burnup calculations", D. Ferraro, M. García, et al., ICONE26.

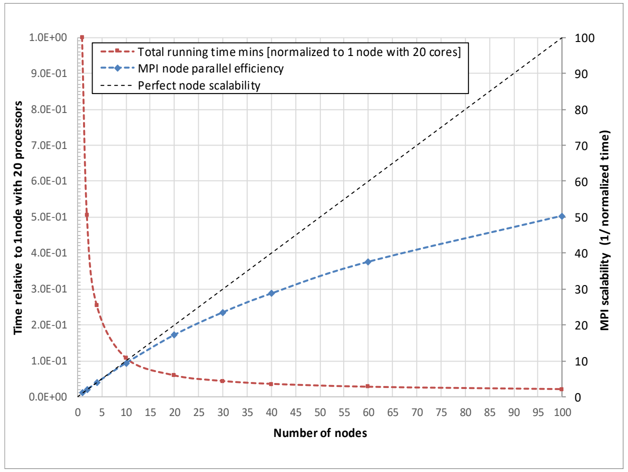
Collision-based Domain Decomposition

- Traditional parallel scheme for Monte Carlo transport:
  - Particle-based parallelism with domain replication
  - Usually excellent speedup, but no memory scalability
- Collision-based domain decomposition:
  - Data decomposition for burnable materials
  - Memory scalability, acceptable speedup

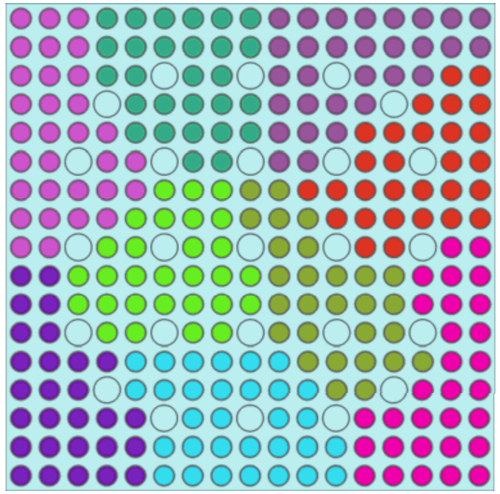




Multithread memory requirement

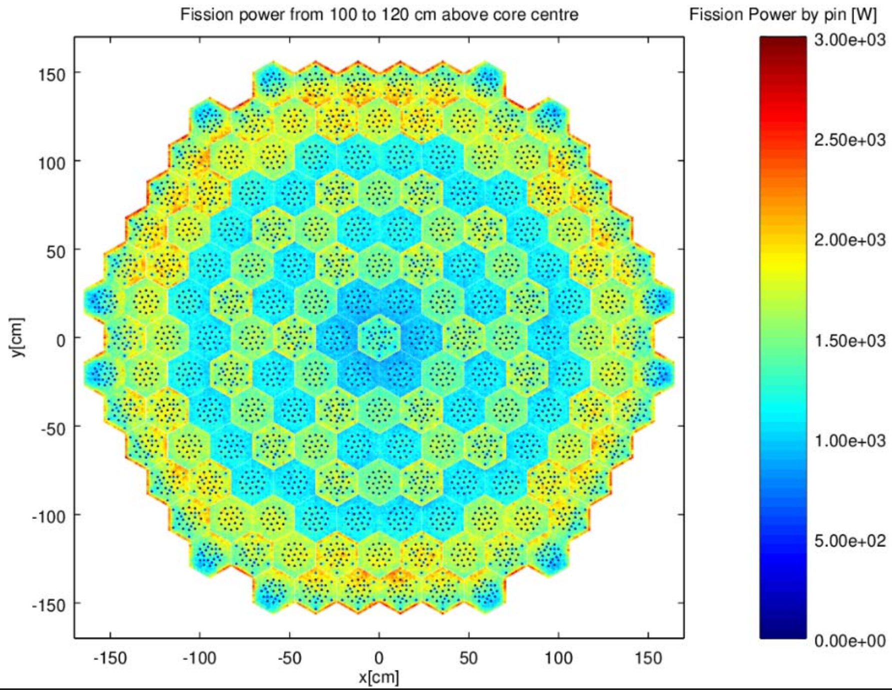


Parallel scalability

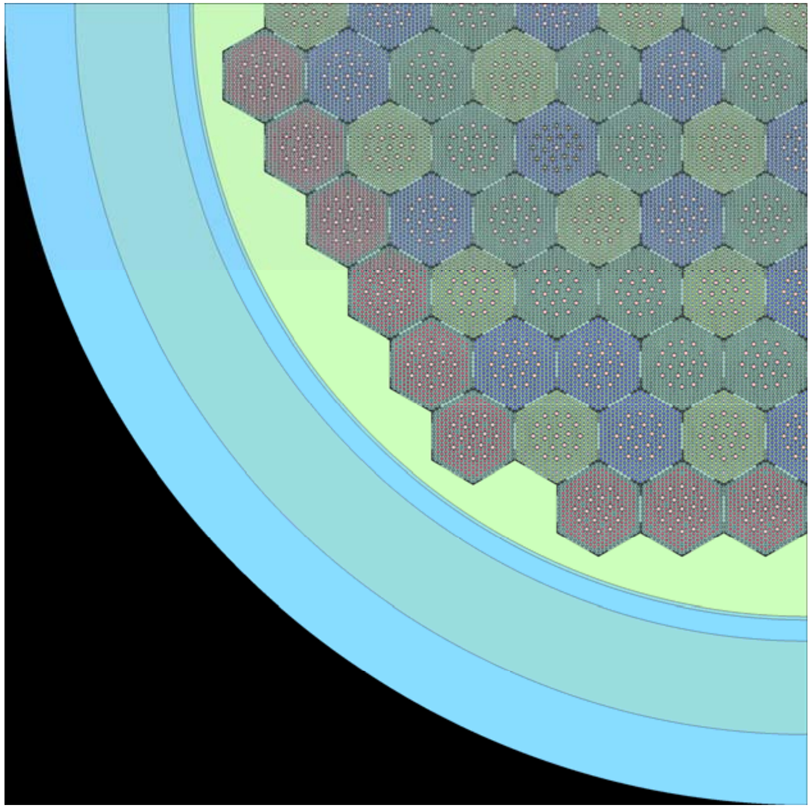


Full-core steady-state calculations

- Verification with the X2 VVER-1000 benchmark [6]:
  - ~150 pcm agreement with measured data at EOC (critical state)
  - Good agreement in global results

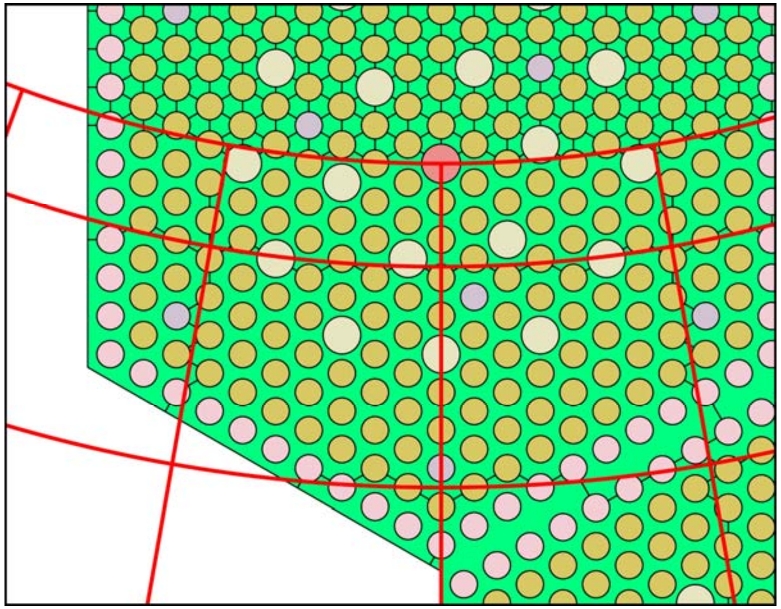


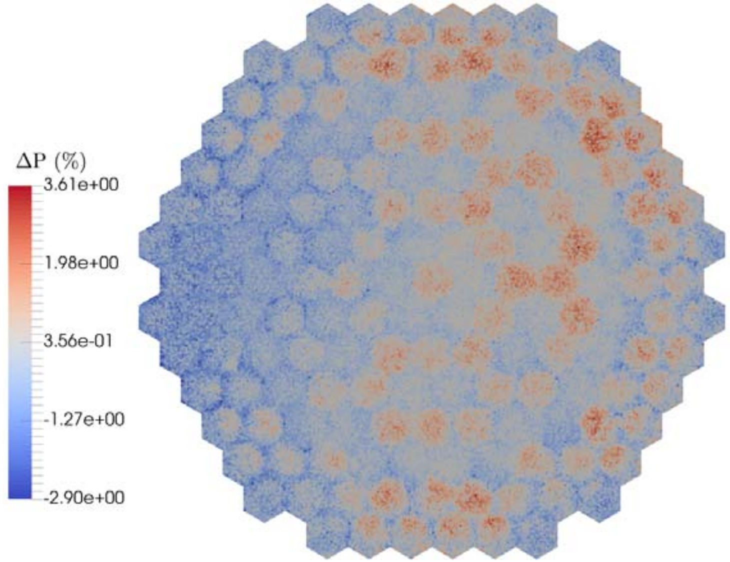
[6] "Serpent/SUBCHANFLOW coupled calculations for a VVER core at hot full power", D. Ferraro, M. García, et al., PHYSOR2020 (submitted).

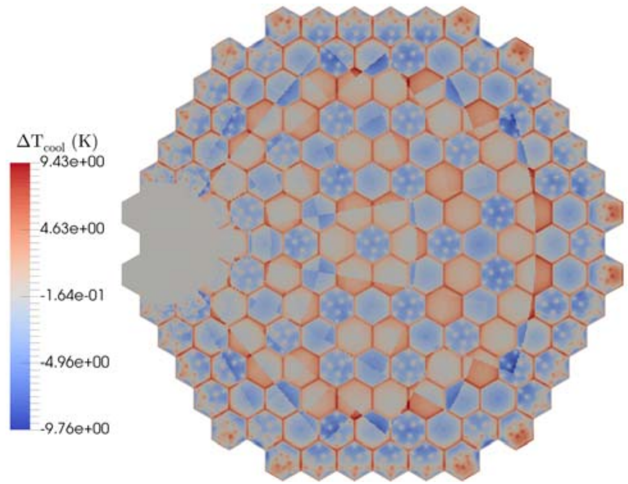


Subchannel coarsening

- Coarsening method [7]:
  - Build the subchannel model
  - Superimpose a mesh defining zones
  - Merge subchannels and condense hydraulic data for each coarse channel







[7] "A subchannel coarsening method for Serpent2-SUBCHANFLOW applied to a full-core VVER problem", M. García, D. Ferraro, et al., PHYSOR2020 (submitted).

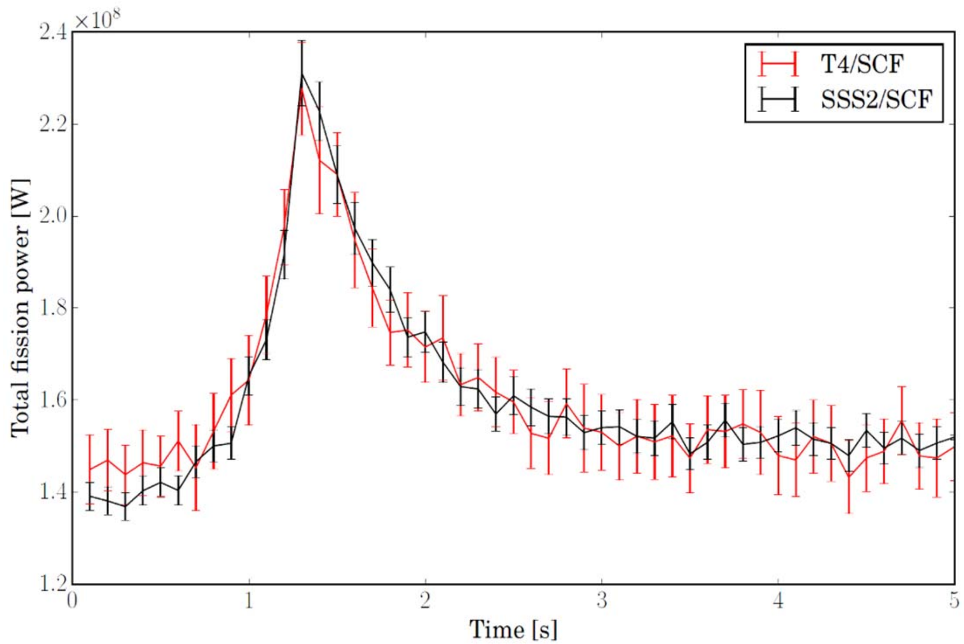
Transient analysis (1/2)

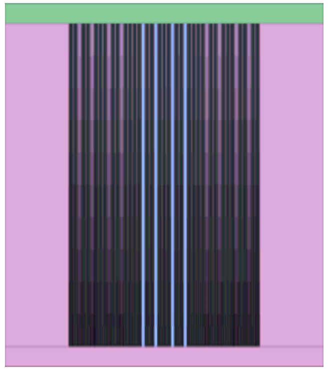
- **Goal:** Monte Carlo simulations of transients with feedback
  → **"move towards high fidelity calculations"**

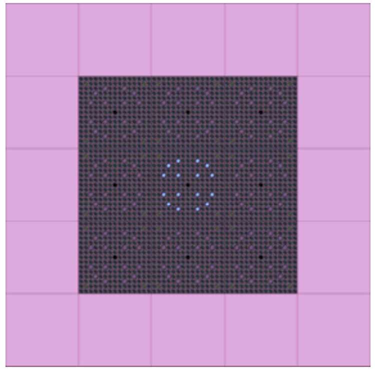
- **Development of dynamic MC-methods for transients analysis**
  - Development of **time-dependent dynSERPENT-SCF** e.g. implementation of methods to account for the prompt neutron and gamma heat deposition in the coolant
  - Development of **time-dependent dynTRIPOLI-SCF**
  - Development of **time-dependent 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 minicore (3x3 FA)

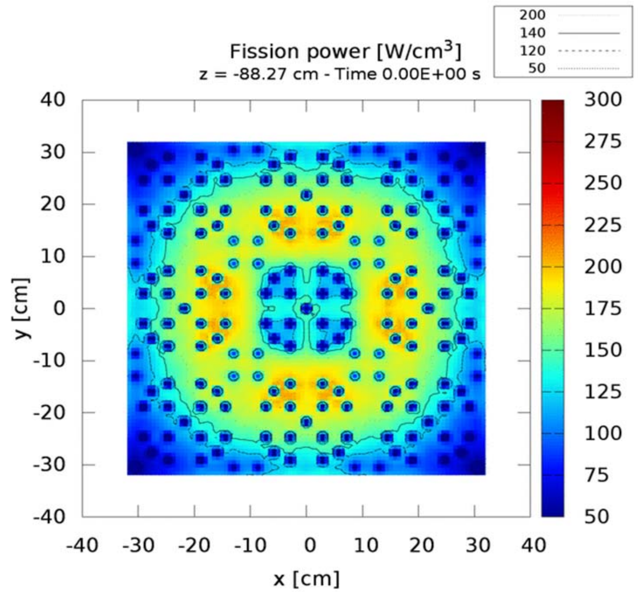
Transient analysis (2/2)

- Code-to-code verification with Tripoli4-SCF [8]









- Validation with SPERT-IIIE experiments [9]

[8] "Serpent/SUBCHANFLOW pin-by-pin coupled transient calculations for a PWR minicore". D. Ferraro, M. García, et al. Annals of Nuclear Energy (in press).

[9] "Serpent/SUBCHANFLOW pin-by-pin coupled transient calculations SPERT-IIIE hot full power tests", D. Ferraro, M. García, et al., Annals of Nuclear Energy (submitted).

Dissemination

- Project web-page: www.mcsafe-h2020.eu
- User Group
- Synthesis reports
- Newsletters
- Training Course
  - March 25-27, 2020 (KIT)

COURSE THEME

The course will focus on the multi-physics coupled tools developed within the McSAFE project and the lectures will cover the following topics:

a. Methods for full-core MC-depletion and optimized thermal-hydraulic feedback
b. Code integration and coupling methods
c. Developments of dynamic MC-methods for transient analysis
d. Validation of MC-based simulations using plant data for depletion, static and dynamic core analysis

COURSE STRUCTURE

The course consists of eighteen lectures (45 min. each) distributed over three days. Lectures will be given by international experts from KIT (Germany), VTT (Finland), CEA (France), DNC (the Netherlands), HZDR (Germany), KTH (Sweden) and UJV (Czech Republic) and will cover both theoretical aspects and practical demonstrations (i.e. solution of multi-physics problems with the developed coupling tools).

LOCATION

Karlsruhe Institute of Technology - Campus Nord, Building 521
Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen (Germany)

FEE

The course is free of charge. Participants have nevertheless to cover their own expenses (travel, food, accommodation).

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Project Website: www.mcsafe-h2020.eu

H2020 McSAFE High Performance Monte Carlo for Safety

- Institute for Neutron Physics and Reactor Technology (INR)
- Campus North, Building 521
- Date: March 25 - 27, 2020

KIT Karlsruher Institut für Technologie

H2020 McSAFE Training Course

(McSAFE: High-Performance Monte Carlo Methods for SAFEty Demonstration-From Proof of Concept to realistic Safety Analysis and Industry Applications)

MAIL GOALS OF THE TRAINING COURSE

Advances in computer capacity and parallel computing are nowadays making possible to use computing-intensive state-of-the-art methods for large-scale problems and realistic reactor geometries in order to cope with the needs of manufacturers, utilities and regulators for optimized nuclear reactor designs and improved safety analyses. Under this framework, highly accurate numerical methods and codes are being developed worldwide in order to predict local safety parameters of reactor cores at steady state and transient conditions. McSAFE (High Performance Monte Carlo Methods for SAFEty Demonstration) is a coordinated H2020 EU research project with the overall objective of the to move the Monte Carlo based stand-alone and coupled solution methodologies (advanced depletion, optimal coupling of MC-codes to thermal-hydraulic solvers, time-dependent Monte Carlo and methods and algorithms for massively parallel simulations) to become valuable and widespread numerical tools for realistic core design, safety analysis and industry-like applications of LWRs of generation II and III. The envisaged McSAFE developments will allow on one hand to reduce the conservatism in the prediction of core safety parameters and on the other hand to increase the reactor performances and the operational flexibility. McSAFE is held in cooperation between code developers, methods developers and industry stakeholders, including twelve partners from eleven institutions of nine different countries around EU. Several calculation tools are being used within the project, including not only the TRIPOLI (CEA), SERPENT (VTT), MONK (WOOD) and MCNP (LANL) Monte Carlo transport codes but also the sub-channel code SUBCHANFLOW (KIT) and the fuel performance code TRANSURANUS (JRC). In order to disseminate the knowledge generated within the McSAFE Project, a Training Course open to young engineers, scientists, as well as professionals coming from the industry, is organized.

Summary

- Development stage (first two years) almost over
- Serpent2-SCF(-TU) coupling implemented and optimized
- Validation stage (last year) beginning, preparation of experimental data and core specifications in progress
- Depletion calculations:
  - Serpent2-SCF-TU fully-coupled depletion scheme:
    - Improvement in the modelling of the fuel during irradiation
    - Minor impact on the neutronic solution
    - Large impact on safety parameters such as gap behavior and fuel temperature
  - Optimization for full-core pin-by-pin problems:
    - Subchannel coarsening methodology for SCF and CDD for Serpent2
- The project will deliver **improved** and **validated high-fidelity numerical simulations tools** that can be used by different end-users to provide **reference solutions to deterministic codes for safety demonstration**