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

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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 scarce 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

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)
High-fidelity multiphysics

- **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

\[ \rho_{\text{cool}}, T_{\text{cool}} \]

\[ P \]

\[ T_{\text{fuel}} \]
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 $\rho_{cool}$, $T_{cool}$ and $T_{fuel}$ used in Serpent2
  - Iterative scheme with pin-by-pin feedback

- Verification with the VERA Core Physics Benchmark (PWR) [1]

<table>
<thead>
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<th>Result</th>
<th>Keff</th>
<th>$\Delta$Keff (pcm)</th>
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<td>RMC-CTF</td>
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<td>Serpent2-SCF (OO)</td>
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<td>Serpent2-SCF (MS)</td>
<td>1.16560±0.00003</td>
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</tbody>
</table>

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]

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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)

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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

![Graph showing temperature changes over burnup (BU) for S2-SCF and S2-SCF-TU, with differences highlighted.](image-url)
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
Fuel-performance results:

- Xe release
- Gap conductance (EOC)

Graph showing Xe release (max.) and Xe release (mean) against BU (MWd/kg).
Takeaways from fully coupled burnup

- **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]:
  - \( \sim 10^9 \) neutrons per transport cycle
  - \( \sim 1-5 \text{TB} \) of memory, mainly for burnable materials

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

Subchannel coarsening

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

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]

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Dissemination

- User Group
- Synthesis reports
- Newsletters
- Training Course
  - March 25-27, 2020 (KIT)
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**