



McSAFE

***High-Performance Monte Carlo Methods for SAFETY Demonstration-
From Proof of Concept to realistic Safety Analysis and Industry
Applications***

Research and Innovation actions

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Generation II and III reactors**

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Summary

In this report the progress and achievements obtained during the period March 2019 till September 2019 of the McSAFE project are presented for interested parties and possible users of the advanced computer codes and methods for accurate nuclear reactor calculations that will be available after completion of the project.

It is demonstrated that reactor core criticality calculations can be executed with thermal-hydraulic and thermo-mechanical feedback. Depletion calculations are now possible with Serpent2 with large numbers of separate zones for depletion. For the Serpent2, TRIPOLI4 and MCNP6 Monte Carlo codes dynamic versions are available and reactor transient calculations are shown taking into account the generation and decay of delayed neutron precursors and including thermal-hydraulic feedback. Variance reduction in the Monte Carlo calculations and methods for increasing the efficiency of parallel execution of the Monte Carlo codes are continuously improving.

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High-Performance Monte Carlo Methods for SAFETY Demonstration-From Proof of Concept to realistic Safety Analysis and Industry Applications




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1. Introduction

The overall objective of the McSAFE project [1] is to move the Monte Carlo based stand-alone and coupled solution methodologies to become valuable and widespread numerical tools for realistic core design, safety analysis and industry-like applications of LWRs of generation II and III. As Monte Carlo codes are very flexible with respect to reactor geometry and composition, the results of the project will also be useful for future types of nuclear reactors as well as to research reactors with complicated geometries and unusual constructions for experimental research applications. Main targets in the development are advanced depletion, optimal coupling of Monte Carlo codes to thermal-hydraulic and thermo-mechanical solvers, time-dependent Monte Carlo and methods for massively parallel simulations.

On one hand, the envisaged developments will permit to predict important core safety parameters with less conservatism than current state-of-the-art methods. On the other hand, they will make possible the increase in performance and operational flexibility of nuclear reactors.

We foster the dissemination of knowledge gained in the project by experienced researchers to become available to any interested party and possible future users of the codes and code systems under development. To that end several actions are planned, like a tailored training course that will be organised in March 2020 in Karlsruhe, Germany, or actions already undertaken, like digital newsletters and synthesis reports. The first newsletter was sent out in August 2018. A second newsletter will be issued in August 2019 and a copy is available via Ref. 2. The first synthesis report was issued in February 2019 and the current report is the second synthesis report. At the end of the project in August 2020 a third newsletter and synthesis report will be issued.

Within this scope of dissemination of results, the synthesis reports are issued to inform interested parties about the goals and progress made in the McSAFE project. This first synthesis report covers the first one and a half year of execution of the McSAFE project. The current second synthesis report covers the next 6 months of the project and the third synthesis report will cover the last 12 months of the project.

Moreover, to boost the exploitation of project results, an exploitation plan was issued as well as a detailed dissemination and communication plan, in which potential users of the McSAFE tools and methods were identified with the help of all project partners.

An overview of the McSAFE project is represented at the international FISA conference in Pitesti, Romania, and will be presented at the Physor conference in Cambridge, UK, March/April 2020. Several presentations about specific parts of the research were given at the ICONE conference in Tsukuba, Japan, May 2019 and the ICAPP conference, Juan-les-Pins, France, May 2019, or are submitted to the Physor conference in Cambridge, UK, March/April 2020. Various papers are published or submitted to international scientific journals like Annals of Nuclear Energy.

2. The McSAFE Project

Monte Carlo methods are nowadays in wide spread use for nuclear reactor calculations. Although their capabilities have increased considerably over the last decades, supported by the increase in computer power, calculation of detailed power distributions throughout the core of a full-size reactor with sufficient statistical accuracy in acceptable computing time is still questionable.

Moreover, for reactor operation evaluation the actual temperature distribution in the reactor core must be taken into account. Hence, coupling of the Monte Carlo calculation with a thermal-hydraulic calculation is necessary, which must normally be executed in an iterative way. Also the thermo-mechanical behaviour of the reactor core must be taken into account. Hence, coupling of the Monte Carlo code with a thermo-mechanical code has become a prerequisite for reactor calculations.

Another challenging task for Monte Carlo is a proper depletion calculation. Most general-purpose codes devoted to reactor physics have an option for depletion calculations, but they take long calculation times and their stability can often be questioned.

For safety analysis not only the static properties of the reactor core are important, but also the dynamic behaviour of the core. This requires the extension of the Monte Carlo code with time dependence. For prompt neutrons this time dependence is often included in the original codes, but for transient reactor calculations delayed neutrons and their precursors are of utmost importance and require a separate treatment in the Monte Carlo code. Transient calculations also require adequate modelling of control rod movements and, for instance, boron dilution.

This gives a sketch of the main lines of the McSafe project [1]: to develop Monte Carlo codes suitable for Monte Carlo calculations coupled with thermal-hydraulics and thermo-mechanics for a full-size reactor core, including depletion (burnup) and time-dependence for reactor transients. Coupled codes can be implemented in the NURESIM computer platform [3,4], which is based on the Salomé platform [5].

Participants in the McSAFE project are:

Karlsruhe Institute of Technology (KIT, coordinator; Germany)

Delft Nuclear Consultancy (DNC; The Netherlands)

Commissariat à l’Energie Atomique et aux Energies Alternatives (CEA; France)

UJV Rez, a.s. (UJV;Czech Republic)

Helmholtz-Zentrum Dresden-Rossendorf (HZDR; Germany)

Wood (Wood; United Kingdom)

Technical Research Centre of Finland (VTT, Finland)

Royal Institute of Technology (KTH; Sweden)

Joint Research Centre (JRC; EU)

E.ON Kernkraft GmbH (EKK; Germany)

CEZ a. s. Nuclear Power Plants (CEZ; Czech Republic)

Electricité de France (EdF; France)

Each partner brings in its typical experience to one or more of the subjects under development in the McSAFE project. This can be a general-purpose Monte Carlo reactor code, a thermo-hydraulics or thermo-mechanics code, experience in coupling codes or in depletion or time-dependent calculations or providing reactor plant data for validation of the developed code combinations.

In the McSAFE project 4 different Monte Carlo codes are considered, 3 of them being developed in Europe: Serpent2 (VTT), Tripoli4 (CEA) and Monk (Wood). The US Monte Carlo code MCNP6 (LANL) is extended and tailored for the project by DNC. The major thermo-hydraulics code used in the project is SubChanFlow (SCF; KIT). The major thermo-mechanics code used in the project is TransUranus (TU, JRC).

The McSAFE projects benefits from the achievements of the former EU HPMC project. Its goals are in line with the priority topics of NUGENIA and the SNETP platform.

3. Progress in Monte Carlo methods and depletion calculations

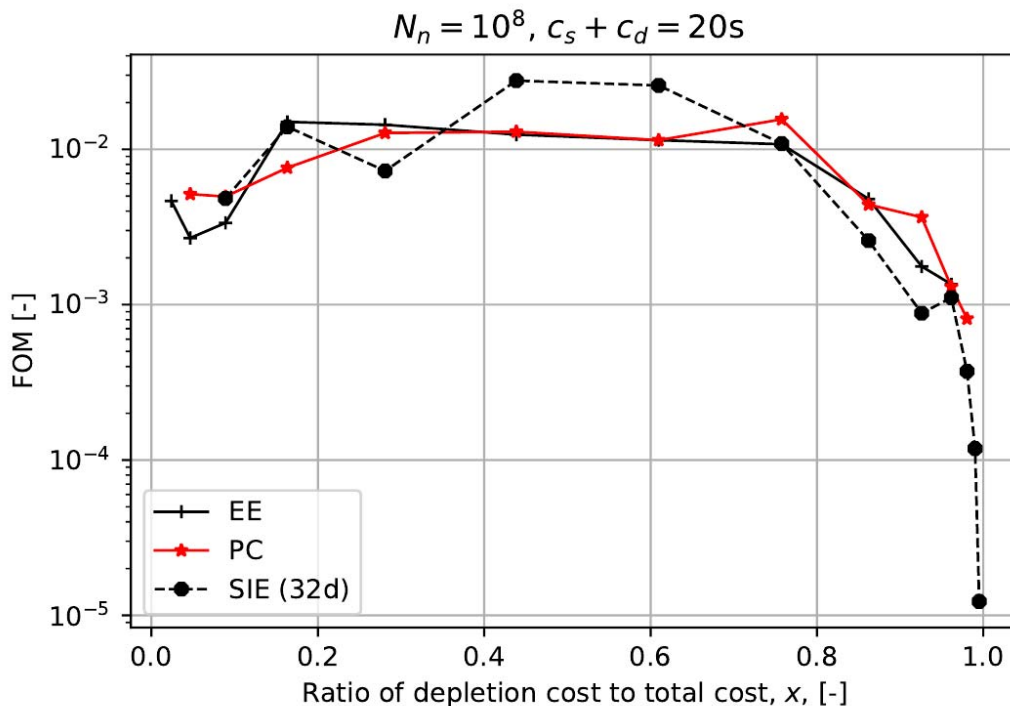
In the McSAFE project the Monte Carlo method is the corner stone for neutron transport. Although each of the Monte Carlo codes used in the project has been developed for a long time and has a history of continuous extensions and improvements, several items are identified for further improvement to achieve the efficiency needed for detailed full-core calculations. Therefore, various participants worked on smaller and larger improvements, which cannot all be discussed in this report. Hence, only a selection of subjects will be detailed here.

3.1 Depletion methodology

In Monte Carlo depletion calculations an important subject is to optimise the time step length and the number of neutron histories simulated at each time step. To solve that issue we developed a special simplified and fast solver to carry out a very large number of test simulations to map the efficiency of depletion simulations with various combinations of parameters.

Since the previous reporting, the final set of test simulations has been completed and results have been analysed. The results suggested that the most efficient simulations spent about equal computing time in Monte Carlo neutron transport simulations as in all other computing procedures (such as in depletion calculations, loading and processing of nuclear cross sections by the Monte Carlo code, processing data, etc.). We also justified this observation theoretically using a simple model of convergence of Monte Carlo depletion simulations.

Fig. 1. Figure of Merit (FoM) for variable cost ratios

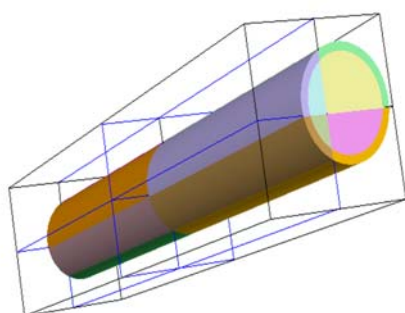


Based on this result, a new methodology was suggested. The methodology automatises the selection of the time step length as well as the number of criticality cycles that must be done at each time step. The new methodology was described in detail in a journal manuscript submitted to Annals of Nuclear Energy [6]. Fig. 1 shows the Figure of Merit (FoM) for one of the test sets as a function of depletion cost to total cost of the calculation, which shows a maximum for a ratio of about 0.5.

3.2 Thermal-hydraulic and depletion mesh interpolation

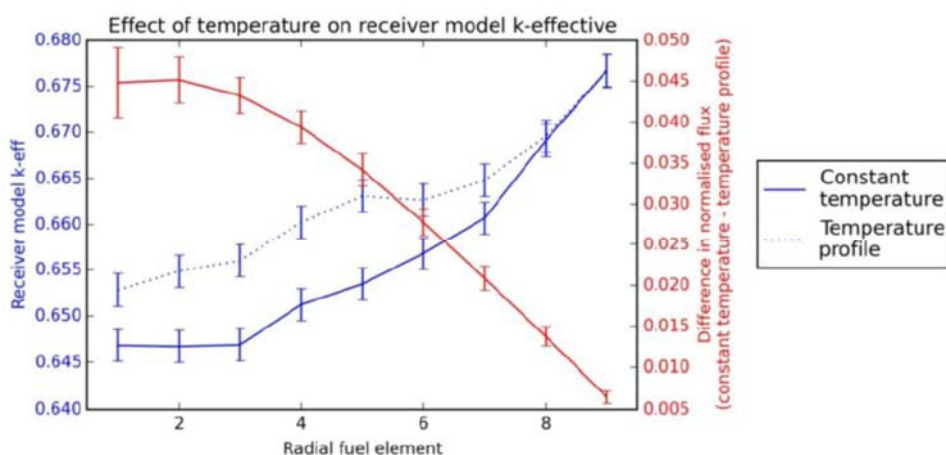
In order to model spatially-dependent depletion of a specific material it is necessary to represent that material by a unique model material in each spatial zone in which unique depletion can be calculated. To achieve this in the MONK code a burnup (BU) mesh is superimposed on the reactor core and an artificial material is automatically assigned in each spatial zone requiring unique burn-up to be calculated – see Fig. 2.

Fig. 2. Section of a fuel pin with sixteen artificial materials resulting from the overlaid mesh



In order to transfer heating, temperature and density data between MONK and a thermal-hydraulic code a spatial mesh (known as the thermal-hydraulics, or TH mesh) is overlaid on the reactor core. MONK merges the BU and TH meshes to form the BUTH mesh and this is used to generate the artificial materials. During tracking MONK tallies the reaction rates in each artificial material, and uses these reaction rates to calculate the heating power in each cell of the TH mesh. The heating powers in the TH mesh are then mapped to the spatial mesh used in the thermal-hydraulic code. The output of the thermal-hydraulic code includes temperatures and densities which are mapped onto the MONK TH mesh. The revised temperatures and densities are applied to the artificial materials in the MONK calculation in the subsequent time-step of the burn-up calculation.

Fig. 3. Effect of applying a realistic temperature profile on k_{eff}

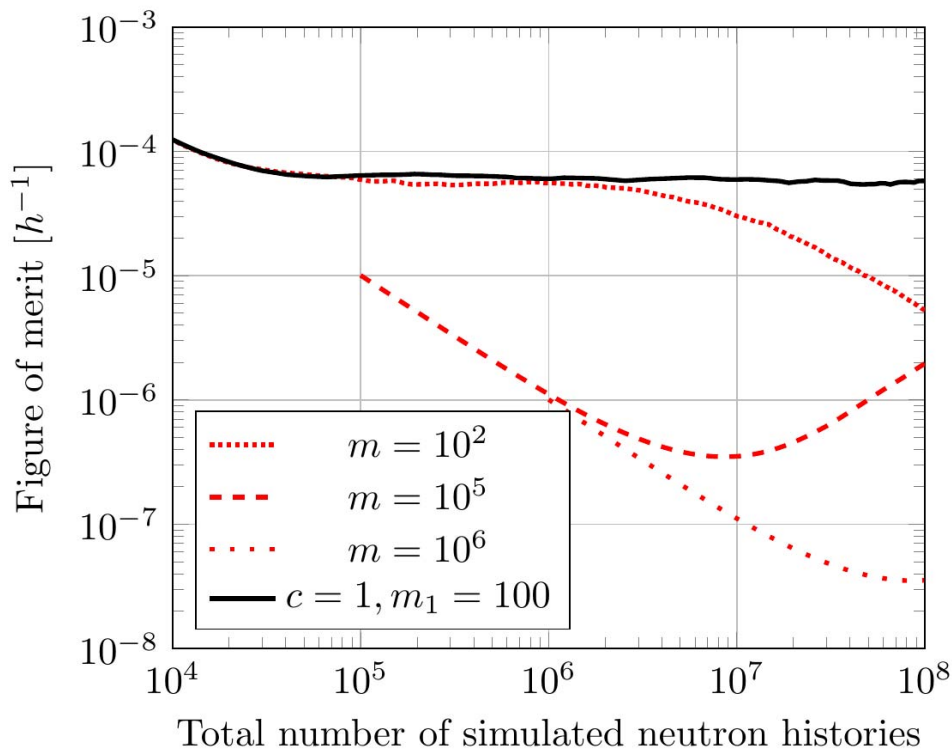


Thermal-hydraulic coupling can have a significant effect on the estimated core reactivity as shown in Fig. 3. The figure displays k -effective in a model core assuming constant temperature and compares this with the case of a temperature profile.

3.3 Optimisation of MC and MC-TH

To optimise Monte Carlo criticality calculations a source convergence acceleration method based on a variable neutron population size over the successive criticality cycles was developed during the first period of the McSAFE project. This work has now been completed and the method is implemented into the SERPENT 2 code and published in a journal article in *Annals of Nuclear Energy* [7]. Fig. 4 shows the Figure of merit as a function of the number of histories for the optimised case and compared with usual strategies.

Fig. 4. Figure of merit for optimised Monte Carlo criticality calculation



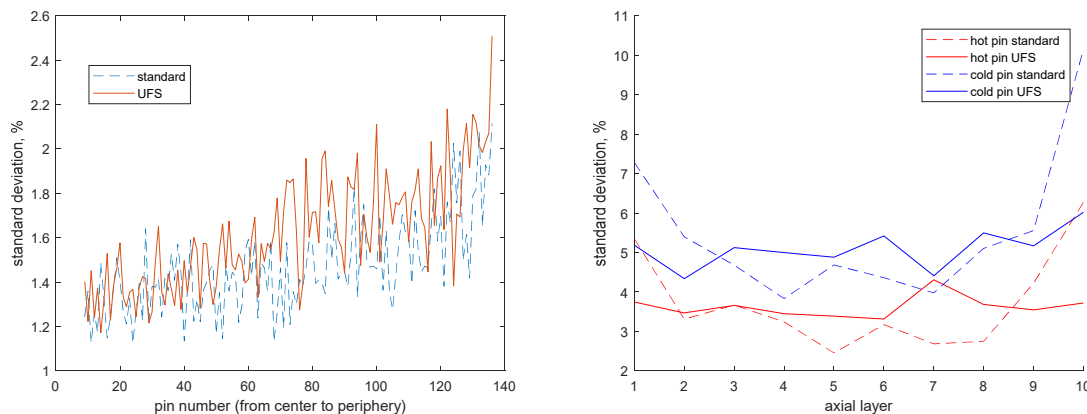
3.4 Multi-physics interface

A new multi-physics interface has been developed for TRIPOLI-4®. Preliminary details have been provided in the previous Synthesis Report. The SALOME-based interface has been extensively tested for the TMI fuel assembly simulations in stationary regime (in collaboration with KIT and VTT) [8] and for the mini-core benchmark in transient regime [9]. This new interface can now be controlled by a C++ supervisor, which allows performing efficient coupling with other simulation codes.

3.5 Uniform Fission Sites (UFS)

In co-operation with VTT, HZDR evaluates the idea of combining the uniform fission sites (UFS) and response matrix methods in order to obtain an acceptable statistical variance in full-core calculations of local parameters throughout the whole reactor core at the same time keeping computation costs as low as possible. Previously it was found that the application of the UFS method to a realistic full-core model (based on fresh BEAVRS HZP configuration) has no significant effect on radial power variance but equalises the axial distribution of variance of local power, decreasing variance in periphery layers and increasing it in central layers (see Fig. 5).

Fig. 5. Effect of UFS on power uncertainty

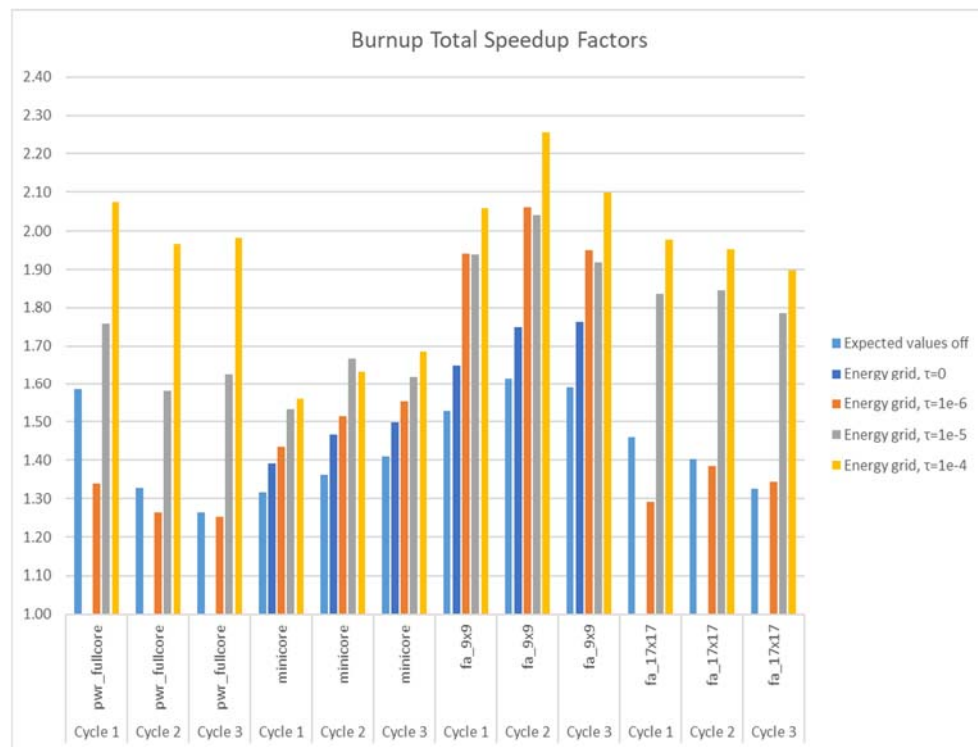


Since last report, VTT has implemented common spatial discretisation for response matrix and UFS methods and direct usage of response matrix results to obtain UFS weight factors. Testing have shown sensitivity of UFS effect on spatial discretisation due to relatively strong fission source gradients on core periphery. On the other hand, to produce a reliable solution, the response matrix solver requires sufficient neutron statistics in each spatial region, which limits common discretisation to relatively coarse meshes.

3.6 Speedup of cross-section lookup

One of the most frequently performed operations in a Monte Carlo radiation transport simulation is to evaluate the nuclear data pertaining to a particle at its current energy. This is particularly important for burnup calculations which require many reactor physics calculations to accurately model fuel depletion. With the advent of continuous energy representations of the nuclear data this has become computationally even more expensive. A number of developments have been implemented and trialled in the MONK code aimed at improving the computational efficiency of this process. This includes the use of a unified energy grid for evaluating the total cross section and turning off some of the $k_{\text{effective}}$ estimators when using the unified energy grid. Four test cases have been used to evaluate the performance of the above measures for three burnup cycles: a 9x9 fuel assembly; a 17x17 fuel assembly; a mini-core; and a PWR core. Figure 6 shows that the above modifications resulted in roughly a factor of two speedup for the chosen test cases.

Fig. 6. Speedup of depletion calculations

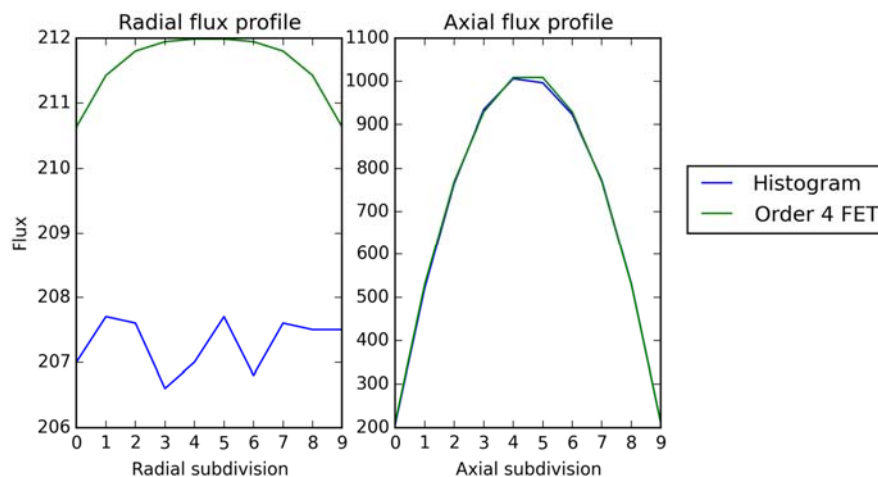


3.7 Functional expansion tallies

In the functional expansion tally (FET) a Monte Carlo simulation is used to calculate the functional expansion coefficients for flux distributions with respect to an orthogonal set of basis functions. The collision density based FET implemented in MONK involves calculating an expansion for the quantity of interest, in this case the neutron flux, in terms of Legendre polynomials.

A test case used a single PWR pin cell in an infinite lattice, based on the Hoogenboom and Martin benchmark. Figure 7 shows comparisons between the classic histogram tally and the FET for the axial and radial variation of the neutron flux in the pin cell model. These were scored simultaneously using exactly the same samples. In the axial direction the FET and the histogram methods give very similar results except that the FET respects the inherent symmetry in the

Figure 7: Comparison of radial and axial flux profile along a line for the pin cell model



problem. On the other hand, in the radial direction only the functional expansion tally is able to give a more meaningful representation of the neutron flux spatial distribution.

3.8 Validation for a VVER reactor

High-fidelity investigations have been performed for the modelling of hexagonal VVER fuel assemblies in Serpent2 coupled with the thermal-hydraulics code SubChanFlow. Coupling is on a pin-by-pin bases. Structural components are explicitly modelled, like stiffeners and grid spacers.

Various test calculations show that the impact of fuel-centered subchannels amounts to 4 K in coolant temperature and 0.2 % in power. The impact of the stiffeners amounts to 2 K in the local coolant temperature and is negligible for the power.

To benchmark the calculations the fuel assembly models are scaled up to a full-core VVER-1000 reactor. The calculated effective multiplication factor is 1.00149 ± 0.00008 . Hence the agreement is up to about 150 pcm.

Fig. 8. Horizontal and vertical cross section of the VVER-1000 core

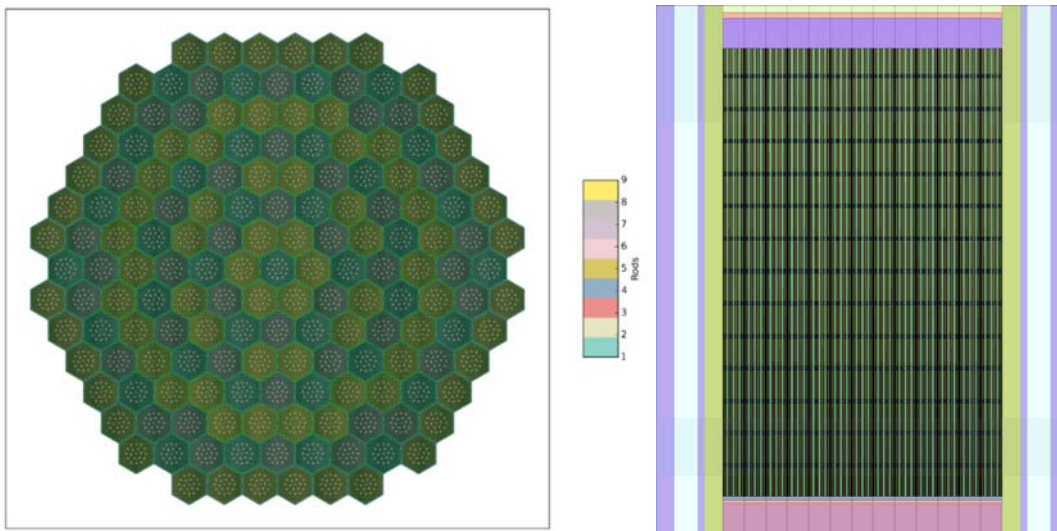
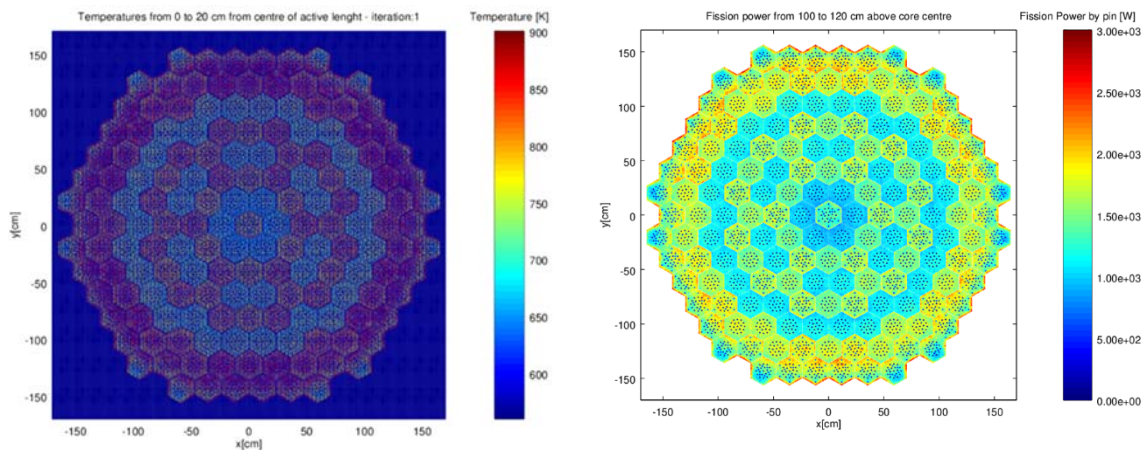


Fig. 8 shows the detailed horizontal and vertical cross section of the reactor core with all fuel assemblies and radial and axial reflector and construction parts. Fig. 9 (left) shows the horizontal distribution of fuel temperatures through the core just above the core midplane. The figure at the right shows the generated fission power at higher positions in the ore. The figures illustrate the detailed information used for the thermal-hydraulic feedback calculations.

As a next step in this type of calculations the complete depletion cycle of the core is tested. Considering memory requirements domain decomposition becomes mandatory.

Fig. 9. Fuel temperature distribution (left) and fission power distribution(right) through the core



4. Progress in coupling codes

For realistic reactor core calculations the effects of the temperature distribution in the core at full power operation must be taken into account, as well as thermo-mechanical effects due to temperature and pressure. To that end the Monte Carlo (MC) code for neutron transport must be coupled with a thermal-hydraulics (TH) code and a thermo-mechanical (TM) code.

For running externally coupled codes the Salomé computer platform [5] is adopted. Salomé is open-source software that provides a generic pre- and post-processing platform for numerical simulation. The SubChanFlow code (KIT, Karlsruhe) is used for the thermal-hydraulics calculation. The TransUranus code (JRC, Karlsruhe) is used for the thermo-mechanical calculations.

The TransUranus code describes the thermo-mechanical behaviour of a nuclear fuel rod during normal operation up until design basis accident conditions such as a LOCA or RIA. A solution is provided for distribution of the TransUranus code to the McSAFE partners that have a user licence. All the TransUranus input files for those benchmark problems defined in McSAFE for the demonstration of the coupling of TransUranus with Serpent and SubChanFlow are composed on the basis of simplified test cases.

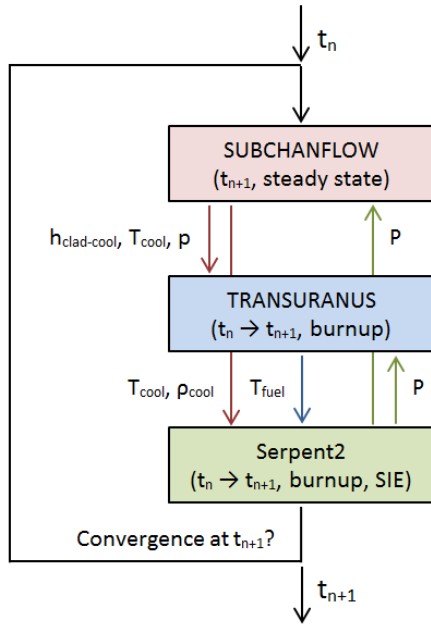
4.1 Coupling scheme for codes integrated in the Salomé platform

A new multi-physics interface has been developed for TRIPOLI-4®. Preliminary details have been provided in the first Synthesis Report. The Salomé-based interface has been extensively tested for the TMI fuel assembly simulations in stationary regime (in collaboration with KIT and VTT) [8] and for the mini-core benchmark in transient regime [9]. This new interface can now be controlled by a C++ supervisor, which allows performing efficient coupling with other simulation codes.

4.2 Testing fully coupled calculations

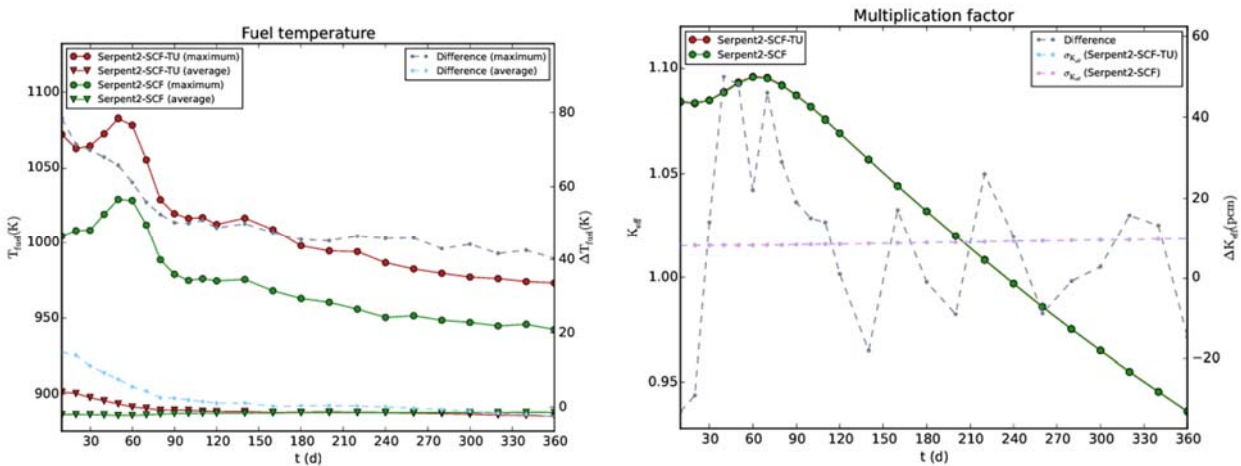
In order to test the full coupling of codes, calculations are performed both for PWR and VVER type reactors with the Serpent2 Monte Carlo code coupled to the thermal-hydraulics code SubChanFlow and the thermo-mechanics code TransUranus. Moreover, large-scale depletion cal-

Fig. 10. Iteration scheme for fully coupled calculations



calculations are included with in each step the full feedback of thermal-hydraulics and thermo-mechanics. For depletion the semi-implicit scheme is chosen. The thermo-mechanics calculate the fuel performance parameters like fission-gas release and detailed fuel-cladding gap behaviour. Improvement of the modelling of the fuel-cladding gap was possible using the sophisticated thermo-mechanical models in TransUranus. Fig. 10 shows schematically the iteration scheme for the coupled calculations. Fig. 11 shows some results. The figure at the left shows the fuel temperature as a function of depletion days for a number of options. The figure at the right shows the effective multiplication factor and the difference between the calculation with and without thermo-mechanical feedback.

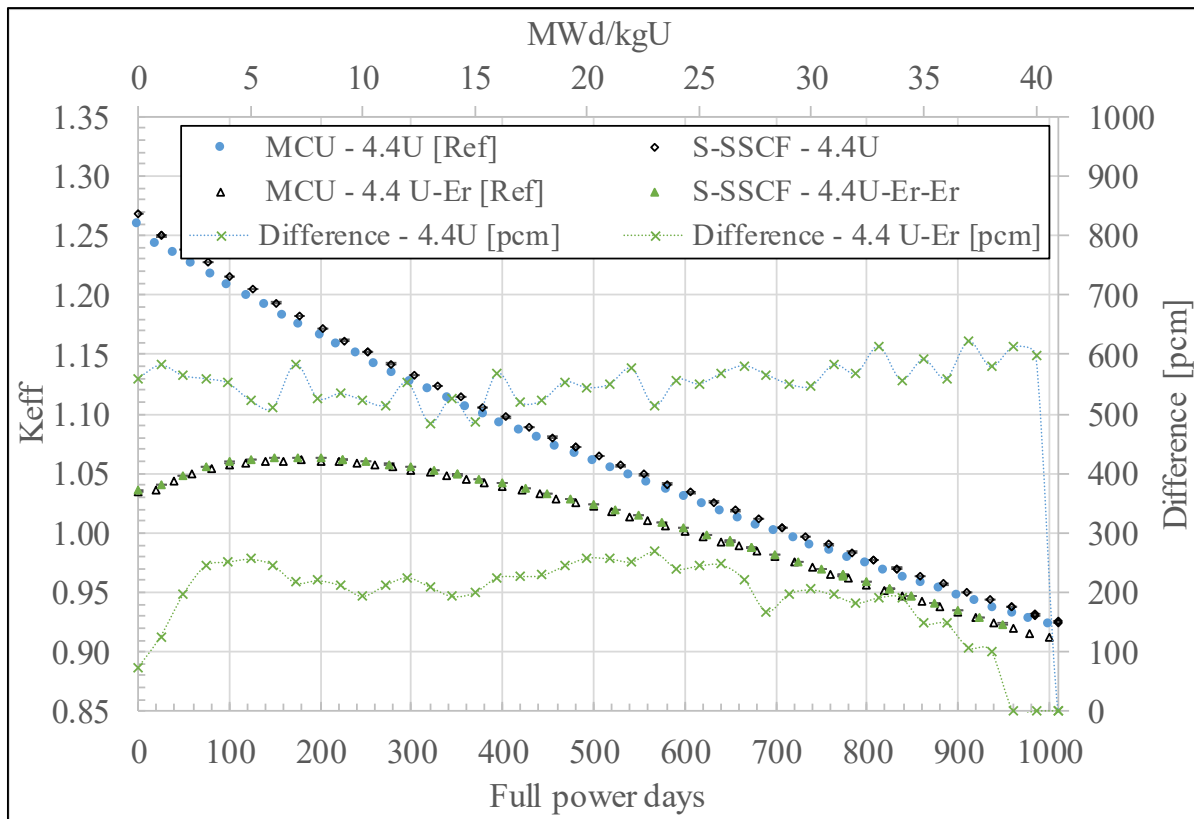
Fig. 11. Fuel temperature (left) and effective multiplication factor (right) as a function of depletion



For comparison with results of external high-fidelity projects (especially with the MCU code), a benchmark for a single fuel assembly of a VVER-1000 reactor is considered for Serpent2 with thermal-hydraulic feedback by the SubChanFlow code. Two types of fuel assemblies are calculated: with and without the burnable poison Erbium. Depletion is calculated with a predictor-corrector scheme with thermal-hydraulic feedback in each depletion step.

Fig. 12 shows the results for the effective multiplication factor as a function of full power days for depletion for the two types of fuel assemblies. Both the results for the MCU code are shown and for the Serpent2-SubChanFlow coupling. Also the differences in pcm are indicated (scale at the right).

Fig. 12. Effective multiplication factor for a depletion calculation of two types of VVER fuel assemblies and comparison with the MCU code.



A benchmark for testing fully coupled calculations

As explained in the previous report, the coupling of the three codes Serpent, SubChanFlow and TransUranus under the European reactor simulation platform NURESIM [3,4] was accomplished successfully. Test cases with single pins as well as single fuel assemblies in rectangular and hexagonal geometry were used for testing the coupling. The next step is now benchmarking of the coupling and the comparison to the coupling of the three codes using the multi-physics interface of the Monte Carlo code Serpent. For that purpose, a benchmark was defined for each of the geometry options. Both cases consider mini-cores (see Fig. 13) at hot full power at equilibrium Xenon concentration in order to test the interaction of the three codes in the two different environments (NURESIM platform and direct interface). The following parameters will be compared:

- critical boron concentration in moderator
- relative powers of fuel assemblies (2D distribution)
- relative powers of the fuel pins in the central fuel assembly (2D distribution)
- averaged axial power distribution of fuel assemblies
- axial power distribution of fuel pins in the central fuel assembly
- outlet temperatures from the subchannels of central fuel assembly (2D distribution)
- averaged fuel pin temperatures of the central fuel assembly (2D distribution)

The disadvantage of the newly defined benchmarks is the lack of reference data for comparison: indeed, the high performance calculations themselves should serve as a reference and there is no other means to obtain the results of comparable accuracy if experimental data are not available. In

order to be able to check the results of coupled calculations better than in a qualitative way we have developed the mini-core model for the deterministic code ANDREA and the alternative subchannel analysis code SUBCAL. Results of these calculations are being used for the coupled codes inputs debugging and basic output verifications.

Currently the coupled codes calculations are in progress. Preliminary results for the subchannel output temperatures and the fuel pin temperatures as predicted by the Serpent-SubChanFlow-TransUranus coupled codes is shown in Fig. 14.

Fig. 13. Layout of the benchmark cases for testing the three-codes-coupling

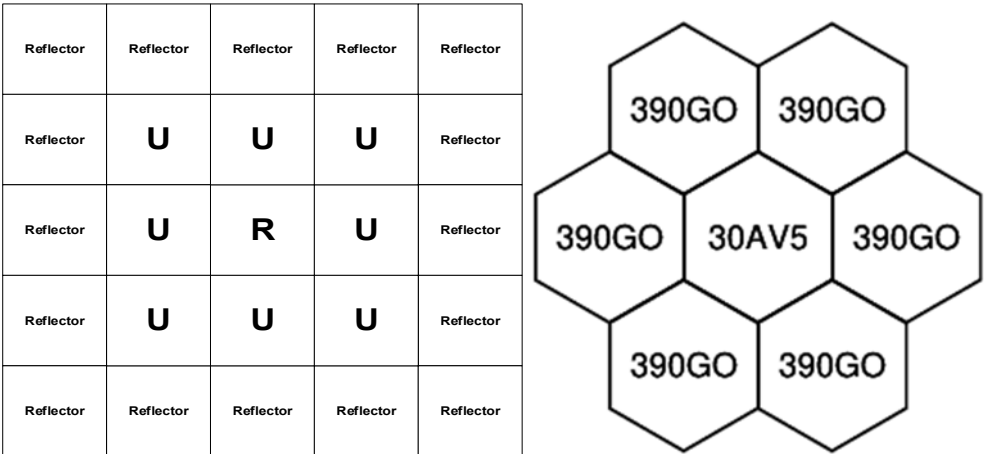
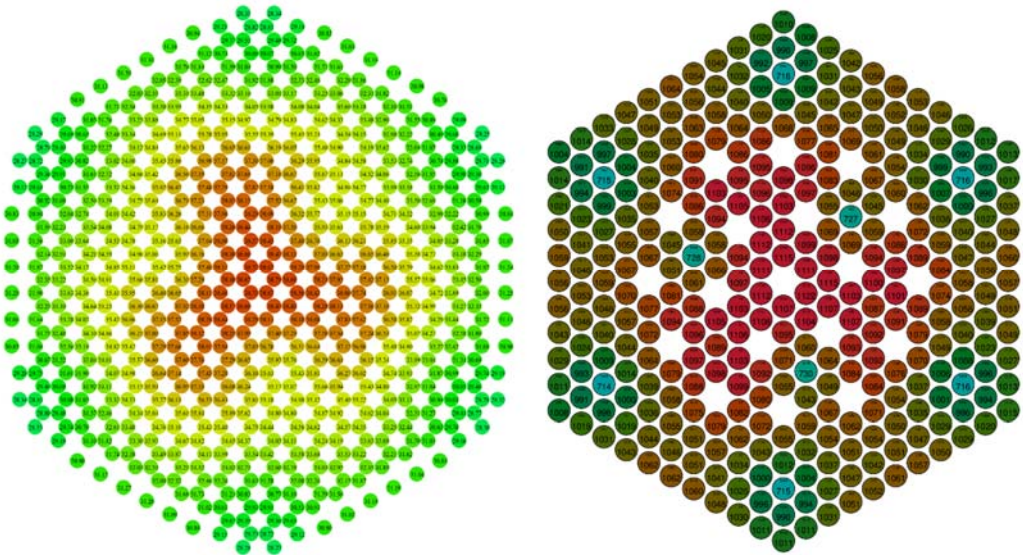


Fig. 14. Subchannel output temperatures (left) and fuel pin temperatures (right) in the central fuel assembly in the VVER mini-core



5. Progress in time-dependent Monte Carlo calculations

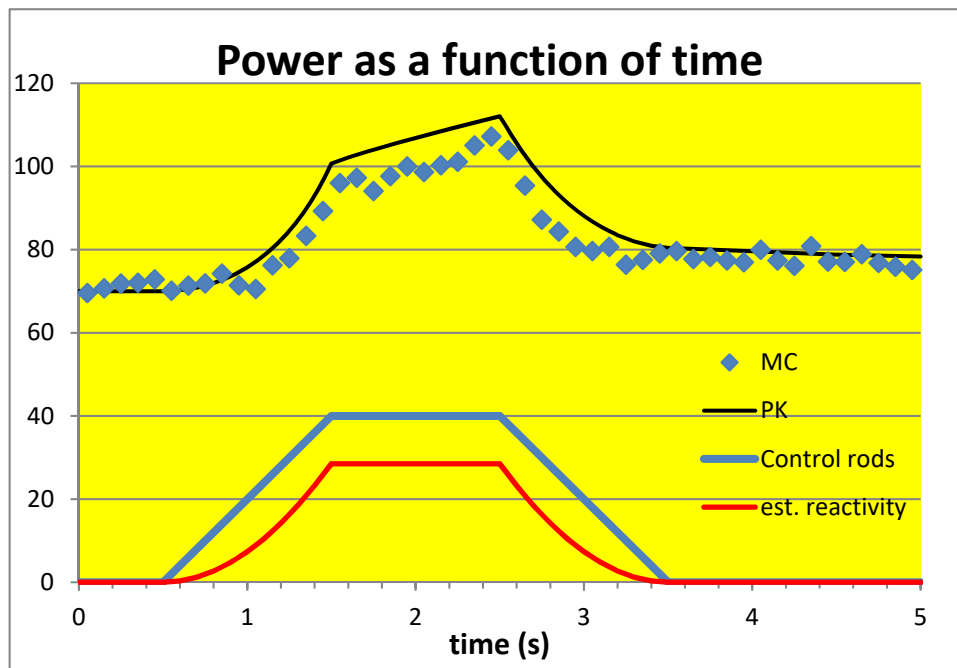
5.1 Development of dynamic Monte Carlo codes

To simulate reactor transient behaviour the generation and decay of delayed neutron precursors was already implemented in the Serpent2 and TRIPOLI4 codes. Now this is also completed for the MCNP6 code, leading to the dynMCNP code.

To overcome the problems arising from very different time scales of prompt neutrons and delayed neutron precursors, each neutron precursor is forced to decay in each time interval with appropriate statistical weight, to ensure that in each time interval for determining the average reactor power sufficient neutron chains with successive new prompt fission events in their history start.

Fig. 15 illustrates the estimated reactor power as a function of time for a mini-core reactor consisting of 3x3 PWR type fuel assemblies. The central fuel assembly contains 16 control rods, which are fully inserted into the core in the stationary situation (control rod tip at $z=0$ cm) and are moved upwards linearly in time to $z=40$ cm and later on moved down again to their original position, hence inducing a power transient. The movement of the control rods in time are also indicated in Fig. 15, as well as the estimated reactivity during control rod movement. With this reactivity behaviour the transient power was also calculated with a point-kinetics calculation, also shown in Fig. 15.

Fig. 15. Power behaviour in a mini-core reactor due to control rod movement

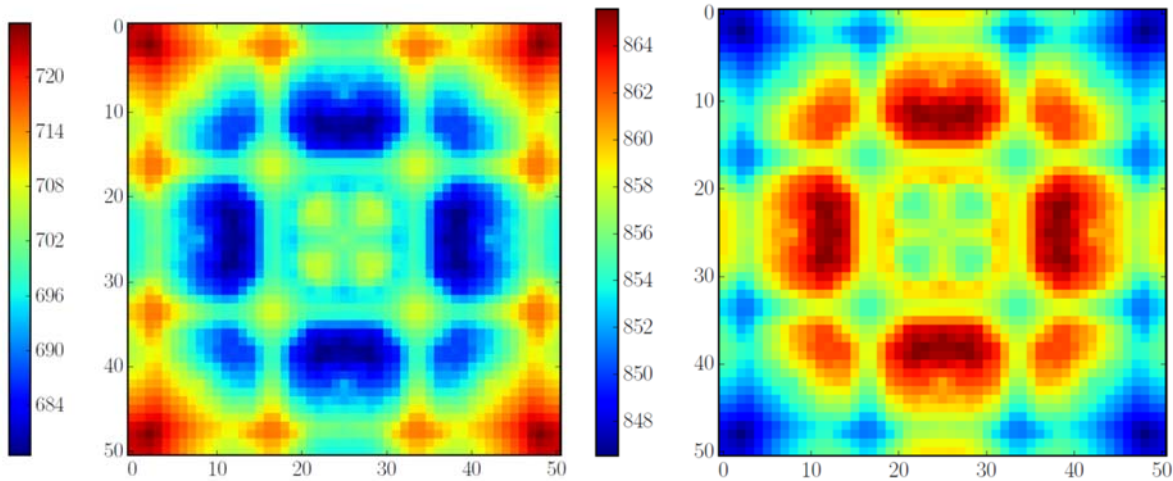


5.2 Further testing of time dependent Monte Carlo codes

In the previous Synthesis Report, we have detailed coupled simulations of a fuel assembly taken from the TMI-1 benchmark model in stationary conditions, which was intended as a preliminary test for the newly developed multi-physics interface of TRIPOLI-4®. Building upon these findings, we

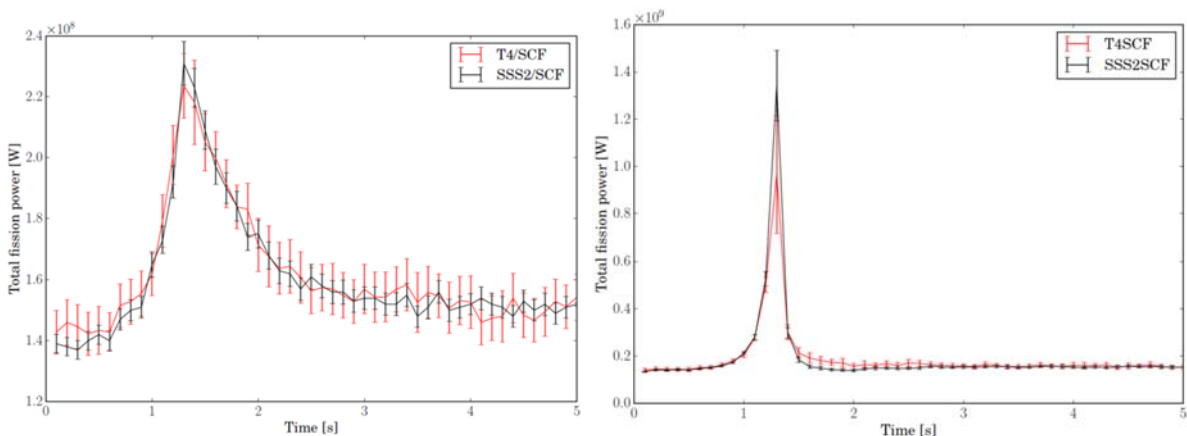
have extended the perimeter of our verification to the case of a larger configuration, namely, the mini-core benchmark, in non-stationary conditions with a pin-by-pin description. The system is first prepared for a critical state with a criticality calculation with thermal-hydraulics feedback. Different

Fig.16. Stationary state simulations (system configuration at time $t=0$) of the mini-core benchmark, with thermal-hydraulics feedback. Left. moderator density across the core. Right. moderator temperature across the core.



reactivity excursion transients, initiated by control-rod movement, have been simulated starting from the critical state. Simulations with and without feedback are compared in order to assess the effects of thermal-hydraulics on the neutron power. We have also discussed the computational and memory requirements, in particular for massively parallel calculations. The numerical results have been submitted to Physor 2020 [9]. A few representative cases are illustrated in Figs. 16 and 17.

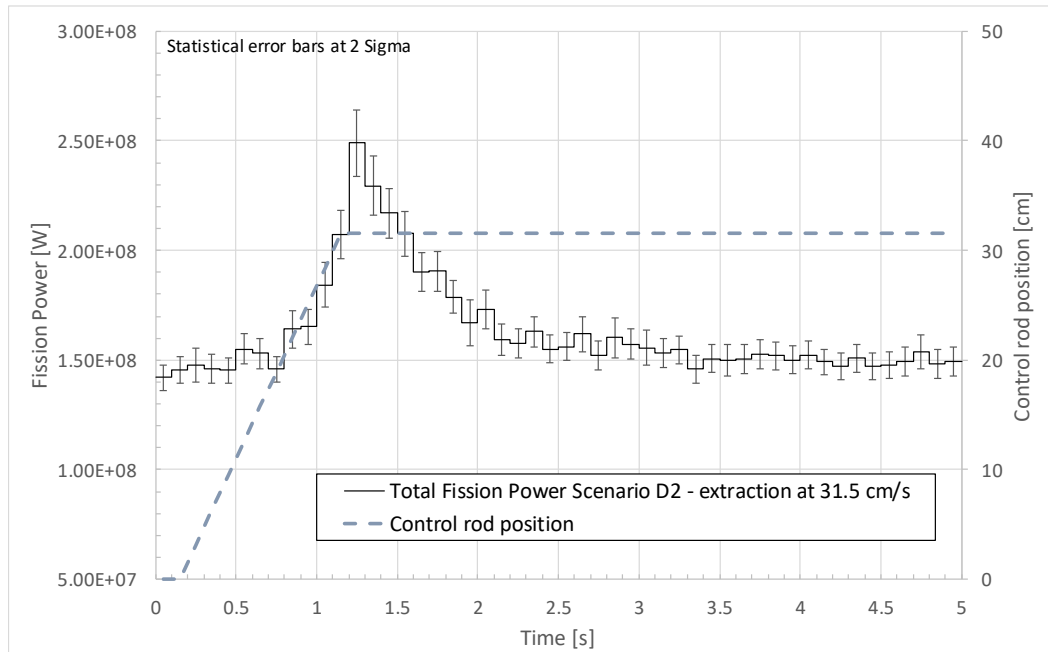
Fig. 17. Time-dependent simulations of the mini-core benchmark with thermal-hydraulic feedback. Left. A transient corresponding to 30 cm rod extraction. Right. A transient corresponding to 40 cm rod extraction. Results obtained with TRIPOLI-4® are contrasted to those of Serpent2.



The simulations reported here are extremely time-consuming (several tens of thousands of CPU hours) and have thus been carried out by resorting to parallel calculations. In the context of the McSAFE project, the native (distributed) parallel simulation scheme of TRIPOLI-4® has been extended in order to accommodate the dispatch of updated temperatures and densities across the

processors. Extensive tests concerning the scaling and efficiency of the parallelisation scheme are ongoing.

Fig. 18. Transient power behaviour due to control rod extraction (dotted line) with temperature feedback.



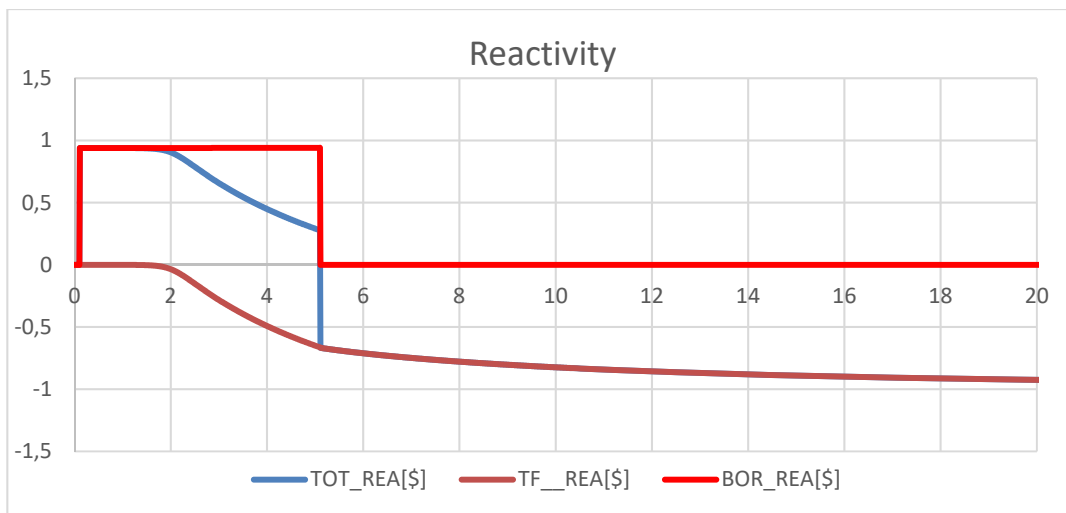
Also the Serpent2 code with thermal-hydraulic feedback from-SubChanFlow is further tested for a transient power behaviour due to control rod extraction. The calculations are performed for the mini-core reactor with 3x3 PWR-type fuel assemblies. Fig. 18 shows the time-dependent behaviour of the reactor power for this transient with temperature feedback.

These tests confirm that the time-dependent codes are well capable of calculating the transient reactor behaviour including thermal-hydraulic feedback.

5.3 Other test cases for time-dependent calculations

A fast-running test case was defined to provide a robust and reliable reference solution for testing new variance reduction techniques in time-dependent Monte Carlo calculations. This reference solution is provided by the deterministic multi-group diffusion solver DYN3D. In the past, steady-state Monte Carlo calculations by the Serpent code were used to provide reference solutions for the DYN3D code. Here, we go the way around. By help of the Serpent code a two-group cross section library with three points in boron concentration (0, 1000, 2000 ppm) and six points in fuel temperature (300, 600, 900, 1200, 1500, 1800 K) was created for one material. The test case consists of a 2D reflected PWR fuel assembly in real geometry and content. The perturbation is an artificial reduction of the boron concentration with one time-step. Only the Doppler feedback is considered in the DYN3D calculation. Two cases have been calculated with DYN3D: one with reactivity increase below 1\$ and the second one above 1\$. With these two options a test case is provided which can be calculated relatively fast by Monte Carlo codes and contains sufficient complexity to serve as a good test for the newly developed methods. Fig. 19 shows the reactivity behaviour due to the boron dilution and the fuel temperature, as well as the total reactivity.

Fig. 19. Reactivity contributions during the test run (delayed critical case)



5.4 Variance reduction for transient calculations

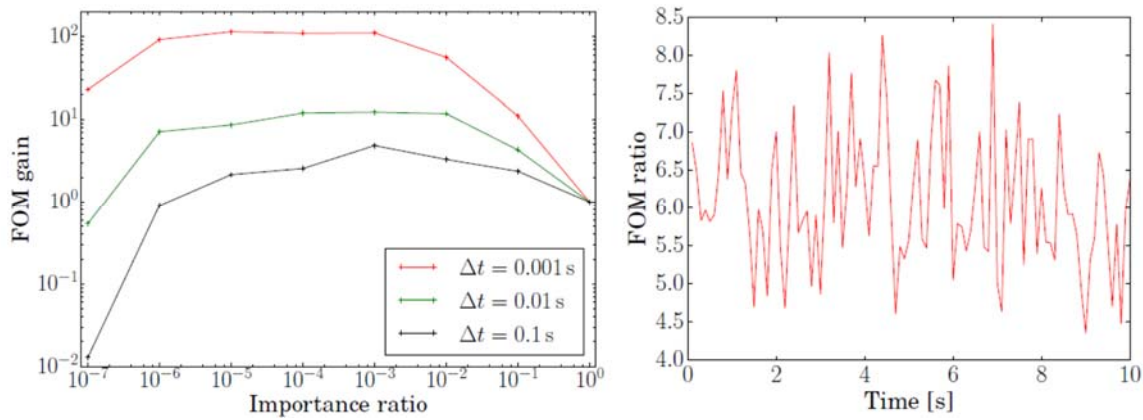
Time-dependent Monte Carlo transport simulations involve very different time scales for neutrons and precursors, which demand distinct variance reduction techniques with respect to stationary simulations. Additionally, the delayed neutron fraction (stemming from precursor decay) is very small, which might lead to serious under-prediction biases. In order to cope with these issues, we have implemented several strategies in TRIPOLI-4®, namely:

- forced precursor decay, to produce at least one additional delayed neutron per time step;
- branchless collisions, in order to enforce a single descendant neutron per collision event and thus mitigate the dispersion of the statistical weights due to the fission chains;
- importance sampling of the neutron and precursor populations, in order to ensure a better representation of the delayed neutrons when the size of the time steps is small with respect to the precursor lifetime (as required, e.g., by the simulation of RIA accidents);
- several population control techniques, including Russian Roulette and splitting and the so-called “combing” (this latter enabling the neutron and precursor populations to be constant in size, while preserving the average statistical weight).

These strategies have been extensively investigated in the framework of a benchmark configuration based on a TMI fuel assembly: these findings have been published in [10] and are illustrated in Fig. 20.

Furthermore, investigations are ongoing concerning the feasibility of zero-variance schemes for time-dependent transport, including the contribution of precursors. A paper has been submitted to Physor 2020 [11].

Fig. 20. Time-dependent simulations of the TMI fuel assembly. Left. Gains in Figures of merit (FoM) for different ratios of the neutron importance to the precursor importance. Red: $\Delta t = 0.001$ s. Green: $\Delta t = 0.01$ s. Black: $\Delta t = 0.1$ s. Right. FoM ratio between simulations with/without branchless collisions

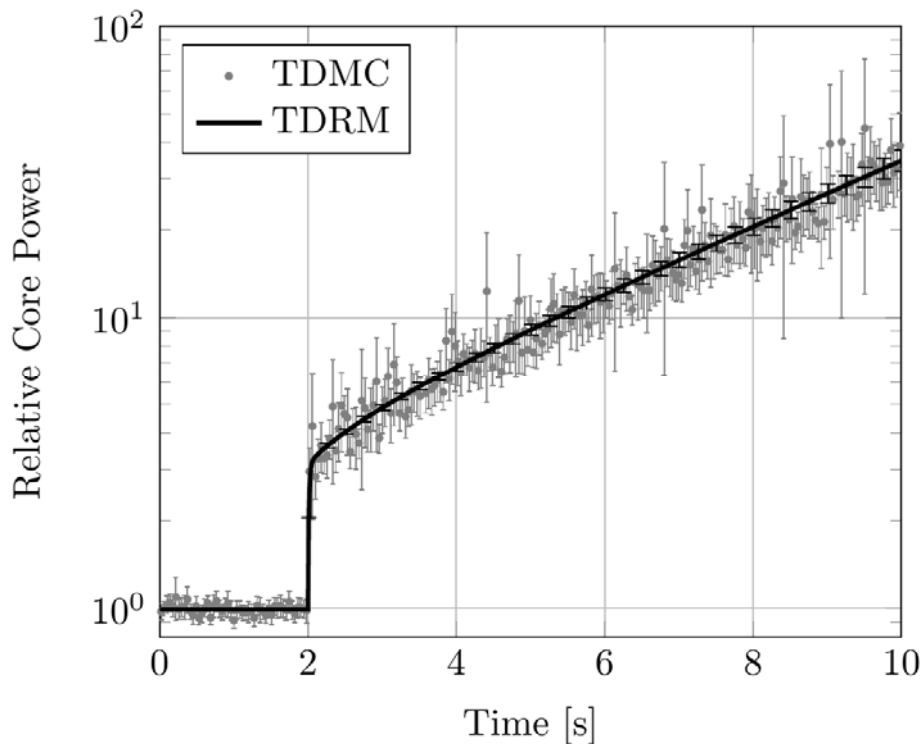


5.5 Time-dependent response matrix

Since the last synthesis report we have been working on developing a time-dependent response matrix method. A static response matrix solver was successfully applied for accelerating the fission source convergence in Monte Carlo criticality calculations. We have extended the static method to include time-dependence and developed a stochastic-deterministic, time-dependent response matrix (TDRM) method for transient analyses of nuclear systems.

The TDRM method describes a system by a set of response functions, which are pre-computed during a Monte Carlo criticality calculation and are later used to formulate a deterministic set of equations for solving a space-time dependent problem. Application of the response matrix formalism results in a set of loosely connected equations which leads to a favourable linear scaling of the problem, compared to the fission matrix based methods which scale quadratically. The developed method may be used as a stand-alone solver, or, possibly, as a variance reduction tool in time-dependent Monte Carlo simulations. The latter application merits further investigation. A manuscript describing the method is submitted to the journal *Annals of Nuclear Energy* [12]. Fig. 21 shows the results for a stepwise introduction of reactivity.

Fig. 21. Transient power behaviour after a stepwise reactivity introduction. Comparison of the Time-Dependent Response Matrix method with normal time-dependent Monte Carlo



5.6 Parallelisation of time-dependent calculation

As Monte Carlo calculations for a full-size reactor and especially time-dependent calculations require long computer run times, parallelisation of the Monte Carlo runs is inevitable. All our Monte Carlo codes have options for parallel execution with MPI and OpenMP. However, to complete such calculations in a reasonable time, say one day, with acceptable statistical accuracy massively parallel execution with large numbers of processor cores is needed, which is not always available in local computer clusters of our participants.

Therefore, access is requested to a supercomputer of the European PRACE organisation. Access is obtained for 6 months to the Joliot-Curie supercomputer of the Very Large Computing Centre (TGCC) of CEA, France. This access will be used to test and improve the parallel efficiency of the Serpent2 and dynMCNP codes when using large numbers of processor cores.

6. Outlook

The current synthesis report, together with the first synthesis report, show that important steps have been realised in the McSAFE project. This regards the optimisation of Monte Carlo criticality runs, the coupling of Monte Carlo codes with thermal-hydraulics and thermo-mechanics (externally coupled in the Salomé platform or internally coupled), optimisation of depletion calculations, extensions for hexagonal lattices (VVER type), availability of time-dependent Monte Carlo calculations, improvements in variance reduction, improved scalability for parallel processing and many detailed improvements that support the calculations.

The progress is regularly communicated with all interested parties via newsletters, synthesis reports, presentations at international conferences and articles in scientific journals.

In the remaining time of the project (up to September 2020) further steps are needed and foreseen to reach the final goal of the McSAFE project, namely to demonstrate that accurate and realistic calculations of full-size reactor cores based on the Monte Carlo method with thermal-hydraulic and thermo-mechanical feedback are possible for safety analysis, not only for criticality but also for transient reactor behaviour and reactivity incidents and for depletion.

Based on the results achieved so far, the final step will be the validation of the static and dynamic simulations against the experimental datasets available for the Konvoi PWR and VVER-1000 reactors and the reactor power excursions of SPERT III E-core. The neutronics models have been built and thoroughly verified. Work is ongoing concerning the construction of a reliable thermal-hydraulics model for the SPERT III E reactor core.

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