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HIGH ACCURACY LARGE SCALE MONTE CARLO AND DETERMINISTIC TRANSPORT CALCULATIONS FOR CRITICAL SYSTEMS

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ABSTRACT

The Monte Carlo method with nuclear point data currently offers the possibility for the most accurate description of the neutronics of critical systems, since practically no approximations are required. However, for many problems deterministic methods are applied for performance reasons and the advantage of the absence of statistical uncertainties. In the present paper, the results of high accuracy Monte Carlo and deterministic S_N transport calculations with pin cell resolution for two recent benchmark problems, namely the VENUS-7 series of critical experiments with LWR-type lattice and the stationary part of the PWR MOX/UO2 core transient benchmark, are presented. Very good agreement between the results for multiplication constants, reactivity values, and pin-wise fission rate distributions is obtained, thereby demonstrating the adequacy of the S_N method including the necessary approximations, like energy group condensation and spatial homogenization over pin cells, to perform large-scale neutronics calculations.

Key Words: Neutron transport, Monte Carlo, discrete ordinates, critical benchmarks

1. INTRODUCTION

Currently, most 3-D neutronics full-core LWR calculations are performed with codes based on the diffusion approximation to the Boltzmann transport equation, using nuclear data homogenized over large spatial zones (typically fuel assembly sections) and collapsed to very few energy groups (typically two), generated in advance by cell codes. With the capabilities of high performance computers available today, it has already become possible to perform such large scale calculations within the S_N formulation of the transport theory or similar methods, without the necessity of the diffusion approximation, and a much finer resolution concerning geometry and energy. Nevertheless, to be able to perform these calculations in reasonable computer time, especially for transient problems where a large series of calculations equivalent to stationary problems have to be performed, certain approximations are advantageous. These are the homogenization of cross sections over small spatial zones (typically pin cells) and the condensation to an appropriate number of energy groups. The adequacy of these solution methods should be assessed by comparing the calculation results with measurements and with results obtained with reference calculation methods. Such a reference is the Monte Carlo method with nuclear point data, within which it is possible to model the problem geometry at an arbitrary level of accuracy without a substantial influence on the computing time needed. With modern high performance computers, it is possible to reduce the statistical uncertainties inherent in the Monte Carlo

method to a level that enables a sufficiently precise determination of local quantities like pin-wise reaction rates even for full-core models, and small reactivity differences for calculations of similar stationary states.

In this paper, we compare results of deterministic S_N and Monte Carlo calculations for the VENUS-7 series of critical experiments, and the uncontrolled and controlled stationary states of the PWR MOX/UO_2 core transient benchmark.

2. THE VENUS-7 CRITICAL EXPERIMENTS

The VENUS-7 [1] series of critical experiments is currently evaluated within an OECD/NEA benchmark activity for the validation of nuclear data and codes for MOX fuel. The VENUS-7 cores are cold square lattices differing in their radial shapes; the configurations 7/0 and 7/1 are approximately cylindrical, while 7/3 is square-shaped. They consist of an inner MOX and an outer UO_2 radial zone, and are moderated and reflected by light water. The measured quantities are the multiplication factors, reactivity differences caused by substitution or removal of fuel pins, and radial pin-wise fission rate distributions. Sketches of the arrangements of fuel pins are given in Figure 1.

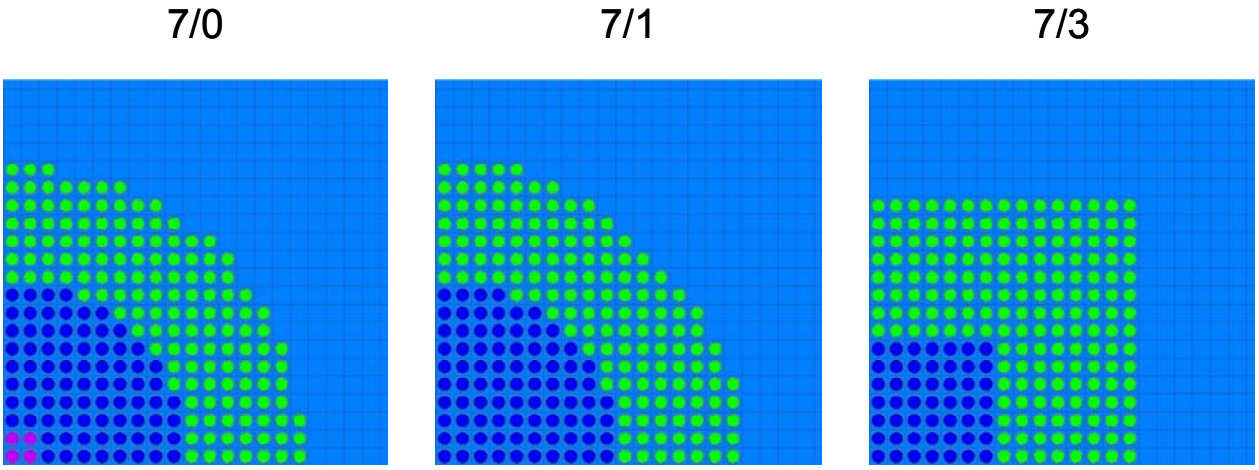

Figure 1. Horizontal cut through one quarter of the VENUS-7 assemblies. Blue pins: MOX fuel; green pins: UO_2 fuel. In assembly 7/0, the central pins for the substitution experiments are displayed in magenta.

We have calculated the various configurations with the Monte Carlo code MCNP-4C [2] with JEF-2.2 based nuclear point data and with the S_N code THREEDANT [3] with 18 group P_3 cross sections for the homogenized pin cells, S_8 quadrature order, and 2x2 meshes per pin cell in the x-y plane. The calculations were performed in 3-D representation and in 1/4 core geometry.

For the S_N calculations, the 18 group data were pre-calculated for the individual pin cells with the 1-D collision probability code RESMOD [4] from a JEF-2.2 master library with 292 energy groups and a hyperfine representation in the resolved resonance region. In these pin cell

calculations, the actual dimensions of the cell were used for all positions, thus not considering any effects of additional moderation for the cells close to the core boundary.

The MCNP calculations were performed with 200 million neutron histories (20,000 active generations and 10,000 neutrons per generation, with 100 discarded generations), thus obtaining a very high accuracy in the results, with relative statistical uncertainties not larger than $5.0\ 10^{-5}$ in the multiplication factors, and $1.0\ 10^{-3}$ in the pin-by-pin fission rates. The CPU time required for each of these calculations was about 32 hours on a single processor of a Cray XD1 computer (all CPU times given in the following will refer to this computer). In the THREEDANT calculations, the convergence criterion for the point fluxes was $1.0\ 10^{-5}$; this accuracy was obtained within a CPU time in the range of 2 – 4 hours. It should be noted, however, that the actual execution time strongly depends on the performance of the data storage system and the transfer rates.

Table I. Multiplication factors for the VENUS-7 configurations, calculated with MCNP and THREEDANT.

	MCNP	THREEDANT	Difference
VENUS-7/0	0.99248	0.99447	0.00199
VENUS-7/1	0.99354	0.99554	0.00200
VENUS-7/3	0.99300	0.99585	0.00285

In Table I, the calculated multiplication factors for the three VENUS-7 configurations are given. Firstly one notes that the experimental multiplication factors, which are very close to 1.0 for all configurations, are clearly underestimated. However, this is observed in all Monte Carlo and deterministic solutions contributed to the benchmark so far. The size of the underestimation depends on the nuclear data libraries and calculation methods used. The origin of this deviation is still not resolved. Comparing the MCNP and THREEDANT results, good agreement is obtained, with differences of 200 pcm for the approximately cylindrical configurations 7/0 and 7/1. For the square-shaped configuration 7/3, the difference is slightly larger; this is compatible with the fact that the deviations from an infinite lattice, for which the 1-D spectral calculations were performed, are largest for corner pins.

Table 2. Differences in the multiplication factors for the VENUS-7/0 fuel pin substitutions and the VENUS-7/1 fuel pin removal; values are given in %.

	Experiment	MCNP	THREEDANT
VENUS-7/0, Subst. UO_2	+0.094 ± 0.004	+0.125 ± 0.01	+0.145
VENUS-7/0, Subst. MOX type 2	–0.058 ± 0.004	–0.090 ± 0.01	–0.073
VENUS-7/0, Subst. MOX type 3	–0.092 ± 0.004	–0.075 ± 0.01	–0.074
VENUS-7/1, pin removal	–0.016 ± 0.003	–0.015 ± 0.0025	–0.013

Table 2 shows the calculated differences in the multiplication factors for different fuel pin substitutions in the centre of the VENUS-7/0 core and for the removal of a peripheral fuel pin from the VENUS-7/1 core. The substitutions are performed by replacing 16 central MOX pins by UO_2 pins, or by MOX pins with different fuel diameters and cladding thicknesses (type 2) or different U-235-enrichment and Pu content (type 3). For calculating the worth of the removal of a peripheral pin, the outmost pin in the 45° direction was chosen. It should be noted that the position of the pin removed for the measurement is not specified in the experimental documentation which introduces a larger uncertainty than the experimental error given. In comparison to the measured values for the multiplication factor differences, the calculated values have the correct sign and magnitude, but the differences are slightly outside the intervals covered by the documented experimental errors and the statistical uncertainties of the Monte Carlo calculations. When comparing the values calculated with MCNP and THREEDANT, the differences are significantly smaller, thus giving very satisfactory agreement between the results obtained with both methods.

Figure 2 displays the radial fission rate distribution for the VENUS-7/0 assembly resulting from the MCNP calculation, and a comparison between the MCNP and THREEDANT distributions. The agreement is quite satisfactory, with a noticeable difference of up to 3.5 % at the core boundary, and therefore a slight tilt in the MCNP/THREEDANT ratio in the radial direction. The larger difference at the core boundary is due to the cross section homogenization in the 1-D spectral calculation which cannot adequately take the core boundary into account. For the 7/3 configuration, the observations are quite similar; however, for the corner pin the relative difference between the MCNP and THREEDANT results is somewhat larger (approx. 5 %), as expected.

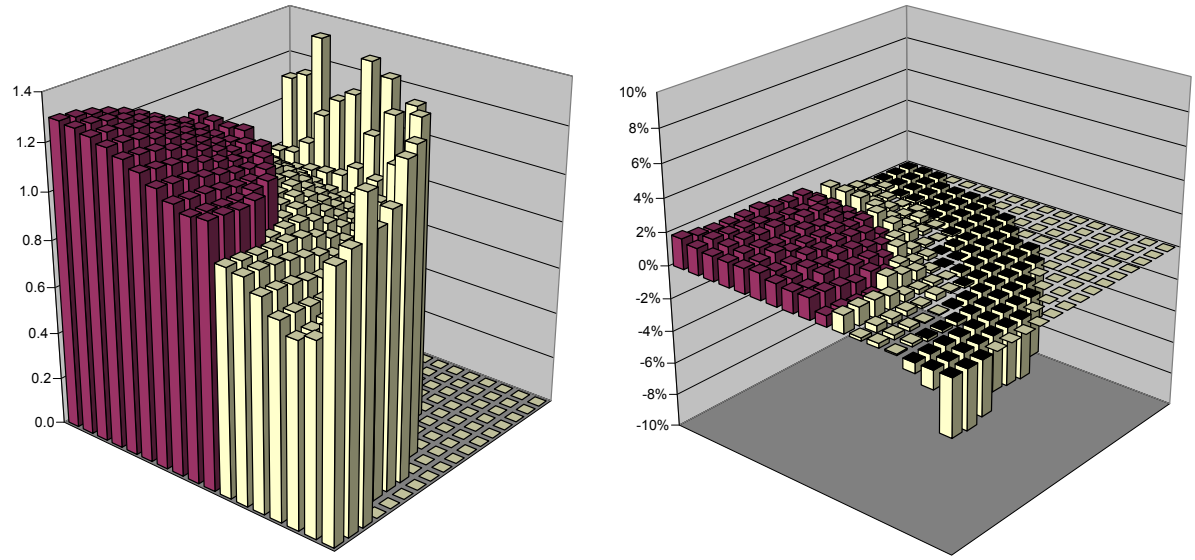

Figure 2. Radial fission rate distribution for one quarter of the VENUS-7/0 configuration. Left: Pin fission rates calculated with MCNP. Right: Relative differences between the MCNP and THREEDANT results. The values for the inner MOX and the outer UO2 zones are displayed in different colors.

3. THE PWR MOX/UO_2 CORE TRANSIENT BENCHMARK

The PWR MOX/UO_2 core transient benchmark [5] was defined by U.S. NRC and OECD/NEA with the purpose to assess the ability of modern reactor kinetics codes to simulate a control rod ejection in a MOX/UO_2 core. The specification describes a Westinghouse PWR core with 30 % MOX loading. It consists of 193 UO_2 and MOX 17x17 fuel assemblies with different enrichments and Pu contents, respectively, at several burn-up states up to 37.5 GWd/t HM. The fresh fuel assemblies contain burnable absorbers. For the stationary calculations, the core can be represented in 2-D geometry with 90° rotational symmetry. The core and fuel assembly layouts are displayed in Figure 3. Detailed results were discussed in [6].

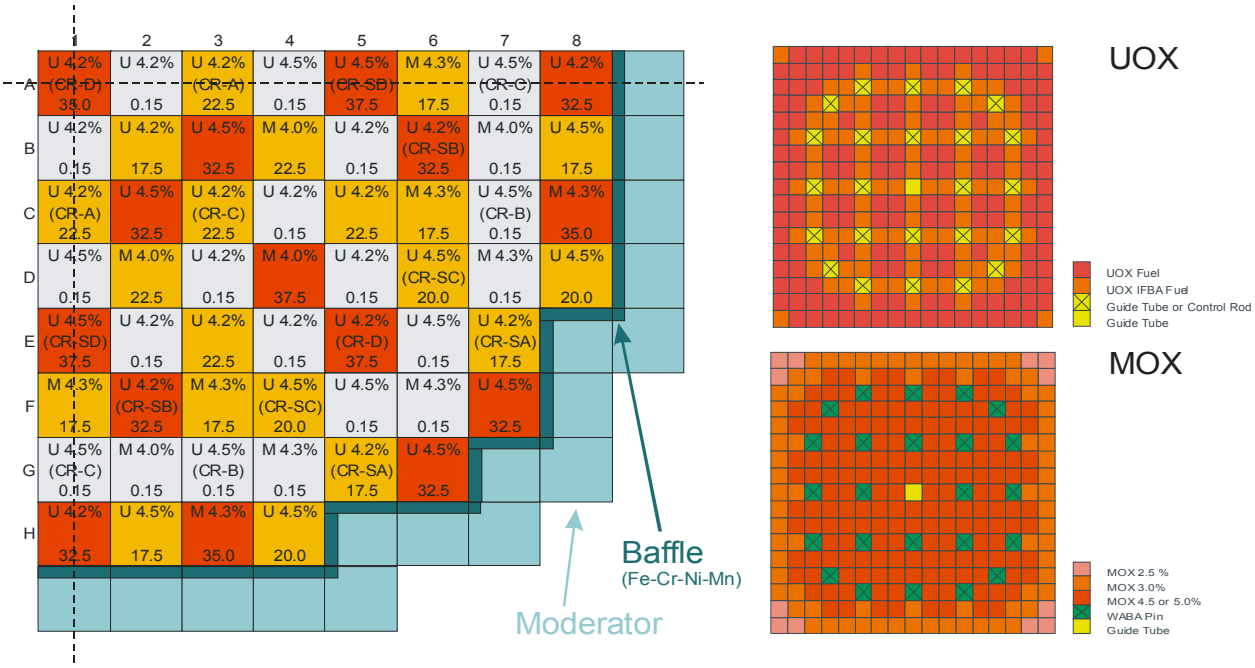

Figure 3. Core configuration and fuel assembly layout for the UO_2 and MOX assemblies of the PWR MOX/UO_2 core transient benchmark. In the core configuration, CR-A to CR-D denote four different control rod banks, and CR-SA to CR-SD refer to four shutdown rod banks. Reflective boundary conditions apply along the dashed symmetry lines.

For the deterministic transport calculations of the stationary case, we used the S_N code DORT with a set of 16 group cross sections, homogenized for individual pin cells. These cross sections were generated in preceding burn-up calculations for each of the different fuel assemblies with the 2-D cell and depletion code HELIOS-1.8 in P_1 scattering expansion. For most of the materials contained in the baffle surrounding the core, the HELIOS library contains P_0 data only. In the course of the analysis, it turned out that this is not sufficient to describe the baffle adequately, and leads to a significant deficiency in the radial flux distribution. Therefore, a set of group cross sections up to P_1 order was generated for the baffle material with the RESMOD code. For the DORT calculations, each homogenized pin cell was divided into 2x2 meshes. For the final calculations, S_4 was chosen for the angular discretization because the results are practically independent of the quadrature order when varying between S_4 and S_{16}. For the problem as discussed, the CPU time is about ½ hour.

The nuclide densities for each material in each burn-up state resulting from the HELIOS calculation were used for MCNP calculations with JEF-2.2 based nuclear point data. These calculations were performed with an exact representation of the 2-D geometry as described in the benchmark specification. Almost 200 million neutron histories were sampled (three independent calculations, each with 13,000 active generations and 5,000 neutrons per generation with 500 discarded generations). In earlier calculations for whole core systems, we had observed errors in the calculated neutron distributions resulting from a slow convergence which is much larger than the estimated statistical uncertainties [7]; therefore, the calculations were split up in three independent runs to make sure, by a comparison of the resulting distributions, that a sufficient convergence was obtained. The CPU time required for the whole problem is about 50 hours.

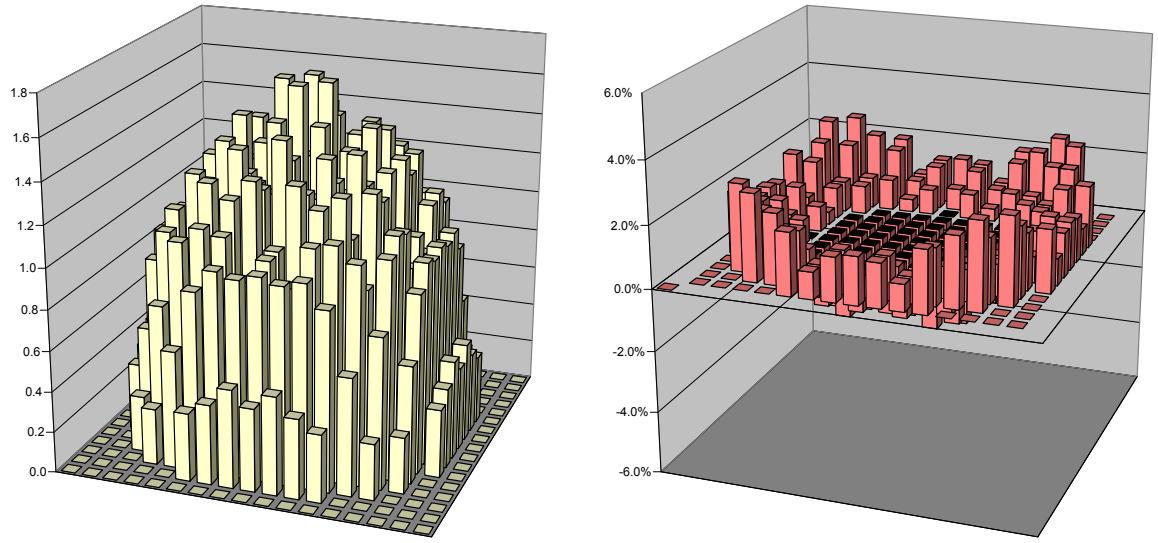

Figure 4. Left: Normalized whole core assembly power distribution of the ARO reactor state obtained from the MCNP solution with JEF-2.2 point data. Right: Relative deviations between the distribution from the DORT S_4-P_1 calculation using pin cell homogenized 16-group cross sections and the MCNP solution.

For the uncontrolled state of the reactor (ARO – all rods out), we find a very good agreement between the multiplication factors, which are 1.06065 ± 0.00005 for the MCNP and 1.06036 for the DORT calculation, the assembly-wise power distributions, and the pin-wise power distributions in selected fuel assemblies calculated with MCNP and DORT. The assembly-wise power distribution and the pin-wise power distribution for a peripheral fuel assembly from the MCNP calculation, along with the relative differences between the corresponding DORT and MCNP solutions, are displayed in Figures 4 and 5. The relative differences have absolute values of up to 3 % for both assembly and pin powers. A similar agreement is achieved with results of the method of characteristics code DeCART, which are available on the benchmark web-site. For the reactor state with all control rods inserted, the differences become somewhat larger. This is due to the fact that for generating pin cell homogenized cross sections, a pure flux-volume weighting for the individual cells is performed in HELIOS. This is not sufficient for strong absorber cells, and further corrections like the SPH method [8] should be applied.

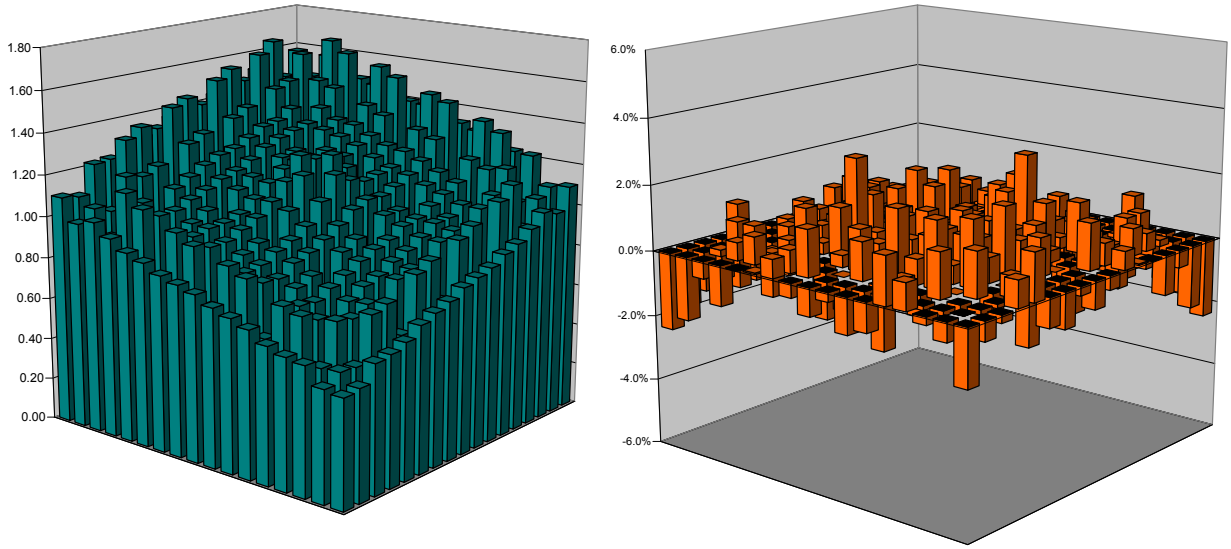

Figure 5. Left: Normalized pin-wise power distribution of assembly F6 of the ARO reactor state obtained from the MCNP solution with JEF-2.2 point data. Right: Relative deviations between the distribution from the DORT S_4-P_1 calculation using pin cell homogenized 16-group cross sections and the MCNP solution.

4. CONCLUSIONS

The Monte Carlo method with nuclear point data, which currently provides the highest level of accuracy for neutronics calculations of critical systems, without the necessity for significant restrictions in the geometrical modeling, or for performing preceding spectral calculations for cross section preparation, was applied for obtaining reference solutions for a series of benchmark problems. It was demonstrated that the S_N method using multi-group cross sections homogenized on the pin cell level, is suitable to describe large-scale critical systems within reasonable computing times, by comparing the results for multiplication factors and fission rate distributions. In the presence of strong heterogeneities, like inserted control rods, special measures have to be taken in generating appropriate cell cross sections. The findings described in the present paper make us confident that when necessary for heterogeneous reactor configurations, S_N calculations with pin cell homogenized cross sections can be used in future for the efficient solution of stationary and also time-dependent reactor problems.

ACKNOWLEDGMENTS

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