

A PROPOSAL FOR A BENCHMARK TO MONITOR THE PERFORMANCE OF DETAILED MONTE CARLO CALCULATION OF POWER DENSITIES IN A FULL SIZE REACTOR CORE

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ABSTRACT

Current computers and Monte Carlo codes are not yet able to calculate the power density map in a full size reactor core with sufficient statistical accuracy. This is only expected in 10 to 20 years from now. To monitor the improvement in efficiency of Monte Carlo codes over the years a benchmark test is proposed with emphasis on the estimation of the power density in a large number of axial regions of each fuel pin. The modeling of the full size reactor core is kept simple but with sufficient geometrical detail for a realistic Monte Carlo calculation. The main aim of the benchmark is to determine the execution time for a Monte Carlo calculation of the power density with sufficient statistical accuracy in as many regions as possible and to monitor the efficiency of the calculation over the years considering improvements in Monte Carlo codes and computers. In this paper full specifications for geometry and composition are provided. Preliminary results with the MCNP5 code indicate that for a 1 % statistical uncertainty in the local power density more than 10^{10} neutron histories must be simulated. The computing time will increase substantially with the number of tallies for power density estimation in separate regions. For the time being this will limit the number of regions for which the power density can be estimated. There may also be memory problems when using very large numbers of tallies. It is expected that the number of available computer nodes and CPU cores for a parallel calculation will increase enormously in the coming decades. However, the noted decrease in efficiency when using more CPU cores will require more advanced programming of Monte Carlo simulation for parallel processing. Hence, the proposed benchmark will stimulate improvement in practical Monte Carlo calculations for reactor cores in many ways.

Key Words: Monte Carlo, benchmark, efficiency, power density

1. INTRODUCTION

Monte Carlo codes are capable of calculating integral parameters such as the effective multiplication factor or a reactivity coefficient, even when all geometrical detail of each individual fuel pin of each fuel assembly is modeled. However, when more detailed information is required such as the local power density, possibly for small regions of a fuel pin in the axial

and/or radial directions, it is much more difficult to get acceptable results with respect to the standard deviation within a reasonable computation time. This becomes even more difficult if results for a large number of tallies are required, for instance the local power densities in all fuel pins, subdivided in a number of axial and possibly radial regions. Nonetheless, this is the requirement for current design calculations of a nuclear reactor core.

In his invited lecture at the M&C 2003 conference in Gatlinburg, Kord Smith [1] formulated the challenge for future Monte Carlo simulation as the calculation of the local power of each of the fuel pins in a fuel assembly when subdivided in 100 axial and 10 radial zones for burnup calculations. The number of fuel pins in a fuel assembly of a PWR core is about 300 while the number of fuel assemblies in a reactor core is around 200. This results in total of perhaps 60 million tallies. For an acceptable result, Smith specified the standard deviation in each local power region should be 1 % or less. In addition, Smith considered 100 different nuclides for which the reaction rate is needed, bringing the total number of tallies to 6 billion. These huge numbers of tallies not only pose a problem in CPU time but also in computer memory. Smith estimated on the basis of Moore's law that it will be 2030 before such a full core Monte Carlo calculation could be done in less than one hour on a single CPU.

Bill Martin [2] analyzed the situation in some detail in his invited lecture at the M&C 2007 conference in Monterey. Assuming that Moore's law manifests itself as *only* more cores in a desktop computer, Martin estimated that it would be 2019 before a full reactor core calculation with 40,000 fuel pins and 100 axial regions and 1 % statistical accuracy for local power estimates could be accomplished. In this case, the desktop computer would have a 1500 core processor at that time. It was also assumed that perfect speedup could be obtained with a 1500 core processor but this assumption would need to be verified.

There are several reasons why the advances in efficiency of full core Monte Carlo reactor calculations may be better or worse than estimated above. No improvements in single processor speed is taken into account, nor advances in other types of processing units. In addition, no progress in Monte Carlo variance reduction techniques is assumed. On the other hand, it is not guaranteed that Moore's law, in whatever form, will continue to hold over a period of 10 years, although it did hold over a longer period in the past. Also, the assumption that Moore's law will be manifested only in the number of processor cores was only made for convenience to allow the 1500 cores to be counted as a single CPU. Moreover, the performance of a Monte Carlo calculation will not scale linearly with the number of cores in a processor. And as noted above, the handling of very large numbers of tallies may also slow down the Monte Carlo calculation. For all these reasons it will be useful to monitor the performance of Monte Carlo full core calculations over the next 1 or 2 decades to assess the progress towards meeting the "Kord Smith challenge". Therefore, a suitable benchmark test which exhibits sufficient realistic detail for a modern full core calculation is needed.

2. SPECIFIC AIM OF THE BENCHMARK TEST

The aim of the proposed benchmark test is to monitor over the coming years the (increase in) performance of Monte Carlo calculations of a full size reactor core. To address the above mentioned issues, the key quantity to be estimated is not the effective multiplication factor, but the local power densities in small regions of the fuel. Moreover, the value of the power density itself is not the most important quantity, although it should be estimated correctly, but rather its standard deviation in relation to the number of neutron histories and computer time. In this

respect the total number of tallies, i.e. the total number of fuel regions for which the power density is calculated, is relevant for the execution time. On the other hand, the number of tallies may be restricted by the Monte Carlo code used and/or the available computer memory, especially if multiple processors consisting of multiple cores are used. Hence, besides the power density of a number of specifically denoted fuel regions spread over the full core and their standard deviation, the number of other tallies used in the calculation, without quoting their specific results, is a parameter which should be chosen as large as reasonably possible.

In addition to the number of neutron histories simulated (as a product of the nominal number of histories per cycle and the number of active cycles) and the resulting standard deviation in the power density at specific fuel volumes, the computing time is, of course, an important measure in this benchmark. It is challenging to compare execution times (this quantity has to be defined more precisely and in an operational way) on different computers. Specifically, with parallel processing the CPU time is not a suitable measure for comparison. Therefore, it will be useful to include relative comparisons using the same Monte Carlo code and on the same computer but starting with a single processor core and multiple processor cores, measuring the wall clock time for each configuration. Care should be taken to ensure that these single and multiple core configurations are running only the Monte Carlo simulation.

This benchmark is a Monte Carlo calculation for the routine design or analysis of a nuclear reactor core, and it is not our intention to find the fastest execution of the benchmark using one of the most advanced computer systems like IBM's Roadrunner or Blue Gene supercomputers, which will be available only to a select group of scientists for specific projects and not to the wider community of engineers doing routine reactor calculations. (These comparisons would not be rejected as they will be of interest to the community, but such expensive and exclusive platforms are outside the spirit of the Kord Smith challenge.) Therefore, the aim is directed to the performance of computers readily available, such as systems we have at our desk or available to a small work group. The capacity of such systems will change over the years, but that is what we want to monitor.

In view of the specific aim of this benchmark to measure the performance of a full-core Monte Carlo simulation, issues such as fission source convergence, while important for practical application of Monte Carlo reactor calculations, are not important for this benchmark. Therefore, we propose to look only at active cycles for which source convergence is already achieved, no matter what it takes to reach that state. Moreover, we will not consider temperature dependence or evolution of burnup. To avoid inconsistencies in this respect, the fuel compositions in terms of nuclide densities and temperatures should be explicitly defined. There will be, of course, differences in outcome of the local power densities due to differences in nuclear data, but such differences are not the subject of this benchmark test, rather it is the efficiency of the calculation that is being measured.

A secondary aim of the benchmark test is to stimulate improvements in Monte Carlo codes and their implementation. This not only refers to improving the random walk of a neutron in a full core nuclear reactor, but also to improving methods for dealing with large numbers of tallies (i.e., local power densities in many small fuel regions) and efficiency improvements in parallel computing using current and future computer architectures generally available for researchers and engineers. Another issue is the quality of the high performance programming of the Monte Carlo code and the performance of the compiler. All these items are implicitly part of the benchmark test.

3. DEFINITION OF THE BENCHMARK TEST

As the aim of the proposed benchmark test is not to get detailed information about one specific reactor core, the details of the geometry and composition of the reactor core and fuel assemblies are not that important, as long as they require the Monte Carlo code to do realistic neutron history simulation with most of the features encountered in current reactor design. We therefore define the reactor core as shown in Fig. 1. It consists of 241 fuel assemblies arranged in a regular pattern with a maximum of 17 fuel assemblies in the x - and y -directions. The core is contained in a 20 cm thick steel reactor vessel with inner radius of 203 cm. There is borated water between the core and the vessel. No other reactor internals are modeled. The core height is 400 cm with additional 20 cm of water above and below the core. For simplicity vacuum boundary conditions are assumed at the outer radius of the reactor vessel and at the outer boundaries of the axial water reflector.

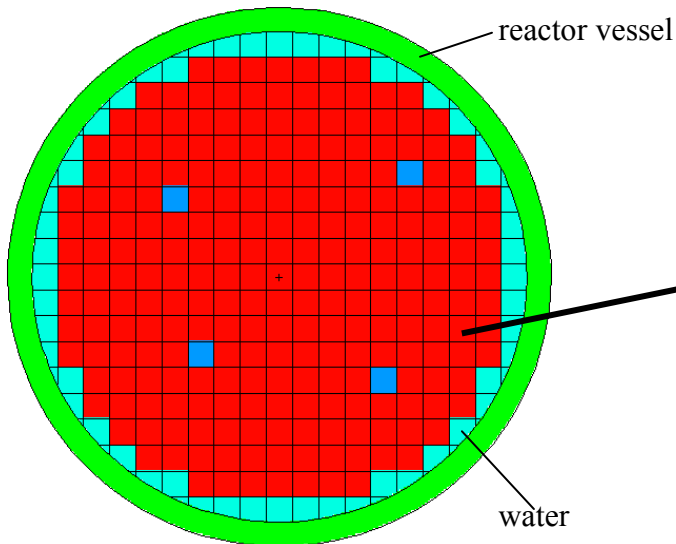


Figure 1. Arrangement of fuel assemblies in the reactor core.

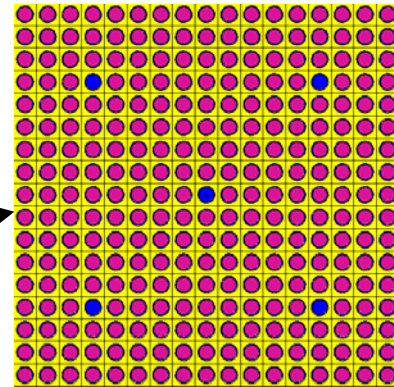


Figure 2. Fuel assembly with 5 Gd-UOX pins.

The fuel assemblies are shown in Fig. 2. They consist of 17x17 fuel pin positions without any fuel assembly structures. No control rods are modeled. Fuel pins have a pin radius of 0.41 cm over the full height of the core. The zirconium cladding has an outer radius of 0.475 cm. No gap between the fuel and the cladding is modeled. The pins are surrounded by borated water. The pitch of the fuel lattice is 0.61 cm. The composition of the fuel pins in an assembly may differ from position to position but to avoid complicating the geometry input, only two types of fuel composition are used. One type contains UOX fuel with a number of U and Pu isotopes and some fission products to simulate a certain burnup stage (roughly corresponding to a burnup of 24,000 MWd/ton). The fuel assemblies concerned are indicated in red in Fig. 1 and the fuel pins concerned are indicated in purple in Fig. 2. Table I specifies the nuclide composition of this type of fuel. The total atom density is $0.06823 \cdot 10^{24} \text{ cm}^{-3}$ resulting in a mass density of this fuel type of 10.063 g/cm^3 . The second fuel type also contains Gd as a burnable absorber in order not to have a strictly regular fuel pin arrangement in a fuel assembly. The positions of the 5 fuel pins with Gd

in each assembly are indicated in blue in Fig. 2. The nuclide densities for this type of fuel are also specified in Table I. The total atom density is $0.066564 \times 10^{24} \text{ cm}^{-3}$, resulting a mass density of 9.6574 g/cm^3 .

To deter codes taking advantage of possible symmetry in the geometry of the fuel assemblies in the core, the composition (density) of the fuel pins is different for a number of fuel assemblies at asymmetric positions in the core. These 4 fuel assemblies are indicated in blue in Fig. 1. Their geometry is the same as for the other fuel assemblies, including the 5 fuel pins with Gd.

However, the density of the fuel in these assemblies, except that of the fuel pins with Gd, is $0.06500 \times 10^{24} \text{ cm}^{-3}$, which is 4.734 % less than the density as specified in Table I. Hence, for these assemblies the densities of Table I should be reduced by this percentage (Monte Carlo codes may allow to input the total atom density for a material and will renormalize the atom densities per nuclide automatically so that the same nuclide composition specification can be used). In order to introduce a further asymmetry in the axial direction, the above fuel composition applies to the fuel below the core midplane. For the fuel above the core midplane the reduced densities apply to the fuel pins in the 4 fuel assemblies indicated in red in Fig. 1. Also, the densities specified in Table I apply to the fuel assemblies indicated in blue in Fig. 1. For all Gd containing fuel rods only one density as specified in Table I applies.

The nuclide density of the borated water in the fuel assemblies is specified in Table II. This corresponds to a mass density of 0.7164 g/cm^3 . For the axial reflector above and below the core

Table I. UOX fuel composition

nuclide	atom density x 10^{-24} cm^{-3}	
	without Gd	with Gd
$^{234}_{92}\text{U}$	4.8797×10^{-6}	4.3381×10^{-6}
$^{235}_{92}\text{U}$	4.8339×10^{-4}	4.2973×10^{-4}
$^{236}_{92}\text{U}$	8.7108×10^{-5}	7.7439×10^{-5}
$^{238}_{92}\text{U}$	2.1500×10^{-2}	1.9114×10^{-2}
$^{237}_{93}\text{Np}$	7.0455×10^{-6}	6.2634×10^{-6}
$^{238}_{94}\text{Pu}$	1.4224×10^{-6}	1.2823×10^{-6}
$^{239}_{94}\text{Pu}$	1.4137×10^{-4}	1.2568×10^{-4}
$^{240}_{94}\text{Pu}$	3.5710×10^{-5}	3.1746×10^{-5}
$^{241}_{94}\text{Pu}$	2.0974×10^{-5}	1.8646×10^{-5}
$^{242}_{94}\text{Pu}$	3.4772×10^{-6}	3.0912×10^{-6}
$^{241}_{95}\text{Am}$	4.5517×10^{-7}	4.0465×10^{-7}
$^{242}_{95}\text{Am}$	6.8986×10^{-9}	6.1329×10^{-9}
$^{243}_{96}\text{Am}$	4.4008×10^{-7}	3.9123×10^{-7}
$^{242}_{96}\text{Cm}$	9.6383×10^{-8}	8.5684×10^{-8}
$^{243}_{96}\text{Cm}$	1.3937×10^{-9}	1.2390×10^{-9}
$^{244}_{96}\text{Cm}$	8.3445×10^{-8}	7.4183×10^{-8}
$^{245}_{96}\text{Cm}$	3.5335×10^{-9}	3.1413×10^{-9}

⁹⁵ ₄₂ Mb	2.6784 10 ⁻⁵	2.3811 10 ⁻⁵
⁹⁹ ₄₃ Tc	3.3255 10 ⁻⁵	2.9564 10 ⁻⁵
¹⁰¹ ₄₄ Ru	3.0895 10 ⁻⁵	2.7466 10 ⁻⁵
¹⁰³ ₄₄ Ru	1.6724 10 ⁻⁵	1.4868 10 ⁻⁵
¹⁰⁹ ₄₇ Ag	1.9932 10 ⁻⁶	1.7720 10 ⁻⁶
¹³³ ₅₅ Cs	3.4680 10 ⁻⁵	3.0831 10 ⁻⁵
¹⁴³ ₆₀ Nd	2.6401 10 ⁻⁵	2.3470 10 ⁻⁵
¹⁴⁵ ₆₀ Nd	1.9992 10 ⁻⁵	1.7773 10 ⁻⁵
¹⁴⁷ ₆₂ Sm	1.6362 10 ⁻⁶	1.4546 10 ⁻⁶
¹⁴⁹ ₆₂ Sm	1.2997 10 ⁻⁷	1.1554 10 ⁻⁷
¹⁵⁰ ₆₂ Sm	7.5391 10 ⁻⁶	6.7023 10 ⁻⁶
¹⁵¹ ₆₂ Sm	5.5617 10 ⁻⁷	4.9444 10 ⁻⁷
¹⁵² ₆₂ Sm	3.0387 10 ⁻⁶	2.7014 10 ⁻⁶
¹⁵³ ₆₃ Eu	2.6708 10 ⁻⁶	2.3743 10 ⁻⁶
¹⁵⁴ ₆₄ Gd	1.8490 10 ⁻⁹	5.1473 10 ⁻⁵
¹⁵⁵ ₆₄ Gd		3.5035 10 ⁻⁴
¹⁵⁶ ₆₄ Gd		4.9864 10 ⁻⁴
¹⁵⁷ ₆₄ Gd		3.7045 10 ⁻⁴
¹⁵⁸ ₆₄ Gd		5.7501 10 ⁻⁴
¹⁶⁰ ₆₄ Gd		5.1722 10 ⁻⁴
¹⁶ ₈ O	4.5737 10 ⁻²	4.4205 10 ⁻²

Table II. Nuclide density specification of borated water and cladding material

material	nuclide	atom density x 10 ⁻²⁴ cm ⁻³
borated water in fuel cells	¹ ₁ H	4.7818 10 ⁻²
	¹⁶ ₈ O	2.3909 10 ⁻²
	¹⁰ ₅ B	1.3974 10 ⁻⁵
	¹¹ ₅ B	6.0087 10 ⁻⁵
cladding	^{nat} ₄₀ Zr	3.8090 10 ⁻²

and radial reflector between the reactor vessel and the core the borated water density is 0.9500 g/cm³ with the same relative nuclide distribution as in Table II. For simplicity the cladding material is taken as natural Zirconium with a mass density of 5.77 g/cm³. The composition of the stainless steel reactor vessel is specified in Table III. The total atom density is 0.086657 10²⁴ cm⁻³ resulting in a mass density of 7.9145 g/cm³.

Table III. Nuclide density specification of reactor vessel material

material	nuclide	atom density x 10 ⁻²⁴ cm ⁻³
reactor vessel	¹² ₆ C	9.7043 10 ⁻⁵
	²⁷ ₁₃ Al	1.2872 10 ⁻⁵
	⁵⁰ ₂₄ Cr	7.4610 10 ⁻⁴
	⁵² ₂₄ Cr	1.4388 10 ⁻²
	⁵³ ₂₄ Cr	1.6314 10 ⁻³
	⁵⁵ ₂₅ Mn	1.372810 ⁻³
	⁵⁴ ₂₆ Fe	3.4068 10 ⁻³
	⁵⁶ ₂₆ Fe	5.3480 10 ⁻²
	⁵⁷ ₂₆ Fe	1.2817 10 ⁻³
	⁵⁸ ₂₆ Fe	1.6437 10 ⁻⁴
	⁵⁹ ₂₇ Co	1.6170 10 ⁻⁴
	⁵⁸ ₂₈ Ni	5.4240 10 ⁻³
	⁶⁰ ₂₈ Ni	2.0893 10 ⁻³
	⁶¹ ₂₈ Ni	9.0829 10 ⁻⁵
	⁶² ₂₈ Ni	2.8954 10 ⁻⁴
	⁶⁴ ₂₈ Ni	7.3779 10 ⁻⁵
	⁶³ ₂₉ Cu	1.1942 10 ⁻⁴
	⁶⁵ ₂₉ Cu	5.3226 10 ⁻⁵
^{nat} ₄₂ Mo	1.7867 10 ⁻⁴	

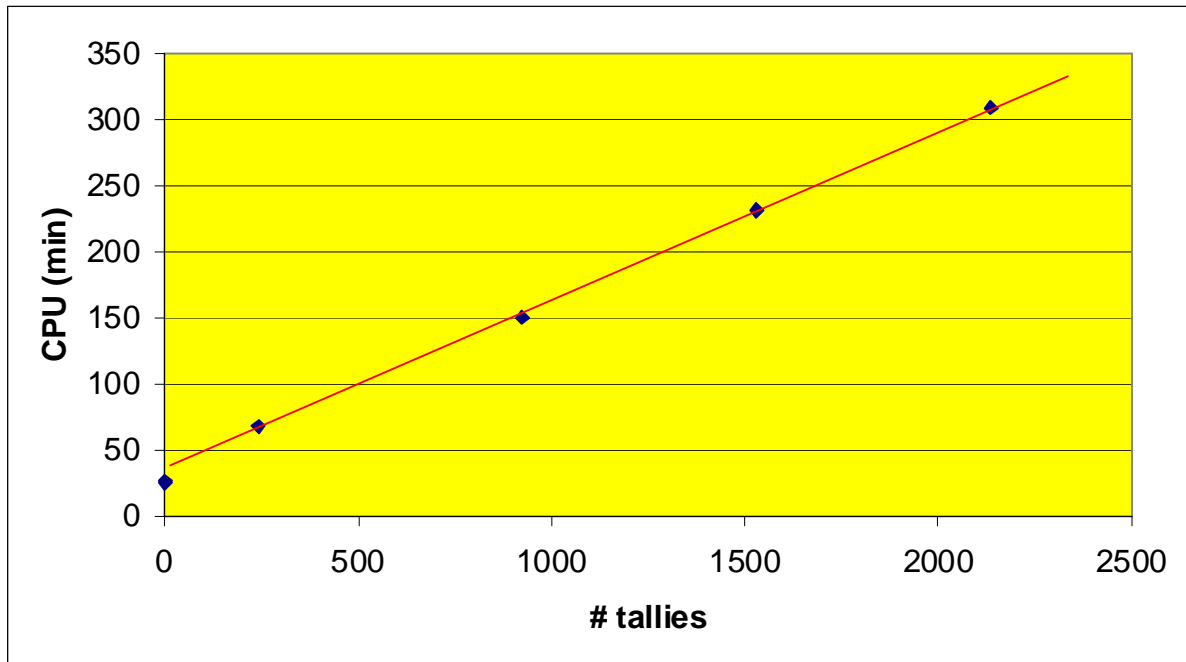
To avoid generating cross sections for all relevant nuclides in this benchmark test at different temperatures, all cross section are to be taken at room temperature. For water in the pin cells and the radial and axial reflectors the $S(\alpha,\beta)$ thermal scattering law at room temperature is to be applied.

Since the first calculations for this benchmark test have been done with the MCNP5 code [3], the input file for MCNP5 is available [4] and will be made public in order to ease the work for other participants and to concentrate on the efficiency of the calculation rather than the geometry modeling. Publication of input files for other general purpose Monte Carlo codes will be encouraged. The NEA Nuclear Data Bank is asked to adopt this benchmark and to serve as the place where the benchmark specifications and possibly input files for specific codes can be downloaded and results can be collected.

4. PRELIMINARY RESULTS

With the reactor geometry and detailed material composition given in Tables I-III, a criticality run with MCNP5.1.51 was made with 5,000 neutrons per cycle and 500 active cycles (+ 100 inactive cycles). The effective multiplication factor was $k_{eff}=1.00856 \pm 0.00044$. The run took 30.2 min CPU time (including the inactive cycles) on a 2.7 GHz single processor. Whether 100 inactive cycles are sufficient for source convergence also depends on the source distribution chosen for the first cycle. Fig. 3 shows that the CPU time with MCNP5 is linearly dependent on the number of tallies (used for estimating the power in various fuel volumes) and indicates that the processing time for each tally is considerable in MCNP5. All calculations in this figure are done with 500 active cycles with 5000 neutrons per cycle. This figure underlines the need for more efficient tallying as the number of tallies can be very large if the power in each separate fuel pin (or even in separate regions within each fuel pin) has to be obtained. It also turns out that the additional CPU time per tally relative to the CPU time for the Monte Carlo run without tallies may strongly depend on the computer system used or the specific implementation of MCNP5.

Fig. 3. CPU time dependence on number of tallies in MCNP5



In Table IV a few results are shown for the power produced per starting neutron in a few fuel assemblies, a few pins in a specific fuel assembly, and a few regions in a specific pin of a specific fuel assembly. For these results the F7 tally in MCNP (“fission energy deposition averaged over a cell”) was used for all considered fuel volumes but expressed in units of MeV per starting neutron. The fuel assemblies are identified by two numbers indicating their position relative to the central fuel assembly, which is identified as (0,0). Also the fuel pins in an assembly are identified relative to the center pin in the assembly. The axial regions are chosen to

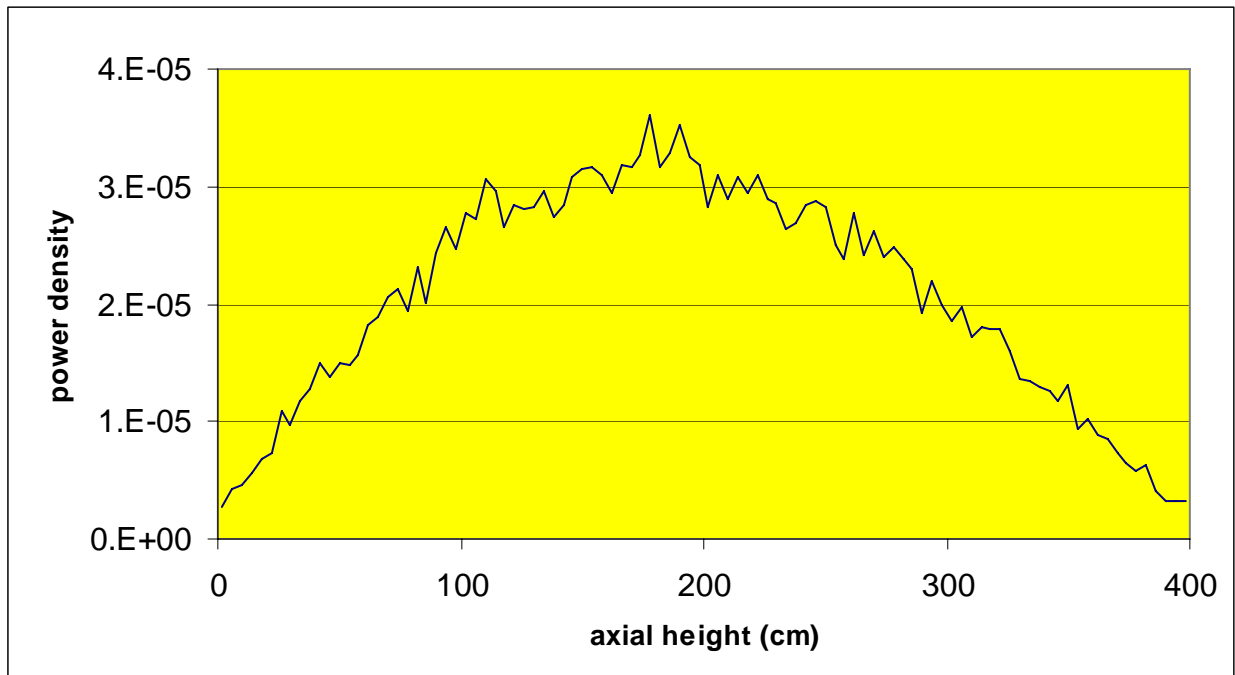
Table IV. Local power densities for a few fuel regions

Fuel assembly	Fuel pin	Axial region	Power	standard deviation	comment
(0, 0)	all	all	$6.359 \cdot 10^{-1}$	0.06 %	central FA
(2, 1)	all	all	$5.819 \cdot 10^{-1}$	0.06 %	
(-3, -8)	all	all	$5.333 \cdot 10^{-2}$	0.2 %	corner FA
(2, 1)	(-8, -8)	all	$2.183 \cdot 10^{-3}$	0.6 %	pin at corner of FA
(2, 1)	(0, 0)	all	$7.056 \cdot 10^{-4}$	0.6 %	central pin with Gd
(2, 1)	(-5, -3)	all	$2.070 \cdot 10^{-3}$	0.6 %	
(2, 1)	(-5, -3)	1	$2.77 \cdot 10^{-6}$	16 %	region at core bottom
(2, 1)	(-5, -3)	50	$2.83 \cdot 10^{-5}$	11 %	region at core midplane
(2, 1)	(-5, -3)	100	$3.30 \cdot 10^{-6}$	17 %	region at core top

be 4 cm high and are numbered from 1 at the bottom of the fuel pin to 100 at the top. All power results are in MeV per neutron history. The results are derived from a MCNP5 calculation with 100,000 cycles of 5,000 neutrons per cycle using a computer cluster of various nodes each consisting of 2 quad core AMD Opteron processors running at 2.7 GHz.

The power results for a complete fuel assembly are very accurate (0.06–0.2 %). The result for a fuel pin over its full length is also very accurate (~0.6 %). However, the standard deviations for the power in specific axial regions are 5 to 17 % and the power per region is therefore not always reliable. If the power distribution over a pin were flat, one can expect a standard deviation of about $\sqrt{400/4} \times 0.6\% = 6\%$. In fact, in a region at the core midplane the standard deviation is about 5 % for a fuel assembly near the core center. If a standard deviation of 1 % is required, about 25 times more neutron histories are needed! If this accuracy were required for the power in a 4 cm fuel region at the top or bottom of the core, the computational cost would be even greater. The above mentioned MCNP5 run was executed in parallel using 24 different computer cores. This calculation with 100,000 cycles of 5,000 neutrons using 634 tallies took 21.9 h execution time with a 82 % efficiency over the use of the 24 cores. This efficiency will further decrease when more computer cores are used. Hence, there is a need for optimizing the parallelization of the Monte Carlo calculation.

Fig. 4 shows the axial power profile per region of $\Delta z = 4$ cm for pin (-5, -3) in fuel assembly (2, 1). As the standard deviations for the power in a single axial region ranges from 5 to 17 % the individual results are not always statistically reliable, but the overall axial profile is clear.

Fig. 4. Axial power profile over a specific fuel pin

5. DISCUSSION AND CONCLUSIONS

The proposed benchmark test aims at monitoring the efficiency of Monte Carlo calculations over the coming years and possibly decades for the detailed estimation of local power densities. It was shown that the number of tallies included in the calculations is a major factor in determining the calculation time. This will make it prohibitive to include a power density tally for each axial region of every fuel pin. Therefore, it is of great importance to design estimators that can collect the scores for the power density much more efficiently. The cause of the relatively large time for obtaining a tally contribution is the fact that MCNP considers at each neutron collision site in a fuel zone the separate contribution of all nuclides comprising the fuel material, whether a nuclide is fissionable or not. It will be more efficient if for each fuel containing material the total contribution to the power as a function of energy is calculated in advance of the Monte Carlo calculation in order to avoid looking up individual contributions of all nuclides in the fuel.

In general there is a need to obtain cross section data more efficiently during the Monte Carlo calculation. Simplifying the energy grid for which cross sections are stored in order to retrieve specific data at a certain energy faster will be a possibility that is already practiced in some codes. A separate paper at this conference [5] discusses a promising new method for performing Doppler broadening of neutron cross sections "on the fly" during the random walk process, obviating the need to generate or store cross section sets at different temperatures, with negligible additional computational expense.

Apart from speeding up the Monte Carlo calculation and the tallying processes, variance reduction of the Monte Carlo process is desirable. This can be realized more easily for an

integral parameter as k_{eff} than for a local power density. Hence, developing theory to realize variance reduction for local flux/power estimates is an important and challenging goal.

As mentioned before the efficiency of parallel Monte Carlo simulations of neutron histories, especially for criticality calculations with many computer nodes and computational cores, needs further attention when implementing a parallel Monte Carlo algorithm. Considerable execution time can be saved if all computer cores can be maximally loaded.

To meet the challenges put forward by various authors Monte Carlo specialists should not just wait for faster computers with more cores, but should strive to improve many aspects of the Monte Carlo simulation itself.

REFERENCES

1. Kord Smith, "Reactor Core Methods," Invited lecture at the *M&C 2003 International Conference*, April 6-10, 2003, Gatlinburg, TN, USA (2003) <http://wwwtest.iri.tudelft.nl/~jhoogenb>.
2. William R. Martin, "Advances in Monte Carlo Methods for Global Reactor Analysis," Invited lecture at the *M&C 2007 International Conference*, April 15-19, 2007, Monterey, CA, USA (2007) <http://wwwtest.iri.tudelft.nl/~jhoogenb>.
3. X-5 Monte Carlo Team, "MCNP – A General Monte Carlo N-particle Transport Code, Version 5", Los Alamos National Laboratory (2003).
4. J. Eduard Hoogenboom, MCNP5 input file for the Monte Carlo efficiency monitoring benchmark (2008) <http://wwwtest.iri.tudelft.nl/~jhoogenb>.
5. G. Yesilyurt, W.R. Martin, and F.B. Brown, "On-The-Fly Doppler Broadening for Monte Carlo Codes," this conference.

APPENDIX. Input file for MCNP5

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PWR core for performance benchmark
c FAs filled with 17x17 cells with UOX (including 5 rods with Gd)
c cell cards
1 1 0.068230 -10          u=10 imp:n=1 $ fuel pin
2 2 -5.77      +10 -20    u=10 imp:n=1 $ cladding
3 3 -0.7164    +20          u=10 imp:n=1 $ borated coolant
14 like 1 but mat=5 u=14 rho=0.066564 $ UOX with Gd
15 like 2 but u=14
16 like 3 but u=14
17 like 1 but u=17 rho=0.065 $ UOX with reduced density
18 like 2 but u=17
19 like 3 but u=17
21 4 -0.95      -102    u=21          imp:n=1 $ radial reflector
20 0 -22 21 -24 23 imp:n=1 lat=1 u=25 fill=-8:8 -8:8 0:0
c note that this "map" below should be interpreted as from bottom to top
c col-8 -7 -6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6 7 8
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row -8
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row -7
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row -6
    10 10 10 14 10 10 10 10 10 10 10 10 10 14 10 10 10 $row -5
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row -4
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row -3
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row -2
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row -1
    10 10 10 10 10 10 10 10 14 10 10 10 10 10 10 10 10 $row 0
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row 1
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row 2
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row 3
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row 4
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    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row 7
    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 $row 8
24 0 -22 21 -24 23 imp:n=1 lat=1 u=27 fill=-8:8 -8:8 0:0
c col-8 -7 -6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6 7 8
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row -8
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row -7
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row -6
    17 17 17 14 17 17 17 17 17 17 17 17 17 14 17 17 17 $row -5
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row -4
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row -3
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row -2
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row -1
    17 17 17 17 17 17 17 17 14 17 17 17 17 17 17 17 17 $row 0
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row 1
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row 2
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row 3
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row 4
    17 17 17 14 17 17 17 17 17 17 17 17 17 14 17 17 17 $row 5
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row 6
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row 7
    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 $row 8

```

Monte Carlo benchmark proposal

```

40 0  -32 31  -34 33  imp:n=1  lat=1  u=40  fill=-9:9  -9:9  0:0
c col  -9 -8 -7 -6  -5 -4 -3 -2 -1  0  1  2  3  4  5  6  7  8  9
      21 21 21 21  21 21 21 21 21  21 21 21 21 21  21 21 21 21  $row -9
      21 21 21 21  21 21 25 25 25  25 25 25 25 21 21  21 21 21 21  $row -8
      21 21 21 21  25 25 25 25 25  25 25 25 25 25  21 21 21 21  $row -7
      21 21 21 25  25 25 25 25 25  25 25 25 25 25  25 21 21 21  $row -6
      21 21 25 25  25 25 25 25 25  25 25 25 25 25  25 25 21 21  $row -5
      21 21 25 25  25 25 25 25 25  25 25 25 27 25  25 25 21 21  $row -4
      21 25 25 25  25 25 27 25 25  25 25 25 25 25  25 25 25 21  $row -3
      21 25 25 25  25 25 25 25 25  25 25 25 25 25  25 25 25 21  $row -2
      21 25 25 25  25 25 25 25 25  25 25 25 25 25  25 25 25 21  $row -1
      21 25 25 25  25 25 25 25 25  25 25 25 25 25  25 25 25 21  $row 0
      21 25 25 25  25 25 25 25 25  25 25 25 25 25  25 25 25 21  $row 1
      21 25 25 25  25 25 25 25 25  25 25 25 25 25  25 25 25 21  $row 2
      21 25 25 25  25 27 25 25 25  25 25 25 25 25  25 25 25 21  $row 3
      21 21 25 25  25 25 25 25 25  25 25 25 25 27  25 25 21 21  $row 4
      21 21 25 25  25 25 25 25 25  25 25 25 25 25  25 25 21 21  $row 5
      21 21 21 25  25 25 25 25 25  25 25 25 25 25  25 21 21 21  $row 6
      21 21 21 21  25 25 25 25 25  25 25 25 25 25  21 21 21 21  $row 7
      21 21 21 21  21 21 25 25 25  25 25 25 25 21 21  21 21 21 21  $row 8
      21 21 21 21  21 21 21 21 21  21 21 21 21 21  21 21 21 21  $row 9
41 0  -32 31  -34 33  imp:n=1  lat=1  u=41  fill=-9:9  -9:9  0:0
c col  -9 -8 -7 -6  -5 -4 -3 -2 -1  0  1  2  3  4  5  6  7  8  9
      21 21 21 21  21 21 21 21 21  21 21 21 21 21  21 21 21 21  $row 1
      21 21 21 21  21 21 27 27 27  27 27 27 27 21 21  21 21 21 21  $row 2
      21 21 21 21  27 27 27 27 27  27 27 27 27 27  21 21 21 21  $row 3
      21 21 21 27  27 27 27 27 27  27 27 27 27 27  27 21 21 21  $row 4
      21 21 27 27  27 27 27 27 27  27 27 27 27 27  27 27 21 21  $row 5
      21 21 27 27  27 27 27 27 27  27 27 27 27 25 27  27 27 21 21  $row 6
      21 27 27 27  27 27 25 27 27  27 27 27 27 27  27 27 27 21  $row 7
      21 27 27 27  27 27 27 27 27  27 27 27 27 27  27 27 27 21  $row 8
      21 27 27 27  27 27 27 27 27  27 27 27 27 27  27 27 27 21  $row 9
      21 27 27 27  27 27 27 27 27  27 27 27 27 27  27 27 27 21  $row 10
      21 27 27 27  27 27 27 27 27  27 27 27 27 27  27 27 27 21  $row 11
      21 27 27 27  27 27 27 27 27  27 27 27 27 27  27 27 27 21  $row 12
      21 27 27 27  27 25 27 27 27  27 27 27 27 27  27 27 27 21  $row 13
      21 21 27 27  27 27 27 27 27  27 27 27 27 25  27 27 21 21  $row 14
      21 21 27 27  27 27 27 27 27  27 27 27 27 27  27 27 21 21  $row 15
      21 21 21 27  27 27 27 27 27  27 27 27 27 27  27 21 21 21  $row 16
      21 21 21 21  27 27 27 27 27  27 27 27 27 27  21 21 21 21  $row 17
      21 21 21 21  21 21 27 27 27  27 27 27 27 21 21  21 21 21 21  $row 18
      21 21 21 21  21 21 21 21 21  21 21 21 21 21  21 21 21 21  $row 19
45 0  -42 41  imp:n=1  lat=1  u=45  fill=-50:49  0:0  0:0  40 49r 41 49r
50 0  -101 202 -203  fill=45  imp:n=1
60 7  0.086657 -102 101 201 -204  imp:n=1 $ vessel
70 4 -0.7164 -101 201 -202  imp:n=1 $ lower reflector
71 4 -0.7164 -101 203 -204  imp:n=1 $ upper reflector
99 0 102:-201:204  imp:n=0  $ outside

```

```

c surfaces
10  cz  0.41  $ pellet radius/cladding inner radius
20  cz  0.475 $ cladding outer radius
21  px -0.63
22  px  0.63
23  py -0.63
24  py  0.63
31  px -10.71

```

```

32 px 10.71
33 py -10.71
34 py 10.71
41 pz 0
42 pz 4      $ axial layer
101 cz 203
102 cz 223
201 pz -220
202 pz -200
203 pz 200
204 pz 220

c data cards
kcode 5000 1. 100 600      $ 500 active cycles + 100 inactive cycles
sdef x=d1 y=d2 z=d3 erg=2
si1 -140 140
sp1 0 1
si2 -140 140
sp2 0 1
si3 -180 180
sp3 0 1
print -160 -178 -110 -128 -10 -30 -40 -50 -70 -72 -98 -120 -130 -140 -102
c tally cards
vol 0.5 19r      $ in order not to divide joint tally by volume
f7:n (1 14 17)   $ total power
c note that for the following power tallies
c only a very limited number of segments have been included for brevity
f37:n $ all FAs
((1 14 17)<(40[-3 -8 0]41[-3 -8 0])) ((1 14 17)<(40[-2 -8 0]41[-2 -8 0]))
((1 14 17)<(40[-1 -8 0]41[-1 -8 0])) ((1 14 17)<(40[ 0 -8 0]41[ 0 -8 0]))
((1 14 17)<(40[ 1 -8 0]41[ 1 -8 0])) ((1 14 17)<(40[ 2 -8 0]41[ 2 -8 0]))
((1 14 17)<(40[ 3 -8 0]41[ 3 -8 0]))
((1 14 17)<(40[-5 -7 0]41[-5 -7 0])) ((1 14 17)<(40[-4 -7 0]41[-4 -7 0]))
c etc.
((1 14 17)<(40[ 3 8 0]41[ 3 8 0]))
t
f57:n $all pins in FA[202]=FA[2 1 0]
((1 14 17)<(20[ 1]24[ 1])<(40[202]41[202]))
((1 14 17)<(20[ 2]24[ 2])<(40[202]41[202]))
((1 14 17)<(20[ 3]24[ 3])<(40[202]41[202]))
c etc.
((1 14 17)<(20[289]24[289])<(40[202]41[202])) t
c
f307:n $ axial regions in single pin (-5 -3) of FA[2 1 0]
((1 14)<20[-5 -3 0]<40[2 1 0]
<45[1]45[2]45[3]45[4]45[5]45[6]45[7]45[8]45[9]45[10]45[11]45[12]45[13]
45[14]45[15]45[16]45[17]45[18]45[19]45[20]45[21]45[22]45[23]45[24]45[25]
45[26]45[27]45[28]45[29]45[30]45[31]45[32]45[33]45[34]45[35]45[36]45[37]
45[38]45[39]45[40]45[41]45[42]45[43]45[44]45[45]45[46]45[47]45[48]45[49]
45[50] )
((17 14)<24[-5 -3 0]<41[2 1 0]
<45[51]45[52]45[53]45[54]45[55]45[56]45[57]45[58]45[59]45[60]45[61]45[62]
45[63]45[64]45[65]45[66]45[67]45[68]45[69]45[70]45[71]45[72]45[73]45[74]
45[75]45[76]45[77]45[78]45[79]45[80]45[81]45[82]45[83]45[84]45[85]45[86]
45[87]45[88]45[89]45[90]45[91]45[92]45[93]45[94]45[95]45[96]45[97]45[98]
45[99]45[100] ) t
c

```

```

m1  $ UOX
    92234 4.8797E-06
    92235 4.8339E-04
    92236 8.7108E-05
    92238 2.1500E-02
    93237 7.0455E-06
    94238 1.4424E-06
    94239 1.4137E-04
    94240 3.5710E-05
    94241 2.0974E-05
    94242 3.4772E-06
    95241 4.5517E-07
    95242 6.8986E-09
    95243 4.4008E-07
    96242 9.6383E-08
    96243 1.3937E-09
    96244 8.3445E-08
    96245 3.5335E-09
    42095 2.6784E-05
    43099 3.3255E-05
    44101 3.0895E-05
    44103 1.6724E-05
    47109 1.9932E-06
    55133 3.4680E-05
    60143 2.6401E-05
    60145 1.9992E-05
    62147 1.6362E-06
    62149 1.2997E-07
    62150 7.5391E-06
    62151 5.5617E-07
    62152 3.0387E-06
    63153 2.6708E-06
    64155 1.8490E-09
    8016 0.045737
m2  40000 1.          $ cladding material
m3  $ borated water
    1001 0.047818
    8016 0.023909
    5010 1.3974e-5    $ B-concentration tuned for a reasonable k_eff
    5011 6.0087e-5
mt3 lwtr.60t          $ room temperature S(a,b)
m4  $ borated water for radial and axial reflector
    $ in fact identical to m3 (but used with a different density)
    1001 0.047818
    8016 0.023909
    5010 1.3974e-5
    5011 6.0087e-5
mt4 lwtr.60t          $ room temperature S(a,b)
m5  $ UOX with Gd burnable absorber
    92234 4.3381E-06
    92235 4.2973E-04
    92236 7.7439E-05
    92238 1.9114E-02
    93237 6.2634E-06
    94238 1.2823E-06
    94239 1.2568E-04
    94240 3.1746E-05

```

94241 1.8646E-05
 94242 3.0912E-06
 95241 4.0465E-07
 95242 6.1329E-09
 95243 3.9123E-07
 96242 8.5684E-08
 96243 1.2390E-09
 96244 7.4183E-08
 96245 3.1413E-09
 42095 2.3811E-05
 43099 2.9564E-05
 44101 2.7466E-05
 44103 1.4868E-05
 47109 1.7720E-06
 55133 3.0831E-05
 60143 2.3470E-05
 60145 1.7773E-05
 62147 1.4546E-06
 62149 1.1554E-07
 62150 6.7023E-06
 62151 4.9444E-07
 62152 2.7014E-06
 63153 2.3743E-06
 64154 5.1473E-05
 64155 3.5035E-04
 64156 4.9864E-04
 64157 3.7045E-04
 64158 5.7501E-04
 64160 5.1722E-04
 8016 4.4205E-02

m7

\$ SS vessel

6000.60c 9.7043E-05 26054.60c 3.4068E-03 26056.60c 5.3480E-02
 26057.60c 1.2817E-03 26058.60c 1.6437E-04 14000.60c 1.1894E-03
 28058.60c 5.4240E-03 28060.60c 2.0893E-03 28061.60c 9.0829E-05
 28062.60c 2.8954E-04 28064.60c 7.3779E-05 25055.60c 1.3728E-03
 24050.60c 7.4610E-04 24052.60c 1.4388E-02 24053.60c 1.6314E-03
 24054.60c 4.0610E-04 29063.60c 1.1942E-04 29065.60c 5.3226E-05
 27059.60c 1.6170E-04 13027.60c 1.2872E-05 42000.60c 1.7867E-04