## Comparison of multigroup eigenvalue solvers: Monte Carlo versus diffusion

K. Mikityuk, Paul Scherrer Institut, Villigen PSI

16.08.2021

Case 8 of a 3D Superphenix Sodium Fast Reactor static neutronic benchmark is used for comparing efficiencies of eigenvalue solvers based on two methods: neutron diffusion and Monte Carlo in a framework of the ROOSTER code.

A structured mesh is used with a hexagonal prism representing an axial layer of a subassembly. The geometry of subassemblies are not explicitly simulated, but the materials are homogenized in every node. In case of the neutron diffusion solver, each hexagonal prism is subdivided in six triangular prisms and the net current between neighbouring nodes are calculated by using finite-difference representation of the Fick's law. A more accurate modeling of the neutron leakage can improve the results.

In case of the Monte Carlo solver, a delta-tracking formalism is used for random walk simulation and scattering angle is not sampled but taken equal to its average value. A more accurate modeling of the anisotropic scattering can improve the results.

Five sets of multigroup microscopic cross sections prepared with NJOY21 are used for the following number of energy groups: 7, 13, 25, 50 and 100 groups.

Three parameters are selected for the comparison:

- 1) k-effective and its deviation from the reference value of 0.99894;
- 2) deviation of subassembly-wise power peaking factors from the reference one;
- 3) wall time.

The second parameter is presented via four values (appearing in Table 1):

- A) fraction of subassemblies (%) in which the power peaking factor deviation is less than 2%;
- B) fraction of subassemblies (%) in which the power peaking factor deviation is from 2% to 5%;
- C) fraction of subassemblies (%) in which the power peaking factor deviation is higher than 5%;
- D) maximum deviation of power peaking factor (%).

The diffusion solver results are presented in Table 1 and Figs. 1, 2 and 3a. An increase of the number of groups does not show a consistent decrease in the k-effective deviation, but rather a piece-wise linear function. The improvement of the power distribution prediction is more consistent with the growing number of groups although there are some minor anomalies in the trend. The bias in k-effective can be explained by a homogenized modeling of the absorber present in the core (CSD rods are inserted by 40 cm in the fissile region). The absolute values of the wall time is not particularly representative because they depend on the computer power, parallelization efficiency and can be strongly improved by implementation of a nodal scheme, but the relative growth of the wall time with the number of groups is more representative and should be taken into account while comparing with the Monte Carlo method.

The Monte Carlo solver results are presented in Table 2 and Figs. 1, 2 and 3b. 100 inactive and 1000 active cycles with 50000 neutrons each cycle were simulated, allowing for a one standard deviation of about 10 pcm in k-effective. As in the case of the diffusion solver, the bias in k-effective can be explained by a homogenization of materials and first of all of the absorber. The improvement of the

power distribution prediction is consistent with the increase of the number of groups. An interesting and expected finding is an almost constant wall time.

The comparison of the two methods shows slightly improved prediction of k-effective by the diffusion solver (Fig. 1) and of power distribution by the Monte Carlo method (Fig. 3) as well as a fast increase of the wall time with increase of the number of groups in the diffusion solver case and almost complete independence of the wall time on the number of groups in case of the Monte Carlo solver. The piece-wise linear shape of the k-effective dependence on the number of group is identical for two methods and can be explained by the selection of the group boundaries, the detailed study being out of scope.

An overall conclusion can be that the Monte Carlo solver is an interesting alternative to the diffusion solver in particular for an IQS method because it can provide improvements in the power distribution by increasing the number of groups and stay fast running.

Finally all 13 benchmark cases were calculated with three methods: 1) diffusion with 1 node per subassembly (ROOSTER DIF1); 2) diffusion with 6 nodes per subassembly (ROOSTER DIF6); 3) Monte Carlo (ROOSTER MC). In all cases 25 energy groups were used. The calculated k-effective values are compared with the reference Serpent solution in Table 3 and Fig. 4. As expected the deeper absorber is inserted in the core the higher the discrepancies in k-effective. Selected reactivity effects are compared in Table 4. The conclusion of the final part of the study is that both diffusion and Monte Carlo methods allows predicting the reactivity effects with reasonable accuracy.

Table 1. Diffusion solver results

# of groups	k-eff	δk-eff, pcm	A, %	В, %	C, %	D, %	Wall time, s
7	0.99410	-484	70	21	9	13	77
13	0.99383	-511	80	15	5	9	167
25	0.99324	-570	79	16	5	8	425
50	0.99597	-297	78	13	9	9	2106
100	0.99494	-400	82	16	2	7	12334

Table 2. Monte Carlo solver results

# of groups	k-eff	δk-eff, pcm	A, %	В, %	С, %	D, %	Wall time, s
7	0.99107	-787	75	22	3	11	50
13	0.99066	-828	82	16	2	9	60
25	0.99034	-860	88	12	0	7	58
50	0.99365	-529	89	10	1	6	65
100	0.99288	-606	88	11	1	6	64

Table 3. k-effective for all benchmark cases calculated by different methods

	SERPENT REF	ROOSTER DIF1	ROOSTERDIF6	ROOSTER MC	ROOSTER DIF1	ROOSTERDIF6	ROOSTER MC
	K-eff	k-eff	k-eff	k-eff	δk-eff	δk-eff	δk-eff
1	1.04365	1.04694	1.04228	1.04190	329	-137	-175
2	1.04246	1.04602	1.04135	1.04077	356	-111	-169
3	1.03670	1.04043	1.03572	1.03515	373	-98	-155
4	0.95119	0.97380	0.94018	0.93198	2261	-1101	-1921
5	1.04080	1.04410	1.03943	1.03895	330	-137	-185
6	1.00824	1.01664	1.00314	1.00001	840	-510	-823
7	1.03053	1.03350	1.02875	1.02830	297	-178	-223

8	0.99894	1.00666	0.99324	0.99034	772	-570	-860
9	1.03139	1.03426	1.02951	1.02938	287	-188	-201
10	1.02886	1.03204	1.02727	1.02710	318	-159	-176
11	0.99742	1.00552	0.99208	0.98909	810	-534	-833
12	1.02483	1.02765	1.02282	1.02256	282	-201	-227
13	1.01903	1.02186	1.01693	1.01656	283	-210	-247

Table 4. Selected reactivity effect calculated by different methods

	100100 100011111	errede carcaratea sy arrierent metrious				
Case	SERPENT REF	ROOSTER DIF1	ROOSTERDIF6	ROOSTER MC		
#5-#7	1027	1060	1068	1065		
#5-#12	1597	1645	1661	1639		
#5-#9	941	984	992	957		
#6-#8	930	998	990	967		
#10-#3	-784	-839	-845	-805		
(#5-#2) + (#5-#7)	861	868	876	883		
(#5-#2) + (#6-#8)	764	806	798	785		
#5-#2	-166	-192	-192	-182		

0.99700 0.99600 0.99500 k-effective 0.99400 0.99300 0.99200 Diffusion 0.99100 Monte Carlo 0.99000 0 25 50 75 100 Number of groups

Fig. 1. K-effective versus number of groups for diffusion and Monte Carlo solvers

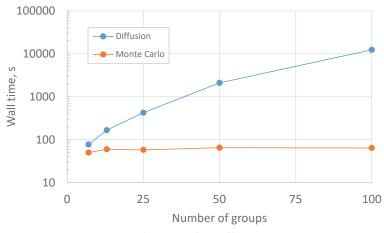


Fig. 2. Wall time versus number of groups for diffusion and Monte Carlo solvers

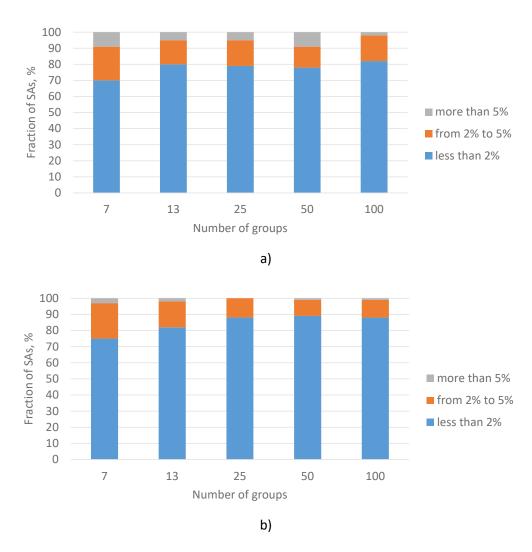


Fig. 3. Deviation of power peaking factor distribution versus number of groups for (a) diffusion and (b) Monte Carlo solvers

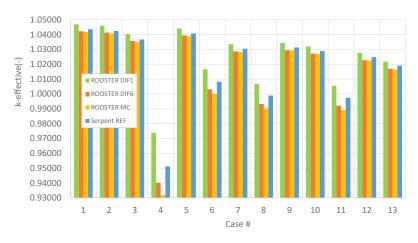


Fig. 4. k-effective calculated by various methods