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A NEW ASSEMBLY-LEVEL MONTE CARLO NEUTRON TRANSPORT CODE FOR REACTOR PHYSICS CALCULATIONS

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ABSTRACT

This paper presents a new assembly-level Monte Carlo neutron transport code, specifically intended for diffusion code group-constant generation and other reactor physics calculations. The code is being developed at the Technical Research Centre of Finland (VTT), under the working title "Probabilistic Scattering Game", or PSG. The PSG code uses a method known as Woodcock tracking to simulate neutron histories. The advantages of the method include fast simulation in complex geometries and relatively simple handling of complicated geometrical objects. The main drawback is the inability to calculate reaction rates in optically thin volumes. This narrows the field of application to calculations involving parameters integrated over large volumes.

The main features of the PSG code and the Woodcock tracking method are introduced. The code is applied in three example cases, involving infinite lattices of two-dimensional LWR fuel assemblies. Comparison calculations are carried out using MCNP4C and CASMO-4E. The results reveal that the code performs quite well in the calculation cases of this study, especially when compared to MCNP. The PSG code is still under extensive development and there are both flaws in the simulation of the interaction physics and programming errors in the source code. The results presented here, however, seem very encouraging, especially considering the early development stage of the code.

KEYWORDS: Monte Carlo, Neutron Transport, Group Constant, Reactor Physics

1. INTRODUCTION

1.1. Background

Several applications in nuclear reactor physics and dynamics require three-dimensional modelling of the core neutronics. Such calculations are presently carried out using few-group nodal diffusion codes. The geometry in the diffusion calculation consists of homogenised material regions, or nodes. The input data for the calculation includes spectrum-averaged cross sections, kinetic parameters and other group constants, which are generated in such way that the integral reaction rate balance is preserved within each node.

The group constant data are generated in detailed two-dimensional assembly-level calculations. In order to collect a sufficient set of data, all fuel types and various thermal hydraulic and burnup conditions need to be covered. The impacts of control rods and soluble absorber used for

reactivity control must be included as well. The number of parameter combinations becomes extremely large and the generation process may consist of several thousands of runs.

Due to the large number of parameter combinations, deterministic fine-group transport calculation codes, such as CASMO and HELIOS, are traditionally used for the group constant generation. The other alternative would be to use Monte Carlo codes, which at present computing resources are far too slow for the job. There are, however, some significant advantages in Monte Carlo over deterministic transport calculation methods, such as the direct access to evaluated nuclear data. Presently, Monte Carlo codes, such as MCNP, KENO and TRIPOLI, are routinely used for criticality safety analyses and other reactor physics calculations requiring the detailed modelling of geometry and core neutronics. It can be foreseen that the range of applications will broaden along with the increase of raw computing power.

1.2. Project Objective

This paper presents a new Monte Carlo neutron transport calculation code, specifically intended for diffusion code group constant generation and other assembly-level reactor physics calculations. The code is being developed at the Technical Research Centre of Finland (VTT). The development is at a very early stage and the code has been given the working title "Probabilistic Scattering Game", or PSG.

The objective of the project is to develop a fast Monte Carlo neutron transport code to meet the future needs in reactor physics calculations. The code should be able to calculate group-wise cross sections, kinetic parameters, pin-wise power distributions, discontinuity factors and all the other parameters needed for nodal diffusion calculations. The next version of the code should also be able to perform burnup calculation. The use of the Monte Carlo method brings some additional functionality compared to deterministic lattice codes and new fields of application may arise during the development.

Although it may take a while before the available computer capacities allow a Monte Carlo code to be used as the primary production tool for group constant generation, it is always good to have both redundancy and diversity in the calculation methods. At the early stage, the PSG code is primarily intended as a research tool to be used in parallel with the deterministic lattice codes. Another very important aspect is educational. Code development is one of the best means for training a new generation of experts in reactor physics.

The following sections introduce the main features of the Monte Carlo transport method used by the PSG code, as well as some general issues related to group constant generation. Some comparison calculations using PSG, MCNP4C and CASMO-4E are presented in Section 4.

2. CALCULATION METHODS

2.1. Overview

The PSG code uses the static k-eigenvalue method and analog Monte Carlo game to simulate neutron transport in a three-dimensional geometry. The methodology is mainly based on two

references – the textbook by Lux and Koblinger [1] and the MCNP4C manual [2]. The code is written from scratch for the Linux environment using the standard C-language.

The most significant difference to most of the other similar codes lies in the method used for neutron tracking. In order to clarify the main differences, some of the basic principles of Monte Carlo transport calculation are shortly reviewed.

2.2. Neutron Transport

The method applied in most Monte Carlo transport calculation codes is to simulate neutron histories by tracking each neutron through homogeneous material regions in the geometry and stopping at each material boundary. The distance to the next collision site is randomly sampled according to the total interaction probability in the material. This probability is exponentially distributed and depends on the macroscopic total cross section. The distance to the next collision site is sampled using:

$$\ell = -\frac{\ln(\xi)}{\Sigma_{\mathrm{t}}(E,\mathbf{r})}\,, \tag{1}$$

where ξ is a random variable uniformly distributed between 0 and 1. The interaction is sampled at the collision site according to the partial cross sections of the available reaction channels. The probability of reaction i is simply

$$P_i = \frac{\Sigma_i(E,\mathbf{r})}{\Sigma_{\mathrm{t}}(E,\mathbf{r})}\,. \tag{2}$$

Since the geometry usually consists of various material regions, the collision distance has to be adjusted each time the neutron enters a new region with higher or lower interaction probability. In practise this means that the distance to the nearest boundary surface has to be calculated each time the next collision site is sampled. If the collision site lies beyond the material boundary, the neutron is stopped at the surface and the remaining part of the flight path is re-sampled or modified according to the new collision probability. The calculation of the surface distances may take a significant fraction of the computing time in complex systems, especially if the neutron mean free path is long compared to the characteristic dimensions of the geometry.

The PSG code uses another approach, developed by Woodcock et al. in the 1960's [3]. The Woodcock tracking method uses the concept of a *virtual* collision, which actually means that there is no collision at all. It is relatively easy to see, even by intuition, that an arbitrary virtual collision cross section, $\Sigma_0(E,\mathbf{r})$, can be added to the material total in Eqs. 1 and 2 without affecting the statistics. The reason to do so is to have the same total cross section for all the materials in the geometry. This eliminates the need to adjust the length of the flight path each time the neutron enters a new material, and eventually, the need to calculate the surface distances.

In practise, the flight distance is sampled using a (material-independent) *majorant cross section*, $\Sigma_{\mathrm{m}}(E)$, which at each energy point is equal to the maximum of all the macroscopic total cross sections in the system. The probability of a virtual collision in a material with total cross section $\Sigma_{\mathrm{t}}(E,\mathbf{r})$ is then:

$$P_0 = \frac{\Sigma_0(E,\mathbf{r})}{\Sigma_{\mathrm{m}}(E)} = \frac{\Sigma_{\mathrm{m}}(E)-\Sigma_{\mathrm{t}}(E,\mathbf{r})}{\Sigma_{\mathrm{m}}(E)} = 1-\frac{\Sigma_{\mathrm{t}}(E,\mathbf{r})}{\Sigma_{\mathrm{m}}(E)}\,. \tag{3}$$

The tracking is simply continued until a real collision is sampled with probability $1 - P_0$. After that, the reaction channel is sampled and the procedure continues in the conventional way.

The main advantage of the Woodcock tracking method is that there is no need to calculate the surface distances, which will speed-up the calculation in complex geometries. Since the total collision probability remains unchanged throughout the geometry, non-uniform material compositions can be modelled with only minor modifications in the tracking procedure. This enables some interesting new features, for example, the simulation of continuous coolant void distributions in the axial direction of a BWR fuel assembly.

The main disadvantage of the method is that the track-length estimator of neutron flux is not available and reaction rates have to be calculated using the (less efficient) collision estimator[1]. Surface currents and fluxes can be determined only at the outer boundaries of the geometry and the method loses some of its efficiency when high-absorbing burnable absorbers or control rods are present. The first two limitations are not too significant for calculations involving reaction rates integrated over large volumes, but they do rule out some of the applications for which Monte Carlo codes are traditionally used.

Despite some of its advantages, the Woodcock method has not been very popular among the developers of modern Monte Carlo neutron transport codes. This is probably due to the loss of generality when the method is applied. In addition to the new PSG code, the method is used in the MONK and MCBEND codes to track neutrons in some complex parts of the geometry [4].

2.3. Geometry Description

Since boundary surfaces are used only to determine whether a neutron is inside a material region or not, complicated objects, such as square and hexagonal channel boxes with rounded corners or cruciform control rod shapes can be handled quite easily. Presently the PSG code handles three-dimensional objects bounded by planes, spheres, cylinders and various derived surface types. Square and hexagonal fuel pin lattices are described as separate objects, for which the pin layout is given and each pin type is defined by concentric cylindrical regions.

2.4. Interaction Physics

The nuclear interaction data are stored and used in a tabular point-wise form. Cross sections are read from ACE-format data libraries, which are also used by the MCNP code [2]. There are several advantages of using this format. The calculations can be directly compared to MCNP results without uncertainties originating from the nuclear data. Several extensively tested and widely used cross section libraries are available through public channels and new libraries can be easily generated using the NJOY nuclear data processing system.

Since the data format is shared with MCNP, most of the interaction physics is very similar as well. The available reaction channels at this stage are fission, capture[2] and two-body scattering

[1] The difference in the efficiency becomes apparent in optically thin material regions with low overall collision probability.
[2] All (n,0n)-reactions are handled in a similar manner.

collisions. Anisotropic angular distributions are used for elastic scattering and inelastic level scattering. For these reactions the emission energy is fixed by the collision kinematics together with the reaction Q-value, and no secondary energy distributions are needed. Continuum inelastic scattering is incorrectly simulated as an isotropic level scattering event with a fixed Q-value. It is yet unclear what is the impact of this deficiency. There are, however, some more significant flaws in the interaction physics, such as the total omission of the (n,2n)-reactions.

The emission energies of fission neutrons are sampled from distributions given in the ACE-format data. If available, delayed neutron fractions, decay constants and emission energy distributions are used appropriately for 6 or 8 precursor groups.

A free-gas model is used to simulate the scattering of thermal neutrons. It is a well-known fact that this treatment is insufficient to accurately describe thermal scattering in high-moderated LWR conditions. The development of a proper thermal scattering model for hydrogen atoms bound in water will hence have the highest priority in future code development.

3. COMPARISON CALCULATIONS

3.1. Calculated Parameters

The results of the comparison calculations presented in this paper are related to input parameters used by nodal diffusion codes. The underlying theory presents itself in the form of two-group diffusion equations, which in the time-independent form can be written as:

$$\begin{aligned} -D_1\nabla^2\Phi_1 + \left(\Sigma_{\mathrm{a},1}+\Sigma_{\mathrm{r}}\right)\Phi_1 &= \frac{1}{k}\left(\overline{\nu}_1\Sigma_{\mathrm{f},1}\Phi_1 + \overline{\nu}_2\Sigma_{\mathrm{f},2}\Phi_2\right) \\ -D_2\nabla^2\Phi_2 + \Sigma_{\mathrm{a},2}\Phi_2 &= \Sigma_{\mathrm{r}}\Phi_1\,, \end{aligned} \tag{4}$$

where group index 1 refers to the fast energy group and index 2 to the thermal group. The group boundary is set to 0.625 eV.

It is not possible to go into the details of the nodal diffusion method and group constant generation within the scope of this paper. Instead, it is considered sufficient to give a brief description of each parameter included in the comparison.

Group-wise reaction cross sections are calculated for each nodal region in such way that the integral reaction rate balance is preserved. The macroscopic cross section of reaction i in group g is given by:

$$\Sigma_{i,g} = \frac{R_{i,g}}{\Phi_g} = \frac{\int_V \int_{E_g}^{E_{g-1}} \Sigma_i(E,\mathbf{r})\phi(E,\mathbf{r})dV\,dE}{\int_V \int_{E_g}^{E_{g-1}} \phi(E,\mathbf{r})dV\,dE}\,. \tag{5}$$

In other words, $\Sigma_{i,g}$ is the flux- and volume-weighted average taken from the energy-dependent cross section data. The strength of the Monte Carlo method is in that the integrals in Eq. 5 can be estimated directly, without explicitly solving for the flux distribution, $\phi(E,\mathbf{r})$.

The removal cross section, Σ_{r}, defines the net rate at which neutrons are scattered from the fast group to the thermal group. This parameter is given by the group-wise scattering cross sections and the group-transfer probabilities:

$$\Sigma_{\mathrm{r}} = \Sigma_{\mathrm{s},1} P_{1\to 2} - \frac{\Phi_2}{\Phi_1} \Sigma_{\mathrm{s},2} P_{2\to 1} \,. \tag{6}$$

The probability of transfer $1 \to 2$ is simply the fraction of scattering reactions, in which a neutron, initially above the group threshold, is emitted at an energy below it. The up-scattering probability ($2 \to 1$) is defined in a similar manner.

The diffusion coefficients are the result of the diffusion approximation, which essentially states that the neutron current is proportional to the flux gradient. The most common practise is to define the group-wise diffusion coefficients using the transport cross sections, $\Sigma_{\mathrm{tr},g}$, which are determined by the reaction cross sections and the average scattering cosines, $\overline{\mu}_g$:

$$D_g = \frac{1}{3\Sigma_{\mathrm{tr},g}} = \frac{1}{3\left(\Sigma_{\mathrm{t},g} - \overline{\mu}_g \Sigma_{\mathrm{s},g}\right)} \,. \tag{7}$$

The effective multiplication factor, k, is calculated using the so-called absorption estimator, which in an infinite geometry is basically the ratio of the total neutron production rate to the total rate of neutron absorption.

Advanced nodal diffusion codes use so-called assembly discontinuity factors to allow a difference between the heterogeneous and the homogeneous neutron flux at nodal boundaries and corners. If the assembly is assumed to be surrounded by an infinite lattice of similar cells, the discontinuity factor for a surface s can be defined as the ratio of the surface group flux to the average group flux in the node:

$$f_{s,g} = \frac{\Phi_{s,g}}{\Phi_g} = \frac{V \int_S \int_{E_g}^{E_{g-1}} \phi(E,\mathbf{r}) dS dE}{S \int_V \int_{E_g}^{E_{g-1}} \phi(E,\mathbf{r}) dV dE} \,. \tag{8}$$

Again, the integrals in Eq. 8 can be estimated directly. In practise, the surface and corner fluxes are calculated as volume-averaged integral values in a thin surface layer around the node boundary.

Reactor dynamics codes require information on the kinetic behaviour of the neutron flux for transient analysis. The kinetic parameters included in the comparison are the total (β_{tot}) and the effective (β_{eff}) delayed neutron fractions in six precursor groups. The total delayed neutron fraction is simply the fraction of all fission neutrons emitted as delayed in the respective precursor group. The effective fraction is related to the importance of the delayed neutrons with respect to the fission chain reaction. The calculation of β_{eff} using the Monte Carlo method is discussed in Ref. [5]. The method used by the PSG code is copied from there.

3.2. Calculation Tools

The results of the PSG code are compared to MCNP4C and CASMO-4E calculations in three test cases. MCNP [2] is a general-purpose Monte Carlo radiation transport code developed at Los Alamos National Laboratory. The code is widely used in both research and industry for various problems in reactor physics. CASMO [6] is a two-dimensional deterministic lattice code developed by Studsvik Scandpower. The code uses the method of characteristics to solve the fine-group Boltzmann transport equation and also has the capability to perform burnup calculation. CASMO is widely used in the industry to calculate group constant data for nodal diffusion reactor physics and dynamics codes. Both codes are routinely used at VTT.

3.3. Calculation Cases

The comparison calculations are divided into three cases, each chosen for a specific reason. All geometries consist of an infinite array of two-dimensional fuel assemblies:

Case 1: A non-profiled VVER-440 fuel assembly.
Case 2: A heterogeneous 17×17 PWR fuel assembly with three types of MOX fuel pins.
Case 3: An asymmetric 10×10 BWR fuel assembly with 10 burnable absorber pins.

The VVER-440 assembly represents a rather typical uranium-fuelled PWR case from the neutronics point-of-view. This case was included also in order to show that the PSG code can handle the geometrically more tedious hexagonal pin lattice. The MOX-fuelled PWR assembly is physically more complicated due to the large number of epithermal resonance peaks and high thermal absorption of the plutonium isotopes. The BWR fuel assembly is more asymmetric than the other cases and contains high-absorbing burnable absorber pins. The geometry has two unique boundary surfaces and three unique corners, which is convenient for testing the consistency of the assembly discontinuity factors.

4. RESULTS

4.1. Criticality Calculation and Computing Time

Table I shows the effective multiplication factors calculated by each code. The differences are relative and in the units of pcm. The results of MCNP4C and PSG are fairly consistent, although the differences can be considered statistically significant. The differences between CASMO-4E and PSG are of the same order in magnitude, except in the PWR MOX case.

A few general remarks need to be made on the calculations, before further discussing the differences in the results. First, the lack of a proper thermal scattering model in the PSG code has a significant impact on the results. For the sake of consistency, all MCNP calculations were run without any thermal scattering libraries for light water. The molecular effects are, however, included in the CASMO calculations. Second, although the same cross section libraries were used for both MCNP and PSG, the CASMO-4E libraries are of a different origin, which results in an additional source of uncertainty. Finally, the calculation methods used by CASMO-4E are completely different from the other two codes. Although the geometry models are consistent, it can not be guaranteed that all the physics are treated in a consistent manner.

Table I. Effective multiplication factors calculated using CASMO-4E, MCNP4C and PSG. The differences between the results are in units of reactivity (pcm). Column "diff1" refers to differences between CASMO-4E and PSG and column "diff2" to differences between MCNP4C and PSG. Statistical uncertainties are given as standard deviations.

	CASMO	MCNP	PSG	diff1	diff2
VVER-440	1.29429	1.29401±0.00029	1.29591±0.00025	125	147
PWR MOX	1.21392	1.22674±0.00031	1.22922±0.00028	1245	202
BWR + Gd	1.11043	1.10961±0.00028	1.11341±0.00032	268	341

A comparison of calculation times shows that the PSG code runs approximately 6 to 8 times faster than MCNP in the VVER-440 and the PWR MOX cases. The factor is reduced to about 2 in the BWR case with burnable absorbers. This is due to the fact that the majorant cross section at thermal energies is dominated by the high capture cross sections of the gadolinium isotopes. Since the probability of a neutron actually hitting one of the burnable absorber rods is relatively low, the fraction of virtual collisions becomes high (approximately 92% compared to 36% in the VVER-440 case) and computing time is wasted in the tracking procedure. There are some relatively simple means to overcome this problem in geometries with localised heavy absorbers. Such methods are to be included in the near future.

The comparison of calculation times between CASMO and PSG is not very practical for a single run. If it is assumed, however, that the group constants were generated for a large number of parameter combinations and that the running time for a single run remains relatively constant, it can be estimated that the calculation times differ by factors of 240, 70 and 1800 in the three test cases. It should be noted, however, that the parallelisation of the Monte Carlo calculation may reduce the differences quite significantly in an efficient multi-processor environment.

4.2. Comparison with MCNP4C

Table II shows the comparison of two-group capture, fission and scattering cross sections calculated using MCNP4C and PSG. It can be seen that the consistency is quite good for the fast energy group. In the thermal group, however, there seems to be some systematic few-percent discrepancies in the first and the third calculation case. This is possibly due to some programming error in the thermal free-gas model or in the scattering routines of the PSG code. The comparison of neutron spectra supports this assumption, since there is a clearly visible difference in the Maxwell-Boltzmann peaks in each case.

The total and effective delayed neutron fractions are compared in Table III. The consistency is quite good in general, although there are some clear exceptions as well. There is a possible convergence problem in the calculation of the effective delayed neutron fractions using the PSG code. The number of scores used for the estimates is relatively small and the statistical accuracy of the results can be significantly over-estimated. This is another topic that needs further investigation before making any final conclusions.

Table II. Group-wise cross sections calculated using MCNP4C and PSG. The differences between the results are relative. Values are in 1/cm. Statistical uncertainties are given as relative errors.

	fast group			thermal group		
	MCNP	**PSG**	**diff.**	**MCNP**	**PSG**	**diff.**
VVER-440						
Σ_c	0.007 (0.0007)	0.007 (0.0005)	-1.18%	0.038 (0.0010)	0.038 (0.0002)	2.19%
Σ_f	0.003 (0.0006)	0.003 (0.0004)	0.29%	0.077 (0.0010)	0.079 (0.0004)	2.22%
Σ_s	0.516 (0.0012)	0.513 (0.0001)	-0.66%	0.908 (0.0011)	0.917 (0.0002)	0.96%
PWR MOX						
Σ_c	0.012 (0.0007)	0.012 (0.0005)	-1.40%	0.152 (0.0015)	0.153 (0.0006)	0.83%
Σ_f	0.006 (0.0006)	0.006 (0.0004)	-0.11%	0.212 (0.0015)	0.213 (0.0007)	0.83%
Σ_s	0.516 (0.0012)	0.511 (0.0001)	-1.13%	1.016 (0.0015)	1.023 (0.0003)	0.67%
BWR + Gd						
Σ_c	0.005 (0.0008)	0.005 (0.0006)	-1.03%	0.038 (0.0010)	0.039 (0.0006)	2.34%
Σ_f	0.002 (0.0006)	0.002 (0.0005)	0.13%	0.042 (0.0009)	0.044 (0.0005)	3.10%
Σ_s	0.447 (0.0016)	0.444 (0.0001)	-0.69%	0.920 (0.0011)	0.931 (0.0002)	1.19%

The same number of neutron histories were simulated in all calculations. It should be noted that the statistical uncertainties in the MCNP4C results are quite conservative, since they are evaluated as combined errors without assuming any correlation between the flux and the reaction rate. In reality, the values are strongly correlated. The PSG code calculates the group constants by evaluating the ratio in Eq. 5, not after the simulation, but after each neutron generation. This gives a direct estimate for the group constants and their related standard deviations.

4.3. Comparison with CASMO-4E

Table IV shows some of the parameters included in the CASMO vs. PSG comparison. The nodal boundary surfaces in hexagonal geometries are not defined consistently in the two codes. For this reason the VVER-440 case lacks the comparison of assembly discontinuity factors.

Again, the fast-group reaction cross sections (not given in Table IV) are fairly consistent, but there are larger discrepancies in the thermal values. Removal cross sections and discontinuity factors in the fast group are also in a relatively good agreement. The discrepancies in the diffusion coefficients and some thermal-group discontinuity factors, however, are unacceptably large.

Since the thermal scattering of neutrons in water is not properly modelled in the PSG code, it is difficult to assess the reasons for these differences. It is certain that the inclusion of molecular binding effects would change the results quite significantly, but would it be enough to explain the large differences in the values?

Table III. Effective and total delayed neutron fractions calculated using MCNP4C and PSG. The differences between the results are relative. Values are in pcm. Statistical uncertainties are given as relative errors.

	effective fraction			total fraction		
	MCNP	**PSG**	**diff.**	**MCNP**	**PSG**	**diff.**
VVER-440						
tot.	714.3 (0.0067)	734.0 (0.0073)	2.69%	734.7 (0.0053)	736.8 (0.0002)	0.29%
β_1	23.2 (0.0345)	23.1 (0.0407)	-0.25%	24.0 (0.0292)	23.9 (0.0000)	-0.51%
β_2	125.8 (0.0159)	127.5 (0.0179)	1.34%	126.4 (0.0127)	127.0 (0.0001)	0.45%
β_3	118.7 (0.0160)	119.0 (0.0182)	0.26%	123.4 (0.0130)	123.3 (0.0001)	-0.05%
β_4	277.1 (0.0108)	285.3 (0.0118)	2.88%	283.8 (0.0085)	284.8 (0.0002)	0.37%
β_5	118.4 (0.0160)	124.7 (0.0178)	5.07%	124.3 (0.0129)	125.5 (0.0003)	0.98%
β_6	51.3 (0.0253)	54.3 (0.0281)	5.57%	52.7 (0.0190)	52.3 (0.0003)	-0.79%
PWR MOX						
tot.	379.5 (0.0087)	387.1 (0.0092)	1.97%	403.5 (0.0069)	410.0 (0.0006)	1.58%
β_1	9.6 (0.0521)	9.5 (0.0572)	-1.19%	10.2 (0.0490)	9.9 (0.0003)	-3.40%
β_2	76.3 (0.0197)	76.7 (0.0212)	0.56%	79.3 (0.0164)	79.8 (0.0004)	0.59%
β_3	59.6 (0.0218)	60.5 (0.0244)	1.41%	63.1 (0.0174)	62.8 (0.0005)	-0.52%
β_4	134.0 (0.0149)	135.8 (0.0160)	1.31%	142.4 (0.0119)	144.6 (0.0007)	1.52%
β_5	72.6 (0.0207)	78.9 (0.0198)	7.96%	79.8 (0.0163)	83.3 (0.0008)	4.22%
β_6	27.3 (0.0330)	25.8 (0.0353)	-5.82%	28.6 (0.0280)	29.7 (0.0009)	3.63%
BWR + Gd						
tot.	722.1 (0.0072)	721.0 (0.0077)	-0.16%	742.9 (0.0052)	741.7 (0.0002)	-0.16%
β_1	22.6 (0.0398)	22.7 (0.0420)	0.36%	23.6 (0.0297)	23.9 (0.0000)	1.09%
β_2	122.3 (0.0172)	124.7 (0.0184)	1.91%	126.0 (0.0127)	127.2 (0.0001)	0.98%
β_3	117.2 (0.0179)	122.9 (0.0181)	4.63%	120.7 (0.0133)	123.8 (0.0001)	2.51%
β_4	278.4 (0.0115)	276.4 (0.0124)	-0.74%	287.6 (0.0083)	286.7 (0.0002)	-0.31%
β_5	128.3 (0.0171)	121.6 (0.0180)	-5.53%	131.8 (0.0121)	127.2 (0.0004)	-3.65%
β_6	53.2 (0.0263)	52.7 (0.0277)	-0.86%	53.2 (0.0188)	52.9 (0.0004)	-0.50%

Another concern is that there are large differences, not only in the thermal values, but in the fast diffusion coefficients as well. This may be due to the fact that the average scattering angle is calculated incorrectly in the PSG code. It is also possible that the definition of the transport cross section in CASMO-4E differs from that in Eq. 7, or that there are other differences in the physics treatment that may affect the results. These uncertainties need to be resolved before making further conclusions on the results.

Table IV. Removal cross sections and group-wise diffusion coefficients and discontinuity factors calculated using CASMO-4E and PSG. The differences between the results are relative. Statistical uncertainties are given as relative errors.

	fast group			thermal group		
	CASMO	**PSG**	**diff.**	**CASMO**	**PSG**	**diff.**
VVER-440						
Σ_r	0.015	0.015 (0.0004)	3.07 %	N/A	N/A	N/A
D	1.410	1.261 (0.0001)	-11.78 %	0.408	0.548 (0.0002)	25.57 %
PWR MOX						
Σ_r	0.010	0.011 (0.0006)	2.73 %	N/A	N/A	N/A
D	1.433	1.330 (0.0001)	-7.75 %	0.306	0.389 (0.0004)	21.34 %
f_s	0.992	0.997 (0.0008)	0.49 %	1.258	1.212 (0.0030)	-3.72 %
f_c	0.982	1.004 (0.0062)	2.19 %	1.647	1.638 (0.0183)	-0.56 %
BWR + Gd						
Σ_r	0.015	0.015 (0.0003)	1.08 %	N/A	N/A	N/A
D	1.664	1.530 (0.0001)	-8.70 %	0.384	0.574 (0.0002)	33.12 %
f_{s1}	0.915	0.929 (0.0012)	1.53 %	2.051	1.832 (0.0017)	-11.93 %
f_{s2}	0.965	0.977 (0.0012)	1.27 %	1.386	1.312 (0.0020)	-5.65 %
f_{c1}	0.862	0.873 (0.0077)	1.21 %	2.853	2.494 (0.0078)	-14.40 %
f_{c2}	0.895	0.917 (0.0075)	2.35 %	2.240	1.995 (0.0086)	-12.31 %
f_{c3}	0.953	0.971 (0.0078)	1.87 %	1.683	1.545 (0.0105)	-8.93 %

The calculation, or even the definition of the transport quantities is a complex topic when the Monte Carlo method is concerned. The approach taken here is not necessarily the best way to calculate these quantities and alternative methods will be considered in the future.

5. SUMMARY AND CONCLUSIONS

5.1. Summary

A new Monte Carlo neutron transport code is being developed at the Technical Research Centre of Finland (VTT). The code is specifically intended for various lattice-level reactor physics calculations, such as group constant generation for nodal diffusion codes. The PSG code uses a method called Woodcock tracking to simulate neutron transport in the geometry. This procedure differs quite significantly from the methods used by most of the other similar codes. The advantages of the Woodcock method include reduced computing time and relatively simple handling of complex geometrical objects. The main drawback is the inability to calculate reaction rates in optically thin volumes, which rules out some of the applications for which Monte Carlo codes are traditionally used.

Group constant calculation and comparison to MCNP4C and CASMO-4E results shows that the code performs quite well in the test cases of this study. There are, however, some indications of errors in the transport procedure. This can be seen as systematic few-percent discrepancies in some of the thermal-group reaction cross sections. Several open questions need to be answered and extensive validation and benchmarking performed before the quality of the new code can be fully assessed. The preliminary results presented here, however, seem very encouraging, especially considering the early development stage of the code.

5.2. Future Plans

The list of ideas for long- and intermediate-term development is endless, but several short-term goals can be identified as well. The first priority is clearly to develop a method for modelling the thermal scattering of neutrons in water. Without this capability, the code has no use in practical calculations. Other plans for code development in the near future include parallelisation using the Message Passing Interface (MPI), improvements and extensions in the geometry description and special procedures to handle the efficiency problems related to localised heavy absorbers. Another important topic is the general problem of calculating transport cross sections and diffusion coefficients using the Monte Carlo method.

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