Monte Carlo Simulation of Joint Transport of Neutrons and Photons

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The approaches used at VNIIEF to simulate transport of neutrons and photons in standard (with surface description of region interfaces) and grid geometries are considered in the paper. Summary of TDMCC code intended for solving dynamic problems of operation of water reactors is presented.

Introduction

RFNC-VNIIEF has been using Monte Carlo methods for neutron and photon transport computations for almost fifty years. Yu.N.Dmitriyev and Yu.N.Kondyurin carried out the first Monte Carlo computations in 1958. Those were the computations of temporal neutron multiplication constant for systems with spherical symmetry. The codes developed later, such as C-2 (1960), C-20 (1962), C-30 (1964), C-60 (1969), C-90 (1989), and C-95 (1995), successively extended both the categories of problems solved and the accuracy of description of processes to be simulated. The currently available codes allow solution of problems in complex 3D geometries with the use of the recent versions of particle/material interaction constants. The codes use algorithms allowing significant improvement of the efficiency of computations. A number of issues concerning the VNIIEF efforts in this area during recent years will be considered further in the paper.

C-95 Code

Code C-95 is the last version of the code intended for Monte Carlo computation of neutron and photon transport equations (Kochubey et al., 2000). The code has been developed for solution of problems of joint transport of neutrons and photons in 3D systems using both spectral and multigroup constants. C-95 is a multiple-purpose code. It can be used for protection problems, calculation of critical parameters (K_{eff} and temporal neutron multiplication constant), nuclear safety problems, as well as reactor problems. One more application of C-95 code is solution of problems in grid geometries.

The original data for a problem to be solved (geometry, compositions of regions, sources of particles, results to be obtained, and methods to be used to improve the computation efficiency) are specified in the text form using a syntactically oriented input language allowing a rather simple description of the required data.

Geometry

A key entity in specification of geometric data is a geometric block. It looks like a set of regions and surfaces of certain types. The following block types are distinguished:

- Plane (surfaces are parallel planes, regions are layers between them),
- Spherical (surfaces are concentric spheres, regions are spherical layers between the),
- Axially symmetric (surfaces and regions are surfaces of revolution and bodies of revolution round some axis, respectively),
- Three-dimensional (arbitrary surfaces of the second order can be boundaries of the block regions).

A problem can have descriptions of a random number of blocks. They are considered as independent "building" components that have to be positioned so as to provide the required geometry. A global space (void) is considered to be the original repository, it has only a coordinate system (and can be considered as an ever existing block of the zero nesting order). It contains blocks (of the 1st nesting order), which, in their turn, can contain other blocks (of the 2nd nesting order), etc. The depth of block nesting is not limited, in general.

The geometry composed of nested blocks looks like a "matreshka" (a set of nesting dolls). The only difference is that not one, but several (both similar to each other and different) blocks can be nested. It is important, however, that the nested blocks don't overlap and don't exceed the bound of the repository block. Unfortunately, the code is not able to check, whether this requirement is met, or not. That's why the data on blocks positioning must be specified carefully.

A graphic output program significantly facilitates verification of the constructed geometry. It allows obtaining images of cross-sections, both for separate blocks and for the entire specified geometry cut by planes. Since this code uses the algorithm to construct cross-sections that is similar to the one used to simulate trajectories of particles during computation, graphic representations of cross-sections provide a rather high confidence of the constructed geometry validity. Besides, the printed graphics can be used as illustrations to the problem.

Compositions and constants

The initial data for regions of geometric blocks can be specified by descriptions of their isotope compositions, densities and initial temperatures and energies. There are several possible ways of specifying isotope compositions:

- Specification of concentrations of nuclei,
- Specification of densities and molecular compositions of materials,
- Specification of densities and weight compositions of materials.

The code allows using various systems of constants describing particle/material interactions.

The following libraries can be used for neutron transport computations: BAS-78 developed at VNIITF (Vasilyev et al, 1979), ENDL-82, ENDF/B-V, ENDF/B-V, and JENDL-3.

The libraries used to simulate photon-generation processes are: NJMC based on the data on photon-generation cross-sections for fast neutrons (developed at VNIIEF) and on libraries ENDL-82 and JENDL-3 for low-energy neutrons; ENDL-82, ENDF/B-V, ENDF/B-VI, and JENDL-3.

Transport of photons is simulated using the library formed basing on the data from the papers (Storm and Israel, 1970) and (Veigele, 1973) and EPDL92 library (Cullen et al., 1989).

Source

The problem allows specification of a random number of elementary sources. An elementary source (or, simply, a source) can emit either neutrons, or photons. Besides, for each source it is required to specify weight, percentage, as well as space, energy, angular and time distribution of the emitted particles.

The distribution in space characterizes configuration of a source and its position in the system geometry and is determined by the source geometry type. The following geometries of sources are possible: sphere and spherical layers, cylinder and cylindrical layers, bar, point, rectangle, trapezium, a surface of an arbitrary shape, or a system region.

The distribution in energy establishes a spectrum of simulated particles of a source that can be monoenergetic, or specified in a tabular form, or a Maxwell spectrum.

The angular distribution (indicatrix) specifies the distribution of cosine of the angle between a particle flight direction and a specified direction of radiation (a normal to surface, if it is a surface source). The following types of indicatrix are possible: mono-directional, tabular, isotropic, or Lambertian.

The distribution in time determines the time of birth for particles. It can be specified either in tabular form, or in δ-wise form. There are several ways of the time distribution specification in tabular form: piecewise constant (bar graph), piecewise linear, or discrete.

The distribution of characteristics of particles emitted by a source in their initial parameters can be either independent, or more complex (when the time, energy and angular distributions depend on each other).

There is a possibility to specify a source as an ensemble of particles, i.e. a set of particles with their specified coordinates, directions of flight and energies.

Results

The problem computation results are subdivided into standard and requested results. Standard results are calculated and given out each time, in contrast to the requested results, which are given out on demand.

Standard results include:

- Number of reactions,
- Number of born and absorbed particles,
- Integral arrivals/departures of particles and energies in regions,
- Integral flights of particles and energy through surfaces.

Standard results are given out both for the problem, as a whole and for each region and each surface separately.

The results given out on demand can be either regional, or surface results. The former are calculated in regions, the latter are calculated at points of intersection of surfaces by simulated particles.

The requested results can be given out as results distributed over sets of values of variables called parameters. About 20 key parameters are provided for in the code, they include energy, time, coordinates of particle, various possible angles, reaction numbers, collision numbers, generation numbers, etc.

Results can be also calculated using additional convolution with function of one variable.

Simulation and Tactics of Computations

The currently operated version of the code simulates processes of neutron and photon transport, as well as generation of photons on neutron collisions and generation of neutrons on photon collisions.

Simulation of transport of neutrons and photons is performed in accordance with the chosen system of constants of interactions between the corresponding particles and material.

The scheme of maximum piecewise-constant cross-sections is used to draw a free range (a stopping range) and select a material, on which collision takes place. Consideration of thermal motion of the medium nuclei is possible either by consideration of chemical bonds (the so-called *S(α, β model)*, or in free Maxwell gas approximation. During simulation with consideration of chemical bonds, interaction cross-sections and the energy-angular distribution at a given temperature are used.

If the free gas model is used, simulation of the neutron distribution is performed on cold cross-sections of material. Consideration of thermal motions of nuclei lays in the algorithm foundation and this feature is very useful, because no calculations of constants at a given temperature are required (Ivanov N. and Ivanov A., 2003).

Generation of photons takes place with each neutron collision over all photon-generation channels for the material, on which neutrons collided.

Several methods improving the computation efficiency has been introduced into the code, they are:

- Splitting and roulette;
- Two types of surface reflection – mirror reflection and Lambertian reflection; the reflection factor is a probability of event of a particle reflection from a given surface;
- Weight windows that allow smoothing of weights of particles crossing a given surface;
- The value of particles in the system regions;
- Exponential transformation.

The method of trial particles (Kochubey et al., 2000) used to calculate a particle flux into a small volume of space is one of the key methods allowing improvement of the computation efficiency.

A particle trajectory may be broken off in any of the parameters provided for in the code by specifying the break-off conditions.

One important feature of the computation tactics is a possibility to impose a set of requirements (usually, these are the ranges of space coordinates of a particle), if the requirements are met, the given tactics can be applied to the particle to be simulated.

It is not always convenient to specify the computation tactics in real system geometry. In C-95 code, introduction of an additional block called a control block is possible. This block is superimposed onto the main system and its geometry is built to provide easier specification of the computation tactics and obtainment of results.

Bremsstrahlung account in photon transport problems

When solving photon transport problems, it is usually assumed that electrons and positrons resultant from photon/material interactions are absorbed at the point of birth, with a positron being annihilated with generation of two annihilation photons. In so doing, it is not

taken into account that during their motion charged particles interact with the material atoms and this process results in bremsstrahlung radiation of photons. Neglect of this fact leads to underestimation (sometimes, significant) of the yield of photons, for example, if the problem of deep penetration across the barriers of heavy materials is solved. However, finding the solution to such problems with consideration of electron and positron transport requires much time.

In 1990 MCNP code (Briesmeister, 2000) was added by TTB model considering bremsstrahlung photons in case, when simulation of electrons and positrons is not performed. This model supposes that all electrons and positrons fly in the direction of the primary photon flight and are absorbed locally with emission of bremsstrahlung photons also flying in the direction of the primary photon flight. The main disadvantage of TTB model is that it doesn't take into consideration the angular and space distribution of the points of birth of bremsstrahlung photons.

To eliminate such disadvantage, VNIIEF proposed TTBIAS model (Donskoy and Zalyalov, 2003) for bremsstrahlung consideration in problems of photon transport in "thick" regions. This model supposes local absorption of electrons and positrons and emission of all the generated bremsstrahlung photons. The number of photons, the spectrum-angular and space distributions of energy of bremsstrahlung photons per one event of interaction of the primary photon are calculated beforehand using ELIZA code (Donskoy, 1993) with taking account of electron and positron transport and the calculated data is placed in tables. In terms of the photon transport equation, the proposed model is reduced to adding one more integral term to the right-hand side of this equation, so the photon transport equation has the form

$$\begin{aligned}&\frac{\partial f(\vec{r},\vec{E},t)}{\partial t}+\vec{v}\frac{\partial f(\vec{r},\vec{E},t)}{\partial \vec{r}}+\sigma(\vec{r},E)v(E)f(\vec{r},\vec{E},t)=\\&=\iint f(\vec{r}',\vec{E}',t)\sigma(\vec{r}',E')v(E')N_{brem}(E')\mathcal{K}_{brem}(\vec{r}',\vec{E}'\to\vec{r},\vec{E})d\vec{r}'d\vec{E}'+\\&+\int f(\vec{r},\vec{E}',t)\sigma(\vec{r},E')v(E')K(\vec{r};\vec{E}'\to\vec{E})d\vec{E}'+g(\vec{r},\vec{E},t).\end{aligned} \qquad [1]$$

Here, $f(\vec{r},\vec{E},t)$ is the photon distribution function at time t at space point $\vec{r}$ in energies E and directions $\vec{\omega}$; $\vec{E}=E\cdot\vec{\omega}$; $\vec{v}=v\cdot\vec{\omega}$; v is velocity; $\sigma(\vec{r},E)$ is the full interaction cross-section; $K(\vec{r};\vec{E}'\to\vec{E})$ is the transition kernel at interaction; $g(\vec{r},\vec{E},t)$ is the source of photons; $N_{brem}(E')$ is the number of bremsstrahlung photons generated by the photon of energy E'; $\mathcal{K}_{brem}(\vec{r}',\vec{E}'\to\vec{r},\vec{E})$ is the spectral angular and space distribution of bremsstrahlung per one event of interaction at point $\vec{r}'$ of the photon (hereinafter, a primary photon) of energy E' and direction $\vec{\omega}'$.

We managed to describe the spectral angular and space distributions of the energy of bremsstrahlung as a function of three variables: energy E, cosine of angle μ between the direction of flight of a bremsstrahlung photon and the direction of flight of the primary photon, and distance z in the primary photon flight direction from the point of interaction of the primary photon to the point of birth of the bremsstrahlung photon (longitudinal displacement).

To improve the accuracy of computations, the model accounting the distribution in space of the points of birth of annihilation photons was added to TTBIAS. In this model the space distribution of the points of birth of annihilation photons is calculated beforehand in the cylindrical coordinate system using ELIZA code and tabulated in the same fashion, as the space distribution of the points of birth of bremsstrahlung photons in TTBIAS model (only longitudinal displacement).

Comparative computations of photon transport in thick lead plates were carried out. It has been demonstrated that the problem run-time using TTBIAS model is less than the run-time of the problem of joint transport of photons and charged particles by several orders of magnitude, however, it is several times longer than the run-time of the problem of photon transport without bremsstrahlung consideration. It has been found in computations with lead plates that the values of photon yield forwards and backwards from the lead plates calculated using TTBIAS model are in good agreement with the values of photon yield calculated with taking account of transport of charged particles.

Tables 1 and 2 below give data on the yield of photons forwards and backwards from a lead plate of thickness 10cm. All the values are normalized per one photon of the source. The statistical error doesn't exceed 1% (1σ) for the problems of joint transport of photons, electrons and positrons and 0.1% for other problems.

Table 1. Yield of photons forwards.

Source energy, MeV	$\gamma + e^- + e^+$	$\gamma + TTBIAS$	γ	MCNP $(\gamma + TTB)$	ELIZA $(\gamma + TTB)$
100	0.36748	0.37324	0.00022367	0.655449	0.64093
50	0.14645	0.14831	0.00065050	0.293417	0.28793
20	0.04480	0.04481	0.0034089	0.100999	0.09894
10	0.02564	0.02565	0.011524	0.050011	0.04817

Table 2. Yield of photons backwards.

Source energy, MeV	$\gamma + e^- + e^+$	γ+TTBIAS	γ+TTBIAS+ annihilation model	γ	MCNP $(\gamma + TTB)$
100	0.73203	0.94920	0.74851	0.27238	0.52134
50	0.55738	0.69756	0.56908	0.24093	0.34223
20	0.37729	0.42794	0.37386	0.18459	0.20653
10	0.22865	0.24796	0.22832	0.13411	0.13866

Parallelization algorithms

Parallelizartion algorithms are based on the model with message passing implemented in MPI library of interpocessor communications.

For linear transport problems, when trajectories of particles are absolutely independent, the parallel algorithm of asynchronous computations of trajectory batches has been developed. It allows achievement of almost 100% efficiency on any number of processors. In this algorithm, each of the started computational processes is independent, it simulates trajectories using its own sub-chains of random numbers and communicates with the rest processes upon certain time intervals.

To solve the eigenvalue problems, some other algorithms have been developed, because trajectories of neutrons in this case are not absolutely independent (simulation of the ensemble of neutrons obtained at a current step continues during the next step).

For such problems, we use a parallel algorithm, in which one process is considered to be a master process. This process performs distribution of data on the neutron ensemble at the beginning of the simulation step over the working processes (slaves) and acquires data from these processes at the end of this step. The slave processes directly simulate the trajectories received at the current step. Such algorithm is used, if up to 50 processors are operated. With further increase of the number of processors the efficiency of parallelization using this algorithm becomes significantly lower.

For this reason, a special parallelization algorithm has been developed for efficient solution of the eigenvalue problems on a large number of processors. The main idea of this algorithm is that one more level is introduced to control distribution of initial parameters of an ensemble of neutrons over processors. This major control process (host-process) controls several master-processes of a lower level; each of them, in its turn, controls its own sub-set of slave processes using the above-described method.

Computations Using Grid Geometry

C-95 code complex has a possibility to use an entity determined by a grid geometry (i.e. a set of cells filled with some material of a certain density) as one of the blocks. It is possible to use either regular grids specified by coordinates of node points, or irregular grids specified by a set of coordinates of vertexes for each grid cell.

Since a typical simulation of particle trajectories using Monte Carlo method includes calculation of the distance between a particle position and a cell boundary and re-calculation of this particle coordinates after it has crossed the boundary, the increased number of cells necessarily causes a sharp increase of the time spent for simulation of one trajectory. For this reason, C-95 uses another approach to simulation of trajectories inside entities with grid geometries.

The algorithm is based on the method of maximum piecewise-constant cross-sections. In contrast to a typical simulation algorithm, in which a stopping range of a particle is drawn basing on the valid cross-section of interaction of the particle with the material contained in the cell, our algorithm simulates particle trajectories using a maximum for each energy group cross-section. This maximum cross-section is calculated for all cells of the system.

A stopping range of a particle of energy corresponding to the j-th energy group is drawn using the cross-section $\Sigma^{j}_{\max}$. To simplify the procedure of determining the particle position inside the entity with grid geometry, the code re-interpolates the grid values using a finer uniform cylindrical, spherical, or cubic grid. It is assumed, that the interpolation grid's cell is filled with material contained in the cell of grid geometry, which the center of the interpolation grid's cell gets into. Since a grid uniform in each direction is used, the number of the grid-geometry cell, which a particle has got into, can be found quite easily. The determined cell number is used to find the valid interaction cross-section for the material from this cell. Then the method of rejections is used, i.e. with a probability proportional to the valid cross-section of material in cell we accept a collision event, otherwise it is considered to be false. Thus, there is no need in calculations of distances to boundaries of each cell and re-calculation of coordinates after particles have crossed these boundaries.

It is clearly seen that in terms of computational burden such algorithm is almost independent on the number of cells in an entity with grid geometry, because the procedure of determining the number of the cell, at which a collision took place, remains the same with any increase in the total number of cells.

At the same time, in systems having significant density differences the method may appear to be inefficient. So, the following scheme is used to simulate particle trajectories. When specifying the initial data describing the original system, a control block is additionally

specified. This is a virtual entity to be superimposed on a real geometry, which allows using various methods improving the computation efficiency. If there is an entity with grid geometry in the system of interest, the control block geometry is used to divide the space into some geometric regions with no density differences inside them. The maximum cross section is calculated in this case separately for each region of the control geometry. The method of cross sections being piecewise constant in energy for the system materials allows easy calculation of the maximum cross sections for the regions determined by the control geometry. Simulation of trajectories is performed using the old scheme, however, with regard to the maximum cross-section calculated for each region.

Such approach allows significant reduction in the time spent for simulation of particle trajectories, as compared to the method of maximum cross sections calculated for the system, as whole, due to the reduced number of false collisions.

TDMCC Code

TDMCC code (Zhitnik et al., 2004) developed on the base of C-95 code complex is intended for model computations of the dynamics of neutrons in water reactor cores.

The data on the reactor geometry and compositions of regions is formed using «Reactor Setting» interface module according to the rule of initial data specification used in C-95. Its own number is assigned to each fuel rod of the heat-generating system (HGS) that characterizes its location in the reactor core. The rods are virtually divided into layers along their height and it is assumed that each layer has a constant composition and concentration of delayed neutrons. To describe data on the compositions of the rods at a current time of reactor operation, a file resultant from computation of the neutron-nuclei kinetics is used.

The adopted computational model for the neutron dynamics uses time-step computations Prompt and delayed neutrons are simulated separately.

The number of simulated particles in ensemble is constant. Data on neutrons released at time T_0 and survived at time $T = T_0 + \Delta t$ is the input data for simulation of the next batch. If the number of particles survived at time T is larger than the ensemble size, data on the rest particles is not recorded (however, their weights are taken into account); if the number of survived particles is lower than the ensemble size, the batch is supplemented to reach the original value by drawing particles from the already available ones.

The space-and-energy distribution of neutrons at the beginning of the current time step is transferred from the previous step via an array containing data on the phase coordinates of neutrons to be simulated. Such data describes each neutron location in the ensemble and its characteristics and, hence, completely determines the distribution of particles in the system. The size of simulated particle ensemble is specified in initial data and determines the computation accuracy.

In addition to prompt neutrons, delayed neutrons emitted by a separate source uniformly within a time step are also simulated. Data on the initial distribution of the delayed neutron sources in the system is generated as a result of preliminary computations using C-95 code (computation of critical parameters). Diminution of the source of delayed particles related to emission of particles during a time step is compensated due to generation of new sources of delayed neutrons, which are fragments of nuclei resultant from fission reactions.

The time of occurrence of delayed neutrons is related to the half-decay periods of their predecessors (fragments of nuclei). With regard to this feature, the delayed neutrons are divided into six groups in the current version of this code. Highlighting of the delayed neutrons during a time step is performed in accordance with the probabilities of grouping neutrons into divisions. Prompt and delayed neutrons differ only in the way they occur in the

system, however, simulation of their trajectories is the same. The method of maximum cross-sections is used to simulate trajectories and thermal motion of medium nuclei is taken into account.

The weight of the delayed neutrons per one prompt neutron per one time step depends on the time step duration. So, the rate of emission of delayed neutrons during the ensemble simulation process varies depending on the time step duration.

The above-described scheme operation results in stepwise computation of the number of neutrons available in the system normalized per one initial neutron.

There has been implemented a capability of TDMCC code to promptly change the regulating rod position that leads to its reactivity changes.

A parallel version of the code for neutron dynamics computations in reactor cores has been also implemented.

The below given are the results of test computations for some model heat-generating system using TDMCC code. The first computation corresponds to achievement of the steady-state conditions in a model HGS.

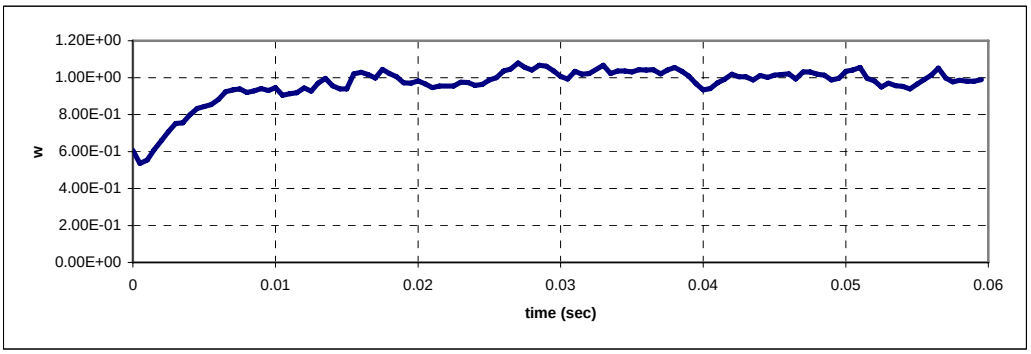

Figure 1. Phase I. Achievement of the steady-state conditions

The second computation corresponds to the time of prompt rise of the regulating rod up to some altitude causing the system reactivity increase by a factor of 0.5 β .

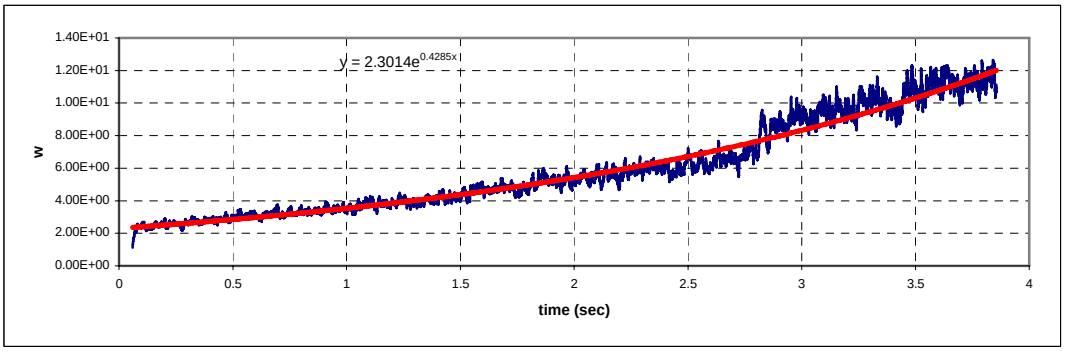

Figure 2. Phase II. The system dynamics after its reactivity has been increased**.**

Conclusion

The VNIIEF efforts on the development of neutron and photon transport simulation algorithms allowed significant extension of the range of problems that could be solved using this method. These problems are solved both in geometries specified by ordinary surfaces and

grid geometries. Parallel versions of codes have been developed, they can be operated with a high enough efficiency using a rather large number of processors. The model computations of the dynamic processes in water reactors have been carried out.

Acknowledgements

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