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Time-Dependent Integral Equations of Neutron Transport for Calculating the Kinetics of Nuclear Reactors by the Monte Carlo Method

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Abstract—Integral equations for the shape functions in the adiabatic, quasi-static, and improved quasi-static approximations are presented. The approach to solving these equations by the Monte Carlo method is described.

Keywords: neutron kinetics, integral equation, Monte Carlo method, quasi-static approximation
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INTRODUCTION

In this work, we present the time-dependent integral neutron transport equations, for solution of which the KIR and KIR-P codes, based on the Monte Carlo method and intended for calculating the kinetics of nuclear reactors, are being developed. In the KIR code, two algorithms for simulating the kinetics by the analog Monte Carlo method are implemented. The KIR-P code implements the classical adiabatic, quasi-static, and improved quasi-static approximations. The Monte Carlo method in the KIR-P code is used for calculating the parameters of point kinetics and finding the shape function. The main aspects of solving these integral equations by the Monte Carlo method are presented.

To date, the analysis of the kinetics and dynamics of reactors is based on algorithms for solving the approximate equations of point or distributed kinetics.

Only recently did works describing programs in which the neutron transport equation with a time dependence of the neutron flux density (NFD) is solved by the Monte Carlo method appear [1–11]. Such programs became possible owing to the intensive development of multiprocessor computers [12].

Preliminary estimates show that the use of supercomputers with a capacity of ~10 petaflops will make possible the simulation of fast dynamic processes with a duration of tens of seconds for both thermal- and fast-neutron reactors. Recall that 1 petaflop equals 10^{15} floating-point operations per second and 1 exaflop equals 10^{18} operations per second. The most powerful computer in the world (information for June 2014 [12]), the Chinese Tianhe-2 (MilkyWay-2), has more than 3 100 000 computing cores with a clock frequency of 2.2 GHz and has a capacity of ~33.9 petaflops; in second place is the Titan (USA) (560 000 cores with a clock frequency of 2.2 GHz and a capacity of ~17.6 petaflops); in third place is the Sequoia (USA) (more than 1.5 million cores with a clock frequency of 1.6 GHz and a capacity of ~17.2 petaflops); and in fourth place is the Japanese K (more than 700000 cores with a clock frequency of 2.0 GHz and a capacity of more than 10 petaflops). By 2020, Japan is going to build a computer with a capacity of 1 exaflop.

It should be noted that all programs mentioned in [1–11] employ either the approximate or direct approach. In addition, although these works describe programs based on the Monte Carlo method, they present only the time-dependent neutron transport equation in the integro-differential form.

Using the Monte Carlo method, the statistics of the processes in the phase space are collected and, in this manner, the integral neutron transport equation, which will be analyzed in the present paper, is solved. Here, we do not present the proof of the possibility to pass from the integro-differential equation to the Peierls integral equation [13]—it is presented in the monograph by Vladimirov [14]. The general transport equation has the form of the Fredholm equation of the second kind,

$$f(\mathbf{x}) = p_1(\mathbf{x}) + \int\limits_X p(\mathbf{x}')p(\mathbf{x}' \to \mathbf{x})d\mathbf{x}'.$$

The analog method for solving the neutron transport equation by the Monte Carlo method naturally simulates the random processes in the reactor, which, in

turn, are described by the neutron transport equation without regard for any variations in time. Therefore, to find a way to implement approximate methods, it is necessary to find out how the time-dependent parameters are reflected in the kinetic equation.

THE COMPUTATIONAL METHOD AND THE INTEGRAL EQUATIONS

The simulation of the distributed neutron kinetics consists in the repeated solution by the Monte Carlo method of the inhomogeneous neutron transport equation in the time intervals into which the time of the dynamic processes under consideration is divided.

The inhomogeneous neutron transport equation in the integro-differential form reads [15]

$$\frac{1}{\upsilon}\frac{\partial\Phi(\mathbf{r},\mathbf{\Omega},E,t)}{\partial t}+\mathbf{\Omega}\nabla\Phi+\Sigma\Phi=q(\mathbf{r},\mathbf{\Omega},E,t), \quad (1)$$

where

$$\begin{aligned} q(\mathbf{r},\mathbf{\Omega},E,t) &= \int\int\sum_{x\neq f}\Sigma_x f_x\Phi' d\mathbf{\Omega}' dE' \\ &+ \int\int\tilde{\chi}_p(1-\beta)\nu\Sigma_f\Phi' d\mathbf{\Omega}' dE' \\ &+ \sum_f \lambda_j C_j(\mathbf{r},t)\tilde{\chi}_j + Q(\mathbf{r},\mathbf{\Omega},E,t), \end{aligned} \quad (2)$$

$$\begin{aligned} &\frac{\partial C_j(\mathbf{r},t)}{\partial t}+\lambda_j C_j = \int\int\beta_j\nu\Sigma_f\Phi' d\mathbf{\Omega}' dE', \\ &\Sigma\equiv\Sigma(\mathbf{r},E,t); \quad \Sigma_x\equiv\Sigma_x(\mathbf{r},E',t) \\ &\text{for} \quad x\neq f; \quad \Sigma_f\equiv\Sigma_f(\mathbf{r},E',t); \\ &f_x\equiv f_x(\mathbf{r};\mathbf{\Omega}',E'\to\mathbf{\Omega},E;t); \\ &\Phi'\equiv\Phi(\mathbf{r},\mathbf{\Omega}',E',t); \quad \nu\equiv\nu(\mathbf{r},E'). \end{aligned} \quad (3)$$

In the book by Bell and Glasstone [15, p. 21], the equation for the NFD in the integral form is derived by the standard method of characteristics. The total derivative of the NFD is introduced as follows:

$$\frac{d\Phi}{ds}=\frac{\partial\Phi}{\partial x}\frac{dx}{ds}+\frac{\partial\Phi}{\partial y}\frac{dy}{ds}+\frac{\partial\Phi}{\partial z}\frac{dz}{ds}+\frac{\partial\Phi}{\partial t}\frac{dt}{ds}, \quad (4)$$

where s is the distance in the direction of the displacement $\mathbf{\Omega}$.

From Eq. (1), it is easy to see that

$$dt/ds = 1/\nu \Rightarrow t = t_0 + s/\nu, \quad (5)$$

$$d\mathbf{r}/ds = \mathbf{\Omega} \Rightarrow \mathbf{r} = \mathbf{r}_0 + s\mathbf{\Omega}. \quad (6)$$

As a result, the equation for the NFD is reduced to the integral form:

$$\begin{aligned} &\Phi(\mathbf{r},\mathbf{\Omega},E,t) \\ &= \int_0^\infty \exp\left(-\int_0^{s'}\Sigma_{\text{tot}}\left(\mathbf{r}-s''\mathbf{\Omega},E,t-\frac{s''}{\nu}\right)ds''\right) \\ &\times q\left(\mathbf{r}-s'\mathbf{\Omega},\mathbf{\Omega},E,t-\frac{s'}{\nu}\right)ds', \end{aligned} \quad (7)$$

where q is defined by formulas (2) and (3).

Formally representing the neutron flux $\Phi(\mathbf{r}, \mathbf{\Omega}, E, t)$ as the product of the amplitude factor $n(t)$ and the shape function $\psi(\mathbf{r}, \mathbf{\Omega}, E, t)$, i.e.,

$$\Phi(\mathbf{r},\mathbf{\Omega},E,t) = n(t)\psi(\mathbf{r},\mathbf{\Omega},E,t), \quad (8)$$

one can obtain the neutron transport equation for the shape function [16, p. 414]:

$$\begin{aligned} &\left[\frac{1}{\upsilon}\frac{\partial\Phi(\mathbf{r},\mathbf{\Omega},E,t)}{\partial t}+\mathbf{\Omega}\nabla\psi(\mathbf{r},\mathbf{\Omega},E,t)\right] \\ &+\left[\frac{1}{\upsilon}\frac{1}{n(t)}\frac{\partial n(t)}{\partial t}+\Sigma_{\text{tot}}(\mathbf{r},E,t)\right]\psi(\mathbf{r},\mathbf{\Omega},E,t) \\ &= \int\int\sum_{x\neq f}\Sigma_x(\mathbf{r},E,t)f(\mathbf{r},\mathbf{\Omega}',E' \\ &\to\mathbf{\Omega},E)\psi(\mathbf{r},\mathbf{\Omega}',E',t)d\mathbf{\Omega}' dE \\ &+\int\int\frac{\chi_p(E)}{4\pi}(1-\beta)\upsilon\Sigma_f(\mathbf{r},E,t)\psi(\mathbf{r},\mathbf{\Omega}',E',t)d\mathbf{\Omega}' dE' \\ &+\frac{1}{n(t)}\sum_j\frac{\chi_j(E)}{4\pi}\lambda_j C_j(\mathbf{r},E,t)+\frac{Q(\mathbf{r},\mathbf{\Omega},E,t)}{n(t)}, \end{aligned} \quad (9)$$

where $f(\mathbf{r}, \mathbf{\Omega}', E' \to \mathbf{\Omega}, E)$ is the probability that, upon collision at point $\mathbf{r}$ of a neutron having the direction of motion $\mathbf{\Omega}'$ and energy E', a neutron with the direction of motion $\mathbf{\Omega}$ and energy E will appear.

Solving differential equation (3), one can obtain an expression for the density of delayed neutron emitters:

$$\begin{aligned} C_j(\mathbf{r},t) = \int_{-\infty}^{t}\int\int_{E',\Omega'} &\beta_j\nu_f\Sigma_f(\mathbf{r},E',t')n(t')\psi(\mathbf{r},\mathbf{\Omega}',E',t) \\ &\times\exp(-\lambda_j(t-t'))d\mathbf{\Omega}' dE' dt'. \end{aligned}$$

When writing the neutron flux as the product of two factors, it is assumed that the amplitude factor $n(t)$ describes the main time dependence, while the shape function ψ slowly varies with time. The methods employing the representation of the flux in form (8) are referred to as factorization methods.

Expanding each term for the neutron source q and dividing Eq. (2) by $n(t)$, one can obtain the equation for the shape function without approximations:

$$\Psi(\mathbf{r},\mathbf{\Omega},E,t)=\frac{1}{n(t)}\int_0^\infty \exp\left[-\int_0^{s'}\Sigma_{\rm tot}\left(\mathbf{r}-s''\mathbf{\Omega},E,t-\frac{s''}{v}\right)ds''\right]$$
$$\times\left\{\iint\limits_{E',\mathbf{\Omega}'}\left(\begin{array}{c}\dfrac{\chi_p(E)}{4\pi}v_f(1-\beta)\Sigma_f\left(\mathbf{r}-s'\mathbf{\Omega}',E,t-\dfrac{s'}{v}\right)\\ +\displaystyle\sum_{x\neq f}\Sigma_x\left(\mathbf{r}-s'\mathbf{\Omega}',E',t-\frac{s'}{v}\right)f(\mathbf{r},\mathbf{\Omega}',E'\to\mathbf{\Omega},E)\end{array}\right)n\left(t-\frac{s'}{v}\right)\psi\left(\mathbf{r}-s'\mathbf{\Omega}',\mathbf{\Omega}',E',t-\frac{s'}{v}\right)d\mathbf{\Omega}'dE'\right.$$
$$\left.+\sum_j\frac{\chi_j(E)}{4\pi}\lambda_jC_j\left(\mathbf{r}-s'\mathbf{\Omega}',E,t-\frac{s'}{v}\right)+Q\left(\mathbf{r}-s'\mathbf{\Omega},\mathbf{\Omega},E,t-\frac{s'}{v}\right)\right\}ds'. \quad (10)$$

For the adiabatic and quasi-static approximations, either this shape function is time-independent or its time dependence is expressed by linear or other approximations. Therefore, the derivative of the shape function with respect to the parameter s is introduced as follows:

$$\frac{d\psi}{ds}=\frac{\partial\psi}{\partial x}\frac{dx}{ds}+\frac{\partial\psi}{\partial y}\frac{dy}{ds}+\frac{\partial\psi}{\partial z}\frac{dz}{ds}. \quad (11)$$

In this case, the change of variables (6) is performed and the change of variables (5) is removed.

By analogy with [15, p. 21], by the method of characteristics, the integral equations for the shape function (rather than for NFD) are derived in three approximations: adiabatic, quasi-static, and improved quasi-static.

The adiabatic approximation implies three simplifications [16, p. 415–416]. In this approximation, the shapes of the distributions of the delayed and prompt neutron sources are identical and, therefore, the time shift in the direction of precursors of delayed neutrons is neglected. In addition, both terms with the time derivatives are neglected in Eq. (1).

The integral equation in the adiabatic approximation reads

$$\psi(\mathbf{r},\mathbf{\Omega},E,t)=\frac{1}{n(t)}\int_0^\infty \exp\left[-\int_0^{s'}\Sigma_{\rm tot}\left(\mathbf{r}-s''\mathbf{\Omega},E,t\right)ds''\right]$$
$$\times\left\{\iint\limits_{E',\mathbf{\Omega}'}\left(\begin{array}{c}\dfrac{\chi_p(E)}{4\pi}v_f(1-\beta)\Sigma_f\left(\mathbf{r}-s'\mathbf{\Omega}',E,t\right)+\displaystyle\sum_j\frac{\chi_j(E)}{4\pi}v_j\,\beta_j\Sigma_f\left(\mathbf{r}-s'\mathbf{\Omega}',E',t\right)\\ +\displaystyle\sum_{x\neq f}\Sigma_x\left(\mathbf{r}-s'\mathbf{\Omega}',E',t\right)f(\mathbf{r},\mathbf{\Omega}',E'\to\mathbf{\Omega},E)\end{array}\right)n(t)\right.$$
$$\left.\times\,\psi\left(\mathbf{r}-s'\mathbf{\Omega}',\mathbf{\Omega}',E',t\right)d\Omega'dE'+Q\left(\mathbf{r}-s'\mathbf{\Omega},\mathbf{\Omega},E,t\right)\right\}ds'. \quad (12)$$

The expression in the exponent in (12) will be called the attenuation factor.

The prompt and delayed neutron sources can be combined, and in the absence of an external source, the eigenfunction corresponding to the eigenvalue $K_{\rm eff}$ can be calculated.

This equation is successfully solved by precise codes based on the Monte Carlo method.

In the quasi-static approximation, only the time derivative of the shape function, $d\psi(\mathbf{r}, \mathbf{\Omega}, E, t)/dt$, in Eq. (1) is set to zero. The integral equation for the shape function in the quasi-static approximation reads

$$\psi(\mathbf{r},\mathbf{\Omega},E,t)=\frac{1}{n(t)}\int_0^\infty \exp\left[-\int_0^{s'}\left(\Sigma_{\rm tot}\left(\mathbf{r}-s''\mathbf{\Omega},E,t\right)+\frac{1}{\upsilon n(t)}\frac{dn(t)}{dt}\right)ds''\right]$$
$$\times\left\{\iint\limits_{E',\mathbf{\Omega}'}\left(\begin{array}{c}\dfrac{\chi_p(E)}{4\pi}v_f(1-\beta)\Sigma_f\left(\mathbf{r}-s'\mathbf{\Omega}',E,t\right)\\ +\displaystyle\sum_{x\neq f}\Sigma_x\left(\mathbf{r}-s'\mathbf{\Omega}',E',t\right)f(\mathbf{r},\mathbf{\Omega}',E'\to\mathbf{\Omega},E)\end{array}\right)n(t)\psi\left(\mathbf{r}-s'\mathbf{\Omega}',\mathbf{\Omega}',E',t\right)d\mathbf{\Omega}'dE'\right.$$
$$\left.+\sum_j\frac{\chi_j(E)}{4\pi}\lambda_jC_j\left(\mathbf{r}-s'\mathbf{\Omega}',t\right)+Q\left(\mathbf{r}-s'\mathbf{\Omega},\mathbf{\Omega},E,t\right)\right\}ds'. \quad (13)$$

It is readily seen from Eqs. (12) and (13) that, for the numerical solution of Eq. (13) by the Monte Carlo method, when calculating the attenuation term, one should take into account the term $\frac{1}{v n(t)}\frac{dn(t)}{dt}$, which can be calculated in the point-kinetics approximation. In the stationary problem, delayed neutrons are emitted immediately and are described in Eq. (12) by the term $\sum_j \frac{\chi_j(E)}{4\pi} v_j \beta_j \Sigma_f(\mathbf{r} - s'\mathbf{\Omega}', E', t)$, which, in the quasi-static approximation, should be eliminated; this can be done relatively easily when calculating the number of neutrons of the next generation. At the same time, the delayed neutron source described in Eq. (13) by the term $\sum_j \frac{\chi_j(E)}{4\pi}\lambda_j C_j(\mathbf{r} - s'\mathbf{\Omega}', t)$ should be distributed.

In the improved quasi-static approximation, it is a common practice to use the following linear approximation of the derivative of the shape function:

$$[\psi(\mathbf{r},\mathbf{\Omega},E,t) - \psi(\mathbf{r},\mathbf{\Omega},E,t-\Delta t)]/\Delta t,$$

where $t - \Delta t$ is the time for which the shape function was recalculated the last time.

There are also other approximations of the shape function [17, p. 61], such as exponential and quadratic ones, which can be easily used in calculations. The integral equation for the improved quasi-static approximation reads

$$\psi(\mathbf{r},\mathbf{\Omega},E,t) = \frac{1}{n(t)}\int_0^\infty \exp\left[-\int_0^{s'}\left(\Sigma_{\text{tot}}(\mathbf{r} - s''\mathbf{\Omega},E,t) + \frac{1}{\upsilon\Delta t} + \frac{1}{\upsilon n(t)}\frac{dn(t)}{dt}\right)ds''\right]$$
$$\times\left\{\iint_{E',\mathbf{\Omega}'}\left(\begin{array}{l}\dfrac{\chi_p(E)}{4\pi}\nu_f(1-\beta)\Sigma_f(\mathbf{r} - s'\mathbf{\Omega}', E, t) \\ +\sum\limits_{x\neq f}\Sigma_x(\mathbf{r} - s'\mathbf{\Omega}', E', t) f(\mathbf{r},\mathbf{\Omega}', E' \to \mathbf{\Omega}, E)\end{array}\right) n(t)\psi(\mathbf{r} - s'\mathbf{\Omega}', \mathbf{\Omega}', E', t)\, d\mathbf{\Omega}' dE'\right.$$
$$\left. + \sum_j \frac{\chi_j(E)}{4\pi}\lambda_j C_j(\mathbf{r} - s'\mathbf{\Omega}', t) + Q(\mathbf{r} - s'\mathbf{\Omega}, \mathbf{\Omega}, E, t) + \frac{n(t)}{\upsilon\Delta t}\psi(\mathbf{r} - s'\mathbf{\Omega}', \mathbf{\Omega}', E', t - \Delta t)\right\} ds'. \quad (14)$$

Besides the operations that must be carried out for the quasi-static approximation, it is evident from Eqs. (13) and (14) that, when calculating the attenuation factor for the numerical solution by the Monte Carlo method, one should take into account the term $\frac{1}{v\Delta t}$. At the same time, neutron sources should be distributed by the distribution in the previous time step, which are expressed in Eq. (14) by the term $\frac{n(t)}{v\Delta t}\psi(\mathbf{r} - s'\mathbf{\Omega}', \mathbf{\Omega}', E', t - \Delta t)$. This functional is supposed to be estimated in the previous time interval.

CONCLUSIONS

On the basis of the integral equations derived, some aspects of the method for calculating fast transient processes in nuclear reactors in different approximations have been considered.

Presently, programs implementing the Monte Carlo method for solving time-dependent integral equations of neutron transport are being developed. These programs are supposed to be used in a program complex intended for simulating the dynamic processes in the cores of liquid-metal cooled reactors.

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