

SOME OUTSTANDING PROBLEMS IN NEUTRON TRANSPORT COMPUTATION

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This article provides selects of outstanding problems in computational neutron transport, with some suggested approaches thereto, as follows: i) ray effect in discrete ordinates method, ii) diffusion synthetic acceleration in strongly heterogeneous problems, iii) method of characteristics extension to three-dimensional geometry, iv) fission source and k_{eff} convergence in Monte Carlo, v) depletion in Monte Carlo, vi) nuclear data evaluation, and vii) uncertainty estimation, including covariance data.

KEYWORDS : Transport Computation, Deterministic Method, Monte Carlo Method, Ray Effect, Acceleration, Depletion, Nuclear Data Evaluation, Nuclear Interaction Model, Covariance

1. INTRODUCTION

As more applications are required of the radiations (e.g., neutrons and photons), be it a nuclear reactor, shielding facility, or a radiation treatment apparatus, the demands on the capability and accuracy of design and analysis are increasing ever to a very high degree. One (perhaps the ultimate) task in designing such a nuclear system is to determine the distribution of the neutrons (and/or photons) in the system under design accurately. For that, we have to take into account the motion of the neutrons and their interactions with the host nuclei of various kinds. Thus, we need a mathematical model or theory to describe this particle transport phenomena.

As a high-level model that describes the distribution of neutrons in a medium such as a reactor, we usually consider the following Boltzmann transport equation :

$$\begin{aligned} & \frac{1}{v} \frac{\partial}{\partial t} \varphi(\mathbf{r}, E, \boldsymbol{\Omega}, t) + \boldsymbol{\Omega} \cdot \nabla \varphi(\mathbf{r}, E, \boldsymbol{\Omega}, t) + \sigma_t(\mathbf{r}, E) \varphi(\mathbf{r}, E, \boldsymbol{\Omega}, t) \\ &= \int_{4\pi} d\boldsymbol{\Omega}' \int_0^\infty dE' \sigma_s(\mathbf{r}, E' \rightarrow E, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) \varphi(\mathbf{r}, E', \boldsymbol{\Omega}', t) \\ &+ \frac{\chi(E)}{4\pi} \int_{4\pi} d\boldsymbol{\Omega}' \int_0^\infty dE' v \sigma_f(\mathbf{r}, E') \varphi(\mathbf{r}, E', \boldsymbol{\Omega}', t) + q_{ex}(\mathbf{r}, E, \boldsymbol{\Omega}, t), \end{aligned} \quad (1.1)$$

with appropriate initial and boundary conditions provided. In Eq.(1.1), the angular neutron flux φ is defined as

$$\varphi(\mathbf{r}, E, \boldsymbol{\Omega}, t) = v n(\mathbf{r}, E, \boldsymbol{\Omega}, t), \quad (1.1a)$$

where

$$v = \left(\frac{2E}{m} \right)^{1/2}$$

and the angular neutron density n has the following meaning :

$$\begin{aligned} & n(\mathbf{r}, E, \boldsymbol{\Omega}, t) dr dE d\boldsymbol{\Omega} = \\ & \text{expected number of neutrons in } dr, dE, d\boldsymbol{\Omega} \\ & \text{around the phase space point } \mathbf{r}, E, \boldsymbol{\Omega} \text{ at time } t. \end{aligned} \quad (1.1b)$$

Other notations are standard, except that the lower case σ stands for macroscopic cross sections.

In writing down Eq.(1.1), we have assumed that i) the medium is isotropic (e.g., the medium exhibits no polarization to neutrons), ii) the fission neutrons are emitted isotropically, and iii) all fission neutrons are emitted promptly (this can be relaxed by considering that some neutrons are delayed). It is also based on the assumption that the neutron is a point particle that is described classically by its position and velocity. The cross sections (the degrees of various reactions) are given by experimental data or by theoretical calculations, if experimental data are not available, with the help of quantum mechanics. The problem of finding solutions to Eq.(1.1) is nontrivial or defies elementary approaches of analytical methods, but requires sophisticated numerical methods. This is due to i) the complicated energy and

space-dependency of the cross sections, ii) the angular dependency of the scattering cross section $\sigma_s(\Omega', \Omega)$, and iii) complexity due to the $\Omega \cdot \nabla \varphi$ term, particularly in curvilinear coordinates.

It is customary to first represent the differential scattering cross section in Legendre components:

$$\sigma_s(\mathbf{r}, E' \rightarrow E, \mu_0) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sigma_{sl}(\mathbf{r}, E' \rightarrow E) P_l(\mu_0). \quad (1.2)$$

In the case of time-independent or steady-state situation, Eq.(1.1) becomes

$$\begin{aligned} & \Omega \cdot \nabla \varphi(\mathbf{r}, E, \Omega) + \sigma_t(\mathbf{r}, E) \varphi(\mathbf{r}, E, \Omega) \\ &= \int_{4\pi} d\Omega' \int_0^{\infty} dE' \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sigma_{sl}(\mathbf{r}, E' \rightarrow E) P_l(\mu_0) \varphi(\mathbf{r}, E', \Omega') \\ &+ \frac{\chi(E)}{4\pi} \int_{4\pi} d\Omega' \int_0^{\infty} dE' \nu \sigma_f(\mathbf{r}, E') \varphi(\mathbf{r}, E', \Omega') + q_{ex}(\mathbf{r}, E, \Omega). \end{aligned} \quad (1.3)$$

The transport equation (1.3) is of continuous form in independent variables. Except for extremely simple cases, it is not feasible to find exact solutions for them. We need to call for a variety of methods by which the governing equations are discretized and solved numerically. The first discretization we consider is the energy variable ; called multigroup approximation, that is common to virtually all deterministic methods.

The discretization of the energy variable in the transport equation may proceed from Eq.(1.3). Following the well-studied procedure [1-3], we can obtain an approximation to the transport equation in terms of the group angular flux defined by

$$\varphi_g(\mathbf{r}, \Omega) = \int_g dE \varphi(\mathbf{r}, E, \Omega), \quad g = 1, 2, \dots, G, \quad (1.4)$$

as follows:

$$\begin{aligned} \Omega \cdot \nabla \varphi_g(\mathbf{r}, \Omega) + \sigma_g(\mathbf{r}) \varphi_g(\mathbf{r}, \Omega) &= \sum_{g'=1}^G \sum_{l=0}^{\infty} \sigma_{l g g'}(\mathbf{r}) \sum_{m=-l}^l Y_{lm}(\bar{\Omega}) \phi_{g'}^m(\mathbf{r}) \\ &+ \chi_g \sum_{g'=1}^G \nu \sigma_{f g'}(\mathbf{r}) \phi_{g'}(\mathbf{r}) + q_g^e(\mathbf{r}, \Omega), \end{aligned} \quad (1.5)$$

where

$$\phi_{g'}^m(\mathbf{r}) = \int d\Omega' Y_{lm}^*(\Omega') \varphi_{g'}(\mathbf{r}, \Omega'). \quad (1.6)$$

Being renewed interest in their capability, stochastic methods such as the Monte Carlo method can treat

continuous energy variable, thus avoiding the complexities incurring from the multigroup approximation, e.g., resonance absorption and self-shielding. In addition, the continuous treatment of the space and angle also avoids approximations due to discretizations in these variables. The Monte Carlo methods solve, in effect, Eq.(1.3) by simulating events of particle histories represented by each term.

The coefficients appearing in Eqs.(1.3) and (1.5) are nuclear data and cross sections, whose accuracy affects of course the accuracies of the solutions of the respective equations. As the computational methods and numerical algorithms in the computer codes advance and the computing power increases, the computational errors continue to diminish (of course if the computer codes are used correctly) and the effect of uncertainty in the nuclear data becomes more conspicuous.

This review article provides discussion on select unresolved (to the views of the authors) problems in the computation of the transport equations. The topics chosen are obviously limited, neither comprehensive nor exhaustive. They reflect the authors' limited experience, interests and taste.

The article is organized as follows. Section 2.1 and Section 2.2 provide the ray effect and the diffusion synthetic acceleration, respectively, in the discrete ordinates method which is most popular and widely used among deterministic transport methods. Section 2.3 discusses the method of characteristics and its applicability to three-dimensional problems. Section 2.4 provides discussion on the Monte Carlo method in two areas : i) convergence in k_{eff} -eigenvalue problems, and ii) spectrum effect in Monte Carlo depletion. Section 3 discusses the processes involved in the nuclear data evaluation and associated issues. Finally, Section 4 provides a summary.

2. SOLUTIONS OF TRANSPORT EQUATION

2.1 Ray Effect in Discrete Ordinates Method

In discrete ordinates (S_N) method, the angular flux in Eq. (1.3) is evaluated only in a finite number (say, M) of discrete angles and the scattering source term in the right hand side of Eq.(1.3), i.e., Eq.(1.6) is approximated by the following quadrature :

$$\phi_{g'}^m(\mathbf{r}) = \sum_{n=1}^M w_n Y_{lm}^*(\Omega_n) \varphi_{g'}(\mathbf{r}, \Omega_n), \quad (2.1)$$

rendering scattering source iteration (SI). This solution procedure allows "sweep" operation, which is a very nice feature of the discrete ordinates method. However, this method can exhibit two drawbacks depending on the problem situations. First, the source iteration becomes extremely slow if the problem medium is scattering-dominant, i.e., if the scattering ratio (σ_s/σ) is close to unity.

In such a case, the source iteration requires a good acceleration scheme, which is the subject in the next section. Second, if the problem is multi-dimensional and absorption-dominant with isolated source, the scalar flux calculated by Eq.(2.1) shows unphysical spatial distortions, i.e., anomalous bumps, even for a quite large number of discrete ordinates M . Simply increasing M is not cost-effective. There have been several approaches in the past to remedy this ray effect, such as the use of piece-wise continuous polynomials [4] or spherical harmonics [5] for the angular variable, the introduction of Legendre function-represented fictitious source term [6], and the use of region-dependent angular quadrature [7]. They all show only a varying degree of success in mitigating the ray effect. An interesting approach to mitigate the ray effect significantly with an easy implementation is to use the ideas in the streaming rays method [8,9], where the angular flux φ_n is decomposed into uncollided φ_n^0 and collided φ_n^c components as

$$\varphi_n = \varphi_n^0 + \varphi_n^c, \quad (2.2)$$

resulting in, for example for cell (i, j) , $\mu_n > 0$, $\eta_n > 0$,

$$\boldsymbol{\Omega}_n \cdot \nabla \varphi_{n,i,j}^0 + \sigma_{i,j} \varphi_{n,i,j}^0 = 0, \quad (2.3)$$

$$\varphi_{n,i-1/2,j}^0 = \varphi_{n,i-1/2,j}, \quad \varphi_{n,i,j-1/2}^0 = \varphi_{n,i,j-1/2}, \quad (2.3a)$$

and

$$\boldsymbol{\Omega}_n \cdot \nabla \varphi_{n,i,j}^c + \sigma_{i,j} \varphi_{n,i,j}^c = q_{n,i,j}, \quad (2.4)$$

$$\varphi_{n,i-1/2,j}^c = \varphi_{n,i,j-1/2}^c = 0, \quad (2.4a)$$

in two-dimensional problem representation.

Eq.(2.3) can be integrated analytically along the streaming rays. We can solve this without source iteration, thus we may use very high quadratures, mitigating the ray effect. Eq.(2.4) is solved using an usual discrete ordinates method.

2.2 Diffusion Synthetic Acceleration

The within-group transport equation either in the discrete ordinates method or in the method of characteristics is solved by iterative methods. A simple iterative method is scattering source iteration (SI) that can be symbolically written as

$$\boldsymbol{\Omega} \cdot \nabla \varphi^{l+1}(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r}) \varphi^{l+1}(\mathbf{r}, \boldsymbol{\Omega}) = \sigma_s(\mathbf{r}) \phi^l(\mathbf{r}) + q(\mathbf{r}, \boldsymbol{\Omega}), \quad (2.5)$$

$$\phi^{l+1}(\mathbf{r}) = \int d\boldsymbol{\Omega} \varphi^{l+1}(\mathbf{r}, \boldsymbol{\Omega}), \quad (2.6)$$

where l is an iteration index.

For problems in which neutrons undergo few collisions or for problems that are “leaky”, the SI method converges rapidly. However, for problems that contain diffusive regions that are optically thick and scattering-dominated ($c = \sigma_s / \sigma \rightarrow 1$), the SI method converges very slowly. To accelerate the convergence, various acceleration methods are used in the following structure :

$$\boldsymbol{\Omega} \cdot \nabla \varphi^{l+1/2}(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r}) \varphi^{l+1/2}(\mathbf{r}, \boldsymbol{\Omega}) = \sigma_s(\mathbf{r}) \phi^l(\mathbf{r}) + q(\mathbf{r}, \boldsymbol{\Omega}), \quad (2.7)$$

$$\phi^{l+1}(\mathbf{r}) = H[\varphi^{l+1/2}(\mathbf{r}, \boldsymbol{\Omega})]. \quad (2.8)$$

Eq.(2.7) is called high-order equation, which is the original transport equation for which solution is sought. The solution $\varphi^{l+1/2}$ is usually obtained by transport sweep. Eq.(2.8) is called acceleration or low-order equation, which is simpler than high-order equation. The solution ϕ^{l+1} is then substituted in the right-hand side of Eq.(2.7) and the process continues until ϕ^{l+1} converges. For details, see a recent review paper by Adams & Larsen [10].

The most widely used acceleration method is diffusion synthetic acceleration (DSA) and based on the diffusion type operation for H . In continuous form, they are given as follows :

Transport sweep (High-order equation) :

$$\boldsymbol{\Omega} \cdot \nabla \varphi^{l+1/2}(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r}) \varphi^{l+1/2}(\mathbf{r}, \boldsymbol{\Omega}) = \sigma_s(\mathbf{r}) \phi^l(\mathbf{r}) + q(\mathbf{r}, \boldsymbol{\Omega}), \quad (2.7)$$

$$\phi^{l+1/2}(\mathbf{r}) = \int d\boldsymbol{\Omega} \varphi^{l+1/2}(\mathbf{r}, \boldsymbol{\Omega}). \quad (2.9)$$

DSA equation (Low-order equation) :

$$-\nabla \cdot \frac{1}{3\sigma(\mathbf{r})} \nabla F^{l+1}(\mathbf{r}) + \sigma_a(\mathbf{r}) F^{l+1}(\mathbf{r}) = \sigma_s(\mathbf{r}) [\phi^{l+1/2}(\mathbf{r}) - \phi^l(\mathbf{r})], \quad (2.10)$$

where

$$\sigma_a(\mathbf{r}) = \sigma(\mathbf{r}) - \sigma_s(\mathbf{r}),$$

$$F^{l+1}(\mathbf{r}) = \phi^{l+1}(\mathbf{r}) - \phi^{l+1/2}(\mathbf{r}).$$

Thus, $\phi^l(\mathbf{r})$ is updated by

$$\phi^{l+1}(\mathbf{r}) = \phi^{l+1/2}(\mathbf{r}) + F(\mathbf{r}). \quad (2.11)$$

The discretization in Eq. (2.10) must be “consistent” with that in Eq. (2.7) for unconditional stability (convergence of solutions for all mesh sizes, including optically thick meshes). The spatially differenced diffusion equation must be derived directly from the spatially differenced S_N equation. The consistent derivation of such diffusion difference schemes is algebraically complicated in multidimensional geometries and non-diamond difference schemes and potentially difficult to solve.

Moreover, recent studies [11,12] show that the computation efficiency of S_N calculations with DSA methods lose their effectiveness when the problem contains strong discontinuities in the material properties. There is an indication and evidence that the reason for this is due to the DSA’s intrinsic limitation in strongly transport problems which call for direction-dependent low-order equation such as the coarse-mesh angular dependent rebalance method (CMADR) [13]. But when used to precondition a Krylov subspace method, as opposed to accelerating some iteration, a DSA method can be applied efficiently even if the discretization is not fully consistent [14].

2.3 Method of Characteristics

The method of characteristics (MOC) [15-17] is similar to the discrete ordinates method in that it considers only a finite number of discrete directions (usually with product quadrature sets) and calculates mesh-average angular flux by sweeping. The key difference is in the way of calculating the mesh-average flux.

In MOC, for a given ordinate (direction of neutron travel traced), each of several rays parallel to the ordinate (that encompass the mesh) is traced to provide mesh-average ray angular flux and outgoing mesh-edge ray angular flux by analytic integration. These mesh-average ray angular fluxes are then summed for all the rays that pass through the mesh to provide mesh-average angular flux. The ray-wise integration allows flexibility of the mesh shapes. The meshes can take any shape and mixture of shapes as in Monte Carlo methods. This is in contrast to the discrete ordinates method.

To provide key element of the method of characteristics, let us start from the within-group transport equation with the scattering term truncated after $l = L$ from Eq.(1.5) with the right hand side written as $q_{g,n}(\mathbf{r})$ in a set of M discrete directions or rays.

If we now assume that $q_{g,n}(\mathbf{r})$ is constant in a computational cell (flat source approximation), then we have by analytic integration of the within-group transport equation along the characteristic ray,

$$\phi_{g,n,l}^{out} = \phi_{g,n,l}^{in} e^{-\sigma_g L_{n,l} / \sin \theta_n} + \frac{q_{g,n}}{\sigma_g} (1 - e^{-\sigma_g L_{n,l} / \sin \theta_n}), \quad (2.12)$$

where $L_{n,l}$ is the track length of the l 'th ray for direction Ω_n in mesh (i, j) , projected to the x-y plane in x-y-z (z-uniform, infinite) geometry. The mesh-average angular flux for the scattering source iteration is obtained by

$$\bar{\phi}_{g,n} = \frac{q_{g,n}}{\sigma_g} + \frac{\sin \theta_n}{A_{ij} \sigma_g} \sum_{l \in ij\text{'th mesh}} \delta_n (\phi_{g,n,l}^{in} - \phi_{g,n,l}^{out}), \quad (2.13)$$

where δ_n is the spacing between adjacent rays for direction Ω_n and A_{ij} is the area of cell (i, j) . To preserve the area A_{ij} , the projected track length $L_{n,l}$ is renormalized as follows :

$$L_{n,l}^* = L_{n,l} \frac{A_{ij}}{\sum_l \sum_n L_{n,l} \delta_n w_n^\varphi}, \quad (2.14)$$

where w_n^φ are the weights for azimuthal angles. Then Eqs.(2.12) and (2.13) and a general geometric tracking module are complete for transport calculation with MOC.

The above computational procedure applies to the 2-D x-y geometry problems (x-y-z problems where properties are independent of z coordinate). Further, if the x-y properties form certain periodic structures such as the fuel pin cells in most of the reactor cores, modular ray tracing is possible, saving computer memory requirements and floating-point operations.

During the last several years, MOC has been revisited and refined to apply to 2-D whole-core calculations [18,19]. A direct extension of MOC to 3-D problems may be possible, but it will take tremendous amount of memory and long computer time, and a practical method is yet to be devised. A more modest approach is the 2D/1D fusion method [20-22], where MOC is used for radial 2-D calculation, coupled with S_N -like method for axial 1-D calculation. This approach takes advantage of the structure of a core that is usually simpler in axial direction than in radial direction. Similar works are some hybrid methods [23,24].

2.4 Monte Carlo Methods

2.4.1 Convergence in k_{eff} -Eigenvalue Problems

Compared to the deterministic transport methods based on multigroup approximation, the Monte Carlo method has advantages due to its capability of treating continuous energy and complex geometry. But it is still difficult to apply to realistic eigenvalue problems. The difficulty comes from the necessity of guessing fission source distribution to start iteration (generation), superimposed on statistical uncertainty in each iteration. Thus, it leads to biased k_{eff} with variance not easily quantified [25-27].

Especially in loosely-coupled fissile systems, the convergence of fission source distribution is not achieved or slow at best, even under apparent convergence of k_{eff} [28,29]. Wielandt acceleration has been proposed and

tested [30,31], but the overall effectiveness (in terms of convergence and computer time) is not definitive. Preliminary results of the Monte Carlo anchoring method [32,33], in which the fission source term is decomposed into a conventional fission distribution and an “anchoring” distribution updated by a deterministic method, indicate that convergence of the fission source distribution is faster and stabilized and that eigenvalue is obtained with faster convergence and significantly reduced bias, if a proper anchoring factor is chosen.

2.4.2 Monte Carlo Depletion

In conventional deterministic depletion codes, e.g., CASMO or HELIOS, a critical spectrum (or leakage corrected spectrum) is used for the depletion of fuel and burnable nuclides and the buildup of actinides and fission products. The critical spectrum is obtained by a critical buckling search such as the B1 method.

In recent papers, due to the advantages of the Monte Carlo method in its capability, the number of depletion studies done by Monte Carlo codes is increasing. An example of the most widely used code is MONTEBURNS [34]. In some Monte Carlo depletion calculations [35,36], the errors on the calculated results are obtained through propagation of the errors in the input parameters such as the cross sections. However, the current Monte Carlo depletion codes do not use the critical spectrum [37]. A recent study [38] introduced an approach to Monte Carlo depletion with leakage corrected spectrum, in which the streaming (leakage) term of the transport equation is treated as an eigenvalue term and transformed into an extended albedo boundary condition problem. This approach was implemented in the MONTEBURNS code, modifying the MCNP engine. Preliminary numerical results on a representative PWR assembly problem showed considerable differences in buildup and depletion of nuclides between the leakage corrected case and the conventional case.

3. NUCLEAR DATA

Modern nuclear data evaluation is based on the nuclear interaction model. However, no universal theory which is based on the first principle has been found yet. So, practical nuclear data evaluation is done by adjusting various model parameters to reproduce the measured data well. The model computer codes are usually developed for different energy regions where the major interaction mechanisms are different. For this situation, the covariance methods based on Bayesian principle or Kalman filter is widely used nowadays. After Gandini's successful work on GPT (Generalized Perturbation Theory) for nuclear engineering problems, various computer tools were developed for application. Uncertainty estimation was also applied for the pressure vessel life time estimation, the neutron metrology where only partial reaction cross sections are

important, and the fast reactor core analysis where resonance region is relatively insignificant. However, the recent trend of licensing demands the uncertainty prediction before starting construction of a new nuclear facility. The methodology development and the application of uncertainty estimation become important with growing capacity of computing power and with recent release of nuclear data with covariance for most transport calculation.

3.1 Nuclear Data Evaluation

To find a solution of the neutron transport equation, it is necessary to know the scattering and reaction cross sections, neutron emission spectrum accompanying various nuclear reactions such as fission, (n,2n), etc. The cross section data is generally provided by a nuclear data evaluation process which is based on the measurements and the nuclear reaction theories. Since the nuclear reaction is not well understood until now, the evaluation process relies on the reaction model which is valid only in some energy range and has some adjustable parameters.

When the incident neutrons energy is below few MeV energy, the interaction is well described by the interaction between a neutron and the potential well of a target nuclide [39]. The interactions among nucleon become important when the incident energy rises above few tens of MeV. At the higher energy region, the nuclear interaction models based on intra nucleon force are developed. However, such high energy is less interesting for the energy application problem.

For low energy region, the discrete nature of quantum energy level allows us to use a formally accurate R-matrix formalism. But R-matrix is not simple enough for practical usage; a Reich-Moore resonance formula [40] or the Multi Level Breit Wigner resonance formula is used for actual nuclear data evaluation. The resonances are completely described by the parameter sets of a level energy, a level spin, an orbital angular momentum, resonance widths for each reaction channel such as neutron width, radiative width, fission width, alpha width, etc [41]. These resonance parameters are derived by fitting the measured transmission coefficient [42] or the measured reaction cross section from the time of flight experiment.

For neutron energy of keV range, it become practically impossible to distinguish individual resonances. A statistical approach extended from the resolved resonance analysis [43,44] is used to fit experimental data in unresolved energy range. Spin dependent wave strengths are also derived from the resolved resonance parameters and the optical model calculation.

For high energy region where cross section becomes smooth and inelastic scattering begins, an optical model approach is used [45]. The neutron potential of a nuclide is described by a Wood-Saxon well type potential. The depth, radius, and boundary width are adjustable parameters to describe the shape of complex potential well. The quantum mechanical wave equation is directly solved to

find the scattering and absorption cross sections. The potential well shape are adjusted to reproduce the measured total cross section and the absorption cross sections such as the capture cross section, the inelastic scattering cross sections, etc. The compound nuclide which is formed by a neutron absorption decays with emission of various particles. The compound nuclide decay is described by Hauser-Feshbach model in which the level densities are adjustable parameters. An optical model code such as ABAREX [46] or ECIS [47] is used for this region.

For higher energy region above few MeV, the reaction is not adequately described by the compound model and various pre-equilibrium models[48] are developed to describe the reaction particularly for the energy and angle distribution of emitting particles [49].

Several comprehensive computer code systems such as EMPIRE [50] and TALYS [51] which can handle wide energy range by coupling the nuclear model codes consistently were developed.

3.2 Uncertainty Estimation

Measurement of nuclear cross section accompanies errors due to statistical nature of nuclear reaction or due to systematic deviation introduced from non-ideal experimental setup. We need to know the estimate from the observed value.

For a multivariate system such as energy dependent cross section, the uncertainty is represented as a matrix, known as the covariance, whose off-diagonal element does not vanish. For a simultaenously measured quantity, i.e. using a time of flight and/or measuring relative value against the well known standard cross section, the best estimate of observables \bar{x} can be defined as follows:

$$\bar{x} = E[x] = \int xP(x)dx, \quad (3.1)$$

when we know the multi-variate probability density fuction (PDF) $P(x)$. The associated covariance C_x is defined as

$$C_x = E[(x - \bar{x})(x - \bar{x})^T] = \int (x - \bar{x})(x - \bar{x})^T P(x)dx. \quad (3.2)$$

The PDF of error can be derived from the maximum entropy principle [51]. In the most case of white noise, the PDF follows the Gaussian error distribution:

$$P\left(x \in (\bar{x}, \bar{x} + dx)\right) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x - \bar{x}}{\sigma}\right)^2\right] dx. \quad (3.3)$$

The estimation of uncertainty due to model parameter can be done when we know the PDF. When an observable

value can be expressed in a function of parameters as $R=f(p)$, we can determine the variance of R from the variance of p as follows, using the Taylor expansion,

$$\delta R = \frac{\partial R}{\partial p} \delta p:$$

$$C_R = E[\delta R' \delta R] = S' C_p S, \quad (3.4)$$

where

$$S_{ij} \equiv \frac{\partial R_j}{\partial p_i}.$$

The sensitivity matrix can be obtained by perturbing each parameter p_j , by a perturbation theory calculation, or by a random selection of a set of parameters p . When the number of parameters is small and the linearity is good, perturbation of each parameter is suitable. However, when the number of parameters is large, one has to use suitable perturbation theory which requires one forward and several adjoint calculations. When the number of parameters is large and nonlinear, a random variation in the set of parameter is acceptable.

For the neutron transport problem which is linear in flux, the well-known GPT [52, 53] can be used to derive the sensitivity matrix. As an example, the sensitivity of eigenvalue due to cross section uncertainty can be derived easily. For a linear system with a given source S ,

$$A(x)\phi(x) = S(x), \quad (3.5)$$

an estimation of a response R_j such as the reaction rate of a dosimeter, is given as

$$R_j \equiv \int \sum_i (x) \phi(x) dx \equiv \langle \sum_i \phi \rangle, \quad (3.6)$$

where \sum_i is reaction cross section of the dosimeter. Using the GPT, a row of sensitivity matrix can be calculated as [54]

$$\frac{\partial R_j}{\partial p_j} = \int \left[\frac{\partial \sum_i}{\partial p_j} \phi + \phi^* \left(\frac{\partial A}{\partial p_j} \phi + \frac{\partial S}{\partial p_j} \right) \right] dx, \quad (3.7)$$

where p_j are the cross sections, or any other parameters, used in the transport equation. The adjoint flux ϕ^* is defined as a solution of the corresponding adjoint system:

$$A^*(x)\phi^*_i(x) = \sum_i (x). \quad (3.8)$$

When there is no source which is a linear eigenvalue problem, the neutron transport equation is written as

$$A(x)\phi(x) = \lambda B(x)\phi(x). \quad (3.9)$$

We can create the corresponding adjoint equation as

$$A^*(x)\phi^*(x) = \lambda B^*(x)\phi^*(x). \quad (3.10)$$

For a multi-group problem, the adjoint matrix is a transpose of the original matrix A and B . Sensitivity on the eigenvalue λ can be expressed as [55-57]

$$\frac{\partial \lambda}{\partial p_j} = \frac{\int \phi^* \left(\frac{\partial A}{\partial p_j} - \lambda \frac{\partial B}{\partial p_j} \right) \phi dx}{\int \phi^* B \phi dx}. \quad (3.11)$$

Similar method can be applied to estimate error in the burnup calculation [58]. For the depletion calculation, the variance associating the number density can be expressed as the contributions from the variance from the initial number density, the cross sections, and the calculated flux.

The uncertainty estimation can guide to select the experiments from existing experimental database or to construct a new experiment for the design and validation of a new nuclear reactor system by defining a representative factor [59].

3.3 Model Parameter Update

Model parameter update using the measured value is necessary for the nuclear data evaluation where the knowledge of intra-nucleus physics is not sufficient for the first principle approach. Bayes has established a theoretical background for parameter estimation problem using the probability theory. The Bayes' theorem states that the probability of observing A when B is observed is the same as the probability of observing B after observing A,

$$P(A|B)P(B) = P(B|A)P(A). \quad (3.12)$$

When we determine the PDF using the maximum entropy principle or heuristically adopt the Gaussian error distribution, we can obtain the following problem to find \mathbf{p} and \mathbf{R} :

$$\min. = (\mathbf{R}^{(meas)} - \mathbf{R})' \mathbf{C}_R^{-1} (\mathbf{R}^{(meas)} - \mathbf{R}) + (\mathbf{p}^{(meas)} - \mathbf{p})' \mathbf{C}_p^{-1} (\mathbf{p}^{(meas)} - \mathbf{p}), \quad (3.13)$$

with the constraints $\mathbf{R} - \mathbf{R}^{(0)} = \mathbf{S}'(\mathbf{p} - \mathbf{p}^{(0)})$ where suffix (0) stands for the calculated value. A solution can be found using the Lagrangian multiplier method as follows:

$$\mathbf{p}^{(new)} = \mathbf{p}^{(0)} + \mathbf{C}_p \mathbf{S} \mathbf{V}_R^{-1} (\mathbf{R}^{(meas)} - \mathbf{R}^{(0)}), \quad (3.14)$$

and the associated covariance matrix

$$\mathbf{C}_p^{(new)} = \mathbf{C}_p^{(0)} + \mathbf{C}_p \mathbf{S} \mathbf{V}_R^{-1} \mathbf{S}' \mathbf{C}_p', \quad (3.15)$$

where $\mathbf{V}_R \equiv \mathbf{C}_R^{(meas)} + \mathbf{S}' \mathbf{C}_p \mathbf{S}$.

Using the above expression, we can update the model parameter reflecting the measured value successively when we have the covariance matrices associating the measured value. Quality and consistency of the updated parameter can be expressed by a scalar quantity χ^2 which should be the same as the degree of freedom (or the number of measured values):

$$\chi^2 = (\mathbf{p}^{(new)} - \mathbf{p}^{(0)})' \mathbf{C}_p^{-1} (\mathbf{p}^{(new)} - \mathbf{p}^{(0)}) + (\mathbf{R}^{(meas)} - \mathbf{R}^{(0)})' (\mathbf{S}' \mathbf{C}_p \mathbf{S})^{-1} (\mathbf{R}^{(meas)} - \mathbf{R}^{(0)}) \quad (3.16)$$

The Kalman filter [60] results in the same formula as Bayesian approach for linear systems with the Gaussian error distribution. For the cross section evaluation, the method described above is widely used to determine the nuclear physics parameters as well as the cross sections [61]. Even when the Gaussian error distribution is not suitable, a direct Monte-Carlo sampling method [62] with the Bayesian principle can be applied.

3.4 Update of Prediction Using Measured Data

By applying the sensitivity equation, we can update the calculated value as follows [63]:

$$\mathbf{R}^{(new)} = \mathbf{R}^{(0)} + \mathbf{S}' \mathbf{C}_p \mathbf{S} \mathbf{V}_R^{-1} (\mathbf{R}^{(meas)} - \mathbf{R}^{(0)}), \quad (3.17)$$

and

$$\mathbf{C}_R^{(new)} = \mathbf{S}' \mathbf{C}_p^{(0)} \mathbf{S} + \mathbf{S}' \mathbf{C}_p \mathbf{S} \mathbf{V}_R^{-1} \mathbf{S}' \mathbf{C}_p'. \quad (3.18)$$

Above formula are useful when we know the covariance of parameters (e.g., cross sections and that of the measured data).

3.5 Covariance Data Library

There is a long history of development and application of the uncertainty estimation methodology. To estimate the fluence of nuclear reactor pressure vessel which is critical for life-time assessment of a nuclear power plant, a standard method was already applied to the uncertainty estimation including the experimental database [64].

Dosimetry cross section libraries [65], which are required to neutron metrology and pressure vessel surveillance, are usually distributed with associated covariance matrices. Recently, there are some published cross section covariance data libraries suitable for transport calculation such as the low fidelity BOLNA library [66].

4. SUMMARY

This article provided (at least partially) the major outstanding problem areas in neutron transport computational field, with some promising approaches to resolve them. The outstanding or unresolved problems we considered important and relevant to the design and analysis of nuclear systems are i) the ray effect in the discrete ordinates method, ii) the diffusion synthetic acceleration in strongly heterogeneous problems, iii) practical method to extend the method of characteristics to 3-D problems, iv) convergence in k_{eff} -eigenvalue problem in the Monte Carlo method, v) Monte Carlo depletion, and vi) nuclear data evaluation requirement and uncertainty estimation, including covariance information.

The problem areas in the list above are not of course comprehensive and not necessarily in order of importance of priority. As a key and core activity for the design of nuclear systems involving radiations, the discipline of computational transport will continue to play an important role as it did in the past. The outstanding problems identified above should serve as potential research and development items of immediate future.

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