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Physics-oriented optimization strategy for the energy lookup algorithm in continuous energy Monte Carlo neutron transport simulation

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ABSTRACT

The continuous energy Monte Carlo method is a most high-fidelity and high-resolution method for neutron transport simulations in reactor physics with minimal approximations. However, one of the major disadvantages is that it is very time-consuming and computational-intensive for large scale whole-core simulations, especially for coupling with depletion analysis for realistic reactors. Some recent researches indicate that one of the principle performance bottlenecks for the problem lies in the energy lookup algorithm during the calculation of energy-dependent material cross sections. Therefore, two physics-oriented optimization strategies, based on making use of the physical characteristics of neutron transport behaviors, are developed to optimize the run-time performance of the algorithm for accelerating the energy lookup without any loss in precision and accuracy. The first optimization strategy is called Neighbored Material Cascade Grid (NMCG) which is a hybrid approach utilizing the key features of the cascade grid and double indexing method. The second optimization strategy is called Adaptive Optimal Logarithmic Grid (AOLG) which is a variation of the conventional logarithmic energy grid method utilizing the advantages of energy hash tables. The strategies are incorporated into a continuous energy Monte Carlo neutron transport code and tested on realistic whole-core reactor systems. The computational performance as measured by memory usage, elapsed runtime and overall speedup, associated with each of the optimization strategies are demonstrated in the whole-core Monte Carlo simulations. Depending on the complexity of the models, the number of nuclides in the material compositions and the utilization of different optimization strategies, overall speedup ratios of 1.2-1.7, relative to the conventional binary lookup algorithm, are routinely observed. Furthermore, the numerical results indicate that the run-time performance of the new physics-oriented optimization strategies performs a bit better than that of conventional optimization methods with existing approaches.

1. Introduction

The Monte Carlo method is a kind of brute-force computational method that can be particularly well-suited for multidegree-of-freedom coupling problems in physics [1]. With the development of reactor physics, the reactor physicists immediately realized that the Monte Carlo method would be a most potential way to solve the neutron transport problems for its distinct characteristics. The most advantages of Monte Carlo method to simulate neutron transport in whole-core reactors include essentially exact representation of geometrical configurations and physical phenomena that are important for reactor physics analysis. Theoretically, it means that the Monte Carlo method is capable of analyzing complicated neutron transport problems in whole-core reactors with arbitrary geometrical complexities and arbitrary physical complexities. One of the most commonly-used strategies is the so-called continuous energy Monte Carlo neutron transport method, which utilizes the pointwise nuclear data library to treat the neutron energy-dependence nuclear reactions with essentially no approximations as comparing with the deterministic multi-group theory [2]. These key features and advantages indicate that the Monte Carlo method is a most high-resolution and high-fidelity method for neutron transport simulations, which makes it to be a potential candidate for the next-generation advanced reactor physics methods [3]. Therefore, the Monte Carlo method is developed rapidly and becomes a common and reference tool for neutron transport simulations. In recent years, many Monte Carlo codes over different

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countries have been developed, such as MCNP6 (USA) [4], Serpent2 (Finland) [5], TRIPOLI4 (France) [6], PRIZMA (Russia) [7], McCARD (South Korea) [8] and SuperMC2 (China) [9], to perform neutron transport simulations in the applications of reactor physics.

The basic principle of the Monte Carlo method is to simulate a neutron from its birth (i.e. initial emission from a neutron source) to death (i.e. absorption or escaping outside of the system), which is called a neutron history. Each history consists of a series of nuclear reactions resulting from the neutron with target nuclides. When a large number of neutron histories are simulated with a Monte Carlo code, multiple response quantities (i.e. effective multiplication factor, neutron flux spectrum, nuclear reaction rate, etc.) could be obtained with a detailed simulation of the neutron transport process at a tremendous cost in computer resources (i.e. computational runtime and memory usage). In particle physics, the microscopic cross section is used to depict the probability of a neutron interacting with a target nuclide (i.e.^{1}H,^{235}U, etc.) of the material (i.e. nuclear fuel, cladding, moderator, etc.). Actually, the cross section strongly depends on the kinetic energy of the incident neutron for every nuclide and for every type of nuclear reaction. Therefore, Monte Carlo codes utilize cross section, which is the foundation of the neutron scattering and reaction theory, to simulate the neutron's behaviors during its transport in the system. Generally, the cross section utilized in continuous energy Monte Carlo method is the ACE (A Compact ENDF) format data libraries that can be generated from the ENDF (Evaluated Nuclear Data File) [10] by using an open-source NJOY nuclear data processing code [11]. The nuclear data stored in the ACE format libraries are organized in so-called pointwise, continuous energy form which consists of tabulated energy-cross section pairs. It means that, for each nuclide in a Monte Carlo simulation, there is a one-dimensional grid of energies and its corresponding one-dimensional grid of microscopic cross sections for each type of reaction (i.e. scattering (n,n), absorption (n, γ), fission (n, f), etc.).

In Monte Carlo neutron transport simulation, the microscopic total cross section describes the neutron interaction probability with a single nuclide and the macroscopic total cross section is the interaction probability per unit path length travelled by the neutron. Thus, due to the nuclide- and energy-dependence of cross section values, every time that a neutron crosses over the boundary of materials (i.e. moves into a new material region) or changes its energy, the macroscopic total cross section must be computed for the new material at the current neutron energy so that the free path length between the neutron's current location and the next collision site can be sampled with an exponential-based probability distribution function (PDF) of the free path length [12]:

$$f(l) = \Sigma_t(\vec{r} + l\vec{\Omega}, E)\exp\left\{-\int_0^l \Sigma_t(\vec{r} + l'\vec{\Omega}, E)dl'\right\}, \quad l \in (0, \infty) \tag{1}$$

where Σ_t is the macroscopic total cross section for a specific material at current neutron energy E, and l is the free path length, $\vec{\Omega}$ is the flying direction of the neutron, $\vec{r}$ is the spatial coordinate of the neutron. Additionally, various kinds of nuclide-dependence microscopic cross sections need to be computed frequently at collision sites and material boundaries for the sampling of which nuclide the neutron interacting with and the corresponding reaction type associated with the sampled nuclide, and material-dependence macroscopic cross sections are also needed for the purpose of accumulation of different tallies (i.e. nuclear reaction rate, energy deposition, etc.).

As mentioned above, the continuous energy Monte Carlo codes use ACE format pointwise cross section libraries consisting of energy-cross section pairs (E, σ). In Monte Carlo simulation, when the nuclide-dependence cross section is needed, the value will be computed by linear interpolation between the cross section values corresponding to the energies that bound the neutron's current energy. Therefore, the nuclide-dependence microscopic cross section, $\sigma_{x,m}(E)$, at neutron energy, E, for some type of reaction, x, of the nuclide, m, is given by:

$$\sigma_{x,m}(E) = \sigma_{x,m}(E_k) + j_m(E)(\sigma_{x,m}(E_{k+1}) - \sigma_{x,m}(E_k)), \quad j_m(E) \in [0, 1) \tag{2}$$

$$j_m(E) = \frac{E - E_k}{E_{k+1} - E_k}, \quad E \in [E_k, E_{k+1}) \tag{3}$$

where E_k and E_{k+1} are the nearest lower and upper bounding energies on the nuclide's energy grid which bounds the current neutron energy E, and k is the energy index on the nuclide's energy grid, and $j_m(E)$ is the linear interpolation factor. Then, the calculation of material-dependence macroscopic cross section, $\Sigma_x(E)$, requires summation over all the nuclide-dependence microscopic cross sections, $\sigma_{x,m}(E)$, of the constituent nuclides of the material by:

$$\Sigma_x(E) = \sum_{m=1}^{M} \Sigma_{x,m}(E) = \sum_{m=1}^{M} \sigma_{x,m}(E)N_m \qquad x = s, a, f, t \ldots \tag{4}$$

where N_m is the nuclide concentration (i.e. atomic density) for the mth nuclide and M is the total number of the constituent nuclides for the material. Finally, the cross sections, $\Sigma_x(E)$, $\sigma_{x,m}(E)$, can be utilized for sampling of the free path length and nuclear reaction type, and for accumulation of different response quantities.

In Monte Carlo simulation, every nuclide has its own unique grid of energy values (i.e. energy grid) as well as a grid of microscopic cross section values (i.e. cross section grid) corresponding to each energy value on the energy grid. In order to calculate the nuclide-dependence cross section, $\sigma_{x,m}(E)$, a lookup on the nuclide's energy grid must be performed to determine the energy index, k, so that the current neutron energy E is bounded within the energy interval denoted by [E_k, E_{k+1}). Then the nuclide- or material-dependence cross sections can be achieved using the Eqs. (2)–(4). Therefore, each time the energy index k corresponding to energy E must be found using an iterative lookup algorithm, which is called the energy lookup process. Traditionally, a binary lookup (i.e. non-optimization) on the nuclide's energy grid is employed for this process. Since the nuclide's energy grids are nuclide-specific and arbitrarily distributed, every time the calculation of nuclide-dependence microscopic cross section must be determined by performing a binary lookup on the nuclide's energy grid. Although this algorithm takes only $O(\log(N_{\text{grid}}))$ scaling for an energy grid of length N_{grid}, the energy lookup must be repeatedly performed for each nuclide within a material each time the material-dependence macroscopic cross section need to be computed.

Historically, the binary lookup for energy-cross section data treatment has been widely utilized in many developed Monte Carlo codes, such as MCNP5 [13], SuperMC2 [14], etc. Its chief advantage is that all of the original physical information contained in an ACE file can be preserved without any loss of data. However, its main disadvantage is that, to calculate the nuclide-specific energy-dependence cross sections whenever they are required, the energy lookups must be performed repeatedly and frequently. Particularly, the repeated energy lookups have a noticeable detrimental effect on computational performance when the nuclide's energy grid consists of a large number of energy values, which typically has between 10^2 and 10^5 values. Besides, since the calculation of material-dependence macroscopic cross sections requires summation over all the constituent nuclides, as a result, M times of binary lookup for each material need to be performed, where M is the total number of the constituent nuclides of the material.

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