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Theory and applications of the fission matrix method for continuous-energy Monte Carlo

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ABSTRACT

The fission matrix method can be used to provide estimates of the fundamental mode fission distribution, the dominance ratio, the eigenvalue spectrum, and higher mode forward and adjoint eigenfunctions of the fission distribution. It can also be used to accelerate the convergence of power method iterations and to provide basis functions for higher-order perturbation theory. The higher-mode fission sources can be used to determine higher-mode forward fluxes and tallies, and work is underway to provide higher-mode adjoint-weighted fluxes and tallies. These aspects of the method are here both theoretically justified and demonstrated, and then used to investigate fundamental properties of the transport equation for a continuous-energy physics treatment. Implementation into the MCNP6 Monte Carlo code is also discussed, including a sparse representation of the fission matrix, which permits much larger and more accurate representations. Properties of the calculated eigenvalue spectrum of a 2D PWR problem are discussed: for a fine enough mesh and a sufficient degree of sampling, the spectrum both converges and has a negligible imaginary component. Calculation of the fundamental mode of the fission matrix for a fuel storage vault problem shows how convergence can be accelerated by over a factor of ten given a flat initial distribution. Forward fluxes and the relative uncertainties for a 2D PWR are shown, both of which qualitatively agree with expectation. Lastly, eigenmode expansions are performed during source convergence of the 2D PWR problem for two initial distributions; observed decay rates of coefficients agree closely with expectation.

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1. Introduction

Continuous-energy Monte Carlo codes simulate neutron behavior using the best available nuclear data, accurate physics models, and detailed geometry models. Reactor criticality calculations for k_{eff} and the power distribution are carried out iteratively, using the power method, where batches of neutrons are simulated for a single generation. The first-generation fission neutrons produced in a batch become the starting neutron sites for the next batch. A suitable number of "inactive" initial batches are required to converge to the fundamental mode eigenvalue and eigenfunction, and then succeeding iterations with "active" batches are used to accumulate Monte Carlo tallies for estimating desired reaction rate distributions.

Most Monte Carlo codes perform the power iteration without acceleration and can sometimes exhibit very slow convergence. Statistical noise for batch results precludes the use of common outer iteration acceleration methods (e.g. Chebyshev). An additional limitation of standard Monte Carlo codes is the inability to directly calculate higher eigenmodes.

The fission matrix approach was proposed in the earliest works on Monte Carlo criticality calculations (Morton, 1956; Kaplan, 1958; Hammersely and Handscomb, 1964) and has been tried by many researchers over the years (Urbatsch, 1992; Kitada and Takeda, 2001; Dufek and Gudowski, 2009; Wenner and Haghighat, 2011). The present work provides a rigorous derivation of the forward and adjoint forms of the fission matrix treatment for *K*-eigenvalue problems. The method is then used to investigate fundamental properties of the transport equation for a continuous-energy physics treatment, for both forward and adjoint modes. The eigenvalue spectrum of a 2D PWR problem is examined in terms of its convergence with mesh refinement and the diminishment of its complex part with larger sampling.

Implementation in the MCNP6 Monte Carlo code (Goorley et al., 2013) and the sparse storage methodology is discussed, as well as the ability to compute higher mode eigenfunctions for fission

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sources, fluxes, and reaction rates (e.g. a higher mode capture rate for use in second-order perturbation theory calculations). Results from these higher mode calculations are shown, in addition to two applications relevant to criticality calculations: source convergence acceleration and modal expansion. Using forward source modes from the fission matrix, the first 30 forward flux modes are calculated from a 2D PWR problem by running fixed source calculations, and reasonable relative variances are found. Convergence acceleration is demonstrated for a fuel storage vault problem: from a flat initial distribution, the number of iterations required for convergence is reduced by over a factor of ten. Eigenmode expansions of converging fission sources for the 2D PWR problem are discussed for two different initial distributions: a point in the center of the core and a point in the corner. The decay rates of significant expansion coefficients are shown to agree with expectations calculated directly from the fission matrix. This paper will summarize and extend work reported in Carney et al. (2012, 2013a,b) and Brown et al. (2013).

2. Theory

The following sections provide derivations of the K-effective form of the integral transport equations for the forward and adjoint fission sources, for continuous-energy problems using a rigorous Green's function approach (Sections 2.1–2.3). The integral equations are then integrated over spatial regions to provide an exact prescription for the fission matrix elements and resulting equations for the regionwise sources (Sections 2.4 and 2.5). The solution to the fission matrix equations, both forward and adjoint, is shown to be exact if the within-region weighting functions are known (as in the case of a converged fission source distribution), or in the limit of vanishingly small region size (Section 2.6). The basis for higher eigenmode calculation is then mentioned (Section 2.7), followed by a discussion of the method's implementation into MCNP6 (Sections 2.8–2.11). Lastly, the expansion of the iterative fission source into fission source eigenmodes is introduced (Section 2.9).

2.1. Integral equation for neutron source

The K-eigenvalue form of the neutron transport equation is

$$\mathbf{M}\cdot\Psi(\vec{r},E,\hat{\Omega}) = \frac{1}{K}\frac{\chi(E)}{4\pi}S(\vec{r}), \tag{1}$$

where $\mathbf{M}$ is the net loss operator defined by

$$\mathbf{M}\cdot\Psi(\vec{r},E,\hat{\Omega}) = \hat{\Omega}\cdot\nabla\Psi(\vec{r},E,\hat{\Omega}) + \Sigma_T(\vec{r},E)\Psi(\vec{r},E,\hat{\Omega}) - \iint dE'd\hat{\Omega}'\Sigma_S(\vec{r},E'\to E,\hat{\Omega}'\to\hat{\Omega})\Psi(\vec{r},E',\hat{\Omega}'), \tag{2}$$

which contains leakage, collision, and scattering terms, respectively. $S(\vec{r})$ is the fission neutron source, defined by

$$S(\vec{r}) = \iint dE'd\hat{\Omega}'\nu\Sigma_F(\vec{r},E')\Psi(\vec{r},E',\hat{\Omega}'), \tag{3}$$

and $\chi(E)$ is the emission energy spectrum of fission neutrons. Fission neutron emission is assumed to be isotropic. To simplify the analysis that follows, $\chi(E)$ is assumed to be independent of space and the energy of the neutrons causing fission (see Appendix A for discussion).

The Green's function for this problem is defined by the equation

$$\mathbf{M}\cdot G(\vec{r}_0,E_0,\hat{\Omega}_0\to\vec{r},E,\hat{\Omega}) = \delta(\vec{r}-\vec{r}_0)\delta(E-E_0)\delta(\hat{\Omega}-\hat{\Omega}_0), \tag{4}$$

where the "0" subscript denotes an initial point in phase space, and δ is the Dirac delta function. Then, based on linearity of the transport equation and the superposition principle, it follows that

$$\Psi(\vec{r},E,\hat{\Omega}) = \frac{1}{K}\iiint d\vec{r}_0 dE_0 d\hat{\Omega}_0\frac{\chi(E_0)}{4\pi}\cdot S(\vec{r}_0)G(\vec{r}_0,E_0,\hat{\Omega}_0\to\vec{r},E,\hat{\Omega}). \tag{5}$$

Eq. (5) is the K-eigenvalue form of the Peierls equation. Now multiply Eq. (5) by $\nu\Sigma_F(\vec{r},E)$ and integrate over all E and $\hat{\Omega}$:

$$S(\vec{r}) = \frac{1}{K}\int d\vec{r}_0 S(\vec{r}_0)H(\vec{r}_0\to\vec{r}), \tag{6}$$

where the kernel $H(\vec{r}_0\to\vec{r})$ represents the energy-angle averaged Green's function,

$$H(\vec{r}_0\to\vec{r}) = \iint\iint dEd\hat{\Omega}dE_0d\hat{\Omega}_0\nu\Sigma_F(\vec{r},E)\cdot\frac{\chi(E_0)}{4\pi}G(\vec{r}_0,E_0,\hat{\Omega}_0\to\vec{r},E,\hat{\Omega}). \tag{7}$$

Eq. (6) is an integral equation for the neutron source at $\vec{r}$ expressed in terms of the kernel H. H is the Green's function integrated over angles and energies, weighted by the initial spectrum and final fission neutron production. It can readily be evaluated by either continuous-energy or multigroup Monte Carlo without approximation. That is, the Green's function G is provided directly by the transport simulation in a Monte Carlo code; the energy-angle integration to produce H in Eq. (7) is a tally in the Monte Carlo simulation, binned according to the initial and final spatial positions. No approximations were made in obtaining Eqs. (6) and (7).

2.2. Integral equation for adjoint neutron source

The K-eigenvalue form of the adjoint neutron transport equation can be written as

$$\mathbf{M}^\dagger\cdot\Psi^\dagger(\vec{r},E,\hat{\Omega}) = \frac{1}{K}\nu\Sigma_F(\vec{r},E)S^\dagger(\vec{r}), \tag{8}$$

where $\mathbf{M}^\dagger$ is the operator adjoint to $\mathbf{M}$, defined by

$$\mathbf{M}^\dagger\cdot\Psi^\dagger(\vec{r},E,\hat{\Omega}) = -\hat{\Omega}\cdot\nabla\Psi^\dagger(\vec{r},E,\hat{\Omega}) + \Sigma_T(\vec{r},E)\Psi^\dagger(\vec{r},E,\hat{\Omega}) - \iint dE'd\hat{\Omega}'\Sigma_S(\vec{r},E\to E',\hat{\Omega}\to\hat{\Omega}')\Psi^\dagger(\vec{r},E',\hat{\Omega}'), \tag{9}$$

$S^\dagger(\vec{r})$ is the adjoint source, defined by

$$S^\dagger(\vec{r}) = \iint dE'd\hat{\Omega}'\frac{\chi(E')}{4\pi}\Psi^\dagger(\vec{r},E',\hat{\Omega}'), \tag{10}$$

Bell and Glasstone (1970) and others have shown that the eigenvalue K in Eq. (8) is identical to the eigenvalue K in Eq. (1), hence the analysis below will just use K, rather than K and $K^\dagger$.

The Green's function for this problem is defined by the equation

$$\mathbf{M}^\dagger\cdot G^\dagger(\vec{r}_0,E_0,\hat{\Omega}_0\to\vec{r},E,\hat{\Omega}) = \delta(\vec{r}-\vec{r}_0)\delta(E-E_0)\delta(\hat{\Omega}-\hat{\Omega}_0). \tag{11}$$

It then follows that

$$\Psi^\dagger(\vec{r},E,\hat{\Omega}) = \frac{1}{K}\iiint d\vec{r}_0 dE_0 d\hat{\Omega}_0\nu\Sigma_F(\vec{r}_0,E_0)\cdot S^\dagger(\vec{r}_0)G^\dagger(\vec{r}_0,E_0,\hat{\Omega}_0\to\vec{r},E,\hat{\Omega}). \tag{12}$$

Now multiply Eq. (12) by $\chi(E)/4\pi$ and integrate over all E and $\hat{\Omega}$:

$$S^\dagger(\vec{r}) = \frac{1}{K}\int d\vec{r}_0 S^\dagger(\vec{r}_0)H^\dagger(\vec{r}_0\to\vec{r}), \tag{13}$$

where the kernel $H^\dagger(\vec{r}_0\to\vec{r})$ represents the energy-angle averaged adjoint Green's function (now weighted by the final spectrum and initial fission neutron production),

$$H^\dagger(\vec{r}_0\to\vec{r}) = \iint\iint dEd\hat{\Omega}dE_0d\hat{\Omega}_0\frac{\chi(E)}{4\pi}\cdot\nu\Sigma_F(\vec{r}_0,E_0)G^\dagger(\vec{r}_0,E_0,\hat{\Omega}_0\to\vec{r},E,\hat{\Omega}). \tag{14}$$