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Verification and validation of the maximum entropy method for reconstructing neutron flux, with MCNP5, Attila-7.1.0 and the GODIVA experiment

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ABSTRACT

Verification and validation of reconstructed neutron flux based on the maximum entropy method is presented in this paper. The verification is carried out by comparing the neutron flux spectrum from the maximum entropy method with Monte Carlo N Particle 5 version 1.40 (MCNP5) and Attila-7.1.0-beta (Attila). A spherical 100% ^{235}U critical assembly is modeled as the test case to compare the three methods. The verification error range for the maximum entropy method is 15–21% where MCNP5 is taken to be the comparison standard. Attila relative error for the critical assembly is 20–35%. Validation is accomplished by comparing a neutron flux spectrum that is back calculated from foil activation measurements performed in the GODIVA experiment (GODIVA). The error range of the reconstructed flux compared to GODIVA is 0–10%. The error range of the neutron flux spectrum from MCNP5 compared to GODIVA is 0–20% and the Attila error range compared to the GODIVA is 0–35%. The maximum entropy method is shown to be a fast reliable method, compared to either Monte Carlo methods (MCNP5) or 30 multi-energy group methods (Attila) and with respect to the GODIVA experiment.

1. Introduction

The method of moments is a very useful approach in the solution of transport equations for density distributions (Marchisio et al., May 2003). This procedure however smoothes much of the information contained in the continuous distribution. The resulting moments are useful for providing integral information about a distribution such as the mean number of particles and their mean size; it is useful to recover the full distribution. In the case of neutron flux moments would provide the average number of neutrons and their average energy but it is desirable to calculate the continuous energy neutron flux distribution itself (Duderstadt and Hamilton, 1976).

The maximum entropy method provides an elegant means of reconstructing a density distribution given a finite number of moments. In general, there are infinitely many continuous distributions whose moments match the known moments. This is commonly known as the moment problem (Bandyopadhyay et al., May 2005). The precise statement of this problem is as follows: given a finite number of moments, is it possible to find a unique distribution that gives rise to these moments? Additional constraints are then required to guide the process of finding a continuous distribution that fits the known moments. The maximum entropy method is one such constraint.

2. Overview of the maximum entropy method for reconstruction of density distributions

The maximum entropy method is based on the concept that the distribution that maximizes the information entropy is the statistically most likely to occur. In the context of information theory, the information entropy S, of a distribution $p(x)$, is given by the integral in Eq. (1), where Ω is the support of the distribution. $M(x)$ is the invariant measure function and is generally a known a priori probability density function (PDF) based on the problem being solved (Uhlenbeck et al., 1963).

$$S = -\int_{\Omega} p(x) \ln \frac{p(x)}{M(x)} dx \tag{1}$$

The problem becomes a search to find a $p(x)$ that maximizes the information entropy S subject to the known moments (Eq. (2)), where the number of known moments is $(N+1)$.

$$\mu_k = \int_{\Omega} x^k p(x) dx, \quad k = 0, 1, 2, \ldots, N \tag{2}$$

To further the search for a $p(x)$, the method of Lagrangian multipliers is used by multiplying the definition of the entropy functional with Lagrangian multipliers, λ_k.

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$$H \equiv S + \sum \lambda_k \left(\int_\Omega x^k p(x) dx \right)$$
$$= -\int_\Omega p(x) \ln \frac{p(x)}{M(x)} dx + \sum \lambda_k \left(\int_\Omega x^k p(x) dx \right) \tag{3}$$

The maximum of Eq. (1) may be found when the derivatives of Eq. (3) are zero.

$$\frac{\partial H}{\partial \lambda_k} = 0 \tag{4}$$

$$\frac{\partial H}{\partial p(x)} = 0 \tag{5}$$

Eq. (4) gives the moment constraint back. The mathematical results of carrying out Eq. (5) are seen in the following equation:

$$\frac{\partial H}{\partial \lambda_k} = -\int_\Omega \left(\ln \frac{p(x)}{M(x)} + 1 \right) dx + \sum_{k=0}^{N} \lambda_k \int_\Omega x^k dx = 0 \tag{6}$$

The integrals in Eq. (6) must be valid on an arbitrary domain (Ω), so the integrand must be zero, Eq. (7) shows this.

$$-\ln \frac{p(x)}{M(x)} - 1 + \sum \lambda_k x^k = 0 \tag{7}$$

After some algebra, Eq. (8) shows the functional form of $p(x)$.

$$p(x) = M(x) \exp \left(-1 + \sum_{k=0}^{N} \lambda_k x^k \right) \tag{8}$$

The maximum entropy solution is found by solving for the Lagrangian multipliers λ_k with a system of nonlinear equations based on finding λ_k such that $(\tilde{\mu}_k - \mu_k)$ is below a certain specified precision. The moments based on the reconstructed distribution are $\tilde{\mu}_k$ in the following equation:

$$\tilde{\mu}_k = \int_\Omega M(x) x^k \exp \left(-1 + \sum_{k=0}^{N} \lambda_k x^k \right) dx, \quad k = 0, 1, 2, \ldots, N \tag{9}$$

The moments (μ_k) based on the distribution are known via the method of moments, some other numerical solution or by experiment. Gauss quadrature coupled with Newton's method can be used to solve this system of nonlinear equations for $(\tilde{\mu}_k - \mu_k) <$ tolerance value.

3. Application of the maximum entropy method to reconstruct neutron flux spectrum

The maximum entropy method is applied to the reconstruction of neutron flux spectrum within a 100% enriched ^{235}U critical assembly and to the GODIVA experiment. Neutron moments are obtained from the method of neutron energy moments. Neutron energy moments have been verified (Crawford and Ring, 2012a, 2012b) and validated (Crawford and Ring, 2012a, 2012b) for the cases in this paper, GODIVA and the 100% ^{235}U critical assembly. The maximum entropy reconstruction method is verified for neutron flux with the spherical 100% ^{235}U critical assembly modeled in Monte Carlo N Particle 5 version 1.40 (MCNP5) and Attila-7.1.0-beta version (Attila) and validated with neutron flux calculated from foil activation measurements (McElroy et al., 1969) from the GODIVA experiment (INL NEA/NSC DOC(95)03, September 2010).

Eqs. (1)–(9) can be quickly rewritten in the terms of energy dependent neutron moments following the same mathematical approach. Energy dependent neutron flux $\phi(\vec{r}, E)$ is taken to be the density distribution sought after i.e. $p(x)$ is replaced with $\phi(\vec{r}, E)$ as the distribution to solve for at a specific distance $\vec{r}$. The moments, $\mu_k$are replaced with the energy and position dependent neutron moments (m_k). The neutron moments, m_k's are known functions for any given $\vec{r}$ (Crawford and Ring, 2012a, 2012b). The derivation of the maximum entropy approach for neutrons is shown with Eqs. (10)–(15), (18).

$$S = -\int_\Omega \phi(\vec{r}, E) \ln \frac{\phi(\vec{r}, E)}{M(E)} dE \tag{10}$$

$$m_k = \int_\Omega E^k \phi(\vec{r}, E) dE, \quad k = 0, 1, 2, \ldots, N \tag{11}$$

$$H = -\int_\Omega \phi(\vec{r}, E) \ \ln \frac{\phi(\vec{r}, E)}{M(E)} dE + \sum \lambda_k \left(\int_0^\infty E^k \phi(\vec{r}, E) dE \right) \tag{12}$$

$$\frac{\partial H}{\partial \lambda_k} = 0 \tag{13}$$

$$\frac{\partial H}{\partial \phi(\vec{r}, E)} = 0 \tag{14}$$

$$\frac{\partial H}{\partial \lambda_k} = -\int_\Omega \left(\ln \frac{\phi(\vec{r}, E)}{M(E)} + 1 \right) dE + \sum_{k=0}^{N} \lambda_k \int_\Omega E^k dE = 0 \tag{15}$$

$$-\ln \frac{\phi(\vec{r}, E)}{M(E)} - 1 + \sum \lambda_k E^k = 0 \tag{16}$$

$$\phi(\vec{r}, E) = M(E) \exp \left(-1 + \sum_{k=0}^{N} \lambda_k E^k \right) \tag{17}$$

$$\tilde{m}_k = \int_\Omega E^k M(E) \exp \left(-1 + \sum_{k=0}^{N} \lambda_k E^k \right) dE, \quad k = 0, 1, 2, \ldots, N \tag{18}$$

Gauss Quadrature was used for integrating the moments in conjunction with Newton's Method to solve for the Lagrangian multipliers $(\tilde{m}_k - m_k) <$ tolerance value. The tolerance for the Newton solver is 1E−6 and it is extremely sensitive to the initial guesses. The initial guesses ranged: 1.79E−02 for λ_0, −1.83E+00 for λ_1, 8.57E−01 for λ_2, −2.02E−01 for λ_3, 2.27E−02 for λ_4 and −9.30E−04 for λ_5. The invariant measure function $M(E)$ is chosen to satisfy the condition $\phi(\vec{r}, E = 0) = 0$ and is a previously known possible PDF for the distribution of the neutrons in the system. Many functions can satisfy the condition just mentioned but $M(E)$ also needs to be a possible known spectrum. The Watt fission spectrum i.e. $\chi = a \exp(-\frac{E}{b}) \sinh(\sqrt{cE})$ where a, b and c are constants based on the fissile isotope (Shultis and Faw, 2002, pp. 176–177) matches the conditions mentioned. The constants a, b and c were chosen to match the isotope mix of GODIVA.

4. Results and discussion

The reconstructed neutron flux is compared to the MCNP5 and Attila neutron flux spectrum at two different radii within the spherical critical assembly. The energy range in Figs. 1–3 for the spectrum plots is 1E−10 to 10 MeV. The flux spectrum at the center of the GODIVA experiment was determined with foil activation measurements (McElroy et al., 1969). The data for the GODIVA spectrum can be found in the McElroy reference in the reference section in this paper. Plots 1 and 2 compare the flux spectrum of the three computational methods at a 1 cm radius within the spherical critical assembly and at the sphere edge, 8.35 cm. Fig. 3 compares the neutron flux spectrum from the three computational methods with the flux spectrum from the GODIVA experiment.

The MCNP5 spectrum in Figs. 1 and 2 has 1000 data points, based on the energy bins used in conjunction with an f2 tally.