

LA-UR-18-31280

Approved for public release; distribution is unlimited.

Title:	Computing Alpha Eigenvalues Using the Fission Matrix
Author(s):	Josey, Colin James Brown, Forrest B.
Intended for:	M&C 2019 - International Conference and Computational Methods Applied to Nuclear Science and Engineering, 2019-08-25/2019-08-29 (Portland, Oregon, United States)
Issued:	2018-12-03

Disclaimer: Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness. technical correctness.

COMPUTING ALPHA EIGENVALUES USING THE FISSION MATRIX

Colin Josey and Forrest B. Brown

Los Alamos National Laboratory P.O. Box 1663 MS A143, Los Alamos, NM 87545 cjosey@lanl.gov, fbrown@lanl.gov

ABSTRACT

In this paper, a technique to compute α eigenvalues from a time-dependent fission matrix is demonstrated. A matrix is formed that computes the next time step source using the source vectors from the last *n* time steps. The matrix also shifts these source vectors one index back. The result is a matrix that tracks the multiplication over time instead of over generation. The eigenvalues of this matrix can then be converted into logarithmic time derivatives, which correspond to the α -eigenvalues. This process is tested on a simple rod geometry. Results indicate the convergence is $\mathcal{O}(h^2)$ until statistical noise sets in. A mesh with 190 time bins and 190 space bins results in a primary α -eigenvalue within 0.6% of the analytic solution.

KEYWORDS: fission matrix, alpha eigenvalues, Monte Carlo

1. INTRODUCTION

The fission matrix is a spatially discretized Green's function in which the probability of a source starting in phase space region i and creating a new source in phase space region j is tallied in \mathbf{F}_{ji} [1]. The discretization most commonly used is over the space dimension. The eigenvalues of the \mathbf{F} matrix converge to the k-eigenvalues of the model as the discretization is refined.

Recently, research has been undertaken on time-dependent fission matrices [2]. In that paper, the dimension of time is added to phase space. This expansion then allows one to analyze the evolution of geometries in time. Nonlinear effects can be added by computing multiple fission matrices and interpolating as the geometry evolves.

In this paper, the fission matrix will be converted into a form useful for computing the α -eigenvalues. The α -eigenvalues correspond to the asymptotic logarithmic derivative of the flux. The equations are typically formulated through a separation of variables:

$$\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \psi(\mathbf{r}, E, \hat{\mathbf{\Omega}})e^{\alpha t}$$
$$\frac{d}{dt}\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \alpha\psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t)$$

If one can estimate the time derivative of the flux, it can be used to estimate α . The fission source is linear to the flux. It is through this route that α can be computed from the fission matrix.

2. THEORY

Let us assume that one has a series of time-dependent fission matrices G_k . The [j, i] index of this matrix corresponds to the probability that a particle born in phase space region i in time bin t_0 created a source particle in region j in time bin t_k . For this discussion, it is assumed that the geometry is constant. As a result, G_k can also represent the relationship for any pair of time bins t_x and t_{x+k} .

Particles can be created within a time step through three processes. First, particles can come from previous time steps. This initial population can be computed from the fission matrices as follows:

$$s_{k0} = \sum_{i=1}^{N} \mathbf{G}_i s_{k-i} \tag{1}$$

An approximation is made that N is finite. Second, particles born in the current time step can create more particles in the current time step. This process can repeat indefinitely. Assuming that the probability of fission in the same bin is constant for each successive generation, the source is given by Eq. (2).

$$s_k = \left(\mathbf{I} + \mathbf{G}_0 + \mathbf{G}_0^2 + \ldots + \mathbf{G}_0^\infty\right) s_{k0}$$
⁽²⁾

If the absolute value of the eigenvalues of matrix G_0 are strictly below one, this source is bounded and Eq. (2) can be simplified to Eq. (3).

$$s_k = \left(\mathbf{I} - \mathbf{G}_0\right)^{-1} s_{k0} \tag{3}$$

The time step can be adjusted to enforce that the eigenvalues are within the unit disk.

It is not relevant to α -eigenvalue problems, but the third possible source is an external source. As it is possible for the external source neutrons to undergo a fission during the same time step in which they are introduced, these particles should be treated the same as the initial source and added to Eq. (1). However, care must be taken if the external source spectrum substantially deviates from the fission spectrum.

In order to compute s_k , one needs the previous N source vectors. The source update matrix F can be computed as follows:

$$\begin{pmatrix} s_{k-N+1} \\ \vdots \\ s_{k-2} \\ s_{k-1} \\ s_k \end{pmatrix} = \begin{pmatrix} \mathbf{I} & & & \\ & \mathbf{I} & & \\ & & \mathbf{I} & \\ & & & (\mathbf{I} - \mathbf{G}_0)^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{0} & \mathbf{I} & & & \\ & & \ddots & & \\ & & & & \mathbf{I} & \\ \mathbf{G}_N & \mathbf{G}_{N-1} & \dots & \mathbf{G}_2 & \mathbf{G}_1 \end{pmatrix} \begin{pmatrix} s_{k-N} \\ s_{k-N+1} \\ \vdots \\ s_{k-2} \\ s_{k-1} \end{pmatrix}$$

$$\mathbf{s}_k = \mathbf{F} \mathbf{s}_{k-1}$$

$$(4)$$

The bottom row of both matrices is equivalent to Eq. (3). The identity matrices are then used to shift the sources one position further into the past. The result is that repeated operation of the matrix F will evolve the source distribution forward in time by h.

The eigenvalues of F, λ_i , correspond to the multiplicative growth rate of the source distribution over time step h. Asymptotically, the growth rate will be governed by the largest such eigenvalue.

As the flux is linear to the source distribution, the growth of the flux also corresponds to these eigenvalues. One could then compute the logarithmic growth rate through the following relation:

$$\alpha_i = \frac{\log(\lambda_i)}{h}$$

A bit of care must be taken with regard to the complex logarithm. The principle value yields $\Im \alpha \in \left(-\frac{\pi}{h}, \frac{\pi}{h}\right]$. However, equally valid solutions occur at $\alpha + k \frac{2\pi i}{h}$ for all integer k. For this reason, comparisons will be performed on e^{α} . However, at the limit of $h \to 0$, this issue disappears. Additionally, the dominant α -eigenvalue will have no imaginary component.

3. TESTING

In order to test the algorithm, a rod reactor model as described in [3] was used. Particles can only scatter forwards or backwards and fly at a constant velocity v. On each collision, ν particles are created. The rod is length L and the material has cross section Σ . For this test, $\nu = 1.5$, $\Sigma = 1$, v = 1, and L = 2.7. The α eigenvalues are given by the roots of Eq. (5) [4].

$$\cosh\left(z\sqrt{\chi\left(\chi-\nu\right)}\right) + \frac{\left(\chi-\frac{\nu}{2}\right)\sinh\left(z\sqrt{\chi\left(\chi-\nu\right)}\right)}{\sqrt{\chi\left(\chi-\nu\right)}} = 0, \qquad \chi = \frac{\alpha}{v\Sigma} + 1 \tag{5}$$

For the Monte Carlo simulation, particles were started in the rod uniformly in space and in the first time step. The initial direction was also uniform. The particle was moved to its first collision. If it was still inside the geometry, the end time was calculated and ν was added to the corresponding position in the fission matrix. The particle was then terminated. This was repeated 10^{10} times.

The fission matrix was partitioned into n space regions, $x \in [0, 2.7]$ and n time regions, $t \in [0, 2.7]$. This resulted in a maximum tally size of n^3 . As particles could only traverse at one velocity, the array was sparse and was stored as such. The matrix in Eq. (4) was then formed as an operator and the largest 11 eigenvalues by magnitude were computed using implicitly restarted Arnoldi [5].

These eigenvalues were then compared to the analytic solution for differing values of n in Fig. 1. Only the odd eigenvalues beyond α_0 are plotted, as the even ones are complex conjugates of the odd ones. As the step size decreased, all of the eigenvalues are converging proportional to h^2 until h becomes quite small. At this point, the solution becomes affected by stochastic noise. The most accurate value of α_0 occurred at n = 190, with $\alpha = -0.000614144$. The reference $\alpha = -0.000610374$, for a relative error of 0.6%.

4. CONCLUSIONS

Through the approach shown in this paper, it is possible to compute the α -eigenvalues from a time-dependent fission matrix. Numerical results indicate that the convergence of the algorithm on a smooth geometry is $\mathcal{O}(h^2)$ for multiple eigenvalues up until the point where stochastic noise affects the result. Further analysis involving the impact of a finite time limit, as well as the impact on a real model is warranted.



Figure 1: The Convergence of e^{α} as Compared to Analytic

ACKNOWLEDGEMENTS

This work was supported by the US-DOE-NNSA programs for Nuclear Criticality Safety and Advanced Simulation & Computing.

REFERENCES

- F. B. Brown, S. E. Carney, B. C. Kiedrowski, and W. R. Martin. "Fission Matrix Capability for MCNP, Part I - Theory." Technical Report LA-UR-13-20429, Los Alamos National Laboratory (2013).
- [2] A. Laureau, M. Aufiero, P. Rubiolo, E. Merle-Lucotte, and D. Heuer. "Transient Fission Matrix: Kinetic Calculation and Kinetic Parameters βeff and Λeff Calculation." Annals of Nuclear Energy, volume 85, pp. 1035–1044 (2015).
- [3] B. Montagnini and V. Pierpaoli. "The Time-Dependent Rectilinear Transport Equation." *Transport Theory and Statistical Physics*, volume 1(1), pp. 59–75 (1971).
- [4] A. Zoia, E. Dumonteil, A. Mazzolo, and S. Mohamed. "Branching exponential flights: travelled lengths and collision statistics." *Journal of Physics A: Mathematical and Theoretical*, **volume 45**(42), p. 425002 (2012).
- [5] R. B. Lehoucq, D. C. Sorensen, and C. Yang. ARPACK Users' Guide: Solution of Large-Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods, volume 6. Siam (1998).