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Solving eigenvalue response matrix equations with nonlinear techniques

Jeremy A. Roberts [a,*], Benoit Forget [b]

[a] Department of Mechanical and Nuclear Engineering, Kansas State University, 3002 Rathbone Hall, Manhattan, KS 66506, USA
[b] Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, 24-107, Cambridge, MA 02139, USA

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ABSTRACT

This paper presents new algorithms for use in the eigenvalue response matrix method (ERMM) for reactor eigenvalue problems. ERMM spatially decomposes a domain into independent nodes linked via boundary conditions approximated as truncated orthogonal expansions, the coefficients of which are response functions. In its simplest form, ERMM consists of a two-level eigenproblem: an outer Picard iteration updates the k-eigenvalue via balance, while the inner λ-eigenproblem imposes neutron balance between nodes. Efficient methods are developed for solving the inner λ-eigenvalue problem within the outer Picard iteration. Based on results from several diffusion and transport benchmark models, it was found that the Krylov–Schur method applied to the λ-eigenvalue problem reduces Picard solver times (excluding response generation) by a factor of 2–5. Furthermore, alternative methods, including Picard acceleration schemes, Steffensen's method, and Newton's method, are developed in this paper. These approaches often yield faster k-convergence and a need for fewer k-dependent response function evaluations, which is important because response generation is often the primary cost for problems using responses computed online (i.e., not from a precomputed database). Accelerated Picard iteration was found to reduce total computational times by 2–3 compared to the unaccelerated case for problems dominated by response generation. In addition, Newton's method was found to provide nearly the same performance with improved robustness.

1. Introduction and background

Fundamental to reactor modeling is analysis of the steady-state balance of neutrons, described concisely as

$$\mathbf{T}\phi(\vec{\rho}) = \frac{1}{k}\mathbf{F}\phi(\vec{\rho}), \tag{1}$$

where the operator $\mathbf{T}$ describes transport processes, $\mathbf{F}$ describes neutron generation, ϕ is the neutron flux, $\vec{\rho}$ represents the relevant phase space, and k is the eigenvalue, the ratio of the number of neutrons in successive generations.

Since the late 1970s, full core analyses for light water reactors (LWR) have been performed using relatively low fidelity nodal methods based on clever homogenization of phase-space with proven success. However, as current reactors become increasingly heterogeneous due more aggressive fuel loadings and longer cycle lengths in existing LWR's, nodal methods are becoming less applicable, and for new, highly heterogeneous reactor designs, even less so. Although advances in production nodal codes, including use of generalized multigroup SP_3 transport with subassembly resolution, address issues related to more complicated designs (Bahadir and Lindahl, 2009), there likely is limited room for further improvement of the underlying approach. Consequently, a move toward full core analysis techniques that can leverage the high fidelity methods typically used for smaller problems is desired.

1.1. The eigenvalue response matrix method

One such approach is the response matrix method (RMM), which is based on a spatial decomposition of the global problem of Eq. (1) into local fixed source problems connected by approximate boundary conditions. The response matrix method has been used in various forms since the early 1960s (Shimizu et al., 1963). Using the terminology of Lindahl and Weiss (1981), the method can be formulated using explicit volume flux responses, called the "source" RMM, or by using current responses that include fission implicitly and hence are functions of k, known as the "direct" RMM. Although both forms are used in various nodal methods, the source RMM is more widespread. This work is on

* Corresponding author. Tel.: +1 7855327182.
E-mail address: jaroberts@ksu.edu (Jeremy A. Roberts).

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the direct RMM, which shall be referred to as the *eigenvalue* response matrix method (ERMM).

Several formulations of ERMM have been proposed since its first use in the 1960s. Here, a rather general approach is described based on expansions of the boundary conditions that couple subvolumes of the global problem, a formalism introduced as early as the work of Lindahl (1976) and studied more recently by several authors (Mosher and Rahnema, 2006; Roberts and Forget, 2011, 2012).

Suppose the global problem of Eq. (1) is defined over a volume V. Then a local homogeneous problem can be defined over a subvolume V_i subject to

$$\mathbf{T}\phi(\vec{\rho}_i) = \frac{1}{k}\mathbf{F}\phi(\vec{\rho}_i), \tag{2}$$

and

$$J_-^{\text{local}}(\vec{\rho}_{is}) = J_-^{\text{global}}(\vec{\rho}_{is}), \tag{3}$$

where $J_-^{\text{local}}(\vec{\rho}_{is})$ is a function of the incident boundary flux, typically the partial current, which quantifies net flows through a surface.

To represent the local problem numerically, an orthogonal basis, P_n, over the relevant phase space is defined

$$P_n(\vec{\rho}_{is}), \quad n = 0, 1, \ldots, N, \tag{4}$$

subject to

$$\int P_m(\vec{\rho}_{is})P_n(\vec{\rho}_{is})\,d\rho_{is} = \delta_{mn}. \tag{5}$$

A response equation is defined

$$\mathbf{T}\phi_i^{ms}(\vec{\rho}_i) = \frac{1}{k}\mathbf{F}\phi_i^{ms}(\vec{\rho}_i) \tag{6}$$

subject to

$$J_-^{\text{local}}(\vec{\rho}_{is}) = P_m(\vec{\rho}_{is}). \tag{7}$$

The resulting outgoing currents $J_-(\vec{\rho}_{is})$ are used to define response functions

$$r_{im's'}^{ms} = \int P_{m'}(\vec{\rho}_{is'})J_{i+}^{m}(\vec{\rho}_{is'})\,d\rho_{is'}. \tag{8}$$

The quantity $r_{im's'}^{ms}$ has a simple physical interpretation: it is the m'th order response out of surface s' due to a unit incident mth order condition on surface s of subvolume i.

The incident and outgoing currents are expressed as truncated expansions using the same basis

$$J_{is\pm}(\vec{\rho}_{is}) \approx \sum_{n=0}^{N} j_{is_\pm}^{n} P_n(\vec{\rho}_{is}), \tag{9}$$

where

$$j_{is_\pm}^{n} = \int P_n(\vec{\rho}_{is})J_\pm(\rho_{is})\,d\rho_{is}. \tag{10}$$

These coefficients are then represented in vector form as

$$\mathbf{J}_{i\pm} = \left(j_{i1_\pm}^0, j_{i1_\pm}^1, \ldots, j_{i2_\pm}^0, j_{i2_\pm}^1, \ldots, j_{iS_\pm}^N\right)^{\mathsf{T}}, \tag{11}$$

and using these together with Eq. (8) yields the nodal balance equation

$$\mathbf{J}_{i+} = \begin{bmatrix} r_{i01}^{01} & r_{i01}^{11} & \cdots \\ r_{i11}^{01} & r_{i11}^{11} & \cdots \\ & & \ddots \end{bmatrix} \begin{bmatrix} j_{i1_-}^0 \\ j_{i1_-}^1 \\ \vdots \end{bmatrix} = \mathbf{R}_i\mathbf{J}_{i-}. \tag{12}$$

Global balance is defined by the eigenvalue response matrix equation

$$\mathbf{MR}(k)\mathbf{J}_- = \lambda\mathbf{J}_-, \tag{13}$$

where $\mathbf{R}$ is the block diagonal response matrix of $\mathbf{R}_i$, $\mathbf{J}_-$ are vectors containing all incident current coefficients, $\mathbf{M} = \mathbf{M}^{\mathsf{T}}$ is the connectivity matrix that redirects outgoing responses as incident responses of neighbors, superscript T represents the matrix transpose, and λ is an eigenvalue that represents the global balance of neutron currents through all nodal surfaces. If the response matrix $\mathbf{R}$ is conservative (i.e. it strictly maintains neutron balance),

$$\lim_{k\to k^*}\lambda = 1, \tag{14}$$

where k^* is the true eigenvalue. For nonconservative response expansions, the deviation of λ from unity measures discontinuities introduced across node boundaries and may be used to evaluate accuracy of the expansions used (with respect to an infinite expansion).

The k-eigenvalue can be interpreted physically as the ratio of neutrons produced in one generation to the previous generation. Alternatively, k can be viewed as the ratio of gains to losses in a given generation, and when applying this interpretation to the response matrix formalism, k can be updated via the process

$$k_{n+1} = \frac{\mathbf{F}(k_n)\mathbf{J}_-}{\mathbf{A}(k_n)\mathbf{J}_- + \mathbf{L}(k_n)\mathbf{J}_-}, \tag{15}$$

where $\mathbf{F}(k)\mathbf{J}_-$ is the global fission rate, $\mathbf{A}(k)\mathbf{J}_-$ is the global absorption rate, and $\mathbf{L}(k)\mathbf{J}_-$ is the total leakage rate from global boundaries.

1.2. Survey of ERMM implementations

The method defined by Eqs. (2)–(15) originates from the work of Shimizu (1963,), which appears to be the first work on response matrix methods (although the authors acknowledged a connection between their work and the earlier and more general theory of invariant imbedding as developed by Bellman et al. (1960)). The method was originally based on 1-D diffusion in slab geometry. Aoki and Shimizu extended the approach to two dimensions, using a linear approximation in space to represent boundary currents (Aoki and Shimizu, 1965). A shortcoming of this early work was an assumed value (unity) of the k-eigenvalue when evaluating responses, following which Eqs. (13) and (15) were solved just once to compute k. Typically $k \approx 1$ for nuclear reactors, so the errors observed were only tens of pcm, which may have been deceptively small and not representative of more general cases. In the later 2-D analysis (Aoki and Shimizu, 1965), the results compared favorably to fine mesh diffusion calculations.

Weiss and Lindahl generalized ERMM by considering arbitrarily high order expansions of the boundary currents in Legendre polynomials (Weiss and Lindahl, 1975) and introducing an iterative sceheme for the k-eigenvalue equivalent to Eq. (15). Lindahl also studied expansions of the current, comparing Legendre expansions to an approach that divides the boundary in several segments in which the current is assumed flat (Lindahl, 1976). A more complete overview of these approaches can be found in the review by Lindahl and Weiss (1981).

These diffusion-based methods rely on semi-analytic solutions to the diffusion equation and hence require homogeneous nodes. Previous scoping studies examined diffusion-based responses using discretized operators (Roberts and Forget, 2011). By numerically integrating the diffusion equation, heterogeneous nodes are treated naturally, though no diffusion models with heterogeneous nodes were studied.

In addition to methods based on diffusion theory, previous work applied transport theory for generating responses. Pryor et al. used a hybrid stochastic–deterministic approach based on Monte Carlo and the collision probability method to generate responses (Pryor and Graves, 1973; Pryor, 1975; Sicilian and Pryor,