A Davidson Method for the k-Eigenvalue Problem

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INTRODUCTION

The development of efficient solution strategies for the k-eigenvalue formulation of the neutron transport equation is an area of significant interest in the design and analysis of nuclear reactors. The availability of rapidly convergent and robust methods becomes even more vital when radiation transport is only a single component of a larger multiphysics computation. Current strategies almost invariably suffer from either poor convergence behavior or a lack of stability for many problems of interest. Additionally, existing methods rely on a nested iteration structure that requires selection of multiple convergence tolerances, leading to possible degradation in performance or even a loss in the accuracy of computed quantities. We proprose a strategy based on a generalized Davidson eigensolver that alleviates many of these issues. Although subspace methods (such as Arnoldi's method) have been investigated previously, to our knowledge this is the first use of a Davidson solver for the transport k-eigenvalue problem. Numerical results using the NEWT transport solver demonstrate the effectiveness of this approach.

DAVIDSON EIGENSOLVER

The k-eigenvalue formulation of the discrete first order neutron transport equation can be written in operator notation as

$$(\mathbf{L} - \mathbf{MSD})\psi = \frac{1}{k}\mathbf{MFD}\psi, \tag{1}$$

where $\mathbf{L}$ is the discretization of the streaming and collision term, $\mathbf{S}$ and $\mathbf{F}$ are the scattering and fission matrices, and $\mathbf{D}$ and $\mathbf{M}$ are angular restriction and prolongation operators. In the current study, we consider a discrete ordinates discretization in angle, a multigroup discretization in energy, and an arbitrary linear discretization in space, though the underlying strategy is not limited to these choices. A corresponding integral equation in terms of the scalar flux ϕ is obtained by multiplying Eqn. (1) by $\mathbf{DL^{-1}}$:

$$(\mathbf{I} - \mathbf{DL^{-1}MS})\phi = \frac{1}{k}\mathbf{DL^{-1}MF}\phi. \tag{2}$$

Mathematically, this equation is a generalized eigenvalue problem. Standard techniques (e.g. power method and Arnoldi's method) approach this problem by first converting it to the standard eigenvalue problem

$$\left(\mathbf{I} - \mathbf{DL^{-1}MS}\right)^{\mathbf{-1}}\mathbf{DL^{-1}MF}\phi = k\phi. \tag{3}$$

The drawback to these approaches is that each iteration requires applying the inverse of (in practice, solving a linear system with) the matrix $(\mathbf{I} - \mathbf{DL^{-1}MS})$, which is equivalent to solving a full fixed point multigroup transport problem. This problem would generally be solved using either a block Gauss-Seidel iteration or with a Krylov subspace method applied to the full problem[2;6].

As an alternative, we apply a generalized Davidson method[1] (for brevity we simply call it a Davidson method) directly to Eqn. (2). The Davidson method is a subspace approach which proceeds by projecting the full eigenproblem onto a low dimensional subspace as

$$\mathbf{V^T AV}y = \mu\mathbf{V^T BV}y, \tag{4}$$

where, for our purposes, $\mathbf{A} = (\mathbf{I} - \mathbf{DL^{-1}MS})$ and $\mathbf{B} = \mathbf{DL^{-1}MF}$. Forming this projected problem requires multiplying by transport matrices but does not involve solving any linear systems. Full space quantities can then be approximated using the solution to this small problem ($\phi \approx \mathbf{V}y$ and $k \approx \frac{1}{\mu}$). In the Davidson method, the subspace $\mathbf{V}$ is expanded at each iteration by applying a preconditioner to the eigenvalue residual, i.e.

$$v^{k+1} = \mathbf{M}^{-1}r^k, \tag{5}$$

where $r^k = \mathbf{A}x^k - \mu^k\mathbf{B}x^k$ and v^{k+1} is the vector to be added to the current subspace. It is important to note that although the rate of convergence of the Davidson solver will depend on the quality of the preconditioner, the accuracy of computed eigenvalues and eigenvectors is entirely independent of $\mathbf{M}$. This is in contrast to Arnoldi's method, where inaccuracies in applying the operator can result in inaccurate final solutions despite apparent convergence. In the present study, we use a multigrid in energy preconditioning strategy with a damped Richardson iteration as the smoother.

There is a cost associated with the use of the Davidson method for the k-eigenvalue problem. Because the problem is being treated as a generalized eigenproblem and the subspace that is formed has no particular structure (in contrast to the Krylov subspace formed in, for instance, Arnoldi's method which has a very rich structure), it is generally necessary to store three sets of vectors (with each set containing as many as 20 vectors) that are the length of the eigenvector. For large problems, this memory cost may potentially be prohibitive, although restarting strategies can significantly alleviate such issues with only a modest reduction in the overall effectiveness of the solver[5].

RESULTS AND CONCLUSION

In order to demonstrate the effectiveness of the proposed strategy, we compare a variety of eigensolvers for two test problems within the NEWT radiation transport code which uses a step characteristics spatial discretization. The first test problem is modeling a single fuel block of the HTTR research reactor. The geometry, shown in Fig. 1, consists of a hexagonal array of 6.3% enriched UO_2 fuel rods inside a graphite block with an instrumentation tube at the center and burnable poison rods at three corners. The spatial mesh is formed by overlaying a 108×96 Cartesian grid over the problem. White boundary conditions are applied on all external boundaries. The second test problem is a slightly modified version of the 2D C5G7-MOX benchmark problem[4]. The only change from the original specification is that 16-group cross sections produced by the SCALE package are used rather than the particular 7-group cross sections specified in the original benchmark. The geometry consists of two UO_2 and two MOX PWR assemblies surrounded by a water reflector on two sides. Reflecting boundaries are applied along the boundaries that don't have a reflector. A 102×102 Cartesian mesh is used to discretize the problem in space (a finer mesh is produced within the fuel pins). For both problems an S_8 level symmetric quadrature is used in angle and P_1 scattering is used for all materials.

Several eigensolvers were used to solve this problem. The pre-existing eigensolver in NEWT is the power method with optional coarse mesh finite difference (CMFD) acceleration (the power method implementation uses a block Gauss-Seidel iteration in energy with source iteration for the within-group problems). Implementations of Arnoldi's method, Rayleigh quotient iteration (RQI), and the Davidson method with multigrid in energy preconditioning (Dav/MGE) have been added to the code. The Arnoldi and RQI implementations use GMRES with the multigrid in energy preconditioner for solving the necessary multigroup transport problems.

The convergence results for all of the solvers for the two test problems are shown in Table 1. As expected, power iteration with no acceleration performs very poorly for these problems. CMFD acceleration greatly improves the performance, although it should be noted that these results depend very strongly on problem parameters (such as the size of the coarse mesh) that have been manually selected in these cases to achieve optimal performance. Such selections would generally not be available to the user a priori. The remaining three methods all offer improved performance relative to power method, with the Davidson method even outperforming CMFD for both problems. It is interesting to note that, although RQI converges extremely rapidly in terms of the number of outer iterations, the cost of each iteration is so large that the Davidson method displays a much lower computational cost.

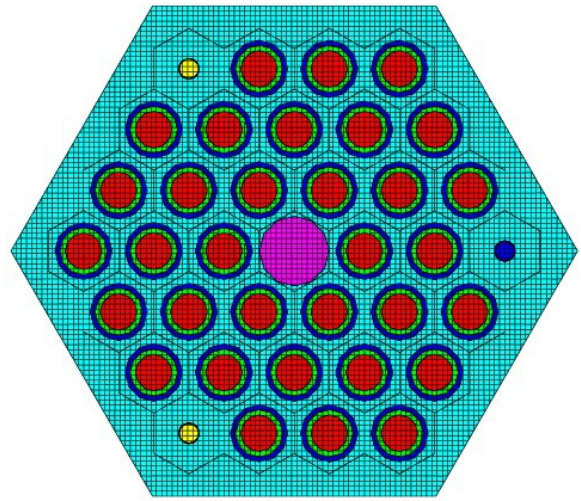

Figure 1: Geometry for HTTR Problem

Table 1: Eigensolver convergence and timings (seconds) for test problems.

	HTTR		C5G7	
Solver	Iters	Time (s)	Iters	Time (s)
Power	103	1752	320	4494
CMFD	14	184	11	248
Arnoldi	5	640	10	1375
RQI	2	244	4	675
Dav/MGE	14	157	16	236

In this study it has been shown that the Davidson eigensolver is a potentially viable alternative to standard approaches that have typically been used to solve the k-eigenvalue problem. In particular, because the Davidson method avoids first converting the problem to a standard eigenvalue problem, the nested iteration structure that plagues other solvers can be avoided. The performance of the Davidson method is competitive with (and frequently better than) nonlinear acceleration schemes; because its convergence does not depend strongly on discretization parameters, it is a much more robust solver.

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