Generalized Partitioned Matrix Acceleration of Variational Nodal Method

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INTRODUCTION

Like most other neutron transport methods, variational nodal method (VNM) codes, such as VARIANT [1-3] and PANX [4], employ at least two levels of iterations: inner (or within group) and outer (or fission source) iterations. In these codes, partitioned matrix (PM) acceleration has successfully accelerated the inner iterations, making it feasible to employ only one computationally intense red-black sweep of the full response matrix equations per energy group. To accelerate the outer iteration legacy methods, such as Chebyshev or Wielandt acceleration, have been employed, but they often result in only marginal improvements. Thus for high dominance ratio problems inordinate numbers of outer iterations are still required.

The PM acceleration iterations are performed only on the lowest order partial current terms (one per nodal interface) while the higher space-angle terms are held constant from the previous outer iteration. This is followed by one full matrix red-black sweep. In the generalized partitioned matrix (GPM) acceleration introduced in this work, iterations on the lowest order flux and fission source (one per node) terms also are performed while the higher order spatial moments are retained from the preceding outer iteration.

GPM acceleration is a module inserted within the standard format of each VNM outer iteration. Other recent work [5] employs more generalized partitioning as well, but in a different framework. It divides outer iterations into un-accelerated, which requires several full matrix sweeps per energy group per outer iterations, and accelerated, which has a somewhat similar structure to our GPM module. Our intent is to develop a method applicable to VNM neutron transport codes. As a first step, we here formulate GPM for diffusion theory and present results.

THEORY

Variational nodal methods result in the following set of three multi-group equations for energy group g and node n: the group source, the response matrix and the flux equations.

$$\underline{q}_{gn} = \sum_{g' \neq g} \underline{\underline{\sigma}}_{sgg'n} \underline{\phi}_{g'n} + \frac{1}{k} \chi_g \underline{f}_n , \tag{1}$$

$$\underline{j}^{+}_{gn} = \underline{\underline{R}}_{gn} \underline{j}^{-}_{gn} + \underline{\underline{B}}_{gn} \underline{q}_{gn} , \tag{2}$$

$$\underline{\phi}_{gn} = \underline{\underline{V}}_{gn} \underline{q}_{gn} - \underline{\underline{C}}_{gn} \left(\underline{j}^{+}_{gn} - \underline{j}^{-}_{gn} \right), \tag{3}$$

where the fission source can be expressed as

$$\underline{f}_n = \sum_{g'} \nu \underline{\underline{\sigma}}_{fg'n} \underline{\phi}_{g'n} . \tag{4}$$

The response matrices $\underline{\underline{R}}_{gn}$ as well as the matrices $\underline{\underline{B}}_{gn}$, $\underline{\underline{V}}_{gn}$ and $\underline{\underline{C}}_{gn}$ must be evaluated for each unique node type and they are pre-calculated before performing outer iterations. $\underline{q}_{gn}$ is the group source, $\underline{j}^{\pm}_{gn}$ are the partial current vectors coupling the nodes, and $\underline{\phi}_{gn}$ is the scalar flux. $\underline{\underline{\sigma}}_{s}$ is the neutron scattering cross section matrix and $\nu \underline{\underline{\sigma}}_{f}$ is the production cross section vector; χ is the fission spectrum.

In VNM diffusion theory, the flux, partial current and source are expanded by orthogonal trial functions [1-3,5]. We divide their expansion coefficients into low-order and high-order parts:

$$\underline{\phi}_{gn} = \begin{bmatrix} \underline{\phi}^{\alpha}_{gn} \\ \underline{\phi}^{\beta}_{gn} \end{bmatrix}, \underline{j}^{\pm}_{gn} = \begin{bmatrix} \underline{j}^{\pm,\alpha}_{gn} \\ \underline{j}^{\pm,\beta}_{gn} \end{bmatrix}, \underline{q}_{gn} = \begin{bmatrix} \underline{q}^{\alpha}_{gn} \\ \underline{q}^{\beta}_{gn} \end{bmatrix}, \tag{5}$$

where α and β indicate the low- and high-order parts, respectively. The low-order part is composed of the average values of the corresponding unknowns. We write Eq. (1) through (3) into partitioned form as (the node notation is omitted):

$$\begin{bmatrix} \underline{q}_g^{\alpha} \\ \underline{q}_g^{\beta} \end{bmatrix} = \sum_{g' \neq g} \underline{\underline{\sigma}}_{sgg'} \begin{bmatrix} \underline{\phi}_{g'}^{\alpha} \\ \underline{\phi}_{g'}^{\beta} \end{bmatrix} + \frac{1}{k} \chi_g \begin{bmatrix} \underline{f}^{\alpha} \\ \underline{f}^{\beta} \end{bmatrix} \tag{6}$$

$$\begin{bmatrix} \underline{j}_g^{+,\alpha} \\ \underline{j}_g^{+,\beta} \end{bmatrix} = \begin{bmatrix} \underline{\underline{R}}_g^{\alpha\alpha}\Pi^{\alpha} & \underline{\underline{R}}_g^{\alpha\beta}\Pi^{\beta} \\ \underline{\underline{R}}_g^{\beta\alpha}\Pi^{\alpha} & \underline{\underline{R}}_g^{\beta\beta}\Pi^{\beta} \end{bmatrix} \begin{bmatrix} \underline{j}_g^{+,\alpha} \\ \underline{j}_g^{+,\beta} \end{bmatrix} + \begin{bmatrix} \underline{\underline{B}}_g^{\alpha\alpha} & \underline{\underline{B}}_g^{\alpha\beta} \\ \underline{\underline{B}}_g^{\beta\alpha} & \underline{\underline{B}}_g^{\beta\beta} \end{bmatrix} \begin{bmatrix} \underline{q}_g^{\alpha} \\ \underline{q}_g^{\beta} \end{bmatrix} \tag{7}$$

$$\begin{bmatrix} \underline{\varphi}_g^{\alpha} \\ \underline{\varphi}_g^{\beta} \end{bmatrix} = -\begin{bmatrix} \underline{\underline{C}}_g^{\alpha\alpha} & \underline{\underline{C}}_g^{\alpha\beta} \\ \underline{\underline{C}}_g^{\beta\alpha} & \underline{\underline{C}}_g^{\beta\beta} \end{bmatrix} \begin{bmatrix} \underline{\underline{I}} - \underline{\underline{\Pi}}^{\alpha} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{I}} - \underline{\underline{\Pi}}^{\beta} \end{bmatrix} \begin{bmatrix} \underline{j}_g^{+,\alpha} \\ \underline{j}_g^{+,\beta} \end{bmatrix} + \begin{bmatrix} \underline{\underline{V}}_g^{\alpha\alpha} & \underline{\underline{V}}_g^{\alpha\beta} \\ \underline{\underline{V}}_g^{\beta\alpha} & \underline{\underline{V}}_g^{\beta\beta} \end{bmatrix} \begin{bmatrix} \underline{q}_g^{\alpha} \\ \underline{q}_g^{\beta} \end{bmatrix} \tag{8}$$

where $\underline{\underline{\Pi}}$ is the Boolean connectivity matrix [7] mapping the partial currents crossing internal interfaces from outgoing to incoming:

$$\begin{bmatrix} \underline{j}_g^{-,\alpha} \\ \underline{j}_g^{-,\beta} \end{bmatrix} = \begin{bmatrix} \underline{\underline{\Pi}}^{\alpha} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{\Pi}}^{\beta} \end{bmatrix} \begin{bmatrix} \underline{j}_g^{+,\alpha} \\ \underline{j}_g^{+,\beta} \end{bmatrix}. \tag{9}$$

To apply GPM acceleration, a module is inserted into a standard VNM outer iteration as indicated in Fig. 1. The contents of the GPM module are indicated in Fig. 2. In the figures, $\left(\underline{\underline{I}} - \underline{\underline{R}}_g\underline{\underline{\Pi}}\right)^{-1}$ indicates an iterative solution of the response matrix equations. In the standard method, PM acceleration is followed by a single red-black sweep of the full response matrices. In the GPM module, we make several passes through the energy group loop, updating the spatial distribution of the low-order fission source terms (as well as flux and current) while retaining the higher order space-angle terms from the previous outer iteration.

Up-scattering iterations are not presented in these figures and are implemented in the usual way: if there is no up-scattering, we only go through the energy groups once every fission source iteration; if there is up-scattering, we perform iterations over the corresponding energy groups.

NUMERICAL RESULTS

Based on the above theory and formulas, GPM is implemented in the NODAL code, a new version of the

$k^{(1)} = 1.0,\ \underline{\phi}_g^{(1)} = 1.0,\ \underline{f}^{(1)} = \sum_{g'} \nu\underline{\underline{\sigma}}_{fg'}\underline{\phi}_{g'}^{(1)},\ g = 1,..., G$

Do $l = 1, L$ *! Outer iteration*

IF(GPM acceleration) Insert GPM module here

Do $g = 1, G$ *! Energy group loop*

$$\underline{q}_g^{(l+1)} = \sum_{g'<g} \underline{\underline{s}}_{sgg'}\underline{f}_{g'}^{(l+1)} + \sum_{g'>g} \underline{\underline{s}}_{sgg'}\underline{f}_{g'}^{(l)} + \frac{1}{k^{(l)}} c_g \underline{f}^{(l)}$$

IF(PM acceleration) Then

$\underline{s}_g^{j} = \underline{\underline{R}}_g^{\alpha\beta}\underline{\underline{\Pi}}^{\beta}\underline{j}_g^{+\beta}$

! Within-group iteration

$\underline{j}_g^{+\alpha,(l+1)} = \left(\underline{\underline{I}} - \underline{\underline{R}}_g^{\alpha\alpha}\underline{\underline{\Pi}}^{\alpha}\right)^{-1} (\underline{\underline{B}}_g^{\alpha}\underline{q}_g^{(l+1)} + \underline{s}_g^{j})$

! Full matrix sweep

$\underline{j}_g^{+(l+1)} = \underline{\underline{R}}_g\underline{j}_g^{-(l)} + \underline{\underline{B}}_g\underline{q}_g^{(l+1)}$

Else

$\underline{j}_g^{+,(l+1)} = \left(\underline{\underline{I}} - \underline{\underline{R}}_g\underline{\underline{\Pi}}\right)^{-1} \underline{\underline{B}}_g\underline{q}_g^{(l+1)}$

End if

! Calculate the flux

$\underline{f}_g^{(l+1)} = \underline{\underline{C}}_g\left(\underline{\underline{I}} - \underline{\underline{\mathrm{P}}}\right)\underline{j}_g^{+,(l+1)} + \underline{\underline{V}}_g\underline{q}_g^{(l+1)}$

End Do *! Energy group loop*

$\underline{f}^{(l+1)} = \sum_{g'} n\underline{\underline{s}}_{fg'}\underline{f}_{g'}^{(l+1)},\ k^{(l+1)} = k^{(l)} \left\|\underline{f}^{(l+1)}\right\|_2 / \left\|\underline{f}^{(l)}\right\|_2$

End Do *! Outer iteration*

Figure 1. Standard VNM Outer Iteration with Location of GPM Module Indicated

VARIANT developed at Argonne National Laboratory as one of the solvers in the PROTEUS package [6]. A 2D problem derived from the C5G7 benchmark [8] is tested. As NODAL can only treat homogeneous nodes, we employ 7-group pin-cell homogenized cross sections in the calculation. To examine the performance of the method, three calculations are presented: 1. without any PM accelerations; 2. with within-group PM acceleration; 3. with GPM acceleration.

In all calculations, we traverse the energy groups once within every outer iteration (with up-scattering iterations added for thermal systems), and the maximum number of within-group iteration is set to 10. In within-group PM acceleration, the maximum number of low-order iteration is also set to 10, and it is followed by one full-order sweep. In GPM acceleration, we set the maximum number of fission source iterations for the low-order system to 5. Additionally, to make a fair comparison, the convergence criterions are the same in all

the calculations: 1.0×10^{-6} for eigenvalue errors, 1.0×10^{-7} for fission source errors and 1.0×10^{-8} for flux errors.

! Initialization

$\tilde{k}^{(1)} = k^{(l)}$, $\underline{\tilde{f}}^{\alpha,(1)} = \underline{f}^{\alpha,(l)}$, $\underline{\tilde{f}}^{\beta,(1)} = \underline{f}^{\beta,(l)}$

Do g = *1,G*

$\underline{\tilde{\phi}}_g^{\alpha,(1)} = \underline{\phi}_g^{\alpha,(l)}$, $\underline{\tilde{\phi}}_g^{\beta,(1)} = \underline{\phi}_g^{\beta,(l)}$

$\underline{\tilde{j}}_g^{\pm\alpha,(1)} = \underline{j}_g^{\pm\alpha,(l)}$, $\underline{\tilde{j}}_g^{\pm\beta,(1)} = \underline{j}_g^{\pm\beta,(l)}$

End do

! calculate the high-order source

Do g = *1,G*

$$\underline{q}_g^{\beta} = \sum_{g'<g} \underline{\underline{\sigma}}_{sgg'} \underline{\tilde{\phi}}_{g'}^{\beta,(1)} + \sum_{g'>g} \underline{\underline{\sigma}}_{sgg'} \underline{\tilde{\phi}}_{g'}^{\beta,(1)} + \frac{1}{k^{(l)}} \chi_g \underline{\tilde{f}}^{\beta,(1)}$$

$$\underline{s}_g^{j} = \underline{\underline{R}}_g^{\alpha\beta} \underline{\underline{\Pi}}^{\beta} \underline{\tilde{j}}_g^{+\beta} + \underline{\underline{B}}_g^{\alpha\beta} \underline{q}_g^{\beta}$$

$$\underline{s}_g^{\phi} = -\underline{\underline{C}}_g^{\alpha\beta} \left(\underline{\underline{I}} - \underline{\underline{\Pi}}^{\beta} \right) \underline{\tilde{j}}_g^{+\beta} + \underline{\underline{V}}_g^{\alpha\beta} \underline{q}_g^{\beta}$$

End Do

Do m = 1, M *! Low-order fission source iteration*

Do g = 1, G *! Energy group loop*

$$\underline{q}_g^{\alpha,(m+1)} = \sum_{g'<g} \underline{\underline{\sigma}}_{sgg'} \underline{\tilde{\phi}}_{g'}^{\alpha,(m+1)} + \sum_{g'>g} \underline{\underline{\sigma}}_{sgg'} \underline{\tilde{\phi}}_{g'}^{\alpha,(m)} + \frac{1}{\tilde{k}^{(m)}} \chi_g \underline{\tilde{f}}^{\alpha,(m)}$$

! Within group iteration

$$\underline{\tilde{j}}_g^{+\alpha,(m+1)} = \left(\underline{\underline{I}} - \underline{\underline{R}}_g^{\alpha\alpha} \underline{\underline{\Pi}}^{\alpha} \right)^{-1} \left(\underline{\underline{B}}_g^{\alpha\alpha} \underline{q}_g^{\alpha,(m+1)} + \underline{s}_g^{j} \right)$$

! Calculate the flux

$$\underline{\tilde{\phi}}_g^{\alpha,(m+1)} = -\underline{\underline{C}}_g^{\alpha\alpha} \left(\underline{\underline{I}} - \underline{\underline{\Pi}}^{\alpha} \right) \underline{\tilde{j}}_g^{+\alpha,(m+1)} + \underline{\underline{V}}_g^{\alpha\alpha} \underline{q}_g^{\alpha,(m+1)} + \underline{s}_g^{\phi}$$

End Do *! Energy group loop*

$$\underline{\tilde{f}}^{\alpha,(m+1)} = \sum_{g'} \nu\underline{\underline{\sigma}}_{fg'} \underline{\tilde{\phi}}_{g'}^{\alpha,(m+1)}, \tilde{k}^{(m+1)} = \tilde{k}^{(m)} \frac{\left\| \underline{\tilde{f}}^{\alpha,(m+1)} \right\|_2}{\left\| \underline{\tilde{f}}^{\alpha,(m)} \right\|_2}$$

End Do *! Low-order fission source iteration*

! put eigenvalue and low-order solution back into full system

$k^{(l)} = \tilde{k}^{(M+1)}$, $\underline{f}^{\alpha,(l)} = \underline{\tilde{f}}^{\alpha,(M+1)}$

Do g = *1,G*

$\underline{\phi}_g^{\alpha,(l)} = \underline{\tilde{\phi}}_g^{\alpha,(M+1)}$

$\underline{j}_g^{\pm\alpha,(l)} = \underline{\tilde{j}}_g^{\pm\alpha,(M+1)}$

End do

Figure 2. The GPM Module

The polynomial expansions of the flux and source in the node are both 6th order and that of the partial current is 2nd order. This leads to 28 degrees of freedoms (DOFs) in each node and 3 DOFs on each nodal surface. We define the flat terms of their expansions as low-order part.

The calculation results for this problem are shown in Table I. First, note that the same eigenvalue (1.18627) and pin power distributions are obtained with three different acceleration methods (not shown here), which demonstrate the correct implementation of GPM. Second, the number of outer iterations is significantly reduced from 72 to 11 by applying GPM. More precisely, there are 11 outer iteration and 55 partitioned matrix fission iterations in the GPM calculation. Third, an acceleration factor of 4.6 (in computational time) is achieved with GPM, while with traditional within-group PM method, the acceleration factor is only 1.88. The relative errors of eigenvalue versus the CPU time are shown in Fig. 3. (The three lines do not terminate at the convergence criterion 1.0×10^{-6} because fission source and flux are not yet converged. The code stops when eigenvalue, flux and fission source are all converged.)

Table I. Comparison of Different Acceleration Methods

	No. of Outer Iterations	CPU Time (s)	Acceleration Ratio
No Acceleration	72	9.96	/
With WG PM	72	5.31	**1.88**
With GPM	11	2.15	**4.63**

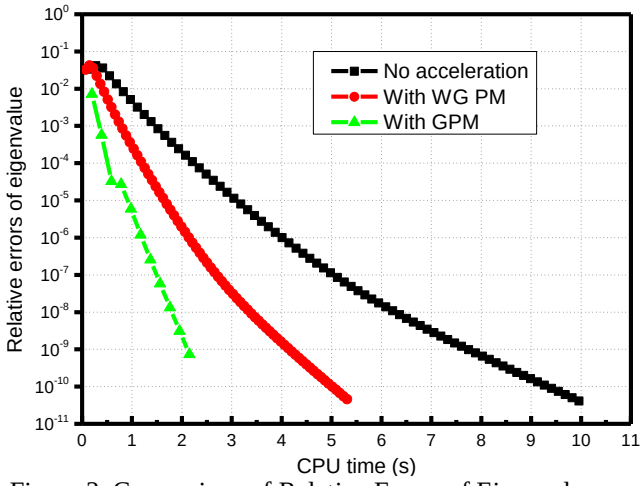

Figure 3. Comparison of Relative Errors of Eigenvalues through CPU Time

CONCLUSION

The Generalized Partitioned Matrix acceleration is formulated and implemented for the diffusion approximation in the NODAL code. For the 2D C5G7 benchmark, results show the number of outer iterations

and CPU time are substantially reduced and an acceleration ratio of 4.6 in computational time is obtained. Similar improvements are obtained for 3D benchmarks and are included in the presentation. Future work will focus on applying the method to transport VNM methods.

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