Implementation of Generalized Coarse-Mesh Rebalance in NEWTRNX for Acceleration of Parallel Block-Jacobi Transport

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I. INTRODUCTION

The NEWTRNX [1] transport module solves the multigroup, discrete-ordinates source-driven or k-eigenvalue transport equation in parallel on a 3-D unstructured tetrahedral mesh using the extended step characteristics (ESC) [2], also known as the slice-balance approach (SBA), spatial discretization. The spatial domains are decomposed using METIS [3]. NEWTRNX is under development for nuclear reactor analysis on computer hardware ranging from clusters to massively parallel machines, like the Cray XT4. Transport methods that rely on full sweeps across the spatial domain have been shown to display poor scaling for thousands of processors. The Parallel Block-Jacobi (PBJ) algorithm allows each spatial partition to sweep over all discrete-ordinate directions and energies independently of all other domains, potentially allowing for much better scaling than possible with full sweeps [4]. The PBJ algorithm has been implemented in NEWTRNX using a Gauss-Seidel iteration in energy and an asynchronous communication by an energy group, such that each partition utilizes the latest boundary solution available for each group before solving the within-group scattering in a given group. For each energy group, the within-group scattering converges with a generalized minimum residual (GMRES) solver [5], preconditioned with beta transport synthetic acceleration (β-TSA) [6].

Reactor analysis software has utilized nonlinear methods for acceleration of the transport equation for almost three decades. Homogenization theory, using lattice-physics transport and full-core diffusion, produce a low-order problem (in space, energy, and direction) with "discontinuity factors" that produce the exact transport solution if the boundary conditions for the lattices are exactly correct. Coarse-mesh finite difference diffusion (CMFD) homogenizes the high-order solution over spatial domains and uses discontinuity factors to formulate a low-order eigen-problem that exactly replicates the high-order solution, averaged over coarse-mesh regions, when converged.

The generalized coarse-mesh rebalance (GCMR) methodology formulates a CMFD-like problem without the structured mesh that is traditionally used with CFMD and has been shown (in one dimension) to provide a more robust method than CMFD [7].

The GCMR methodology has been implemented in NEWTRNX for solving the 3-D parallel transport equations on the nonconvex, unstructured METIS spatial domains.

I.A. Generalized Coarse-Mesh Rebalance

For a given problem (in this case source-driven transport, but could also applied to an eigen-problem as well):

$$A\psi = b \tag{1}$$

With a given iteration procedure of

$$\psi^{(l+1)} = \left[I - MA\right]\psi^{(l)} + Mb \tag{2}$$

Where ψ is the high-order solution (volumetric and surface of each spatial domain), A is the high-order matrix, and M is a preconditioner (e.g., PBJ source iteration). A low-order (coarse-mesh) region of phase space (space and neutron direction) is defined and homogenization is used as the restriction operation (R) over each region. Similarly, the surface solution is reduced to the neutron current and flux on the interface of partitions:

$$\Phi^{(l)} = R\psi^{(l)} \tag{3}$$

Where R is the homogenization operator. Given R, a prolongation operator (P) is defined to preserve the high-order solution after a restriction and prolongation operation:

$$\psi^{(l)} = P\Phi^{(l)} = P\left[R\psi^{(l)}\right]. \tag{4}$$

R and P are used to define a low-order problem such that, when converged, is equal to the integral of the fine-mesh solution over coarse-mesh regions:

$$P^{(l)} \ s.t. \ \psi^{(l)} = P^{(l)}R\psi^{(l)}. \tag{5}$$

$$A_{LO} = RAP^{(l)} \tag{6}$$

Given the low order problem, we solve for $\Phi^{(l+1/2)}$:

$$A_{LO}\Phi^{\left(l+\frac{1}{2}\right)} = Rb \qquad (7)$$

Then calculate the high-order solution:

$$\psi^{\left(l+\frac{1}{2}\right)} = P^{(l)}\Phi^{\left(l+\frac{1}{2}\right)} \qquad (8)$$

$$\psi^{(l+1)} = \left[I - MA\right]\psi^{\left(l+\frac{1}{2}\right)} + Mb \qquad (9)$$

I.B. Surface Prolongation on a METIS Domain

The prolongation operator for the volumetric solution is straightforward—the ratio of the fine-mesh flux moments to the scalar flux integrated over the coarse-mesh. In three dimensions, the angular flux for every face on the interface of partitions is reduced to the scalar flux and net current (and algebraically eliminated). However, the prolongation operator is defined for the half-range (incident and outgoing) solution to preserve the net current and flux from the low-order problem.

$$\Psi^{(l)}_{\substack{inc\\out}} = \sum_{\left(\overline{\Omega_m}\bullet\overline{n_s}\right)^{<}_{>}0} w_m \sum_{surfaces} A_s\psi^{(l)}_{m,s} \qquad (10)$$

$$P^{(l)}_{\substack{inc\\out}} = \left[\frac{\psi^{(l)}_{m,s}}{\Psi^{(l)}_{\substack{inc\\out}}}\right]_{\left(\overline{\Omega_m}\bullet\overline{n_s}\right)^{<}_{>}0} \qquad (11)$$

The low-order, half-range surface solution can be defined using the initial half-range current to flux ratio $\left(\mu_{out}, \mu_{inc}\right)$:

$$\mu^{(l)}_{\substack{inc\\out}}\Psi^{(l)}_{\substack{inc\\out}} = \sum_{\left(\overline{\Omega_m}\bullet\overline{n_s}\right)^{<}_{>}0} w_m \sum_{surfaces} A_s\psi^{(l)}_{m,s}\left|\overline{\Omega_m}\bullet\overline{n_s}\right| \qquad (12)$$

$$\begin{bmatrix} \mu^{(l)}_{out} & -\mu^{(l)}_{inc} \\ 1 & 1 \end{bmatrix}\begin{bmatrix} \Psi^{\left(l+\frac{1}{2}\right)}_{out} \\ \Psi^{\left(l+\frac{1}{2}\right)}_{inc} \end{bmatrix} = \begin{bmatrix} J^{\left(l+\frac{1}{2}\right)} \\ \Phi^{\left(l+\frac{1}{2}\right)} \end{bmatrix} \qquad (13)$$

II. RESULTS

A partial height 3-D LMFBR fuel pincell was analyzed to demonstrate the performance of the GCMR nonlinear acceleration of the PBJ algorithm in space (with Gauss-Seidel in energy). This single assembly (shown in Figure 1) contains 6984 tetrahedral elements (~3.5 slices per element). The SCALE computer code was used to generate a 44-group cross section library, and a product quadrature set with 16 polar and 36 azimuthal angles was used— a total of 500 million degrees of freedom. Figure 2 displays the convergence of the PBJ algorithm with and without GCMR by iteration for 4 and 16 spatial domains.

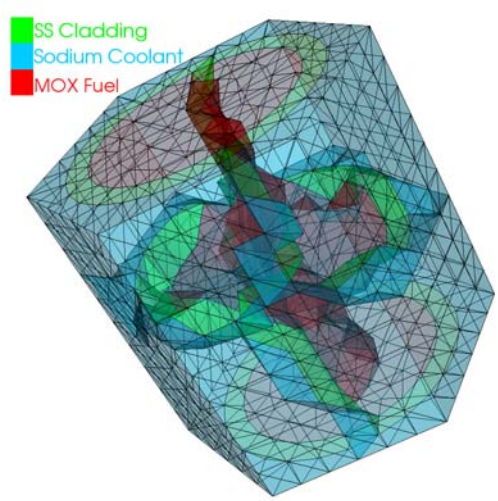

Fig. 1. Axial slice of an LMFBR pincell with mesh and 4 spatial partitions displayed..

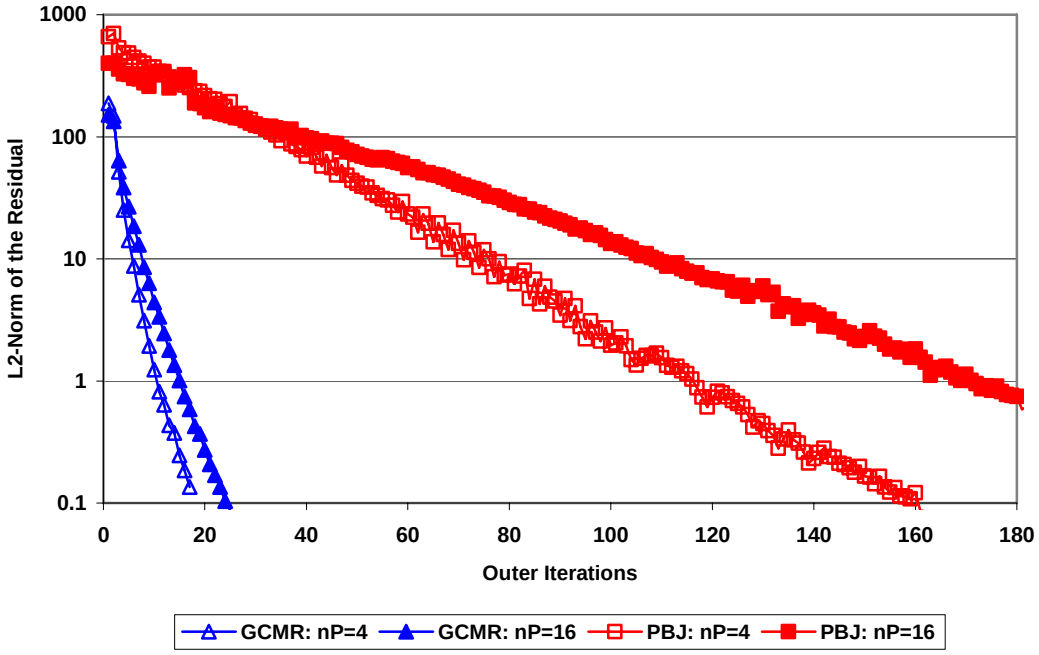

Fig. 2. Convergence by outer iteration for PBJ alone SI and with GCMR using 4 and 16 processors.

III. CONCLUSIONS

The PBJ algorithm has been shown to parallelize well for multigroup algorithms, but the rate of convergence is substantially improved with the nonlinear GCMR algorithm. The rate of convergence is not affected by the implementation of the GCMR nonlinear acceleration. In addition, the computational burden of the GCMR solver is negligible with respect to the transport sweeping. Additional problems will be analyzed and scaling studies for larger domains with many more processors will be considered in the near future.

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