Implementation of Transport Synthetic Acceleration in NEWTRNX

Seth R. Johnson, *Oak Ridge National Laboratory, Nuclear Science and Technology Division*
Oak Ridge, Tennessee 37831-6370, sethjohnson@aggienetwork.com

Kevin T. Clarno, *Oak Ridge National Laboratory, Nuclear Science and Technology Division*
Oak Ridge, Tennessee 37831-6370, clarnokt@ornl.gov

INTRODUCTION

NEWTRNX [1] is a 3-D deterministic transport solver under development to solve large problems using spatial partitioning with Parallel Block Jacobi iteration structure [2]; it employs the Slice-Balance Approach to sweep across a tetrahedral mesh on each partition independently. The innermost iteration, operating on a single partition, solves a one-group transport equation that stores only the volumetric flux moments and the angular flux on boundary faces.

When solved with source iteration (SI), this one-group problem may converge arbitrarily slowly. The Generalized Minimal RESidual method (GMRES) [3], a Krylov iterative solver, is used as an alternative to SI. The beta Transport Synthetic Acceleration (β-TSA) method [4] is implemented as a standard synthetic accelerator for SI and as a preconditioner for GMRES.

Because the solution of a multigroup problem requires iteration over each energy group, the group with the highest self-scattering ratio will be a limiting factor. Using this group with a simple geometry provides a practical test of the acceleration implementation.

The two 3-D geometries chosen to test the acceleration method are slices from standard nuclear reactor pin cells: one is a square-pitch pin from a pressurized water reactor (PWR), and the other is a triangular-pitch pin from a liquid metal fast breeder reactor (LMFBR). Each problem uses fully reflecting boundaries and is executed on one processor.

ANALYSIS

Solution of the Transport Equation

The inner iteration of NEWTRNX solves the one-group transport equation (Eq. 1).

$$\mathbf{W}(\mathbf{I}-\mathbf{EV})\mathbf{x} = \mathbf{WEq} \tag{1}$$

$$\mathbf{x} = \begin{bmatrix} \boldsymbol{\varphi} \\ \boldsymbol{\psi}_\mathbf{b} \end{bmatrix}, \mathbf{V} = \begin{bmatrix} \mathbf{S} & \mathbf{0} \\ \mathbf{0} & \mathbf{H} \end{bmatrix}, \mathbf{q} = \begin{bmatrix} \mathbf{q_m} \\ \mathbf{0} \end{bmatrix} \tag{2}$$

Here **E** is the transport operator, which transforms the angular moments of the source to an ordinate-based source, and performs a transport sweep over all ordinates (given an incident boundary source) to calculate new moments of the volumetric flux and boundary angular flux. **V** is the scattering/reflecting operator, **x** is the solution vector comprised of the volume and exiting boundary fluxes, and $\mathbf{q_m}$ contains the volumetric source moments (Eq. 2). Synthetic acceleration acts as a left preconditioner **W** which can be directly applied to the result of an SI iteration, or used on a swept search vector in GMRES.

The synthetic method implemented in NEWTRNX is modified to operate on the residual of a source iteration and update the old scalar flux and boundary angular flux with a correction **e** (Eq. 3). This reformulation removes the extra source iteration that is present in the traditional method, allowing a description as a preconditioner to be more simply stated and applied to GMRES.

$$\begin{aligned} \mathbf{x}^{(l+1/2)} &= \mathbf{EVx}^{(l)} + \mathbf{Eq} \\ \mathbf{e} &= \mathbf{W}\left(\mathbf{x}^{(l+1/2)} - \mathbf{x}^{(l)}\right) \\ \mathbf{x}^{(l+1)} &= \mathbf{x}^{(l)} + \mathbf{e} \end{aligned} \tag{3}$$

Transport Synthetic Acceleration

The β-TSA method approximates a correction to the problem with a low-order quadrature set and uses a parameter β that modifies the scattering ratio. Other parameters affect the performance of the TSA scheme, including the number of iterations to run and an execution criterion.

Formulated as the preconditioner **W**, TSA acts as an approximation of the inverse of a scatter-sweep operation (Eq. 4). $\mathbf{E}_{\beta,lo}$ and $\mathbf{V}_{\beta,lo}$ are the low-order operators that modify the scattering ratio (Eq. 5), and **P** and **R** are the angular prolongation and restriction operators that operate on the boundary angular flux.

$$\mathbf{z} = \mathbf{Wy} = \left(\mathbf{I} - \mathbf{PE}_{\beta,lo}\mathbf{V}_{\beta,lo}\mathbf{R}\right)^{-1}\mathbf{y} \tag{4}$$

$$\mathbf{V}_{\beta,lo} = \begin{bmatrix} (1-\beta)\mathbf{S} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{lo} \end{bmatrix} \tag{5}$$

To solve the preconditioned vector **z**, it is desirable not to prolongate and restrict inside every inner iteration,. Therefore, an alternate solution method is used (Eq. 6-8).

$$\tilde{\mathbf{y}} = \mathbf{Ry}, \qquad \tilde{\mathbf{z}}^{(0)} = \mathbf{0} \tag{6}$$

$$\tilde{\mathbf{z}}^{(m+1)} = \mathbf{E}_{\beta,lo}\mathbf{V}_{\beta,lo}\tilde{\mathbf{z}}^{(m)} + \tilde{\mathbf{y}} \tag{7}$$

$$\mathbf{z} = \mathbf{P}\left(\tilde{\mathbf{z}}^{(converged)} - \tilde{\mathbf{y}}\right) + \mathbf{y} \tag{8}$$

The use of GMRES to solve the inner iteration (Eq. 1) imposes limits on the use of the β-TSA preconditioner. If the TSA iteration (Eq.7) is also solved with GMRES, it

must be converged to a tighter tolerance than that of the inner iterations in order to function correctly [5]. If the β-TSA preconditioner uses SI, it must be iterated a set number of times in order to be a linear operator.

The use of a low-order quadrature set with boundary conditions requires angular restriction and prolongation operators [6]. For the product quadrature set, which is used in problems with mirror boundaries in a hexagonal geometry, each octant is collapsed into three ordinates. The level-symmetric quadrature set uses S_2 as its low-order quadrature set.

One definition of the angular restriction **R** may preserve the zeroth angular moment, the scalar flux (Eq. 9). An alternate definition preserves the first angular moment; that is, the partial current with respect to the outward normal of each boundary face (Eq. 10). Note that this definition requires that no surface normal can be parallel to any low-order ordinate direction. In Eqs. 9 and 10, *m* is each high-order ordinate, inside each section *s*, which is collapsed to ordinate *n* for each boundary face *i*.

$$\psi_{i,n} = \frac{\sum_{m \in s} w_m \psi_{i,m}}{w_n} \tag{9}$$

$$\psi_{i,n} = \frac{\sum_{m \in s} w_m \left(\vec{n}_i \bullet \vec{\Omega}_m\right) \psi_{i,m}}{w_n \left(\vec{n}_i \bullet \vec{\Omega}_n\right)} \tag{10}$$

The prolongation operator **P** similarly preserves the zeroth or first moment by giving each high-order ordinate an equal share of the scalar flux or partial current.

Test Problems

Two simplified problems were chosen to test the implementation of β-TSA. A product quadrature set with a multiple of three azimuthal directions is chosen with an LMFBR pin's hexagonal geometry, and a level-symmetric quadrature set is used with a PWR pin's square geometry. The LMFBR and PWR meshes contain 1583 and 1420 tetrahedra, respectively (Fig. 1). SCALE 5.1 [7] is used to generate 44-group cross sections, and the group with the highest self-scattering ratio is extracted to provide the basis for the one-group test problem (Table I).

A Perl script is used to run NEWTRNX and process the many permutations of parameters needed to optimize and generate data for the test problems.

RESULTS

The choice of prolongation and restriction method had little effect on the solution or convergence rate. Because the literature [6] suggests that conserving partial currents is the more correct method, that option was chosen for all further tests.

Testing of the scattering parameter β on a variety of cases showed little effect on the overall computational

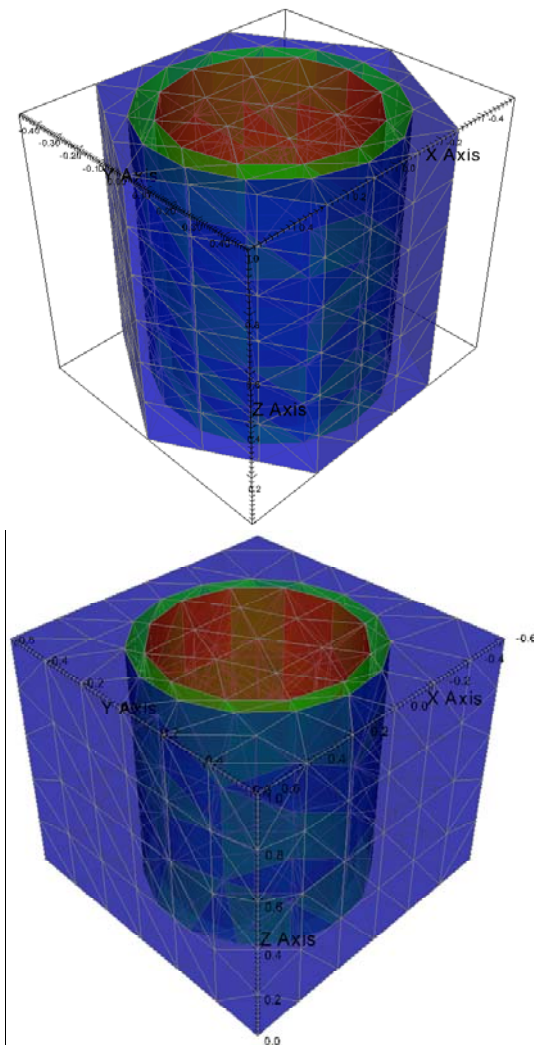

Fig. 1. LMFBR (top) and PWR (bottom) test geometries. The red region is fuel; the green, cladding; and the blue, coolant. Each problem geometry is 1.0 cm tall with fully reflecting boundary conditions.

TABLE I. Cross sections used in the PWR and LMFBR test problems (cm^{-1}).

Problem	*Material*	Σ_t	Σ_s	$\nu\Sigma_f$
LMFBR	*Fuel*	5.64E-01	4.56E-01	1.31E-01
	Cladding	5.98E-01	5.93E-01	0.00E+00
	Coolant	7.12E-02	3.35E-04	0.00E+00
PWR	*Fuel*	4.36E-01	4.15E-01	2.00E-03
	Cladding	3.82E-01	3.78E-01	0.00E+00
	Coolant	5.35E-01	2.91E-01	0.00E+00

time. The typical value of 0.3 was used.

The number of inner iterations was varied from 5 to 50 on the PWR problem using the S_{12} quadrature set. It had little effect when GMRES was used to solve the inner iterations, since GMRES converged very quickly. When using source iterations, however, 20 was close to the

TABLE II. Computational time (in seconds) required for solution of test problems. The product quadrature set for the LMFBR is written as (number of azimuthal directions)x(number of polar directions). Bold entries indicate an improvement relative to the unaccelerated method.

Outer Method	*Inner Method*	**LMFBR**						**PWR**			
		6x3	6x6	12x3	12x6	18x3	18x6	S_4	S_8	S_{12}	S_{16}
SI	----	426.81	849.88	881.09	1740.53	1313.07	2663.83	5.28	17.59	36.71	62.58
SI	*SI*	678.63	959.29	1020.13	2048.84	1356.25	**2346.6**	11.54	**15.45**	**30.08**	**50.33**
SI	*GMRES*	595.99	913.69	943.32	1791.38	1564.13	**2483.7**	9.1	19.24	**27.02**	**48.38**
GMRES	----	37.19	53.12	47.78	109.9	78.75	172.9	2.04	8.2	18.33	31.38
GMRES	*SI*	73.37	149.73	140.64	242.54	221.75	311.76	15.47	21.17	33.79	50.31
GMRES	*GMRES*	49.08	102.23	97.55	196.27	166.69	257.91	7.72	15.14	24.09	40.9

optimal value.

These optimized parameters were used in the execution of the problem set (Table II). TSA accelerated the higher-order sets modestly when SI was used to solve the outer iterations. However, in all other cases, TSA caused the solution time to increase relative to the unaccelerated method.

CONCLUSIONS AND FUTURE WORK

The overhead required to use TSA makes the acceleration method inefficient for quadrature sets smaller than S_8 when SI is used to solve the outer iterations. It is expected that similar inefficiency may occur with a product quadrature set with a small number of high-order ordinates. However, the use of TSA with GMRES solving the outer iterations requires more computational time. In fact, using GMRES alone to solve the problem is more computationally efficient than any application of TSA.

Overall, the TSA implementation when applied to the test problems performs poorly. This is likely caused by the opposing reflecting boundaries on a highly scattering, optically thin medium. In order to more accurately simulate a single partition, the test problem should be reformulated to be a section of a fuel assembly with vacuum boundaries.

ACKNOWLEDGEMENTS

Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

REFERENCES

1. K. T. CLARNO, V. F. DE ALMEIDA, E. D'AZEVEDO et. al., "GNES-R: Global Nuclear Energy Simulator for Reactors Task 1 - High-Fidelity Neutron Transport," PHYSOR-2006, American Nuclear Society's Topical Meeting on Reactor Physics, September 10–14, Vancouver, B.C. Canada (2006).
2. J.S. WARSA, K.G. THOMPSON, J.E. MOREL, et al., "Preconditioning a Parallel, Inexact Block-Jacobi Splitting of the SN Algorithm," Proceedings of the International Topical Meeting on Mathematics and Computation, Super Computing, Reactor Physics, and Nuclear Biological Applications, 2005 September 12-15, Avignon, France.
3. Y. SAAD and M. H. SCHULTZ, "GMRES: A Generalized Minimal Residual Algorithm for Solving Nonsymmetric Linear Systems," *SIAM J. Sci. Stat. Comput*., **7**, 856 (1986).
4. M. L. ADAMS and E. W. LARSEN, "Fast Iterative Methods for Discrete-Ordinates Particle Transport Calculations," Prog. Nucl. Energy, 40, 3 (2002).
5. A. BOURAS and V. FRAYSSÉ, "A Relaxation Strategy for Inexact Matrix-Vector Products for Krylov Methods," CERFACS TR0PA000015, European Centre for Research and Advanced Training in Scientific Computation (2000).
6. M. R. ZIKA and M. L. ADAMS, "Transport Synthetic Acceleration for Long-Characteristics Assembly-Level Transport Problems," *Nucl. Sci. Eng.* **134**, 135 (2000).
7. *SCALE: A Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluations*, ORNL/TM-2005/39, Version 5.1, Vols. I–III, Oak Ridge National Laboratory, Oak Ridge, Tennessee, November 2006. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-732.