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Original Article

# Multilevel acceleration of scattering-source iterations with application to electron transport

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ABSTRACT

Acceleration/preconditioning strategies available in the SCEPTRE radiation transport code are described. A flexible transport synthetic acceleration (TSA) algorithm that uses a low-order discrete-ordinates ($S_N$) or spherical-harmonics ($P_N$) solve to accelerate convergence of a high-order $S_N$ source-iteration (SI) solve is described. Convergence of the low-order solves can be further accelerated by applying off-the-shelf incomplete-factorization or algebraic-multigrid methods. Also available is an algorithm that uses a generalized minimum residual (GMRES) iterative method rather than SI for convergence, using a parallel sweep-based solver to build up a Krylov subspace. TSA has been applied as a preconditioner to accelerate the convergence of the GMRES iterations. The methods are applied to several problems involving electron transport and problems with artificial cross sections with large scattering ratios. These methods were compared and evaluated by considering material discontinuities and scattering anisotropy. Observed accelerations obtained are highly problem dependent, but speedup factors around 10 have been observed in typical applications.



## 1. Introduction

Electron transport is characterized by a large number of collisions before removal from the scattering source, which makes the source iterations (SIs) in a sweep-based solution method slowly convergent. The SCEPTRE radiation transport code [1] has several alternative solvers that do converge rapidly for electron transport in many circumstances. In these alternative solvers, a discretized linear system is constructed involving both the spatial and angular variables, including the scattering source, which is then solved in parallel with Krylov iterative methods. In SCEPTRE, the space/angle linear system is solved by making use of capabilities contained in the Trilinos project [2], which includes iterative solvers and preconditioners developed for the efficient parallel solution of discretized linear systems for large-scale, scientific applications. Convergence of the Krylov methods depends on the condition number of the system matrix and the clustering of the eigenvalues, rather than on the scattering ratio, so that rapid convergence may be obtained even when highly scattering media are present in the problem. A main drawback of these methods is that they can be memory intensive.

In this work, a method is described that combines the two solution approaches, using a coarse-level (low-order-in-angle) space/angle solve to accelerate a fine-level (high-$S_N$-order) SI solve. Preferably, a method is used for the coarse-level solve that converges rapidly for problems containing highly scattering media and that effectively speeds up convergence of the SI of the fine-level problem. If Trilinos tools are used for the coarse-level solves, it is possible to attain further acceleration by applying off-the-shelf incomplete-factorization (IF) [3] or algebraic multigrid (AMG) [4] algorithms. This work is basically generalized transport synthetic acceleration (TSA) [5] with great flexibility in performing the coarse-level solves.

In addition, capability has been added to SCEPTRE by applying a generalized minimum residual (GMRES) algorithm for convergence as an alternative to SI. Krylov iterative methods have been effectively applied to radiation transport problems for some time [6–9]. In this approach, sweep solves are used to build up a Krylov subspace that is used to minimize a residual and converge to a solution. This method is shown to be effective for electron transport and other applications with large scattering ratios. TSA has been applied as a preconditioner to accelerate the convergence of the GMRES iterations. The GMRES algorithm implemented in SCEPTRE will be described in the following section.

The next section will provide more details about the TSA methods, and then results will be provided for modeling electron

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transport in a twisted-pair electrical cable, and a three-material-block cylinder with various combinations of uniform and nonuniform cross sections. Observed accelerations obtained are highly problem dependent, but speedup factors around 10 have been observed in typical applications.

## 2. Background

Acceleration methods such as diffusion synthetic acceleration (DSA) and TSA have been very effective at reducing the number of iterations and/or solve time for a wide range of applications [10–13]. However, partially consistent DSA may perform poorly for certain applications, and fully consistent DSA and TSA may effectively reduce the iteration count, while shifting much of the work to the coarse-level solves. The effectiveness of acceleration methods tends to be very problem dependent. In general, for problems with highly scattering regions, some type of acceleration is effective, but practical problems often have highly scattering regions and streaming regions, so some flexibility is desired in applying a preconditioner.

The SCEPTRE radiation transport code has a unique ability of allowing for any number of different types of solvers to be defined within a single transport calculation [1]. The primary application of SCEPTRE is coupled photon/electron transport, so this flexibility was needed because the convergence properties for problems involving neutral particles are so different from those involving charged particles, and even among different energy groups, convergence behavior may be quite variable. As noted previously, SCEPTRE includes a sweep-based SI solver as well as a number of solvers that use a Krylov iterative method to solve the space/angle dependence simultaneously.

A wide variety of space/angle solvers are available in SCEPTRE, such as those based on the first-order (FO) form of the transport equation using discontinuous finite elements (DFEs), for both the spherical-harmonics ($P_N$) and discrete ordinates ($S_N$) treatment of the angular variable. A DFE spatial discretization always results in a nonsymmetric positive definite (non-SPD) linear system, so GMRES is used for these solvers. Also available are several solvers that result in a SPD linear system, so that the highly efficient conjugate gradients (CGs) algorithm may be used. These methods include the self-adjoint angular flux (SAAF) method and the least-squares (LSs) method, using continuous finite elements (CFEs), again for both $P_N$ and $S_N$ [14,15]. In particular [14], describes the $P_N$ method applied to the FO transport equation with DFE spatial discretization, which in this work is shown to be one of the most effective TSA methods tested. The use of spatial DFE results in a nonsymmetric linear system, regardless of the form of the transport equation used, so only CFE spatial approximation is available for use with the SAAF and LS solvers.

As noted earlier, due to huge memory requirements, the space/angle solvers are not generally practical except for fairly small problems. However, these methods are very effective as coarse-level accelerators for a SI solver. Because the space/angle linear systems are built using Trilinos [2] data structures, the rich assortment of preconditioners included in the Trilinos project, including AMG and IF, is accessible.

Mapping from the fine-level to coarse-level problem is basically angular multilevel (AML) optionally combined with an algebraic preconditioner, either IF [3] or AMG [4]. AMG is not expected to perform well for hyperbolic problems, as encountered in this work. AMG results are included for completeness, and results confirm the expected poor performance of AMG for this application. For AML, the restriction and prolongation operators involve the moment-to-discrete and discrete-to-moment operators, as will be described in the next section. For AMG, the restriction and interpolation operators and number of levels are handled by the Trilinos/MueLu package, and for IF the preconditioning is handled by the Trilinos/Ifpack2 package. For the SAAF and LS coarse-level solves, which use CFE, the mapping back and forth between the DFE and CFE representations of the spatial dependence is handled by Trilinos/Tpetra tools [2]. In SCEPTRE, the basic representation of the internal angular flux, fixed source, and boundary angular flux is based on a DFE representation in space. In constructing a linear system, a mapping is set up using Trilinos/Tpetra mapping tools to transfer the DFE information to a CFE representation in the FE assembly phase. After obtaining the solution in the CFE space, the resulting angular flux solution is mapped back to a DFE representation using the Import/Export tools in Tpetra.

### 2.1. Description of the TSA algorithm

The mono-energetic transport equation is

$$\boldsymbol{\Omega}\cdot\nabla\psi + \sigma_t\psi(\boldsymbol{r},\boldsymbol{\Omega}) = \int \sigma_s\left(\boldsymbol{\Omega}'\rightarrow\boldsymbol{\Omega}\right)\psi\left(\boldsymbol{r},\boldsymbol{\Omega}'\right)d\boldsymbol{\Omega}' + \mathrm{Q}(\boldsymbol{r},\boldsymbol{\Omega}) \tag{1}$$

with an imposed surface-source boundary condition

$$\psi(\boldsymbol{r},\boldsymbol{\Omega}) = \psi_b(\boldsymbol{r},\boldsymbol{\Omega}),\ \boldsymbol{r}\in\Gamma,\ \boldsymbol{\Omega}\cdot\boldsymbol{n}<0 \tag{2}$$

where $\boldsymbol{r}$ is the spatial position, $\boldsymbol{\Omega}$ is the particle direction of motion, $\sigma_t$ is the total cross section, $\sigma_s$ is the scattering cross section, $\psi$ is the angular flux, and Q is a known distributed fixed source. $\Gamma$ is the external spatial boundary and $\boldsymbol{n}$ is the unit outward normal on $\Gamma$. $\psi_b$ is the imposed surface boundary condition for incoming directions.

Defining the transport operator $\mathcal{T}$ as

$$\mathcal{T}\circ\ = \boldsymbol{\Omega}\cdot\nabla\circ + \sigma_t\circ \tag{3}$$

and the scattering operator $\mathcal{S}$ as

$$\mathcal{S}\circ\ = \int \sigma_s\left(\boldsymbol{\Omega}'\rightarrow\boldsymbol{\Omega}\right)\circ\, d\boldsymbol{\Omega}' \tag{4}$$

the transport equation can be written compactly as

$$\mathcal{T}\psi(\boldsymbol{r},\boldsymbol{\Omega}) = \mathcal{S}\psi(\boldsymbol{r},\boldsymbol{\Omega}) + \mathrm{Q}(\boldsymbol{r},\boldsymbol{\Omega}) \tag{5}$$

The transport equation can be solved by SI

$$\mathcal{T}\psi^{(k+1)} = \mathcal{S}\psi^{(k)} + \mathrm{Q} \tag{6}$$

where $\psi^{(k)}$ is the known $k$th iterate of the angular flux, and $\psi^{(k+1)}$ is the computed $(k+1)^{\mathrm{st}}$ iterate, with the iterations continuing until convergence. With an $S_N$ discretization in angle and a DFE discretization in space, the $(k+1)^{\mathrm{st}}$ iterate of the angular flux is obtained by an efficient sweeping algorithm.

In the TSA algorithm, the $(k+1)^{\mathrm{st}}$ iterate of the angular flux is obtained by a two-step process: (1) a sweep solve, and (2) computation and application of a correction term. Reindexing the result of a sweep solve as the $(k+½)^{\mathrm{th}}$ iteration

$$\mathcal{T}\psi^{\left(k+\frac{1}{2}\right)} = \mathcal{S}\psi^{(k)} + \mathrm{Q} \tag{7}$$

the goal is to determine a correction to the $(k+½)^{\mathrm{th}}$ iterate of the solution to accelerate convergence. The residual at the $(k+½)^{\mathrm{th}}$ iteration is

$$r^{\left(k+\frac{1}{2}\right)} = \mathrm{Q} - (\mathcal{T}-\mathcal{S})\psi^{\left(k+\frac{1}{2}\right)} \tag{8}$$