Denovo-A New Parallel Discrete Transport Code for Radiation Shielding Applications

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INTRODUCTION

We have developed a new, three-dimensional, discrete ordinates (S_N) radiation transport code named Denovo for radiation shielding applications and analysis. Denovo was designed for two primary purposes:

1. to serve as the deterministic solver module in the SCALE MAVRIC sequence, and
2. to replace TORT as the principal three-dimensional (3D) deterministic transport code for nuclear technology applications at Oak Ridge National Laboratory (ORNL).

The code features multiple spatial differencing schemes, state-of-the-art linear solvers, and a modern, novel code framework that supports straightforward integration of new features. Denovo uses the Koch-Baker-Alcouffe (KBA) [1] parallel-wavefront sweeping algorithm. It also features a new multilevel energy decomposition for massive k-eigenvalue calculations.

As opposed to traditional S_N codes that use source iteration, Denovo uses nonstationary Krylov methods to solve the within-group equations. Krylov methods are far more efficient than stationary schemes. Additionally, classic acceleration schemes (Diffusion Synthetic Acceleration) do not suffer stability problems when used as a preconditioner to a Krylov solver [2]. Users have the option of running traditional source iteration instead of Krylov iteration. Multigroup upscatter problems can be solved using Gauss-Seidel iteration with transport, two-grid acceleration. A parallel first-collision source is also available. Denovo has been verified against a number of problems, including several from the Kobayashi benchmark set.

The features of Denovo are summarized in the following list:

1. 3D, Cartesian orthogonal structured (nonuniform) grids
2. fixed source and eigenvalue problems
3. domain decomposition (DD) parallelism using the Koch-Baker-Alcouffe (KBA) sweep algorithm
4. Krylov and source-iteration within-group solvers;
5. multigroup with optional thermal upscattering
6. Diffusion Synthetic Acceleration (DSA) preconditioning of within-group solves and transport two-grid acceleration of Gauss-Seidel iteration for upscatter groups
7. forward and adjoint modes
8. multiple spatial differencing schemes: diamond difference, diamond difference with linear-zero flux fixup, theta-weighted diamond difference, step characteristics (slice balance), linear-discontinuous finite element, trilinear-discontinuous finite element
9. reflecting, vacuum, and surface source boundary conditions
10. first collision and distributed external fixed sources
11. multiple input front-ends, including Python bindings
12. support for multiple outputs, including HDF5.

In this paper we will highlight specific, novel features of the Denovo code.

COMPUTATIONAL METHODS AND RESULTS

Denovo solves the multigroup S_N equation that can be written in operator form as

$$\mathbf{L}\psi = \mathbf{MS}\phi + q \,, \tag{1}$$

where ψ are the discrete angular fluxes and ϕ are moments of the angular flux. Operating on Eq. (1) with $\mathbf{DL}^{-1}$ and using $\phi = \mathbf{D}\psi$, we get

$$(\mathbf{I} - \mathbf{DL}^{-1}\mathbf{MS})\phi = \mathbf{DL}^{-1}q \,. \tag{2}$$

Writing Eq. (1) in this form makes it amenable to solution by Krylov iteration, in which only the matrix-vector products need to be specified. In the S_N method the matrix-vector multiply operations are transport sweeps. Krylov iterative methods are very efficient when applied to the S_N transport equation (even without preconditioning) as shown in Fig. 1. Furthermore, Krylov methods provide a uniformly stable platform for DSA preconditioning and have a very small per iteration performance overhead.

For multigroup S_N problems with thermal neutron upscatter or photoneutron physics, Denovo provides a new, transport two-grid (TTG) acceleration method that is highly efficient and uniformly stable [3]. Table 1 shows results using the TTG method in a neutron well-logging problem. The TTG method gives performance increases of greater

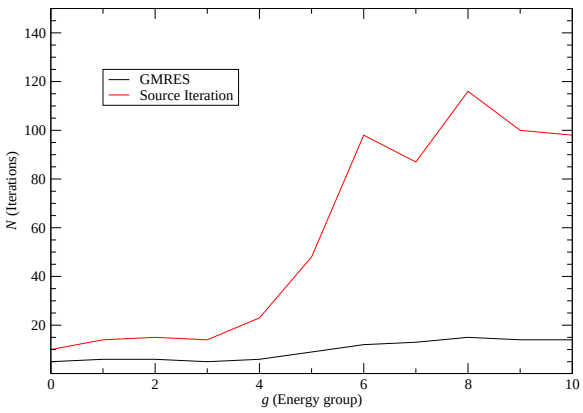

Figure 1: Unpreconditioned Krylov iteration versus source iteration in a multigroup S_N problem.

Table 1: Comparison of traditional Gauss-Seidel (GS) and TTG for a neutron well-logging problem.. All timing results are normalized to the unaccelerated Gauss-Seidel (GS) iteration time.

Method	Acc. S_N order	GS iterations	Time
GS	-	175	1.0
TTG	8	15	0.113
TTG	4	14	0.097
TTG	2	13	0.086

than 10 in runtime for this class of problems. In problems with graphite or heavy water, the improvements can be greater than 500.

As seen in Eq. (2) each Krylov matrix-vector multiply requires a transport sweep. Denovo uses the KBA algorithm to decompose the space-angle sweeps. Additionally, Denovo has efficient parallel input/output algorithms that allow the setup, initialization, and output of the massive data sets required by large problems. Denovo is used extensively on the National Center for Computational Sciences (NCCS) Cray XT5 supercomputer (Jaguar). The direct inversion of **L** by KBA allows for good weak-scaling on Jaguar as shown in Fig. 2. Furthermore, Denovo has demonstrated the ability to run massive problems in reasonable runtimes as shown in Table 2. This problem featured a full PWR modeled at 10 cm spatial resolution. The mesh for this problem contained greater than one billion zones. Nonetheless, Denovo was able to generate a solution on Jaguar in just over one hour of runtime.

CONCLUSIONS

Denovo is a new S_N code that has been used to perform shielding analysis on a wide variety of problems.

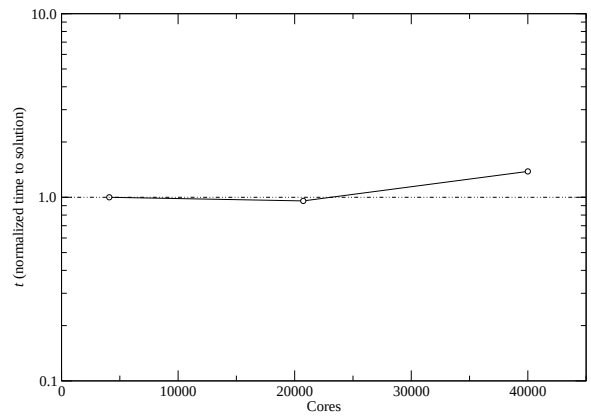

Figure 2: Weak-scaling of Denovo on the Jaguar XT5 at NCCS.

Table 2: Problem sizes for a PWR full-facility shielding analysis using Denovo. Both calculations used S_{24}/P_3 and 27 energy groups.

Zones	State (GB)	Cores	Runtime (min)
103.7M	333.8	4,096	47
1,047M	3,372.8	40,000	79

Denovo uses state-of-the-art Krylov solvers that provide excellent performance and robustness. Denovo's parallel KBA implementation and solvers have demonstrated excellent weak-scaling up to 20,000 cores and good scaling up to 40,000 cores on the JAGUAR XT5 supercomputer. These features of Denovo enable deterministic shielding analysis of three-dimensional problems at a previously unattainable resolution.

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