Deterministic Transport Capability for HEU Sources in Cargo Containers

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Background

In a closed Senate hearing room sometime in the year after the bomb was tested, a senator asked Robert Oppenheimer, "What instrument would you use to detect an atomic bomb hidden somewhere in the city?" Oppenheimer quipped, "A screwdriver. To open each and every crate or suitcase."

The signature of highly-enriched uranium is very minute. Shipping ports undergo thousands of false alarms every day ranging from ceramics to cathode-ray televisions to kitty litter. Current detector models are excellent for detecting dirty-bomb sources such as cesium-137 but struggle with the weak radiation footprint of highly-enriched uranium. To provide the most accurate and detailed data for detecting weapons-grade uranium we have developed a deterministic transport capability based on the discrete ordinates (S_n)method.

Our Code

Parallel Deterministic Transport (PDT) is a massively parallel deterministic transport code which can handle large number angular discretizations, perform uncollided flux calculations, and custom-refine energy groups.

Problems with S_n

The Monte Carlo Method (MCM) is the principle method for accurate computation. However, the MCM is computationally costly and slow to converge, on the order of $N^{-1/2}$, where N is the number of particles. The discrete-ordinates method is more efficient but with a trade-off in accuracy for small quadrature sets. To improve angular accuracy, we have used a recently developed quadrature technique (LDFE) to allow for very large numbers of angles to be simulated (at present, we have performed calculations with over 32,000 angles).

Description of Quadrature

- LDFE: Every triangle has 4 data points - a center point and a point between each vertex and the center point.
  - Starting with octants, every triangle is locally re-finable into 4 subsequent triangles
- Level Symmetric: number of points per octant is n(n+2)/8
  - All points are arranged with n/2 different levels and [n/2 - i + 1] points on the ith level.

Uncollided Flux Treatment

- The discrete ordinates solution for problems with large streaming gaps can be greatly improved by exactly tracking particles from the source to their first collision.
  - This is known as an uncollided flux treatment
- Uncollided flux treatment can be expensive because a straight forward implementation requires O(N^2) work for N sources.
  - Also, load balancing can be an issue when the source is localized
- We have developed and implemented a method to track uncollided particles across domain decomposed meshes that scales to a large number of processors

Energy Group Manipulation

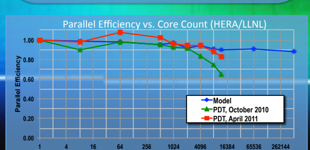
- PDT has the ability to custom-refine the energy group boundaries around spectral lines of interest. Using cross-section libraries from SCALE, such as a combined 200 neutron group/47 gamma group library or a single 238 neutron group library, there are two options for manipulating group bounds:
  - SPLIT : Insert a group boundary. If available, appropriate weights are collected for splitting quantities. These quantities are integrated over groups and the actual weight function data is split.
  - COMBINE : Two separate groups are combined into a single group. A weighted average is used for new cross-section values.

Performance/Scaling

- PDT Solves the time-dependent/steady-state neutral particle Boltzmann transport equation in three dimensions on general polyhedral meshes using multiple time discretizations, the Sn angular discretization, the multigroup energy discretization, and a piecewise-linear-discontinuous Galerkin spatial discretization.
- It also solves time-dependent thermal radiative transfer problems.
- PDT utilizes the Standard Template Adaptive Parallel Library (STAPL) - developed at TAMU.
  - STAPL provides parallel data structures and offers various services and capabilities utilizing upon both MPI and threading.
- We are now running on Blue Gene/L and run on 32,000 processors.
- We believe our current algorithm can get us out to about 250,000 processors with about 80% efficiency using a simple partition.

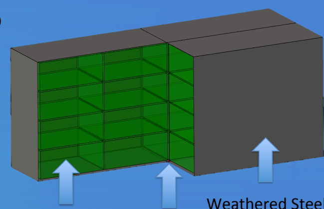
Parallel Efficiency

- We have developed a parallel efficiency model for any such partitioning that assumes optimal parallel scheduling and include a simple communications model (latency and bandwidth parameters)
- Performance tracks model reasonably well
- On BG/L, we can easily run on 32,768 processors, but are constrained by the amount of available memory per processor. We are actively addressing this memory limitation.

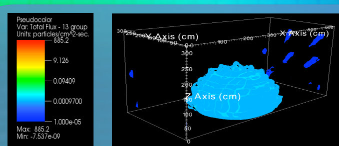


Problem Description

- Cargo container of dimensions 20 ft. x 8 ft. by 8.5 ft.
- 32 total boxes: 4 boxes across in the 20 ft. [X] dimension, 4 boxes stacked in the 8.5 ft. [Z] dimension, 2 boxes deep in the 8 ft. [Z] dimension.
- Containment material is 3 mm thick weathered steel.
- 3 cm air gaps on every side of 32 interior compartments.
- Boxes filled with a variety of contents, for example, balsa wood.
- HEU source (70% U-235, 18.95 g/cm3) is not encapsulated and located at the bottom of the cargo container in the center filling a 3 cm x 3 cm x 3cm area.
- An extra 2 ft. of air was added to the positive X, positive Y, positive Z directions for detector modeling.
- The energy group structure has been modified to fit +/-5 eV of five spectral lines of interest:
  - 1.001 MeV (U-238)
  - 786.3 keV (U-238)
  - 766.4 keV (U-238)
  - 742.8 keV (U-238)
  - 186 keV (U-235)

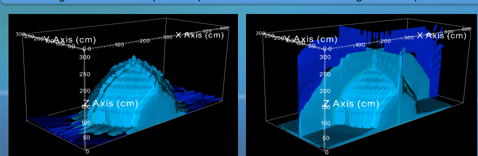


Results

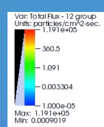


Isosurface representation of Level Symmetric Level 10 Cargo Container filled with balsa wood

Isosurface Comparison of LDFE Level 3 (Left) and Level 4 (Right) - Cargo Container filled with balsa wood
Higher order LDFE computations produce more accurate results along streamline paths



Cargo container filled with balsa wood (LDFE - 32768 angles)



Empty cargo container (LDFE - 2048 angles) Blue spots are indicative of too few angles