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 bands were 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 suitcase.” The signature of highly-enriched uranium is very minute. Scoping parts undergo thousands of false alarms every day ranging from ceramics to carbon-ray televisions to kiddie litter. Count 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 capture off-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^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 calculated (at present, we have performed calculations with over 32,768 angles).

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.
  o This is known as an uncollided flux treatment.
  o Uncollided flux treatment can be expensive because a straightforward implementation requires O(N^2) work for N sources.
  o 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 construct the energy group boundaries around spectral lines of interest. Using cross sections libraries from SCALE, such as a combined 2460 neutron reaction library, or a single 288 section group library, there are two options for manipulating group broads:
  o 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.
  o COMBINE - Two separate groups are combined into a single group. A weighted average is used for new cross-section values.

Performance/Scalability
• PDT solves the three-dimensional steady-state neutral particle Boltzmann transport equation in three dimensions on general polyedral meshes using multiple time discretizations, the Sn angular discretization, the multipole 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.
  o STAPL provides parallel data structures and offers various services and capabilities that allow users both MPI and threading.
• We are now running on杉杉 Gene and run on 64,384 processors.
• We believe our current algorithm can get us to about 130,000 processors with about 85% efficiency using a single partition.

Parallel Efficiency
• We have developed a parallel efficiency model for any such partitioning that ensures optimal parallel scheduling and isolate a communicaions model (Qthreads and breakdowns parameters).
• Performance models work reasonably well.
• On STAPL, we can scale out on 448 processors, but not 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 6.5 ft.
• 32 total boxes: 4 boxes across in the 20 ft. (4) dimension, 4 boxes stacked in the 8.5 ft. (2) dimension, 3 boxes deep in the 8.2 ft. (2) dimension.
• Containment material is 3 mm thick weathered steel.
• 2 cm air gaps on every side of 12 interior compartments.
• Boxes filled with a variety of contents, for example, balsa wood.
• HEU source (76% U-235, 18.95 g/cm3) is not encapsulated and located at the bottom of the cargo container in the center filling a 2 cm x 2 cm x 2 cm 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 N +5/6 of five spectral lines of interest:
  o 1.05 MeV (U-238)
  o 766.4 keV (U-238)
  o 766.4 keV (U-238)
  o 762.8 keV (U-238)
  o 586 keV (U-235)

Results
•貨物容器内にディレイドフロント（LDFE）レベル3（左）とレベル4（右）: 貨物容器にバラスウッドで作られた高濃度ウランソースの比較。LDFE計算はより正確な結果を生成する沿線の分化パスを示しています。
• Cargo container filled with balsa wood (LDFE - 32,768 angles).
• Cargo container filled with balsa wood (LDFE - 2048 angles).
• 含まれる箱は、さまざまなオプションで構成され、検出器の性能を向上させることが可能です。
• サースの周囲は、3 mm厚のコンクリートで構成されます。
• 所定の配置が必要である場合、サンプリングが適切に行われます。
• 目標は、特定の方向へのraysを追跡し、最初の干渉点までを正確に計算することです。