$S_N$ on Unstructured Meshes

using the

Slice Balance Approach (SBA)

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SBA (Slice Balance Approach) Introduction

- What’s a Slice Balance Approach?
  - Discrete ordinates ($S_N$) deterministic transport method
  - General geometry description of problem
  - Arbitrary polyhedral (polygonal) mesh
  - Angle-dependent, characteristic-based spatial decomposition of mesh cells
  - Multiple balance mathematical framework
  - Coefficient-based solution framework; multiple solution schemes
  - Face-based (or traditional cell-based) mesh sweep ordering

- Goal
  Provide accurate, efficient, flexible, and full-featured 3D general-geometry deterministic transport capability to complement Monte Carlo capability for large, geometrically-complex, neutral-particle transport problems

- Motivation
  Solve larger, more complicated problems, in less time, with fewer engineering and computing resources
## Background

<table>
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<tr>
<th>Author(s)</th>
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<td>Morel &amp; Larsen [1990]</td>
<td>Multiple Balance Approach</td>
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<td>Azmy [1992]</td>
<td>Arbitrarily High Order Transport - Characteristic</td>
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also, in 1996, Adams pointed out
Voronkov & Sychugova [1993] CDS\textsubscript{N} Methods

Primary reference:
SBA Transport Solution

Discretize the transport problem
- Angle (discrete ordinates)
- Energy (multi-group, ultra-fine-group, etc.)
- Space (characteristic-based decomposition)

Solve the discretized transport problem
- Standard source iteration
- **Mathematical approach (multiple balance):**
  - exact spatial moments on *whole cells*
  - exact spatial moments on *slices*
  - approximations on *slices*
- Cast solution schemes in coefficient-based framework
- Sweep the *polyhedral mesh* (face-based sweep)

The crux is the “inner iteration” mesh sweep. This will set the computational efficiency.
The Slice Balance Approach

- an approach for $S_N$ transport on arbitrary meshes
- in the context of an $S_N$ inner iteration
- angle-dependent subdivision of 3D polyhedra (polygons in 2D) into slices:

  * This is a “natural” spatial decomposition; the exact $S_N$ transport solution with smooth sources and boundary conditions contains this subdivision.
  * SBA decomposes a complex problem into a sum of simple “slab-like” problems.
  * SBA provides a clear path for extending $S_N$ spatial differencing schemes to arbitrarily complex two- and three-dimensional geometries.
SBA Mathematical Framework

... remains unchanged in 1D, 2D, and 3D

1D slab problem

\[ \Omega \rightarrow s \rightarrow u \]

2D polygonal mesh decomposes into a sum of “slab-like” problems

\[ \Omega \rightarrow s(u) \rightarrow u \rightarrow v \]

3D polyhedral mesh decomposes into a sum of “slab-like” problems

\[ \Omega \rightarrow s(u,v) \rightarrow u \rightarrow v \rightarrow w \]
Consider an arbitrary uniform material region, $V_I$, bounded by the surface $\partial I$.

We write the transport equation for neutral particles at the point $r$ within $V_I$, within a given energy group, traveling in the direction $\Omega$:

$$\Omega \cdot \nabla \psi(r, \Omega) + \sigma_t(r, \Omega)\psi(r, \Omega) = Q(r, \Omega), \quad r \in V_I,$$

$$\psi(r', \Omega) = \psi_b(r', \Omega), \quad r' \in \partial I, \quad n(r', \Omega) \cdot \Omega < 0,$$

where:
- $\psi(r, \Omega)$ is the angular flux,
- $Q(r, \Omega)$ is the angular source,
- $\sigma_t$ is the total macroscopic cross section,
- $\psi_b(r', \Omega)$ is a prescribed angular flux incident on the surface $\partial I$,
- $n(r', \Omega)$ is the outward directed unit normal of the surface.
SBA Mathematical Framework

... characteristic-based, multiple balance approach

Cell Balance Equation (exact)

\[ \sum_i A_i \psi_i + \sum_j A_j \psi_j + \sigma_{tl} V_i \psi_i = V_i Q_i. \]

Slice Balance Equation (exact)

\[ A_{\text{in},ij} \psi_{\text{in},ij} + A_{\text{out},ij} \psi_{\text{out},ij} + \sigma_{tl} V_{1,ij} \psi_{1,ij} = V_{1,ij} Q_{1,ij}. \]

Other relations (exact)

\[ A_j \psi_j = \sum_{i \neq j} A_{\text{out},ij} \psi_{\text{out},ij} \]

Auxiliary Equations (approximate)

\[ A_{\text{out},ij} \psi_{\text{out},ij} = \begin{cases} \text{step} \\ \text{step characteristic} \\ \text{linear (diamond - difference - like)} \\ \text{linear characteristic} \\ \text{etc.} \end{cases} \]
**SBA Inner Iteration Solution Framework**

\[ A_j \psi_j = \sum_{i*} A_{ij} \psi_i K_{i \rightarrow j} + A_j Q_1 K_{I \rightarrow j}, \]

Face angular fluxes for each discrete direction are computed in the inner iteration.

Two contribution types: incoming face \( \rightarrow \) outgoing face \((i \rightarrow j)\)

\[ \text{cell} \rightarrow \text{outgoing face } (I \rightarrow j) \]

**Properties of the solution framework:**

- Superposition of slab-like solutions; same in 1D/2D/3D; many schemes
- Only the \((i \rightarrow j)\) contributions require a sweep order
- Can use cell-based, face-based, structured, or unstructured sweeps

**Properties of the coefficients:**

- Coefficients & sweep order isolate problem geometry & solution
- Decomposition (into slices) gives coefficient & sweep order info
- Coefficients can be precomputed (before the mesh sweep)
- Cells with same shape & material have same coefficients

The properties of the framework & coefficients provide flexibility that should lead to efficient algorithms.
SBA Solution Schemes

\[ A_j \psi_j = \sum_{i^* j} A_{ij} \psi_i K_{i \rightarrow j} + A_j Q_1 K_{l \rightarrow j} , \]

SC (Step-characteristic):

\[ A_{ij} K_{i \rightarrow j}^{SC} = \frac{1}{\sigma_t \Delta b_{ij}} \sum_{p=1}^{n} e^{-\sigma_t \Delta w_{ij,p}} \left[ \frac{\Delta V_p}{\Delta t_p} - \frac{\Delta V_{p+1}}{\Delta t_{p+1}} \right] \]

\[ A_j K_{i \rightarrow j}^{SC} = \frac{1}{\sigma_t} \left[ A_j - \sum_{i^* j} A_{ij} K_{i \rightarrow j}^{SC} \right] , \]

\[ \Delta b_{ij} = -\left[ (A_{out,ij})_{vw} - (A_{in,ij})_{vw} \right] / A_{ij} . \]

DDL (Diamond-Difference-Like):

\[ A_{ij} K_{i \rightarrow j}^{DDL} = A_{ij} \left( \frac{2 - \alpha_{ij}}{2 + \alpha_{ij}} \right) , \]

\[ A_j K_{i \rightarrow j}^{DDL} = \sum_{i^* j} A_{ij} K_{i \rightarrow j}^{DDL} = \sum_{i^* j} -2 V_{I,ij} / (2 + \alpha_{ij}) , \]

\[ \alpha_{ij} = \sigma_t V_{I,ij} / A_{ij} . \]
Rectangular-Mesh Diamond-Difference

Cell-average $S_4$ Scalar Flux in One Quadrant of System Composed of a Uniform Source (2x2mfp) Centered in a Uniform Shield (12x12mfp) Scattering Ratio, $c=0.5$
Traditional DD vs. SBA-DDL

TWODANT

CENTAUR123 (SBA-DDL)

Cell-average $S_4$ Scalar Flux in One Quadrant of System Composed of a Uniform Source (2x2mfp) Centered in a Uniform Shield (12x12mfp) Scattering Ratio, $c=0.5$
Unstructured Mesh Sweeps

Unstructured Mesh Sweeps:

Cell-based (finite element) vs. Face-based
Unstructured Mesh Sweeps


- Sweep-ordering based on low-complexity list-ordering heuristics
- Observed nearly linear speedups on up to 126 processors

$\Rightarrow$ Step toward efficient parallel $S_N$ unstructured mesh sweeps
- Focused on obtaining good sweep-ordering
- Deferred optimizing spatial decomposition (both needed for best results)

$\Rightarrow$ Casts $S_N$ mesh sweep problem as a scheduling problem
- Scheduling: task distribution + ordering among processors
  (accounting for data dependencies between tasks)
- Dependency graphs depict tasks and dependencies

Dependency graphs provide a clear medium for illustrating the additional flexibility provided by SBA for unstructured mesh sweep algorithms
Unstructured Mesh Sweeps:
Cell-based (Finite-Element) Cell Dependency

(a) Unstructured mesh. (b) Cell-based cell dependency graph for $\Omega$.

Note: This figure is from S. D. Pautz, "An Algorithm for Parallel Sn Sweeps on Unstructured Meshes," Nucl. Sci. Eng., 140, 111 (2002).
Unstructured Mesh Sweeps:
Cell-based (Finite-Element) Face Dependency

(a) Unstructured mesh.

(b) Cell-based face dependency graph for $\Omega$.

Note that with cell-based coupling, within a cell, each "outgoing" face is coupled to all of the "incoming" faces.
Unstructured Mesh Sweeps:
Face-based (SBA) Face Dependency

(a) Unstructured mesh.

(b) Face-based face dependency graph for Ω.

Note that with face-based (or "slice"-based) coupling, an "outgoing" face is coupled only to physically reasonable "incoming" faces.
Unstructured Mesh Sweeps:
SBA Face-based Sweep Removes Cyclic Dependencies

(b) Cell-based face dependency graph for Ω.

(b) Face-based face dependency graph for Ω.

SBA face-based sweep removes cyclic dependencies and reduces complexity
Unstructured Mesh Sweeps:
Cell-based & Face-based Sweeps

SBA face-based sweep removes cyclic dependencies and reduces complexity
**Unstructured Mesh Sweeps:**

**Cyclic Dependencies**

Twisted Ring Mesh 1

- Cell-based sweep:
  - cyclic dependencies
  - break cycle with approx. solution on a face

- Face-based sweep (SBA):
  - no cyclic dependency for SBA
  - slices penetrate the ring

Twisted Ring Mesh 2

- Cell-based sweep (as in Twisted Ring Mesh 1)

- Face-based sweep (SBA):
  - cyclic dependencies
  - slices don’t penetrate the ring
  - break cycle with a new face (penetrate ring) (no approximation!)

**SBA face-based sweep reduces cyclic dependencies; cycles are easily broken without approximation**
Unstructured Mesh Sweeps:
Cell-based vs. Face-based Dependency

Cell-based cell dependency graph

Cell-based face dependency graph

Face-based face dependency graph
Unstructured Mesh Sweeps:
Angle-dependent spatial decomposition

(a) Unstructured mesh.

(b) Face-based face dependency graph for $\Omega$.

SBA permits an angle-dependent spatial decomposition that can completely decouple spatial regions of a mesh.
Summary

- Complex problem ➔ superposition of simple “slab-like” problems
- Clear path to extend $S_N$ spatial schemes to 2D/3D geometries
- Cell-local decomposition permits arbitrary polyhedral (polygonal) cells
- Mathematical framework: characteristic-based, multiple balance approach
- Coefficient-based solution framework remains unchanged in 1D/2D/3D
- Coefficients encapsulate solution scheme differences
- Coefficients & sweep ordering encapsulate cell topological information
- Face-based sweep ordering reduces or removes cyclic dependencies & reduces complexity
- Permits an angle-dependent spatial decomposition that can completely decouple spatial regions of a problem

SBA provides additional flexibility for new 2D/3D unstructured mesh $S_N$ algorithms