Iterative Methods for Parallel Transport

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Outline

- Transport Equation
- Solution Methods
- Parallel Implementations

The transport equation in operator notation leads naturally to "source iteration" and "synthetic acceleration."

$$\left[\vec{\Omega}\bullet\vec{\nabla}+\sigma_t\left(\vec{r},E\right)\right]\psi\left(\vec{r},E,\vec{\Omega}\right)=\int dE'\int d\Omega'\sigma_s\left(\vec{r},E'\rightarrow E,\vec{\Omega}'\bullet\Omega\right)\psi\left(\vec{r},E',\vec{\Omega}'\right)+q_{ext}\left(\vec{r},E,\vec{\Omega}\right)$$

Transport Equation: $L\psi = S\psi + q$

Source Iteration: $L\psi^{(l+1/2)} = S\psi^{(l)} + q$

Converged Solution: $\psi = \psi^{(l+1/2)} + \left(L-S\right)^{-1} S\left(\psi^{(l+1/2)} - \psi^{(l)}\right)$

"Low-order" Operator: $M \approx \left(L-S\right)^{-1}$

"Synthetic" Iteration: $\psi^{(l+1)} = \psi^{(l+1/2)} + MS\left(\psi^{(l+1/2)} - \psi^{(l)}\right)$

Different choices of low-order operator (M) give different synthetic methods.

- Diffusion synthetic acceleration (DSA)
  - Low-order operator is a diffusion approximation.
  - If discretized consistently, unconditionally convergent for all spatial meshes. (spectral radius < 1)
  - Effective for uniform meshes and homogeneous material properties (spectral radius << 1)
  - Efficiency of solving the diffusion approximation is a question.
- Transport synthetic acceleration (TSA)
  - Low-order operator is a simplified transport approximation.
  - Contains adjustable parameters:
    - Parameters determine spectral radius.
    - Parameters determine difficulty of low-order solution.
    - For many neutronics problems, parameters can be found to give effective and efficient scheme for uniform homogeneous problems.
  - Effectiveness degrades for optically thick problems.

TSA uses a simple transport operator to accelerate source iteration.

$$\vec{\Omega}_m \bullet \vec{\nabla} \psi_m^{(l+1/2)}(\vec{r}) + \sigma_t(\vec{r}) \psi_m^{(l+1/2)}(\vec{r}) = \frac{\sigma_s(\vec{r})}{4\pi} \phi^{(l)}(\vec{r}) + \frac{q(\vec{r})}{4\pi}$$

$$\phi^{(l+1/2)}(\vec{r}) = \sum_{m=1}^{M} w_m \psi_m^{(l+1/2)}(\vec{r})$$

$$\vec{\Omega}_n \bullet \vec{\nabla} f_n^{(k+1/2)}(\vec{r}) + \left[\sigma_t(\vec{r}) - \beta \sigma_s(\vec{r})\right] f_n^{(k+1/2)}(\vec{r})$$
$$= \frac{\sigma_s(\vec{r})(1-\beta)}{4\pi} F^{(k)}(\vec{r}) + \frac{\sigma_s(\vec{r})}{4\pi}\left[\phi^{(l+1/2)}(\vec{r}) - \phi^{(l)}(\vec{r})\right],$$

$$F^{(k+1)}(\vec{r}) = \sum_{n=1}^{N} w_n f_n^{(k+1/2)}(\vec{r})$$

$$\phi^{(l+1)}(\vec{r}) = \phi^{(l+1/2)}(\vec{r}) + F^{(k+1/2)}(\vec{r})$$

- Parameters:
  - β
  - N
  - k

If we keep the diffusion length constant between high and low order problems, we have the stretched TSA.

$$\vec{\Omega}_m \bullet \vec{\nabla} \psi_m^{(l+1/2)}(\vec{r}) + \sigma_t(\vec{r}) \psi_m^{(l+1/2)}(\vec{r}) = \frac{\sigma_s(\vec{r})}{4\pi} \phi^{(l)}(\vec{r}) + \frac{q(\vec{r})}{4\pi}$$

$$\phi^{(l+1/2)}(\vec{r}) = \sum_{m=1}^{M} w_m \psi_m^{(l+1/2)}(\vec{r})$$

$$\left(\vec{\Omega}_n \bullet \vec{\nabla}_n\right) f_n^{(k+1/2)} + \frac{\sigma_t}{\varepsilon} f_n^{(k+1/2)} = \frac{\frac{\sigma_t}{\varepsilon} - \varepsilon(\sigma_t - \sigma_s)}{4\pi} F^{(k+1/2)} + \frac{\varepsilon \sigma_s}{4\pi}\left(\phi^{(l+1/2)} - \phi^{(l)}\right)$$

$$F^{(k+1/2)} = \sum_{n=1}^{N} w_n f_n^{(k+1/2)}$$

$$\phi^{(l+1)} = \phi^{(l+1/2)} + F^{(k+1)}$$

To damped the high frequency error modes, filtering steps were introduced.

$$\left(\vec{\Omega}_n \bullet \vec{\nabla}_n\right) f_n + \sigma_t \sqrt{1-c}\, f_n = \frac{\sigma_s}{4\pi\sqrt{1-c}} \left(\phi^{(l+1/2)} - \phi^{(l)}\right)$$

$$F = \sum_{n=1}^{N} w_n f$$

$$\pm\alpha \frac{\partial g_{x,\pm}}{\partial x} + \sigma_t g_{x,\pm} = \frac{\sigma_t}{2} F \qquad G_x = g_{x,+} + g_{x,-}$$

$$\pm\alpha \frac{\partial g_{y,\pm}}{\partial y} + \sigma_t g_{y,\pm} = \frac{\sigma_t}{2} G_x \qquad G_y = g_{y,+} + g_{y,-}$$

$$\phi^{(l+1)} = \phi^{(l+1/2)} + G_y$$

Wrapping a Krylov method around existing transport methods may improve convergence.

- Finds the "best" linear combination of previous iterates.
- Use DSA or TSA as a preconditioner to a Krylov iterative solvers.
- Easy to implement over existing transport codes.
- Conjugate gradient, BiCG, or GMRES.

Implementing transport sweeps in parallel.

- Problem decomposition
  - Angle
  - Space
  - Energy
- Communication
- Synchronization
- Scheduler
- Partitioner

GMRES in parallel

- Parallel implementation of inner products and norms
- Global reduce and broadcast
- DSA uses CG to solve the diffusion problem (low-order problem).

We use pArrays to implement GMRES.

- Use GMRES to solve the within groupset problem.
- pArray – parallel array
  - STAPL container
  - Built in parallel functions and operators, e.g. dot products and norms
  - Distribution of data handled automatically
- Independent of spatial discretization
  - Source iteration
  - TSA