Simplified P_N Equations

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DTK Update

- M & C paper accepted - recommended for journal
- Corresponding with MOOSE team lead at INL
    - Really happy with DTK performance for Geometry/Mesh code-to-code coupling
    - Building new solver framework around DTK in MOOSE
    - Includes moving data between hierarchies in hierarchal solve system
    - Details to come - seems to be based on domain decomposition methods
    - Interested in more complex communicator structures
    - Core DTK functionality should remain unmodified
    - Higher-level MIMD support required - INL framework

MCLS Update

- M & C paper accepted for domain leakage approximations for Markov chains
- Trilinos linear solver abstract numerical algorithm interfaces completed and tested
- Incorporated into Exnihilo with tests - can now be used as a linear solver
- Now we have to study the linear system...

Neutron Transport Solution Methods

$$\hat{\Omega} \cdot \vec{\nabla}\psi(\vec{r}, \hat{\Omega}, E) + \sigma(\vec{r}, E)\psi(\vec{r}, \hat{\Omega}, E) = \int\int \sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega})\psi(\vec{r}, \hat{\Omega}', E')d\Omega' dE' + q(\vec{r}, \hat{\Omega}, E) \quad (1)$$

- S_N transport is expensive
  - Difficult to parallelize: sweeps in space, pipelining in angle, energy decoupling
  - Large storage requirements
  - Ray effects
- P_N equations still expensive
  - Complicated system: $(N + 1)^2$ equations in 3D
  - Coupling of equations through both angular moments and spatial derivatives

SP_N Approximation

- Ad-hoc generalization of planar P_N equations by Gelbard in the 1960's
- Rigorous formulation through asymptotic and variational analysis in 1990's and 2000's
- Simpler system $(N+1)/2$ equations in $3D$
- Yields elliptic, diffusion-like equations
- Applicable when diffusion theory is applicable: reasonable flux gradients, full-core transport
- Typically does not converge to transport solution as $N \rightarrow \infty$
- **Can build the full linear operator**
- **Parallelism through the linear solver**

Legendre Polynomials

$$P_l(\mu) = \frac{1}{2^l l!}\frac{d^l}{d\mu^l}(\mu^2 - 1)^l \, . \tag{2}$$

Orthogonality:

$$\int_{-1}^{1} P_l(\mu)P_{l'}(\mu)d\mu = \frac{1}{2l+1}\delta_{ll'} \, , \tag{3}$$

Recurrence:

$$\mu P_l(\mu) = \frac{1}{2l+1}[(l+1)P_{l+1}(\mu) + lP_{l-1}(\mu)] \, , \tag{4}$$

Addition theorem:

$$P_l(\hat{\Omega}\cdot\hat{\Omega}') = \frac{1}{2n+1}\sum_{m=-l}^{l} Y_{lm}(\hat{\Omega})Y^*_{lm}(\hat{\Omega}') \, , \tag{5}$$

Planar addition theorem:

$$P_l(\hat{\Omega}\cdot\hat{\Omega}') = P_l(\mu)P_l(\mu') \, . \tag{6}$$

P_N Derivation

Monoenergetic, planar 1D transport equation:

$$\mu \frac{\partial}{\partial x}\psi(x,\mu) + \sigma(x)\psi(x,\mu) = \int d\Omega' \sigma_s(x, \hat{\Omega}' \rightarrow \hat{\Omega})\psi(\vec{r}, \hat{\Omega}') + \frac{q(x)}{4\pi} \ . \quad (7)$$

Angular discretization:

$$\psi(x,\mu) = \sum_{n=0}^{\infty}(2n+1)P_n(\mu)\phi_n(x) \ , \quad (8)$$

$$\sigma_{sm}(x) = \sum_{m=0}^{\infty}(2m+1)P_m(\mu)\sigma_s(x) \ , \quad (9)$$

P_N Derivation

Insert expansions:

$$\frac{\partial}{\partial x}\Big[\sum_{n=0}^{\infty}(2n+1)\phi_n\mu P_n(\mu)\Big] + \sigma\sum_{n=0}^{\infty}(2n+1)\phi_n P_n(\mu) = \int_{-1}^{1}\sum_{m=0}^{\infty}(2m+1)\sigma_{sm}P_m(\mu_0)\sum_{n=0}^{\infty}(2n+1)\phi_n P_n(\mu')d\mu' + q\,, \quad (10)$$

Use legendre polynomial properties to reduce:

$$\sum_{n=0}^{\infty}\frac{\partial}{\partial x}\frac{1}{2n+1}\Big[(n+1)\phi_{n+1}+n\phi_{n-1}\Big] + \sum_{n=0}^{\infty}\sigma\phi_n = \sum_{n=0}^{\infty}\sigma_{sn}\phi_n + q\delta_{n0}\,. \quad (11)$$

P_N Equations

$$\frac{1}{2n+1}\frac{\partial}{\partial x}\Big[(n+1)\phi_{n+1} + n\phi_{n-1}\Big] + \Sigma_n\phi_n = q\delta_{n0}\,, \tag{12}$$

with $\Sigma_n = \sigma - \sigma_{sn}$ and $n = 0, 1, \ldots, N$ and closure: $\phi_{N+1} = 0$

Example:P5 Equations

$$\frac{\partial}{\partial x}\phi_1 + \Sigma_0\phi_0 = q\,, \tag{13a}$$

$$\frac{1}{3}\frac{\partial}{\partial x}\Big[2\phi_2 + \phi_0\Big] + \Sigma_1\phi_1 = 0\,, \tag{13b}$$

$$\frac{1}{5}\frac{\partial}{\partial x}\Big[3\phi_3 + 2\phi_1\Big] + \Sigma_2\phi_2 = 0\,, \tag{13c}$$

$$\frac{1}{7}\frac{\partial}{\partial x}\Big[4\phi_4 + 3\phi_2\Big] + \Sigma_3\phi_3 = 0\,, \tag{13d}$$

$$\frac{1}{9}\frac{\partial}{\partial x}\Big[5\phi_5 + 4\phi_3\Big] + \Sigma_4\phi_4 = 0\,, \tag{13e}$$

$$\frac{1}{11}\frac{\partial}{\partial x}5\phi_4 + \Sigma_5\phi_5 = 0\,. \tag{13f}$$

Use odd-order moments in even-order equations to eliminate them:

$$\phi_n = \frac{1}{\Sigma_n}\left[q\delta_{no} - \frac{\partial}{\partial x}\left(\frac{n}{2n+1}\phi_{n-1} + \frac{n+1}{2n+1}\phi_{n+1}\right)\right] \quad n = 1, 3, \cdots N, \quad (14)$$

$$\begin{aligned} &-\frac{\partial}{\partial x}\left[\frac{n}{2n+1}\frac{1}{\Sigma_{n-1}}\frac{\partial}{\partial x}\left(\frac{n-1}{2n-1}\phi_{n-2} + \frac{n}{2n-1}\phi_n\right)\right. \\ &\qquad \left. + \frac{n+1}{2n+1}\frac{1}{\Sigma_{n+1}}\frac{\partial}{\partial x}\left(\frac{n+1}{2n+3}\phi_n + \frac{n+2}{2n+3}\phi_{n+2}\right)\right] \\ &\qquad\qquad + \Sigma_n\phi_n = q\delta_{n0} \qquad n = 0, 2, 4, \cdots, N\,. \quad (15)\end{aligned}$$

SP_N Approximation

- Replace spatial derivatives with general multidimensional gradient operators:

SP_N Equations

$$
\begin{aligned}
-\nabla \cdot \Bigg[& \frac{n}{2n+1}\frac{1}{\Sigma_{n-1}}\nabla\left(\frac{n-1}{2n-1}\phi_{n-2} + \frac{n}{2n-1}\phi_n\right) \\
& + \frac{n+1}{2n+1}\frac{1}{\Sigma_{n+1}}\nabla\left(\frac{n+1}{2n+3}\phi_n + \frac{n+2}{2n+3}\phi_{n+2}\right)\Bigg] \\
& + \Sigma_n\phi_n = q\delta_{n0} \qquad n = 0, 2, 4, \cdots, N\,, \qquad (16)
\end{aligned}
$$

SP_7 Example

$$-\nabla \cdot \frac{1}{3\Sigma_1} \nabla(\phi_0 + 2\phi_2) + \Sigma_0 \phi_0 = q \tag{17a}$$

$$-\nabla \cdot \left[\frac{2}{15\Sigma_1} \nabla(\phi_0 + 2\phi_2) + \frac{3}{35\Sigma_3} \nabla(3\phi_2 + 4\phi_4) \right] + \Sigma_2 \phi_2 = 0 \tag{17b}$$

$$-\nabla \cdot \left[\frac{4}{63\Sigma_3} \nabla(3\phi_2 + 4\phi_4) + \frac{5}{99\Sigma_5} \nabla(5\phi_4 + 6\phi_6) \right] + \Sigma_4 \phi_4 = 0 \tag{17c}$$

$$-\nabla \cdot \left[\frac{6}{143\Sigma_5} \nabla(5\phi_4 + 6\phi_6) + \frac{7}{195\Sigma_7} \nabla(7\phi_6) \right] + \Sigma_6 \phi_6 = 0\,. \tag{17d}$$

SP_7 Example

Change variables:

$$u_1 = \phi_0 + 2\phi_2 \tag{18a}$$
$$u_2 = 3\phi_2 + 4\phi_4 \tag{18b}$$
$$u_3 = 5\phi_4 + 6\phi_6 \tag{18c}$$
$$u_4 = 7\phi_6 \ , \tag{18d}$$

$$\phi_0 = u_1 - \frac{2}{3}u_2 + \frac{8}{15}u_3 - \frac{16}{35}u_4 \tag{19a}$$
$$\phi_2 = \frac{1}{3}u_2 - \frac{4}{15}u_3 + \frac{8}{35}u_4 \tag{19b}$$
$$\phi_4 = \frac{1}{5}u_3 - \frac{6}{35}u_4 \tag{19c}$$
$$\phi_6 = \frac{1}{7}u_4 \ . \tag{19d}$$

SP_7 Example

$$-\nabla \cdot \frac{1}{3\Sigma_1}\nabla u_1 + \Sigma_0\left[u_1 - \frac{2}{3}u_2 + \frac{8}{15}u_3 - \frac{16}{35}u_4\right] = -q \tag{20a}$$

$$-\nabla \cdot \left[\frac{2}{15\Sigma_1}\nabla u_1 + \frac{3}{35\Sigma_3}\nabla u_2\right] + \Sigma_2\left[\frac{1}{3}u_2 - \frac{4}{15}u_3 + \frac{8}{35}u_4\right] = 0 \tag{20b}$$

$$-\nabla \cdot \left[\frac{4}{63\Sigma_3}\nabla u_2 + \frac{5}{99\Sigma_5}\nabla u_3\right] + \Sigma_4\left[\frac{1}{5}u_3 - \frac{6}{35}u_4\right] = 0 \tag{20c}$$

$$-\nabla \cdot \left[\frac{6}{143\Sigma_5}\nabla u_3 + \frac{7}{195\Sigma_7}\nabla u_4\right] + \Sigma_6\left[\frac{1}{7}u_4\right] = 0\,. \tag{20d}$$

SP_7 Example

Rearrange so that we only have 1 divergence operation in each equation:

$$-\nabla \cdot D_n \nabla u_n + \sum_{m=1}^{4} A_{nm} u_m = q_n \qquad n = 1, 2, 3, 4 \,, \tag{21}$$

D the vector of effective diffusion coefficients:

$$\mathbf{D} = \begin{pmatrix} \frac{1}{3\Sigma_1} & \frac{1}{7\Sigma_3} & \frac{1}{11\Sigma_5} & \frac{1}{15\Sigma_7} \end{pmatrix}^T , \tag{22}$$

q the vector of source terms where the 0^{th} moment source has now been distributed through the system:

$$\mathbf{q} = (q \quad -\frac{2}{3}q \quad \frac{8}{15}q \quad -\frac{16}{35}q)^T \,, \tag{23}$$

and **A** a matrix of angular scattering terms:

$$\mathbf{A} = \begin{bmatrix} (\Sigma_0) & (-\frac{2}{3}\Sigma_0) & (\frac{8}{15}\Sigma_0) & (-\frac{16}{35}\Sigma_0) \\ (-\frac{2}{3}\Sigma_0) & (\frac{4}{15}\Sigma_0 + \frac{1}{3}\Sigma_2) & (-\frac{16}{45}\Sigma_0 - \frac{4}{9}\Sigma_2) & (\frac{32}{105}\Sigma_0 + \frac{8}{21}\Sigma_2) \\ (\frac{8}{15}\Sigma_0) & (-\frac{16}{45}\Sigma_0 - \frac{4}{9}\Sigma_2) & (\frac{64}{225}\Sigma_0 + \frac{16}{45}\Sigma_2 + \frac{9}{25}\Sigma_4) & (-\frac{128}{525}\Sigma_0 - \frac{32}{105}\Sigma_2 - \frac{54}{175}\Sigma_4) \\ (-\frac{16}{35}\Sigma_0) & (\frac{32}{105}\Sigma_0 + \frac{8}{21}\Sigma_2) & (-\frac{128}{525}\Sigma_0 - \frac{32}{105}\Sigma_2 - \frac{54}{175}\Sigma_4) & (\frac{256}{1225}\Sigma_0 + \frac{64}{245}\Sigma_2 + \frac{324}{1225}\Sigma_4 + \frac{13}{49}\Sigma_6) \end{bmatrix} . \quad (24)$$

Multigroup SP_N equations

Multigroup, planar, 1D transport equation:

$$\mu \frac{\partial}{\partial x}\psi^g(x,\mu) + \sigma^g(x)\psi^g(x,\mu) = \sum_{g'=0}^{G} \int \sigma_s^{gg'}(x,\hat{\Omega}' \rightarrow \hat{\Omega})\psi^{g'}(x,\hat{\Omega}')d\Omega' + \frac{q^g(x)}{4\pi}\ , \tag{25}$$

Multigroup P_N Equations:

$$\frac{1}{2n+1}\frac{\partial}{\partial x}\left[(n+1)\phi^g_{n+1} + n\phi^g_{n-1}\right] + \sum_{g'}(\sigma^g \delta_{gg'} - \sigma_{sn}^{gg'})\phi^g_n = q\delta_{n0}\ , \tag{26}$$

Scattering Matrix:

$$\mathbf{\Sigma}_n = \begin{bmatrix} (\sigma^0 - \sigma_{sn}^{00}) & -\sigma_{sn}^{01} & \dots & -\sigma_{sn}^{0G} \\ -\sigma_{sn}^{10} & (\sigma^1 - \sigma_{sn}^{11}) & \dots & -\sigma_{sn}^{1G} \\ \vdots & \vdots & \ddots & \vdots \\ -\sigma_{sn}^{G0} & -\sigma_{sn}^{G1} & \dots & (\sigma^G - \sigma_{sn}^{GG}) \end{bmatrix}. \tag{27}$$

Multigroup SP_N equations

Multigroup SP_N equations:

$$
\begin{aligned}
-\nabla \cdot \Bigg[& \frac{n}{2n+1}\mathbf{\Sigma_{n-1}}^{-1}\nabla\Big(\frac{n-1}{2n-1}\mathbf{\Phi_{n-2}} + \frac{n}{2n-1}\mathbf{\Phi_n}\Big) \\
& + \frac{n+1}{2n+1}\mathbf{\Sigma_{n+1}}^{-1}\nabla\Big(\frac{n+1}{2n+3}\mathbf{\Phi_n} + \frac{n+2}{2n+3}\mathbf{\Phi_{n+2}}\Big)\Bigg] \\
& + \mathbf{\Sigma_n}\mathbf{\Phi_n} = \mathbf{q}\delta_{n0} \qquad n = 0, 2, 4, \cdots, N\,.
\end{aligned} \tag{28}
$$

Change variables and rearrange again:

$$
-\nabla \cdot \mathbb{D}_n \nabla \mathbb{U}_n + \sum_{m=1}^{4} \mathbb{A}_{nm}\mathbb{U}_m = \mathbb{Q}_n\,, \tag{29}
$$

Spatial discretization

- Equations to this point ignored spatial discretization
- All are valid in the domain anywhere (but not necessarily on the boundary)
- Exnihilo uses a finite volume discretization on a rectilinear grid
- Discretization is constistent, based on a conservation law approach
- Flux is balanced in a cell, currents continuous across cell/material boundaries

SP_N Numerical Spectral Analysis

- Monte Carlo methods for have strong restrictions on the eigenvalues of the operator for convergence
- MCSA has the same restrictions on the outer stationary iteration
- We need to compute these eigenvalues for various forms of the SP_N equations to verify convergence of these methods.

We need eigenvalues for $\mathbf{A}$, $\mathbf{H_J}$, and $\mathbf{H_{GS}}$ with:

$$\mathbf{H_J} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{A} \tag{30}$$

where $\mathbf{D} = diag(\mathbf{A})$ and

$$\mathbf{H_{GS}} = (\mathbf{L} + \mathbf{D})^{-1}\mathbf{U} \tag{31}$$

SP_7, P_3, 3 groups, reflecting boundaries

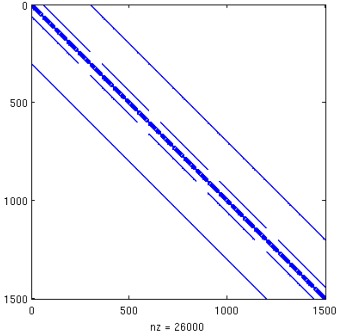

Figure: **Linear operator sparsity pattern**

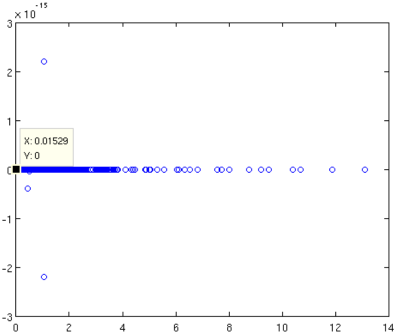

Figure: **Linear operator eigenvalues**

SP_7, P_3, 3 groups, reflecting boundaries

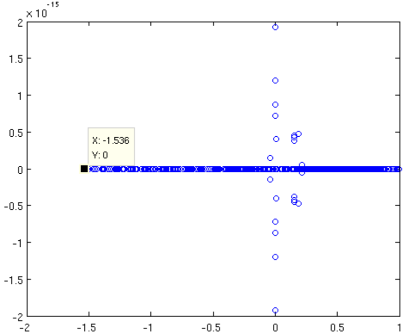

Figure: **Jacobi iteration matrix eigenvalues**

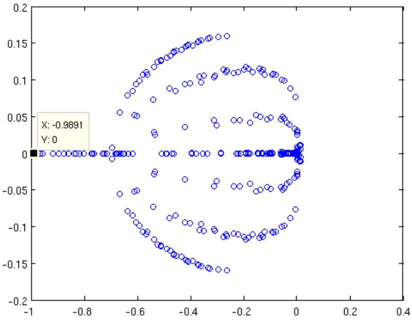

Figure: **Gauss-Seidel iteration matrix eigenvalues**

Oh No!

- The Jacobi method won't converge - all that stuff I said in my prelim won't work

Some solutions

There are some solutions to this problem...

- Use Gauss-Seidel for the outer stationary iteration in MCSA
- Alternative matrix scalings - Dimov 1998
- Resolvent Monte Carlo
  - Spectral mapping of the Neumann series into the unit circle of the complex plane
  - Requires some a priori knowledge about the linear system
  - Many Dimov papers including 2001
- Stochastic projection methods
  - Simple forms always converge for nonsingular systems
  - Simple forms yield a stationary methods
  - Stationary methods yield Neumann series
  - The matrices are more complicated
- All of these options fit in the MCLS framework
- Focusing on studying them to solve the above problems for the SP_N equations

Conclusions

- The SP_N equations are a great system to use for my work (assymetry, have to make some system-specific convergence adjustments)
- Recent results using convential Krylov and multigrid methods suggest we can perform better
- Real implications for full-core neutron transport solutions
- A much better challenge problem