Preconditioning Strategies for Particle Transport Simulations

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What this talk is (and isn't)

- I'll discuss preconditioning issues for discrete ordinates methods for particle transport simulations.
- Some details are omitted for brevity, namely anisotropic scattering and eigenvalue (criticality) calculations.
- My aim is to provide a tutorial for how these calculations are done in practice to foster collaboration between our transport group at Texas A&M and the solver/preconditioning experts at University of West Bohemia.

The dependent variables

In transport simulations we the equations are cast in terms of an intensity, usually called an angular flux, $\psi(x, \Omega, v, t)$ where

- The spatial variable $x \in \mathbb{R}^3$
- The angular variable $\Omega \in \mathbb{S}_2$ (i.e., Ω is a point on the unit sphere).
- The speed variable $v \in [0, \infty)$ or equivalently an energy variable E.
- A time variable $t \in [0, \infty)$.

Physically, ψ is the phase space density times the particle speed. Often the quantity that we actually want to solve for is the scalar flux (or scalar intensity) ϕ:

$$\phi(x, v, t) = \int_{4\pi} d\Omega \, \psi(x, \Omega, v, t).$$

The importance of ϕ comes from the fact that it is required to compute the reaction rate which is directly related to the power level in a nuclear reactor or the dose in a medical physics application.

The physical processes

A neutron can leave a given volume of phase space by streaming out or by having a collision with a nucleus. A neutron can enter a given volume of phase space centered about (x, Ω, v, t)

- By scattering from speed v' and angle Ω'. The total rate density is found by integrating over all v' and Ω':

$$\int_0^\infty dv' \int_{4\pi} d\Omega' \, \sigma_{\mathrm{s}}(x, \Omega' \to \Omega, v' \to v)\psi(x, \Omega', v', t).$$

- By a fission event caused by a neutron at speed v' releasing a neutron at speed v. The neutrons are emitted isotropically (with no special Ω). The total rate density of fission neutrons emitted into our phase space volume:

$$\frac{\chi(v)}{4\pi} \int_0^\infty dv' \nu\sigma_{\mathrm{f}}(x, v')\phi(x, v', t).$$

- Being emitted from a source: $Q(x, \Omega, v, t)$.

The linear Boltzmann transport equation

Putting all this together, we can write the linear Boltzmann that we can solve for $\psi(x, \Omega, v, t)$:

$$\frac{1}{v}\partial_t\psi + \Omega \cdot \nabla\psi + \sigma_{\mathrm{t}}\psi = \int_0^\infty dv' \int_{4\pi} d\Omega'\, \sigma_{\mathrm{s}}(x, \Omega' \to \Omega, v' \to v)\psi(x, \Omega', v', t) + \frac{\chi(v)}{4\pi} \int_0^\infty dv' \nu\sigma_{\mathrm{f}}(x, v')\phi(x, v', t) + Q(x, \Omega, v, t).$$

With inflow boundary conditions on ∂V and an initial condition at $t = 0$

$$\psi(x, \Omega, v, t) = f(x, v, \Omega, t) \qquad \text{for } x \in \partial V, \quad \Omega \cdot n < 0$$

$$\psi(x, \Omega, v, 0) = I(x, \Omega, v).$$

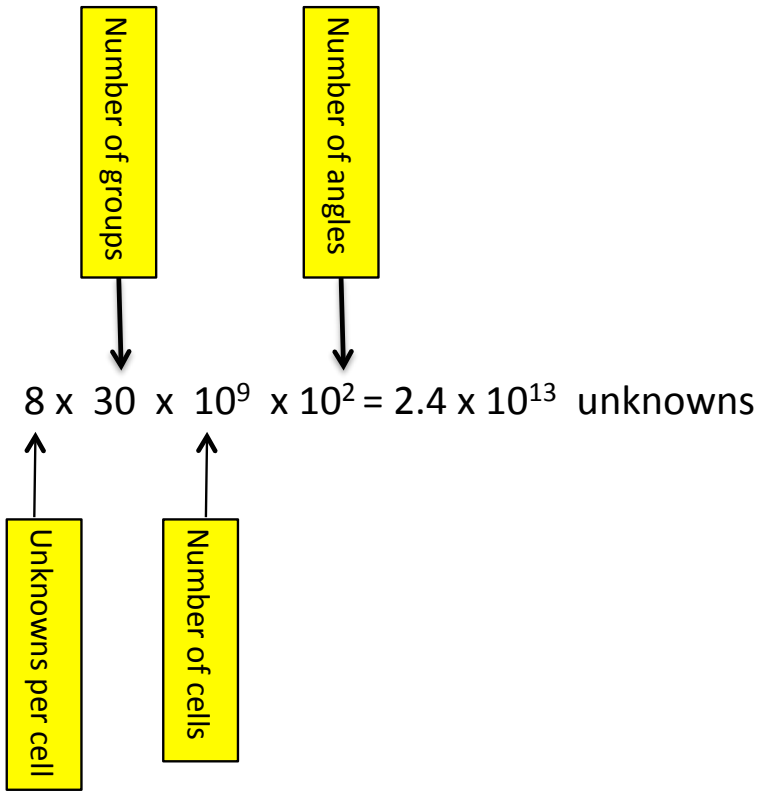
What makes these problems so hard?

There are several difficulties that make solving transport problems hard.

1. The high-dimensional phase space often requires many degrees of freedom per spatial zone. There can be hundreds of angular unknowns and tens of speed unknowns per spatial degree of freedom.
2. Potential high degrees of anisotropy in angle such as shadows or beams.
3. Spatial discontinuities in material properties (σ_{t}, σ_{f}, σ_{t}, and Q).
4. Truly wild energy dependence in the material properties.

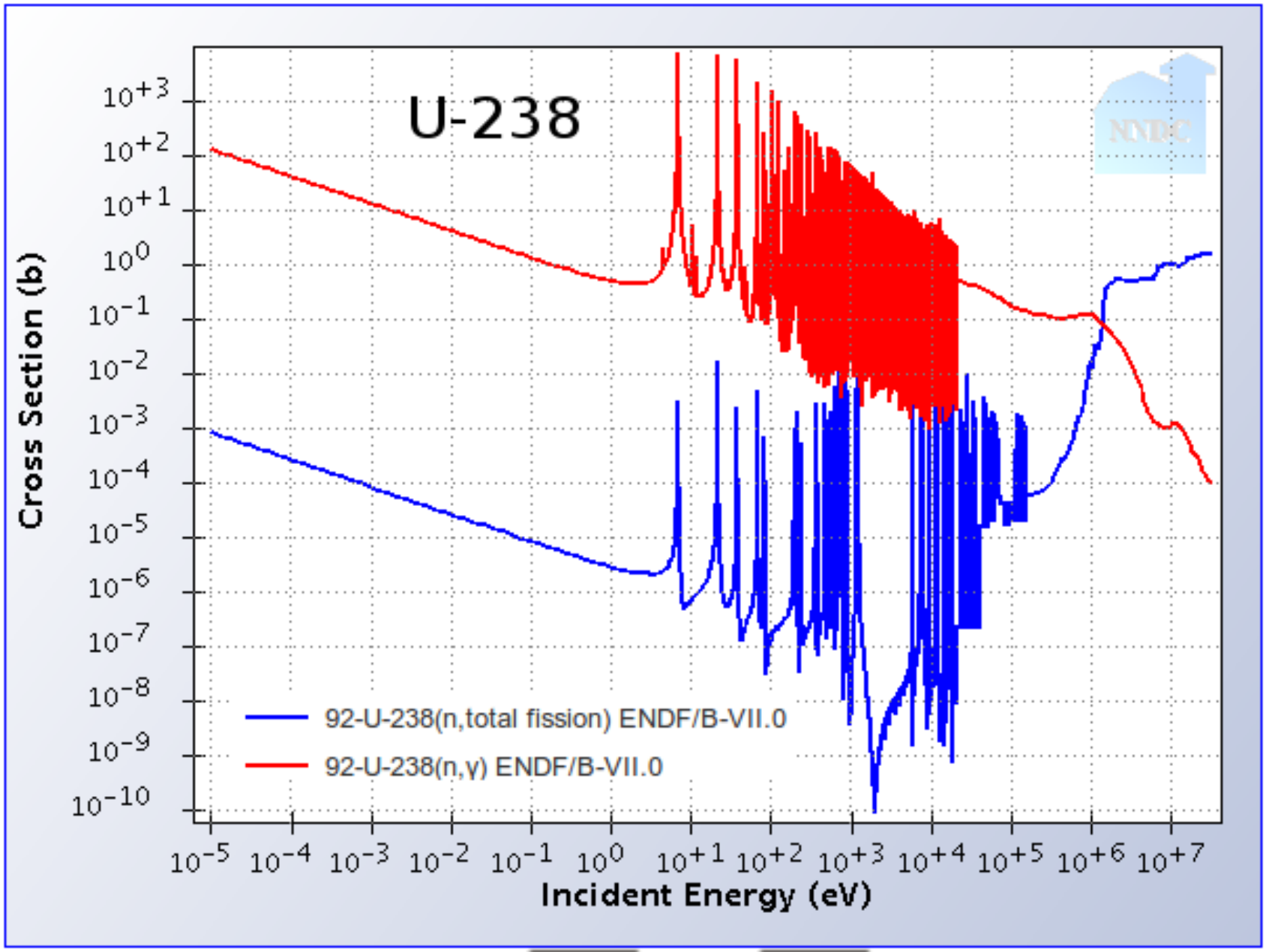
Computational Challenge

A well-resolved, 3D transport calculation would require (per timestep)

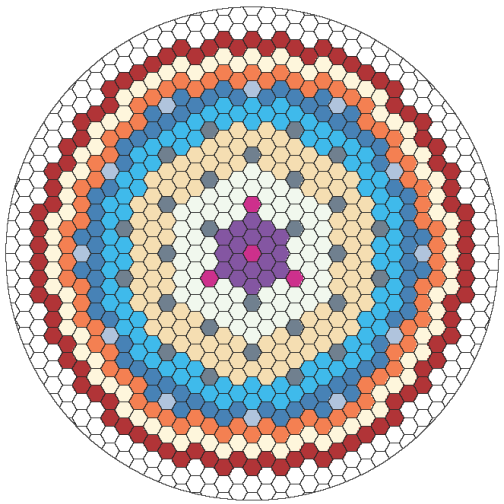


- Rule of thumb is 1 μs per unknown per iteration
- In this case each timestep is going to take about 6000 cpu/hrs.
- This might be reduced by being clever.
- At this cost, compromise might be a necessity.

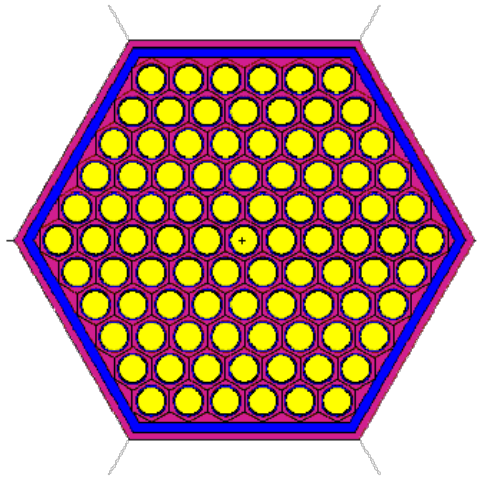
Energy (speed) dependence of σ_t and σ_f.



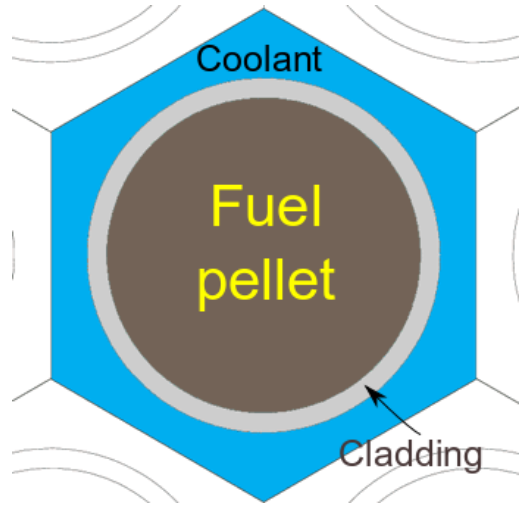
Complex geometries to model (core comprised of assemblies comprised of pins)



Reactor core



Assembly



Pin

The material properties are discontinuous at interfaces between fuel, cladding, and/or coolant.

Some good news

- These problems must not be impossible to solve. After all, we have nuclear reactors that operate as designed. Most of these reactors were developed with minimal computational power.
- These reactors were developed using extensive experimental campaigns as well as very clever multiscale modeling techniques (developed before the term multiscale had been invented). Yet, if we want to provide first principles calculations for accident scenarios, new types of reactors, or to squeeze every drop efficiency out of a reactor, we will have to solve large scale problems.
- As we will see, it is straightforward, and very useful to break the transport problem up into sub-problems regarding particular angles and energies, and iterating on the coupling between the problems.

Multigroup

We create a grid of size G of the speed variable v by partitioning the speed range (from 0 to some max speed). A given range of speeds from v_g to v_{g-1} is called the g^{th} group. Now if we integrate the transport equation from over v_g to v_{g-1} we get

$$\frac{1}{\bar{v}_g}\partial_t\psi_g + \Omega\cdot\nabla\psi_g + \sigma_{\mathrm{t},g}\psi_g = \sum_{g=1}^{G}\int_{4\pi} d\Omega'\,\sigma_{\mathrm{s},g'\to g}(x,\Omega'\to\Omega)\psi_{g'}(x,\Omega',t) + \frac{\chi_g}{4\pi}\sum_{g=1}^{G}\nu\sigma_{\mathrm{f},g'}(x)\phi_{g'}(x,t) + Q_g(x,\Omega,t),$$

where

$$\psi_g(x,\Omega,t) = \int_{v_g}^{v_g-1} dv\,\psi(x,\Omega,v,t),$$

and, for example,

$$\sigma_{\mathrm{f},g'}(x) = \frac{\int_{v'_g}^{v'_g-1} dv\,\sigma_{\mathrm{f}}(x,v)\psi(x,\Omega,v,t)}{\psi_{g'}}.$$

Angular discretizations

The multigroup approximation is standard in the transport community. There are several approaches to treat the angular variable.

- Discrete ordinates methods solve for ψ along particular directions and then use a quadrature rule to compute moments (such as ϕ).
- Spherical harmonics methods expand ψ in a truncated spherical harmonics series and use some closure relation.
- Diffusion methods make a very simple approximation to the angular dependence of ψ so that we can write the transport equation only as a function of ϕ.

All of these methods, and other deterministic transport methods, have issues. The most popular high-fidelity deterministic transport scheme is discrete ordinates. These are the methods we will discuss for the remainder of the talk.

I should also mention Monte Carlo methods which use sampling to treat the emission and interaction of particles. These methods have a lot of nice features, but are even more expensive from a computational point of view.

Discrete ordinates

For ease of notation (believe me), we will treat isotropic scattering here:

$$\sigma_{\mathrm{s},g'\to g}(x, \Omega' \to \Omega) = \sigma_{\mathrm{s},g'\to g}(x).$$

For a given quadrature set, (w_l, Ω_l), $l = 1, \ldots, L$ we write

$$\psi_{l,g}(x,t) = \psi_g(x, \Omega_l, t), \quad \text{and} \quad \phi_g(x,t) \approx \sum_{l=1}^{L} w_l \psi_{l,g}(x,t).$$

This makes the transport equation

$$\frac{1}{\bar{v}_g}\partial_t \psi_{l,g} + \Omega_l \cdot \nabla \psi_{l,g} + \sigma_{\mathrm{t},g}\psi_{l,g} = \sum_{g=1}^{G} \sigma_{\mathrm{s},g'\to g}(x)\phi_{g'}(x,t) + \frac{\chi_g}{4\pi}\sum_{g=1}^{G} \nu\sigma_{\mathrm{f},g'}(x)\phi_{g'}(x,t) + Q_g(x, \Omega_l, t).$$

We can now write this equation in an operator form which greatly simplifies the notation.

Operator form

First we define a discrete to moment operator, that is an operator that takes the discrete ordinates and maps them onto moments (the scalar flux in the isotropic scattering case). Ψ is a vector of length LG:

$$D\Psi = \begin{pmatrix} w_1\psi_{1,1} + w_2\psi_{2,1} + \cdots + w_L\psi_{L,1} \\ w_1\psi_{1,2} + w_2\psi_{2,2} + \cdots + w_L\psi_{L,2} \\ \vdots \\ w_1\psi_{1,G} + w_2\psi_{2,G} + \cdots + w_L\psi_{L,G} \\ \vdots \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \cdots \\ \phi_G \\ \vdots \end{pmatrix} = \Phi;$$

the dots at the end indicate that the vector repeats L times. We also define a scattering operator that acts on each $D\Psi_l$:

$$S = \begin{pmatrix} \sigma_{s,1\to1} & \sigma_{s,2\to1} & \cdots & \sigma_{s,G\to1} \\ \sigma_{s,1\to2} & \sigma_{s,2\to2} & \cdots & \sigma_{s,G\to2} \\ \vdots & & & \\ \sigma_{s,1\to G} & \sigma_{s,2\to G} & \cdots & \sigma_{s,G\to G} \\ \vdots & & & \end{pmatrix}.$$

Operator form (cont.)

For the fission term we define a fission matrix that also acts on $D\Psi_l$:

$$F = \begin{pmatrix} \chi_1\nu\sigma_{\mathrm{f},1} & \chi_1\nu\sigma_{\mathrm{f},2} & \cdots & \chi_1\nu\sigma_{\mathrm{f},G} \\ \chi_2\nu\sigma_{\mathrm{f},1} & \chi_2\ \nu\sigma_{\mathrm{f},2} & \cdots & \chi_2\nu\sigma_{\mathrm{f},G} \\ \vdots & & & \\ \chi_G\nu\sigma_{\mathrm{f},1} & \chi_G\nu\sigma_{\mathrm{f},2} & \cdots & \chi_G\nu\sigma_{\mathrm{f},G} \\ \vdots & & & \end{pmatrix}.$$

The streaming + collision operator acts on Ψ:

$$L\Psi = \begin{pmatrix} \Omega_l \cdot \nabla\psi_{1,1} + \sigma_{\mathrm{t},1}\psi_{1,1} \\ \vdots \\ \Omega_l \cdot \nabla\psi_{1,G} + \sigma_{\mathrm{t},2}\psi_{1,G} \\ \vdots \\ \Omega_l \cdot \nabla\psi_{L,1} + \sigma_{\mathrm{t},1}\psi_{L,1} \\ \vdots \\ \Omega_l \cdot \nabla\psi_{L,G} + \sigma_{\mathrm{t},2}\psi_{L,G} \end{pmatrix}.$$

Operator form (cont.)

The last operator we need to define is the moment to discrete operator M:

$$M\Phi = \frac{1}{4\pi} \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_G \\ \phi_1 \\ \vdots \\ \phi_G \\ \vdots \end{pmatrix}.$$

Now we can write the transport equation in operator form:

$$\frac{1}{\bar{v}}\partial_t \Psi + L\Psi = MSD\Psi + MFD\Psi + \hat{Q}.$$

Here $\hat{Q}$ is the appropriate vector form of Q_g, augmented to include boundary conditions.

Properties of the Operator form

We generally cast time -dependent problems in a quasi-steady form by writing

$$\partial_t \Psi = \frac{\Psi^{n+1} - \Psi^n}{\Delta t},$$

and then writing

$$L^* \Psi^{n+1} = MSD\Psi^{n+1} + MFD\Psi^{n+1} + \hat{Q}^*,$$

where L^* is L with $\sigma_{\mathrm{t},g} \rightarrow \sigma_{\mathrm{t},g} + \Delta t^{-1}$ and $\hat{Q}^* = \hat{Q} + \Delta t^{-1} \Psi^n$. We will drop the $*$ and $(n+1)$ henceforth.
We also note that for a given ordinate, the streaming operator represents a linear advection operator with reaction. Assuming an upwinded method is used in the spatial discretization, the L operator is lower triangular (that is one of the reasons it is denoted as L). A lower triangular operator is simple to invert via a transport sweep (that is by starting at the boundary and then progressively updating spatial cells). Inverting this operator and rearranging gives

$$(I - DL^{-1}M(S+F))D\Psi = DL^{-1}\hat{Q},$$

which we can rewrite as

$$(I - DL^{-1}M(S+F))\Phi = DL^{-1}\hat{Q}.$$

Properties of the Operator form (cont.)

Note that we have effectively reduced our transport problem from a LG dimensional space to a G dimensional space. Though we have reduced the problem to solve for the moments of the angular flux, using this solution we can compute the angular flux:

$$\Psi = L^{-1}M(S+F)\Phi + L^{-1}\hat{Q}.$$

If we solve the transport equation using a Krylov method, usually GMRES, we only need to have the moment variables in the Krylov vector.

The convergence properties of the Krylov method will depend on the structure of the $DL^{-1}M(S+F)$ operator. We will first look at the structure as it relates to the energy variable.

Due to physical effects, most scattering is "downscattering" meaning that particles lose energy in a collision, and importantly only move from groups with lower numbers to higher numbers. For low energy groups, where the particle energy is close to the thermal energy of the background material, up scattering is possible.

This makes the S operator almost triangular:

$$S = \begin{pmatrix} \sigma_{s,1\to1} & 0 & \dots & & \\ \sigma_{s,1\to2} & \sigma_{s,2\to2} & 0 & \dots & \\ \vdots & & & & \\ \sigma_{s,1\to G_u} & \sigma_{s,2\to G_u} & \dots & \dots & \sigma_{s,G\to G_u} \\ \sigma_{s,1\to G} & \sigma_{s,2\to G} & \dots & & \sigma_{s,G\to G} \\ \vdots & & & & \end{pmatrix},$$

here G_u is the group where upscattering begins to be possible.

Properties of the Operator form (cont.)

The fission operator also has a special structure. In many applications, the value of χ_g is non-zero only for a few groups, e.g.

$$\chi_g > 0 \qquad g < G_f \leq G.$$

This makes the fission operator

$$F = \begin{pmatrix} \chi_1 \nu\sigma_{\mathrm{f},1} & \chi_1 \nu\sigma_{\mathrm{f},2} & \cdots & \chi_1 \nu\sigma_{\mathrm{f},G} \\ \chi_2 \nu\sigma_{\mathrm{f},1} & \chi_2 \nu\sigma_{\mathrm{f},2} & \cdots & \chi_2 \nu\sigma_{\mathrm{f},G} \\ \vdots & & & \\ \chi_{G_f} \nu\sigma_{\mathrm{f},1} & \chi_{G_f} \nu\sigma_{\mathrm{f},2} & \cdots & \chi_{G_f} \nu\sigma_{\mathrm{f},G} \\ 0 & \cdots & & \\ \vdots & & & \end{pmatrix}.$$

Also, the fission cross-section is small for many of groups and is largest for the low energy groups (groups near G).This further reduces the spectrum of F.

Gauss-Seidel for energy groups

We can solve the equations for energy dependent transport using a Gauss-Seidel approach where we start with group 1. Specifically, we write the iteration scheme for iterate $m+1$ as

$$\Omega_l \cdot \nabla \psi_{l,g}^{m+1} + \sigma_{\mathrm{t},1} \psi_{l,g}^{m+1} = \frac{\chi_g}{4\pi} \sum_{g'=1}^{g} \sigma_{\mathrm{f},g} \phi_g^{m+1} + \frac{\chi_g}{4\pi} \sum_{g'=g+1}^{G} \sigma_{\mathrm{f},g} \phi_{g'}^{m} + \hat{Q}, \qquad g \in [1, G].$$

For each group we can write this, somewhat ambiguously, as

$$(I + DL^{-1} M (S_g + F_g)) \Phi_g^{m+1} = DL^{-1} \left[(S_{g'<g} + F_{g'<g}) \Phi_{g'<g}^{m+1} + (S_{g'>g} + F_{g'>g}) \Phi_{g'>g}^{m} + \hat{Q} \right].$$

Note that if there is no upscattering (i.e., $\sigma_{\mathrm{s},g' \to g} = 0$ for $g' < g$) and no fission, then this will converge in a single iteration.

An important fact is that each Gauss-Seidel iteration contains the solution to G transport problems of the form

$$(I + DL^{-1} M (S_g + F_g)) \Phi_g^{m+1} = DL^{-1} \tilde{Q}.$$

The solution of these transport problems will require preconditioning of their own. To describe his we first describe an important limit of the transport equation.

The Diffusion Limit

For a small, positive parameter ϵ, if the following holds

- $\sigma_{\mathrm{s}}(v)/\sigma_{\mathrm{t}}(v) \sim O(\epsilon^{-1})$,
- $\nu\sigma_{\mathrm{f}}(v)/\sigma_{\mathrm{t}}(v) \sim O(\epsilon)$,
- $Q \sim O(\epsilon)$,
- $v^{-1}\partial_t\psi \sim O(\epsilon)$,

then the hyperbolic transport equation asymptotically (to second order) limits to a parabolic diffusion equation

$$\frac{1}{v}\partial_t\phi(x,v,t) + \nabla\cdot\frac{1}{3\sigma_{\mathrm{t}}(x,v)}\nabla\phi(x,v,t) + (\sigma_{\mathrm{t}} - \sigma_{\mathrm{s}} - \nu\sigma_{\mathrm{f}})\phi(x,v,t) = \langle Q\rangle,$$

where the angle brackets denote integration over the unit sphere. In operator form, we write this as

$$C\Phi = \langle\hat{Q}\rangle.$$

This relationship between transport and diffusion has been known since at least the 1940's but the asymptotic limit had not been established until the 1970's (Larsen and Keller, 1973).

Diffusion Synthetic Acceleration

The connection between transport and diffusion led to the development of an early, and still used today, solution method for transport problems. Called Source Iteration with Diffusion Synthetic Acceleration. Source Iteration is a form of Richardson iteration for solving mono-energetic transport problems for computing iterations $l+1$

$$\Phi^{l+1} = DL^{-1}MS\Phi^{l} + F\Phi^{l} + DL^{-1}\hat{Q}.$$

Source iteration performs very well when scattering or fission is small. When scattering or fission is large, this process can be arbitrarily slow.

An analysis of the error reduction in successive Source iterations shows that low-frequency (in space) error modes are the slowest to converge. One can show that these slowly converging modes are effectively reduced by applying a diffusion operator to the error. This method is called *Diffusion synthetic acceleration* (DSA):

$$\Phi^{l+1/2} = L^{-1}MS\Phi^{l} + MF\Phi^{l} + DL^{-1}\hat{Q},$$

$$f^{l+1/2} = C^{-1}S\left(\Phi^{l+1/2} - \Phi^{l}\right),$$

$$\Phi^{l+1} = \Phi^{l+1/2} + f^{l+1/2}.$$

Diffusion Synthetic Acceleration

DSA has several issues, the chief of being that if the spatial discretizations of the transport and diffusion operators are not "compatible" the iteration process will diverge. This fact has led to an involved body of literature on developing compatible discretizations.

Thankfully, DSA can be recast as a left preconditioner for a Krylov method:

$$(I + C^{-1}S)(I + DL^{-1}M(S + F))\Phi = (I + C^{-1}S)DL^{-1}\hat{Q}.$$

That is $(I + C^{-1}S)$ is an approximate inverse to $(I + DL^{-1}M(S + F))$.

When used as a preconditioner to the transport system, the issues of compatibility are removed.

Note that between our solution procedure for the energy groups (which requires the solution of several one-group problems), the bulk of the work in solving transport problems is in the solving the diffusion systems used as preconditioners.

Diffusion Synthetic Acceleration

- Diffusion is, in some sense, an angular approximation to the transport operator because it replaces the angular variable with a linear approximation.
- Therefore, DSA can be considered a multigrid in angle preconditioner.
- This is the most extreme multigrid in angle preconditioner.
- Other multigrid in angle preconditioners are possible, say going from an L angle discretization to an L/2 angle discretization, then diffusion.
- However early work on these preconditioners, in the context of an acceleration scheme demonstrated that the cost in solving the intermediate transport operators was too costly to be efficient.

Diffusion Synthetic Acceleration

There was a lot of research into DSA.

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FAST ITERATIVE METHODS FOR DISCRETE-ORDINATES PARTICLE TRANSPORT CALCULATIONS

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ABSTRACT

In discrete-ordinates (S_N) simulations of large problems involving linear interactions between radiation and matter, the underlying linear Boltzmann problem is discretized and the resulting system of algebraic equations is solved iteratively. If the physical system contains subregions that are optically thick with small absorption, the simplest iterative process, Source Iteration, is inefficient and costly. During the past 40 years, significant progress has been achieved in the development of *acceleration* methods that speed up the

The bigger picture

The solution procedure I have describe so far takes an transport problem for neutrons (or other particles) of different energies.

1. Puts those particles into bins (groups) based on there energies
2. As part of a Gauss-Seidel iteration procedure that solves G quasi-mono-energetic transport equations
3. Where each Gauss-Seidel iteration is preconditioned by a diffusion operator.

Of course, in materials with a large amount of upscattering or fission, the Gauss-Seidel procedure can be slow to converge.

Once again, we turn to a diffusive preconditioner (that was originally developed as an acceleration scheme).

The Energy Preconditioning

To precondition the Gauss-Seidel iterations we can use an energy averaged diffusion equation:

$$-\nabla \bar{D} \nabla \phi + \bar{\sigma_{\mathrm{a}}} \phi = D \bar{Q},$$

where

$$\bar{D} = \sum_{g=1}^{G} \frac{\frac{\chi_g \sigma_{\mathrm{f}} + \sigma_{\mathrm{s}}}{\sigma_{\mathrm{t},g}}}{3\sigma_{\mathrm{t},g} \sum_{g'=1} G \frac{\chi'_g \sigma_{\mathrm{f}} + \sigma_{\mathrm{s}}}{\sigma_{\mathrm{t}g'}}},$$

$$\bar{\sigma_{\mathrm{a}}} = \sum_{g=1}^{G} (\sigma_{\mathrm{t},g} - \sigma_{\mathrm{s},g\to g} - \nu\sigma_{\mathrm{f},g}) \frac{\frac{\chi_g \sigma_{\mathrm{f}} + \sigma_{\mathrm{s}}}{\sigma_{\mathrm{t},g}}}{\sum_{g'=1} G \frac{\chi'_g \sigma_{\mathrm{f}} + \sigma_{\mathrm{s}}}{\sigma_{\mathrm{t}g'}}},$$

$$\bar{Q} = \sum_{g=1} G L_g^{-1} Q_g.$$

We re-write this operator as

$$\bar{C}\phi = D\bar{Q},$$

to define the preconditioned system:

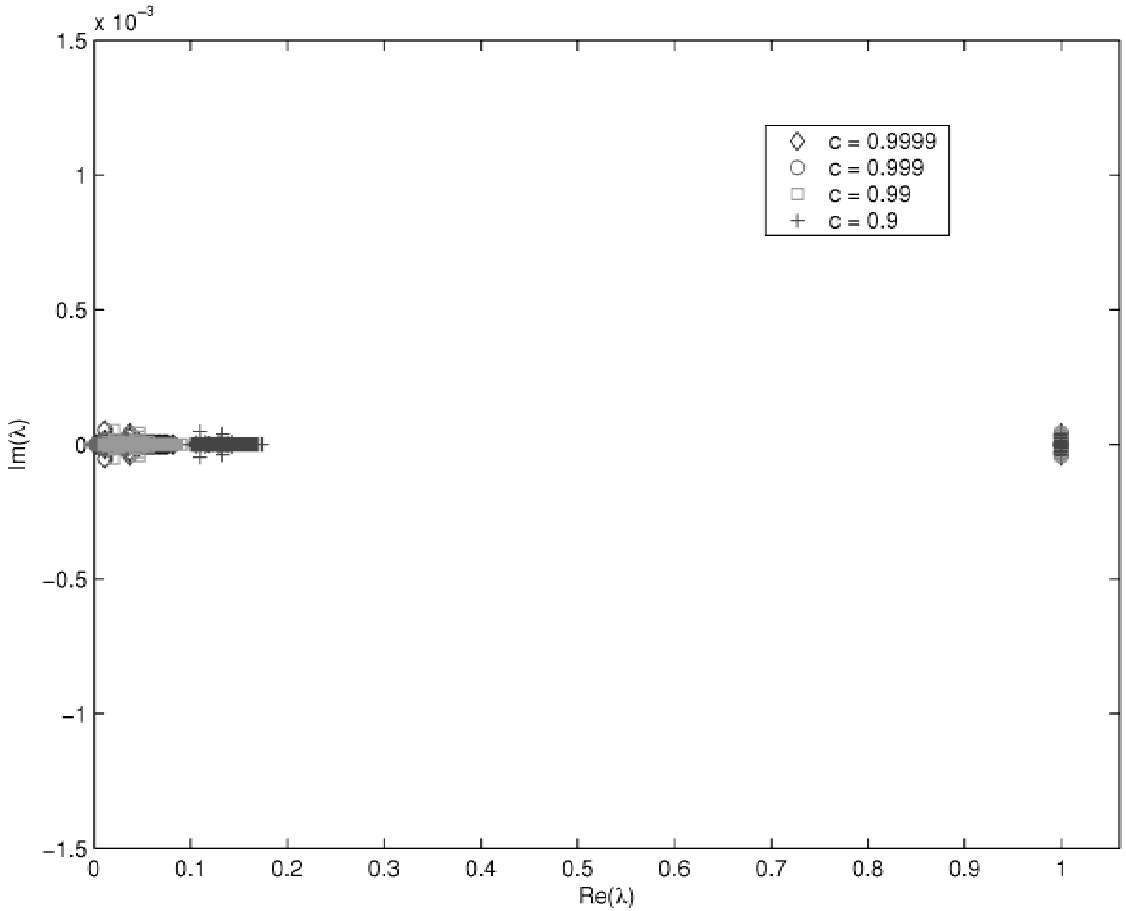
$$(I + \bar{C}^{-1} S)(I + DL^{-1} M(S + F))\Phi = (I + \bar{C}^{-1}) DL^{-1} \hat{Q}.$$

The Energy Preconditioning

- This has been called the Two-Grid acceleration scheme.
- It is based on the multifrequency grey scheme from radiative transfer.
- This method is also the state of the art for preconditioning energy dependent transport problems.
- Once again, it is a multigrid in *energy* preconditioner
  - Go from a grid in energy of G unknowns to 1 unknown.
- There has been almost no work on intermediate preconditioners.

Some results

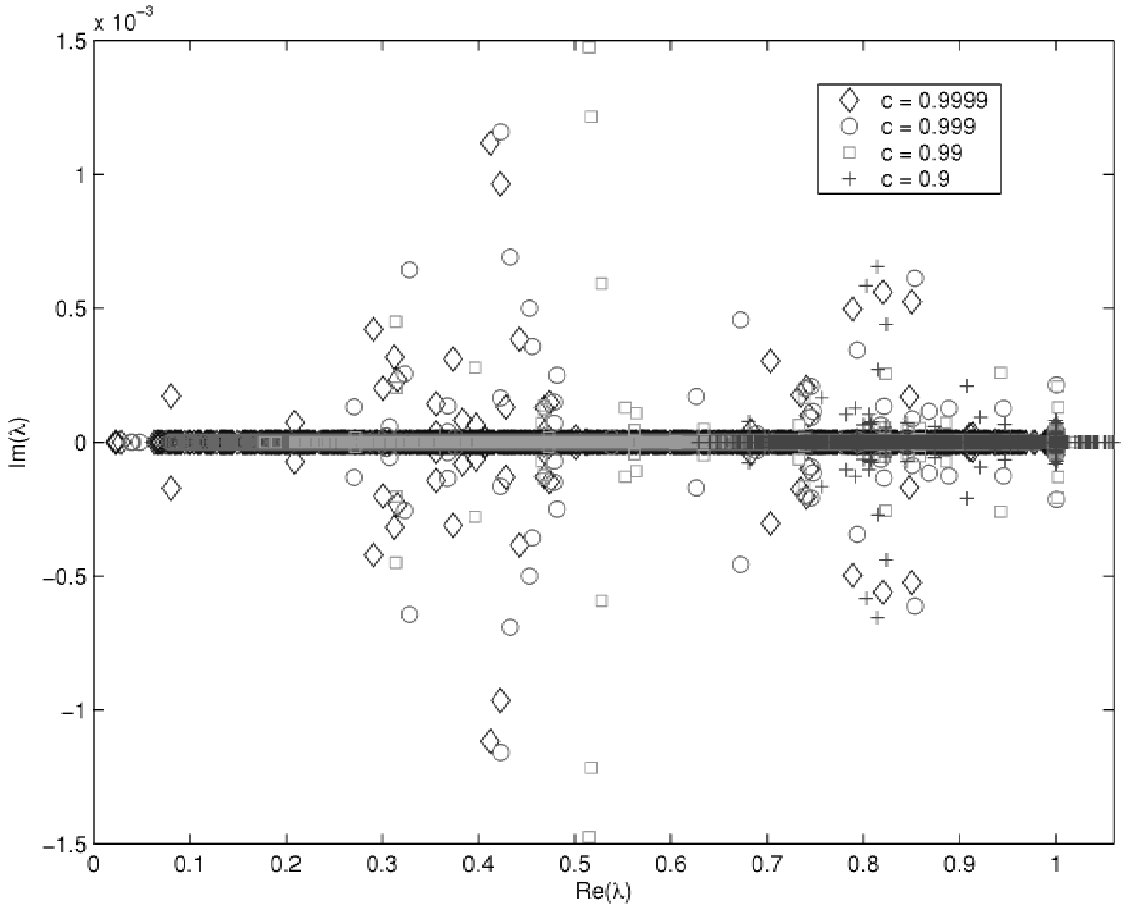
From (Warsa, Wareing, & Morel, 2004) we show some results from a typical 1-group transport problem. Here is the eigenvalue spectrum of the transport operator $(I + DL^{-1}MS)$



Here c is the scattering ratio. Note that the eigenvalues can approach 0 as $c \to 1$.

Some results

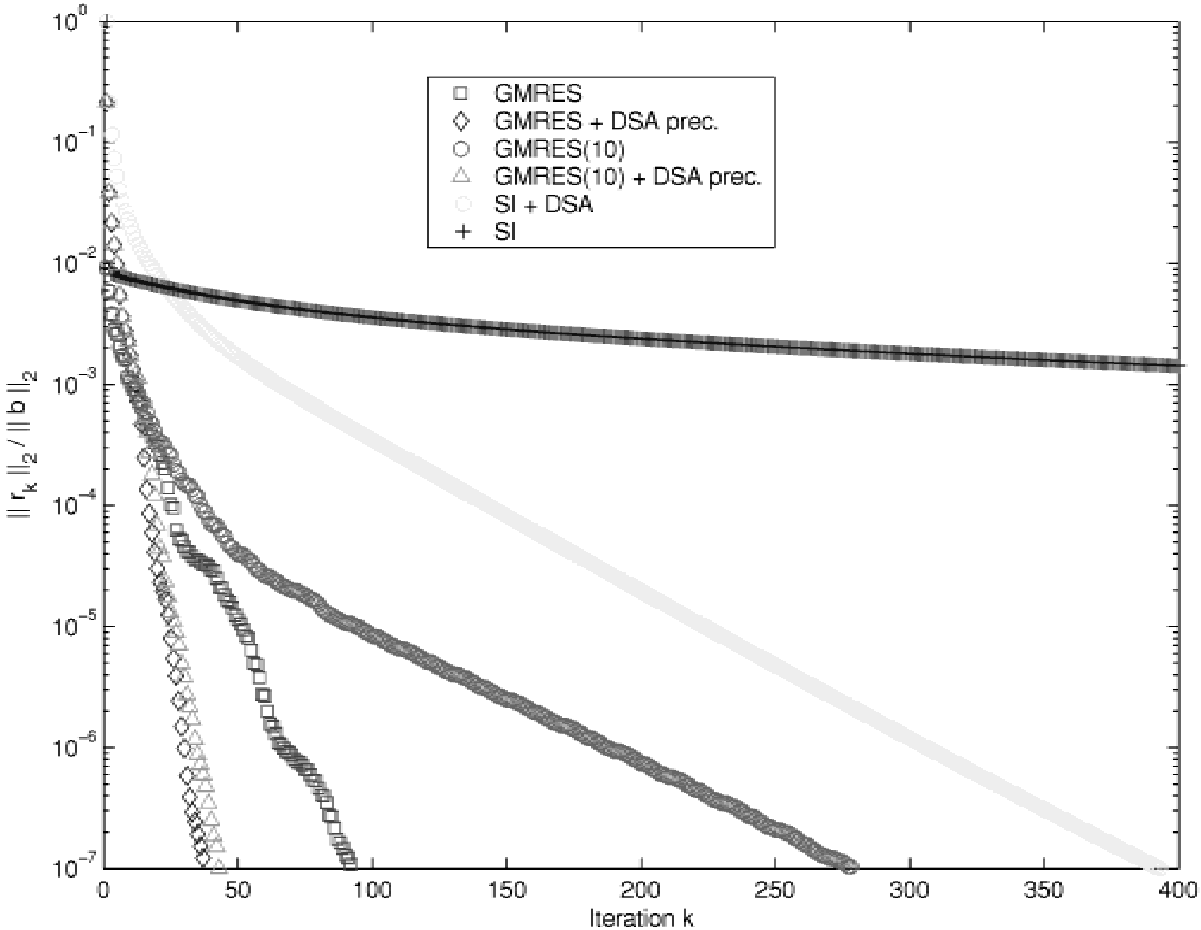
Preconditioning with a DSA type operator corrects the issue at zero, but spreads out the eigenvalues:



This suggests that DSA is not the best preconditioner.

Some results

But it works!



Outstanding Work

- Similar results exist for preconditioning the Gauss-Seidel system for the energy groups
  - The preconditioned form reduces the number of iterations from about 100 to below 50.
  - Still room for improvement.
- We have not even touched on improvements for the diffusion operator.
  - Preconditioned CG is the most common approach to inverting the diffusion operator.
  - Usually we just rely on "standard" multi-level pre conditioners.
  - Still room for improvement.

Summary

- I've touched on just some of the aspects of solving transport problems for nuclear engineering.
- There is more detail to cover for all of this, but I hope this engenders some interest for collaboration.
- There has been a lot of previous work, but there is more work to do.
- I haven't even touched on preconditioners for other types of transport schemes
  - I'm also particularly interested in P_n and SP_n methods.
  - These moment-based methods have different properties, and have *much* less research into their efficient solution methods.

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