Neutron transport - a few mathematical perspectives

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Steady-state neutron transport equation

angular flux $\Psi(\mathbf{r}, E, \Omega)$ describes distribution of neutrons in:
space ($\mathbf{r} \in V \subset \mathbb{R}^3$), energy ($E \in \mathbb{R}^+$), direction ($\Omega \in \mathbb{S}^2$)

- source problem for BTE:

$$\begin{aligned} &\Omega.\nabla\Psi(\mathbf{r}, E, \Omega) + \sigma(\mathbf{r}, E)\Psi(\mathbf{r}, E, \Omega) \\ = &\left\{ \frac{1}{4\pi} \int_{\mathbb{R}+} \int_{\mathbb{S}^2} \sigma_s(\mathbf{r}, E', E, \Omega', \Omega)\Psi(\mathbf{r}, E', \Omega')\, \mathrm{d}\Omega'\, \mathrm{d}E' \right\} \\ &+ \left\{ \frac{\chi(E)}{4\pi} \int_{\mathbb{R}+} \nu(\mathbf{r}, E')\sigma_f(\mathbf{r}, E') \int_{\mathbb{S}^2} \Psi(\mathbf{r}, E', \Omega')\, \mathrm{d}\Omega'\, \mathrm{d}E' \right\} \\ &+ Q(\mathbf{r}, E) \end{aligned}$$

- Abstractly:

$$\mathcal{T}\Psi = \mathcal{S}\Psi + \mathcal{F}\Psi + Q$$

+ boundary condition ($\mathcal{T}$ is a first order hyperbolic operator)

Criticality:

Find the smallest $\lambda > 0$ such that the eigenpair (λ, Ψ) solves

$$(\mathcal{T} - \mathcal{S})\Psi \quad = \quad \lambda \mathcal{F}\Psi \qquad\qquad (*)$$

+ homogeneous boundary conditions

- $\lambda = 1$: system is critical
- $\lambda < 1$: supercritical
- $\lambda > 1$: subcritical

(*) is a generalised EVP for a non-self-adjoint operator!

For simplicity, consider model problems with

- one energy group (no energy dependence):
- isotropic scattering (no dependence on angle):

$$\sigma_s(\mathbf{r}, \Omega, \Omega') = \sigma_s(\mathbf{r})$$

- vacuum boundary condition (zero incoming flux)

$$\Psi(\mathbf{r}, E, \Omega) = 0, \qquad \forall\, \mathbf{r} \in \partial V, \quad \forall\, \Omega \cdot \mathbf{n}(\mathbf{r}) < 0$$

Comment
Many mathematical results in this scenario. Many open problems to extend these...

$$\Omega.\nabla\Psi(\mathbf{r},\Omega) \; + \; \sigma(\mathbf{r})\Psi(\mathbf{r},\Omega) \; = \; (\sigma_S(\mathbf{r}) + \lambda\nu(\mathbf{r})\sigma_f(\mathbf{r})) \underbrace{\frac{1}{4\pi}\int_{\mathbb{S}^2} \Psi(\mathbf{r},\Omega')\,\mathrm{d}\Omega'}_{\text{scalar flux } \phi(\mathbf{r}) \quad (2)} + Q(\mathbf{r}) \qquad (1)$$

Classical Discrete Ordinates (S_N) method:

- apply quadrature with N points $\{\Omega_i\}$ to (2).
- evaluate (1) at $\{\Omega_i\}$: N coupled PDEs
- First order hyperbolic: requires “upwinding”
- modelling geometry? - Discontinuous Galerkin methods
- Linear systems with dimension $\sim 10^8 - 10^{10}$ for accuracy ?

Analogue Monte Carlo: no linear systems

Very important tool

- The source problem

$$\mathcal{T}\Psi(\mathbf{r},\Omega) \;=\; g(\mathbf{r}) \quad + \text{vacuum boundary conditions}$$

can be solved analytically (method of characteristics)

- Average Ψ over angle to get scalar flux:

$$\phi(\mathbf{r}) \;=\; \mathcal{K}_\sigma g(\mathbf{r}) \;=\; \int_V \frac{1}{4\pi}\,\frac{\exp(-\tau(\mathbf{r},\mathbf{r}'))}{\|\mathbf{r}-\mathbf{r}'\|_2^2}\, g(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

$\tau(\mathbf{r},\mathbf{r}')$ = line integral of σ from $\mathbf{r}$ to $\mathbf{r}'$.

$\mathcal{K}_\sigma$ Self-adjoint, positive definite, positive, easy to estimate

Some consequences

- The EVP

$$(\mathcal{T} - \mathcal{S})\Psi(\mathbf{r}, \Omega) = \lambda \mathcal{F}\Psi(\mathbf{r}, \Omega)$$

  is equivalent to a self adjoint generalised EVP for ϕ. This provided an analysis of AMECs algorithms ("method of perturbations")
- The convergence of source iteration

$$\mathcal{T}\Psi^{(i+1)} = \mathcal{S}\Psi^{(i)} + \mathcal{F}\Psi^{(i)} + Q \qquad (3)$$

  can be obtained, implying the convergence of certain analogue MC methods
- Convergence of (3) can be accelerated by inverting $\mathcal{T}$ on subdomains and sharing data on boundaries (domain decomposition)
- diffusion approximation in domains when mean free path is small.

perspective

Very little numerical analysis on BTE since mid-80s

Huge ongoing engineering and physics literatures - Rob J

Huge growth in NA of hyperbolic PDEs in general - adaptivity, DG, multiscale

Huge growth in acceleration of MC for other problems - Rob S

Analysis of MC methods: Probabilistic interpretation of BTE is needed - Andreas