Solving the neutron transport equation within a diffusive regime

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The problem

An important problem in nuclear physics is that of efficiently solving the neutron transport equation. This equation governs the behaviour of neutrons within a nuclear fission reactor. It is used to model reactors for testing and simulation purposes.

$$\Omega \cdot \nabla \psi(x, \Omega) + \sigma_T \psi(x, \Omega) = \frac{\sigma_S}{2} \int_{-1}^{1} \psi(x, \Omega') \, \mathrm{d}\Omega' + q(x, \Omega)$$

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Boundary conditions: $\begin{array}{ll} \psi(a,\mu) = 0, & \mu > 0 \\ \psi(b,\mu) = 0, & \mu < 0 \end{array}$, with $\begin{array}{l} x \in [a,b] \\ \mu \in [-1,1] \end{array}$

Note: $\sigma_T = \sigma_S + \sigma_A$

Operator notation and source iteration

Introduce

$$\mathcal{T}(\cdot) \equiv \mu \frac{\partial}{\partial x}(\cdot) + \sigma_T(\cdot) \quad \text{and define} \quad \phi(x) = \frac{1}{2}\int_{-1}^{1} \psi(x,\mu)\,\mathrm{d}\mu.$$

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Define source iteration as follows

$$\begin{aligned} \mathcal{T}\psi^{(i+1)} &= \sigma_S \phi^{(i)} + q \\ \phi^{(i+1)} &= \tfrac{1}{2}\textstyle\int_{-1}^{1} \psi^{(i+1)}\,\mathrm{d}\mu \end{aligned}$$

This basic iterative method is a contraction, with the difference between successive iterations bounded as (F. Scheben, 2011)

$$\left\|\phi^{(i+1)} - \phi^{(i)}\right\|_2 \leq \frac{\sigma_S}{\sigma_T}\left\|\phi^{(i)} - \phi^{(i-1)}\right\|_2.$$

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$$\sigma_T \equiv \frac{1}{\epsilon}, \quad \sigma_A \equiv \epsilon, \quad \sigma_S \equiv \left[\frac{1}{\epsilon} - \epsilon\right], \quad \text{and} \quad q(x) \equiv \epsilon Q(x)$$

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SPOILER:

$$-\frac{1}{3}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi + \phi = Q + O(\epsilon^2).$$

(boundary conditions: ?)

Implications for source iteration

Looking back to the contraction inequality, we note

$$\begin{aligned}\left\|\phi^{(i+1)}-\phi^{(i)}\right\|_2 &\leq \frac{\sigma_S}{\sigma_T}\left\|\phi^{(i)}-\phi^{(i-1)}\right\|_2 \\ &= \left[1-\epsilon^2\right]\left\|\phi^{(i)}-\phi^{(i-1)}\right\|_2\end{aligned}$$

thus a small ϵ has the potential to cause very slow convergence.
How can we improve on this?

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We want to work with a pair of coupled equations for ψ and ϕ in block operator form, and for this the following will be convenient:

$$\mathcal{P}(\cdot) \equiv \frac{1}{2}\int_{-1}^{1} (\cdot)\, \mathrm{d}\mu, \quad \Sigma(\cdot) \equiv \left[\frac{1}{\epsilon} - \epsilon\right](\cdot).$$

Then $\phi(x) \equiv \mathcal{P}\psi(x, \mu)$

Transport equation as a 2x2 block system

Working from the transport equation in block operator form

$$\begin{pmatrix} \mathcal{T} & -\Sigma \\ -\mathcal{P} & \mathcal{I} \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} = \begin{pmatrix} \epsilon Q \\ 0 \end{pmatrix}$$

Transport equation as a 2x2 block system

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$$\begin{pmatrix} \mathcal{I} & 0 \\ \mathcal{P}\mathcal{T}^{-1} & \mathcal{I} \end{pmatrix} \begin{pmatrix} \mathcal{T} & -\Sigma \\ -\mathcal{P} & \mathcal{I} \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} = \begin{pmatrix} \mathcal{I} & 0 \\ \mathcal{P}\mathcal{T}^{-1} & \mathcal{I} \end{pmatrix} \begin{pmatrix} \epsilon Q \\ 0 \end{pmatrix}$$

where $\mathcal{T}^{-1}$ is defined in F.Scheben, 2011, for the 1D case.

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$$\Rightarrow \qquad \begin{pmatrix} \mathcal{T} & -\Sigma \\ 0 & \mathcal{I} - \mathcal{P}\mathcal{T}^{-1}\Sigma \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} = \begin{pmatrix} \epsilon Q \\ \epsilon \mathcal{P}\mathcal{T}^{-1} Q \end{pmatrix}$$

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Diffusion Approximation Theorem:

$$\frac{1}{\epsilon^2}(\mathcal{I} - \mathcal{P}\mathcal{T}^{-1}\Sigma)\phi = -\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{3}\frac{\mathrm{d}}{\mathrm{d}x}\phi\right) + \phi + O(\epsilon^2)$$

Heuristic proof

We know $\mathcal{T} = \frac{1}{\epsilon}\left(\mathcal{I} + \epsilon\mu\frac{\partial}{\partial x}\right)$, where $\mathcal{I}$ is the identity operator.
Expand:

$$\mathcal{T}^{-1} = \epsilon\left(\mathcal{I} - \epsilon\mu\frac{\partial}{\partial x} + \epsilon^2\mu^2\frac{\partial^2}{\partial x^2} - \dots\right)$$

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Using this expansion

$$\begin{aligned}\mathcal{P}\mathcal{T}^{-1}\Sigma &= \epsilon\mathcal{P}\left(\mathcal{I} - \epsilon\mu\frac{\partial}{\partial x} + \epsilon^2\mu^2\frac{\partial^2}{\partial x^2} - \dots\right)\left[\frac{1}{\epsilon} - \epsilon\right] \\ &= \left[1 - \epsilon^2\right]\left(\mathcal{P} - \epsilon\frac{\partial}{\partial x}\mathcal{P}\mu + \epsilon^2\frac{\partial^2}{\partial x^2}\mathcal{P}\mu^2 - \dots\right).\end{aligned}$$

Note that $\mathcal{P}\mu = 0$, $\mathcal{P}\mu^2 = \frac{1}{3}$ and $\mathcal{P}\phi = \phi$,

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Note that $\mathcal{P}\mu = 0$, $\mathcal{P}\mu^2 = \frac{1}{3}$ and $\mathcal{P}\phi = \phi$, so

$$\begin{aligned}\frac{1}{\epsilon^2}(\mathcal{I} - \mathcal{P}\mathcal{T}^{-1}\Sigma)\phi &= \frac{1}{\epsilon^2}\left(\mathcal{I} - \mathcal{P} - \frac{\epsilon^2}{3}\frac{\partial^2}{\partial x^2}\mathcal{P} + \epsilon^2\mathcal{P} + O(\epsilon^4)\right)\phi \\ &= -\frac{1}{3}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi + \phi + O(\epsilon^2).\end{aligned}$$

Discretise

Transport equation in discrete block matrix form

$$\begin{pmatrix} T & -\Sigma \\ -P & I \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} = \begin{pmatrix} \epsilon Q \\ 0 \end{pmatrix}$$

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$$\Rightarrow \qquad \begin{pmatrix} T & -\Sigma \\ 0 & I - PT^{-1}\Sigma \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} = \begin{pmatrix} \epsilon Q \\ \epsilon PT^{-1}Q \end{pmatrix}$$

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- Form source iteration in block matrix form
- Subtract this from block matrix transport equation
- Conduct the same Gaussian elimination

$$\begin{pmatrix} T & -\Sigma \\ 0 & I - PT^{-1}\Sigma \end{pmatrix} \begin{pmatrix} \psi - \psi^{(i+1)} \\ \phi - \phi^{(i+1)} \end{pmatrix} = \begin{pmatrix} \Sigma(\phi^{(i+1)} - \phi^{(i)}) \\ PT^{-1}\Sigma(\phi^{(i+1)} - \phi^{(i)}) \end{pmatrix}$$

A quick numerical experiment

Iteration	$\|\phi - \phi^{(i)}\|_2$ for $\epsilon = 10^{-3}$
1	1.0e-004
2	1.8e-004
3	9.6e-005
4	4.9e-005
⋮	⋮
14	5.1e-008
15	2.6e-008
16	1.3e-008
17	6.4e-009

Source iteration would take roughly 5 million iterations for the same calculation.

Fynn Scheben.
Iterative Methods for Criticality Computations in Neutron Transport Theory.
PhD thesis, University of Bath, 2011.

Edward W Larsen, J.E Morel, and Warren F Miller Jr.
Asymptotic solutions of numerical transport problems in optically thick, diffusive regimes.
Journal of Computational Physics, 69(2):283 – 324, 1987.