Chapter 1

Recent Work Report, 14:43, Wednesday 5$^{\text{th}}$ June, 2013

1.1 Introduction

In this brief report we will outline some recent work. Notably in section 1.3 we will set up a matrix version of the 1D neutron transport equation under several assumptions (as given in section 1.2). We will use this version to further our understanding of how a diffusion equation can be used to accelerate an iterative solve of the neutron transport equation. In section 1.4 we will give results supporting the suitability of this approximation when working within a *diffusive regime*.

1.2 The Neutron Transport Equation

The 1D, monoenergetic, steady-state form of the neutron transport equation in slab geometry with constant cross-sections (i.e. assuming a homogeneous spatial domain and isotropic scattering) is given by

$$\mu \frac{\partial}{\partial x}\psi(x,\mu) + \sigma_T \psi(x,\mu) = \frac{\sigma_S}{2}\int_{-1}^{1} \psi(x,\mu)\ \mathrm{d}\mu + Q(x), \tag{1.1}$$

with spatial variable $x \in [a,b] \subset \mathbb{R}$ and angular variable $\mu \in [-1,1]$. Here $\psi(x,\mu)$ is known as the *neutron flux* and governs the position and direction of travel of neutrons within a fission reactor. Q is called the *neutron source* and is a non-fission source term of neutrons. We will use vacuum boundary conditions to enforce a requirement for zero incoming neutron flux over the boundary of the spatial domain. These conditions are given by

$$\begin{aligned} \psi(a,\mu) &= 0 \quad \text{for } \mu > 0, \\ \psi(b,\mu) &= 0 \quad \text{for } \mu < 0. \end{aligned} \tag{1.2}$$

So we have that at the left-most end of the domain ($x = a$), the flux in the inward direction (positive μ) is zero, and at the right-most end of the domain ($x = b$), the flux in the inward direction (negative μ) is zero.

Diffusion Theory

Let us define a quantity, $\phi(x) \in L^2[a, b]$, known as the *scalar flux* as follows

$$\phi(x) \equiv \frac{1}{2}\int_{-1}^{1} \psi(x, \mu)\, \mathrm{d}\mu. \tag{1.3}$$

It is known ([5],[4],[3],[2]) that, under certain conditions, the scalar flux can be approximated by a diffusion equation of the form

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{3\sigma_T}\frac{\mathrm{d}}{\mathrm{d}x}\phi(x)\right) + \sigma_A\phi(x) = Q(x), \tag{1.4}$$

with boundary conditions given by

$$\begin{aligned} \phi(a) - \frac{\lambda}{\sigma_T}\phi(a) &= 0, \\ \phi(b) + \frac{\lambda}{\sigma_T}\phi(b) &= 0. \end{aligned} \tag{1.5}$$

To make this approximation several assumptions, given in [5], must be made. These are:

- that the physical medium is several *mean free paths* thick, where a mean free path is the average distance travelled by a neutron between successive collisions,
- that the probability of a neutron collision resulting in a scatter is far higher than it resulting in an absorption, i.e. $\sigma_a \ll \sigma_s$,
- that the neutron flux, cross-sections and source are continuous, and vary by only a 'small amount' in space over the distance of a mean free path.

Unfortunately the third of these assumptions does not hold near boundaries, but the approximation can actually still give accurate predictions by working on a homogenised domain where the cross-sections are averaged spatially (see [6] Chapter 3, p.47).

Asymptotic Formulation

We now move into an asymptotic set up, which will allow us to easily characterise to what extent the above conditions for diffusivity are satisfied. This will be pivotal in understanding how effective a method that relies upon this actually is.

Let us first define a *scale length*, ρ, to be the typical distance over which ψ and q vary by at most an $O(1)$ amount. This value is discussed further in [5], p.288. To

ensure the above conditions for a diffusive regime are satisfied, we can now introduce an asymptotic variable ϵ represents the ratio of a typical mean free path to a scale length. Requiring ϵ to be small now ensures the third condition above holds.

Further specifying $\rho\sigma_A \equiv \epsilon\hat{\sigma}_A$ and that $\rho\sigma_T \equiv \hat{\sigma}_T/\epsilon$ ensures the second diffusive regime condition holds for small ϵ.

From here, nondimensionalising the above diffusion equation in terms of the scale length results in

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{3\hat{\sigma}_T}\frac{\mathrm{d}}{\mathrm{d}x}\phi^\epsilon(x)\right)+\hat{\sigma}_A\phi^\epsilon(x)=\hat{Q}(x). \tag{1.6}$$

with boundary conditions given by

$$\begin{aligned}\phi^\epsilon(a)-\epsilon\frac{\lambda}{\hat{\sigma}_T}\phi^\epsilon(a)=0,\\ \phi^\epsilon(b)+\epsilon\frac{\lambda}{\hat{\sigma}_T}\phi^\epsilon(b)=0.\end{aligned} \tag{1.7}$$

This process is more thoroughly explained in [2] (my 12 month report) and in [5], with boundary conditions given in [3].

Similarly, an asymptotic form of the transport equation, (1.1), is given by

$$\mu\frac{\partial}{\partial x}\psi^\epsilon(x,\mu)+\frac{\hat{\sigma}_T}{\epsilon}\psi^\epsilon(x,\mu)=\frac{1}{2}\left[\frac{\hat{\sigma}_T}{\epsilon}-\epsilon\hat{\sigma}_A\right]\int_{-1}^{1}\psi^\epsilon(x,\mu)\,\mathrm{d}\mu+\epsilon\hat{Q}(x), \tag{1.8}$$

with boundary conditions

$$\begin{aligned}\psi^\epsilon(a,\mu)=0 \quad \text{for } \mu>0,\\ \psi^\epsilon(b,\mu)=0 \quad \text{for } \mu<0.\end{aligned} \tag{1.9}$$

Operator Form

To simplify the notation in (1.8) we can introduce two *operators*, $\mathcal{T}^\epsilon$ and $\mathcal{S}^\epsilon$, that represent the transport and scatter parts of (1.8) respectively. These are defined as follows

$$\begin{aligned}\mathcal{T}^\epsilon(\cdot)&\equiv\frac{1}{\mu}\frac{\partial}{\partial x}(\cdot)+\frac{\hat{\sigma}_T}{\epsilon}(\cdot),\\ \mathcal{S}^\epsilon(\cdot)&\equiv\frac{1}{2}\left[\frac{\hat{\sigma}_T}{\epsilon}-\epsilon\hat{\sigma}_A\right]\int_{-1}^{1}(\cdot)\,\mathrm{d}\mu.\end{aligned} \tag{1.10}$$

These allow for (1.1) to be written in operator form as

$$(\mathcal{T}^\epsilon-\mathcal{S}^\epsilon)\psi^\epsilon=\epsilon\hat{Q}. \tag{1.11}$$

We will take this a little further and define an operator

$$\mathcal{P}(\cdot) = \frac{1}{2}\int_{-1}^{1} (\cdot)\, \mathrm{d}\mu. \tag{1.12}$$

With this the scalar flux can be written as $\phi^\epsilon(x) \equiv \mathcal{P}\psi^\epsilon(x,\mu)$.

The operator notation will be useful in understanding how the structure of the matrix set up represents the neutron transport equation in the next section.

Moving forwards, it is these asymptotic versions of the transport and diffusion equations that we will use.

1.3 Matrix Form of the Neutron Transport Equation

In this section we will formulate (1.11) as a matrix vector system, and then move towards understanding how diffusion theory can be used as a tool when solving the system iteratively. First of all, we will run through the specifics of the discretisation used. Throughout this section we will be working with the asymptotic versions of all variables, though we will drop the $(\cdot)^\epsilon$ to avoid overcrowded notation.

Discretisation

To discretise (1.11) in angle we apply discrete ordinates and specify that the equation holds at $2N$ discrete angular points, $\mu_j \in (-1,1)\backslash\{0\}$ for $1 \leq |j| \leq N$. We choose these to be Gauss quadrature points with corresponding weights ω_j for $1 \leq |j| \leq N$. Then the integral over μ can be represented as a weighted gauss quadrature sum

$$\mathcal{P}\psi(x,\mu) = \frac{1}{2}\sum_{|j|=1}^{N} \omega_j \psi(x,\mu_j).$$

We will use a method known as diamond differencing to discretise in space using $M+1$ uniformly distributed points $x_i in [a,b]$, with $0 \leq i \leq M$. Further define half-points by $2x_{i+1/2} \equiv x_i + x_{i+1}$ for $0 \leq i \leq M-1$. Let us also introduce the notation $\psi(x_i,\mu_j) \equiv \psi_{i,j}$. We then replace the derivative in x by a centred difference at surrounding nodes

$$\frac{\partial}{\partial x}\psi(x_{i+1/2},\mu_j) = \frac{\psi_{i+1,j}-\psi_{i,j}}{x_{i+1}-x_i},$$

and we approximate the flux at zone centres by the average of their values at surrounding nodes

$$\psi(x_{i+1/2},\mu_j) = \frac{\psi_{i,j}+\psi_{i+1,j}}{2}.$$

The Matrix Form

The full details of the matrix set up can be found in [1], chapter 3. Here we will give only the resulting matrix-vector system and say what each block represents. So, first of all the discretised matix-vector formulation of the neutron transport equation described by (1.11) is given by

$$\begin{pmatrix} T & -\Sigma \\ -P & I \end{pmatrix} \begin{pmatrix} \Psi \\ \Phi \end{pmatrix} = \begin{pmatrix} Q \\ 0 \end{pmatrix}. \tag{1.13}$$

Within this form, $\Psi \in \mathbb{R}^{2N(M+1)}$ is a vector containing ψ evaluated at all relevant combinations of discrete points x_i and μ_j. $\Phi \in \mathbb{R}^M$ is also a vector, however it is evaluated at the half-points of the spatial domain and so is only of length M. $T \in \mathbb{R}^{2N(M+1)\times 2N(M+1)}$ is a square, non-symmetric, tridiagonal matrix representation of the transport operator, $\mathcal{T}$, defined above. So this means that $T\Psi$ is a discretised version of $\mathcal{T}\psi$. $\Sigma \in \mathbb{R}^{2N(M+1)\times M}$ implements a 'multiplication by σ_S' of the vector Φ. This means that $\Sigma\Phi$ is a discretised version of $\sigma_S\phi$. $P \in \mathbb{R}^{M\times 2N(M+1)}$ carries out the weighted Gauss quadrature summation specified above. Thus $P\Psi$ is a discretised version of $\mathcal{P}\psi$.

This form contains two systems of equations: the first is a discrete version of the transport equation, and the second imposes the condition $\phi \equiv \mathcal{P}\psi$.

Source Iteration and the Diffusion Error Equation

Source iteration based on 1D transport equation defined in (1.11) is given by

$$\mathcal{T}\psi^{(1/2)} = \mathcal{S}\psi^{(0)} + \epsilon\hat{Q}. \tag{1.14}$$

We are using a basic 'half step' notation here to simplify the set up. From here we can obtain an equation for the current error in our approximation, $\psi - \psi^{(1/2)}$. To do this we subtract the iterative equation (1.14) away from an exact formulation, then rearrange to obtain

$$(\mathcal{T} - \mathcal{S})(\psi - \psi^{(1/2)}) = \left[\frac{\hat{\sigma}_T}{\epsilon} - \epsilon\hat{\sigma}_A\right](\phi^{(1/2)} - \phi^{(0)}). \tag{1.15}$$

Unfortunately solving this is as hard as solving the original problem. Instead we would like to obtain a good and (crucially) easily calculable approximate solution. To this end we look to the diffusion theory introduced above.

To obtain the diffusion approximation to (1.15) we follow the theory developed for (1.6) to approximate (1.11) and obtain

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{3\hat{\sigma}_T}\frac{\mathrm{d}}{\mathrm{d}x}(\phi-\phi^{(1/2)})\right)+\hat{\sigma}_A(\phi-\phi^{(1/2)})=\frac{\left[\frac{\hat{\sigma}_T}{\epsilon}-\epsilon\hat{\sigma}_A\right]}{\epsilon}(\phi^{(1/2)}-\phi^{(0)}). \quad (1.16)$$

We will refer back to this equation later when establishing how the diffusion approximation comes in to a matrix set up.

Matrix Form

To represent source iteration in matrix form, we must split the system (1.13) as follows

$$\begin{pmatrix} T & 0 \\ -P & I \end{pmatrix}\begin{pmatrix} \Psi^{(1/2)} \\ \Phi^{(1/2)} \end{pmatrix}=\begin{pmatrix} 0 & \Sigma \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \Psi^{(0)} \\ \Phi^{(0)} \end{pmatrix}+\begin{pmatrix} Q \\ 0 \end{pmatrix}. \quad (1.17)$$

From this we can easily obtain an equation for the current error in our approximation. To do this we subtract the iterative equation (1.17) away from an exact formulation, then rearrange to obtain

$$\begin{aligned}\begin{pmatrix} T & -\Sigma \\ -P & I \end{pmatrix}\begin{pmatrix} \Psi-\Psi^{(1/2)} \\ \Phi-\Phi^{(1/2)} \end{pmatrix} &= \begin{pmatrix} 0 & \Sigma \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \Psi^{(1/2)}-\Psi^{(0)} \\ \Phi^{(1/2)}-\Phi^{(0)} \end{pmatrix}, \\ &= \begin{pmatrix} \Sigma(\Phi^{(1/2)}-\Phi^{(0)}) \\ 0 \end{pmatrix}.\end{aligned} \quad (1.18)$$

This is an equation for the error in the approximation $\left(\Psi^{(1/2)},\Phi^{(1/2)}\right)^\top$, but solving it is as hard as solving the original problem. Instead we would like to obtain a good and (crucially) easily calculable approximate solution. To this end we look to the diffusion theory introduced above.

Diffusion Synthetic Acceleration and Preconditioning

In a method called *diffusion synthetic acceleration* (DSA) an approximation to the error in (1.14), namely $\phi-\phi^{(1/2)}$, is obtained using the diffusion equation as discussed above. We now want to establish how to bring this into the matrix set up. To this end, we premultiply (1.18) as follows

$$\begin{aligned}&\begin{pmatrix} I & 0 \\ PT^{-1} & I \end{pmatrix}\begin{pmatrix} T & -\Sigma \\ -P & I \end{pmatrix}\begin{pmatrix} \Psi-\Psi^{(1/2)} \\ \Phi-\Phi^{(1/2)} \end{pmatrix}=\begin{pmatrix} I & 0 \\ PT^{-1} & I \end{pmatrix}\begin{pmatrix} \Sigma(\Phi^{(1/2)}-\Phi^{(0)}) \\ 0 \end{pmatrix}, \\ \Rightarrow\quad &\begin{pmatrix} T & -\Sigma \\ 0 & I-PT^{-1}\Sigma \end{pmatrix}\begin{pmatrix} \Psi-\Psi^{(1/2)} \\ \Phi-\Phi^{(1/2)} \end{pmatrix}=\begin{pmatrix} \Sigma(\Phi^{(1/2)}-\Phi^{(0)}) \\ PT^{-1}\Sigma(\Phi^{(1/2)}-\Phi^{(0)}) \end{pmatrix}.\end{aligned} \quad (1.19)$$

The system now contains an equation for the discrete form of the error that we are interested in approximating, namely

$$(I - PT^{-1}\Sigma)(\Phi - \Phi^{(1/2)}) = PT^{-1}\Sigma(\Phi^{(1/2)} - \Phi^{(0)}). \tag{1.20}$$

1.4 Numerical Tests

In this section we aim to numerically justify DSA as a method for solving the neutron transport equation within a diffusive regime (as defined above). We begin by looking at the nature of the matrix $I - PT^{-1}\Sigma$ and try to justify why approximating the solution to its associated inverse problem is a good idea in the first place. We will then look at results which support the use of the diffusion approximation in particular.

Why approximate?

So firstly, why should we approximate the solution to (1.20) when working within a diffusive regime? To answer this we examine the nature of $I - PT^{-1}\Sigma$.

For a value of $M = 64$, it is found that $\left\|(I - PT^{-1}\Sigma) - (I - PT^{-1}\Sigma)^\top\right\|_2 \approx 10^{-16}$. Thus numerically we are justified in assuming this matrix to be symmetric, though this should be analytically justifiable too.

For a symmetric matrix, say A, the Spectral Theorem allows us to choose the eigenvectors to form an orthonormal basis. Hence $A = X\Lambda X^\top$, where the columns of X contain the eigenvectors of A, and Λ is a diagonal matrix of the associated eigenvalues. In this case we have that, up to sign, the eigenvalues equal the singular values of A and so the condition number satisfies

$$\kappa(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)} = \frac{|\lambda_{\max}(A)|}{|\lambda_{\min}(A)|}.$$

The following table contains the absolute values of the maximum and minimum eigenvalues of $I - PT^{-1}\Sigma$ for $M = 64$ corresponding to an orthonormalised basis of eigenvectors. It also contains their ratio, which is the condition number. These values are given as $\epsilon \to 0$, which represents a move into a diffusive regime.

ϵ	$\lvert\lambda_{\max}\rvert$	$\lvert\lambda_{\min}\rvert$	$\kappa(I - PT^{-1}\Sigma)$
10^{-1}	1.0e+000	3.4e-002	2.9e+001
10^{-2}	9.8e-001	4.2e-004	2.3e+003
10^{-3}	8.2e-001	4.3e-006	1.9e+005
10^{-4}	3.0e-001	4.3e-008	6.9e+006
10^{-5}	4.0e-002	4.3e-010	9.2e+007
10^{-6}	4.1e-003	4.3e-012	9.5e+008
10^{-7}	4.1e-004	4.5e-014	9.1e+009
10^{-8}	4.1e-005	3.0e-015	1.4e+010

This table shows that the minimum eigenvalue of $I - PT^{-1}\Sigma$ goes as $O(\epsilon^2)$, whereas the maximum only goes with $O(\epsilon)$. This causes the condition number to behave like $O(\epsilon^{-1})$. As a consequence, the matrix $I - PT^{-1}\Sigma$ becomes more and more poorly conditioned as we move toward a diffusive regime. This suggests that within such a regime, solving an associated matrix system is likely to be inaccurate and so approximating the solution could be a better choice.

Why Diffusion?

This section presents some numerical evidence in support of using a diffusion approximation (as presented above) to approximate the solution of (1.20) when working within a diffusive regime.

DSA as we have presented can be viewed as a 2-step iterative process: the first half of the iteration is one source iteration ($\phi^0 \to \phi^{1/2}$); the second half is one diffusion solve ($\phi^{1/2} \to \phi^1$). We will first see how much each of these steps alters the current approximation, i.e. how much input each step has to the overall progression of the iterative process. The following table contains the 2-norms of the difference made by each step: $\left\|\phi^{1/2} - \phi^0\right\|_2$ for the source iteration difference, and $\left\|\phi^1 - \phi^{1/2}\right\|_2$ for diffusion. These are again given for decreasing ϵ to induce a move toward a diffusive regime. In all cases, these are from the first step of DSA as a whole with $M = 64$, and are found using a random (but consistent throughout) initial guess. Looking at later steps or different values of M did not affect the pattern seen and so have not been included.

ϵ	$\left\|\phi^{1/2}-\phi^{0}\right\|_2$	$\left\|\phi^{1}-\phi^{1/2}\right\|_2$
10^{-1}	1.8e+000	1.6e+000
10^{-2}	9.9e-001	2.4e+000
10^{-3}	2.6e-001	5.6e+000
10^{-4}	6.0e-002	9.8e+000
10^{-5}	8.7e-003	1.2e+001
10^{-6}	9.1e-004	1.2e+001
10^{-7}	9.1e-005	1.2e+001
10^{-8}	9.1e-006	2.5e+001

From this it is clear that as $\epsilon \to 0$ the influence of the source iteration step goes with $O(\epsilon)$, but the influence of the diffusion step remains constant. This means that as the diffusivity of the domain increases, DSA becomes progressively more dominated by the diffusion approximation step.

This supports the use of the diffusion approximation, provided that its influence is productive in reducing the *error* in the solution. To see this we look at another table which gives the *error* in the current approximation, where by error we mean

$$\mathrm{err}(\tilde{\phi}) \equiv \left\|\phi - \tilde{\phi}\right\|_2 .$$

Here ϕ represents the true solution to the problem, and $\tilde{\phi}$ represents our approximation. We look at values for this error both after the source iteration step and after the diffusion step ($\mathrm{err}(\phi^{1/2})$ and $\mathrm{err}(\phi^{1})$ respectively).

ϵ	$\mathrm{err}(\phi^{1/2})$	$\mathrm{err}(\phi^{1})$
10^{-1}	1.8e+000	3.7e-001
10^{-2}	2.9e+000	8.6e-001
10^{-3}	3.3e+000	2.8e+000
10^{-4}	3.3e+000	5.0e+000
10^{-5}	3.3e+000	7.4e+000
10^{-6}	3.3e+000	7.8e+000
10^{-7}	3.4e+000	7.9e+000
10^{-8}	4.3e+000	2.1e+001

I think instead of this table I need to look at the convergence of the whole iteration. Convergence there when almost all of the change is coming from the diffusion part would show a productive influence from the diffusion.

References

[1] J. C. H. Blake. Preconditioning of iterative methods for the transport equation. Master's thesis, University of Bath, 2011.

[2] J. C. H. Blake. 12 month report. Online at people.bath.ac.uk/jchb20/docs.html, December 2012. University of Bath.

[3] FranÃ§ois Golse, Shi Jin, and C. David Levermore. The convergence of numerical transfer schemes in diffusive regimes i: Discrete-ordinate method. *SIAM Journal on Numerical Analysis*, 36(5):1333–1369, 1999.

[4] Edward W. Larsen. Diffusion theory as an asymptotic limit of transport theory for nearly critical systems with small mean free paths. *Annals of Nuclear Energy*, 7(4-5):249 – 255, 1980.

[5] 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.

[6] W.M. Stacey. *Nuclear reactor physics*. Wiley-VCH, 2007.