Radiation Transport Equation

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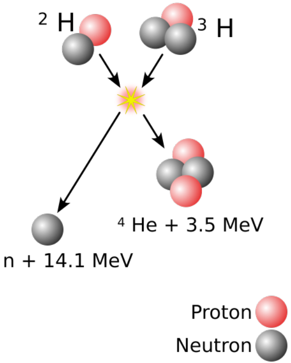
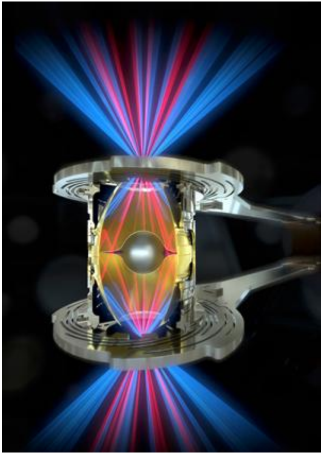
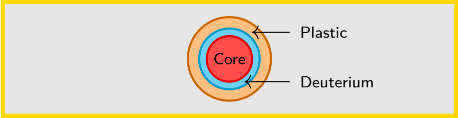
Deuterium-Tritium Fusion





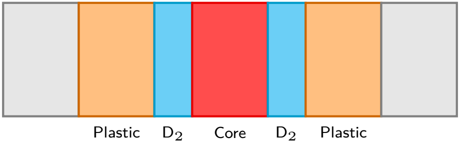
Hohlraum

Gold Foil Wall



$$\begin{cases} \Omega \cdot \nabla_x \psi + \sigma_t \psi = q + \frac{\sigma_s}{4\pi} \int_{S^2} \psi(x, \Omega)\, d\Omega \\ \psi : \mathbb{R}^3 \times S^2 \to \mathbb{R} \quad x \in \mathbb{R}^3, \Omega \in S^2 \quad \psi(x_{inflow}) = \alpha \end{cases}$$

1D Slab Geometry



$$\begin{cases} \mu \partial_x \psi + \sigma_t \psi = q + \frac{\sigma_s}{4\pi} \int_{-1}^{1} \psi(x, \mu) 2\pi\, d\mu \\ \psi : \mathbb{R} \times [-1, 1] \quad x \in \mathbb{R}, \mu = \Omega \cdot \vec{e}_1 \in [-1, 1] \quad \psi(x_{inflow}) = \alpha \end{cases}$$

Discretized Integral

Consider the quadrature of order $\mathcal{L}$:

$$\int_{-1}^{1} \psi(x,\mu)d\mu = \sum_{\ell \in \mathcal{L}} w_\ell \psi(x,\mu_\ell)$$

Then we have the system of equations:

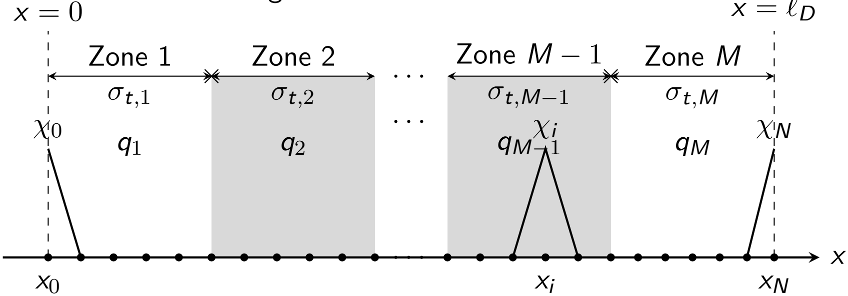
$$\mu_\ell \, \partial_x \psi_\ell + \sigma_t \psi_\ell = q + \frac{\sigma_s}{4\pi} \sum_{\ell \in \mathcal{L}} w_\ell \psi(x,\mu_\ell)$$

so it makes sense to first solve the simplified equation, an advection-reaction PDE:

$$\mu_\ell \psi_\ell'(x) + \sigma_t(x)\psi_\ell(x) = q(x) \quad \forall\, \ell \in \mathcal{L}$$

Setup of Mesh

We assume that σ_t, σ_s, $q(x)$ are constant across zones, and in particular are constant inside a single cell.



Standard hat functions $\chi_i \in \mathbb{V}_h$, $\chi_i : \mathbb{R} \to [0, 1]$,

$$\chi_i = \begin{cases} \frac{x - x_{i-1}}{x_i - x_{i-1}} & x \in [x_{i-1}, x_i] \\ \frac{x_{i+1} - x}{x_{i+1} - x_i} & x \in [x_i, x_{i+1}] \\ 0 & \text{otherwise} \end{cases}$$

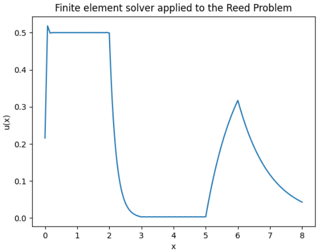
Finite Elements Formulation (Galerkin)

The finite element formulation is:

$$\int_0^{\ell_D} (\mu \partial_x \psi_h) \chi_i \, dx + \int_0^{\ell_D} \sigma_t \psi_h \chi_i dx + \underline{\mu \psi_h(x_{\text{in}}) \chi_i(x_{\text{in}})}$$
$$= \int_0^{\ell_D} q \chi_i \, dx + \underline{\mu \alpha \chi_i(x_{\text{in}})}, \quad \forall i = 0, ..., N_h$$

The underlined terms are our weakly enforced inflow boundary conditions.

Naive Finite Element Solution



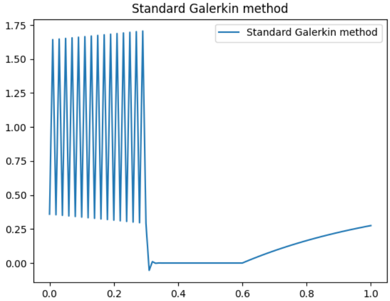
Reed Problem Benchmark					
Length	2	1	2	1	2
Cells	25	25	25	25	25
σ_t	50	5	0	1	1
q	25	0	0	0.5	0
α	0.0				
μ	1.0				

h	L^1 Error	Conv. Rate
4.00×10^{-2}	3.33×10^{-3}	—
2.00×10^{-2}	8.72×10^{-4}	1.93
1.00×10^{-2}	2.21×10^{-4}	1.98
5.00×10^{-3}	5.54×10^{-5}	2.00
2.50×10^{-3}	1.39×10^{-5}	2.00
1.25×10^{-3}	3.47×10^{-6}	2.00
6.25×10^{-4}	8.67×10^{-7}	2.00
3.13×10^{-4}	2.17×10^{-7}	2.00

What Goes Wrong?

Although the numerical method is convergent in $||\cdot||_{L^1}$, the gradient was not bounded and thus there is no control on the oscillations of the solution.

Internal boundary layers appear when σ_t changes rapidly; this leads to instability.



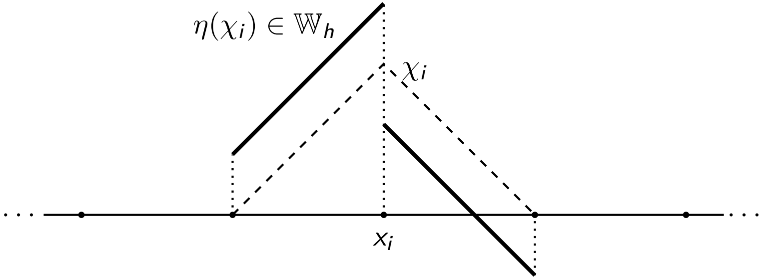
Boundary Value Benchmark			
Length	0.3	0.3	0.4
Cells	30	30	40
σ_t	1.0	1×10^5	2
q	1.0	0.0	1.0
α		1.0	
μ		1.0	

Streamline Upwind Petrov–Galerkin (SUPG)

The Petrov method involves continuing to use $\mathbb{V}_h$ as the trial space where the solution lives, but now the test functions are in:

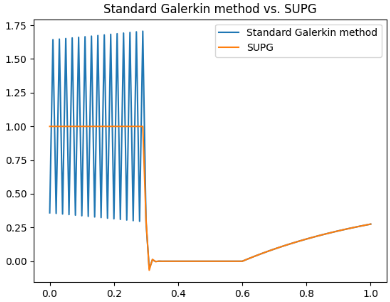
$$\mathbb{W}_h := \mathrm{span}_{i\in\text{Vertices}}\left\{\chi_i(x) + \sum_{K\in\text{Cells}} \tau_K \mu\, \chi'_{|K}(x)\right\},\ \tau_K = \frac{h_K}{2|\mu|}\frac{1}{\max(1, \sigma_t h_K)}$$

Note $\tau_K = 0$ is Galerkin.



SUPG Results

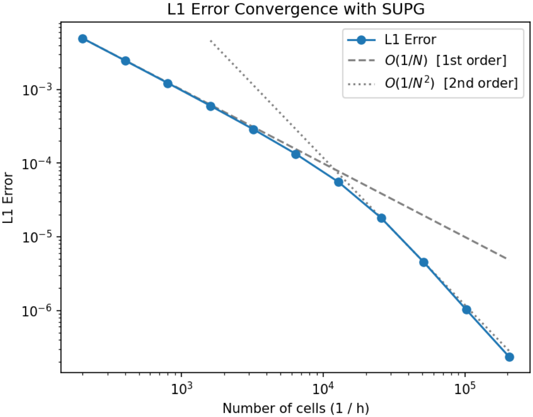
For the previous problem with boundary layers, SUPG performs much better.



Boundary Value Benchmark			
Length	0.3	0.3	0.4
Cells	30	30	40
σ_t	1.0	1×10^5	2
q	1.0	0.0	1.0
α	1.0		
μ	1.0		

SUPG Results

This method is stable around boundary layers (large changes in σ_t), but with a coarse mesh it does not converge quadratically around them.



Reintroducing Integral Term

Now that we can solve each individual Advection-Reaction Equation:

$$\mu_\ell \psi_\ell'(x) + \sigma_t(x)\psi_\ell(x) = q(x) \quad \forall\, \ell \in \mathcal{L}$$

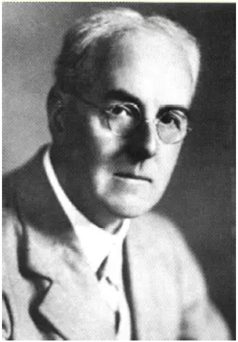
We can return to the system of equations:

$$\mu_\ell\, \partial_x \psi_\ell + \sigma_t \psi_\ell = q + \frac{\sigma_s}{4\pi} \sum_{\ell \in \mathcal{L}} w_\ell \psi(x, \mu_\ell)$$

Thus, the system we want to solve is a system of differential equations (for each $\ell \in \mathcal{L}$) coupled by the RHS.

Richardson Iteration

When we discretize our mesh and use the finite element method to solve the differential equations, we get a very large linear system.



Solving it is impractical, but because the only coupling term is the flux integral, we can use Richardson iteration.

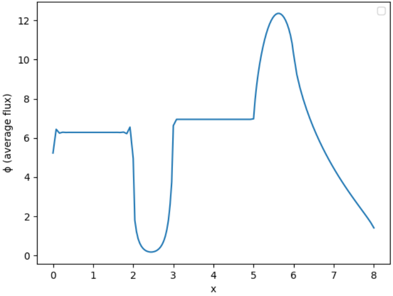
Richardson Iteration (cont.)

Algorithm: Richardson Iteration for Transport

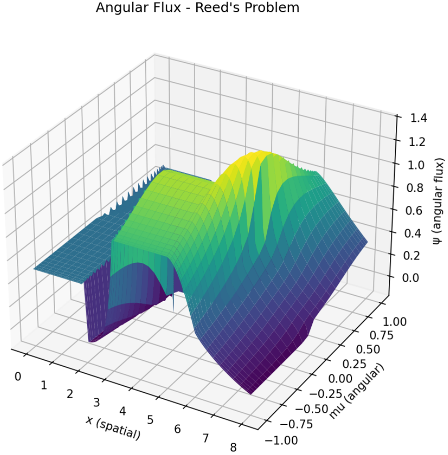
1. Take a scalar flux guess $\phi^{(0)} = 0$
2. Solve the system of differential equations using our scalar flux guess. $\mu_\ell \frac{d\psi^{\ell,(k)}}{dx} + \sigma_t(x)\psi^{\ell,(k)}(x) = q(x) + \frac{\sigma_s(x)}{4\pi}\phi^{(k)}(x)$
3. Calculate a new scalar flux guess using quadrature with our solutions to the system of equations. $\phi^{(k+1)}(x) = \sum_{\ell' \in \mathcal{L}} w_{\ell'} \psi^{\ell',(k)}(x)$
4. Repeat until convergence.

For problems where $\frac{\sigma_t - \sigma_s}{\sigma_t} \approx O(1)$, i.e. sufficiently high absorption, Banach fixed point theorem guarantees convergence, so the algorithm works.

Reed Problem Across All Angles



Reed Problem Benchmark					
Length	2	1	2	1	2
Cells	25	25	25	25	25
σ_t	50	5	0	1	1
σ_s	0	0	0	0.9	0.9
q	25	0	0	0.5	0
α	0.0				
Angles	32				



Preconditioning

In the regime where $\sigma_s >> \sigma_a$, Richardson iteration needs exponentially more steps to converge, which quickly becomes prohibitive.

σ_s/σ_t	Iterations
0.0	1
0.25	14
0.5	27
0.9	174
1.0	57006

Scattering Benchmark	
Length	10
Cells	100
σ_t	10
q	0.05
α	1.0
Angles	8

Preconditioning (cont.)

We assume $\sigma_s \sim 1/\varepsilon$, $\sigma_a \sim \varepsilon$. Via the method of asymptotic expansion, we introduce

$$\psi = \psi^{(0)} + \varepsilon\psi^{(1)} + \varepsilon^2\psi^{(2)} + \cdots \text{ as } \varepsilon \to 0$$

into

$$\Omega \cdot \nabla_x \psi^\varepsilon(x, \Omega) + \frac{\sigma_t}{\varepsilon}\psi^\varepsilon(x, \Omega) = \varepsilon q(x) + \frac{1}{4\pi}\left[\frac{\sigma_t}{\varepsilon} - \sigma_a\varepsilon\right]\int_{S^2} \psi^\varepsilon(x, \Omega')d\Omega'$$

By grouping the $o(1/\varepsilon)$, $o(1)$, $o(\varepsilon)$, ... terms we see that the former dominates, and we obtain a Poisson PDE:

$$-\nabla \cdot \left(\frac{1}{3\sigma_t}\nabla\psi^{(0)}(x)\right) + \sigma_a\psi^{(0)}(x) = 4\pi q(x)$$

Preconditioning (cont.)

Define a mapping $r \mapsto \Phi_h(r)$.

Multiplying by a test function $v_h \in \mathbb{V}_h$ and using integration by parts gives:

$$\int_0^{\ell_D} \frac{1}{3\sigma_t} \Phi_h(r)' v_h' dx + \int_0^{\ell_D} \sigma_a \Phi_h(r) v_h dx \\ + \frac{\overline{\omega}}{4} \{\Phi_h(r)(0) v_h(0) + \Phi_h(r)(\ell_D) v_h(\ell_D)\} = \int_0^{\ell_D} r \, dx$$

We can solve this via classical Finite Element Method.

Preconditioning (cont.)

Let Φ_h be the FEM solution operator for our Poisson problem.

We use $M := \mathbb{I} + \Phi_h$ as a preconditioner for our Richardson iteration!

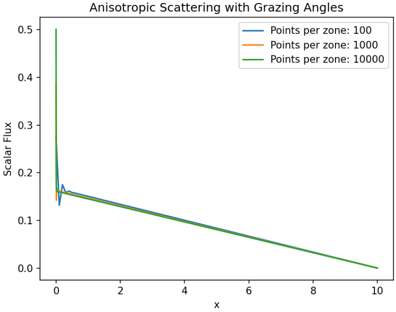
σ_s/σ_t	Iterations
0.0	1
0.25	5
0.5	6
0.9	10
1.0	22

Scattering Benchmark	
Length	10
Cells	100
σ_t	10
q	0.05
α	1.0
Angles	8

Grazing Problem

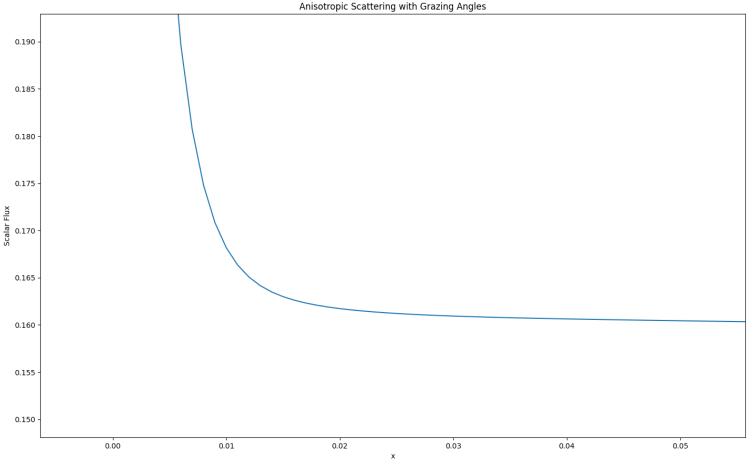
Consider boundary condition imposed on the "grazing" direction:

$$\psi(0,\mu) = \begin{cases} 1 & \mu = \mu_0 \approx 0 \\ 0 & \text{else} \end{cases}$$



Grazing Benchmark	
Length	10
Cells	100
σ_t	100
σ_s	100
q	0.0
$\psi_0(\mu)$	1.0
Angles	8

Internal Boundary Layer - Grazing Problem



Takeaways

- Moving from theory to implementation takes tremendous care
- Good coding practices and test cases are vital
- Organizing code is essential as the project scales
- Rigorous justification of our methods is harder than writing them

Conclusion

1. Radiation Transport Equation
2. Naive Method for Advection-Reaction via Galerkin
3. Improved Method via SUPG
4. Reintroduced Integral Term
5. Richardson Iteration
6. Preconditioning

Acknowledgments

Prof. Guermond

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Appendix A: a priori 1-D energy estimate

$$\mu u'(x) + \sigma_t(x) u(x) = q(x), \quad u(x_{\text{inflow}}) = \alpha$$

$$\mu u' + \sigma_t u + \frac{1}{2}(|\mu \vec{e}_1 \cdot \vec{n}| - \mu \vec{e}_1 \cdot \vec{n}) u = q + \frac{1}{2}(|\mu \vec{e}_1 \cdot \vec{n}| - \mu \vec{e}_1 \cdot \vec{n}) \alpha$$

$$v \left[\mu u' + \sigma_t u + \frac{1}{2}(|\mu \vec{e}_1 \cdot \vec{n}| - \mu \vec{e}_1 \cdot \vec{n}) u \right] = v \left[q + \frac{1}{2}(|\mu \vec{e}_1 \cdot \vec{n}| - \mu \vec{e}_1 \cdot \vec{n}) \alpha \right]$$

$$\int_D \mu v u' \, dx + \int_D \sigma_t v u \, dx + \frac{1}{2} \int_{\partial D} (|\mu \vec{e}_1 \cdot \vec{n}| - \mu \vec{e}_1 \cdot \vec{n}) u v \, dx$$

$$= \int_D v q + \frac{1}{2} \int_{\partial D} (|\mu \vec{e}_1 \cdot \vec{n}| - \mu \vec{e}_1 \cdot \vec{n}) \alpha \, dx, \quad \forall \, v \in \mathbb{V}_h.$$

Now let $v = u$ for the energy estimate and we have

$$\int_D \mu u u' dx + \int_D \sigma_t u u dx + \frac{1}{2}\int_{\partial D}(|\mu\vec{e}_1\cdot\vec{n}| - \mu\vec{e}_1\cdot\vec{n})u^2\,dx$$

$$= \int_D uq + \frac{1}{2}\int_{\partial D}(|\mu\vec{e}_1\cdot\vec{n}| - \mu\vec{e}_1\cdot\vec{n})\alpha u\,dx$$

$$\frac{\mu}{2}\int_D (u^2)' dx + \sigma_t \int_D u^2 dx = \int_D u(x)q(x) \le ||u||_2||q||_2 \le \frac{||u||_2^2}{2\varepsilon} + \frac{\varepsilon||q||_2^2}{2}$$

$$\frac{\mu}{2}\left. u^2\right|_{\partial D} + \sigma_t||u||_2^2 \le \frac{\sigma_t||u||_2^2}{2} + \frac{||q||_2^2}{2\sigma_t} + \frac{1}{2}\int_{\partial D}(|\mu\vec{e}_1\cdot\vec{n}| - \mu\vec{e}_1\cdot\vec{n})\alpha u\,dx$$

$$\frac{\mu}{2}\left. u^2\right|_{\partial D} + \frac{\sigma_t}{2}||u||_2^2 \le \frac{||q||_2^2}{2\sigma_t} + \frac{1}{2}\int_{\partial D}(|\mu\vec{e}_1\cdot\vec{n}| - \mu\vec{e}_1\cdot\vec{n})\alpha u\,dx$$

$$\min\sigma_t||u||_2^2 \le \frac{||q||_2^2}{\min\sigma_t} + |\mu\vec{e}_1\cdot\vec{n}|\alpha^2$$

Appendix B: Energy estimate in $\mathbb{R}^n$

We begin with the following advection-reaction equation with boundary condition:

$$\Omega \cdot \nabla_x u + \sigma_t u = q, \quad u(x_{inflow}) = \alpha$$

We "weakly" incorporate the inflow condition into the PDE:

$$\begin{aligned}\int_D u(\Omega \cdot \nabla_x u) + \int_D \sigma_t u^2 + \int_{\partial D} \frac{1}{2}(|\Omega \cdot \vec{n}| - \Omega \cdot \vec{n})u^2 \\ = \int_D qu + \frac{1}{2}\int_{\partial D}(|\Omega \cdot \vec{n}| - \Omega \cdot \vec{n})\alpha u\end{aligned}$$

$$\int_D u(\Omega \cdot \nabla_x u) = \int_D \Omega \cdot u\nabla_x u = \frac{1}{2}\int_D \nabla_x \cdot (u^2\Omega) = \frac{1}{2}\int_{\partial D} u^2\Omega \cdot \vec{n}\, dS$$

Appendix B (cont.)

$$\int_D \sigma_t u^2 - \int_{\partial D^-} u^2 \Omega \cdot \vec{n} + \frac{1}{2} \int_{\partial D} u^2 \Omega \cdot \vec{n}$$

$$= \int_D \sigma_t u^2 - \frac{1}{2} \int_{\partial D^-} u^2 \Omega \cdot \vec{n} + \frac{1}{2} \int_{\partial D^+} u^2 \Omega \cdot \vec{n}$$

$$= \int_D qu - \int_{\partial D^-} (\Omega \cdot \vec{n}) \alpha u$$

$$\leq \frac{||q||_2^2}{2 \min \sigma_t} + \frac{\min \sigma_t ||u||_2^2}{2} - \int_{\partial D^-} (\Omega \cdot \vec{n}) \alpha u$$

$$\frac{1}{2} \min \sigma_t ||u||_2^2 - \frac{1}{2} \int_{\partial D^-} u^2 \Omega \cdot \vec{n} + \frac{1}{2} \int_{\partial D^+} u^2 \Omega \cdot \vec{n}$$

$$\leq \frac{||q||_2^2}{2 \min \sigma_t} - \int_{\partial D^-} (\Omega \cdot \vec{n}) \alpha u$$

$$\int_{\partial D^-} |\alpha u| \leq ||u||_2 ||\alpha||_2 \leq \frac{||u||_2^2}{2} + \frac{||\alpha||_2^2}{2}$$

$$\int_{\partial D^-} |(\Omega \cdot \vec{n})\alpha u| \leq -\frac{1}{2}\int_{\partial D^-} (\Omega \cdot \vec{n}) u^2 - \frac{1}{2}\int_{\partial D^-} (\Omega \cdot \vec{n})\alpha^2$$

So consider

$$\frac{1}{2}\min \sigma_t ||u||_2^2 - \frac{1}{2}\int_{\partial D^-} u^2 \Omega \cdot \vec{n} + \frac{1}{2}\int_{\partial D^+} u^2 \Omega \cdot \vec{n}$$

once more and notice that we can cancel the leftmost term of the RHS above, also the the other boundary condition on the LHS is strictly positive, and so we have as before

$$\min \sigma_t ||u||_2^2 \leq \frac{||q||_2^2}{\min \sigma_t} - \int_{\partial D^-} (\Omega \cdot \vec{n})\alpha^2$$

Appendix C: Better 1-D Bound and Existence

$$I(x)u' + (\sigma_t/\mu)I(x)u = q/\mu I(x) \iff (I(x)u)' = (q/\mu)I(x)$$

since $I'(x) = \frac{\sigma_t(x)}{\mu}I(x)$. Then,

$$u(x) = \frac{1}{\mu I(x)}\int_0^x qI(s)ds$$

$$= \frac{1}{\mu}\exp\left(-\frac{1}{\mu}\int_0^x \sigma_t(\tau)d\tau\right)\int_0^x q\exp\left(\frac{1}{\mu}\int_0^s \sigma_t(\tau)d\tau\right)ds$$

$$= \frac{1}{\mu}\int_0^x q \exp\left(-\frac{1}{\mu}\int_0^x \sigma_t(\tau)d\tau\right)\exp\left(\frac{1}{\mu}\int_0^s \sigma_t(\tau)d\tau\right) ds$$

$$= \frac{1}{\mu}\int_0^x q \exp\left(-\frac{1}{\mu}\int_s^x \sigma_t(\tau)d\tau\right) ds$$

By assumption $\sigma_t > 0$, so $\exp(\cdots) \leq 1$ and

$$|u(x)| \leq \frac{1}{\mu}\int_0^x q\, ds \leq \frac{1}{\mu}||q||_2\sqrt{x}$$

$$||u||_2^2 = \int_0^L |u|^2\, dx \leq \int_0^L \frac{1}{\mu^2}||q||_2^2 x\, dx \leq \frac{||q||_2^2}{\mu^2}L$$

$$||u||_2 \leq \frac{||q||_2}{\mu}\sqrt{L}$$

Appendix D: Uniqueness

We could use either estimate to show this, but the second is more obvious. Suppose that u_1 and u_2 both satisfy

$$\mu u'(x) + \sigma_t(x)u(x) = q(x), \quad u(x_{\text{inflow}}) = \alpha$$

then $u_1 - u_2 = v$ satisfies

$$\mu v'(x) + \sigma_t(x)v(x) = 0, \quad v(x_{\text{inflow}}) = 0$$

and

$$||v||_2^2 = \int v^2 \leq 0 \implies v = u_1 - u_2 = 0$$