Radiation Transport Material Analysis

MTH 656 - Final Project

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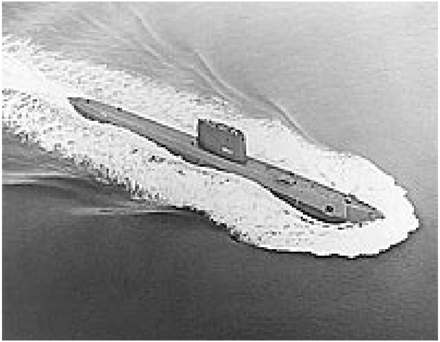
Doug Woods
Tony Alberti

Outline

- Scientific Computing in Nuclear Engineering
- Fundamentals of Reactor Physics
- Purpose and Motivation
- Project Objectives
- Methodology
    - Discretization of “measured data"
    - Objective Function
- Reed-Hill Problem
- Results
- Conclusions and Future Work

Scientific Computing In N.E. - Post WWII

- R&D for nuclear energy in full swing
- Hundreds of reactor designs were created
  - Cost prohibitive to build prototypes
  - Need computational models
- Method development driven by:
  - Naval reactor needs
  - Nuclear power



USS Nautilus - first nuclear powered submarine.

Source:[http://www.ne.anl.gov/About/reactors/lwr3.shtml]

Reactor Physics - Underlying Equation

$$\frac{1}{v}\frac{\partial\psi\left(\boldsymbol{r},E,\boldsymbol{\Omega},t\right)}{\partial t}+\boldsymbol{\Omega}\cdot\nabla\psi\left(\boldsymbol{r},E,\boldsymbol{\Omega},t\right)+\sigma_t\left(\boldsymbol{r},E,t\right)\psi\left(\boldsymbol{r},E,\boldsymbol{\Omega},t\right)$$
$$=\frac{1}{4\pi}\int_{4\pi}d\Omega'\int_0^\infty dE'\sigma_s\left(\boldsymbol{r},E'\rightarrow E,\boldsymbol{\Omega}'\rightarrow\boldsymbol{\Omega},t\right)\psi\left(\boldsymbol{r},E,\boldsymbol{\Omega},t\right)$$
$$+\frac{1}{4\pi}S_0\left(\boldsymbol{r},E,\boldsymbol{\Omega},t\right)$$

Seven independent variables:

$\boldsymbol{r}=\left(x,y,z\right)$ spatial coordinates

$\boldsymbol{\Omega}=\left(\theta,\rho\right)$ = angular components

E = energy dependence (lost and gained through scattering events (think billiards)

t = time dependence

Reactor Physics - What we really want (generally)

Solve for:

$$\int_{\boldsymbol{\Omega}} \psi\left(\boldsymbol{r}, E, \boldsymbol{\Omega}, t\right) d\boldsymbol{\Omega}$$

Gives:

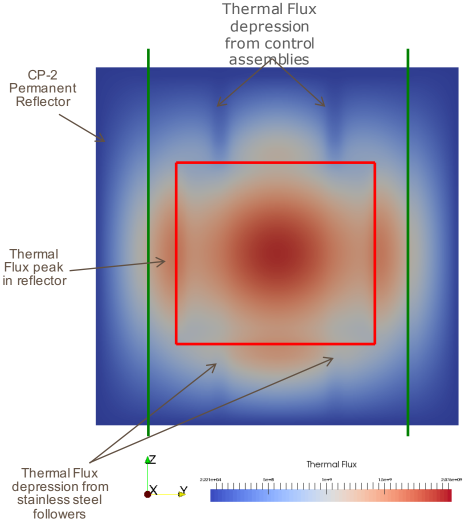
$$\phi\left(\boldsymbol{r}, E, t\right)$$

Scalar Flux - Neutron population as a function of space, energy, and time.

Implications of Flux Distribution

Gives insight into physics of reactor:

- Fission Rate - power, temperature
- Interactions with:
  - Coolant (water, gas, molten metal)
  - Structure
- Mitigation and prevention of nuclear accidents (Fukushima!)



Simplifications

- Solving full transport equation is unrealistic for many cases.
  - Solving small research reactor via FEM can have on the order 10^6 - 10^7 unknowns.
- Need to develop simpler form.
- Can do this by:
  - integrating out angle, $\mathbf{\Omega}$
  - integrating out energy dependence, E
  - making time-independence, $\frac{\partial \psi}{\partial t} = 0$
  - constant source, S.

Integrating out angular dependence

Recall streaming term of neutron transport equation:

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \psi \left(\boldsymbol{r}, E, \boldsymbol{\Omega}, t \right)$$

integrating out angle and energy dependence (generates angular current density):

$$\int_E \int_{4\pi} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \psi \left(\boldsymbol{r}, E, \boldsymbol{\Omega}, t \right) d\boldsymbol{\Omega} dE = \int_E \boldsymbol{\nabla} \cdot \int_{4\pi} \boldsymbol{j} \left(\boldsymbol{r}, E, \boldsymbol{\Omega}, t \right) d\boldsymbol{\Omega} dE$$

Which, when integrated becomes the current density:

$$\boldsymbol{\nabla} \cdot \boldsymbol{J} \left(\boldsymbol{r}, t \right)$$

Leaving us with the following:

$$\boldsymbol{\nabla} \cdot \boldsymbol{J} \left(\boldsymbol{r} \right) + \Sigma_{\boldsymbol{t}} \left(\boldsymbol{r} \right) \phi \left(\boldsymbol{r} \right) = \boldsymbol{S} \left(\boldsymbol{r} \right)$$

In the interest of time.... Some black box derivation

Recognizing that the, above equation has two unknowns, we have more work to do.

We find that we can define the neutron current vector as follows:

$$\boldsymbol{J}(\boldsymbol{r}, E, t) = -\frac{1}{3\Sigma_t}\nabla\phi(\boldsymbol{r}) = -\boldsymbol{D}(\boldsymbol{r})\nabla\phi(\boldsymbol{r})$$

Taking streaming operator approximation, we can arrive at the monoenergetic, steady state diffusion diffusion equation:

$$-\boldsymbol{D}\cdot\nabla^2\phi + \Sigma_{\boldsymbol{t}}\phi = \boldsymbol{S}$$

Which will be the governing equation for the objective function later on.

Project Objectives

- Use inverse methods to solve for the total cross section that defines the diffusion coefficient, D.

$$D = \frac{1}{3\Sigma_t}$$

- Methodology will be on 1-dimensional medium with reflecting and vacuum boundary conditions.
- Use LSQNONLIN function within Matlab to do Levenberg-Marquardt unconstrained optimization problem.

Solution Methods

- Approximate flux in terms of high-order polynomial basis functions for all J_k basis and weight functions

$$\psi\left(\boldsymbol{x},\boldsymbol{\Omega}\right) \approx \sum_{j=1}^{J_k} \psi_{kj}\left(\boldsymbol{\Omega}\right) b_{kj}\left(\boldsymbol{x}\right)$$

Methods

- Steady-state, mono-energetic transport equation

$$\boldsymbol{\Omega} \cdot \nabla \psi(\boldsymbol{x}, \boldsymbol{\Omega}) + \sigma \psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \frac{1}{4\pi} \sigma_s \phi(\boldsymbol{x}) + \frac{1}{4\pi} S_0$$

$$\phi = \sum_i w_i \psi(\boldsymbol{x}, \boldsymbol{\Omega}_i)$$

- Tests spatial discretization, quadrature, boundary conditions, and source iteration implementation
- “Measured data” from forward solve using step characteristics method

Methods

- Parameter estimation using `lsqnonlin`
- Objective function

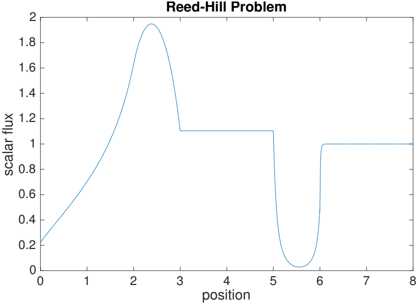
$$T = \frac{1}{2}||\phi_{\text{lsq}}\left(\boldsymbol{x} : \boldsymbol{Q}\right) - \phi_{\text{measured}}\left(\boldsymbol{x}\right)||_2^2$$

$$\boldsymbol{Q} = \begin{bmatrix} \sigma_{t,1} \\ \sigma_{t,2} \\ \sigma_{t,3} \\ \sigma_{t,4} \\ \sigma_{t,5} \end{bmatrix}$$

Reed-Hill Problem

Reed-Hill problem description

	$x \in (0,2)$	$x \in (2,3)$	$x \in (3,5)$	$x \in (5,6)$	$x \in (6,8)$
S_0	0	1.0	0	0	50
σ_t	1.0	1.0	0	5.0	50
σ_s	0	0.9	0	0	0
σ_a	1.0	0.1	0	5.0	50



Reed-Hill solution

- Multiregion 1-D problem
    - Scattering ratio of 0.9 region
    - Void region
    - Strong absorption region
    - Strong absorption and source region
- Sharp flux changes between regions
- Vacuum boundary on left
- Reflecting boundary on right

Reed-Hill Problem - Transport Equation

	$x \in (2,3)$	$x \in (3,5)$
S_0	1.0	0.0
σ_t	1.0	0.0
σ_s	0.9	0.0

Table: True parameters.

	$x \in (2,3)$	$x \in (3,5)$
S_0	1.0	1.2e-5
σ_t	1.0	4.4e-6
σ_s	0.9	4.5e-6
iterations	21	15

Table: Initial guesses of 0.1.

	$x \in (2,3)$	$x \in (3,5)$
S_0	1.0	1406
σ_t	1.0	0.0
σ_s	0.9	1300
iterations	5	19

Table: Initial guesses of 1.0.

- Wrapped parameter estimation around transport solver
- For verification, tested transport equation parameter estimation against itself solving for a particular material: σ_t, σ_s, and S
- Some regions required “better” initial guesses

Reed-Hill Problem - Diffusion Equation

- Diffusion Equation

$$-\nabla D(\boldsymbol{x}) \cdot \nabla \phi(\boldsymbol{x}) + \sigma_a \phi(\boldsymbol{x}) = S(\boldsymbol{x})$$

- General analytical solution where $L^2 = D/\sigma_a$,

$$\phi(x) = c_1 e^{x/L} + c_2 e^{-x/L} + \frac{S}{\sigma_a}$$

- Dirichlet boundary conditions from “measured data”

$$\phi(\boldsymbol{x}_{\text{left}}) = \phi_{\text{transport}}(\boldsymbol{x}_{\text{left}})$$
$$\phi(\boldsymbol{x}_{\text{right}}) = \phi_{\text{transport}}(\boldsymbol{x}_{\text{right}})$$

- Reflecting BC

$$\frac{\partial \phi}{\partial x} = 0$$

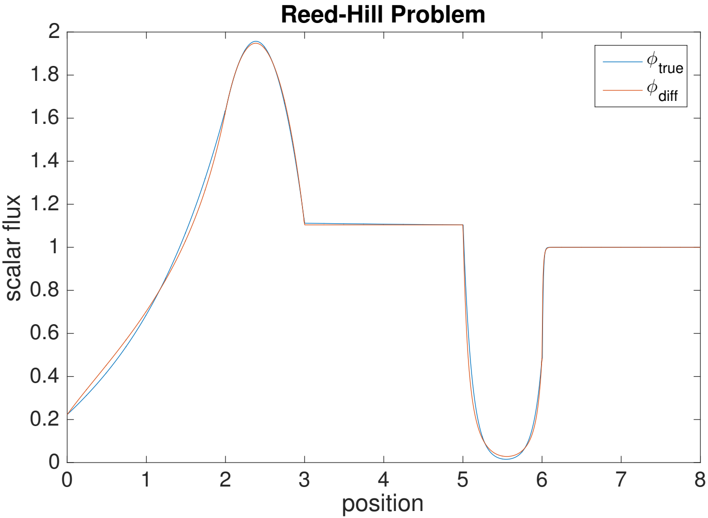
Reed-Hill Problem - Diffusion Equation

- Evaluated 5 different regions for σ_t from diffusion equation
- The values differed from those used in the transport equation
- Differences quantify the diffusion approximation (depends on other assumptions)
- Other material parameters were same as transport equation

	$x \in (0, 2)$	$x \in (2, 3)$	$x \in (3, 5)$	$x \in (5, 6)$	$x \in (6, 8)$
transport σ_t	1.0	1.0	0.0	5.0	50
diffusion σ_t	0.223	1.811	2.155	5.552	52.478

Table: Initial guesses were true values ($\sigma_a = 1e-3$).

Reed-Hill Problem - Diffusion Equation



Conclusions

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Future Work

- Vary σ_a and initial guess for σ_t in diffusion equation parameter estimation
- Sensitivity to initial guesses
- Noisy data

Questions?

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