Advances in Inverse Transport Methods with Applications to Neutron Tomography

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SLB-SDR, 04-26-2010
Bio

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  B.S., Engineering Physics, Tsinghua, China, 1999
  M.S., Engineering Physics, Tsinghua, China, 2001
  M.E., Nuclear Engineering, Texas A&M, 2005
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  Intern, Baker Hughes, Houston, TX, Summer, 2004
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Outline of This Talk

- Introduction
- Analytic Tomography Method
- Deterministic Optimization Method
- Stochastic-based Combinatorial Optimization
- Model Problems and Results
- Summary
Introduction
Radiography vs. Tomography

**Fig:** An idealized facility configuration for radiographic Imaging system

**Simple exponential attenuation method (SEAM)**

\[ I(x) = I_0 e^{-\int_0^x \Sigma_t(s) ds} \]

\[ \Rightarrow \int_0^x \Sigma_t(s) ds = -\ln\left(\frac{I(x)}{I_0}\right) \]
A tomography imaging system deals with reconstructing an internal image of an object based on its peripheral emerging radiations. The cross-sectional image of an object was reconstruction by illuminating the object from many different directions.

“Tomo” means “to cut” in Greek
Forward vs. Inverse

- Forward Transport Problem

\[ \mathbf{\Omega} \cdot \nabla \psi_g(r, \Omega) + \Sigma_{tg}(r) \psi_g(r, \Omega) = \sum_{g'=1}^{G} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[ Y_{lm}(\Omega) \Sigma_{sg' \rightarrow g}(r) \phi_{lm,g'}(r) + S_{ext,g}(r, \Omega) \right] \]

- Inverse Transport Problem

\[ \mathbf{\Omega} \cdot \nabla \psi_g(r, \Omega) + \Sigma_{tg}(r) \psi_g(r, \Omega) = \sum_{g'=1}^{G} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \left[ Y_{lm}(\Omega) \Sigma_{sg' \rightarrow g}(r) \phi_{lm,g'}(r) + S_{ext,g}(r, \Omega) \right] \]

Note: Symbols in red are unknown variables in the problem.
Solve the Inverse Problem

The purpose of our project is to infer material distribution inside an object based upon detection and analysis of radiation emerging from the object.

We are particularly interested in problems in which radiation can undergo significant scattering within the object.
Why we do this?

- Neutron radiography/tomography has unique advantages in nondestructive testing (NDT)
- “Scattering blur” is always a big issue in tomography and there is no best solution to it yet today
- Leverage the expertise we have in computational methods on neutron transport equation to solve practical engineering problems
Tomographic Reconstruction Methods

- **Analytic methods**
  - Line integral (Radon transform),
  - Fourier slice theorem (FST)
  - Back projection reconstruction (BPR)

- **Iteration methods**
  
  forward model & inverse update scheme

  Iteration image reconstruction (IIR) methods mainly differ in their choice of forward model and how the spatial distributions of the optical properties of the medium are updated.
Analytic Tomography Method
Theories\textsuperscript{1}

- **Line Integral (Radon transform)**
  \[
P_\theta(t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x, y) \delta(x \cos \theta + y \sin \theta - t) \, dx \, dy
\]

- **Fourier Slice Theorem (FST)**
  \[
  F(u, v) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x, y) e^{-j2\pi(ux + vy)} \, dx \, dy
  \]
  \[
  S_\theta(\omega) = \int_{-\infty}^{+\infty} P_\theta(t) e^{-j2\pi\omega t} \, dt
  \]
  \[
  S_\theta(\omega) = F(\omega \cos \theta, \omega \sin \theta)
  \]

- **Filter Back Projection (FBP)**
  \[
  f(x, y) = \int_{0}^{\pi} \left[ \int_{-\infty}^{+\infty} S_\theta(\omega) |\omega| e^{j2\pi\omega t} \, d\omega \right] d\theta
  \]

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\textsuperscript{1}A.C. Kak. & M. Slaney, *Principles of Computerized Tomographic Imaging*, IEEE Press, 1987
Obtaining Radiation Projections/Measurements

(a) X-Y View  
(b) X-Z View

Fig: Test problem layout and experimental configuration

10cm x 10cm object; An array of 20 detectors, each 0.5 cm wide, is placed on the other side of the object
**Source Definition**

```
sdef  pos=0 -2 0 vec=0 1 0 dir=1 erg=d2 y=-2 x=d3 z=d4
sp2   -2 2.5e-8 $ Maxwell thermal energy spectrum
si3   h -1.42 1.42 $ Plane source
sp3   d 0 1
si4   h -2 2
sp4   d 0 1
```

**Material Definition**

```
m1    1001 -0.111894 $ Water
     8016 -0.888106
m2    26000 -1.000000 $ Iron
m3    6000 -0.000124 $ C(air)
     7014 -0.755268 $ N
     8016 -0.231781 $ O
     18000 -0.012827 $ Ar
```

---

Fig: Particles transport procedure simulated in the test problem (nps=1000).
**MCNP Tallies**

- **Tally Definition**

  c Tally card section
  fq0 s c $ Change the order of tallies output
  c F1 Tally
  f11:n 4
  fs11 -100 -101 -102 -103 -104 -105 -106
         -107 -108 -109 -110 -111 -112 -113
         -114 -115 -116 -117 -118 -119 -120
  sd11 (1 20r 1)
  c11 0 1
  c F2 Tally
  f12:n 4
  fs12 -100 -101 -102 -103 -104 -105 -106
         -107 -108 -109 -110 -111 -112 -113
         -114 -115 -116 -117 -118 -119 -120
  sd12 (1 20r 1)
  c12 1
  c F5 Tally
  fir15:n 0 5.1 0 7r nd $ Array of point detectors
  c15 -1 1
  fs15 -5 19i 5

**Fig:** Comparison of plots from different tally type (normalized)
Multiple Groups of Projections

Fig: Rotate the object in different angles using mcnp_pstudy.  
Implementation detail: Set mcnp_pstudy parameters in TRn card.

3F. B. Brown et al., Monte Carlo parameter studies and uncertainty analysis with MCNP5, LA-UR-04-0499, LANL, 2004
Fig: Transmitted radiation measured with object rotated in different angle.

Implementation detail: Output is post processed by MATLAB script
Image Reconstruction Results

Total cross section reconstructed with FBP method for the test problem.

Geometry and material configuration of the test problem.
Smaller Version Problem

Total cross section reconstructed with FBP method for a smaller version of the test problem.

Geometry and material configuration of the test problem for a smaller version problem.
Summary to Analytic Tomography Method

- The results we obtained from our experiment demonstrate that the analytic tomography method is not a workable approach to address such problems even with collimated source and detectors applied. This is due to the fact that the basic assumption underlying line-integral methods is violated when the scattering component significantly contributes to the transmitted projections.

- For thick problem undergoing many highly scatterings, we must turn to other methodologies such as iterative based optimization methods. These are the topics we present in the rest of this presentation.
Gradient-based Deterministic Optimization Method
Minimization Based Approaches\textsuperscript{4,5}

- **Objective function**
  \[ \Phi = \frac{1}{2} \sum_{i=1}^{N} \left( \frac{P_i - M_i}{M_i} \right)^2 \]

- Here ‘M’ is experimental measurements provided by MCNP simulation

- ‘P’ is predicted measurements provided by forward model calculation, which is treated as a function of properties of the unknown object
  \[ P = P(\sigma_t, \sigma_s, \sigma_{sl}, \cdots) \]
  \[ \Rightarrow \Phi = \Phi(\sigma_t, \sigma_s, \sigma_{sl}, \cdots) \]

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\textsuperscript{4}V. Scipolo, Scattered neutron tomography based on a neutron transport problem, Master Thesis, Texas A&M, 2004

\textsuperscript{5}A. D. Klose et al., Optical tomography using the time-Independent equation of radiative transfer - part 1: forward model
  J. Quant. Spectrosc. Radiat. Transf. , 72, 691-713, 2002

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Forward and Inverse Model

- **Forward model**: One-group neutron transport equation for a non-multiplying system with linearly anisotropic scattering

\[
\Omega \cdot \nabla \psi (r, \Omega, t) + \Sigma_t (r) \psi (r, \Omega, t) = \frac{1}{4\pi} \Sigma_s (r) \left[ \phi (r, t) + 3g \Omega \cdot J (r, t) \right] + S_{\text{ext}} (r, \Omega, t)
\]

- **Inverse model**: Nonlinear conjugated gradient (CG) based iterative updating scheme

  Initialize variables \( x^{(1)} \), search direction \( d^{(1)} = r^{(1)} \), where \( r^{(1)} \equiv -\nabla \Phi (x^{(1)}) \), \( x = \{ \Sigma_t, \Sigma_s, g \} \)

  Define termination tolerance \( \mathcal{E} \) and set iteration counter \( k = 0 \)

  Start of iteration loop

  Perform line search to find \( \alpha_{\text{min}} \) that minimizes \( \Phi (x^{(k)} + \alpha d^{(k)}) \)

  \[
  x^{(k+1)} = x^{(k)} + \alpha_{\text{min}} d^{(k)}
  \]

  \[
  r^{(k+1)} \equiv -\nabla \Phi \left( x^{(k+1)} \right)
  \]

  \[
  d^{(k+1)} = r^{(k+1)} + \beta_{x} d^{(k)}
  \]

  Exit if \( \left\| \nabla \Phi \left( x^{(k)} \right) \right\| < \mathcal{E} \)

  End of iteration loop
Variable Change Technique

Purpose: Convert constrained optimization to non-constrained optimization

\[ x_i^{(k+1)} = x_i^{(k)} + \alpha_{x,\text{step}} d_i^{(k)}, \quad (x = \Sigma \text{ or } g) \]

\( y_i^{(k+1)} = y_i^{(k)} + \alpha_{y,\text{step}} d_{y,j}^{(k)} \)

(a) \( y_j = \log(\Sigma_j) \Rightarrow \frac{\partial \Phi}{\partial y_j} = \frac{\partial \Phi}{\partial \Sigma_j} \frac{d\Sigma_j}{dy_j} = \frac{\partial \Phi}{\partial \Sigma_j} \Sigma_j \)

(b) \( y_j = \tan\left(\frac{\pi}{2} g_j \right) \Rightarrow \frac{\partial \Phi}{\partial y_j} = \frac{\partial \Phi}{\partial g_j} \frac{dg_j}{dy_j} = \frac{\partial \Phi}{\partial g_j} 2 \frac{1}{\pi + \tan^2\left(\frac{\pi}{2} g_j \right)} \)

Nonlinear CG Updating Scheme with Variable Change Technique Incorporated

Initialize variables $x^{(1)}$, search direction $d^{(1)} = r^{(1)}$, where $r^{(1)} ≡ -\nabla \Phi \left( x^{(1)} \right)$, $x = \{ \Sigma, \Sigma, g \}$

Define termination tolerance $\varepsilon$ and set iteration counter $k = 0$

Start of iteration loop

Change variable $x$ to $y$

Perform line search to find $\alpha_{\text{min}}$ that minimizes $\Phi(y^{(k)} + \alpha d^{(k)})$

$y^{(k+1)} = y^{(k)} + \alpha_{\text{min}} d^{(k)}$

$r^{(k+1)} ≡ -\nabla \Phi \left( y^{(k+1)} \right)$, where $\nabla \Phi \left( y^{(k+1)} \right)$ is calculated based on $\nabla \Phi \left( x^{(k+1)} \right)$

$d^{(k+1)} = r^{(k+1)} + \beta_k d^{(k)}$

Change variable $y$ back to $x$

Exit if $\left\| \nabla \Phi \left( x^{(k)} \right) \right\| < \varepsilon$

End of iteration loop
Model Problem

Table: Physics properties of the materials in the model problem

<table>
<thead>
<tr>
<th>Material</th>
<th>Water</th>
<th>Iron</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma_s$ (1/cm)</td>
<td>0.7362</td>
<td>0.96715</td>
</tr>
<tr>
<td>$\Sigma_t$ (1/cm)</td>
<td>0.7435</td>
<td>1.17883</td>
</tr>
<tr>
<td>$g$ (2/3A)</td>
<td>0.037</td>
<td>0.012</td>
</tr>
<tr>
<td>$\Sigma_{tr}$ (1/cm)</td>
<td>0.7163</td>
<td>1.1672</td>
</tr>
<tr>
<td>$mfp$ (cm)</td>
<td>1.345</td>
<td>0.8483</td>
</tr>
<tr>
<td>$C$</td>
<td>0.9902</td>
<td>0.8204</td>
</tr>
</tbody>
</table>

Fig: Schematic diagram of the one iron inclusion model problem
Forward Calculation Verification

Fig: Comparison of MCNP F1 tally and $S_N$ Transport Solution
Image Reconstruction Results

Fig: Transport cross section ($\Sigma_\nu$) distribution obtained from deterministic CG based iterative search scheme for the one iron problem. (a) The real $\Sigma_\nu$ (background is water and square inclusion is iron). (b) Initial guess for $\Sigma_\nu$. (c) and (d) are results after 100 and 1000 iterations, respectively.

The objective function drastically reduced along iterative process.

The objective function changes after each iteration for one iron problem.
Drawbacks Associated with Deterministic Methods

- Deterministic search method could be trapped into local minima
- Cross-section sets obtained are not constrained to be realistic
- Dimension of unknowns grows fast as the case becomes more realistic

Notes: Number of possible variables (only think of scattering cross sections) in continuous searching scheme:

\[
16 \times 100 \times 100 \times 4 = 640000
\]
Stochastic-based Combinatorial Optimization Method
Advances Devised in This Stage

- Treat unknowns as materials instead of cross sections
- Combine deterministic and stochastic optimization method together
- Hierarchical Approach
  - Mesh refinement
  - High fidelity forward calculation
- Search space dimension reduction techniques
  - Cell grouping
  - Material restriction
- Efficient stochastic-based heuristic optimization scheme
Why Combinatorial Optimization?

- Suppose we divide an object into have a 4x4 cells in a 2-D view and we have 10 material candidates in our material library.

- In each cell, the material in it has 10 possibilities, so over all there’re totally \(10 \times 10 \times \cdots \times 10 = 10^{16}\) possibilities (solutions) to construct the object.

- Call one solution as one combination, it has a limited but discrete space.

- The problem becomes to find the combination/solution to minimize the objective function, i.e. combinatorial optimization.
Cell Grouping Result for Model Problem

3-D show of the $\Sigma_{fr}$ distribution yielded from deterministic optimization in the first stage

Different regions identified by the cell grouping process. (Color in this figure denotes region only, not any particular numerical value.)
Cell Grouping Technique

- Strategies in this stage are based on the results gained from the deterministic optimization process
- Group into regions the cells that are likely to contain the same material
- Devise a criterion to divide the problem into different regions

\[
\begin{align*}
\Sigma_{tr} &> \Sigma_{tr,mean} + \alpha(\Sigma_{tr,max} - \Sigma_{tr,mean}) \Rightarrow \text{Inclusion region} \\
\Sigma_{tr} &< \Sigma_{tr,mean} + \beta(\Sigma_{tr,max} - \Sigma_{tr,mean}) \Rightarrow \text{Background region} \\
\text{otherwise} & \Rightarrow \text{Interface region}
\end{align*}
\]

We chose $\alpha = 0.8$, $\beta = 0.2$ in the implementation to the model problem.
We use MCNP to generate energy collapsed **one group cross sections** for different materials. These information will be used to construct a material candidate library (MCL) for discrete optimization.

\[
\bar{\sigma}_i = \frac{\int_0^{E_{ih}} \sigma_i(E)\phi(E)dE}{\int_0^{E_{ih}} \phi(E)dE} = \frac{(F4 + Fm4) \text{Tally}}{F4 \text{Tally}} \\
\bar{\Sigma}_i = n\bar{\sigma}_i = \rho \frac{N_A}{M} \bar{\sigma}_i
\]

### Current materials in MCL

<table>
<thead>
<tr>
<th>#</th>
<th>Material</th>
<th>(\bar{\Sigma}_i) (1/cm)</th>
<th>(\bar{\sigma}_i) (1/cm)</th>
<th>(g \left( \frac{2}{3\lambda} \right))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Paraffin</td>
<td>0.5669</td>
<td>0.5666</td>
<td>0.0556</td>
</tr>
<tr>
<td>2</td>
<td>B-10</td>
<td>554.0688</td>
<td>0.3197</td>
<td>0.0667</td>
</tr>
<tr>
<td>3</td>
<td>Water</td>
<td>0.7435</td>
<td>0.7362</td>
<td>0.037</td>
</tr>
<tr>
<td>4</td>
<td>Si</td>
<td>0.1101</td>
<td>0.10215</td>
<td>0.0237</td>
</tr>
<tr>
<td>5</td>
<td>Fe</td>
<td>1.1788</td>
<td>0.96715</td>
<td>0.0119</td>
</tr>
<tr>
<td>6</td>
<td>Nitrogen</td>
<td>0.00065</td>
<td>0.00055</td>
<td>0.0476</td>
</tr>
<tr>
<td>7</td>
<td>Cadmium (Cd)</td>
<td>0.30056</td>
<td>0.2472</td>
<td>0.0059</td>
</tr>
<tr>
<td>8</td>
<td>Aluminum (Al)</td>
<td>0.0968</td>
<td>0.0831</td>
<td>0.0247</td>
</tr>
<tr>
<td>9</td>
<td><strong>Natural Uranium</strong></td>
<td><strong>0.82105</strong></td>
<td><strong>0.9208</strong></td>
<td><strong>0.0014</strong></td>
</tr>
<tr>
<td>10</td>
<td><strong>HEU</strong></td>
<td><strong>27.0366</strong></td>
<td><strong>52.4947</strong></td>
<td><strong>3.6114E-05</strong></td>
</tr>
</tbody>
</table>
Material Restriction Result for Model Problem

Our algorithm determined that the background material must be water; thus region 1 was always chosen to be water. Our algorithm determined that the inclusion (region 3) could be any one of four different materials: iron, water, paraffin, natural uranium.

Cell grouping result
Material Restriction Technique

- Restrict the material candidates in the inclusion and background regions by comparing each material’s cross sections to the cross sections that were found in the deterministic search stage.

- Chose the following “error” metric:

\[
e_m = \text{error} = \frac{1}{3} \left( \left| \frac{\Sigma_s^m - \Sigma_s^r}{\Sigma_s + \Sigma_s^r} \right| + \left| \frac{\Sigma_t^m - \Sigma_t^r}{\Sigma_t + \Sigma_t^r} \right| + \left| \frac{\Sigma_{tr}^m - \Sigma_{tr}^r}{\Sigma_{tr} + \Sigma_{tr}^r} \right| \right)
\]

- Restrict the material candidates for the region based on the following criterion:

If exist one and only material that has \( e_m < a \), the region is determined to be that material; Otherwise we include all materials for which \( e_m < b \). Here \( a \) is a relatively small number and \( b \) is a relatively larger number; In the model problem in this research we use \( a = 0.01 \), \( b = 0.5 \).
Combinatorial Optimization (CO) Process

- Make a combinatorial solution
  1. Water assigned to region 1
  2. A choice made in restricted materials for region 3
  3. The material assignment for region 2 began with the cells adjacent to region 3 and marched out to those adjacent to region 1

- Employ material continuity restraint to the combinatorial solution

- Forward calculation

- Loop on the procedure until reaching a minimum objective function

Cell grouping result
**CO Result for Model Problem**

Material distribution from the combinatorial optimization (CO) after 50 iterations and Color in this figure denotes material only, not any particular numerical value.

Quantitative results of the inclusion location and area with comparison to the real problem:

<table>
<thead>
<tr>
<th>Case</th>
<th>Real</th>
<th>CO Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-center (cm)</td>
<td>3.0</td>
<td>2.97</td>
</tr>
<tr>
<td>Y-center (cm)</td>
<td>7.5</td>
<td>7.49</td>
</tr>
<tr>
<td>Area (cm²)</td>
<td>4.0</td>
<td>4.0</td>
</tr>
<tr>
<td>Iron/Water</td>
<td>0.0417</td>
<td>0.0417</td>
</tr>
</tbody>
</table>

Another Model Problem
Model Problem II

Fig: Schematic diagram of the two irons inclusion model problem (X-Y view).
Results for Model Problem II (Deterministic Stage)

Fig: Transport cross section ($\Sigma_{tr}$) distribution obtained from deterministic CG based iterative search scheme for the two irons problem. (a) The real $\Sigma_{tr}$ (background is water and square inclusion is iron). (b) Initial guess for $\Sigma_{tr}$ . (c) and (d) are results after 100 and 1000 iterations, respectively.
Results for Model Problem II (Stochastic Stage)

Different regions identified by the cell grouping process. (Color in this figure denotes region only, not any particular numerical value.)

Material distribution from the combinatorial optimization after 100 iterations. (Color in this figure denotes material only, not any particular numerical value.)

Quantitative result for Inclusion locations and areas with comparison to real problem

<table>
<thead>
<tr>
<th>Case</th>
<th>X-center (cm)</th>
<th>Y-center (cm)</th>
<th>Area (cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inclusion 1</td>
<td>Real</td>
<td>3.0</td>
<td>7.5</td>
</tr>
<tr>
<td></td>
<td>CO Result</td>
<td>2.9485</td>
<td>7.3676</td>
</tr>
<tr>
<td>Inclusion 2</td>
<td>Real</td>
<td>7.25</td>
<td>2.75</td>
</tr>
<tr>
<td></td>
<td>CO Result</td>
<td>7.2893</td>
<td>2.6607</td>
</tr>
</tbody>
</table>
Summary
Summary of This Talk

• We have introduced some advances in inverse transport methods and applied them to solve 2D neutron tomography problems

• We employ multiple steps that work together to dramatically reduce the difficulty of the combinatorial optimization

• We implement a series of novel dimension-reduction techniques and integrate them to achieve the desired result

• Results from simple model problems illustrate the potential power of these ideas and feasibility of the method

• Optically thick problems with a high scattering ratio, in which analytic tomography method generally fails, are solved almost exactly with very modest computational effort
Back up slides
Line Integral
Fourier Slice Theorem

Fourier transform

space domain

frequency domain

projection

object

BACK
Linear Scattering Anisotropy Factor

Also referred to as scattering asymmetry factor or $g$ factor

![Neutron diffracts with angle theta after colliding with a nuclide target]

$$g = \mu_0 = \frac{\int_{-1}^{1} \mu_0 \sigma_s (\mu_0) d\mu_0}{\int_{-1}^{1} \sigma_s (\mu_0) d\mu_0}, \quad \text{where } \mu_0 = \cos \theta.$$
Step Characteristic (SC) Method

Here \( \tau_{j,j}^k = \sigma_t \min \left\{ \frac{\Delta x_i}{\mu_k}, \frac{\Delta y_j}{\eta_k} \right\} \),

\( \alpha_{i,j}^k = \min \left\{ \frac{\mu_k \Delta y_j}{\eta_k \Delta x_i} \right\} \),

\( \nu_{j,j}^k = \min \left\{ \frac{\eta_k \Delta x_i}{\mu_k \Delta y_j} \right\} \).

\[
\begin{align*}
\psi_{k,i,j} &= \frac{q_{k,i,j}}{\sigma_t} + \nu_{i,j}^k \left( \psi_{k,i,j-\frac{1}{2}} - \frac{q_{k,i,j}}{\sigma_t} \right) \left( 1 - e^{-\frac{\tau_{i,j}^k}{\tau_{i,j}^k}} \right) + \left( 1 - \nu_{i,j}^k \right) \left( \psi_{k,i-\frac{1}{2},j} - \frac{q_{k,i,j}}{\sigma_t} \right) e^{-\frac{\tau_{i,j}^k}{\tau_{i,j}^k}} \\
\psi_{k,i,j+\frac{1}{2}} &= \frac{q_{k,i,j}}{\sigma_t} + \alpha_{i,j}^k \left( \psi_{k,i,j-\frac{1}{2}} - \frac{q_{k,i,j}}{\sigma_t} \right) \left( 1 - e^{-\frac{\tau_{i,j}^k}{\tau_{i,j}^k}} \right) + \left( 1 - \alpha_{i,j}^k \right) \left( \psi_{k,i,j-\frac{1}{2}} - \frac{q_{k,i,j}}{\sigma_t} \right) e^{-\frac{\tau_{i,j}^k}{\tau_{i,j}^k}} 
\end{align*}
\]
Adjoint Difference Method

\[
\begin{bmatrix}
\psi_0 \\
\psi_1 \\
\psi_2 \\
\psi_3 \\
\psi_4
\end{bmatrix} = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\psi \\
\sigma_1 \\
\sigma_2 \\
\sigma_3
\end{bmatrix}
\]

\[
A = \begin{bmatrix}
0 & \frac{\partial \psi_2}{\partial \psi_1} & 0 & 0 \\
0 & 0 & \frac{\partial \psi_3}{\partial \psi_2} & 0 \\
0 & 0 & 0 & \frac{\partial \psi_4}{\partial \psi_3} \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\nu = \begin{bmatrix}
0 \\
0 \\
0 \\
\frac{\partial \Phi}{\partial \psi_4}
\end{bmatrix}
\]

\[
B_\sigma = \begin{bmatrix}
\frac{\partial \psi_1}{\partial \sigma_1} & 0 & 0 & 0 \\
0 & \frac{\partial \psi_2}{\partial \sigma_2} & 0 & 0 \\
0 & 0 & \frac{\partial \psi_3}{\partial \sigma_3} & 0
\end{bmatrix}
\]

\[
\frac{\partial \Phi}{\partial \sigma_1} \quad \frac{\partial \Phi}{\partial \sigma_2} \quad \frac{\partial \Phi}{\partial \sigma_3}
\]

\[
= B_\sigma \sum_{i=0}^{3} A_i \nu
\]
Incorporate Multi-beams

\[ \Phi_1 = \frac{1}{2} \sum_{i=1}^{N} (M_{1i} - P_{1i})^2 \]

\[ \Phi_2 = \frac{1}{2} \sum_{i=1}^{N} (M_{2i} - P_{2i})^2 \]

\[ \Phi_3 = \frac{1}{2} \sum_{i=1}^{N} (M_{3i} - P_{3i})^2 \]

\[ \Phi_4 = \frac{1}{2} \sum_{i=1}^{N} (M_{4i} - P_{4i})^2 \]

\[ \Phi = \Phi_1 + \Phi_2 + \Phi_3 + \Phi_4 \]

\[ \frac{\partial \Phi}{\partial \sigma_i} = \frac{1}{\frac{1}{2} \sum_{j=1}^{4} \sum_{i=1}^{N} (M_{ji})^2} \left( \frac{\partial \Phi_1}{\partial \sigma_i} + \frac{\partial \Phi_2}{\partial \sigma_i} + \frac{\partial \Phi_3}{\partial \sigma_i} + \frac{\partial \Phi_4}{\partial \sigma_i} \right) \]
Conjugate Gradient Iteration

• First invented to solve linear equations problem, and later introduced to non-constrained optimization problem.

• Unlike the steepest descent (SD) method, in each iteration step conjugate gradient (CG) method moves along a so-called conjugate direction instead of moving along a direction only orthogonal the previous direction.

• A more understandable point of view, the CG method tries to minimize the residual rather than the objective function itself.

• In order to do that, the new search direction in every iteration step is produced by a linear interpolation between the old direction and the new gradient direction.

\[ d_{k+1} = r_{k+1} + \beta_k d_k \]
Line Search

- Once the search direction is set, you have to know how far to move along this direction to make the objective function minimum. This is the basic conception of line search (1D search).

\[ x_{k+1} = x_k + \alpha_k d_k \]

- The importance of line search is that the accuracy of its result is usually vital to the efficiency of the whole CG method.

- If the objective function could be written as a quadratic function to the unknown variables, it would be easy to find the minimum. Unfortunately our objective doesn’t have such a good quality.

\[ f(x) = \frac{1}{2} x^T A x - b^T + c = \frac{1}{2} (Ax, x) - (b, x) + c \]
A variant of line search methods was applied and tested here, either utilizing trial method such as the golden section search or using only function evaluations such as the quadratic fit method.

\[ x_m = x_0 + \alpha d \]
Fissile Material Treatment

\[ \Omega \cdot \nabla \psi (r, \Omega, t) + \Sigma_t (r) \psi (r, \Omega, t) \]

\[ = \frac{1}{4\pi} \Sigma_s (r) \left[ \phi (r, t) + 3g \Omega \cdot J (r, t) \right] + \frac{1}{4\pi} \nu \Sigma_f (r) \phi (r, t) + S_{ext} (r, \Omega, t) \]

\[
\begin{cases}
\tilde{\Sigma}_s (r) = \Sigma_s (r) + \nu \Sigma_f (r) \\
\tilde{g} = g \frac{\Sigma_s (r)}{\Sigma_s (r) + \nu \Sigma_f (r)}
\end{cases}
\]

\[ \Omega \cdot \nabla \psi (r, \Omega, t) + \Sigma_t (r) \psi (r, \Omega, t) = \frac{1}{4\pi} \tilde{\Sigma}_s (r) \left[ \phi (r, t) + 3\tilde{g} \Omega \cdot J (r, t) \right] + S_{ext} (r, \Omega, t) \]