Advances in Inverse Transport Methods and Applications to Neutron Tomography

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Ph.D. Defense Presentation

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May 4th, 2010

Summary of This Research

- 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 solving the optimization problem
- 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

Outline of This Talk

- Introduction
- Analytic Tomography Method
- Gradient-based Deterministic Optimization
- Stochastic-based Combinatorial Optimization
- Results
- Conclusions

Introduction

Forward vs. Inverse

- **Forward Transport Problem[1]**

$$\underline{\Omega}\bullet\underline{\nabla}\psi_g(\underline{r},\underline{\Omega})+\Sigma_{tg}(\underline{r})\psi_g(\underline{r},\underline{\Omega})=\sum_{g'=1}^{G}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\underline{\Omega})\Sigma_{sg'\to g}^{l}(\underline{r})\phi_{lm,g'}(\underline{r})+S_{ext,g}(\underline{r},\underline{\Omega})$$

- **Inverse Transport Problem**

$$\underline{\Omega}\bullet\underline{\nabla}\psi_g(\underline{r},\underline{\Omega})+\Sigma_{tg}(\underline{r})\psi_g(\underline{r},\underline{\Omega})=\sum_{g'=1}^{G}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Y_{lm}(\underline{\Omega})\Sigma_{sg'\to g}^{l}(\underline{r})\phi_{lm,g'}(\underline{r})+S_{ext,g}(\underline{r},\underline{\Omega})$$

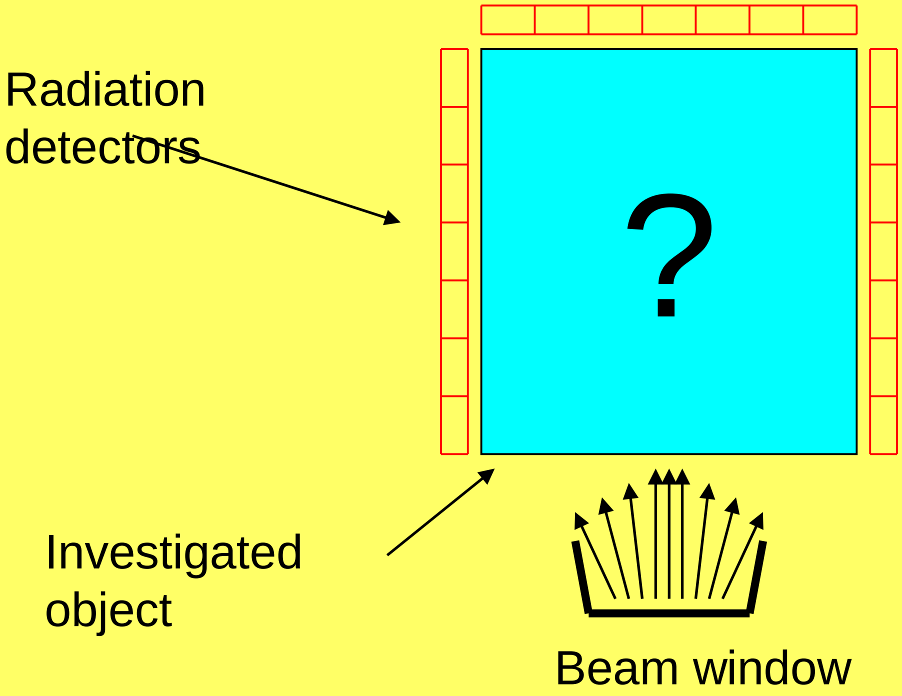
Note: Symbols in red are unknown variables in the problem.

[1]J.J. Duderstadt & L.J. Hamilton, *Nuclear Reactor Analysis*, John Wiley & Sons*, 1976*

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.



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[2]

- <u>Line Integral</u> (Radon transform)

$$P_\theta(t) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y)\delta(x\cos\theta + y\sin\theta - t)dxdy$$

- <u>Fourier Slice Theorem</u> (FST)

$$F(u,v) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y)e^{-j2\pi(ux+vy)}dxdy$$

$$S_\theta(\omega) = \int_{-\infty}^{+\infty} P_\theta(t)e^{-j2\pi\omega t}dt$$

$$S_\theta(\omega) = F(\omega\cos\theta, \omega\sin\theta)$$

- **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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[2] A.C. Kak & M. Slaney, *Principles of Computerized Tomographic Imaging*, IEEE Press, 1987

Model Problem

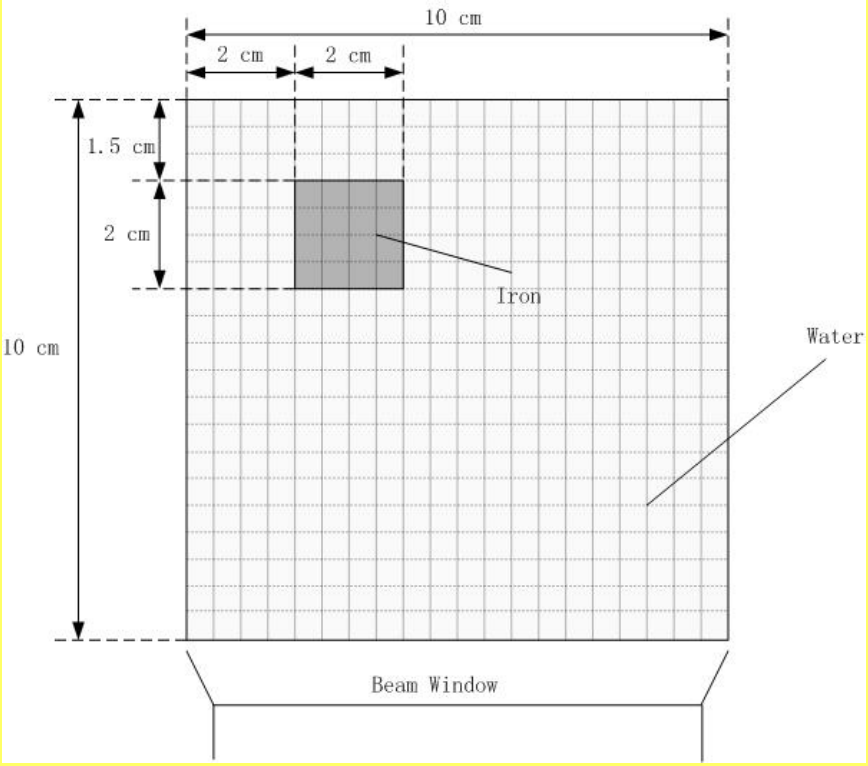


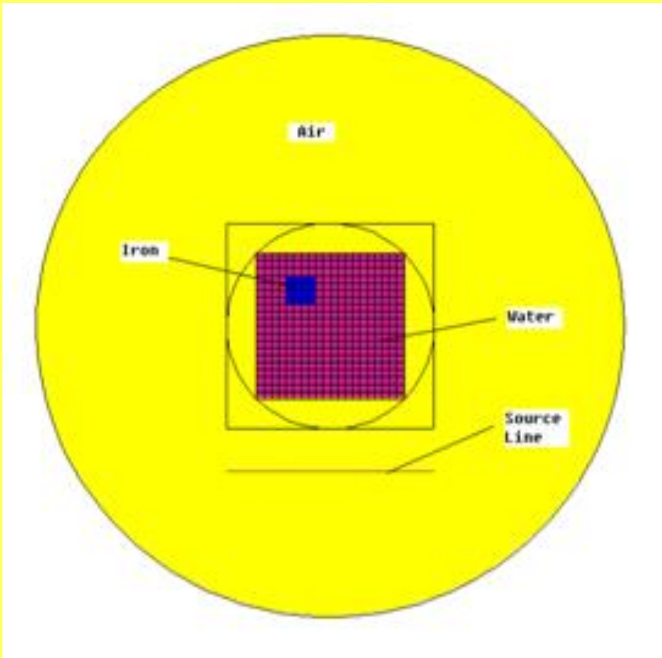
Fig: Schematic diagram of the one iron inclusion model problem (X-Y view).

Table: Physics properties of the materials in the model problem

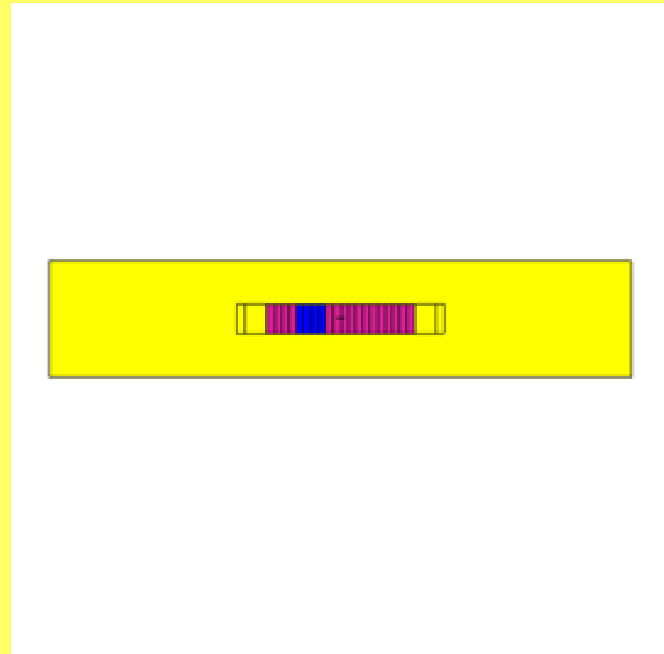
Material	Water	Iron
Σ_s (1/cm)	0.736	0.967
Σ_t (1/cm)	0.744	1.19
g (2/3A)	3.70E-2	1.20E-2
Σ_{tr} (1/cm)	0.716	1.167
mfp (cm)	1.35	0.848
c	0.990	0.820

$$\Sigma_{tr} = \Sigma_t - g\Sigma_s, \quad mfp = \frac{1}{\Sigma_t}, \quad c = \frac{\Sigma_s}{\Sigma_t}$$

MCNP[3] Modeling to Provide Projections



(a) X-Y View



(b) X-Z View

Fig: Test problem layout and experimental configuration

[3]J. Briesmeister ed., MCNP-A general Monte Carlo n-particle transport code, v-5, LA-UR-03-1987, 2003

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
```

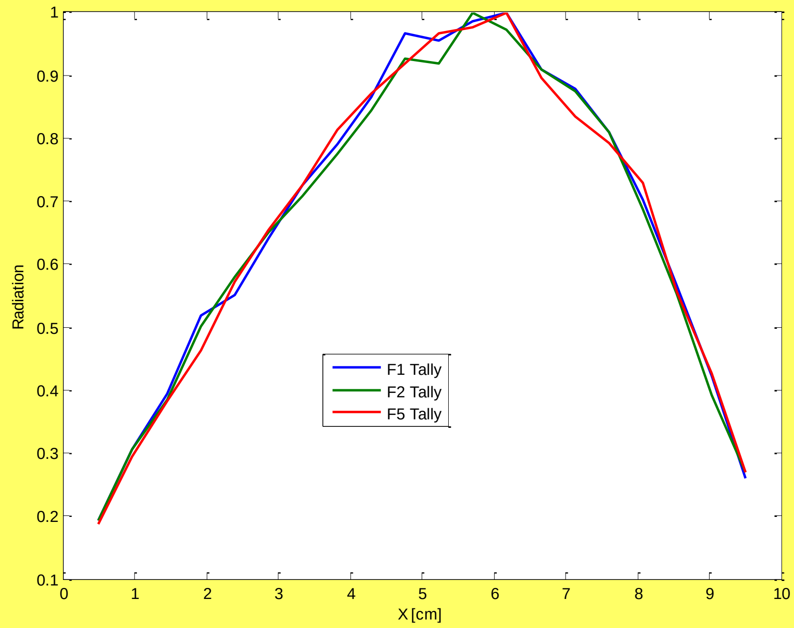


Fig: Comparison of plots from different tally type (normalized)

Multiple Groups of Projections

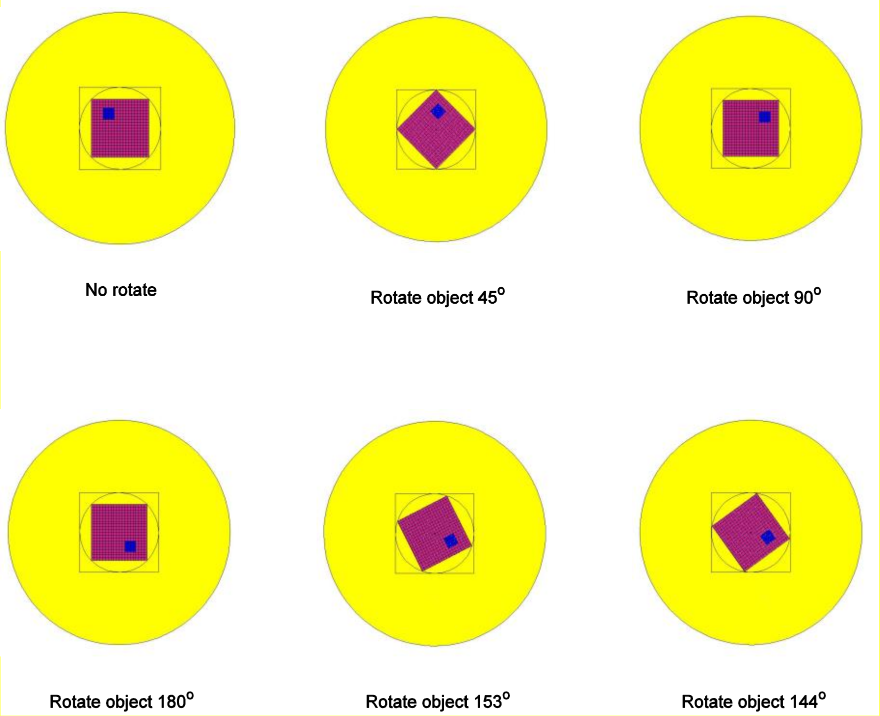


Fig: Rotate the object in different angles using mcnp_pstudy[4].

Implementation detail: Set mcnp_pstudy parameters in TRn card

[4]F. B. Brown et al., Monte Carlo parameter studies and uncertainty analysis with MCNP5, LA-UR-04-0499, LANL, 2004

Plots of Radiation Projections

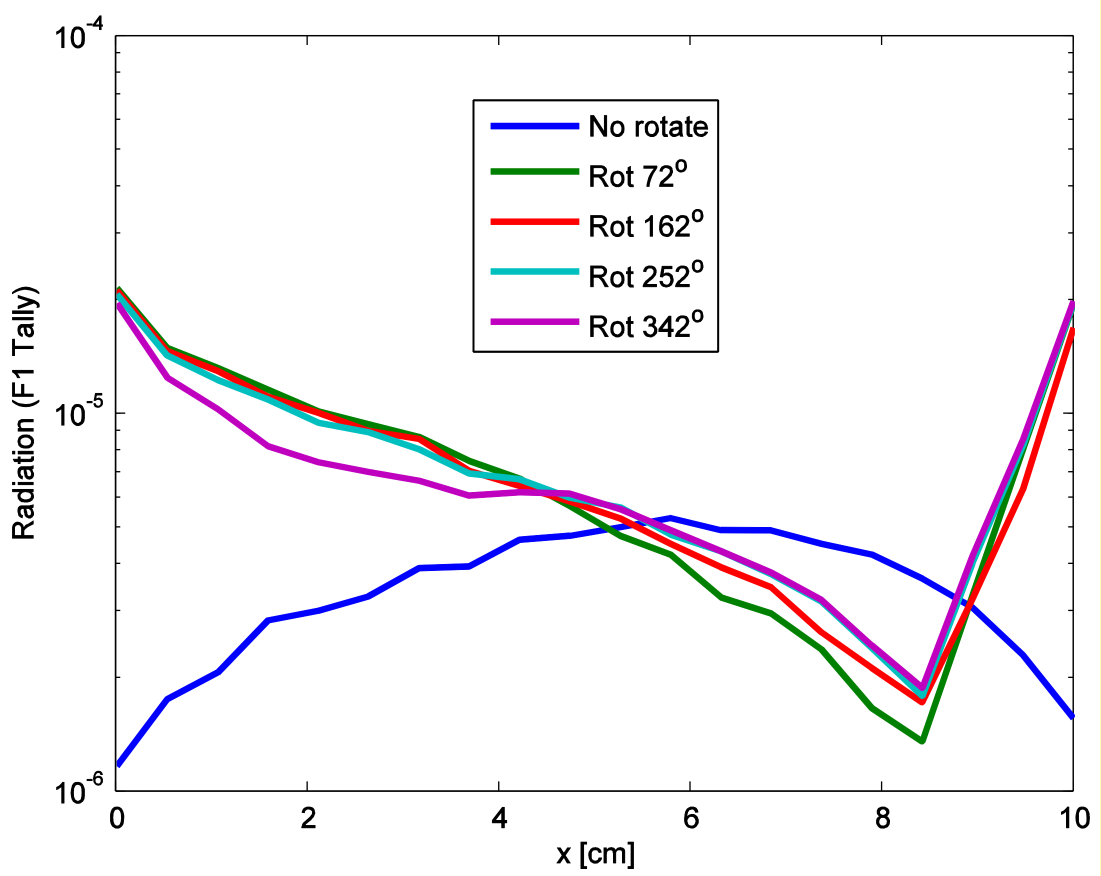
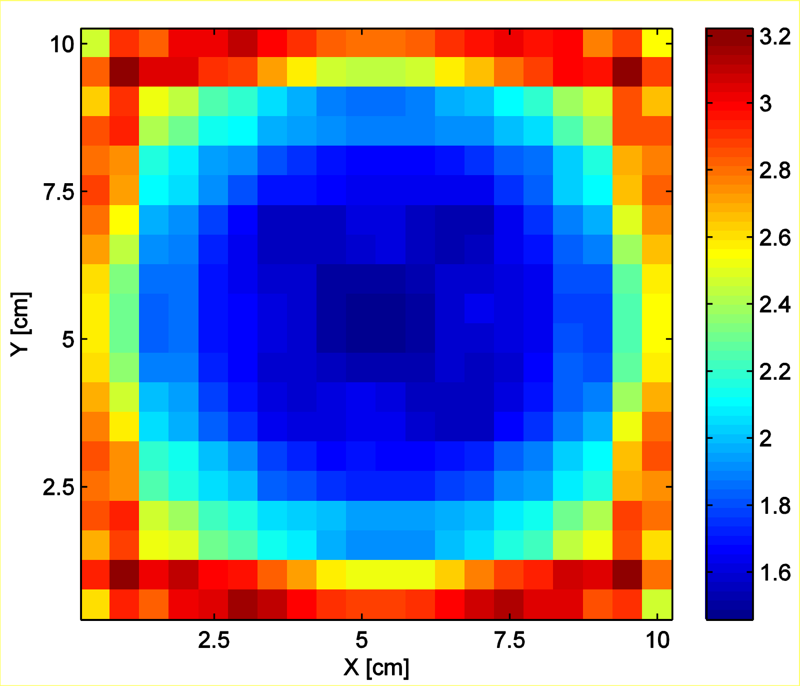


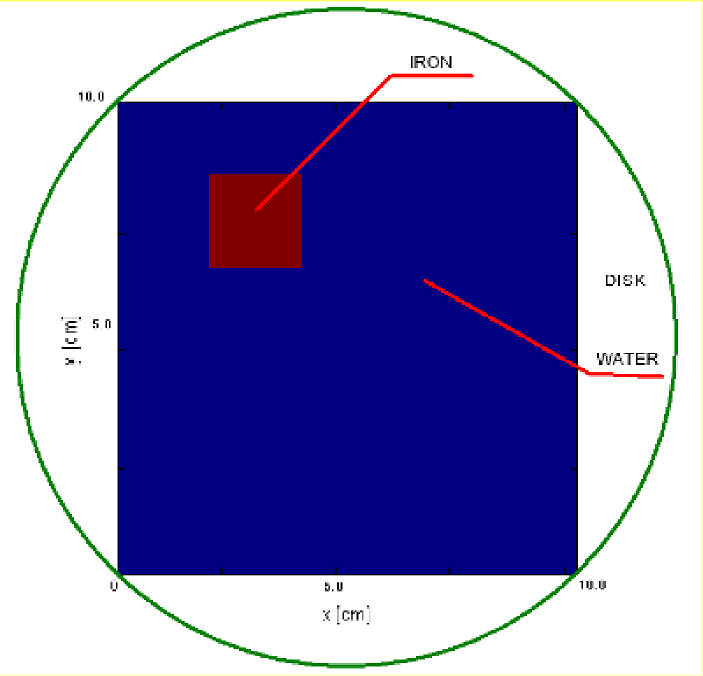
Fig: Transmitted radiation measured with object rotated in different angle.

Implementation detail: Output is post processed by MATLAB script

Image Reconstruction Results

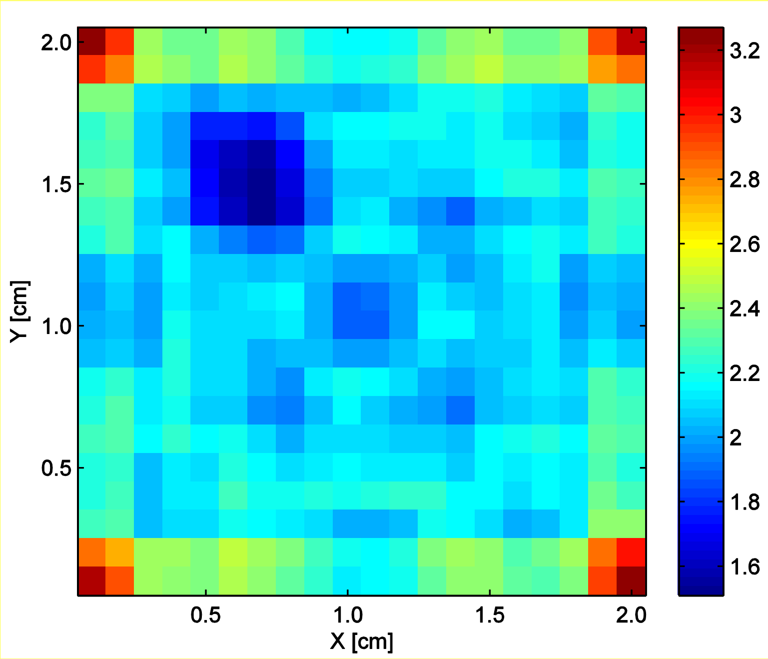


Total cross section reconstructed with FBP method for the test problem.

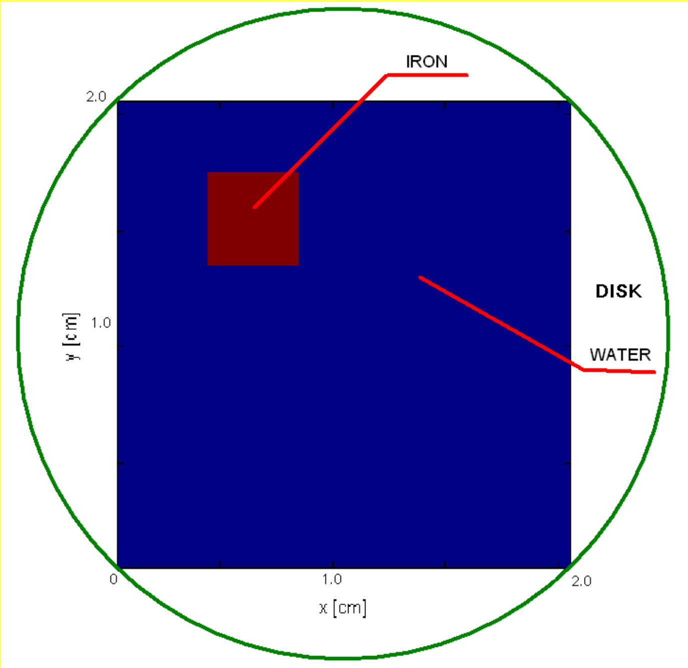


Geometry and material configuration of the test problem .

Smaller Version Problem



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



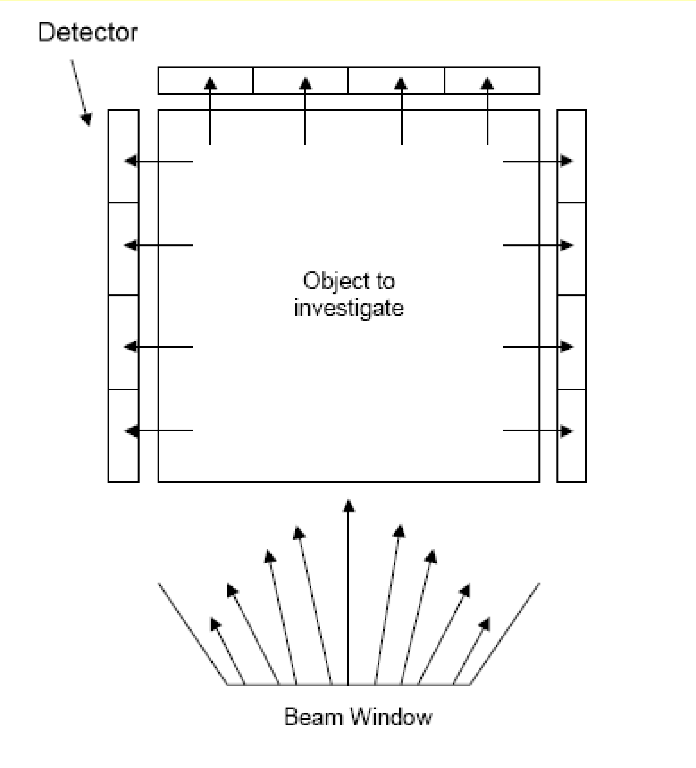
Geometry and material configuration of the test problem for a smaller version problem.

Summary to Analytic Tomography Method

- The analytic tomography method is **not viable** for optically thick and highly scattering problems even with collimated source and detectors.
- The basic assumption of **line-integral** methods is **violated** when the scattering component significantly contributes to the measurements
- 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 talk.

Gradient-based Deterministic Optimization Method

Minimization Based Approaches[5,6]



A schematic diagram of the beam-object-detector system

- **Objective function**

$$\Phi = \frac{1}{2}\sum_{i=1}^{N}\left(P_i - M_i\right)^2$$

- **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**

$$P = P\left(\sigma_t, \sigma_s, \sigma_{s1}, \cdots\right)$$

$$\Rightarrow \Phi = \Phi\left(\sigma_t, \sigma_s, \sigma_{s1}, \cdots\right)$$

[5]V. Scipolo, Scattered neutron tomography based on a neutron transport problem, Master Thesis, Texas A&M, 2004

[6]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

Improvements Introduced in This Stage

- Create a variable change technique to convert constrained optimization to non-constrained optimization
- Apply a Krylov subspace iterative scheme[7] to speed up each forward calculation
- Non-linear conjugate gradient updating scheme with Brent's method integrated to perform 1-D line search
- Allow illumination of the object from all four sides of a rectangular object in 2-D perspective

[7] M.L. Adams & E.W. Larsen, Fast Iterative Methods for Discrete-Ordinates Particle Transport Calculations, Progress in Nuclear Energy, 40, 3-159, 2002

Multi-beams Incorporation

Old objective function:

$$\Phi = \frac{\frac{1}{2}\sum_{i=1}^{N}(P_i - M_i)^2}{\frac{1}{2}\sum_{i=1}^{N}(M_i)^2}$$

New objective function:

$$\Phi = \frac{\Phi_1 + \Phi_2 + \Phi_3 + \Phi_4}{\frac{1}{2}\sum_{k=1}^{4}\sum_{i=1}^{N}\left(M_{ki}\right)^2}$$

Where:

$$\Phi_k = \frac{1}{2}\sum_{i=1}^{N}\left(M_{ki} - P_{ki}\right)^2, \qquad k = 1, 2, 3, 4$$

Modification in gradient calculation:

$$\frac{\partial \Phi}{\partial \sigma_i} = \frac{1}{\frac{1}{2}\sum_{k=1}^{4}\sum_{i=1}^{N}\left(M_{ki}\right)^2}\left(\frac{\partial \Phi_1}{\partial \sigma_i} + \frac{\partial \Phi_2}{\partial \sigma_i} + \frac{\partial \Phi_3}{\partial \sigma_i} + \frac{\partial \Phi_4}{\partial \sigma_i}\right)$$

Forward and Inverse Model

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

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

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

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

Define termination tolerance ε *and set iteration counter* $k=0$

Start of iteration loop

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

$$\mathbf{x}^{(k+1)}=\mathbf{x}^{(k)}+\alpha_{\min}\mathbf{d}^{(k)}$$

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

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

$$k=k+1$$

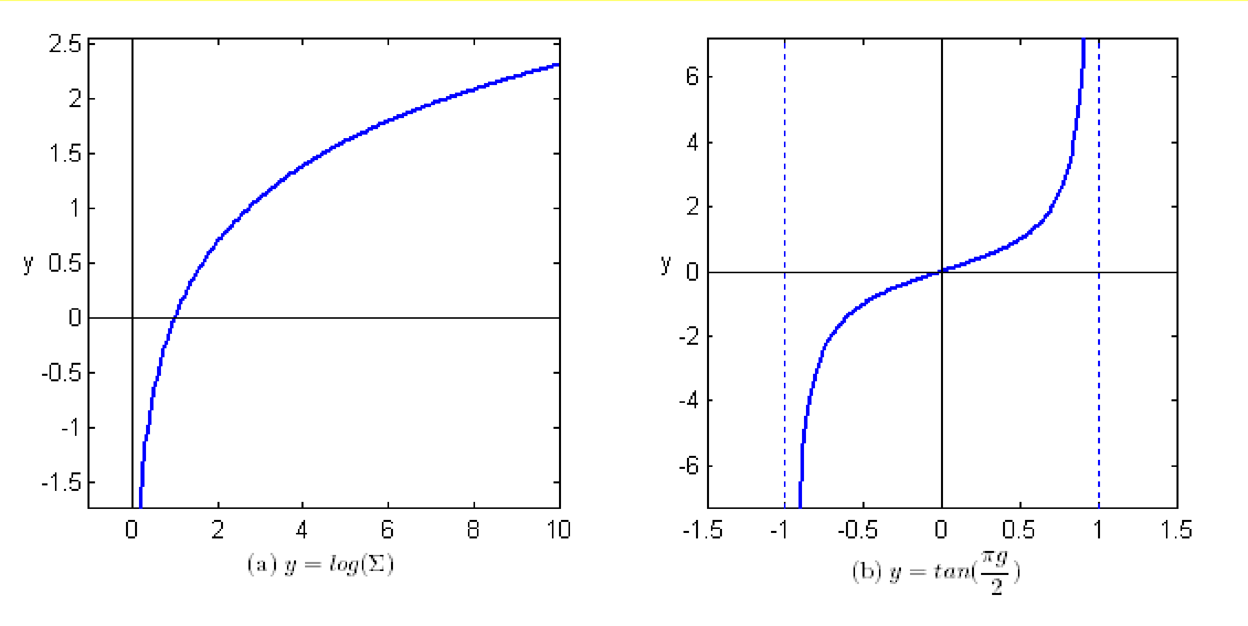
Exit if $\left\|\nabla\Phi\left(\mathbf{x}^{(k)}\right)\right\|<\varepsilon$

End of iteration loop

Variable Change Technique[9]

Purpose: Convert constrained optimization to non-constrained optimization

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



(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) $y_j = \tan\left(\frac{\pi}{2} g_j\right) \Rightarrow$

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

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

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[9]Z. Wu and M.L. Adams, Variable change technique applied in constrained inverse transport applications, Tran. Ame. Nuc. Soc., 102, 2010

Nonlinear CG Updating Scheme with Variable Change Technique Incorporated

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

Define termination tolerance ε *and set iteration counter* $k = 0$

Start of iteration loop

Change variable x to y

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

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

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

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

$$k = k + 1$$

Change variable y back to x

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

End of iteration loop

Deterministic Optimization Results for Model Problem

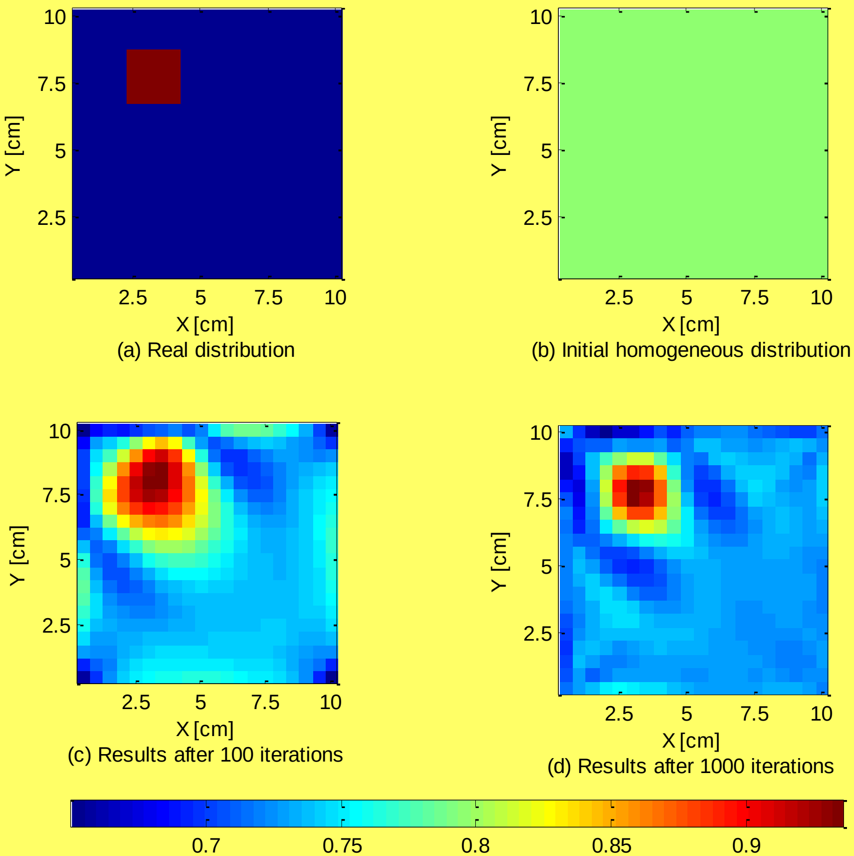
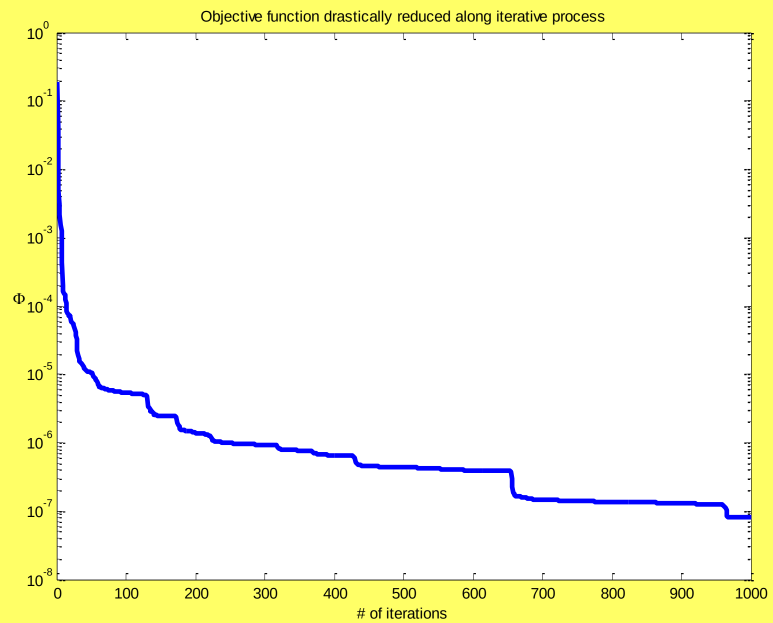
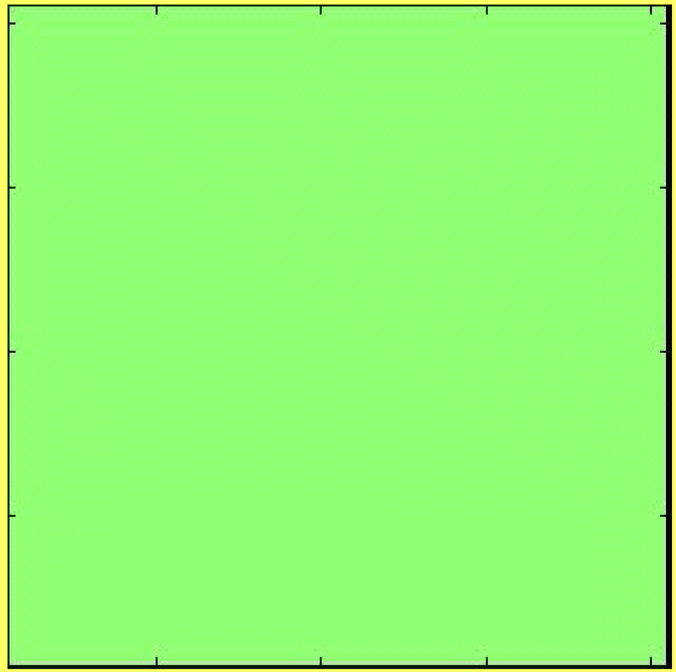


Fig: Transport cross section (Σ_{tr}) distribution obtained from deterministic CG based iterative search scheme for the one iron problem. (a) The real Σ_{tr} (background is water and square inclusion is iron). (b) Initial guess for Σ_{tr} . (c) and (d) are results after 100 and 1000 iterations, respectively.



The objective function changes after each iteration for one iron problem

Animation Show of the Iterative Reconstruction Procedure



Transport cross section (Σ_{tr}) distribution within the object changes after each updating iteration.

Drawbacks Associated with Deterministic Methods

- Deterministic search method could be trapped into local minima; the results are greatly dependent on initial guess
- Each P_i (predicted measurement) is a complicated nonlinear functional of each unknown cross section
- These inverse problems are ill-conditioned: In many cases, there are a wide variety of solutions to produce approximately the same objective function
- 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: $\underset{\text{number of cells}}{\mathrm{n}} \times \underbrace{100\times100}_{\text{100 groups}} \times \underset{P_3\ \text{method}}{4} = n \times 40,000$

Stochastic-based Combinatorial Optimization Method

Advances Devised in This Stage

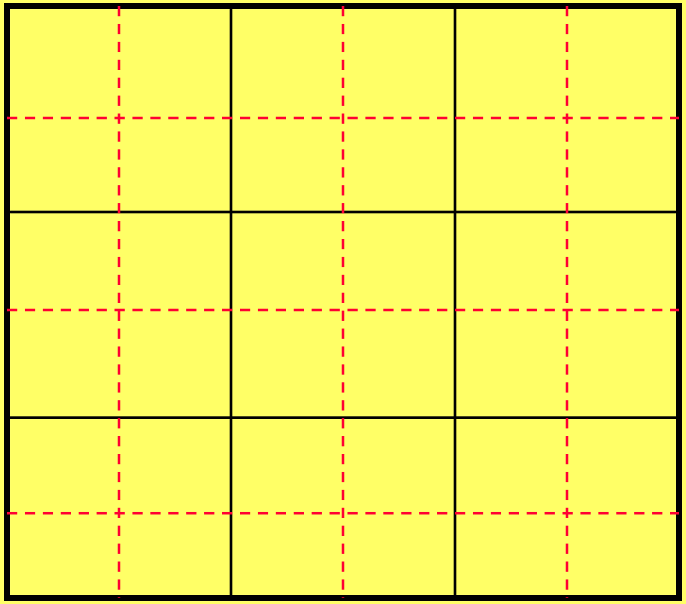
- Treat unknowns as materials instead of cross sections
- Change continuous search to discrete search
- Combine deterministic and stochastic optimization method together
- Hierarchical Approach

  - Mesh refinement

  - High fidelity forward calculation
- Search dimension reduction techniques

  - Cell grouping

  - Material restriction
- Efficient stochastic-based combinatorial optimization (CO) scheme



Material Candidate Library (MCL)

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) which works as search space for the discrete search.

$$\overline{\sigma_i} = \frac{\int_0^{E_{th}} \sigma_i(E)\phi(E)dE}{\int_0^{E_{th}} \phi(E)dE} = \frac{F4(Fm4)\ \text{Tally}}{F4\ \text{Tally}}$$

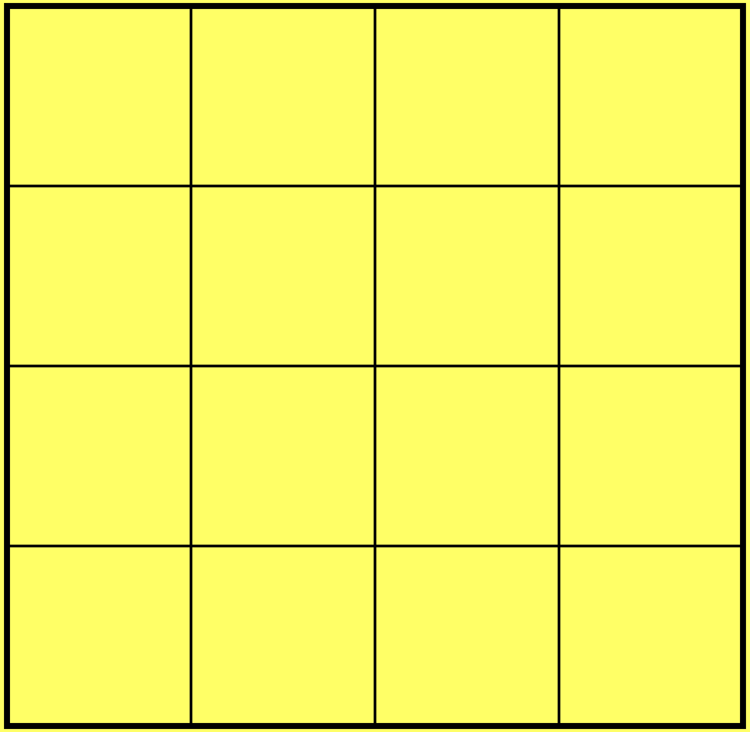
$$\overline{\Sigma_i} = n\overline{\sigma_i} = \rho \frac{N_A}{M}\overline{\sigma_t}$$

Current materials in MCL

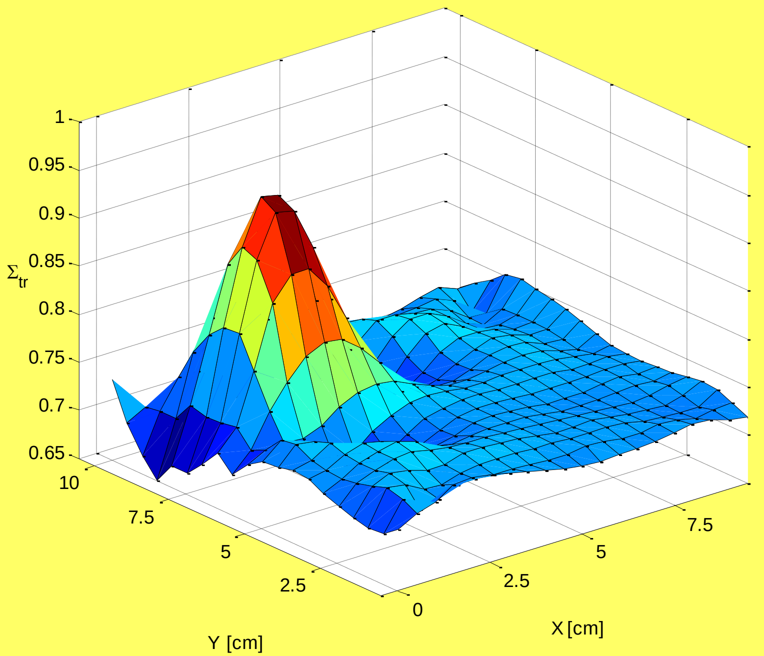
#	Material	Σ_t (1/cm)	Σ_s(1/cm)	g ($\frac{2}{3A}$)
1	Paraffin	0.567	0.567	5.56E-2
2	B-10	5.54E+2	3.20E-1	6.67E-2
3	Water	0.746	0.736	3.70E-2
4	Si	0.110	0.102	2.37E-2
5	Fe	1.18	0.967	1.19E-2
6	Nitrogen	6.50E-4	5.50E-4	4.76E-2
7	Cadmium (Cd)	0.301	0.247	5.90E-3
8	Aluminum (Al)	9.68E-2	8.31E-2	2.47E-2
9	Natural Uranium	0.821	0.921	1.40E-3
10	HEU	2.70E+1	5.25E+1	3.61E-5

Why Combinatorial Optimization?

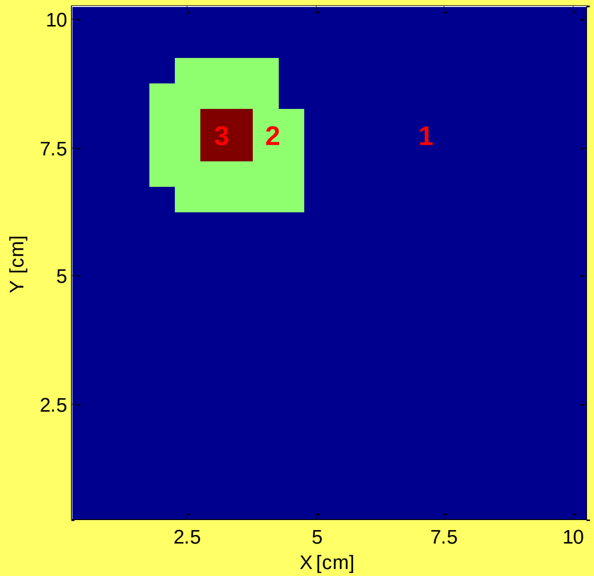
- Suppose we divide an object into have a 4x4 cells in a 2-D view and we have 10 material candidates in our material library.
- In each cell, the material in it has 10 possibilities, so over all there're totally $\underbrace{10\times10\times\cdots\times10}_{16\ \text{times}}=10^{16}$ possibilities (solutions) to construct the object.
- Call one solution as one combination
- The problem becomes to find the combination/solution to minimize the objective function, i.e. combinatorial optimization.



Cell Grouping Result for Model Problem



Surface plot of the Σ_{tr} distribution yielded from deterministic optimization 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**

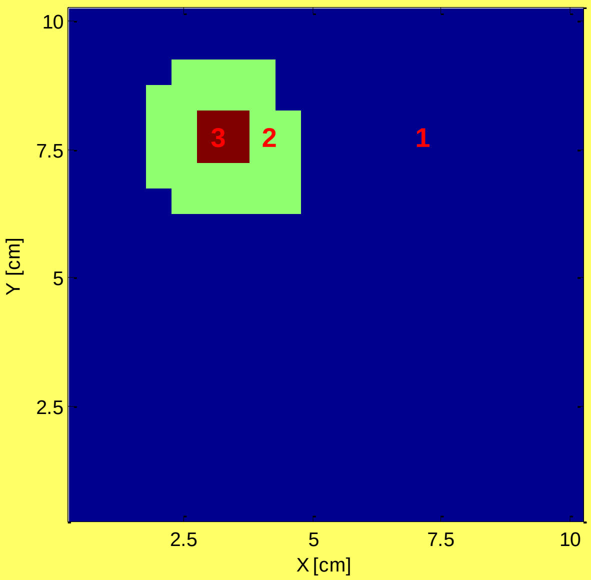
$$\Sigma_{tr} > \Sigma_{tr,mean} + \alpha(\Sigma_{tr,max} - \Sigma_{tr,mean}) \Rightarrow \text{ Inclusion region}$$

$$\Sigma_{tr} < \Sigma_{tr,mean} + \beta(\Sigma_{tr,max} - \Sigma_{tr,mean}) \Rightarrow \text{ Background region}$$

$$\text{otherwise } \Rightarrow \text{ Interface region}$$

We chose $\alpha = 0.8,\ \beta = 0.2$ in the implementation to the model problem.

Material Restriction Result for Model Problem



Cell grouping result

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

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:

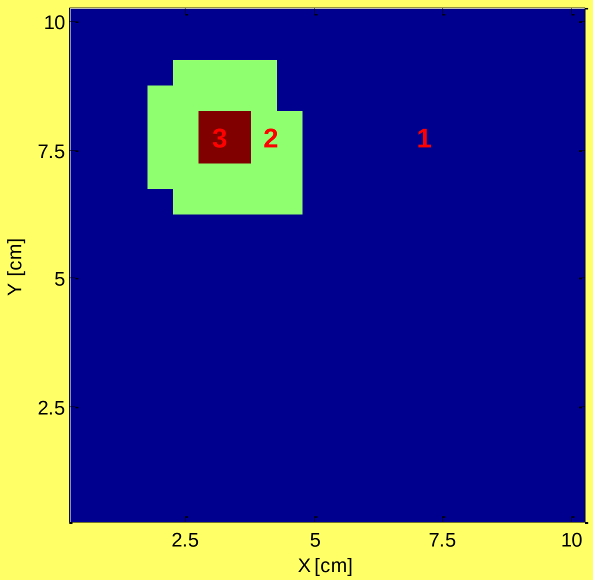
$$e_m = error = \frac{1}{3}\left(\left|\frac{\Sigma_s^m - \Sigma_s^r}{\Sigma_s^m + \Sigma_s^r}\right| + \left|\frac{\Sigma_t^m - \Sigma_t^r}{\Sigma_t^m + \Sigma_t^r}\right| + \left|\frac{\Sigma_{tr}^m - \Sigma_{tr}^r}{\Sigma_{tr}^m + \Sigma_{tr}^r}\right|\right)$$

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

If exist one and only one 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 $a = 0.01,\ b = 0.5$.

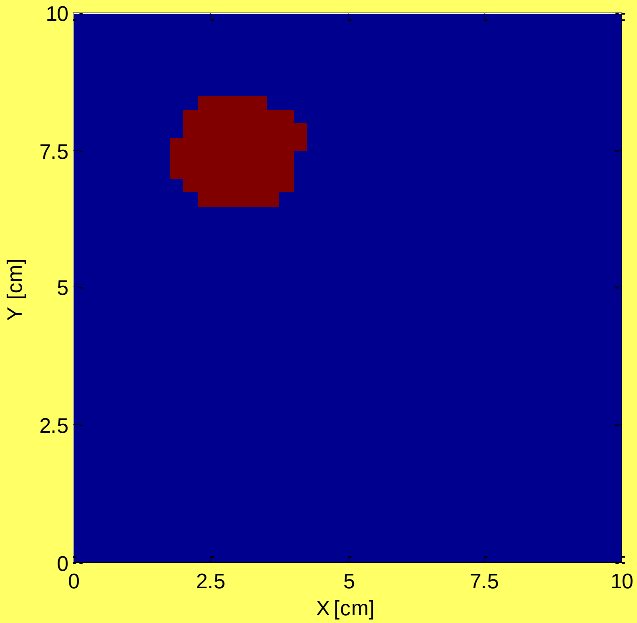
Combinatorial Optimization (CO) Scheme

- **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 some constraints, such as material continuity constraint, to the combinatorial solution**
- **Forward calculation to obtain the objective function**
- **Loop on the procedure until reaching a minimum objective function**



Cell grouping result

CO Result for Model Problem[10]



Material distribution from the combinatorial optimization (CO) after 50 iterations. (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

Parameter	Actual	Opt. Result
Material	Iron	Iron
X-center (cm)	3.00	2.97
Y-center (cm)	7.50	7.49
Area (cm^2)	4.00	4.00
Iron/Water	4.17E-2	4.17E-2

[10] Z. Wu and M.L. Adams, Advances in inverse transport methods, Proceedings of ICONE-18, 2010

Another Model Problem

Model Problem II

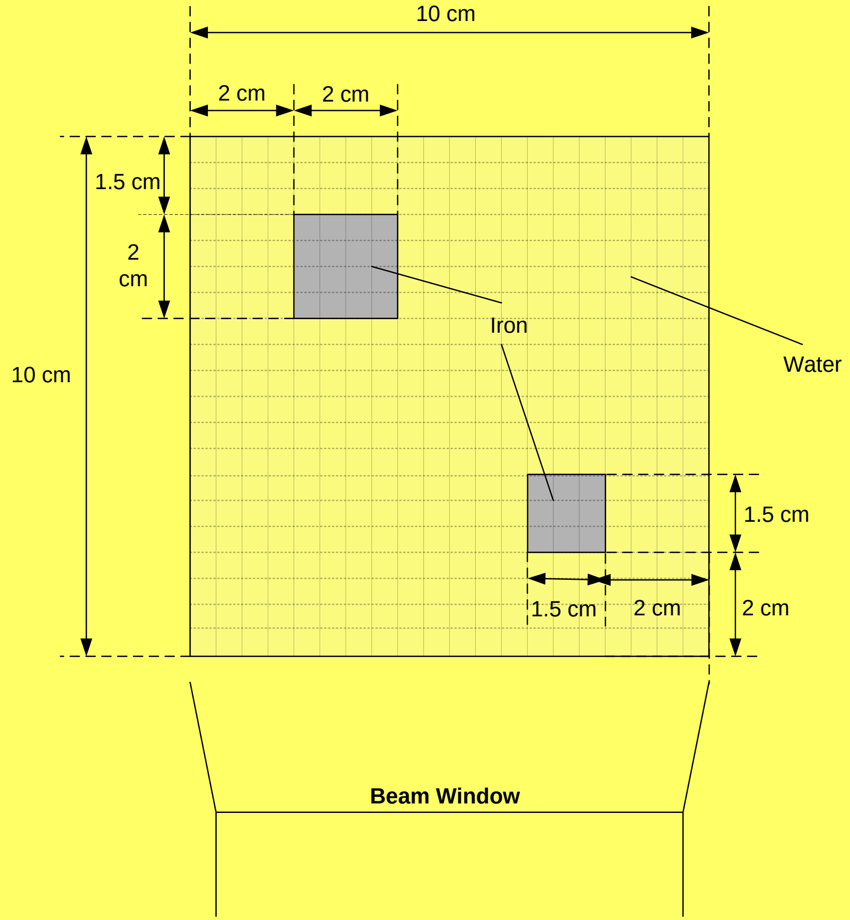


Fig: Schematic diagram of the two irons inclusion model problem (X-Y view).

Results for Model Problem II (Deterministic Stage)

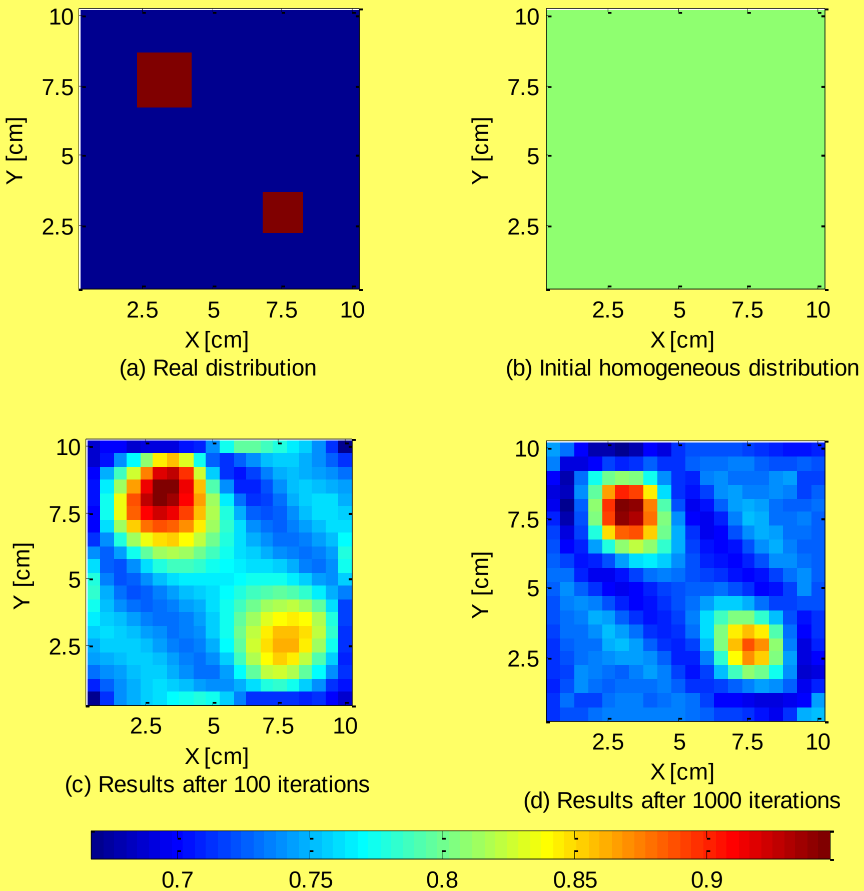


Fig. 1: Transport cross section (Σ_{tr}) distribution obtained from deterministic CG based iterative search scheme for the two irons problem. (a) The real Σ_{tr} (background is water and square inclusions are irons). (b) Initial guess for Σ_{tr} . (c) and (d) are results after 100 and 1000 iterations, respectively.

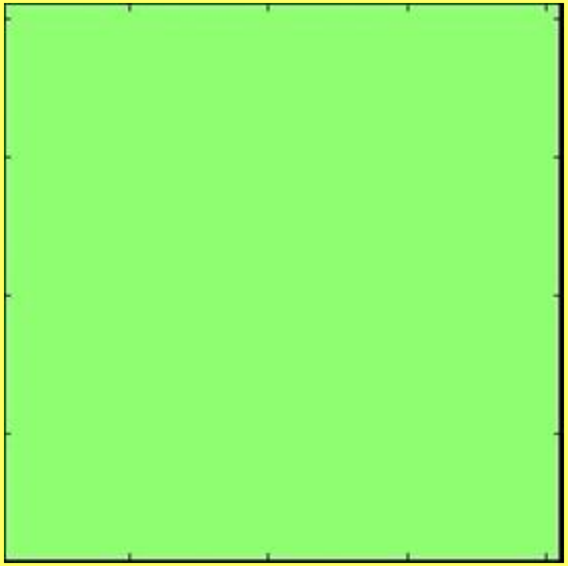
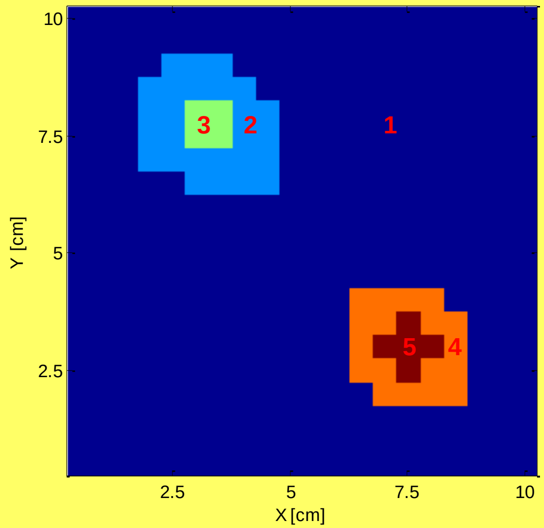
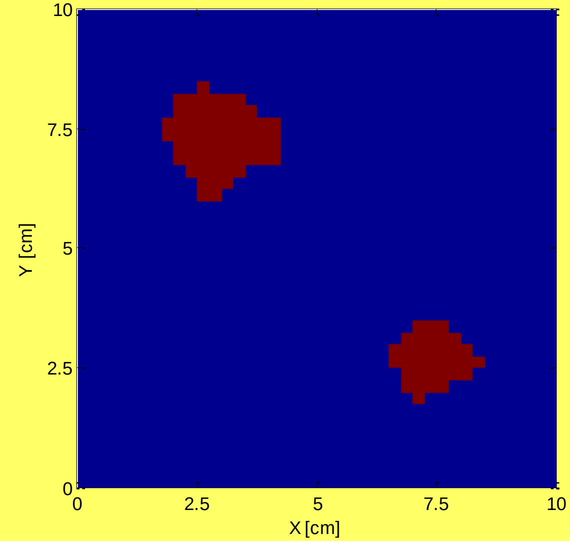


Fig. 2: Animation show of the reconstruction procedure for transport cross section (Σ_{tr}) distribution within the object changes with each iteration.

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

Parameter		Material	X-center (cm)	Y-center (cm)	Area (cm^2)
Inclusion 1	**Actual**	Iron	3.00	7.50	4.00
	Opt. Result	Iron	2.95	7.37	4.25
Inclusion 2	**Actual**	Iron	7.25	2.75	2.25
	Opt. Result	Iron	7.29	2.66	2.19

Conclusions

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

Future Recommendation

- Address measurement noise and model error
- More efficient computation of gradients with explicit ad-joint difference model in deterministic optimization
- Improve the constraints and bias employed in stochastic combinatorial optimization
- Cell grouping and material restriction using multi-group parameters
- Extend general strategies we present in this research to different highly scattering problems and applications

Questions?

Thank You!

Back up slides

Radiography vs. Tomography

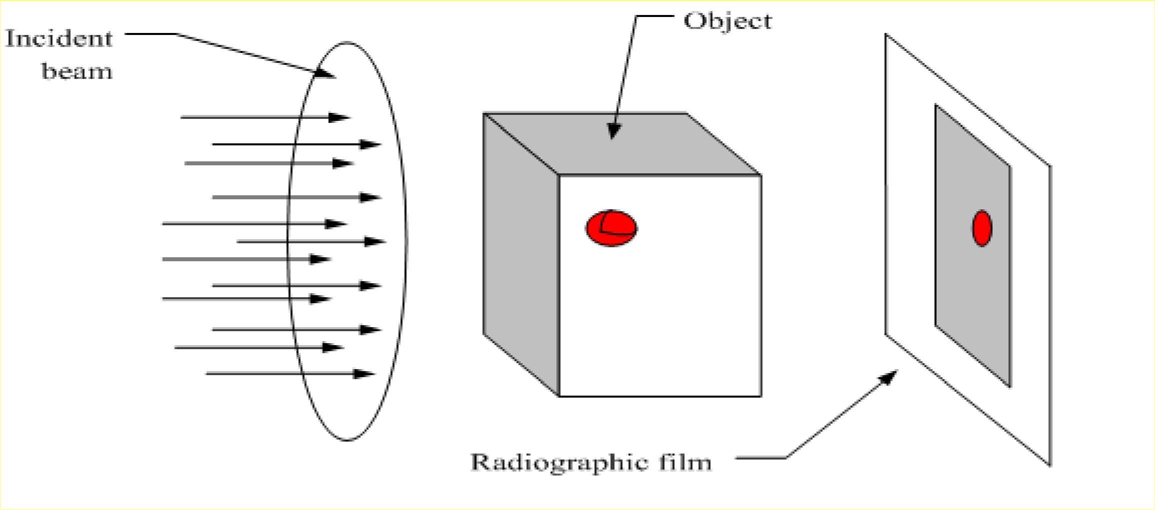


Fig: An idealized facility configuration for radiographic Imaging system

Simple exponential attenuation method (SEAM)

$$I(x) = I_0 e^{-\int_0^x \Sigma_t(s)ds} \quad \Rightarrow \quad \int_0^x \Sigma_t(s)ds = -\ln\left(\frac{I(x)}{I_0}\right)$$

Radiography vs. Tomography (cont.)

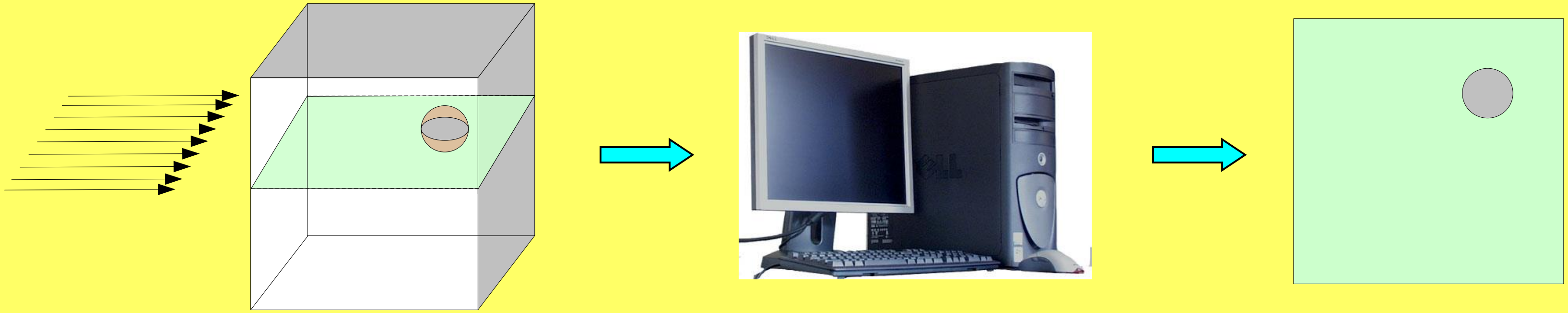
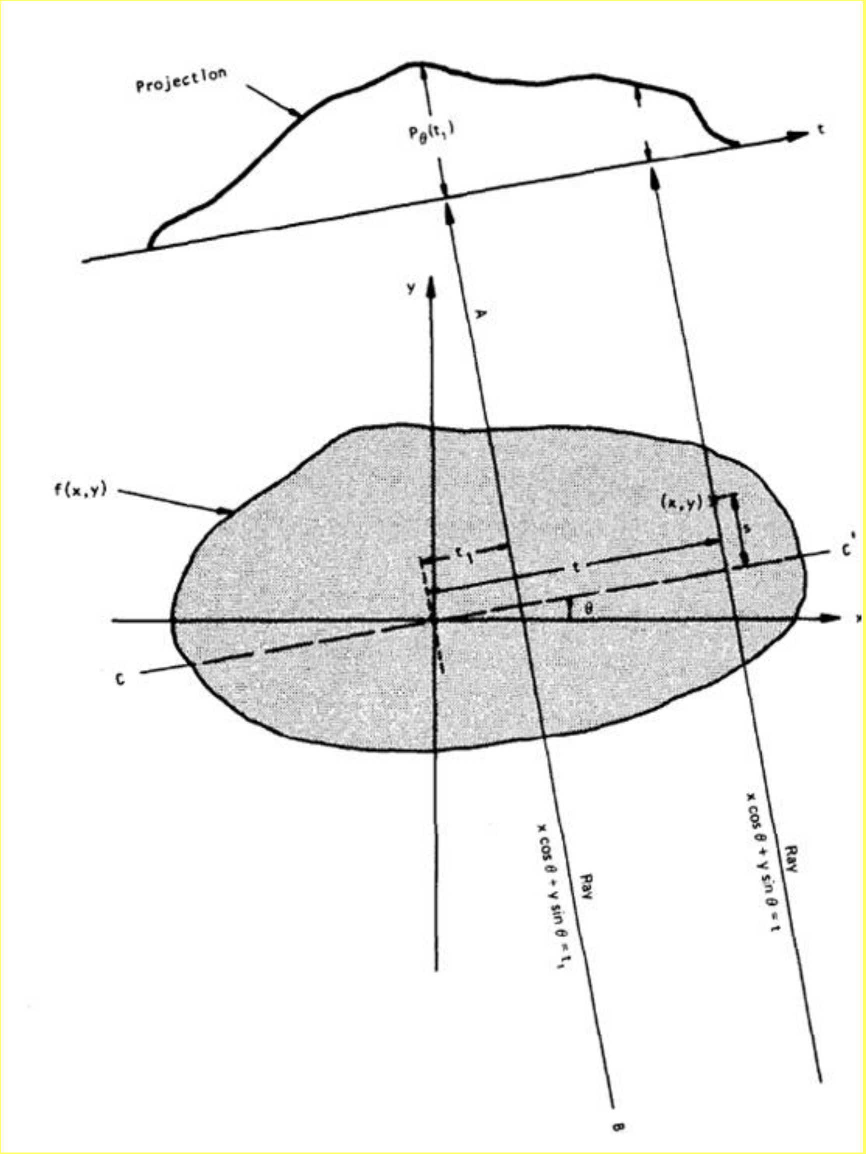


Fig: Traditional Computer Tomography (CT) Procedure

"Tomo" means "to cut" in Greek

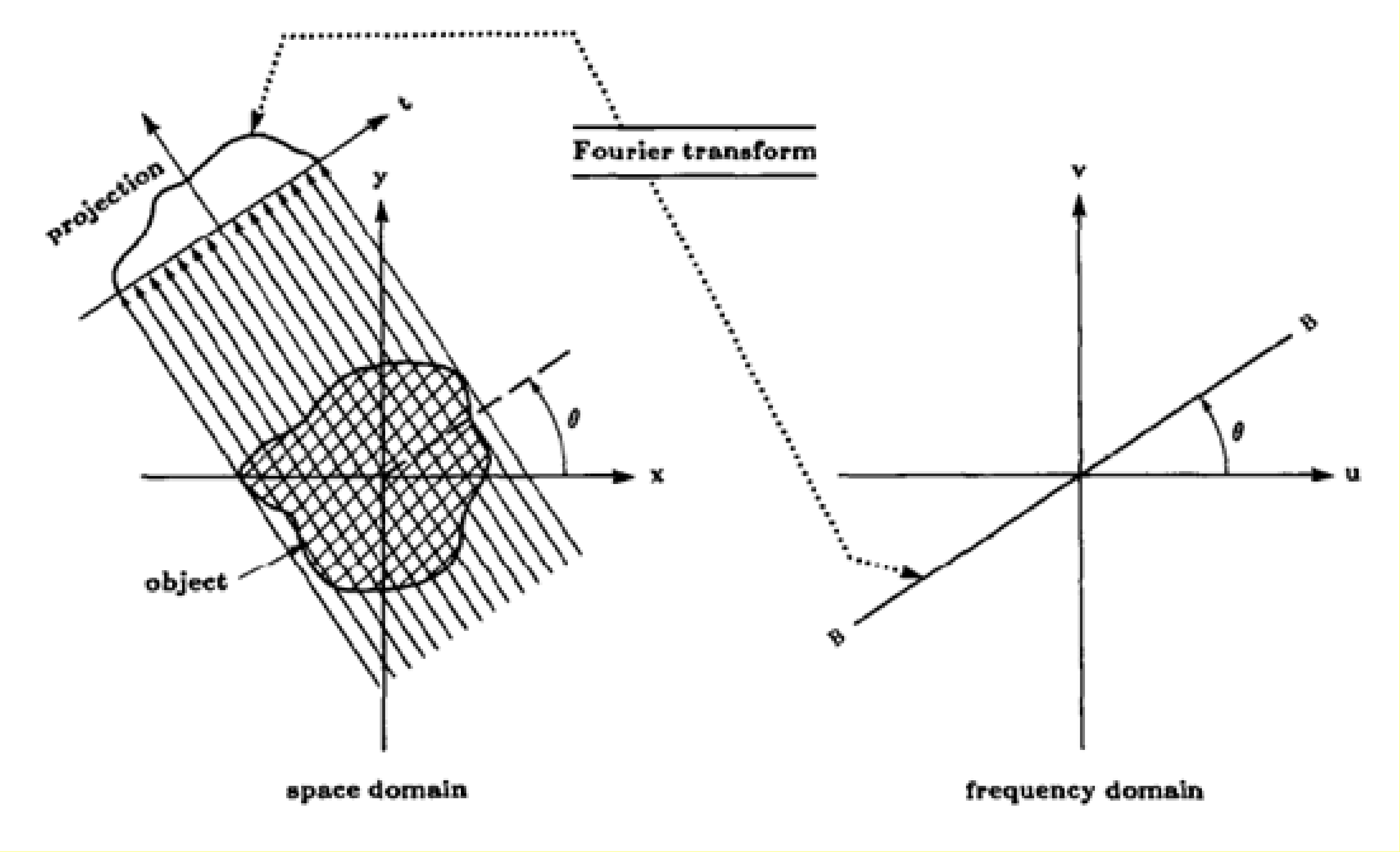
A tomography imaging system deals with reconstructing an internal image of an object based on its peripheral emerging radiations. The cross-sectional image of an object was reconstruction by illuminating the object from many different directions.

Line Integral



BACK

Fourier Slice Theorem



BACK

Linear Scattering Anisotropy Factor

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

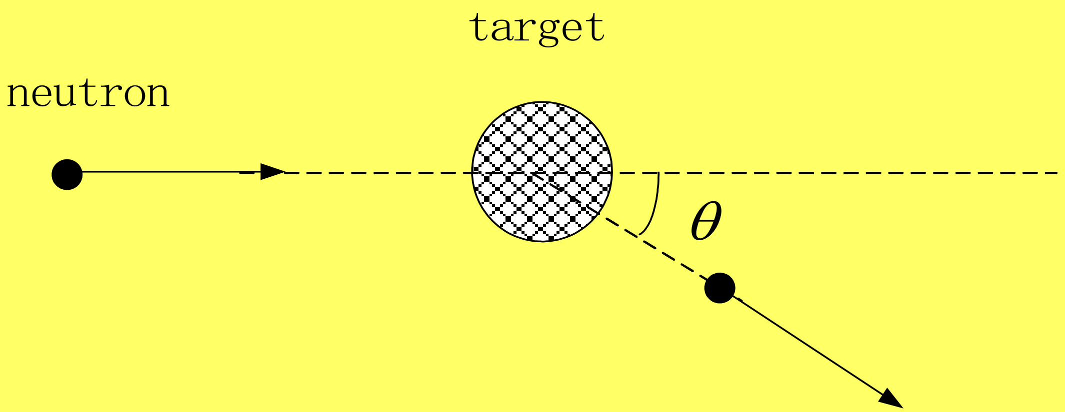
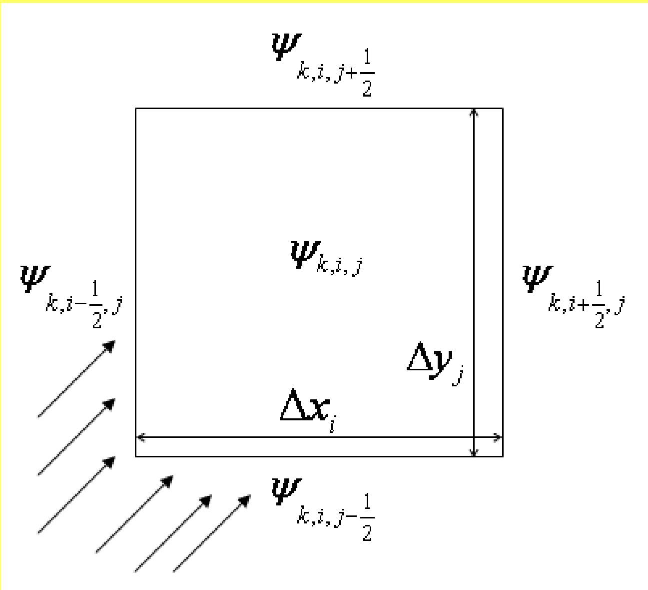


Fig: Neutron diffracts with angle theta after colliding with a nuclide target

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

BACK

Step Characteristic (SC) Method



Here $$\tau^k_{i,j} = \sigma_t \min\left\{\frac{\Delta x_i}{|\mu_k|}, \frac{\Delta y_j}{|\eta_k|}\right\},$$

$$\alpha^k_{i,j} = \min\left\{1, \left|\frac{\mu_k \Delta y_j}{\eta_k \Delta x_i}\right|\right\},$$

$$\nu^k_{i,j} = \min\left\{1, \left|\frac{\eta_k \Delta x_i}{\mu_k \Delta y_j}\right|\right\}$$

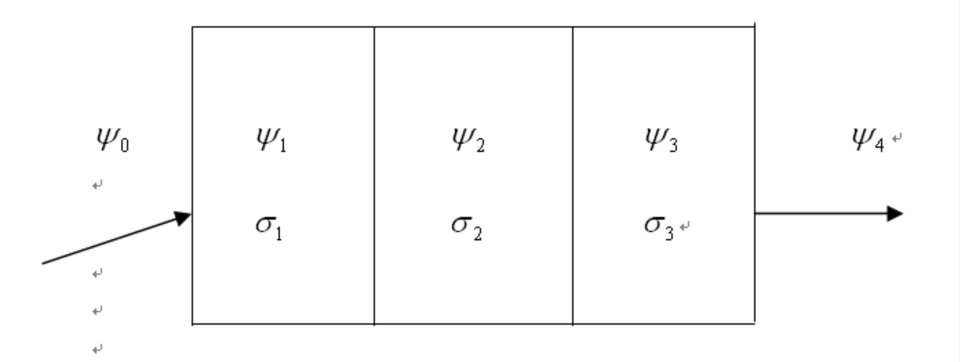
$$\psi_{k,i,j} = \frac{q_{k,i,j}}{\sigma_t} - \mu_k \frac{\psi_{k,i+\frac{1}{2},j} - \psi_{k,i-\frac{1}{2},j}}{\Delta x_i \sigma_t} - \eta_k \frac{\psi_{k,i,j+\frac{1}{2}} - \psi_{k,i,j-\frac{1}{2}}}{\Delta y_j \sigma_t}$$

$$\psi_{k,i+\frac{1}{2},j} = \frac{q_{k,i,j}}{\sigma_t} + \nu^k_{i,j}\left(\psi_{k,i,j-\frac{1}{2}} - \frac{q_{k,i,j}}{\sigma_t}\right)\left(\frac{1-e^{-\tau^k_{i,j}}}{\tau^k_{i,j}}\right) + \left(1-\nu^k_{i,j}\right)\left(\psi_{k,i-\frac{1}{2},j} - \frac{q_{k,i,j}}{\sigma_t}\right)e^{-\tau^k_{i,j}}$$

$$\psi_{k,i,j+\frac{1}{2}} = \frac{q_{k,i,j}}{\sigma_t} + \alpha^k_{i,j}\left(\psi_{k,i-\frac{1}{2},j} - \frac{q_{k,i,j}}{\sigma_t}\right)\left(\frac{1-e^{-\tau^k_{i,j}}}{\tau^k_{i,j}}\right) + \left(1-\alpha^k_{i,j}\right)\left(\psi_{k,i,j-\frac{1}{2}} - \frac{q_{k,i,j}}{\sigma_t}\right)e^{-\tau^k_{i,j}}$$

BACK

Ad-joint Difference Method



$$A = \begin{bmatrix} 0 & \frac{\partial \psi_2}{\partial \psi_1} & 0 & 0 \\ 0 & 0 & \frac{\partial \psi_3}{\partial \psi_2} & 0 \\ 0 & 0 & 0 & \frac{\partial \psi_4}{\partial \psi_3} \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad \nu = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{\partial \Phi}{\partial \psi_4} \end{bmatrix} \qquad B_\sigma = \begin{bmatrix} \frac{\partial \psi_1}{\partial \sigma_1} & 0 & 0 & 0 \\ 0 & \frac{\partial \psi_2}{\partial \sigma_2} & 0 & 0 \\ 0 & 0 & \frac{\partial \psi_3}{\partial \sigma_3} & 0 \end{bmatrix}$$

$$\begin{bmatrix} \frac{\partial \Phi}{\partial \sigma_1} \\ \frac{\partial \Phi}{\partial \sigma_2} \\ \frac{\partial \Phi}{\partial \sigma_3} \end{bmatrix} = \begin{bmatrix} \frac{\partial \Phi}{\partial \psi_4}\frac{\partial \psi_4}{\partial \psi_3}\frac{\partial \psi_3}{\partial \psi_2}\frac{\partial \psi_2}{\partial \psi_1}\frac{\partial \psi_1}{\partial \sigma_1} \\ \frac{\partial \Phi}{\partial \psi_4}\frac{\partial \psi_4}{\partial \psi_3}\frac{\partial \psi_3}{\partial \psi_2}\frac{\partial \psi_2}{\partial \sigma_2} \\ \frac{\partial \Phi}{\partial \psi_4}\frac{\partial \psi_4}{\partial \psi_3}\frac{\partial \psi_3}{\partial \sigma_3} \end{bmatrix} = B_\sigma \sum_{i=0}^{3} A^i \nu$$

BACK

Incorporate Multi-beams

$$\Phi_1 = \frac{1}{2}\sum_{i=1}^{N}\left(M_{1i} - P_{1i}\right)^2$$

$$\Phi_2 = \frac{1}{2}\sum_{i=1}^{N}\left(M_{2i} - P_{2i}\right)^2$$

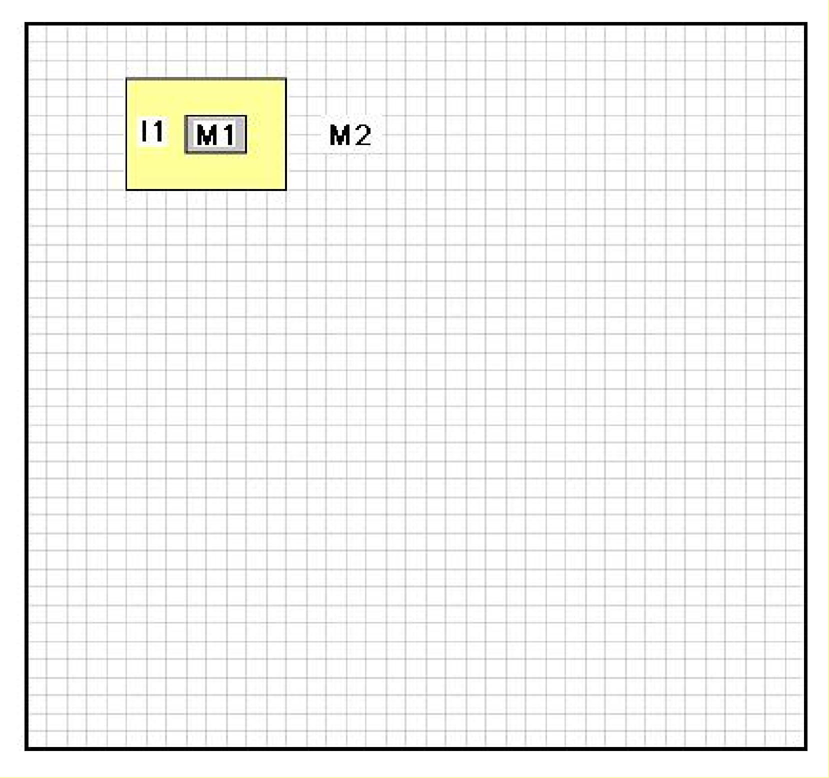
$$\Phi_3 = \frac{1}{2}\sum_{i=1}^{N}\left(M_{3i} - P_{3i}\right)^2$$

$$\Phi_4 = \frac{1}{2}\sum_{i=1}^{N}\left(M_{4i} - P_{4i}\right)^2$$

$$\Phi = \frac{\Phi_1 + \Phi_2 + \Phi_3 + \Phi_4}{\frac{1}{2}\sum_{j=1}^{4}\sum_{i=1}^{N}\left(M_{ji}\right)^2}$$

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

Example of Constraints



Three regions (M1, M2, I1) are determined after cell grouping process in a demonstration problem with 40 x 40 grids discretization.

BACK

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

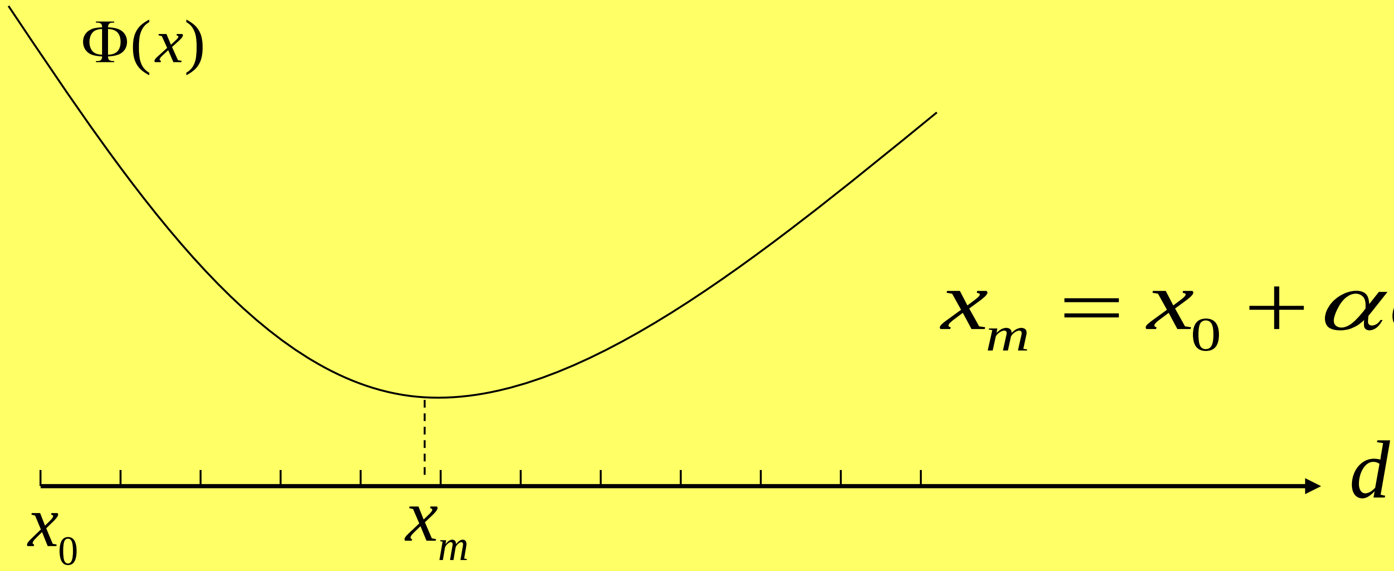
- **Once the search direction is set, you have to know how far to move along this direction to make the objective function minimum. This is the basic conception of line search (1D search).**

$$x_{k+1} = x_k + \alpha_k d_k$$

- **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.**

$$f(x) = \frac{1}{2} x^T A x - b^T + c = \frac{1}{2}(Ax, x) - (b, x) + c$$

Line Search (cont.)



$$x_m = x_0 + \alpha d$$

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.

Fissile Material Treatment

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

$$\boxed{\begin{cases}\Sigma_s(\underline{r})=\Sigma_s(\underline{r})+\nu\Sigma_f(\underline{r})\\ g=g\,\dfrac{\Sigma_s(\underline{r})}{\Sigma_s(\underline{r})+\nu\Sigma_f(\underline{r})}\end{cases}}$$

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

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