Variable Change Technique Applied in Constrained Inverse Transport Applications

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Introduction

Forward vs. Inverse

- Forward Transport Problem[1]

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

- Inverse Transport Problem

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

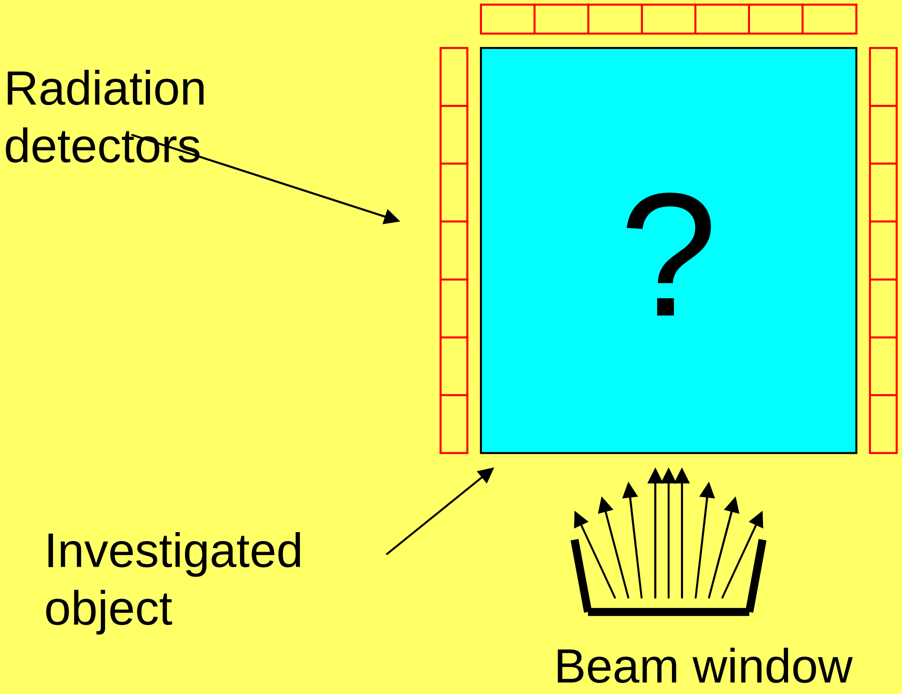
Note: Symbols in red are unknown variables in the problem.

[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. (Neutron tomography)

We are particularly interested in problems in which radiation can undergo significant scattering within the object.



Model Problem

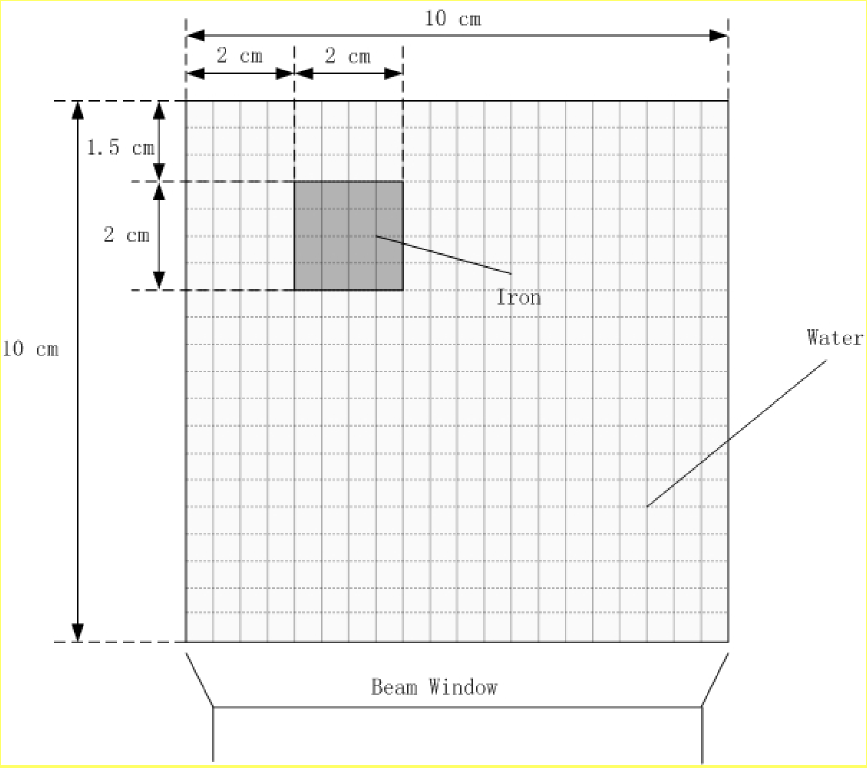


Fig: Schematic diagram of the one iron inclusion model problem (X-Y view).

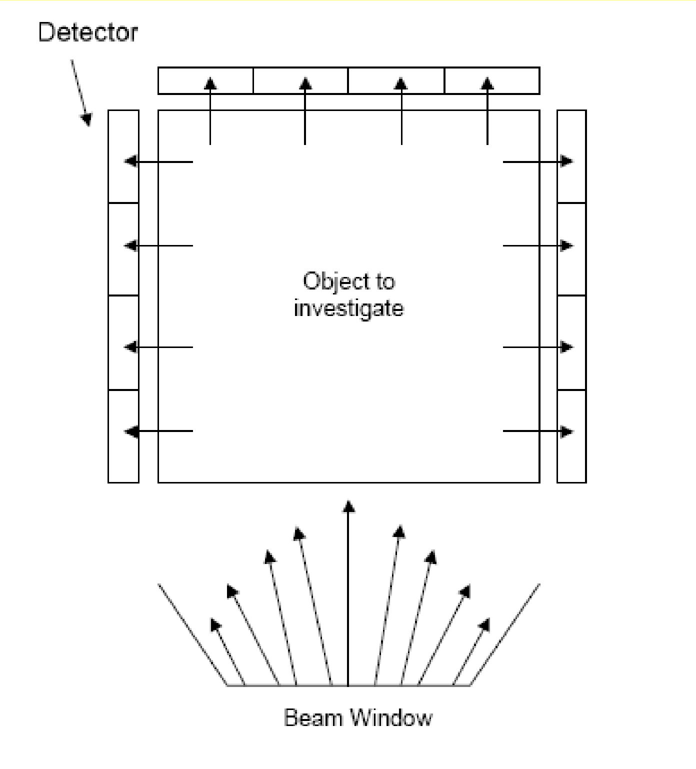
Table: Physics properties of the materials in the model problem

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

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

Gradient-based Iterative Optimization Method

Minimization Based Optimization Approaches[2,3]



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 accurate mathematical model
- 'P' is predicted measurements provided by forward model calculation, which is treated as a function of properties of the unknown object

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

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

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

[3]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

Forward and Inverse Model

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

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

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

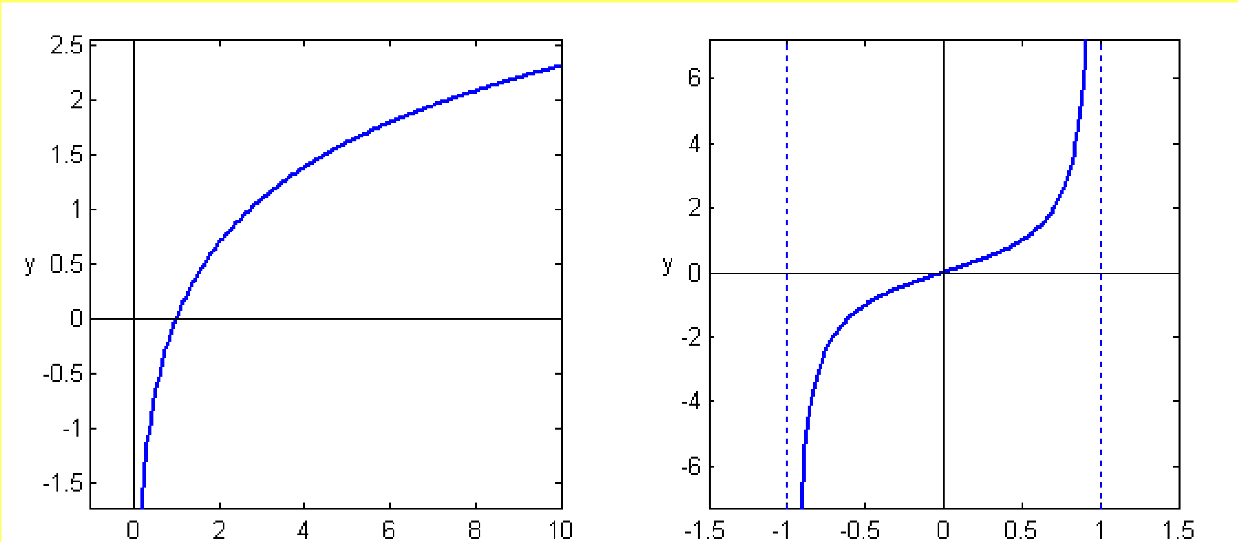
End of iteration loop

Variable Change Technique

Variable Change Technique

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) $y = log(\Sigma)$ (b) $y = tan(\frac{\pi g}{2})$

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

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

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

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

Results

Deterministic Optimization Results for Model Problem

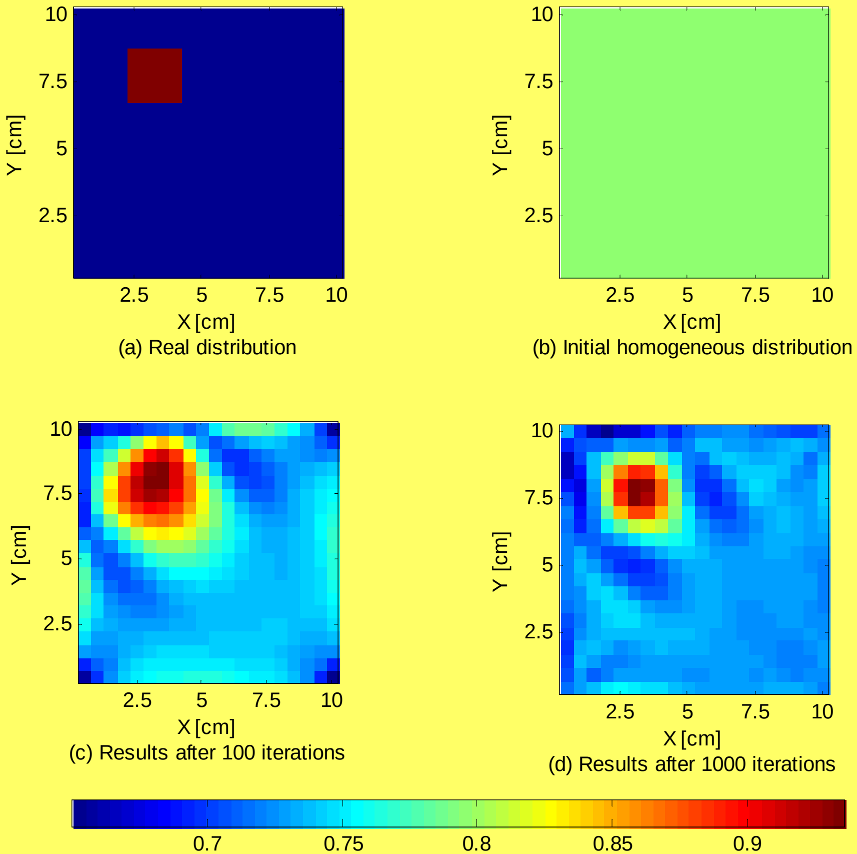
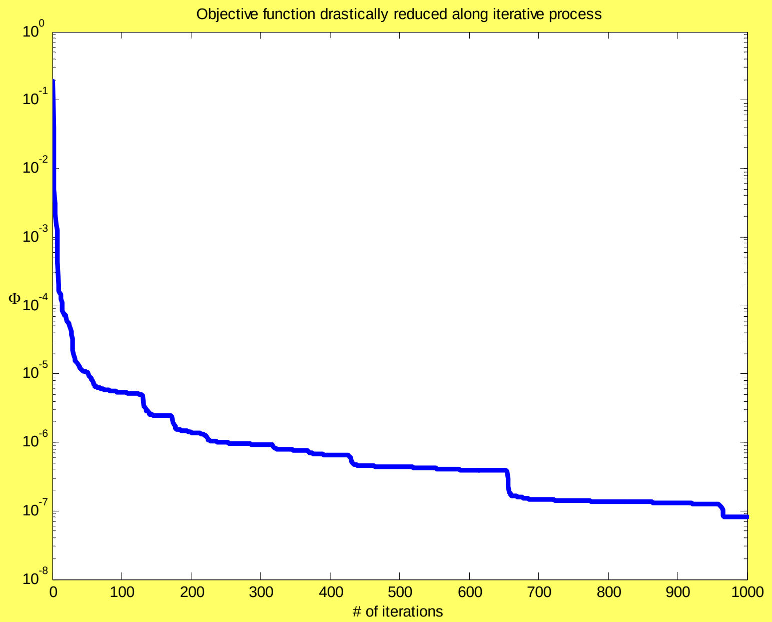
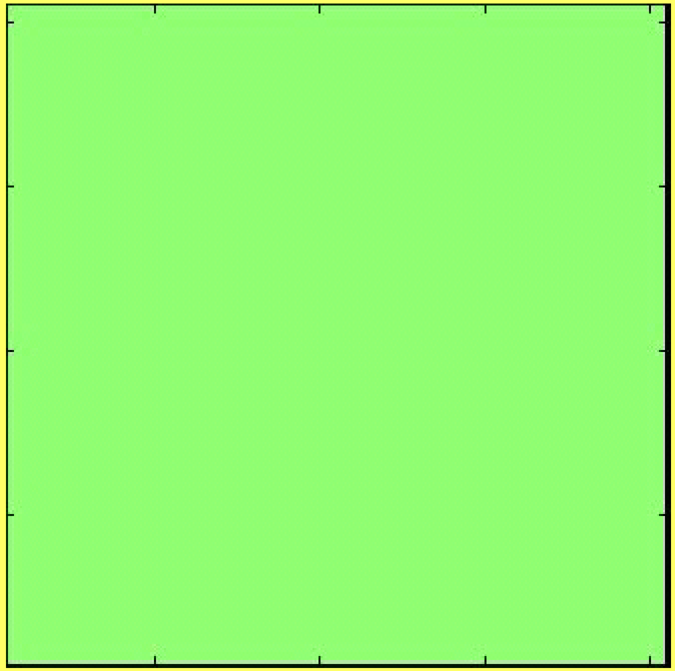


Fig: Transport cross section (Σ_{tr}) distribution obtained from deterministic CG based iterative search scheme for the one iron problem. (a) The real Σ_{tr} (background is water and square inclusion is iron). (b) Initial guess for Σ_{tr} . (c) and (d) are results after 100 and 1000 iterations, respectively.



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.

Another Model Problem

Model Problem II

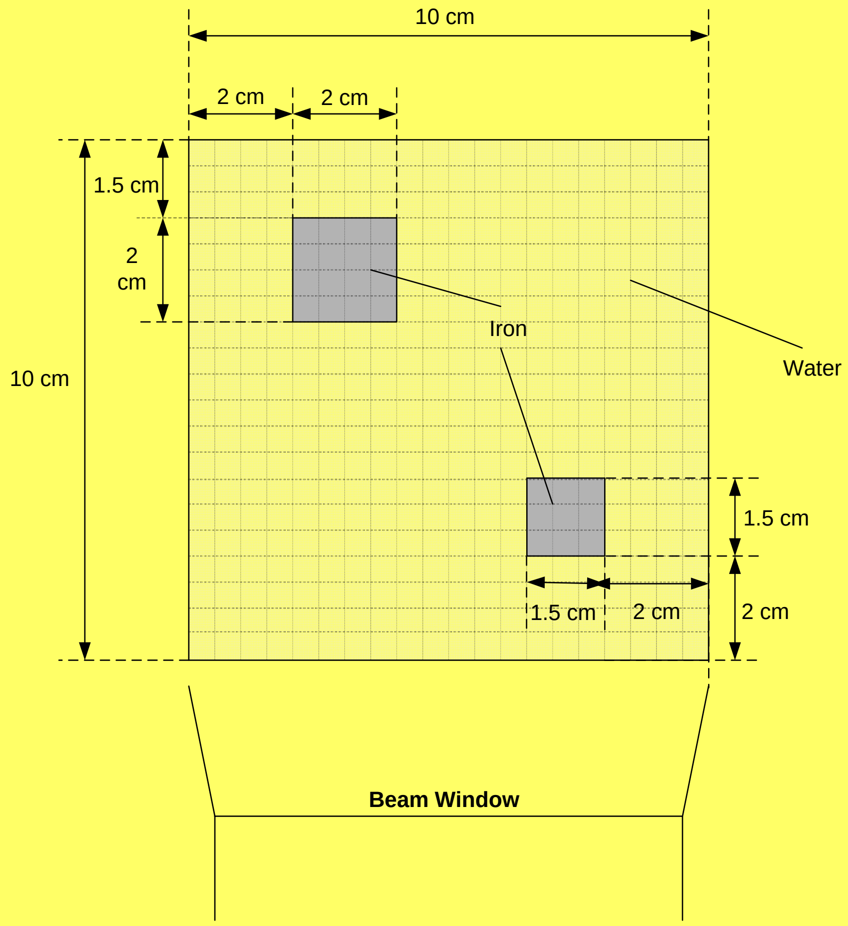


Fig: Schematic diagram of the two irons inclusion model problem (X-Y view).

Results for Model Problem II (Deterministic Stage)

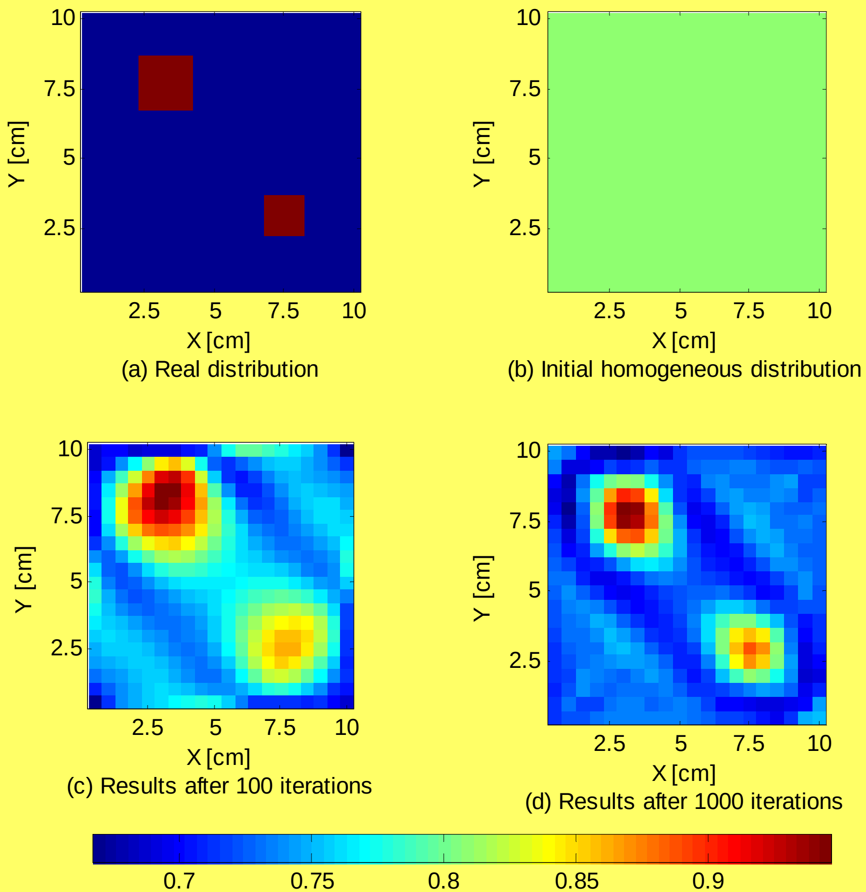


Fig. 1: Transport cross section (Σ_{tr}) distribution obtained from deterministic CG based iterative search scheme for the two irons problem. (a) The real Σ_{tr} (background is water and square inclusions are irons). (b) Initial guess for Σ_{tr} . (c) and (d) are results after 100 and 1000 iterations,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

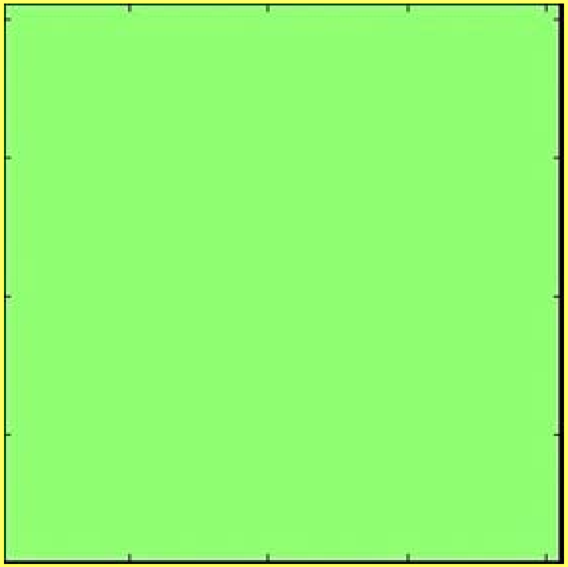


Fig. 2: Animation show of the reconstruction procedure for transport cross section (Σ_{tr}) distribution within the object changes with each iteration.

Conclusions

Summary of This Talk

- We have introduced a variable change technique to convert constrained optimization into unconstrained one in inverse transport applications
- Results from our neutron tomography model problems demonstrate that the method works well and is robust
- The method is very easy to apply
- We believe this technique may be beneficial to many gradient-based iterative optimization problems.

Questions?

Thank You!