## On the Use of Analytical Techniques for Parameter Identification in Radiation and Particle Transport Models

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New Trends in Parameter Identification for Mathematical Models

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## Inverse Particle Transport Problems: Parameters Identification

- Nuclear Safety: source reconstruction
- Optical Thomography : absorption coefficients reconstruction
- Solution of the forward problems: analytical approaches (K. Rui, Programa de Pós Graduação em Engenharia Mecânica, UFRGS)
- Inverse techniques (C. Pazinatto, Programa de Pós Graduação em Matemática Aplicada, UFRGS)


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- On the use of Adjoint Operator to the solution of an Inverse Problem ;
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## Forward Problems

- Absorption coefficient estimation: biological tissues
- Two dimensional transport equation:
(1) 2D Explicit Nodal Formulation [3]
(2) Alternative quadrature schemes $\times$ angular directions representation [4]
(3) Radiative transfer equation: anisotropy effects


## This Talk

- we report some studies and preliminary results we have carried out in this context
- we have considered parameters estimation: coefficients of a proposed expansion
- Isotropic sources
- Tikhonov's Regularization
- Two-dimensional Radiative Transfer Forward Fomulation


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## The Model

- We begin with the time-independent neutron transport equation which considers the distribution of the particles in non-multiplying homogeneous media, with one energy group, written as follows

$\sigma_{t}$ represents the total macroscopic cross section;
$\sigma_{s}\left(\mathbf{r}, \Omega^{\prime} \cdot \boldsymbol{\Omega}\right)$ represents the differential scattering macroscopic cross section;
$\Omega=(\mu, \eta, \xi)$ represents the direction of the particle as a vector on the unit sphere $S$;
$Q(\mathbf{r}, \boldsymbol{\Omega})$ is the fixed neutron source term.;
$\Psi(\mathbf{r}, \boldsymbol{\Omega})$ is the angular flux at $\mathbf{r}=(x, y, z)$ along direction $\Omega$.


## Balance- Phase Space



## Directions



## Variables



Angular variable: discrete directions

## Problem of interest



Figure: Multilayer slab

## Forward Problem

$$
\begin{equation*}
\mathcal{L} \psi=S, \quad \mathcal{L} \quad \text { transport operator } \tag{2}
\end{equation*}
$$

$$
\begin{equation*}
\mathcal{L} \psi(z, \mu)=\mu \frac{\partial}{\partial z} \psi(z, \mu)+\sigma \psi(z, \mu)-\frac{c}{2} \sum_{l=0}^{L} \beta_{l} P_{l}(\mu) \int_{-1}^{1} P_{l}\left(\mu^{\prime}\right) \psi\left(z, \mu^{\prime}\right) d \mu^{\prime} \tag{3}
\end{equation*}
$$

$\psi$ is the angular flux of particles, ; $\mu \in[-1,1]$ is the cosine of the polar angle measured from the positive $z$-axis, $z \in\left(0, z_{0}\right)$. $\sigma$ is the total macroscopic cross-section, $c$ is the mean number of neutral particles emerging from collisions, $\beta_{\text {I }}$ 's are the coefficients of the expansion of the scattering in terms of Legendre's polynomials $P_{l}$ 's.

$$
\begin{gather*}
\psi(0, \mu)=g_{1}(\mu)+\alpha_{1} \psi(z,-\mu)  \tag{4a}\\
\psi\left(z_{0},-\mu\right)=g_{2}(\mu)+\alpha_{2} \psi\left(z_{0}, \mu\right) \tag{4b}
\end{gather*}
$$

$\mu \in[0,1]$, (known) incoming fluxes at the boundaries $g_{1}$ and $g_{2}$, $\alpha_{1}, \alpha_{2} \in[0,1]$, the reflection coefficients.
$\sigma_{d}$ is the absorption macroscopic cross-section of a neutral particles detector located within $\left(0, z_{0}\right)$,

$$
\begin{equation*}
r=\left\langle\psi, \sigma_{d}\right\rangle \equiv \int_{0}^{z_{0}} \int_{-1}^{1} \sigma_{d}(z, \mu) \psi(z, \mu) d \mu d z \tag{5}
\end{equation*}
$$

is a measure of the absorption rate of neutral particles by the detector. In this formulation, $\sigma_{d}$ is defined as a positive constant in a given contiguous region of $\left(0, z_{0}\right)$ and zero outside the region. Thus, $r$ measures the absorption rate of neutral particles within the detector's region migrating from all possible directions.

Closely related to the transport operator $\mathcal{L}$, the adjoint transport operator $\mathcal{L}^{\dagger}$ is defined by [6]

$$
\begin{align*}
\mathcal{L}^{\dagger} \psi^{\dagger}(z, \mu)=-\mu \frac{\partial}{\partial z} \psi^{\dagger}(z, \mu) & +\sigma \psi^{\dagger}(z, \mu) \\
& -\frac{c}{2} \sum_{l=0}^{L} \beta_{l} P_{l}(\mu) \int_{-1}^{1} P_{l}\left(\mu^{\prime}\right) \psi^{\dagger}\left(z, \mu^{\prime}\right) d \mu^{\prime} \tag{6}
\end{align*}
$$

where all physical parameters are the same as the ones in the transport operator $\mathcal{L}$. The rate of absorption of neutral particles defined in Equation (5) might be alternatively computed as [6]

$$
\begin{equation*}
r=\left\langle\psi^{\dagger}, S\right\rangle-P\left(g_{1}, g_{2}, \psi^{\dagger}\right) \tag{7}
\end{equation*}
$$

$\psi^{\dagger}$ computed once
solving the adjoint transport problem

$$
\begin{equation*}
\mathcal{L}^{\dagger} \psi^{\dagger}=\sigma_{d} \tag{8}
\end{equation*}
$$

subjected to boundary conditions prescribed by

$$
\begin{gather*}
\psi^{\dagger}(0,-\mu)=\alpha_{1} \psi^{\dagger}(z, \mu)  \tag{9a}\\
\psi^{\dagger}\left(z_{0}, \mu\right)=\alpha_{2} \psi^{\dagger}\left(z_{0},-\mu\right) \tag{9b}
\end{gather*}
$$

for $\mu \in[0,1]$. The term $P\left(g_{1}, g_{2}, \psi^{\dagger}\right)$ represents a contribution of particles migrating on both inward and outward directions at $z=0$ and $z=z_{0}$ and is given by

$$
\begin{equation*}
P\left(g_{1}, g_{2}, \psi^{\dagger}\right)=-\int_{0}^{1} \mu\left[g_{1}(\mu) \psi^{\dagger}(0, \mu)+g_{2}(\mu) \psi^{\dagger}\left(z_{0},-\mu\right)\right] d \mu \tag{10}
\end{equation*}
$$

Homogeneous solution to the adjoint transport equation [9]

$$
\begin{equation*}
\vec{\psi}_{ \pm, h}^{\dagger}(z)=\sum_{j=1}^{N}\left[a_{j} \vec{\phi}_{ \pm}\left(\nu_{j}\right) e^{-z / \nu_{j}}+b_{j} \vec{\phi}_{\mp}\left(\nu_{j}\right) e^{-\left(z_{0}-z\right) / \nu_{j}}\right], \tag{11}
\end{equation*}
$$

$\vec{\psi}_{ \pm, h}^{\dagger}(z)=\left[\psi_{h}^{\dagger}\left(z, \pm \mu_{i}\right)\right] \in \mathbb{R}^{N}$ and $\vec{\phi}_{ \pm}(\nu)=\left[\phi\left(\nu, \pm \mu_{i}\right)\right] \in \mathbb{R}^{N}$

$$
\begin{equation*}
\vec{\phi}_{ \pm}(\nu)=\frac{1}{2} \vec{M}^{-1}\left(\vec{l} \mp \nu \overrightarrow{B_{+}}\right) \vec{x} \tag{12a}
\end{equation*}
$$

$\vec{M}=\operatorname{diag}\left(\mu_{i}\right) \in \mathbb{R}^{N \times N}$, where $\vec{x} \in \mathbb{R}^{N}$ and $\nu>0$ are such that

$$
\begin{gather*}
B_{-} \vec{B}_{+} x=\frac{1}{\nu^{2}} \vec{x}  \tag{12b}\\
\overrightarrow{B_{ \pm}}=\left(\sigma \vec{l}-\frac{c}{2} \sum_{l=0}^{L} \beta_{l} \vec{\Pi}_{l} \vec{\Pi}_{l}^{T} \vec{W}\left[1 \pm(-1)^{\prime}\right]\right) \vec{M}^{-1} \tag{12c}
\end{gather*}
$$

$\overrightarrow{B_{ \pm}} \in \mathbb{R}^{N \times N} ; \vec{\Pi}_{l}=\left[P_{l}\left(\mu_{i}\right)\right] \in \mathbb{R}^{N} ; \vec{W}=\operatorname{diag}\left(w_{i}\right) \in \mathbb{R}^{N \times N} .2 N$ directions

## Particular Solutions

$S^{\dagger}$ is a constant source

$$
\begin{equation*}
\psi_{p}^{\dagger}(z, \mu)=\frac{S^{\dagger}}{\sigma-c \beta_{0}} \tag{13}
\end{equation*}
$$

$S^{\dagger}$ is an isotropic source Green's functions

$$
\begin{gather*}
\vec{\psi}_{ \pm, p}^{\dagger}(z)=\sum_{j=1}^{N}\left[a_{j}(z) \vec{\phi}_{ \pm}\left(\nu_{j}\right)+b_{j}(z) \vec{\phi}_{\mp}\left(\nu_{j}\right)\right]  \tag{14}\\
a_{j}(z)=c_{j} \int_{0}^{z} S^{\dagger}\left(z^{\prime}\right) e^{-\left(z-z^{\prime}\right) / \nu_{j}} d z^{\prime}  \tag{15a}\\
b_{j}(z)=c_{j} \int_{z}^{z_{0}} S^{\dagger}\left(z^{\prime}\right) e^{-\left(z^{\prime}-z\right) / \nu_{j} d z^{\prime}}  \tag{15b}\\
c_{j}=-\frac{\sum_{i=1}^{N} w_{i}\left[\phi\left(\nu_{j}, \mu_{i}\right)+\phi\left(\nu_{j},-\mu_{i}\right)\right]}{\sum_{i=1}^{N} w_{i} \mu_{i}\left[\phi\left(\nu_{j}, \mu_{i}\right)^{2}-\phi\left(\nu_{j},-\mu_{i}\right)^{2}\right]} \tag{15c}
\end{gather*}
$$

## Source Reconstruction Strategy

- a set of $D$ particle detectors are placed within the physical domain $\left[0, z_{0}\right]$;
- for each detector, the adjoint angular flux that solves $\mathcal{L}^{\dagger} \psi^{\dagger}=\sigma_{d, i}$ is known, with $\sigma_{d, i}$ the absorption macroscopic cross section of the $i$-th detector;
- the original source of neutral particles $S$ might be accurately approximated by the projection of $S$ onto a linear space with known basis function $f_{j}, j=1, \ldots, B$;
$S$ might be approximated by

$$
\begin{equation*}
\hat{S}(z)=\sum_{j=1}^{B} \alpha_{j} f_{j}(z) \tag{16}
\end{equation*}
$$

with constants $\alpha_{j}$ yet to be found, i.e., targets of our source reconstruction process.

In this work, only sectionally constant approximations are considered to the neutral particle source $S$, thus, given $\left[0, z_{0}\right]=\bigcup_{j=1}^{B}\left[z_{j-1}, z_{j}\right]$, a partition of the physical domain, a function basis is defined as [?]

$$
f_{j}(z)= \begin{cases}1, & \text { if } z \in\left[z_{j-1}, z_{j}\right]  \tag{17}\\ 0, & \text { otherwise }\end{cases}
$$

Under these assumptions, the rate of absorption of neutral particles within the $i$-th detector region might be computed by

$$
\begin{equation*}
r_{i}=\psi_{i}^{\dagger} \hat{S}-P\left(g_{1}, g_{2}, \psi_{i}^{\dagger}\right)=\sum_{j=1}^{B} \alpha_{j}\left\langle\psi_{i}^{\dagger}, f_{j}\right\rangle-P\left(g_{1}, g_{2}, \psi_{i}^{\dagger}\right) \tag{18}
\end{equation*}
$$

for $i=1, \ldots, D$. Upon defining $\vec{r}=\left[r_{i}\right] \in \mathbb{R}^{D}, \vec{p}=\left[P\left(g_{1}, g_{2}, \psi_{i}^{\dagger}\right)\right] \in \mathbb{R}^{D}$ and $\vec{A}=\left[\left\langle\psi_{i}^{\dagger}, f_{j}\right\rangle\right] \in \mathbb{R}^{D \times B}$, Equation (18) is rewritten in vector form as

$$
\begin{equation*}
\vec{r}=\vec{A} \vec{\alpha}-\vec{p} \tag{19}
\end{equation*}
$$

with $\vec{\alpha}=\left[\alpha_{j}\right] \in \mathbb{R}^{B}$.
the coefficients $\alpha_{j}$ in Equation (16) are to be estimated by the minimization of the objective function [?]

$$
\begin{equation*}
f(\vec{\alpha})=\left\|\vec{r}^{\prime}-\vec{A} \vec{\alpha}\right\|_{2}^{2}, \tag{20}
\end{equation*}
$$

with $\vec{r}^{\prime}=\vec{r}_{m}-\vec{p}, \vec{r}_{m}=\left[r_{m, i}\right] \in \mathbb{R}^{D}$.
for each neutral particle detector a noisy measurement $r_{m, i}$ is made available, computed by numerical simulation

The well known ill-posedness of inverse problems might negatively affect the quality of the reconstruction. This problem is treated here by searching for Tikhonov regularized solutions of a minimization problem, i.e, looking for solutions that minimize the objective function [5]

$$
\begin{equation*}
f_{\lambda}(\vec{\alpha})=\left\|\vec{r}^{\prime}-\vec{A} \vec{\alpha}\right\|_{2}^{2}+\lambda^{2}\|\vec{\alpha}\|_{2}^{2}, \tag{21}
\end{equation*}
$$

where $\lambda$ is the Tikhonov's regularization parameter, here chosen by the Morozov discrepancy principle [5].

## Test I

$$
\begin{equation*}
S(z)=-\frac{z^{2}}{150}(z-10) \tag{22}
\end{equation*}
$$

- $z_{0}=10 ; c=0.99, \sigma=1, L=6[9]$.
- Vacuum boundary conditions at $z=0$ and $z=10$.
- 10 detectors uniformly distributed within the physical domain
- absorption cross-sections, $i=1, \ldots, 10$

$$
\sigma_{d, i}= \begin{cases}0.1, & z \in[0.4+i-1,0.6+i-1]  \tag{23}\\ 0.0, & \text { otherwise }\end{cases}
$$

For each detector: $r_{m, i}$ (Eq.(5)) solving $\mathcal{L} \psi=S$ by the ADO method, $N=4$, PLUS white noise is applied to the readings in order to generate 5000 different tests to the problem.

Figure shows the distribution of the maximum error imposed on the readings $r_{m, i}$.


Figure: Measurement errors imposed on the readings $r_{m, i}$.

- Partitions 1 and 2 to define the basis functions

$$
[0,10]=\bigcup_{j=1}^{10}[j-1, j] \quad[0,10]=\bigcup_{j=1}^{20}[0.5(j-1), 0.5 j]
$$




Figure: Dashed line: true source $S$; Solid lines: reconstruction $\hat{S}$.

Reconstruction $\hat{S}$ (minimal relative error from all the reconstructions) Figures indicate: reconstruction process was able to recover the shape of the source of neutral particles $S$.

Next, the transport equation $\mathcal{L} \hat{\psi}=\hat{S}$ is solved in order to compute readings $\hat{r}_{m, i}$ with the reconstructed source $\hat{S}$. Relative errors between the noisy free measurements and the reconstructions were computed.



Figure: Relative errors on the reconstructed reading $\hat{r}_{m, i}$ using Partitions 1 and 2.

It was noted similar behavior between the error in the measurements and the reconstruction error. It is also highlighted that the maximum value computed to the Tikhonov's regularization parameter were 0.0680 and 0.0472, respectively.

## Test II

Reconstruction of a localized source piecewisely defined for $z \in[0,30]$ by

$$
S(z)= \begin{cases}0.75, & z \in[17,20),  \tag{25}\\ 1.00, & z \in[20,24), \\ 0.25, & z \in[24,26] \\ 0.00, & \text { otherwise }\end{cases}
$$

Parameters: $c=0.3, \sigma=1$ and $\beta_{0}=1$ (isotropic scattering). As before, it is also assumed that there is no incoming flux at the boundaries $z=0$ and $z=30$.

## Test II

60 detectors are uniformly distributed within the physical domain, absorption cross section

$$
\sigma_{d, i}= \begin{cases}0.1, & z \in[(2 j-11 / 10) / 4,(2 j-9 / 10) / 4]  \tag{26}\\ 0.0, & \text { otherwise }\end{cases}
$$

$i=1, \ldots, 60$. Just as before, for each detector, a reading $r_{m, i}$ is computed and, thereafter, white noise were applied to the readings in order to generate 5000 different tests to the problem.


For the reconstruction, a partition $[0,30]=\bigcup_{j=1}^{60}[0.5(j-1), 0.5 j]$ is considered to define the basis functions.


Figure: True source $S$ : dashed line; Reconstruction $\hat{S}$ : solid line

The transport equation is evaluated using the reconstructed source $\hat{S}$ in order to calculate the relative errors between the exact measurements and the noisy ones.

Figure exhibits the maximum relative errors among the sixty measurements for all 5000 tests.


Figure: Relative errors on the reconstructed reading $\hat{r}_{m, i}$ using partition $[0,30]=\bigcup_{j=1}^{60}[0.5(j-1), 0.5 j]$.

The errors were found to be inferior than the noise added to the measurements as Figure (5) indicates. For this test problem, the maximum value among the Tikhonov's regularization parameters was 0.1221 , a higher value than the ones presented on the previous test problems.

60 particles detectors were first distributed uniformly within the slab, where 18 of these detectors were in $z \in[17,26]$. As a final test, most of the detectors are removed with the exception $4(i=38,41,46$ and 51$)$, resulting in an underdetermined system (objetive-function). The distribution of the maximum error added to the readings $r_{m, i}$ is shown


Figure: Measurement errors imposed on the readings $r_{m, i}$.

Once more (for each reconstructions) the transport equation is evaluated with the reconstructed source and the detectors readings are computed. Figure shows the maximum relative errors among all detectors between the readings calculated using the reconstructions and the original source. The maximum value of the regularization parameter was the same as before, 0.1221 .


## Computational Aspects

(1) tests were performed on a machine equipped with an Intel Core i5-4670 processor with 16 GiB of RAM
(2) minimization of the objective function defined in Equation (21) was performed by the non-negative least squares nnls subroutine, available at Netlib
(3) the first test problem took an average of $6.9 \times 10^{-4}$ seconds per inversion.
(9) second test problem, an average of $1.2 \times 10^{-3}$ seconds was required per inversion
(0) The third and fourth test problems took an average of $9.8 \times 10^{-3}$ and $8.8 \times 10^{-3}$ seconds per inversion

## Source-detector Problems - Energy Dependence

## Forward Transport Problem

- We consider a multilayer slab $[0, Z]=\bigcup_{r=1}^{R}\left[z_{r-1}, z_{r}\right]$
- Energy spectrum divided into $G$ energy groups
- Forward transport operator $\mathcal{L}$ takes the form [6]

$$
\begin{aligned}
\mathcal{L} \psi(z, \mu) & =\mu \frac{\partial}{\partial z} \boldsymbol{\psi}(z, \mu)+\mathbf{S}(z) \psi(z, \mu) \\
& -\frac{1}{2} \sum_{l=0}^{L} P_{l}(\mu) \mathbf{T}_{l}(z) \int_{-1}^{1} P_{l}\left(\mu^{\prime}\right) \psi\left(z, \mu^{\prime}\right) d \mu^{\prime}
\end{aligned}
$$

with $\mu \in[-1,1]$

- Within each region $\left[z_{r-1}, z_{r}\right]$ :
- $\mathbf{S}(z)=\mathbf{S}_{r}, G \times G$ diagonal matrix, macroscopic total cross section of each energy group
- $\mathbf{T}_{l}(z)=\mathbf{T}_{l, r}, G \times G$ matrices, group transfer cross sections
- We also require continuity of $\psi$ on the interface between these regions


## Source-detector Problems

## Forward Transport Problem

- Thus, we write the forward transport equation as

$$
\mathcal{L} \psi=\mathbf{q}
$$

- Where $\mathbf{q}$ is an internal source of neutral particles
- Subjected to boundary conditions at incoming directions

$$
\begin{gathered}
\psi(0, \mu)=\mathbf{f}_{1}(\mu)+\alpha_{1} \boldsymbol{\psi}(0,-\mu) \\
\psi(Z,-\mu)=\mathbf{f}_{2}(\mu)+\alpha_{2} \boldsymbol{\psi}(Z, \mu)
\end{gathered}
$$

with $\mu \in(0,1]$

- $\mathbf{f}_{1}$ and $\mathbf{f}_{2}$ represent incoming fluxes of particles
- $\alpha_{1}, \alpha_{2} \in[0,1]$ are reflective coefficients


## Source-detector Problems

## Absorption Rate of Particles - Forward Formulation

- Particle detector with absorption cross-section $\sigma_{\text {d }}$

- The absorption rate in the detector is given by [10]

$$
r=\left\langle\boldsymbol{\sigma}_{\mathbf{d}}, \boldsymbol{\psi}\right\rangle=\sum_{g=1}^{G} \int_{-1}^{1} \int_{z_{a}}^{z_{b}} \sigma_{d, g}(z, \mu) \psi_{g}(z, \mu) d z d \mu
$$

- New $\mathbf{q}, \mathbf{f}_{1}, \mathbf{f}_{2} \Rightarrow$ new evaluation of $\boldsymbol{\psi}$ in order to compute $r$
- The adjoint (backward) transport equation offers an alternative and a more efficient procedure


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- Particle detector with absorption cross-section $\sigma_{\mathrm{d}}$
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$$

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## ADO Formulation for Adjoint Problems

## Explicit Formulas for the Absorption Rate

- Back to the absorption rate evaluation, we may rewrite it as

$$
r=\left\langle\boldsymbol{\psi}_{\mathbf{h}}^{\dagger}, \mathbf{q}\right\rangle+\left\langle\boldsymbol{\psi}_{\mathbf{p}}^{\dagger}, \mathbf{q}\right\rangle=r_{h}+r_{p}
$$

- $r_{h}$ depends only on the homogeneous solution $\left(\mathbf{f}_{1}=\mathbf{f}_{2}=\mathbf{0}\right)$
$h=\sum_{j=1}^{N G} \nu_{j, r}\left[B_{r, j}\left(e^{-\frac{z_{r}-z_{b}}{\nu_{j, r}}}-e^{-\frac{z_{r}-z_{a}}{\nu_{j, r}}}\right)-A_{r, j}\left(e^{-\frac{z_{b}-z_{r-1}}{\nu_{j, r}}}-e^{-\frac{z_{a}-z_{r-1}}{\nu_{j, r}}}\right)\right] \phi_{j, r}$
- With $\phi_{j, r}$ such that

$$
\phi_{j, r}=\sum_{k=1}^{N} w_{k} \sum_{g=1}^{G} q_{g}\left(\boldsymbol{\Phi}_{+, r}^{j, g, k}+\boldsymbol{\Phi}_{-, r}^{j, g, k}\right)
$$

with $\boldsymbol{\Phi}^{j, g, k}$ being the $k$-th direction of the $g$-th of the $j$-th eigenfunction

- If $\mathbf{q}$ is constant, $r_{p}$ is such that

$$
r_{p}=2\left(z_{b}-z_{a}\right) \sum^{G} \psi_{p, g, r}^{\dagger} q_{g, r}
$$

## Numerical Results for Source-detector Problems

Test Problem, Ref. [?]


$$
\begin{aligned}
& \mathbf{S}_{1}=\operatorname{diag}(1.00,1.20), \mathbf{S}_{2}=\operatorname{diag}(0.90,1.50) \\
& \mathbf{S}_{3}=\operatorname{diag}(1.10,0.85), \mathbf{S}_{4}=\mathbf{S}_{1}
\end{aligned}
$$

- Group transfer cross-sections (isotropic scattering)

$$
\begin{aligned}
& \mathbf{T}_{0,1}=\left[\begin{array}{ll}
0.90 & 0.05 \\
0.20 & 0.80
\end{array}\right], \mathbf{T}_{0,2}=\left[\begin{array}{ll}
0.75 & 0.10 \\
0.30 & 0.99
\end{array}\right], \mathbf{T}_{0,3}=\left[\begin{array}{ll}
0.95 & 0.00 \\
0.60 & 0.20
\end{array}\right] \\
& \mathbf{T}_{0,4}=\mathbf{T}_{0,1}
\end{aligned}
$$

- We compute the absorption rate using both the forward ( $r$ ) and backward $\left(r^{\dagger}\right)$ formulations with ADO method


## Numerical Results for Source-detector Problems

## Test Problem

Table: Absorption rate of neutral particles.

|  | $r^{\dagger}$ | $r$ |
| ---: | :---: | :---: |
| 4 directions | 0.19672070465 | 0.19672070465 |
| 8 directions | 0.19618914572 | 0.19618914572 |
| 16 directions | 0.19618610963 | 0.19618610963 |
| 32 directions | 0.19618610990 | 0.19618610990 |
| 64 directions | 0.19618610982 | 0.19618610982 |
| 128 directions | 0.19618610981 | 0.19618610981 |

- All solutions performed well when increasing the number of directions
- Using explicit formulas, $\left|r-r^{\dagger}\right|=O\left(10^{-16}\right)$
- The same result was not possible to obtain using numerical integration
- ADO took less than a second to run (even at 128 directions)

$$
\# \text { directions }=2 \times N \text { for ADO }
$$

## Source Estimation

## A Model for Estimating the Absorption Rate

- We consider a slab $[0, Z]$ with known physical properties
- and an internal source of particles $\mathbf{q}$, isotropically defined
- A set of $D$ particle detectors is placed within the slab with absorption cross-sections $\sigma_{\mathbf{d} i}$
- In practice, readings are expected to be noisy
- Question: given the readings, are we able to recover $\mathbf{q}$ ?
- Suppose known solutions to $\mathcal{L}^{\dagger} \psi^{\dagger}{ }_{i}=\sigma_{\mathrm{d} i}$ (ADO method)
- We suppose that $\mathbf{q} \approx \tilde{\mathbf{q}}=\left[\begin{array}{lll}\tilde{q}_{1} & \cdots & \tilde{q}_{G}\end{array}\right]^{T}$, with

$$
\tilde{q}_{g}(z)=\sum_{b=1}^{B_{g}} \alpha_{b, g} \tilde{q}_{b, g}(z)
$$

## Source Estimation

## A Model for Estimating the Absorption Rate

- This way, we have

$$
r_{i}=\left\langle\boldsymbol{\psi}^{\dagger}{ }_{i}, \tilde{\mathbf{q}}\right\rangle=\sum_{g=1}^{G}\left\{\sum_{b=1}^{B_{g}} \alpha_{b, g} A_{i, b, g}-p_{i, g}\right\}
$$

- With

$$
A_{i, b, g}=\int_{-1}^{1} \int_{0}^{Z} \psi_{i, g}^{\dagger}(z, \mu) \tilde{q}_{b, g}(z) d z d \mu
$$

- And

$$
p_{i, g}=\int_{0}^{1} \mu\left[\psi_{i, g}^{\dagger}(0, \mu) f_{1, g}(\mu)+\psi_{i, g}^{\dagger}(Z,-\mu) f_{2, g}(\mu)\right] d \mu
$$

- Finally, we write

$$
\mathbf{r}\left(\boldsymbol{\alpha}_{1}, \ldots, \boldsymbol{\alpha}_{G}\right)=\sum_{g=1}^{G}\left[\mathbf{A}_{g} \boldsymbol{\alpha}_{g}-\mathbf{p}_{g}\right]
$$

with $\mathbf{A}_{g}=\left[A_{i, b, g}\right], \boldsymbol{\alpha}_{g}=\left[\alpha_{b, g}\right]$ and $\mathbf{p}_{g}=\left[p_{i, g}\right]$

## Source Estimation

## Inverse Problem

- Given exact measurements $\mathbf{r}\left(\boldsymbol{\alpha}_{1}, \ldots, \boldsymbol{\alpha}_{G}\right)$, we consider additive errors such that

$$
\tilde{\mathbf{r}}=\mathbf{r}\left(\boldsymbol{\alpha}_{1}, \ldots, \boldsymbol{\alpha}_{G}\right)+\boldsymbol{\epsilon}
$$

- If $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{W})$, we might write the probability density function for the error distribution as [5]

$$
\pi(\boldsymbol{\epsilon})=(2 \pi)^{-D / 2}|\mathbf{W}|^{-1 / 2} \exp \left\{-\frac{1}{2}[\tilde{\mathbf{r}}-\mathbf{r}]^{T} \mathbf{W}^{-1}[\tilde{\mathbf{r}}-\mathbf{r}]\right\}
$$

- Which is maximized when

$$
S_{M L}\left(\boldsymbol{\alpha}_{1}, \ldots, \boldsymbol{\alpha}_{G}\right)=[\tilde{\mathbf{r}}-\mathbf{r}]^{T} \mathbf{W}^{-1}[\tilde{\mathbf{r}}-\mathbf{r}]
$$

is minimized

- Since $r$ is linear, a common approach for the minimization is the least squares method


## Numerical Results for Source Estimation Problems

## Test Problem I

- We consider a single layer slab defined for $z \in[0,10]$, total macroscopic cross-sections $\mathbf{S}=\operatorname{diag}(1.0,1.2)$, and group transfer cross-sections

$$
\mathbf{T}_{0}=\left[\begin{array}{ll}
0.90 & 0.05 \\
0.20 & 0.80
\end{array}\right]
$$

- And a particles' source $\mathbf{q}=\left[\begin{array}{ll}q_{1} & q_{2}\end{array}\right]^{T}$, with components given by

$$
q_{1}(z)= \begin{cases}0.6, & z \in[3.0,5.0] \\ 0.0, & \text { otherwise }\end{cases}
$$

and

$$
q_{2}(z)= \begin{cases}0.3, & z \in[6.0,7.0] \\ 0.0, & \text { otherwise }\end{cases}
$$

## Numerical Results for Source Estimation Problems

 Test Problem I- Our minimization problem takes the form

$$
S_{\lambda}(\boldsymbol{\alpha})=\left\|\mathbf{W}^{-1 / 2}[\hat{\mathbf{r}}-\mathbf{A} \boldsymbol{\alpha}]\right\|^{2}+\lambda^{2}\|\boldsymbol{\alpha}\|^{2}
$$

with $\hat{\mathbf{r}}=\tilde{\mathbf{r}}-\mathbf{p}, \mathbf{p}=\left[\begin{array}{ll}\mathbf{p}_{1}^{T} & \mathbf{p}_{2}^{T}\end{array}\right]^{T}, \mathbf{A}=\left[\begin{array}{ll}\mathbf{A}_{1} & \mathbf{A}_{2}\end{array}\right], \boldsymbol{\alpha}=\left[\begin{array}{ll}\boldsymbol{\alpha}_{1}^{T} & \boldsymbol{\alpha}_{2}^{T}\end{array}\right]^{T}$

- Tikhonov regularized solution due to the ill-posedness of the problem


## Numerical Results for Source Estimation Problems

## Test Problem I

- $\mathbf{r}_{\mathbf{0}}=\left[r_{0, i}\right]$ calculated with DD method, considering 128 discrete directions, 100 nodes per cm and tolerance of $10^{-12}$
- Using $\mathbf{r}_{0}$, we compute perturbed measurements $\mathbf{r}_{i}$ with $\mathbf{W}_{1}=\operatorname{diag}\left(\left[0.01 r_{0, i}\right]^{2}\right)$ and $\mathbf{W}_{2}=\operatorname{diag}\left(\left[0.05 r_{0, i}\right]^{2}\right)$
- A is computed using the ADO method to approximate the adjoint fluxes, with $N=4$ (8 discrete directions)
- We searched for non-negative solutions for our minimization problem


## Numerical Results for Source Estimation Problems

Test Problem I - Noisy Measurement

Energy Group 1


## Numerical Results for Source Estimation Problems

Test Problem I-q estimation


Group 2 -- Absolute Error: 0.0012, Relative Error: 0.40\%


## Numerical Results for Source Estimation Problems

Test Problem I - Scalar Flux


## Numerical Results for Source Estimation Problems

Test Problem II - Noisy Measurement


## Numerical Results for Source Estimation Problems

Test Problem II - q estimation

Group 1 -- Absolute Error: 0.1050, Relative Error: 12.37\%


Group 2 -- Absolute Error: 0.0747, Relative Error: 24.89\%


## Numerical Results for Source Estimation Problems

Test Problem II - Scalar Flux


Group 1 -- Absolute Error: 0.1768, Relative Error: 3.33\%


## Concluding Remarks

- method was successfully applied in simple source reconstruction 1D model problems with energy dependence
- yielding good results in the sense that errors on the estimated measurements were found slightly inferior to the noise added to the real readings (one-group)
- solution is fast


## Ongoing Projects and Future Works

- alternative forms of errors
- probabilistic approaches (preliminary results)
- 2D model : inverse (adjoint) and forward problem
(1) Coarser meshes: accuracy improved
(2) Angular discretization error and Ray Effects: use of alternative quadrature schemes up to higher orders
(3) currently: development of the associated eigenvalue problem for more general phase functions
- New Trends ?


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## THANK YOU!

