On the use of the Adjoint Operator in Estimating Neutral Particles Sources

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Motivations

The adjoint flux, the solution of the adjoint transport equation, is an important mathematical tool. In neutral particles transport theory, some applications may benefit from its study, such as

- Nuclear Reactors Analysis [4]:
  - Importance function;
  - Criticality problems.
- Inverse Problems [5, 6]:
  - Applications such as: nuclear safety, non-destructive material identification;
  - In such problems, we are often concerned with estimating the spatial distribution and intensity of internal sources of neutral particles;
  - The adjoint flux frequently appear in iterative schemes, when computing gradients related to minimization procedures, or in the evaluation of detector readings in the so-called source-detector problems.

This way, we need to obtain accurate solutions to the adjoint of transport equation.

- The ADO method (*Analytical Discrete Ordinates* method) was developed and successfully applied to solve problems in:
  - radiative heat transfer [3];
  - rarefied gases dynamic [9];
  - neutral particles transport [1].
- The methodology was extended to the one-dimensional planar geometry adjoint of the transport equation, considering arbitrarily high anisotropy degree [8];
- Then, the formulation was further extended to two-dimensional XY-geometry transport problems in a medium with isotropic scattering [2];
- In such problems, we were able to derive closed form expressions to the averaged fluxes in either x or y directions.

- In this work, the adjoint flux is applied in estimating internal sources of particles, from measurements of internal particles detectors:
  - We use the iterated Tikhonov (IT) algorithm [6];
  - And the Markov Chain Monte Carlo (MCMC) method within the Bayesian framework.
- We consider that all physical properties of the medium and incoming fluxes at the boundaries are known;
- Then, we derive using the adjoint of the transport equation a linear model that relates absorption rate measurements of a series of particle detectors with the coefficients of the source expansion in a given basis.

Transport Equation

Transport Equation

- In steady state, considering two-dimensional Cartesian geometry (XY-geometry), considering isotropic scattering and the monoenergetic approximation, the transport equation takes the form:

$$\boldsymbol{\Omega} \cdot \nabla\psi + \sigma\psi = \int_{\mathbb{S}'} \sigma_s \psi \, \mathrm{d}\boldsymbol{\Omega}' + S,$$

  with $(x, y) \in D = [0, X] \times [0, Y]$ and $\psi = \psi(x, y, \eta, \xi)$;

- This way, we can rewrite the transport equation in a more compact form as:

$$\boldsymbol{\mathcal{L}}\psi = S.$$

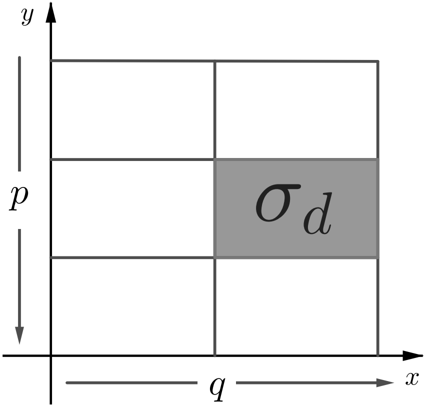
- We also prescribe boundary conditions at the inward directions of the domain:

$$\psi(\cdot, \boldsymbol{\Omega}_{in}) = \psi_b(\cdot, \boldsymbol{\Omega}_{in}) + \rho\psi(\cdot, \boldsymbol{\Omega}_{out});$$

Absorption Rate Measurements

Absorption Rate Measurements

- Rectangular mesh of n_x by n_y rectangles;
- Internal particles detectors with absorption cross section σ_d:



$$\sigma_d(x,y) = \begin{cases} \sigma_{d,p,q}, & (x,y) \in [x_q, x_{q+1}] \times [y_{p+1}, y_p] \\ 0, & \text{otherwise} \end{cases}$$

Absorption Rate Measurements

- We may evaluate the absorption rate of particles migrating from all directions within a region R of the domain using the expression:

$$r = \langle \sigma_d, \psi \rangle \, ;$$

- Where $\langle \cdot, \cdot \rangle$ is the inner product in the phase space:

$$\langle f, g \rangle = \int_{\mathbb{S}'} \int_V f(\boldsymbol{r}, \boldsymbol{\Omega}) g(\boldsymbol{r}, \boldsymbol{\Omega}) dV d\boldsymbol{\Omega};$$

- **Remember:** Our goal is to estimate the spatial distribution and magnitude of an isotropic internal source of particles S from a series of known measurements provided by n_d particles detectors, that is,

$$\boldsymbol{r} = [\ \overbrace{r_1}^{\text{detector 1}} \quad \overbrace{r_2}^{\text{detector 2}} \quad \dots \quad \overbrace{r_{n_d}}^{\text{detector } n_d}\ ]^T.$$

Absorption Rate Measurements

- We also assume that S may be approximated by a function written as:

$$\tilde{S}(x,y) = \sum_{b=1}^{B} \alpha_b \tilde{s}_b(x,y);$$

- Where $\tilde{s}_b(x,y)$, $b = 1,\ldots,B$, corresponds to a set of basis functions defined in D and α_b are the targets of the estimation process;
- If we try to directly relate $\boldsymbol{r}$ with the source $\tilde{S}$, we find out that we end up with a nonlinear relation between them due to the requirement of first solving the transport equation.

Absorption Rate Measurements

- Alternatively, we can use the adjoint of the transport equation to write a new expression for the rate of absorption, which leads us to a linear model that relates $\boldsymbol{r}$ and $\tilde{S}$. Thus, we write [2]:

$$r = \left\langle \psi^\dagger, \tilde{S} \right\rangle - P[\psi, \psi^\dagger];$$

- Where $\psi^\dagger$ is the adjoint flux and satisfy the adjoint transport equation:

$$\boldsymbol{\mathcal{L}}^\dagger \psi^\dagger = \sigma_{\boldsymbol{d}};$$

- With $\mathcal{L}^\dagger$ being the adjoint transport operator defined by:

$$\mathcal{L}^\dagger \psi^\dagger(\boldsymbol{r},\boldsymbol{\Omega}) = -\boldsymbol{\Omega} \cdot \nabla \psi^\dagger + \sigma \psi^\dagger - \int_{\mathbb{S}'} \sigma_{\boldsymbol{s}} \psi^\dagger \, \mathrm{d}\boldsymbol{\Omega}'.$$

Absorption Rate Measurements

- The $P[\psi, \psi^\dagger]$ term depends on the boundary conditions of both transport problems;
- In fact, if we define boundary conditions at the outward directions of the adjoint problem:
$$\psi^\dagger(\cdot, \mathbf{\Omega}_{out}) = \rho\psi^\dagger(\cdot, \mathbf{\Omega}_{in});$$
- Then, the $P\left[\psi, \psi^\dagger\right]$ term will depend only on the boundary conditions of the original transport problem, that is:

$$P\left[\psi, \psi^\dagger\right] = \int_{\partial V} \int_{\mathbf{\Omega} \cdot \boldsymbol{n} < 0} \boldsymbol{n} \cdot \mathbf{\Omega} \psi_b(\boldsymbol{r}, \mathbf{\Omega}) \psi^\dagger(\boldsymbol{r}, \mathbf{\Omega}) \, \mathrm{d}\mu.$$

Absorption Rate Measurements

- The absorption rate measurements vector is rewritten as:

$$\boldsymbol{r}(\boldsymbol{\alpha}) = \boldsymbol{A}\boldsymbol{\alpha} + \boldsymbol{p};$$

- Where $\boldsymbol{A} = [A_{i,b}]$ is a $D \times B$ matrix whose components we write as:

$$A_{b,i} = \left\langle \psi_i^\dagger, \tilde{s}_b \right\rangle;$$

- $\boldsymbol{p} = [p_i]$ is a D-dimensional vector whose components are $p_i = P[\psi,\psi_i^\dagger]$;
- And $\boldsymbol{\alpha} = [\alpha_b]$ is a B-dimensional vector with the targets of the estimation process;
- **Question:** how to solve the adjoint transport equation?

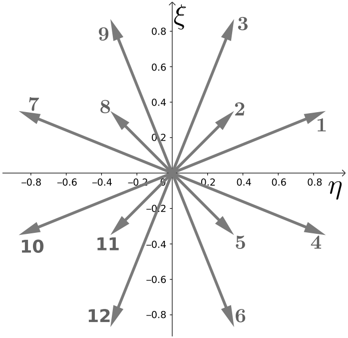
ADO-Nodal Formulation
2D Adjoint Monoenergetic Problems

ADO-Nodal Formulation to the Adjoint Transport Equation

- For each region, we consider the averaged flux with respect to the y variable [2]:

$$\psi_y^\dagger(x,\mathbf{\Omega}) = \frac{1}{h_y}\int_{y_{p+1}}^{y_p} \psi^\dagger(x,y,\mathbf{\Omega})\,\mathrm{d}y;$$

- We use M nodes, $\mathbf{\Omega}_k = (\eta_k, \xi_k)$, and weights, w_k of the projection of the known LQ_n quadrature in the plane $\eta O \xi$ [7];
- We consider discrete directions ordered according to:



ADO-Nodal Formulation to the Adjoint Transport Equation

- Integrating the adjoint transport equation with respect to the y variable, we obtain:

$$\mp\eta_m \frac{d}{dx}\psi_y^\dagger(x,\mathbf{\Omega}_m) + \sigma\psi_y^\dagger(x,\mathbf{\Omega}_m) - \sigma_s \sum_{n=1}^{M/2} w_n \left[\psi_y^\dagger(x,\mathbf{\Omega}_n) + \psi_y^\dagger(x,\mathbf{\Omega}_{n+M/2})\right] = S_y^\dagger(x,\mathbf{\Omega}_m);$$

- Where $S_y^\dagger(x,\mathbf{\Omega}_m)$ is such that:

$$S_y^\dagger(x,\mathbf{\Omega}_m) = \frac{\xi_m}{h_y}\left[\psi^\dagger(x,y_p,\mathbf{\Omega}_m) - \psi^\dagger(x,y_{p+1},\mathbf{\Omega}_m)\right] + \frac{1}{h_y}\int_{y_{p+1}}^{y_p} S_y^\dagger(x,y,\mathbf{\Omega}_m)\,\mathrm{d}y;$$

- We assume that the transversal leakage terms $\psi^\dagger(x,y_p,\mathbf{\Omega}_m)$ and $\psi^\dagger(x,y_{p+1},\mathbf{\Omega}_m)$ are constant for each direction.

ADO-Nodal Formulation to the Adjoint Transport Equation

- We apply the known one-dimensional adjoint ADO methodology to obtain homogeneous solutions [8]:

$$\psi^{\dagger}_{y,h}(x,\boldsymbol{\Omega}_m) = \sum_{j=1}^{M/2} \{ A_j \phi_y(\nu_j,\boldsymbol{\Omega}_m) e^{-(x-x_q)/\nu_j} + A_{j+M/2} \phi_y(\nu_j,\boldsymbol{\Omega}_{m+M/2}) e^{-(x_{q+1}-x)/\nu_j} \},$$

$$\psi^{\dagger}_{y,h}(x,\boldsymbol{\Omega}_{m+M/2}) = \sum_{j=1}^{M/2} \{ A_j \phi_y(\nu_j,\boldsymbol{\Omega}_{m+M/2}) e^{-(x-x_q)/\nu_j} + A_{j+M/2} \phi_y(\nu_j,\boldsymbol{\Omega}_m) e^{-(x_{q+1}-x)/\nu_j} \};$$

- Constant source for each region $\Rightarrow$ constant particular solution for each region:

$$\sigma K_m - \sigma_s \sum_{n=1}^{M} w_n K_n = S^{\dagger}_y + \frac{\xi_m}{h_y} \left(\psi^{\dagger}(x,y_p,\boldsymbol{\Omega}_m) - \psi^{\dagger}(x,y_{p+1},\boldsymbol{\Omega}_m) \right).$$

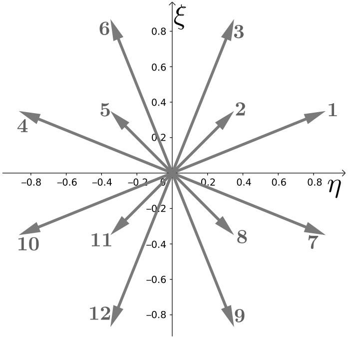
ADO-Nodal Formulation to the Adjoint Transport Equation

- Similarly, we consider the averaged flux with respect to the x variable:

$$\psi_x^\dagger(y,\mathbf{\Omega}) = \frac{1}{h_x}\int_{x_q}^{x_{q+1}} \psi^\dagger(x,y,\mathbf{\Omega})\,\mathrm{d}x;$$

- We still use M nodes, $\mathbf{\Omega}_k = (\eta_k, \xi_k)$, and weights, w_k of the projection of the known LQ_n quadrature in the plane $\eta O \xi$;

- But, this time, we consider discrete directions ordered according to:



ADO-Nodal Formulation to the Adjoint Transport Equation

- This way, integrating the transport equation with respect to x, we obtain:

$$\mp\xi_m \frac{d}{dy}\psi_x^\dagger(y,\mathbf{\Omega}_m) + \sigma\psi_x^\dagger(y,\mathbf{\Omega}_m)$$
$$- \sigma_s \sum_{n=1}^{M/2} w_n \left[\psi_x^\dagger(y,\mathbf{\Omega}_n) + \psi_x^\dagger(y,\mathbf{\Omega}_{n+M/2})\right] = S_x^\dagger(y,\mathbf{\Omega}_m);$$

- Where $S_x^\dagger(y,\mathbf{\Omega}_m)$ is such that:

$$S_x^\dagger(y,\mathbf{\Omega}_m) = \frac{\eta_m}{h_x}\left[\psi^\dagger(x_{q+1},y,\mathbf{\Omega}_m) - \psi^\dagger(x_q,y,\mathbf{\Omega}_m)\right]$$
$$+ \frac{1}{h_x}\int_{x_q}^{x_{q+1}} S_x^\dagger(x,y,\mathbf{\Omega}_m)\,\mathrm{d}x;$$

- We also assume constant transversal leakage terms $\psi^\dagger(x_q,y,\mathbf{\Omega}_m)$ and $\psi^\dagger(x_{q+1},y,\mathbf{\Omega}_m)$

ADO-Nodal Formulation to the Adjoint Transport Equation

- Finally, we apply the one-dimensional ADO methodology to obtain homogeneous solutions:

$$\psi^{\dagger}_{x,h}(y,\mathbf{\Omega}_m) = \sum_{j=1}^{M/2}\{B_j\phi_x(\gamma_j,\mathbf{\Omega}_m)e^{-(y-y_{p+1})/\gamma_j} + B_{j+M/2}\phi_x(\gamma_j,\mathbf{\Omega}_{m+M/2})e^{-(y_p-y)/\gamma_j}\},$$

$$\psi^{\dagger}_{x,h}(y,\mathbf{\Omega}_{m+M/2}) = \sum_{j=1}^{M/2}\{B_j\phi_x(\gamma_j,\mathbf{\Omega}_{m+M/2})e^{-(y-y_{p+1})/\gamma_j} + B_{j+M/2}\phi_x(\gamma_j,\mathbf{\Omega}_m)e^{-(y_p-y)/\gamma_j}\};$$

- Constant source for each region $\Rightarrow$ constant particular solution for each region:

$$\sigma W_m - \sigma_s \sum_{n=1}^{M} w_n W_n = S^{\dagger}_x + \frac{\eta_m}{h_x}\left(\psi^{\dagger}(x_{q+1},y,\mathbf{\Omega}_m) - \psi^{\dagger}(x_q,y,\mathbf{\Omega}_m)\right).$$

ADO-Nodal Formulation to the Adjoint Transport Equation

- To obtain the coefficients A_j and B_j we deduce a linear system obtained by considering:
  (i) Particular solutions for the averaged fluxes within each region:
    (a) Regions that do not contain the boundaries – constant leakage terms;
    (b) Regions that contain the boundaries – boundary conditions.

  (ii) Boundary conditions for the averaged fluxes within each region;
  (iii) Continuity of the averaged fluxes at the interfaces of two contiguous regions.
- We obtain a system of order $4Mn_xn_y$.

Explicit Formulas for the Absorption Rate Measurements

ADO-Nodal Formulation to the Adjoint Transport Equation

Explicit Formulas for the Absorption Rate

- As previously stated, the rate of absorption is given by:

$$r = \left\langle \psi^{\dagger}, \tilde{S} \right\rangle - P\left[\psi, \psi^{\dagger}\right];$$

- Where we may use the explicit expressions for the averaged fluxes to write:

$$\left\langle \psi^{\dagger}, \tilde{S} \right\rangle = \sum_{q=1}^{n_x} \sum_{p=1}^{n_y} \tilde{S}_{p,q} h_{x,p,q} h_{y,p,q} \phi^{\dagger}_{p,q}.$$

- $\phi^{\dagger}_{p,q}$ represents the averaged scalar flux of particles, and is given by either:

$$\phi^{\dagger}_{p,q} = \frac{1}{h_{x,p,q}} \sum_{j=1}^{M/2} \nu_j^{p,q} \left(1 - e^{-(x_{q+1}-x_q)/\nu_j^{p,q}}\right) \times \left(A_j^{p,q} + A_{j+M/2}^{p,q}\right) \phi_{y,j}^{0,p,q} + \phi_{y,j}^{1,p,q};$$

- Or:

$$\phi^{\dagger}_{p,q} = \frac{1}{h_{y,p,q}} \sum_{j=1}^{M/2} \gamma_j^{p,q} \left(1 - e^{-(y_p-y_{p+1})/\gamma_j^{p,q}}\right) \times \left(B_j^{p,q} + B_{j+M/2}^{p,q}\right) \phi_{x,j}^{0,p,q} + \phi_{x,j}^{1,p,q};$$

- Where $\phi_{y,j}^{0,p,q}$, $\phi_{y,j}^{1,p,q}$, $\phi_{x,j}^{0,p,q}$ and $\phi_{x,j}^{1,p,q}$ are closed form terms and depend on the eigenfunctions and internal sources.

ADO-Nodal Formulation to the Adjoint Transport Equation

Explicit Formulas for the Absorption Rate

- Further, We write the boundary term $P[\psi,\psi^{\dagger}]$ as:

$$P[\psi,\psi^{\dagger}] = P_1[\psi,\psi^{\dagger}] + P_2[\psi,\psi^{\dagger}] + P_3[\psi,\psi^{\dagger}] + P_4[\psi,\psi^{\dagger}];$$

- Where:

$$P_1[\psi,\psi^{\dagger}] = -\sum_{q=1}^{n_x}\sum_{m=1}^{M/2} w_m h_{x,n_y,q} f_{n_y,q} \psi^{\dagger}_{x,n_y,q}(0,\mathbf{\Omega}_m),$$

$$P_2[\psi,\psi^{\dagger}] = -\sum_{q=1}^{n_x}\sum_{m=1}^{M/2} w_m h_{x,1,q} f_{1,q} \psi^{\dagger}_{x,1,q}(b,\mathbf{\Omega}_{m+M/2}),$$

$$P_3[\psi,\psi^{\dagger}] = -\sum_{p=1}^{n_y}\sum_{m=1}^{M/2} w_m h_{y,1,q} f_{p,1} \psi^{\dagger}_{y,p,1}(0,\mathbf{\Omega}_m),$$

$$P_4[\psi,\psi^{\dagger}] = -\sum_{p=1}^{n_y}\sum_{m=1}^{M/2} w_m h_{y,p,n_x} f_{p,n_x} \psi^{\dagger}_{y,p,n_x}(a,\mathbf{\Omega}_{m+M/2}).$$

Source Estimation

Source Estimation

- Given exact measurements $\boldsymbol{r}(\boldsymbol{\alpha})$, we consider additive noise such that:

$$\tilde{\boldsymbol{r}}_m = \boldsymbol{r}(\boldsymbol{\alpha}) + \boldsymbol{\epsilon};$$

- If $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{W})$, with $\boldsymbol{W} = \sigma^2 \boldsymbol{I}$, it is possible to write the PDF for $\boldsymbol{\epsilon}$ as [6]:

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

- Which is maximized when the maximum likelihood function

$$S_{ML}(\boldsymbol{\alpha}) = \left[\tilde{\boldsymbol{r}} - \boldsymbol{r}\right]^T \left[\tilde{\boldsymbol{r}} - \boldsymbol{r}\right] = ||\boldsymbol{A}\boldsymbol{\alpha} - \boldsymbol{b}||^2,$$

is minimized.

Source Estimation

- We obtain exact results when using noise free measurements calculated using the ADO method with the same valor of N and the same mesh used to calculate $\boldsymbol{A}$;
- However, as expected, we got oscillations on our estimates when considering noisy measurements;
- Tikhonov regularization: the maximum likelihood function is modified according to:

$$S_\lambda(\boldsymbol{\alpha}) = ||\boldsymbol{A}\boldsymbol{\alpha} - \boldsymbol{b}||^2 + \lambda\,||(\boldsymbol{\alpha} - \boldsymbol{\alpha}_0)||^2\,;$$

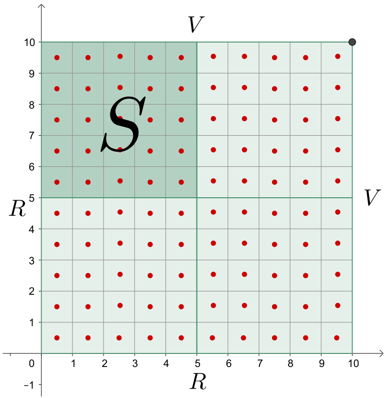
- Iterated Tikhonov to find the best values of λ (discrepancy principle).

Source Estimation
Test Problem I

Source Estimation – Test Problem I

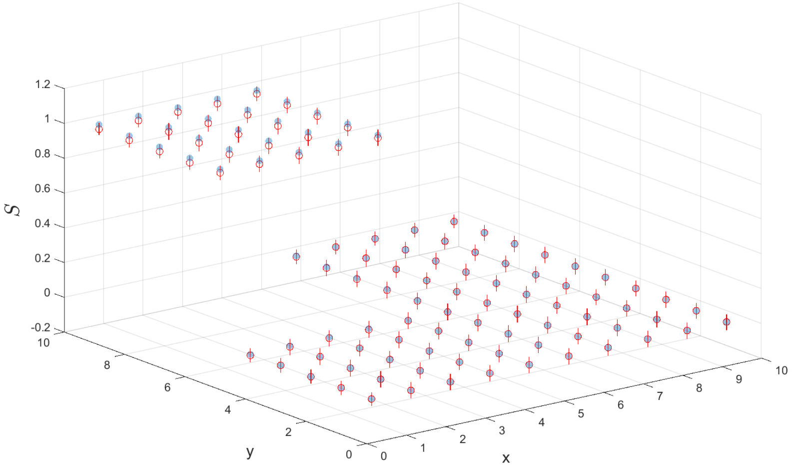
Test Problem I configuration

- Rectangle $(x, y) \in [0, 10] \times [0, 10]$;
- Heterogeneous medium:
  $$\sigma_t(x, y) = \begin{cases} 1.0, & \text{for } (x,y) \in [0,5] \times [0,5], \\ 2.0, & \text{otherwise;} \end{cases}$$
  $$\sigma_s(x, y) = \begin{cases} 0.5, & \text{for } (x,y) \in [0,5] \times [0,5], \\ 0.1, & \text{otherwise;} \end{cases}$$
- Internal source of particles:
  $$S(x, y) = \begin{cases} 1.0, & \text{for } (x, y) \in [0,5] \times [6,10], \\ 0.0, & \text{otherwise;} \end{cases}$$
- Diamond difference to generate "exact" measurements, then add 1% of additive white noise.



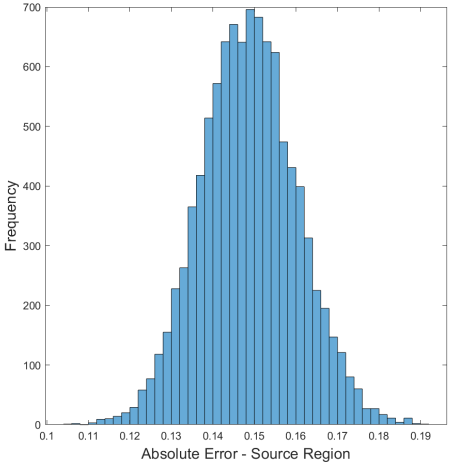
Source Estimation – Test Problem I

Mean value of estimates and confidence intervals



Source Estimation – Test Problem I

Errors



- Minimum, mean, maximum and standard deviation of the absolute errors (L^2 norm):

Errors	Min.	Mean	Max.	Std.
$\left\|\tilde{S} - \hat{S}\right\|$	0.1054	0.1487	0.1914	0.0116

- 99% confidence interval:

$$(0.1193, 0.1796)$$

Source Estimation
Test Problem II

Source Estimation – Test Problem II

Test Problem II configuration

- Rectangle $(x, y) \in [0, 10] \times [0, 10]$;
- Heterogeneous medium:

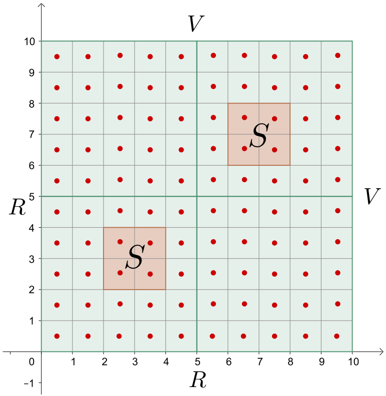
$$\sigma_t(x, y) = \begin{cases} 1.0, & \text{for } (x,y) \in [0,5] \times [0,5], \\ 2.0, & \text{otherwise;} \end{cases}$$

$$\sigma_s(x, y) = \begin{cases} 0.5, & \text{for } (x,y) \in [0,5] \times [0,5], \\ 0.1, & \text{otherwise;} \end{cases}$$

- Internal source of particles:

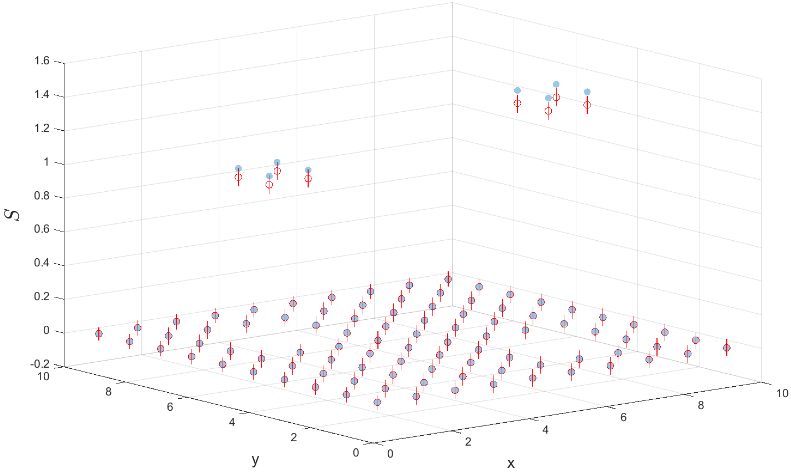
$$S(x, y) = \begin{cases} 1.0, & \text{for } (x, y) \in [2,4] \times [2,4]; \\ 1.5, & \text{for } (x, y) \in [6,8] \times [6,8]; \\ 0.0, & \text{otherwise;} \end{cases}$$

- Diamond difference to generate "exact" measurements, then add 1% of additive white noise.



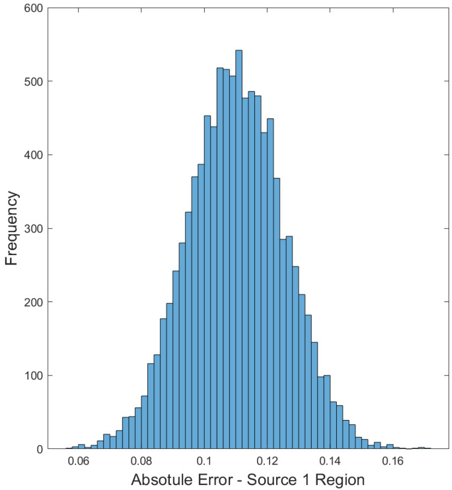
Source Estimation – Test Problem II

Mean value of estimates and confidence intervals



Source Estimation – Test Problem II

Errors – S_1 region



- Minimum, mean, maximum and standard deviation of the absolute errors (L^2 norm) at $S_1 = 1.0$ region:

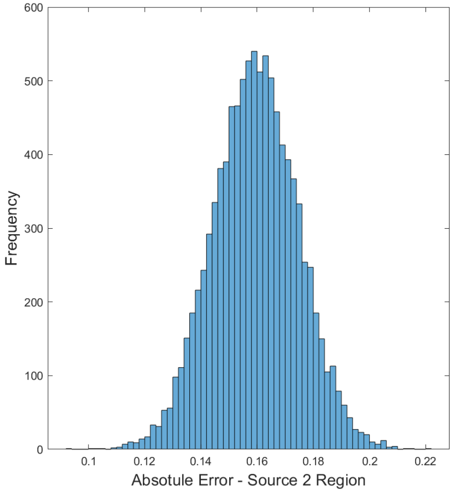
Errors	Min.	Mean	Max.	Std.
$\left\|\left\|\tilde{S}_1 - \hat{S}_1\right\|\right\|$	0.0569	0.1102	0.1717	0.0153

- 99% confidence interval:

$$(0.0701, 0.1488)$$

Source Estimation – Test Problem II

Errors – S_2 region



- Minimum, mean, maximum and standard deviation of the absolute errors (L^2 norm) at $S_2 = 1.5$ region:

Errors	Min.	Mean	Max.	Std.
$\left\|\left\|\tilde{S}_2 - \hat{S}_2\right\|\right\|$	0.0920	0.1595	0.2208	0.0151

- 99% confidence interval:

$$(0.1200, 0.1988)$$

Bayesian Inference Techniques

Bayesian Inference Techniques

- Using Bayes' theorem in $\pi_{post}(\boldsymbol{\alpha}) = \pi(\boldsymbol{\alpha}|\tilde{\boldsymbol{r}})$:

$$\pi_{post}(\boldsymbol{\alpha}) = \frac{\pi(\tilde{\boldsymbol{r}}|\boldsymbol{\alpha})\pi(\boldsymbol{\alpha})}{\pi(\tilde{\boldsymbol{r}})} \propto \pi(\tilde{\boldsymbol{r}}|\boldsymbol{\alpha})\pi(\boldsymbol{\alpha});$$

- Prior distribution $\pi(\boldsymbol{\alpha})$ for the parameters – Gaussian Markov random field;
- Parameter λ treated as a hyperparameter – Rayleigh's distribution;
- Posterior distribution of probability:

$$\pi_{post}(\boldsymbol{\alpha}, \lambda) \propto \lambda^{\frac{N_d+2}{2}} \exp\left\{ -\frac{1}{2} \left[\tilde{\boldsymbol{r}} - \boldsymbol{r}(\boldsymbol{\alpha})\right]^T \boldsymbol{W}^{-1} \left[\tilde{\boldsymbol{r}} - \boldsymbol{r}(\boldsymbol{\alpha})\right] \right.$$
$$\left. -\frac{1}{2}\lambda \left[\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}\right]^T \boldsymbol{Z} \left[\boldsymbol{\alpha} - \tilde{\boldsymbol{\alpha}}\right] - \frac{1}{2}\left(\frac{\lambda}{\lambda_0}\right)^2 \right\}.$$

Bayesian Inference Techniques

- We use the Metropolis-Hastings algorithm [6] to sample the posterior distribution of the source parameters:
  - Consider an initial state $\boldsymbol{\alpha}^{(0)}$, $\lambda^{(0)}$;
  - Given a state $\boldsymbol{\alpha}^{(k-1)}$, $\lambda^{(k-1)}$, we perform a random walk step to find a proposal state $\boldsymbol{\alpha}^{(*)}$, $\lambda^{(*)}$ given by:

$$\boldsymbol{\alpha}^{(*)} = \boldsymbol{\alpha}^{(k-1)} + \boldsymbol{\alpha}, \quad \lambda^{(*)} = \lambda^{(k-1)} + \lambda;$$

  - We accept the new state, that is, we set $\boldsymbol{\alpha}^{(k)} = \boldsymbol{\alpha}^{(*)}$ and $\lambda^{(k)} = \lambda^{(*)}$, if [6]:

$$\min\left\{1, \frac{\pi_{post}(\boldsymbol{\alpha}^{(*)},\lambda^{(*)})}{\pi_{post}(\boldsymbol{\alpha}^{(k-1)},\lambda^{(k-1)})}\right\} \geq \mu,$$

    where $\mu \sim \mathcal{U}(0,1)$;
  - Otherwise, we reject the new state, that is, we set $\boldsymbol{\alpha}^{(k)} = \boldsymbol{\alpha}^{(k-1)}$ and $\lambda^{(k)} = \lambda^{(k-1)}$.

Source Estimation
Test Problem III

Source Estimation – Test Problem III

Test Problem III configuration

- Same physical properties of the Test Problem I;
- Rectangle $(x, y) \in [0, 10] \times [0, 10]$;
- Heterogeneous medium:

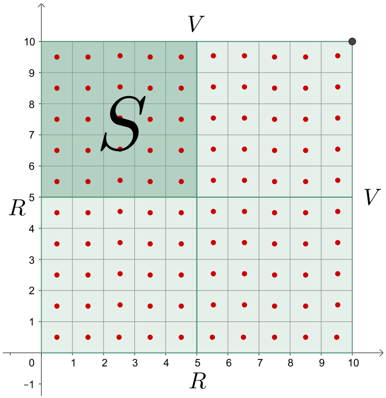
$$\sigma_t(x,y) = \begin{cases} 1.0, & \text{for } (x,y) \in [0,5] \times [0,5], \\ 2.0, & \text{otherwise;} \end{cases}$$

$$\sigma_s(x,y) = \begin{cases} 0.5, & \text{for } (x,y) \in [0,5] \times [0,5], \\ 0.1, & \text{otherwise;} \end{cases}$$

- Internal source of particles:

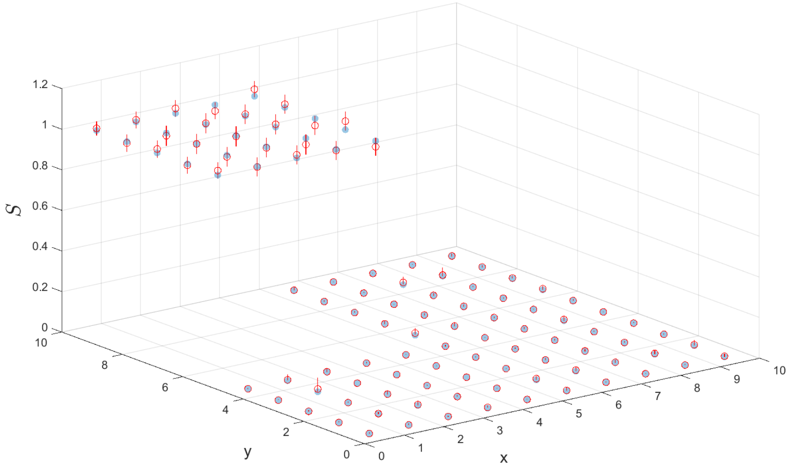
$$S(x,y) = \begin{cases} 1.0, & \text{for } (x,y) \in [0,5] \times [6,10], \\ 0.0, & \text{otherwise;} \end{cases}$$

- Diamond difference to generate "exact" measurements, then add 1% of additive white noise.



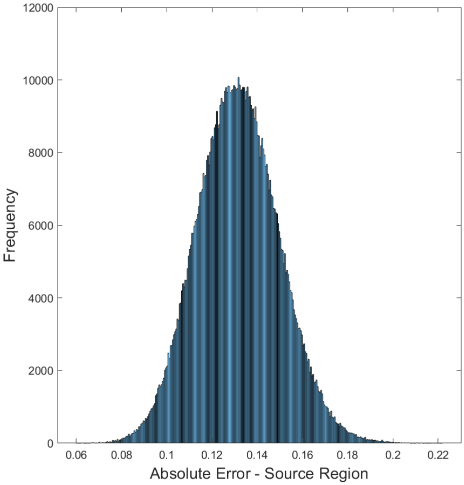
Source Estimation – Test Problem III

Mean value of estimates and credible intervals



Source Estimation – Test Problem III

Errors



- Minimum, mean, maximum and standard deviation of the absolute errors (L^2 norm):

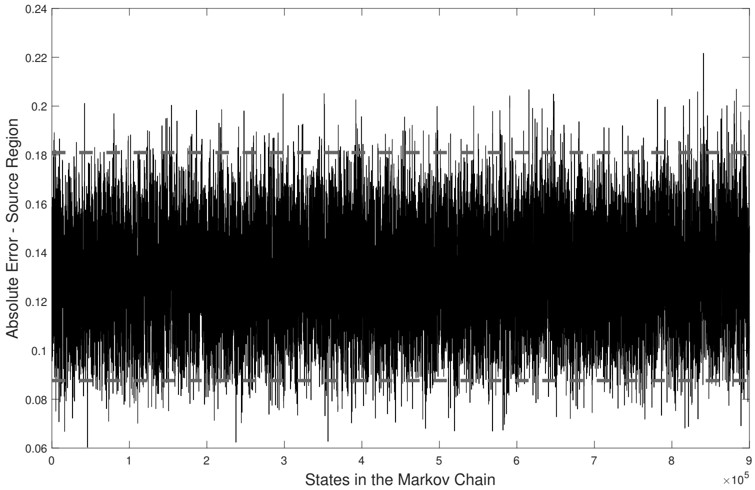
Errors	Min.	Mean	Max.	Std.
$\left\|\left\|\tilde{S} - \hat{S}\right\|\right\|$	0.0603	0.1316	0.2217	0.0181

- 99% credible interval:

$$(0.0876, 0.1810)$$

Source Estimation – Test Problem III

States in the Markov chain and 99% credible interval



Source Estimation
Test Problem IV

Source Estimation – Test Problem IV

Test Problem IV configuration

- Same physical properties of the Test Problem II;
- Rectangle $(x, y) \in [0, 10] \times [0, 10]$;
- Heterogeneous medium:

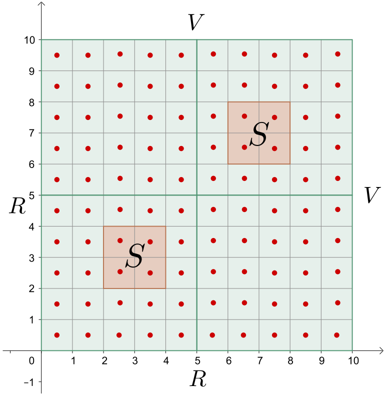
$$\sigma_t(x, y) = \begin{cases} 1.0, & \text{for } (x,y) \in [0,5] \times [0,5], \\ 2.0, & \text{otherwise;} \end{cases}$$

$$\sigma_s(x, y) = \begin{cases} 0.5, & \text{for } (x,y) \in [0,5] \times [0,5], \\ 0.1, & \text{otherwise;} \end{cases}$$

- Internal source of particles:

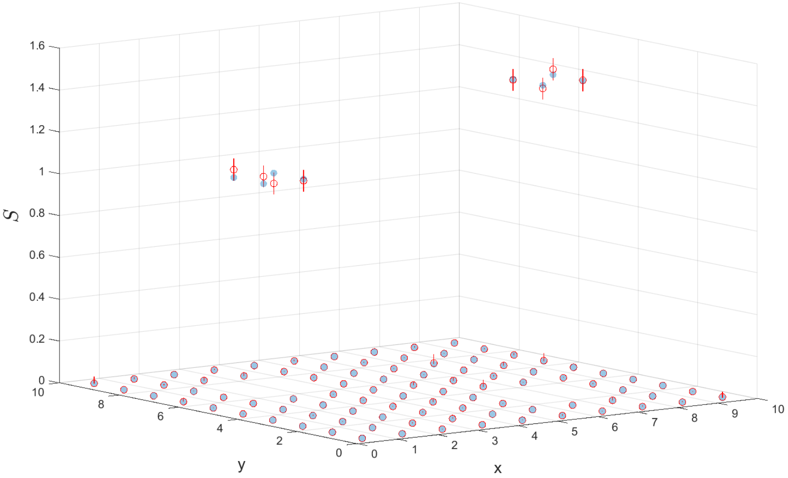
$$S(x, y) = \begin{cases} 1.0, & \text{for } (x, y) \in [2,4] \times [2,4]; \\ 1.5, & \text{for } (x, y) \in [6,8] \times [6,8]; \\ 0.0, & \text{otherwise;} \end{cases}$$

- Diamond difference to generate "exact" measurements, then add 1% of additive white noise.



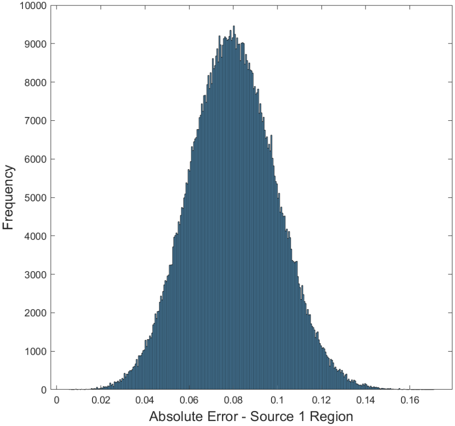
Source Estimation – Test Problem IV

Mean value of estimates and credible intervals



Source Estimation – Test Problem IV

Errors – S_1 region



- Minimum, mean, maximum and standard deviation of the absolute errors (L^2 norm) at $S_1 = 1.0$ region:

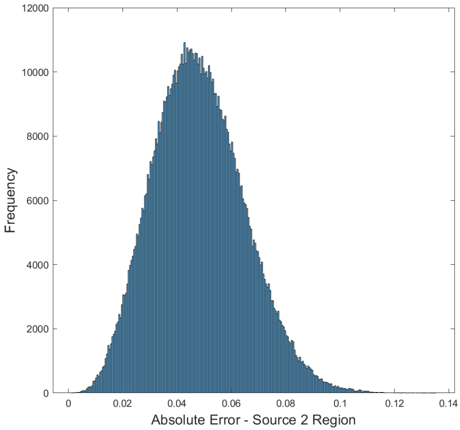
Errors	Min.	Mean	Max.	Std.
$\left\|\tilde{S} - \hat{S}\right\|$	0.0056	0.0799	0.1708	0.0195

- 99% credible interval:

$$(0.0319, 0.1313)$$

Source Estimation – Test Problem IV

Errors – S_2 region



- Minimum, mean, maximum and standard deviation of the absolute errors (L^2 norm) at $S_2 = 1.5$ region:

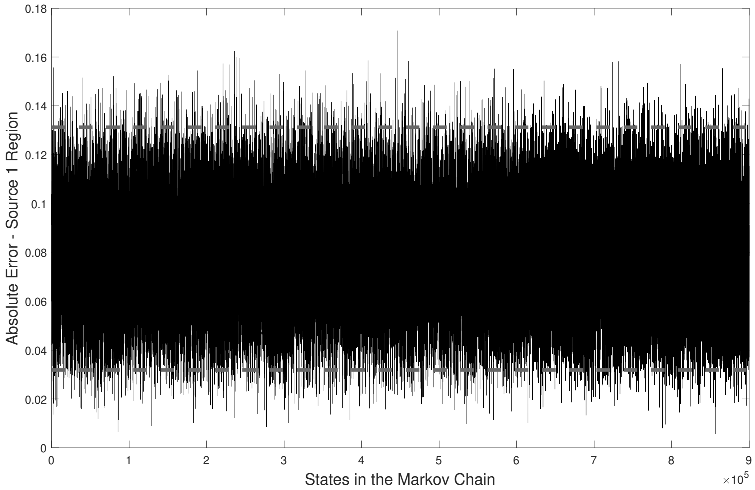
Errors	Min.	Mean	Max.	Std.
$\left\|\tilde{S} - \hat{S}\right\|$	0.0013	0.0481	0.1353	0.0167

- 99% credible interval:

$$(0.0122, 0.0955)$$

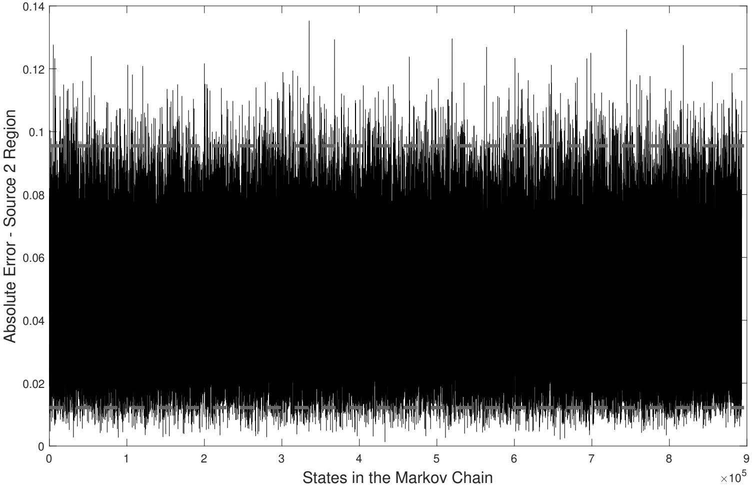
Source Estimation – Test Problem IV

States in the Markov chain and 99% credible interval – S_1 region



Source Estimation – Test Problem IV

States in the Markov chain and 99% credible interval – S_2 region



Conclusions

- We proposed an ADO-Nodal solution fo the adjoint transport equation in a rectangular region, considering the monoenergetic approximation and isotropic scattering;
- Explicit solutions allowed us to derive explicit expressions for r, which lead us to speed and accuracy when estimating the absorption rates;
- With respect to the source estimation problems, we believe to have attained good approximations in all cases;
- We found the results obtained considering the MCMC algorithm to be slightly better than the ones obtained using IT algorithm, in the sense of producing smaller absolute erros;
- Moreover, the estimated magnitudes outside the sources region were also better approximated using the Bayesian formulation;
- Finally, we found that the MCMC algorithm performed at least twice as fast as the IT, though no analysis have yet been performed.

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- L. B. Barichello, C. B. Pazinatto e K. Rui, An analytical discrete ordinates nodal solution to the two-dimensional adjoint transport problem. **Annals of Nuclear Energy**, 2020.

Ongoing works

- More detailed study of Bayesian inference techniques for solving source estimation inverse problems;
- Use of more refined meshes – analysis of the ADO-Nodal matrices;
- Energy dependence – multigroup approximation;
- Arbitrary degree of anisotropy.

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Thank you!

On the use of the Adjoint Operator in Estimating Neutral Particles Sources

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