SEXTO COLÓQUIO DE MATEMÁTICA DA REGIÃO SUL

RNA-MDC: 1D
Um método baseado em dados e modelo de transporte de partículas neutras

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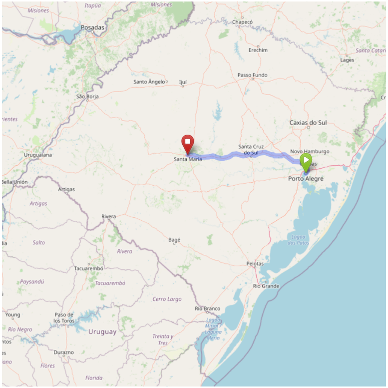
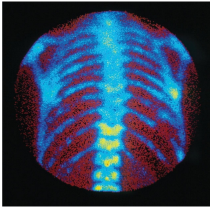
Thank you for having me here!

Porto Alegre, RS, Brazil



Contents

Introduction: Neutral Particle Transport



Introduction: Transport Model

- $\mathcal{D} = (a, b)$, $-1 < \mu < 1, \mu \neq 0$

$$\mu \cdot \frac{\partial}{\partial x} I(x, \mu) + \sigma_t I = \sigma_s \Psi(x) + q(x, \mu; \lambda)$$

- Boundary conditions

$$\forall \mu > 0 : \; I(a, \mu) = I_a$$
$$\forall \mu < 0 : \; I(b, \mu) = I_b$$

- Average scalar flux

$$\Psi(x) := \frac{1}{2} \int_{-1}^{1} I(x, \mu') \, d\mu'$$

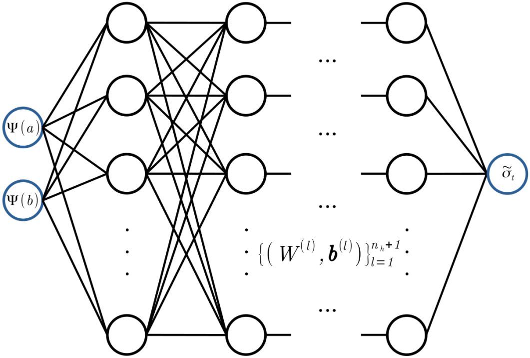
E. Lewis and W. Miller. 1984a. *Computational Methods of Neutron Transport*.

M. Modest. 2013a. *Radiative Heat Transfer*.

Background/Insight: ANN as Regression Models

Data Driven

$$\mathcal{T} = \left\{ \left(\left(\hat{\Psi}^{(m)}(a), \hat{\Psi}^{(m)}(b) \right), \hat{\sigma}_t{}^{(m)} \right) \right\}_{m=1}^{m_s}$$



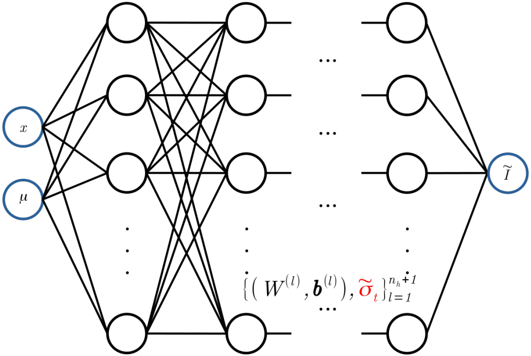
$$\underbrace{\min \frac{1}{m_s} \sum_{m=1}^{m_s} \left\| \tilde{\sigma}_t{}^{(m)} - \hat{\sigma}_t{}^{(m)} \right\|^2}_{\mathcal{L}}$$

Roman, N.G.; Santos, P.C.; Konzen. 2024a. *LAJC*.

Roman, N.; Konzen, P.H.A. 2024b. *CeN*.

Background/Insight: PINNs

Data & Model Driven



(Raissi, Perdikaris & Karniadakis, 2019)

(Mishra & Molinaro, 2021)

$$\mathcal{L} := \frac{1}{m_{\text{in}}} \sum_{m=1}^{m_{\text{in}}} \underbrace{\left\| \mu \tilde{I}_x^{(m)} - \tilde{\sigma}_t \tilde{I}^{(m)} - \sigma_s \tilde{\Psi}^{(m)} - q^{(m)} \right\|^2}_{\text{residual}}$$

$$+ \frac{1}{2} \sum_{y=a,b} \left| \tilde{\Psi}(y) - \hat{\Psi}(y) \right|^2 + \text{b.c.}$$

ANN-MoC Method: DOM + SI

- Discrete Ordinates Method + Source Iteration

$$\mu_i \cdot \frac{\partial}{\partial x} I^{(j)}(x, \mu_i) + \sigma_t I_i^{(j)}(x) = \sigma_s \Psi^{(j-1)}(x) + q(x, \mu_i; \lambda)$$
$$\mu_i > 0: \; I_i^{(j)}(a) = I_a$$
$$\mu_i < 0: \; I_i^{(j)}(b) = I_b$$

- Gauss-Legendre quadrature $\{\mu_i, w_i\}_{i=1}^{N}$

$$\Psi^{(j)}(x) = \frac{1}{2} \sum_{i=1}^{N} w_i I_i^{(j)}(x)$$

ANN-MoC Method: Method of Characteristics

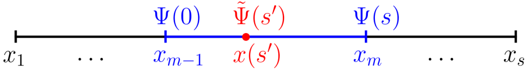
- Change of variables: $x(s) = x_0 + s \cdot \mu_i$

$$\frac{d}{ds} I_i^{(j)}(s) + \sigma_t I_i^{(j)}(s) = \sigma_s \Psi^{(j-1)}(s) + q(s, \mu_i; \lambda)$$

- MoC solution form

$$I_i^{(j)}(s) = I_i^{(j)}(0) e^{-\int_0^s \sigma_t \, ds'} + \int_0^s \left[\sigma_s \tilde{\Psi}^{(j-1)}(s') + q(s'; \lambda) \right] e^{-\int_{s'}^s \sigma_t \, ds''} \, ds'$$

- Internal cell estimations



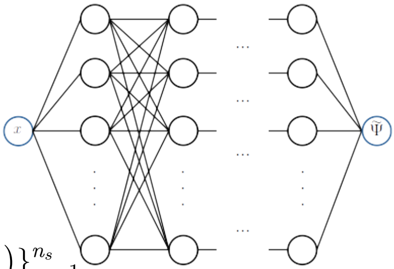
L. Evans. 2010a. *Partial Differential Equations.*

ANN-MoC Method: ANN Scalar Flux Estimations

- Multilayer Perceptron (MLP)

$$\tilde{\Psi}(x) = \mathcal{N}(x)$$

$$\{(W^{(l)}, \boldsymbol{b}^{(l)}, \boldsymbol{f}^{(l)})\}_{l=1}^{n_l}$$



- Training set $\{x^{(m)}, \tilde{\Psi}\left(x^{(m)}\right)\}_{m=1}^{n_s}$

$$\min_{\{(W^{(l)}, \boldsymbol{b}^{(l)})\}_{l=1}^{n_l}} \underbrace{\frac{1}{n_s}\sum_{m=1}^{n_s}\left(\tilde{\Psi}^{(m)} - \Psi^{(m)}\right)^2}_{\mathcal{L}}$$

S. Haykin. 2005a. *Neural Networks: A Comprehensive Foundation.*

ANN-MoC Method: Algorithm

1. Set parameters: mesh, $\Psi^{(0)}(x)$ initial condition, ANN architecture, quadrature, etc.
2. Train ANN to estimate $\Psi^{(0)}(x)$.
3. Source iteration, j-index:

   6.a) For each μ_i, loop over mesh points x_m:

   - If $\mu_i > 0$, then $s = (x^{(m)} - a)/\mu_i$

     $$I_i^{(j)}(x^{(m)}) = I_a e^{-\int_0^s \sigma_t\, ds'} + \int_0^s \left[\mathcal{N}(s') + q(s', \mu_i)\right] e^{-\int_{s'}^s \sigma_t\, ds''}\, ds'$$

   - If $\mu_i < 0$, then $s = (x^{(m)} - b)/\mu_i$

     $$I_i^{(j)}(x^{(m)}) = I_b e^{-\int_0^s \sigma_t\, ds'} + \int_0^s \left[\mathcal{N}(s') + q(s', \mu_i)\right] e^{-\int_{s'}^s \sigma_t\, ds''}\, ds'$$

   6.b) Compute $\Psi^{(j)} = \frac{1}{2}\sum w_i I_i^{(j)}$.

   6.c) Retrain the ANN $\mathcal{N}(x)$ to estimate $\Psi^{(j)}(x)$.

   6.d) Check a given stop criteria.

P. Konzen. 2023a. `https://arxiv.org/abs/2307.03114`.

ANN Training: Backpropagation

Forward

$$\boldsymbol{a}^{(0)} = x$$

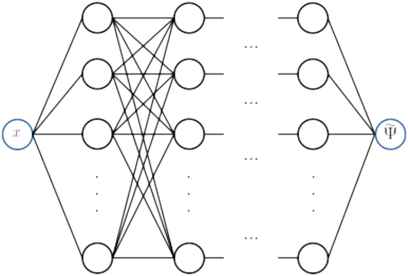
$$\boldsymbol{a}^{(l)} = \boldsymbol{f}^{(l)}\left(W^{(l)}\boldsymbol{a}^{(l-1)} + \boldsymbol{b}^{(l)}\right)$$

$$\boldsymbol{a}^{(n_h+1)} = \tilde{\Psi}(x)$$

$$\mathcal{L} = \frac{1}{n_s}\sum_{m=1}^{n_s}\left(\tilde{\Psi}^{(m)} - \Psi^{(m)}\right)^2$$

Backward

$$(W, \boldsymbol{b}) = (W, \boldsymbol{b}) - l_r \nabla_{(W,\boldsymbol{b})}\mathcal{L}$$



Appl. 1: Direct Model Driven Problem

The Problem

- Exact intensity

$$\hat{I}(x,\mu) = e^{-\alpha\sigma_t x}$$

- Exact scalar flux

$$\hat{\Psi}(x) = e^{-\alpha\sigma_t x}$$

- Equation source

$$q(x,\mu) = \left[(1-\mu\alpha)\sigma_t - \sigma_s)\right] e^{-\alpha\sigma_t x}$$

- $\sigma_s = 0.5$, $\alpha = 5$

The ANN

- Architecture

$$1 - 200 \times 3 - 1$$

- Activation functions

Tanh - Softplus

- Optimizer

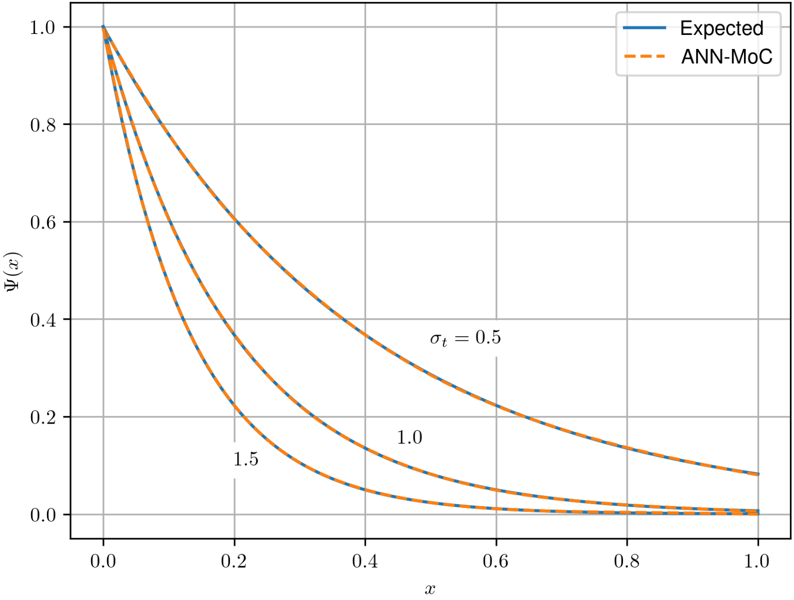
Adam Method

- Training parameters

$$n_s = 100, l_r = 10^{-3}$$

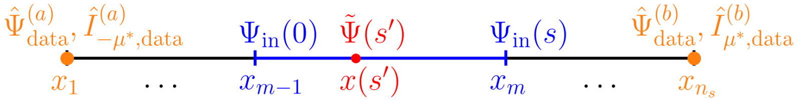
A. Tchantchalam. 2024a. Dissertação de Mestrado, PPGMAp, UFRGS.

Appl. 1: Results



Appl. 2: Direct Data & Model Driven Problem

Data sensors

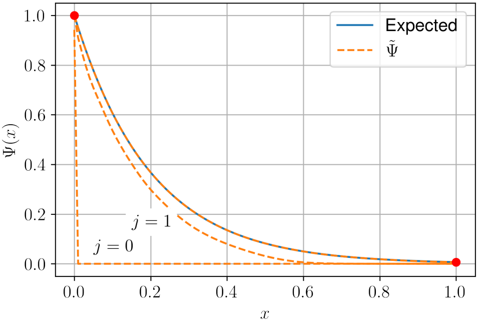


Loss function

$$\mathcal{L}_{\text{DDM}} := \frac{1}{n_{\text{in}}} \sum_{m=1}^{n_{\text{in}}} \left| \tilde{\Psi}^{(m)}_{\text{in}} - \Psi^{(m)}_{\text{in}} \right|^2 + \frac{1}{n_{\text{d}}} \sum_{m=1}^{n_{\text{d}}} \left| \tilde{\Psi}^{(m)}_{\text{data}} - \hat{\Psi}^{(m)}_{\text{data}} \right|^2$$

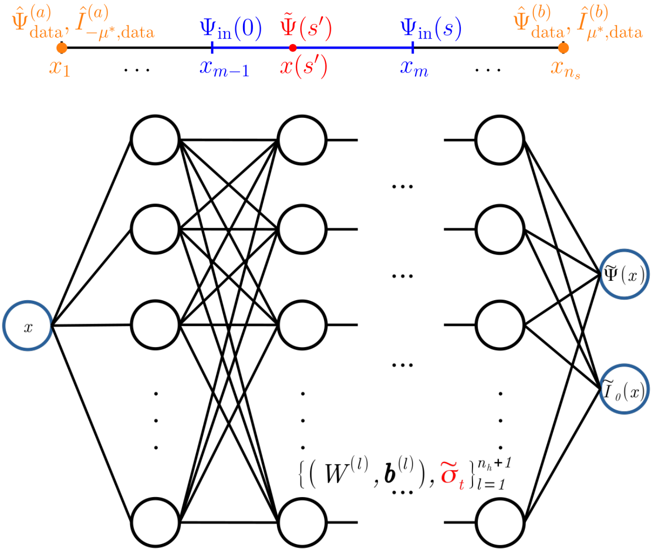
Appl. 2: Results

ANN-MoC	S.I.
$\sigma_t = 1.0,\ \sigma_s = 0.5$	
M	10
DM	11



Appl. 3: Inverse Data & Model Driven Problem

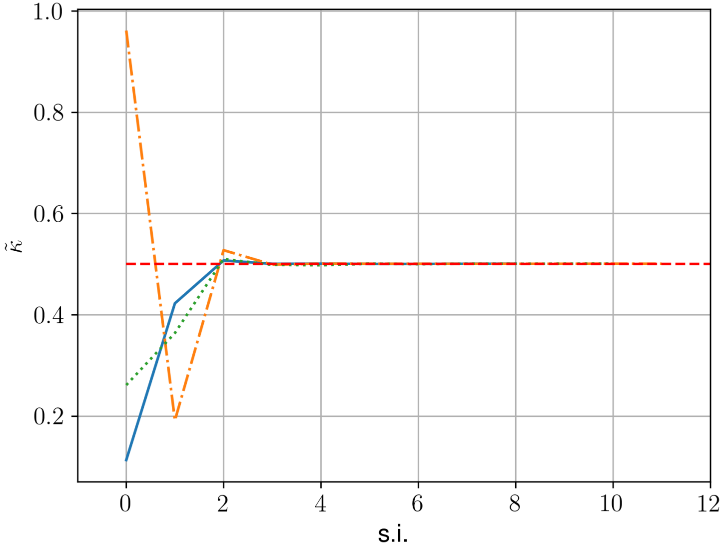
Data sensors & $\sigma_t = ?$



Appl. 3: Loss Function

$$
\begin{aligned}
\mathcal{L}_{\mathrm{IDM}} := & \underbrace{\frac{1}{n_{\mathrm{in}}} \sum_{m=1}^{n_{\mathrm{in}}} \left\| \left(\tilde{\Psi}_{\mathrm{in}}^{(m)}, \tilde{I}_{\mathrm{in}}^{(m)} \right) - \left(\Psi_{\mathrm{in}}^{(m)}, I_{\mathrm{in}}^{(m)} \right) \right\|^2}_{MoC} \\
& + \underbrace{\frac{1}{n_{\mathrm{d}}} \sum_{m=1}^{n_{\mathrm{d}}} \left| \tilde{\Psi}_{\mathrm{data}}^{(m)} - \hat{\Psi}_{\mathrm{data}}^{(m)} \right|^2 + \frac{1}{n_{\mathrm{d}}} \sum_{m=1}^{n_{\mathrm{d}}} \left| \tilde{I}_{\boldsymbol{\mu}^*,\mathrm{data}}^{(m)} - \hat{I}_{\boldsymbol{\mu}^*,\mathrm{data}}^{(m)} \right|^2}_{\text{Data}} \\
& + \underbrace{\frac{1}{n_{\mathrm{d}}} \sum_{m=1}^{n_{\mathrm{d}}} \left| \mu \frac{\partial \tilde{I}_{\boldsymbol{\mu}^*}^{(m)}}{\partial x} + \tilde{\sigma}_t \tilde{I}_{\boldsymbol{\mu}^*}^{(m)} - \sigma_s \hat{\Psi}_{\mathrm{data}}^{(m)} - q_0^{(m)} \right|^2}_{\text{Model}}
\end{aligned}
$$

Appl. 3: Results $\hat{\sigma}_t = \sigma_s + \hat{\kappa}, \sigma_s = 0.5$



Appl. 4: Source localization

The Problem

- Source term

$$q(x, \lambda) = e^{-\frac{(x-\lambda)^2}{\beta^2}}, \quad \beta = 0.1$$

- Vacuum boundary conditions
- Medium properties

$$\sigma_s = 0.5, \sigma_t = 1.0$$

- Sensors ($\mu_0 > 0$)

$$\{I_{-\mu_0}(a), \Psi(a), I_{\mu_0}(b), \Psi(b)\}$$

The ANN

- Architecture

$$1 - 50 \times 4 - 3$$

- Activation functions

Tanh - Identity

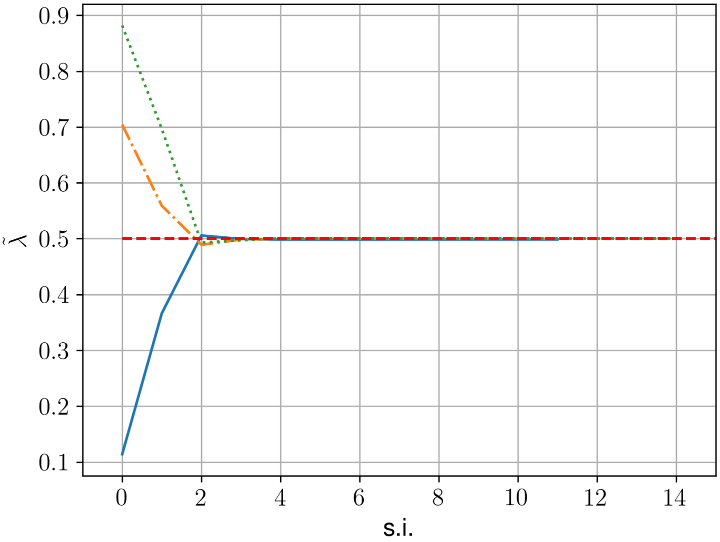
- Optimizer

Adam Method

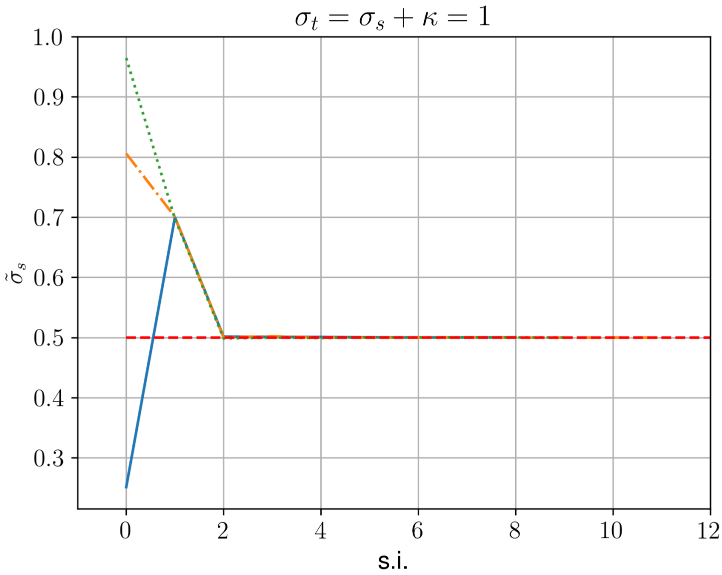
- Training parameters

$$n_s = 100, l_r = 10^{-3}$$

Appl. 4: Results $\hat{\lambda} = 0.5$



Appl. 5: Results $\hat{\sigma}_s = 0.5$



Final Considerations

- ANN-MoC Method for Neutral Particle Transport Problems

  MoC method with ANN estimates of Ψ
- Meshless method
- Framework
  - Direct problems + Data
  - Inverse problems + Data & Model
- Further work
  - Convergence properties and limitations
  - Sensitivity analysis (noisy data)
  - Enhance computational performance
  - More complex models (anisotropy, multidimensional domains, etc.)

Thanks for your attention!

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