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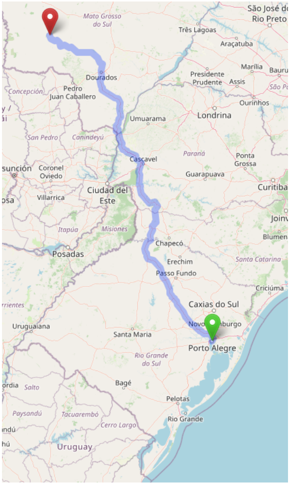
ANN-MoC Method for Solving Unidimensional Neutral Particle Transport Problems

Pedro Henrique de Almeida Konzen

PPGMAp, IME, UFRGS
Porto Alegre, RS

Thank you for having me here!

Porto Alegre, RS, Brazil



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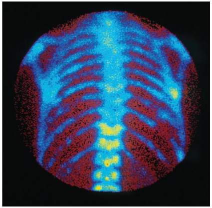


Introduction: Transport Problem

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

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

- 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. 1984. *Computational Methods of Neutron Transport.*

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

ANN-MoC Method: DOM + SI

- Discrete Ordinates Method + Source Iteration

$$\mu_i \cdot \frac{\partial}{\partial x} I^{(j)}(x, \mu_i) + \sigma_t I_i^{(j)}(x) = \sigma_s \Psi^{(j-1)}(x) + q(x, \mu_i)$$

$$\mu_i > 0: \; I_i^{(j)}(a) = I_a$$

$$\mu_i < 0: \; I_i^{(j)}(b) = I_b$$

- Gaussian 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

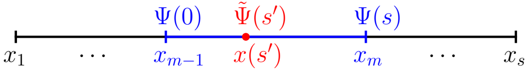
- Change of variables: $x(s) = x_0 + s \cdot \mu_i$

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

- MoC solution form

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

- Internal cell estimations



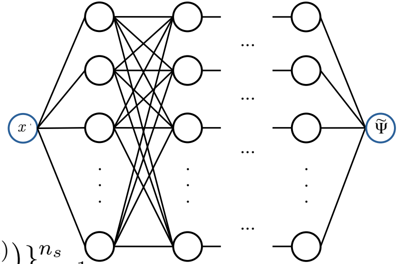
L. Evans. 2010. *Partial Differential Equations.*

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

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

S. Haykin. 2005. *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. 2023. `https://arxiv.org/abs/2307.03114`.

Results - Problem 1: Manufactured Solution

- Exact intensity

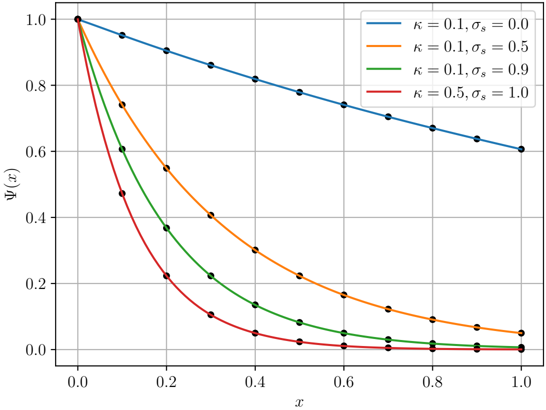
$$\hat{I}(x,\mu) = e^{-\alpha\sigma_t x}$$

- Exact scalar flux

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

- Equation source

$$q(x,\mu) = (\kappa - \alpha\sigma_t\mu)\, e^{-\alpha\sigma_t x}$$



$$\sigma_t = \kappa + \sigma_s$$

Results - Problem 1: Mesh Refinements

Average flux of particles computed at selected points for Problem 1 with $\kappa = 0.1$ and $\sigma_s = 0.5$.

n_s	$\Psi(0.0)$	$\Psi(0.25)$	$\Psi(0.5)$	$\Psi(0.75)$	$\Psi(1.0)$	$\|\tilde{\Psi} - \hat{\Psi}\|_2$
11	1.0000	0.4722	0.2232	0.1051	0.0498	1.98E−4
51	0.9998	0.4726	0.2232	0.1053	0.0498	1.48E−4
101	0.9992	0.4724	0.2231	0.1053	0.0496	1.07E−4
201	0.9995	0.4722	0.2231	0.1054	0.0496	1.22E−4
exact	1.0000	0.4724	0.2231	0.1054	0.0498	-x-

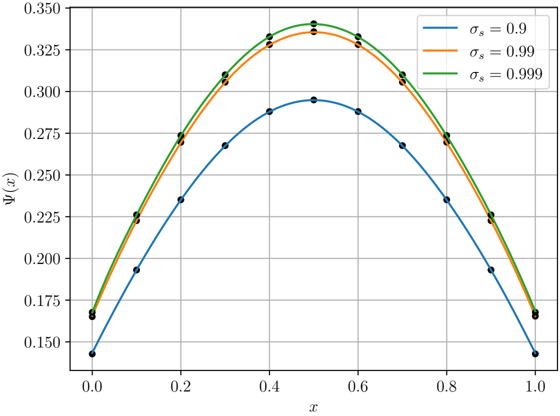
Results - Problem 2: Benchmark Problem

- Equation Source

$$q(x, \mu) = x - x^2$$

- B.Cs.

$$I_a = I_b = 0$$



$$\sigma_t = 1$$

R. Vargas et al. 2017, J. Quant. Spectrosc. Radiat. Transf. **105**, 1-7.

Final Considerations

- ANN-MoC Method for Neutral Particle Transport Problems

  MoC method with ANN estimates of Ψ
- Meshless method
- Provide an ANN that estimates $\Psi = \Psi(x)$
- Good approximations on presented numerical experiments
- Further work
  - More on parameter convergence
  - Enhance computational performance
  - More complex models (anisotropy, multidimensional domains, etc.)

Thanks for your attention!

Research group

Site UFRGS

professor.ufrgs.br/pedro

Lecture Notes

notaspedrok.com.br

Instagram

@notas.pedrok

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Instituto de MATEMÁTICA E ESTATÍSTICA UFRGS