Assessment of the Lagrange Discrete Ordinates Equations for Three-dimensional Neutral Particle Transport

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SIAM CSE 2019

Outline

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- Problem
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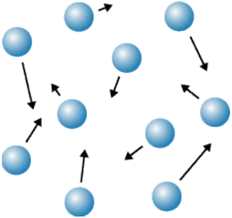
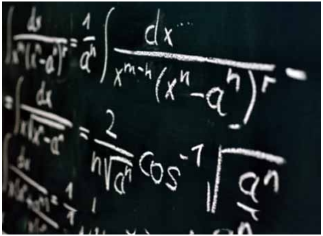
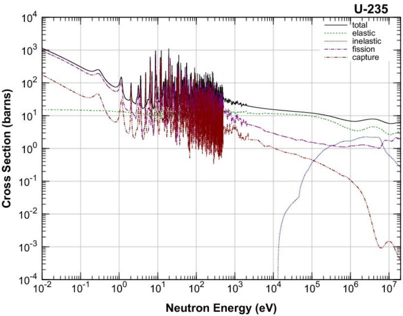
Radiation Transport



Numerical Methods for Radiation Transport

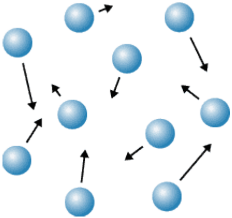
- Predictive simulation
- Translate applied math into code
- Inform algorithm development with physics
- Use high performance computing





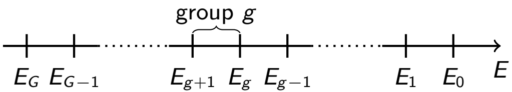
Solving the Transport Equation

$$\mathbf{\Omega} \cdot \nabla \psi(\mathbf{r}, E, \mathbf{\Omega}) + \Sigma_t(\mathbf{r}, E)\psi(\mathbf{r}, E, \mathbf{\Omega}) =$$
$$\int_0^\infty \int_{4\pi} \Sigma_s(\mathbf{r}, E' \to E, \mathbf{\Omega}' \to \mathbf{\Omega})\psi(\mathbf{r}, E', \mathbf{\Omega}') d\mathbf{\Omega}' dE' + Q(\mathbf{r}, E, \mathbf{\Omega})$$

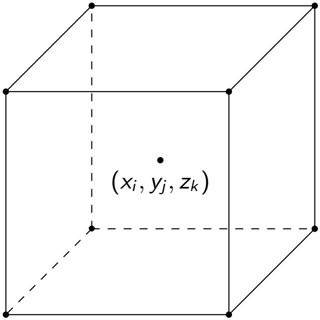


Deterministic Solution Methods

Discretize energy and space:



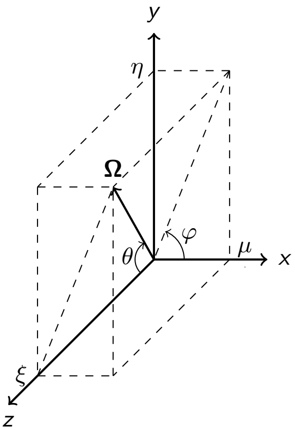
$$g = 0, 1, \ldots, G-1,$$



$$i = 1, 2, \ldots, I,$$
$$j = 1, 2, \ldots, J,$$
$$k = 1, 2, \ldots, K.$$

Angular Discretization

Let μ, η, ξ be the direction cosines of $\mathbf{\Omega}$ with respect to x, y, z.



$$\xi = \cos\theta$$

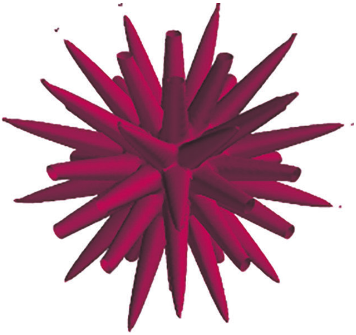
$$\mu = \sqrt{1-\xi^2}\cos\varphi$$

$$\eta = \sqrt{1-\xi^2}\sin\varphi$$

$$\mu^2 + \eta^2 + \xi^2 = 1$$

Discrete Ordinates ("S$_N$") Approximation

$$\mathbf{\Omega}_n \cdot \nabla \psi_n^g(\mathbf{r}) + \Sigma_t^g(\mathbf{r})\psi_n^g(\mathbf{r}) = \sum_{g'=0}^{G-1}\sum_{\ell=0}^{P}\Sigma_{s,\ell}^{g'\to g}(\mathbf{r})\Bigg[Y_{\ell 0}^e(\mathbf{\Omega}_n)\phi_{\ell 0}^{g'}(\mathbf{r}) + \sum_{m=1}^{\ell}\Big(Y_{\ell m}^e(\mathbf{\Omega}_n)\phi_{\ell m}^{g'}(\mathbf{r}) + Y_{\ell m}^o(\mathbf{\Omega}_n)\vartheta_{\ell m}^{g'}(\mathbf{r})\Big)\Bigg] + Q_n^g(\mathbf{r})$$



increasing N

$\longrightarrow$

Lagrange Discrete Ordinates (LDO) Equations

$$\boldsymbol{\Omega}_n \cdot \nabla\psi_n^g(\mathbf{r}) + \Sigma_t^g(\mathbf{r})\psi_n^g(\mathbf{r}) = \sum_{g'=0}^{G-1}\sum_{m=1}^{N}\sum_{n'=1}^{N}\langle L_{n'}, L_m\rangle \Sigma_{s,L}^{g'\to g}(\mathbf{r}, \boldsymbol{\Omega}_m \cdot \boldsymbol{\Omega}_n)\psi_{n'}^{g'}(\mathbf{r}) + Q_n^g(\mathbf{r})$$

increasing N

$\longrightarrow$

Software

- Exnihilo
  - Framework including massively parallel 3D Denovo deterministic transport solver
  - Developed at Oak Ridge National Laboratory
  - C++, Python

Implementation of LDO Equations in Denovo

$\mathbf{S_N}$ Operator Form

$$\mathbf{L}\vec{\psi} = \mathbf{MS}\vec{\phi} + \vec{Q}$$

$$\vec{\phi} = \mathbf{D}\vec{\psi}\,, \quad \mathbf{D} = \mathbf{M}^{\mathsf{T}}\mathbf{W}$$

$$\left(\mathbf{I} - \mathbf{DL}^{-1}\mathbf{MS}\right)\vec{\phi} = \mathbf{DL}^{-1}\vec{Q}$$

LDO Operator Form

$$\mathbf{L}\vec{\psi} = \mathbf{J}\tilde{\mathbf{S}}\vec{\psi} + \vec{Q}$$

$$\left(\mathbf{I} - \mathbf{L}^{-1}\mathbf{J}\tilde{\mathbf{S}}\right)\vec{\psi} = \mathbf{L}^{-1}\vec{Q}$$

$$\mathbf{L}^{-1} = \mathbf{IL}^{-1} \quad \text{and let } \mathbf{D} \equiv \mathbf{I}\text{, then}$$

$$\left(\mathbf{I} - \mathbf{DL}^{-1}\mathbf{J}\tilde{\mathbf{S}}\right)\vec{\psi} = \mathbf{DL}^{-1}\vec{Q}$$

$\mathbf{L}$ = transport operator matrix,

$\mathbf{M}$ = moment-to-discrete matrix,

$\mathbf{S}$ = scattering cross section matrix,

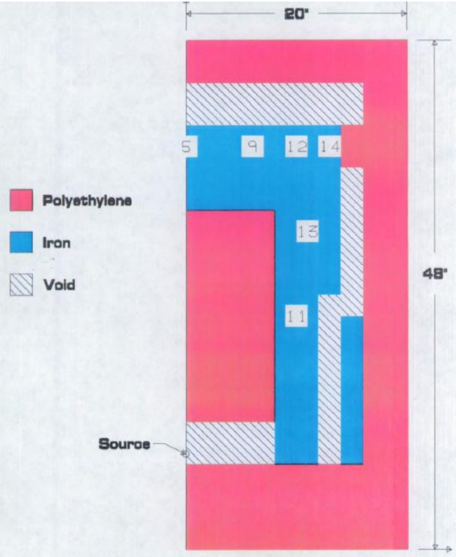
$\mathbf{D}$ = discrete-to-moment matrix,

$\mathbf{W}$ = quadrature weights matrix,

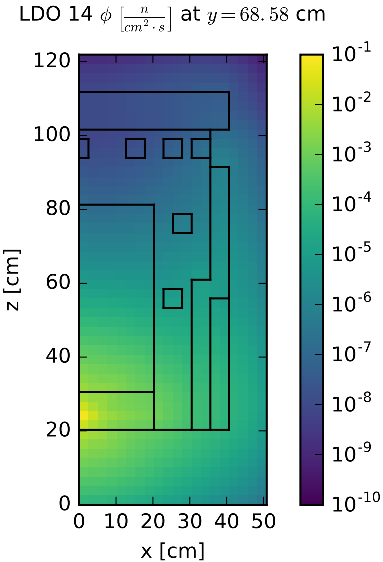
$\mathbf{J}$ = Lagrange expansion matrix

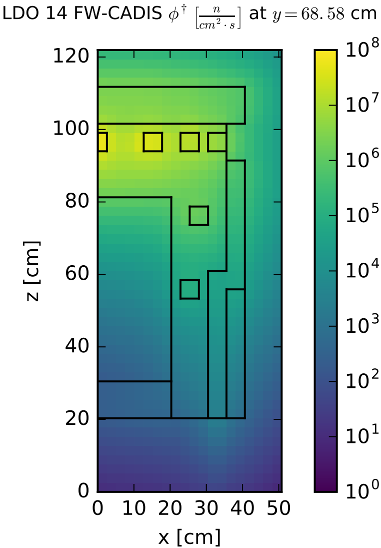
Dog-Legged Void Neutron (DLVN) Benchmark

- Designed to measure neutron streaming in iron with air voids
- Iron and polyethylene
- $40 \times 54 \times 48$ inches
- Cf-252 point source located at center of $x-$ and $y-$directions at $z = 9$ inches
- Symmetric about $y - z$ plane at $x = 0$
- Modeled with vacuum boundary conditions
- **Difficult to solve accurately and quickly**



DLVN Forward and Adjoint Solutions





DLVN Benchmark Comparative Results

Experimental and simulated scalar flux values [n/cm^2/s]:

	Det. 5	Det. 9	Det. 11	Det. 12	Det. 13	Det. 14
Exp.	6.97×10^{-8}	1.57×10^{-7}	8.81×10^{-6}	2.60×10^{-7}	1.42×10^{-6}	2.74×10^{-7}
QR	4.98×10^{-8}	1.68×10^{-7}	8.65×10^{-5}	4.92×10^{-7}	2.71×10^{-6}	1.45×10^{-6}
Galerkin	3.24×10^{-8}	1.47×10^{-7}	8.19×10^{-5}	4.43×10^{-7}	2.95×10^{-6}	9.55×10^{-7}
LDFE	5.12×10^{-8}	1.76×10^{-7}	9.17×10^{-5}	5.14×10^{-7}	2.93×10^{-6}	1.47×10^{-6}
LDO	4.56×10^{-8}	1.39×10^{-7}	7.88×10^{-5}	4.28×10^{-7}	2.37×10^{-6}	1.28×10^{-6}

Percent differences between experimental and simulated scalar flux values:

	Det. 5	Det. 9	Det. 11	Det. 12	Det. 13	Det. 14
QR	**25.58**	6.89	881.94	89.09	90.63	428.81
Galerkin	53.48	**6.37**	829.72	70.56	107.7	**248.42**
LDFE	26.61	12.3	940.41	97.75	106.4	435.01
LDO	34.61	11.2	**794.75**	**64.46**	**66.77**	368.24

Summary

- Many radiation transport problems of interest are difficult to solve quickly with high-quality answers
- For problems with strong particle flux anisotropies, we need novel ways to incorporate angular information into solutions
- LDO equations treat particle scattering differently than traditional discrete ordinates equations and incorporate angular information into scalar flux solutions in a new way

Acknowledgements

This material is based upon work supported under an Integrated University Program Graduate Fellowship as well as supported by the Department of Energy under Award Number(s) DE-NE0008661. This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or limited, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

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Questions?

https://tiny.cc/klr-nse18

https://github.com/kellyrowland/ldo-deterministic

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