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Adjoint Monte Carlo Electron Transport in the Continuous-Slowing-Down Approximation

J. A. Halbleib and J. E. Morel (1980)

Adjoint Electron Transport

- Delayed development paralleling that of forward electron transport
- At the time only one published work
  - T. M. Jordon (1976)
  - Multi-group
  - Green’s function formalism

Overview of Method

- Describes transport of primary electrons
- 1D
- Condensed History method
- Goudsmit-Saunderson Multiple Elastic Scattering Theory for angular deflections
  - Averaged over random walk segments using the method of Spencer
- Continuous Slowing Down Approximation for energy loss and deposition
- The Nearest-Grid-Point (NGP) method
  - Uninterpolated tabular data only

Overview of Method

- Continuous Slowing Down Approximation (CSDA)
  - Ignores energy loss caused by the production of δ-rays, Bremsstrahlung photons, and energy straggling
  - Goudsmit-Sauderson and Moliere multiple scattering theories

Forward-Adjoint Formalism

- Forward $\quad H\varphi = q$
  - H is some linear operator
- Adjoint $\quad H^{\dagger}\varphi^{\dagger} = q^{\dagger}$
- Multiply by $\varphi^{\dagger}$ or φ and subtract

$$H\varphi, \varphi^{\dagger} - \varphi, H^{\dagger}\varphi^{\dagger} = q\varphi^{\dagger} - \varphi q^{\dagger}$$

- Integrate over variable

$$\langle H\varphi, \varphi^{\dagger}\rangle - \langle \varphi, H^{\dagger}\varphi^{\dagger}\rangle = \langle q\varphi^{\dagger}\rangle - \langle \varphi q^{\dagger}\rangle$$

Forward-Adjoint Formalism

Linear Operator for the Boltzmann Equation

- Forward

$$H = \nabla \cdot \Omega + \sigma_T(\boldsymbol{r}, E) - \int_{E'} \int_{\Omega'} d\Omega' dE' \ \sigma_s(\boldsymbol{r}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, E' \rightarrow E)$$

- Adjoint

$$H^{\dagger} = -\nabla \cdot \Omega + \sigma_T(\boldsymbol{r}, E) - \int_{E'} \int_{\Omega'} d\Omega' dE' \, \sigma_s(\boldsymbol{r}, \boldsymbol{\Omega} \rightarrow \boldsymbol{\Omega}', E \rightarrow E')$$

Forward-Adjoint Formalism

- Plug in H and H† and expand the left side

$$\langle H\varphi, \varphi^\dagger\rangle - \langle \varphi, H^\dagger \varphi^\dagger\rangle = \langle q\varphi^\dagger\rangle - \langle \varphi q^\dagger\rangle =$$

$$\int_V \int_E \int_\Omega \left[\left(\nabla \cdot \Omega\varphi(\boldsymbol{r}, \Omega, \boldsymbol{E})\right)\varphi^{\dagger}(\boldsymbol{r}, \Omega, \boldsymbol{E}) + \varphi(\boldsymbol{r}, \Omega, \boldsymbol{E})\left(\nabla \cdot \Omega\varphi^{\dagger}(\boldsymbol{r}, \Omega, \boldsymbol{E})\right)\right] d\Omega dE dr$$

$$+ \int_V \int_E \int_\Omega \left[\sigma_T(\boldsymbol{r}, E)\varphi(\boldsymbol{r}, \Omega, \boldsymbol{E})\varphi^{\dagger}(\boldsymbol{r}, \Omega, \boldsymbol{E}) + \varphi(\boldsymbol{r}, \Omega, \boldsymbol{E})\sigma_T(\boldsymbol{r}, E)\varphi^{\dagger}(\boldsymbol{r}, \Omega, \boldsymbol{E})\right] d\Omega dE dr$$

$$- \int_V \int_E \int_\Omega \int_{E\prime} \int_{\Omega\prime} \sigma_s(\boldsymbol{r}, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}, E' \to E)\ \varphi(\boldsymbol{r}, \Omega, \boldsymbol{E})\varphi^{\dagger}(\boldsymbol{r}, \Omega, \boldsymbol{E})\ d\Omega' dE' d\Omega dE dr$$

$$+ \int_V \int_E \int_\Omega \int_{E\prime} \int_{\Omega\prime} \sigma_s(\boldsymbol{r}, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}, E' \to E)\ \varphi(\boldsymbol{r}, \Omega, \boldsymbol{E})\varphi^{\dagger}(\boldsymbol{r}, \Omega, \boldsymbol{E})\ d\Omega' dE' d\Omega dE dr$$

CSDA Formalism

- CSDA decouples the scattering cross-section

$$\sigma_s(\boldsymbol{r}, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}, E' \to E) =$$

$$\sigma_1(\boldsymbol{r}, \boldsymbol{\Omega} \to \boldsymbol{\Omega}', E \to E')\delta(\mathrm{E}' - \mathrm{E}) + \sigma_2(\boldsymbol{r}, \boldsymbol{\Omega} \to \boldsymbol{\Omega}', E \to E')\delta(\Omega' \cdot \Omega - 1)$$

  - Where σ_1 is the elastic and σ_2 is the inelastic scattering terms

- Expanding the σ_2 in the adjoint Boltzmann equation for n=1

$$-\left[\frac{d}{dE} S(E)\right] + \frac{\partial}{\partial E} S(E)$$

  - Where $\left[\frac{d}{dE} S(E)\right]$ is the effective absorption rate and S(E) is the stopping power

Forward-Adjoint Formalism

Linear Operator for the CSDA Boltzmann Equation

- Forward

$$H = \nabla \cdot \Omega + \sigma_1(\boldsymbol{r}, E) - \int_{\Omega'} d\Omega' \sigma_1(\boldsymbol{r}, E, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) - \frac{\partial}{\partial E} S(E)$$

- Adjoint

$$H^{\dagger} = -\nabla \cdot \Omega + \sigma_1(\boldsymbol{r}, E) - \int_{\Omega'} d\Omega' \sigma_1(\boldsymbol{r}, E, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) + \left[\frac{d}{dE} S(E)\right] - \frac{\partial}{\partial E} S(E)$$

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Forward-Adjoint Formalism

- Plug in H and H† and expand the left side

$$\langle H\varphi, \varphi^{\dagger}\rangle - \langle \varphi, H^{\dagger}\varphi^{\dagger}\rangle = \langle q\varphi^{\dagger}\rangle - \langle \varphi q^{\dagger}\rangle =$$

$$\langle q, \varphi^{\dagger}\rangle - \int_A \int_E \int_{\Omega} \varphi\varphi^{\dagger}(\boldsymbol{\Omega}\cdot\boldsymbol{n})\,d\Omega\,dE\,dA$$

$$+ \int_V \int_{\Omega} \Big[{}_{E_{min}}^{E_{max}} S(E)\varphi(E)\varphi^{\dagger}(E)\Big]\, d\boldsymbol{\Omega}\,dV = \langle \varphi, q^{\dagger}\rangle$$

- Choose $\varphi(E_{min}) = \varphi(E_{max}) = 0$

Transmission Coef for a Slab

For a slab (0 < z < L) with surface source at z = 0

$$\int_E \int_\mu \varphi(L)\varphi^\dagger(L)\mu \, dE d\mu - \int_E \int_\mu \varphi(0)\varphi^\dagger(0)\mu \, dE d\mu$$

$$= \int_z \int_E \int_\mu [\varphi^\dagger(z)q(z) - \varphi(z)q^\dagger(z)] \, d\mu dE dz$$

- The Partial Number Transmission Coefficient is defined

$$J\left(\Delta E^\dagger, \Delta\mu^\dagger\right) = \int_{\Delta E^\dagger,} \int_{\Delta\mu^\dagger} \varphi(L)\mu \, dE d\mu$$

Transmission Coef for a Slab

- Set

$$\varphi^{\dagger}(L) = 1 \text{ for E within } \Delta E^{\dagger} \text{ and, } \mu \text{ within } \Delta\mu^{\dagger}$$
$$= 0 \quad \text{otherwise}$$

- Then

$$\int_{\Delta E}\int_{\Delta\mu} \varphi(0)\varphi^{\dagger}(0)\mu \, dE d\mu = \int_{\Delta E^{\dagger}}\int_{\Delta\mu^{\dagger}} \varphi(L)\mu \, dE d\mu$$

- In terms of currents

$$N\int_{\Delta E}\int_{\Delta\mu} \frac{\psi(0)\psi^{\dagger}(0)}{\mu} dE d\mu = N^{\dagger}J\left(\Delta E^{\dagger}, \Delta\mu^{\dagger}\right)$$

Transmission Coef for a Slab

- Set

$$\varphi^\dagger(L) = 1 \text{ for E within } \Delta E^\dagger \text{ and, } \mu \text{ within } \Delta\mu^\dagger$$
$$= 0 \;\; \text{otherwise}$$

- In terms of currents

$$N \int_{\Delta E} \int_{\Delta\mu} \frac{\psi(0)\psi^\dagger(0)}{\mu} dE d\mu = N^\dagger J(\Delta E^\dagger, \Delta\mu^\dagger)$$

  - Where:

$$N = \left\{\int_{\Delta E} \int_{\Delta\mu} \psi^\dagger(0) dE d\mu\right\}^{-1} \qquad N^\dagger = \left\{\int_{\Delta E^\dagger} \int_{\Delta\mu^\dagger} \psi^\dagger(L) dE d\mu\right\}^{-1}$$

Results

- Results agree well with the forward model
  - Most results agree within 1σ
  - Discrepancies to error in NGP approximation
  - Discrepancies masked with inclusion of angular scattering
- Forward is favorable in calculations with a highly restrictive source (small angle and energy) and distributive response