

Efficient Computation of K-Ratio Profiles in EPMA Using Adjoint Electron Transport

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Adjoint Electron Transport in EPMA

Vision: an efficient computational model for EPMA

Current Approach:

- define a model $\text{🔬}(\text{🍷}) : \{\text{🍷}\} \rightarrow \text{x-ray intens. (e.g. MC or determ.)}$
- loop model $\text{🔬}(\cdot)$ over beam positions \rightarrow expensive

$$\begin{pmatrix} \begin{array}{c} \text{300} \\ \text{250} \\ \text{200} \\ \text{150} \\ \text{100} \\ \text{50} \\ \text{0} \\ \text{-50} \\ \text{-100} \\ \text{-150} \\ \text{-200} \\ \text{-250} \\ \text{-300} \end{array} & \begin{array}{c} \text{300} \\ \text{250} \\ \text{200} \\ \text{150} \\ \text{100} \\ \text{50} \\ \text{0} \\ \text{-50} \\ \text{-100} \\ \text{-150} \\ \text{-200} \\ \text{-250} \\ \text{-300} \end{array} \end{array} \begin{array}{c} \text{mm} \\ \text{mm} \end{array} \right) = \begin{pmatrix} \text{🔬}(\text{🍷}) & \text{🔬}(\text{🍷}) & \dots \\ \text{🔬}(\text{🍷}) & \ddots & \end{pmatrix}$$

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- define a model $\mathcal{M}(\mathbf{y}) : \{\mathbf{y}\} \rightarrow \text{x-ray intens. (e.g. MC or determ.)}$
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$$\begin{pmatrix} \begin{array}{c} \text{mm} \\ \begin{array}{c} 300 \\ 250 \\ 0 \\ -250 \\ -300 \end{array} \\ \begin{array}{c} -500 \quad -250 \quad 0 \quad 250 \quad 500 \\ \text{mm} \end{array} \end{array} \quad \begin{array}{c} \begin{array}{c} 300 \\ 250 \\ 0 \\ -250 \\ -300 \end{array} \\ \begin{array}{c} -500 \quad -250 \quad 0 \quad 250 \quad 500 \\ \text{mm} \end{array} \end{array} \quad \begin{array}{c} \begin{array}{c} 300 \\ 250 \\ 0 \\ -250 \\ -300 \end{array} \\ \begin{array}{c} -500 \quad -250 \quad 0 \quad 250 \quad 500 \\ \text{mm} \end{array} \end{array} \end{pmatrix} = \begin{pmatrix} \begin{array}{c} \text{microscope} \end{array} \begin{array}{c} \begin{array}{c} \text{blue} \\ \text{cup} \end{array} \end{array} \quad \begin{array}{c} \text{microscope} \end{array} \begin{array}{c} \begin{array}{c} \text{blue} \\ \text{cup} \end{array} \end{array} \quad \dots \\ \begin{array}{c} \text{microscope} \end{array} \begin{array}{c} \begin{array}{c} \text{red} \\ \text{cup} \end{array} \end{array} \quad \begin{array}{c} \text{microscope} \end{array} \begin{array}{c} \begin{array}{c} \text{red} \\ \text{cup} \end{array} \end{array} \quad \dots \end{pmatrix}$$

If the model $\mathcal{M}(\cdot)$ is *linear (and bounded)* w.r.t. the beam, then
 → Riesz Representation: *there is a \mathbf{v} such that $\mathcal{M}(\mathbf{u}) = \langle \mathbf{v}, \mathbf{u} \rangle_{\mathcal{H}}$* .





Adjoint Electron Transport in EPMA

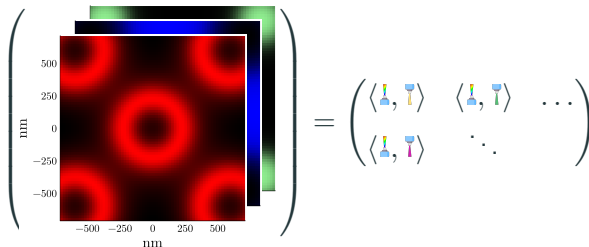






Riesz Representation: *there is a  such that $\mathcal{L}(\text{🍷}) = \langle \text{🍷}, \text{🍷} \rangle_{\{\text{🍷}\}}$.*

Adjoint Electron Transport in EPMA

Riesz Representation: *there is a  such that $\mathcal{A}(\text{) = \langle \text{, \text{} \rangle_{\{\text{$*

Adjoint Approach:

- compute $\text{} = \mathcal{A}^T(\text{)$ [\rightarrow cost comparable to $\mathcal{A}(\text{)$]
- loop $\langle \text{, \cdot \rangle$ over beam positions \rightarrow much cheaper


$$\left(\begin{array}{c} \text{Heatmap} \\ \text{mm} \end{array} \right) = \begin{pmatrix} \langle \text{, \text{} \rangle & \langle \text{, \text{} \rangle & \dots \\ \langle \text{, \text{} \rangle & \ddots & \end{pmatrix}$$

\rightarrow also useful for e.g. 'material derivatives' in inverse modeling

\rightarrow a similar concept accelerates 'training' in AI

[1] Halbleib & Morel (1980). Adjoint Monte Carlo electron transport in the continuous-slowing-down approximation. *Journal of Computational Physics*, 34(2), 211-230.

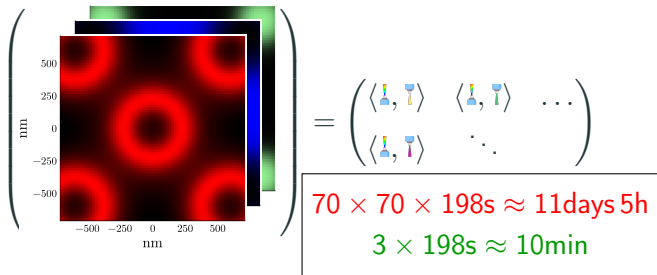
[2] Kuridan (2023). The Adjoint Transport Equation—The Equation of Neutron Importance. In: *Neutron Transport*. Graduate Texts in Physics. Springer, Cham.

Adjoint Electron Transport in EPMA

Riesz Representation: *there is a  such that $\mathcal{A}(\text{red glass}) = \langle \text{blue glass}, \text{red glass} \rangle_{\{\text{red glass}\}}$.*

Adjoint Approach:

- compute $\text{blue glass} = \mathcal{A}^T(\text{red glass})$ [\rightarrow cost comparable to $\mathcal{A}(\text{red glass})$]
- loop $\langle \text{blue glass}, \cdot \rangle$ over beam positions \rightarrow much cheaper


$$\left(\begin{array}{c} \text{500} \\ \text{250} \\ \text{0} \\ \text{-250} \\ \text{-500} \end{array} \begin{array}{c} \text{red glass} \end{array} \begin{array}{c} \text{-500} \\ \text{-250} \\ \text{0} \\ \text{250} \\ \text{500} \end{array} \right) = \begin{pmatrix} \langle \text{blue glass}, \text{red glass} \rangle & \langle \text{blue glass}, \text{red glass} \rangle & \dots \\ \langle \text{blue glass}, \text{red glass} \rangle & \ddots & \end{pmatrix}$$

$$70 \times 70 \times 198\text{s} \approx 11\text{days } 5\text{h}$$
$$3 \times 198\text{s} \approx 10\text{min}$$

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