High-Order Polytopic Discontinuous Galerkin Methods for Radiotherapy Treatment Planning

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Joint work with
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Outline

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- Background
- Boltzmann Problem and DGFEM Discretisation
- Stability and Convergence Analysis
- Implementation Aspects
- Numerical Validation
- Summary and Outlook

Outline

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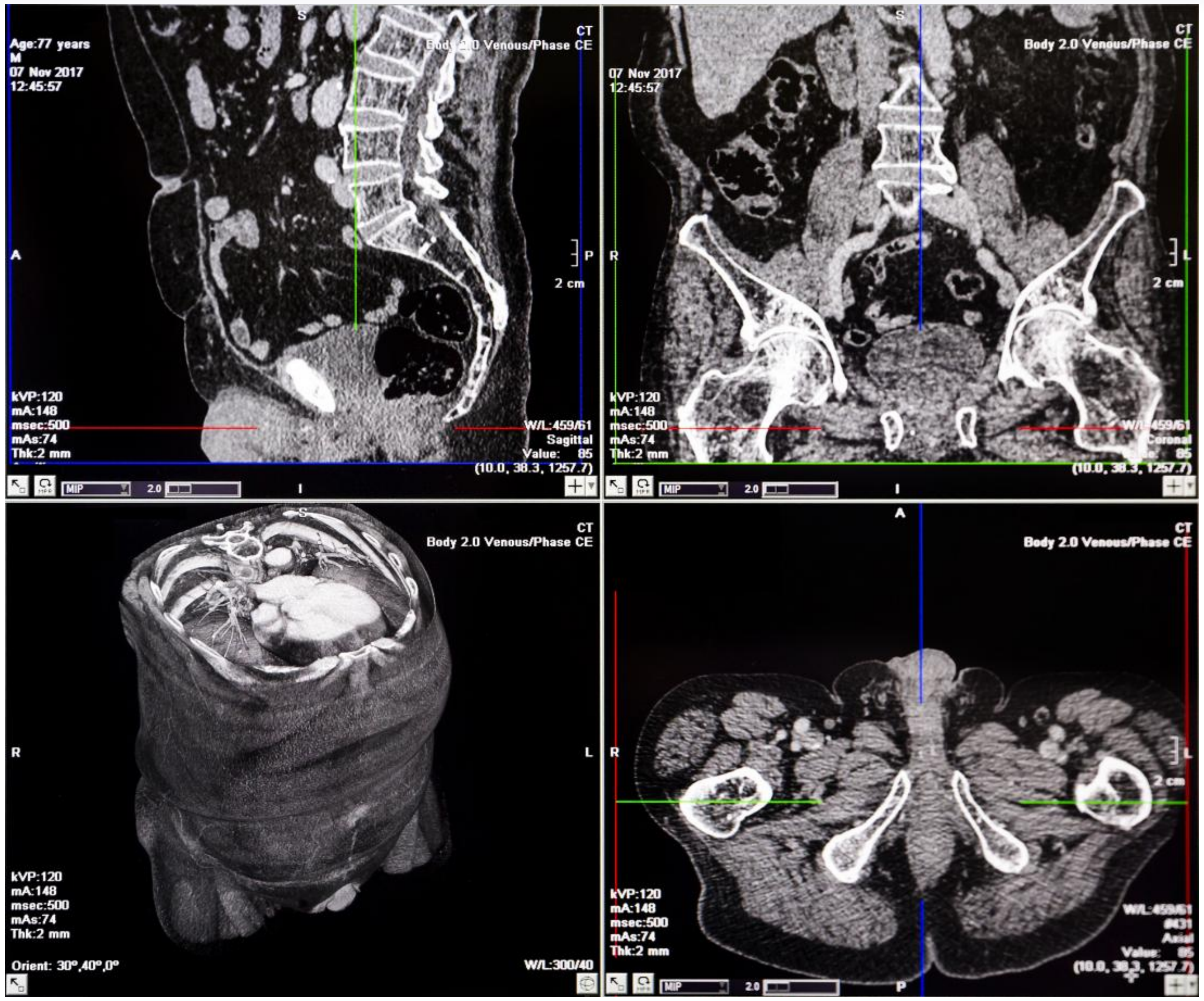
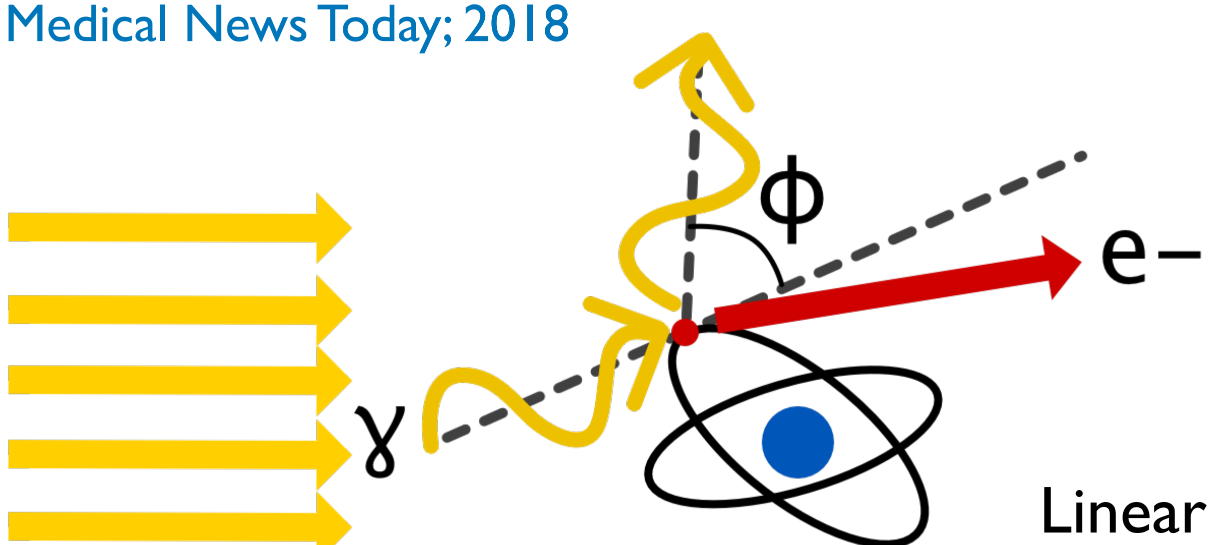
Background



Medical News Today; 2018

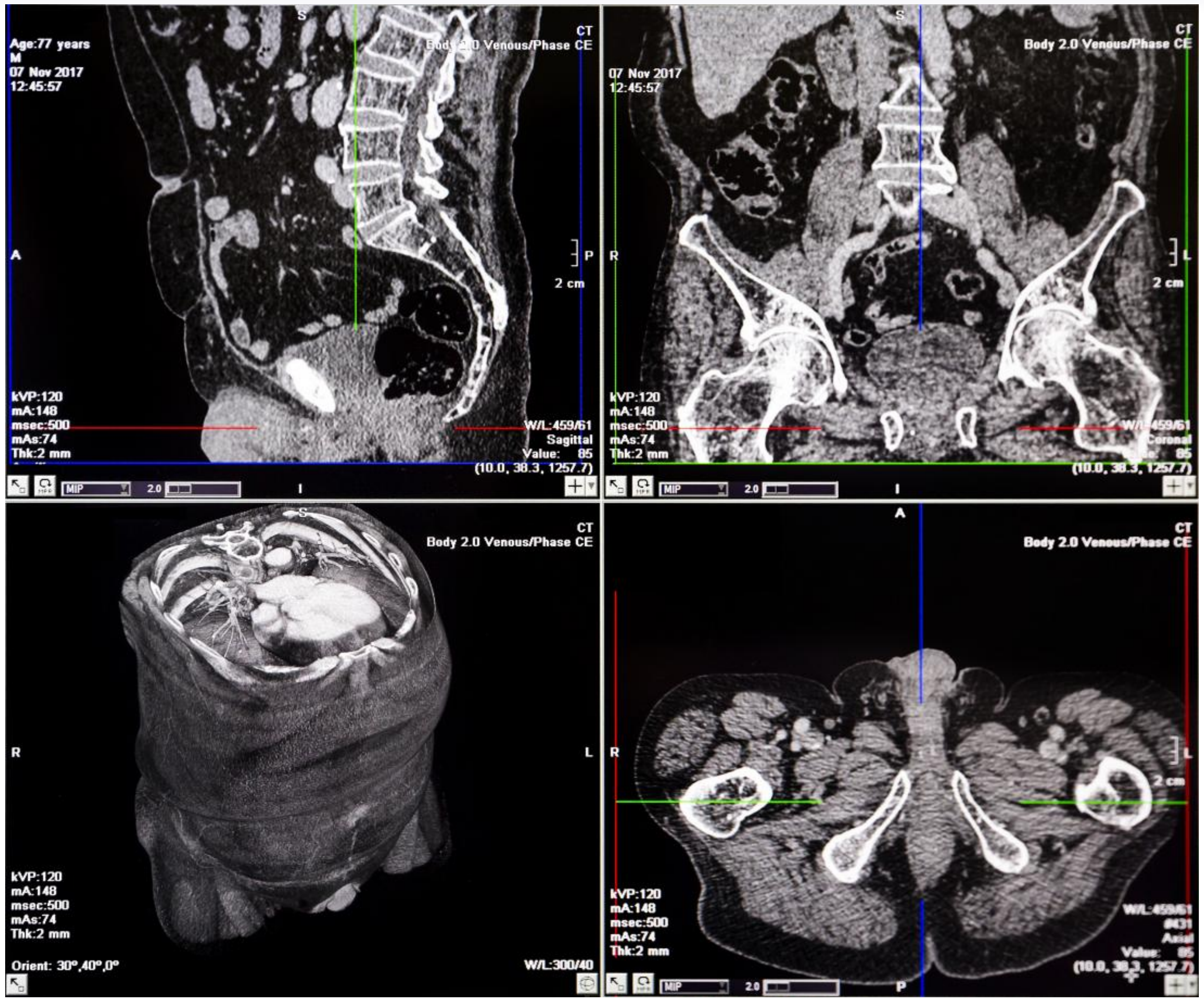
Given a CT scan of a patient and the location of a tumour, optimise the radiotherapy beam placement to:

- Maximise dosage to the tumour
- Minimise dosage to key organs
- 5% error => change in tumour control probability by up to 20%



Linear Particle Accelerator

Radiotherapy Treatment Planning



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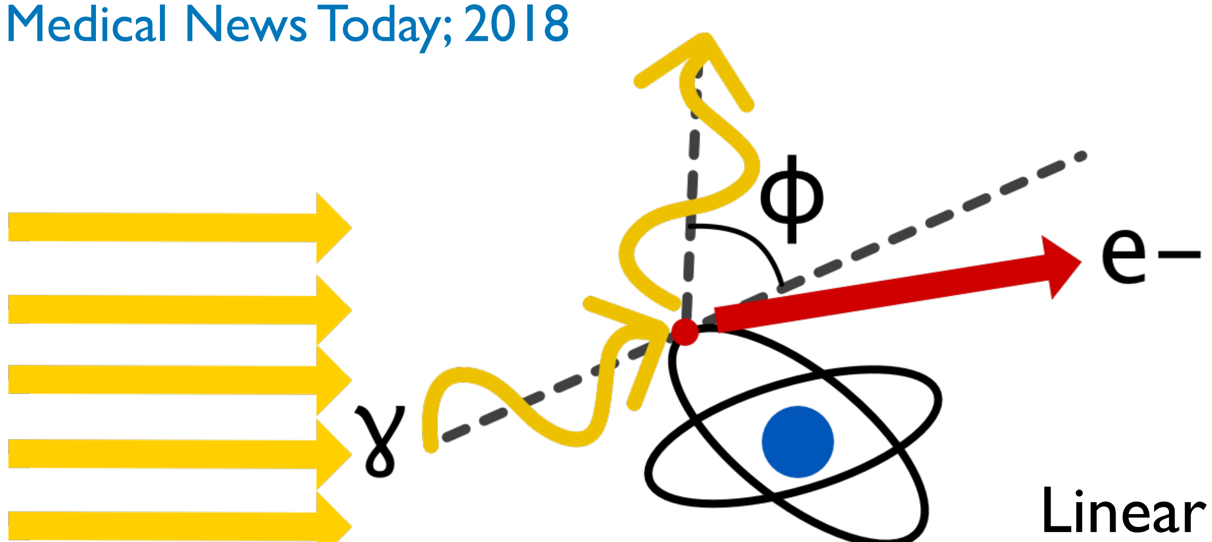
- Pencil beam convolution
- Stochastic Monte Carlo schemes (Slow convergence; complex geometries; heterogeneous tissue)
- Deterministic Boltzmann solvers

➡Varian Acuros system Vassiliev et al. 2010, Bedford; 2019



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Radiotherapy Treatment Planning

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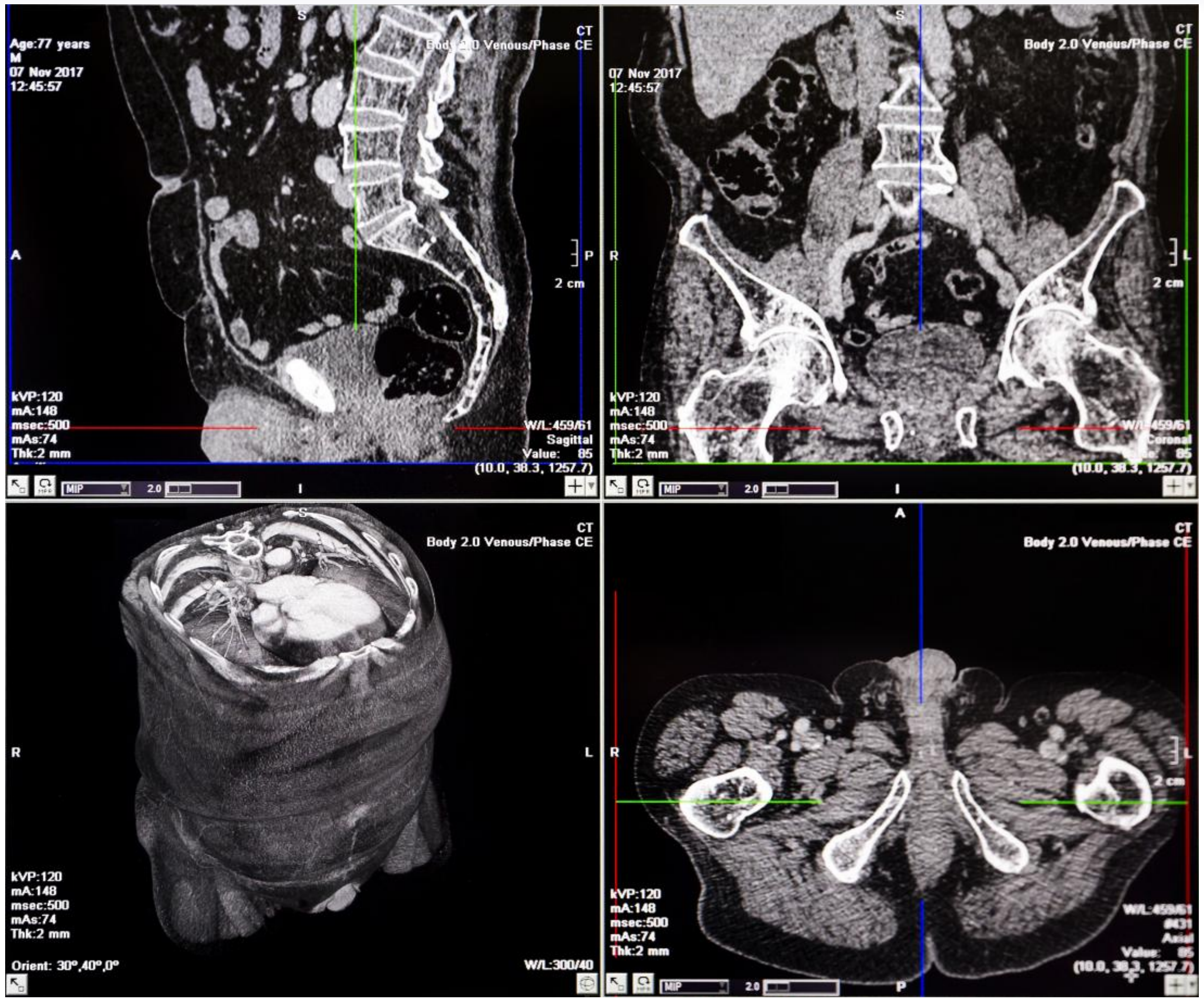

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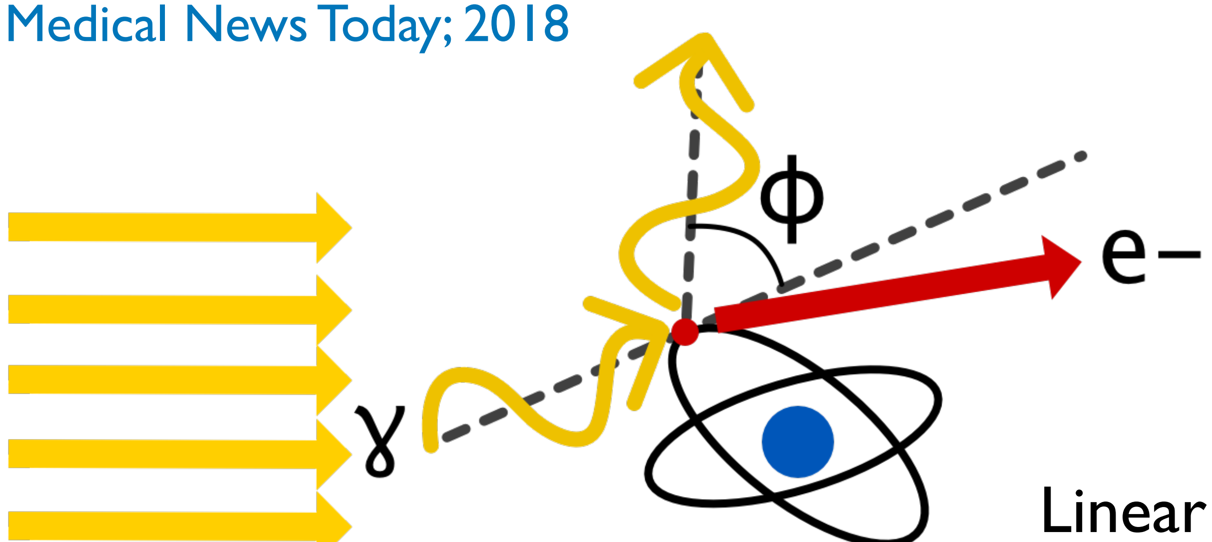
- Monte Carlo vs Deterministic Solvers Borgers 1998, Gifford et al. 2006



Linear Particle Accelerator

Objectives

➡ Develop unified discontinuous Galerkin finite element approximation of the linear Boltzmann problem employing general polytopic meshes in space.

- ✓ Stability and Convergence Analysis
- ✓ Discrete Ordinates Implementation
- ✓ Fast Numerical Integration
- ✓ Development of Robust Solvers

Boltzmann Problem and DGFEM Discretisation

- Space: polytope $\mathbf{x} \in \Omega \subset \mathbb{R}^d$ where $d = 2$ or 3,
- Angle: unit sphere $\boldsymbol{\mu} \in \mathbb{S} = \{\boldsymbol{\mu} \in \mathbb{R}^d$ such that $|\boldsymbol{\mu}| = 1\}$,
- Energy: non-negative reals $E \in \mathbb{E} = \{E \in \mathbb{R}$ with $E \geq 0\}$,
- Full domain: $\mathcal{D} = \Omega \times \mathbb{S} \times \mathbb{E}$
- Inflow boundary: $\Gamma_{\text{in}} = \{(\mathbf{x}, \boldsymbol{\mu}, E) \in \bar{\mathcal{D}} : \mathbf{x} \in \partial\Omega$ and $\boldsymbol{\mu} \cdot \boldsymbol{n} < 0\}$

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Boltzmann Problem

Find $u : \mathcal{D} \to \mathbb{R}$ such that

$$\boldsymbol{\mu} \cdot \nabla_{\mathbf{x}} u(\mathbf{x}, \boldsymbol{\mu}, E) + (\alpha(\mathbf{x}, \boldsymbol{\mu}, E) + \beta(\mathbf{x}, \boldsymbol{\mu}, E))u(\mathbf{x}, \boldsymbol{\mu}, E) = \mathcal{S}[u](\mathbf{x}, \boldsymbol{\mu}, E) + f(\mathbf{x}, \boldsymbol{\mu}, E) \text{ in } \mathcal{D},$$

$$u(\mathbf{x}, \boldsymbol{\mu}, E) = g_{\mathrm{D}}(\mathbf{x}, \boldsymbol{\mu}, E) \text{ on } \Gamma_{\text{in}}.$$

- **Space:** polytope $\mathbf{x} \in \Omega \subset \mathbb{R}^d$ where $d = 2$ or 3,
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Boltzmann Problem

Find $u : \mathcal{D} \to \mathbb{R}$ such that

$$\begin{aligned}\boldsymbol{\mu} \cdot \nabla_{\mathbf{x}} u(\mathbf{x}, \boldsymbol{\mu}, E) + (\alpha(\mathbf{x}, \boldsymbol{\mu}, E) + \beta(\mathbf{x}, \boldsymbol{\mu}, E)) u(\mathbf{x}, \boldsymbol{\mu}, E) &= \mathcal{S}[u](\mathbf{x}, \boldsymbol{\mu}, E) + f(\mathbf{x}, \boldsymbol{\mu}, E) \text{ in } \mathcal{D}, \\ u(\mathbf{x}, \boldsymbol{\mu}, E) &= g_{\mathrm{D}}(\mathbf{x}, \boldsymbol{\mu}, E) \text{ on } \Gamma_{\mathrm{in}}.\end{aligned}$$

Here $f, g_{\mathrm{D}}, \alpha : \mathcal{D} \to \mathbb{R}$ are given data terms, with the scattering operator

$$\mathcal{S}[u](\mathbf{x}, \boldsymbol{\mu}, E) = \int_{\mathbb{E}} \int_{\mathbb{S}} \theta(x, \boldsymbol{\eta} \to \boldsymbol{\mu}, E' \to E) u(\mathbf{x}, \boldsymbol{\eta}, E') \, d\boldsymbol{\eta} \, dE',$$

θ is problem data and $\beta(\mathbf{x}, \boldsymbol{\mu}, E) = \int_{\mathbb{E}} \int_{\mathbb{S}} \theta(x, \boldsymbol{\mu} \to \boldsymbol{\eta}, E \to E') \, d\boldsymbol{\eta} \, dE'$.

Find $u : \mathcal{D} \to \mathbb{R}$ such that

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- $u(\mathbf{x}, \boldsymbol{\mu}, E)$: fluence of particles with energy $E \in \mathbb{E}$, travelling in direction $\boldsymbol{\mu} \in \mathbb{S}$, passing through $\mathbf{x} \in \Omega$.
- $\theta(\mathbf{x}, \boldsymbol{\eta} \to \boldsymbol{\mu}, E' \to E)$: proportion of particles at $\mathbf{x}$ with energy E' travelling in direction $\boldsymbol{\eta}$ which transition to direction $\boldsymbol{\mu}$ and energy E as a result of an instantaneous collision with the medium.
- $\alpha(\mathbf{x}, \boldsymbol{\mu}, E)$: loss of particles absorbed by the medium.
- $\beta(\mathbf{x}, \boldsymbol{\mu}, E)$: loss of particles that are scattered into other directions and energies.

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Find $u : \mathcal{D} \to \mathbb{R}$ such that

$$\boldsymbol{\mu} \cdot \nabla_{\mathbf{x}} u(\mathbf{x}, \boldsymbol{\mu}, E) + (\alpha(\mathbf{x}, \boldsymbol{\mu}, E) + \beta(\mathbf{x}, \boldsymbol{\mu}, E))u(\mathbf{x}, \boldsymbol{\mu}, E) = \mathcal{S}[u](\mathbf{x}, \boldsymbol{\mu}, E) + f(\mathbf{x}, \boldsymbol{\mu}, E) \text{ in } \mathcal{D},$$
$$u(\mathbf{x}, \boldsymbol{\mu}, E) = g_{\mathrm{D}}(\mathbf{x}, \boldsymbol{\mu}, E) \text{ on } \Gamma_{\mathrm{in}}.$$

Assumptions:

- Scattering doesn't gain energy: $\theta(x, \boldsymbol{\eta} \to \boldsymbol{\mu}, E' \to E) = 0$ for $E' < E$.
- Compactly supported data: $supp(f), supp(g_{\mathrm{D}}) \subset \mathbb{E}$.
- Angularly isotropic medium:
  - $\alpha(\mathbf{x}, \boldsymbol{\mu}, E) = \alpha(\mathbf{x}, E)$,
  - $\theta(x, \boldsymbol{\eta} \to \boldsymbol{\mu}, E' \to E) = \theta(x, \boldsymbol{\mu} \cdot \boldsymbol{\eta}, E' \to E)$.
- There exists a constant c_0 such that

$$c(\mathbf{x}, \boldsymbol{\mu}, E) := \alpha(\mathbf{x}, \boldsymbol{\mu}, E) + \frac{1}{2}(\beta(\mathbf{x}, \boldsymbol{\mu}, E) - \gamma(\mathbf{x}, \boldsymbol{\mu}, E)) \geq c_0 > 0,$$

where $\gamma(\mathbf{x}, \boldsymbol{\mu}, E) = \int_{\mathbb{E}} \int_{\mathbb{S}} \theta(\mathbf{x}, \boldsymbol{\eta} \to \boldsymbol{\mu}, E' \to E) \, d\boldsymbol{\eta} \, dE'$.

Energy discretisation

- Multigroup Lewis & Miller 1984

Angular discretisation

- Spherical harmonics in angle (P_N approximation) Spectral Plasma Solver group, Los Alamos, …
- Reformulate as a spatial diffusion problem (simplified P_N approximation) Gelbard, McClarren, …
- Discrete ordinates methods (S_N methods) Chandrasekhar, Carlson, Thurgood, Kanschat, Adams, Ragusa, …
- Wavelet methods Smedley-Stevenson, Dargaville, Pain, …
- Continuous or discontinuous piecewise polynomials or piecewise spherical harmonics Kophazi & Lathouwers 2015, Hall, H., & Murphy 2017, Lau & Adams 2017, Yang 2018, …

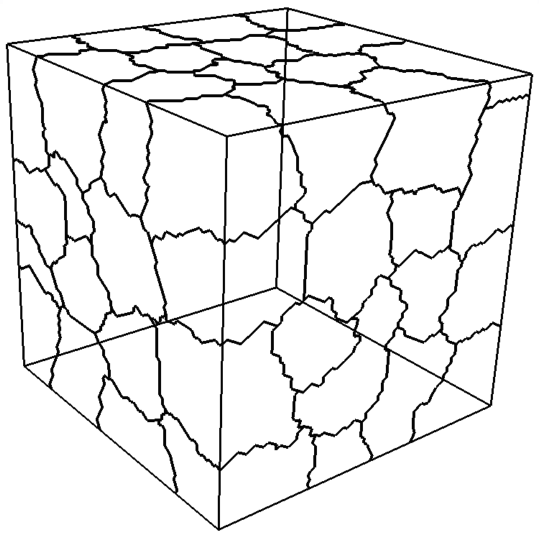
…

Space discretisation

- Finite difference methods (e.g. diamond differences)
- Finite volume methods Adam 1970 …
- Discontinuous Galerkin methods Reed and Hill 1973 …
- Characteristics-based methods Jones, Kunasz, Auer, …

- Space Discretization:
  - Polytopic mesh $\mathcal{T}_\Omega = \{\kappa_\Omega\}$.
  - Discrete Space

$$\mathbb{V}_\Omega^{\mathbf{p}} = \{v \in L^2(\Omega) : v|_{\kappa_\Omega} \in \mathbb{P}_{p_{\kappa_\Omega}}(\kappa_\Omega)\ \forall \kappa_\Omega \in \mathcal{T}_\Omega\}.$$



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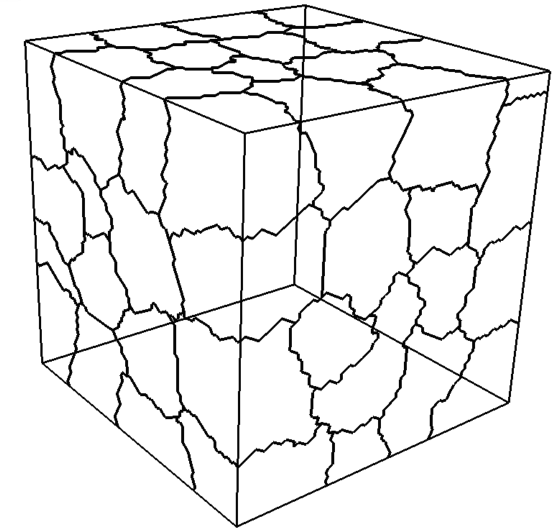
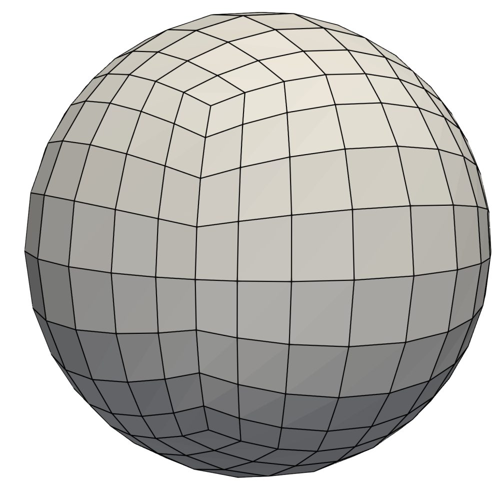


- Angular Discretization:
  - Angle mesh $\mathcal{T}_\mathbb{S} = \{\kappa_\mathbb{S}\}$.
  - Discrete Space

$$\mathbb{V}_\mathbb{S}^{\mathbf{q}} = \{v \in L^2(\mathbb{S}) : v|_{\kappa_\mathbb{S}} \in \mathbb{Q}_{q_{\kappa_\mathbb{S}}}(\kappa_\mathbb{S}) \ \forall \kappa_\mathbb{S} \in \mathcal{T}_\mathbb{S}\}.$$



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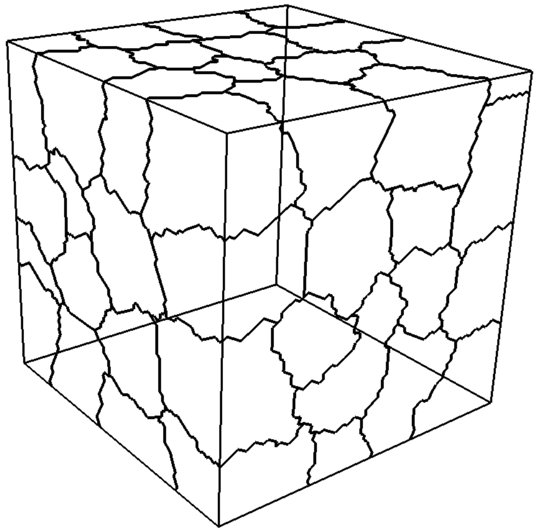

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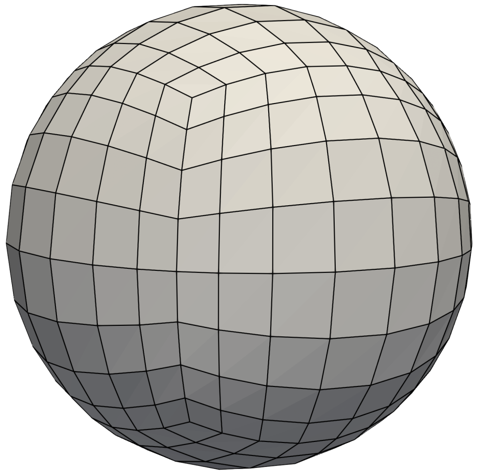

- Energy Discretization:
  - Energy mesh $\mathcal{T}_\mathbb{E} = \{\kappa_g\}$ for $[E_{\min}, E_{\max}]$.
  - Discrete Space

$$\mathbb{V}_\mathbb{E}^{\mathbf{r}} = \{v \in L^2([E_{\min}, E_{\max}]) : v|_{\kappa_g} \in \mathbb{P}_{r_{\kappa_g}}(\kappa_g)\ \ \forall \kappa_g \in \mathcal{T}_\mathbb{E}\}.$$

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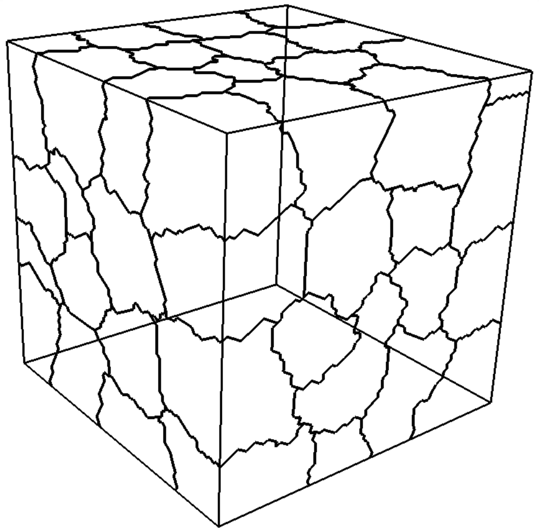

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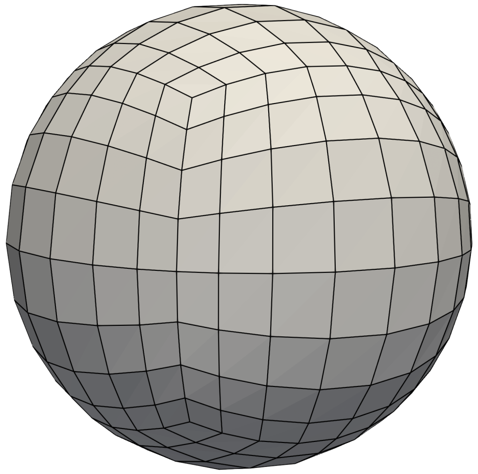

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- Combined DGFEM space: $\mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}} = \mathbb{V}_\Omega^{\mathbf{p}} \otimes \mathbb{V}_\mathbb{S}^{\mathbf{q}} \otimes \mathbb{V}_\mathbb{E}^{\mathbf{r}}$

DGFEM Formulation

- Spatial DGFEM bilinear form and linear functional:

$$a_{\boldsymbol{\mu}}^{E}(w,v) = \sum_{\kappa_\Omega \in \mathcal{T}_\Omega} \int_{\kappa_\Omega} (\boldsymbol{\mu} \cdot \nabla_{\mathbf{x}} wv + (\alpha+\beta)wv)\, d\mathbf{x} - \sum_{\kappa_\Omega \in \mathcal{T}_\Omega} \int_{\partial_- \kappa_\Omega \setminus \partial\Omega} (\boldsymbol{\mu} \cdot \mathbf{n}) \lfloor u \rfloor v^+ \, ds$$

$$- \sum_{\kappa_\Omega \in \mathcal{T}_\Omega} \int_{\partial_- \kappa_\Omega \cap \partial\Omega} (\boldsymbol{\mu} \cdot \mathbf{n}) w^+ v^+ \, ds,$$

$$\ell_{\boldsymbol{\mu}}^{E}(v) = \int_{\Omega} f w \, d\mathbf{x} - \sum_{\kappa_\Omega \in \mathcal{T}_\Omega} \int_{\partial_- \kappa_\Omega \cap \partial\Omega} (\boldsymbol{\mu} \cdot \mathbf{n}) g_{\mathrm{D}} w \, ds.$$

DGFEM Formulation

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$$- \sum_{\kappa_\Omega \in \mathcal{T}_\Omega} \int_{\partial_-\kappa_\Omega \cap \partial\Omega} (\boldsymbol{\mu}\cdot\mathbf{n}) w^+ v^+\,ds,$$
$$\ell_{\boldsymbol{\mu}}^E(v) = \int_\Omega f w\,d\mathbf{x} - \sum_{\kappa_\Omega \in \mathcal{T}_\Omega} \int_{\partial_-\kappa_\Omega \cap \partial\Omega} (\boldsymbol{\mu}\cdot\mathbf{n}) g_{\mathrm{D}} w\,ds.$$

- DGFEM scheme: find $u_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}$ such that

$$b(u_h,v_h) := a(u_h,v_h) - s(u_h,v_h) = \ell(v_h) \quad \forall v_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}},$$

where

$$a(w_h,v_h) = \int_{\mathbb{E}}\int_{\mathbb{S}} a_{\boldsymbol{\mu}}^E(w_h,v_h)\,d\boldsymbol{\mu}\,dE, \quad s(w_h,v_h) = \int_{\mathbb{E}}\int_{\mathbb{S}}\int_\Omega \mathcal{S}[w_h](\mathbf{x},\boldsymbol{\mu},E) v_h\,d\mathbf{x}\,d\boldsymbol{\mu}\,dE,$$
$$\ell(v_h) = \int_{\mathbb{E}}\int_{\mathbb{S}} \ell_{\boldsymbol{\mu}}^E(v_h)\,d\boldsymbol{\mu}\,dE.$$

Stability and Convergence Analysis

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- DGFEM norm:

$$|||v|||_{\mathrm{DG}}^2 = \|\sqrt{c}v\|_{L_2(\mathcal{D})}^2 + \frac{1}{2}\int_{\mathbb{E}}\int_{\mathbb{S}} \sum_{\kappa_\Omega \in \mathcal{T}_\Omega} \left(\|v^+ - v^-\|_{\partial_-\kappa_\Omega \setminus \partial\Omega}^2 + \|v^+\|_{\partial\kappa_\Omega \cap \partial\Omega}^2 \right) d\boldsymbol{\mu}\, dE.$$

where we recall that

$$c(\mathbf{x}, \boldsymbol{\mu}, E) := \alpha(\mathbf{x}, \boldsymbol{\mu}, E) + \frac{1}{2}(\beta(\mathbf{x}, \boldsymbol{\mu}, E) - \gamma(\mathbf{x}, \boldsymbol{\mu}, E)).$$

Lemma (Coercivity)

$$b(v, v) \geq |||v|||_{\mathrm{DG}}^2 \quad \forall v \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}.$$

- Streamline norm:

$$|||v|||_s^2 = |||v|||_{\mathrm{DG}}^2 + \int_{\mathbb{E}} \int_{\mathbb{S}} \sum_{\kappa_\Omega \in \mathcal{T}_\Omega} \tau_{\kappa_\Omega} \|\boldsymbol{\mu} \cdot \nabla_{\mathbf{x}} v\|_{L_2(\kappa_\Omega)}^2 \, d\boldsymbol{\mu} \, dE.$$

Selecting τ_{κ_Ω} as follows:

$$\tau_{\kappa_\Omega} = \frac{h_{\kappa_\Omega}^{\perp}}{p_{\kappa_\Omega}^2},$$

we deduce the following result.

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- Streamline norm:

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we deduce the following result.

Lemma (inf-sup stability)

$$\inf_{v \in \mathbb{V}_h \setminus \{0\}} \sup_{w \in \mathbb{V}_h \setminus \{0\}} \frac{b(v, w)}{|||v|||_s |||w|||_s} \geq \Lambda.$$

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Theorem (H., Hubbard, Radley, Sutton, & Widdowson 2024)

For uniform orders we have that

$$|||u - u_h|||_s \leq C \frac{h^{s-1/2}}{p^{k-1}} \|u\|_{H^k(\mathcal{D})}.$$

for $s = \min\{p+1, k\}$, $k \geq 1$.

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Implementation Aspects

- DGFEM scheme: find $u_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}$ such that

$$\int_{\mathbb{E}} \int_{\mathbb{S}} a_{\boldsymbol{\mu}}^{E}(u_h, v_h)\, d\boldsymbol{\mu}\, dE - \int_{\mathbb{E}} \int_{\mathbb{S}} \int_{\Omega} \mathcal{S}[u_h](\mathbf{x}, \boldsymbol{\mu}, E) v_h \, d\mathbf{x}\, d\boldsymbol{\mu}\, dE = \ell(v_h) \quad \forall v_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}.$$

Implementation

- **DGFEM scheme:** find $u_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}$ such that

$$\int_{\mathbb{E}}\int_{\mathbb{S}} a_{\boldsymbol{\mu}}^{E}(u_h, v_h)\, d\boldsymbol{\mu}\, dE - \int_{\mathbb{E}}\int_{\mathbb{S}}\int_{\Omega} \mathcal{S}[u_h](\mathbf{x}, \boldsymbol{\mu}, E) v_h \, d\mathbf{x}\, d\boldsymbol{\mu}\, dE = \ell(v_h) \quad \forall v_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}.$$

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- **DGFEM scheme:** find $u_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}$ such that

$$\underbrace{\int_{\mathbb{E}}\int_{\mathbb{S}} a_{\mu}^{E}(u_h, v_h)\, d\mu\, dE}_{AU} - \underbrace{\int_{\mathbb{E}}\int_{\mathbb{S}}\int_{\Omega} \mathcal{S}[u_h](\mathbf{x}, \mu, E) v_h\, d\mathbf{x}\, d\mu\, dE}_{SU} = \underbrace{\ell(v_h)}_{F} \quad \forall v_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}.$$

In matrix form, we have: find U such that

$$AU - SU = F$$

➡ S is typically large and dense.

- DGFEM scheme: find $u_h \in \mathbb{V}_h^{\mathbf{p},\mathbf{q},\mathbf{r}}$ such that

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Example: Source iteration (preconditioned Richardson iteration)

Given U^0, find U^n such that

$$AU^n = SU^{n-1} + F, \quad n = 1, 2, \ldots$$

until convergence.

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Theorem (PH, Hubbard, Radley 2024)

The source iteration solution satisfies:

$$|||u_h - u_h^{(n+1)}|||_a \leq \sqrt{q_\beta q_\gamma}\, |||u_h - u_h^{(n)}|||_a$$

for all $n \geq 0$, where

$$q_\beta = \sup_{\mathbf{x}\in\Omega, E\in\mathbb{E}} \frac{\beta(\mathbf{x},E)}{\alpha(\mathbf{x},E)+\beta(\mathbf{x},E)}, \qquad q_\gamma = \sup_{\mathbf{x}\in\Omega, E\in\mathbb{E}} \frac{\gamma(\mathbf{x},E)}{\alpha(\mathbf{x},E)+\beta(\mathbf{x},E)}.$$

Thus, we have the following *a posteriori* solver error bound:

$$|||u_h - u_h^{(n+1)}|||_{DG} \leq \sqrt{r_\gamma}\, ||\sqrt{\beta}(u_h^{(n)} - u_h^{(n+1)})||_{L_2(\mathcal{D})}$$

for all $n \geq 0$, where

$$r_\gamma = \sup_{\mathbf{x}\in\Omega, E\in\mathbb{E}} \frac{\gamma(\mathbf{x},E)}{c(\mathbf{x},E)}.$$

Energy Discretization:

- Divide $\mathbb{E} = [E_{\min}, E_{\max}]$ into *energy groups* $\kappa_g = (E_g, E_{g-1})$ with

$$E_{\max} = E_0 > E_1 > \ldots > E_{N_{\mathbb{E}}-1} > E_{N_{\mathbb{E}}} = E_{\min}.$$

- Assumption on scattering $\left[\theta(\mathbf{x}, \boldsymbol{\mu} \cdot \boldsymbol{\eta}, E' \to E) = 0 \text{ for } E' < E\right]$ implies that $u|_{G_g}$ does not depend on $u|_{G_{g'}}$ for $g' > g$

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Energy & Angular Basis/Quadrature:

- Employ Nodal DGFEM approximation
- Lagrangian basis defined at the Gauss quadrature points (employing $p+1$ points in each direction).
- Discrete ordinates discretization in angle.
- For each energy group, a sequence of uncoupled linear transport problems must be computed for each angular quadrature (ordinate) point.

Algorithm 1 High order multigroup algorithm for the DGFEM scheme

Initialise solution vectors $U^0_{\mu_m,E_l} = 0 \in \Re^{N_\Omega}$ for each angle and energy quadrature point μ_m and E_l

for energy group κ_g with $g \in \{1,\dots,N_\mathbb{E}\}$ **do**

  for source iteration $t \in \{1,\dots,N\}$ **do**

    ▷ *Compute scattering*

    for (PAR) Energy quadrature points $E_l \in \texttt{GaussLegendre}(\kappa_g, r_{\kappa_g}+1)$ **do**

      for (PAR) Angular quadrature points $\mu_m \in \bigcup_{\kappa_\mathbb{S}\in\mathcal{T}_\mathbb{S}} \texttt{GaussLegendre}(\kappa_\mathbb{S}, q_{\kappa_\mathbb{S}}+1)$ **do**

        Evaluate scattering: $S^E_{\boldsymbol{\mu}} \in \Re^{N_\Omega}$, $(S^E_{\boldsymbol{\mu}})_i = s(u_h^{t-1}, \varphi^i_\Omega\varphi^l_g\varphi^m_{\kappa_\mathbb{S}})$

    ▷ *Compute streaming*

    for (PAR) Energy quadrature points $E_l \in \texttt{GaussLegendre}(\kappa_g, r_{\kappa_g}+1)$ **do**

      for (PAR) Angular quadrature points $\mu_m \in \bigcup_{\kappa_\mathbb{S}\in\mathcal{T}_\mathbb{S}} \texttt{GaussLegendre}(\kappa_\mathbb{S}, q_{\kappa_\mathbb{S}}+1)$ **do**

$$\text{Assemble}\begin{cases}\text{transport matrix} & A^E_{\boldsymbol{\mu}} \in \Re^{N_\Omega\times N_\Omega} \text{ with } (A^E_{\boldsymbol{\mu}})_{i,j} = a^E_{\boldsymbol{\mu}}(\varphi^i_\Omega, \varphi^j_\Omega),\\ \text{source vector} & F^E_{\boldsymbol{\mu}} \in \Re^{N_\Omega} \text{ with } (F^E_{\boldsymbol{\mu}})_i = \ell^E_{\boldsymbol{\mu}}(\varphi^i_\Omega\varphi^l_g\varphi^m_{\kappa_\mathbb{S}}).\end{cases}$$

        Solve $A^E_{\boldsymbol{\mu}} U^t_{\mu_m,E_l} = \texttt{weight}(E)^{-1}\texttt{weight}(\boldsymbol{\mu})^{-1}(F^E_{\boldsymbol{\mu}} + S^E_{\boldsymbol{\mu}})$

Output: Angular flux vectors $U^t_{\mu_m,E_l}$ for each μ_m, E_l.

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Spatial Discretization:

- Apply Tarjan's strongly connected components algorithm.

Tarjan 1972, Hall, H, & Murphy 2017

- Matrix free implementation.

- Quadrature free evaluation of integrals over general polytopes.

Lasserre 1998, Chin, Lasserre, & Sukumar 2015, Antonietti, H., & Pennesi 2018,
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$\Rightarrow$ Highly parallelizable efficient algorithm

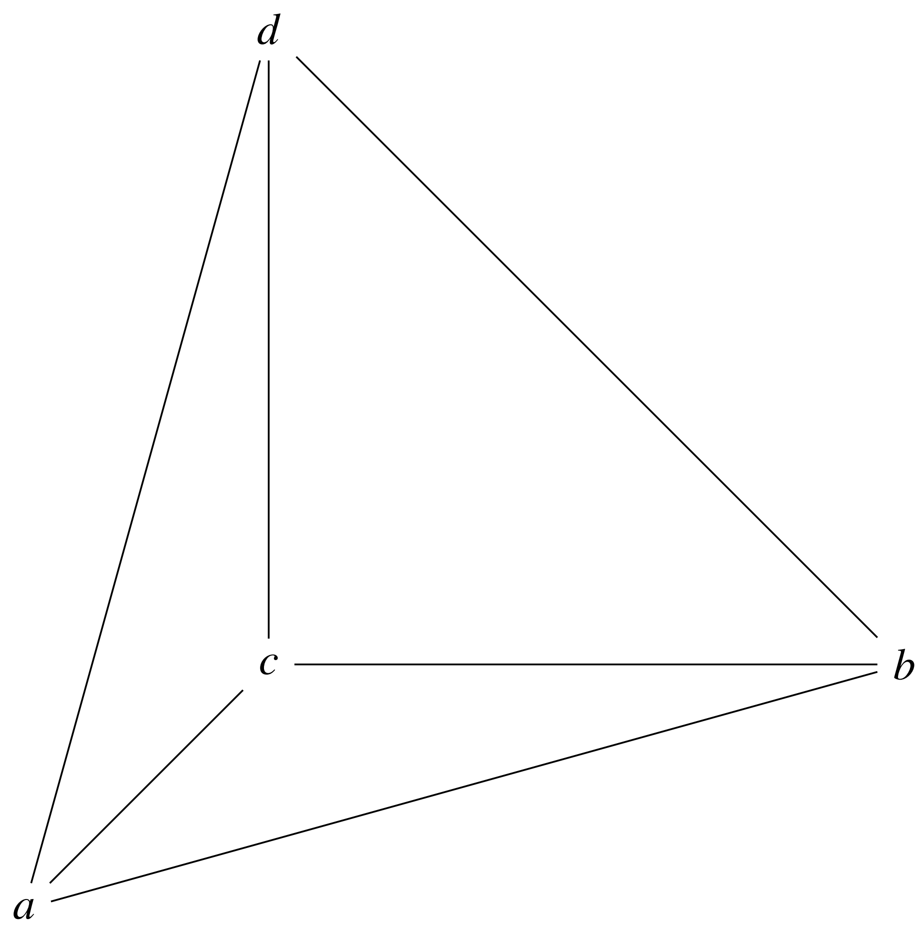
Quadrature Free Implementation

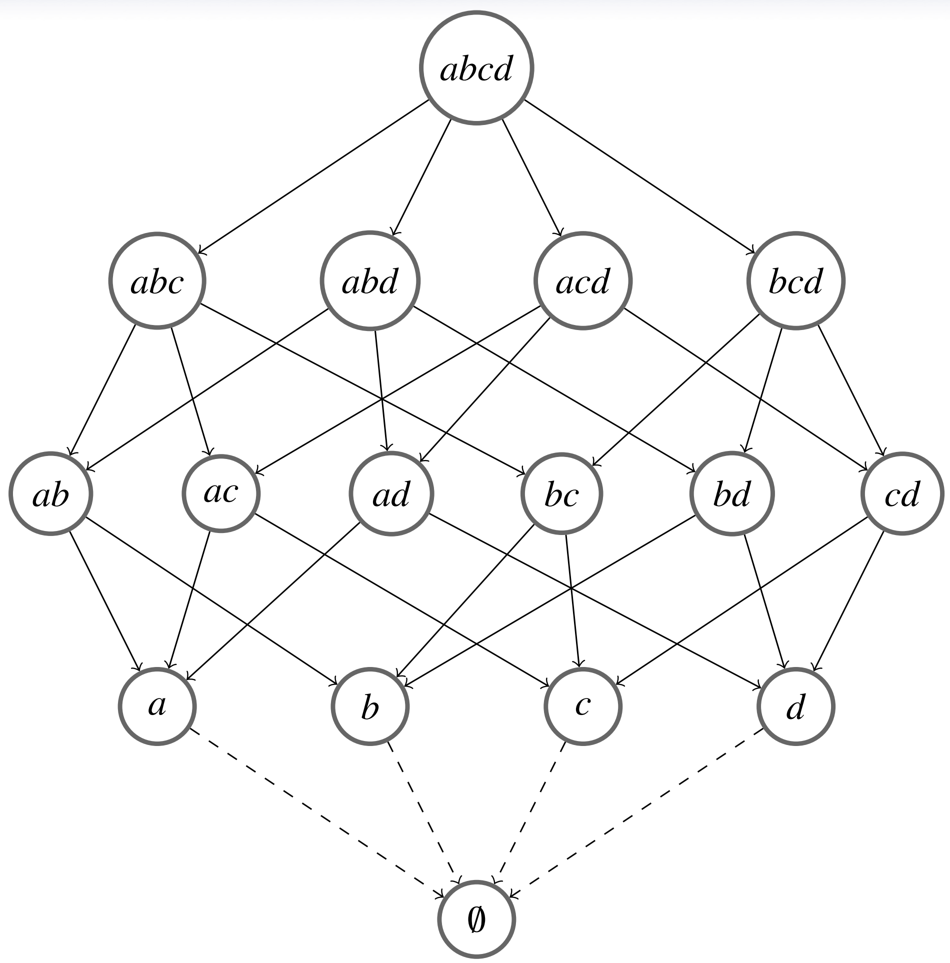
- $f : \mathcal{F} \to \mathbb{R}$ denotes a *(positively) homogeneous function* of degree $q \in \mathbb{R}$.
- $\mathcal{F}$ is a k-dimensional facet, $0 \leq k \leq d$, with $\partial\mathcal{F} = \{\partial\mathcal{F}_i\}_{i=1}^{m(\mathcal{F})}$.
- $\mathbf{x}_\mathcal{F}$ is an arbitrary point contained in $\mathcal{F}$ (or the k-dimensional hyperplane containing $\mathcal{F}$).

$$\int_\mathcal{F} f(\mathbf{x})\, ds = \frac{1}{\dim \mathcal{F} + q} \left[\sum_{i=1}^{m(\mathcal{F})} \mathrm{dist}(\partial\mathcal{F}_i, \mathbf{x}_\mathcal{F}) \int_{\partial\mathcal{F}_i} f(\mathbf{x})\, d\xi + \int_\mathcal{F} \mathbf{x}_\mathcal{F} \cdot \nabla f(\mathbf{x})\, ds \right]$$

Lasserre 1998, Chin, Lasserre, & Sukumar 2015, Antonietti, H., & Pennesi 2018, Radley, H., & Hubbard 2024

Quadrature Free Implementation: Effects of Pruning





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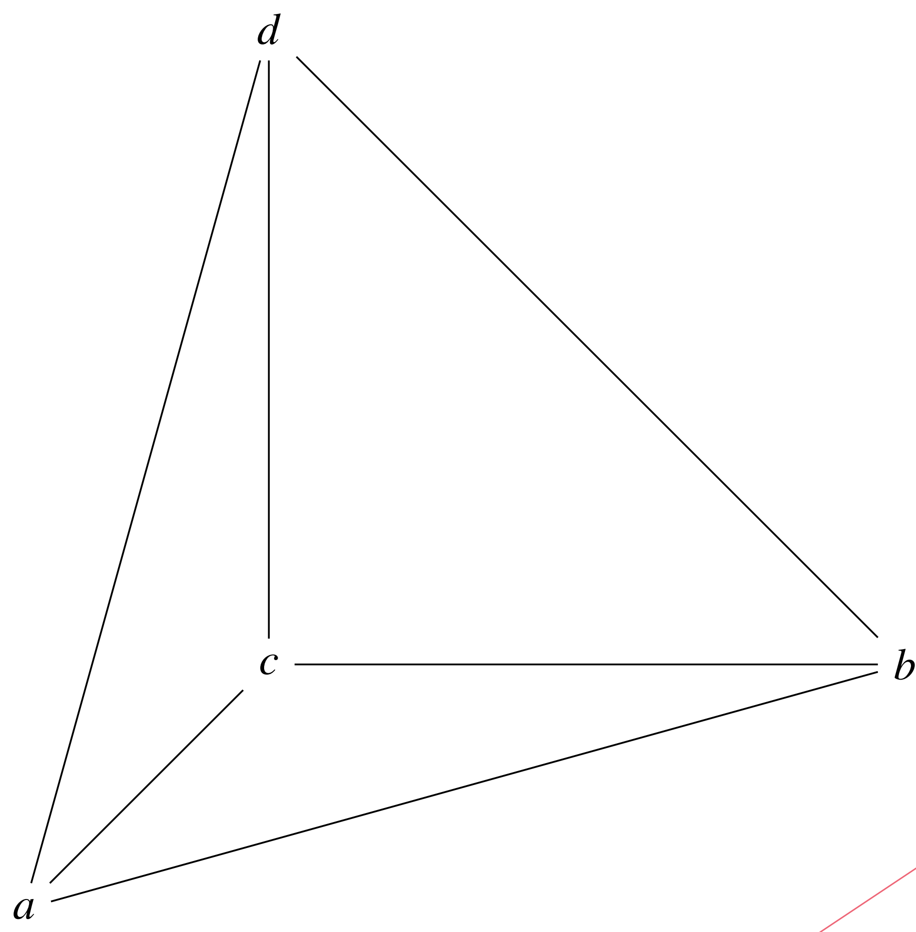
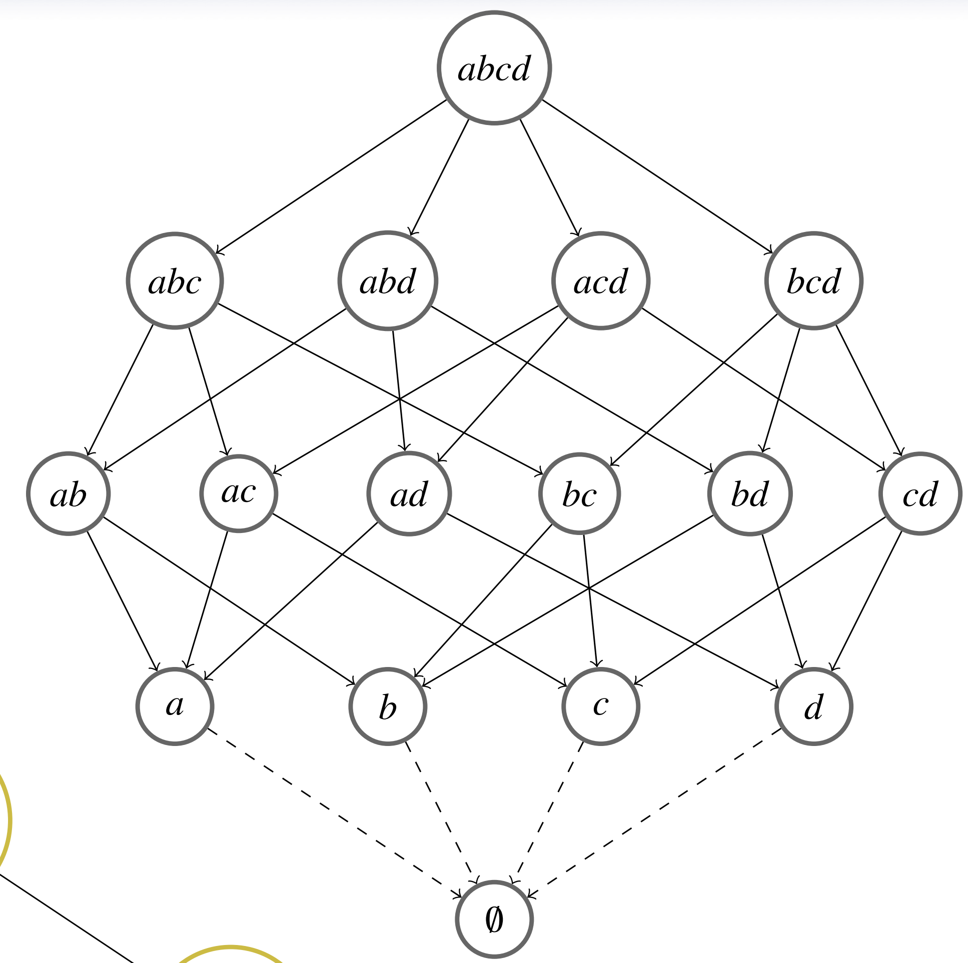
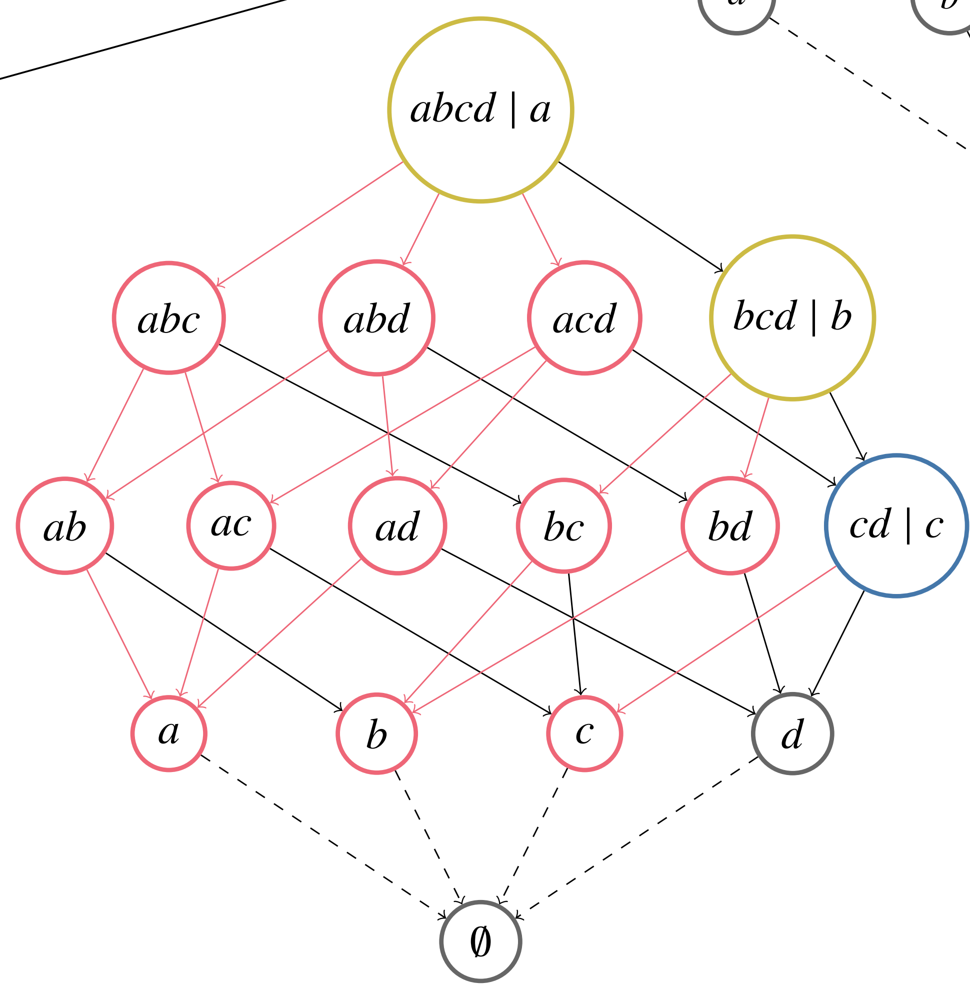






Numerical Validation

Example: Compton Scattering in Water

[2 Spatial dimensions + 1 angular dimension + 1 energy dimension]

- Let $\Omega = (0, 1)^2$ (in units of m) and $\mathbb{E} = (500\text{keV}, 1000\text{keV})$.
- Macroscopic total absorption cross-section: $\alpha = 0$.
- Differential scattering cross-section:

$$\theta(\mathbf{x}, \boldsymbol{\mu}' \to \boldsymbol{\mu}, E' \to E) = \rho(\mathbf{x})\sigma_{KN}(E', E, \boldsymbol{\mu}\cdot\boldsymbol{\mu}')\delta(F(E', E, \boldsymbol{\mu}\cdot\boldsymbol{\mu}')),$$

where $\rho(\mathbf{x}) \approx 3.34281 \times 10^{29}\text{e/m}^3$ is the electron density of water.

- Here, σ_{KN} is the Klein-Nishina differential scattering cross-section defined by

$$\sigma_{KN}(E, E', \cos\phi) = \frac{1}{2}r_e^2\left(\frac{E'}{E}\right)^2\left(\frac{E'}{E} + \frac{E}{E'} - \sin^2\phi\right),$$

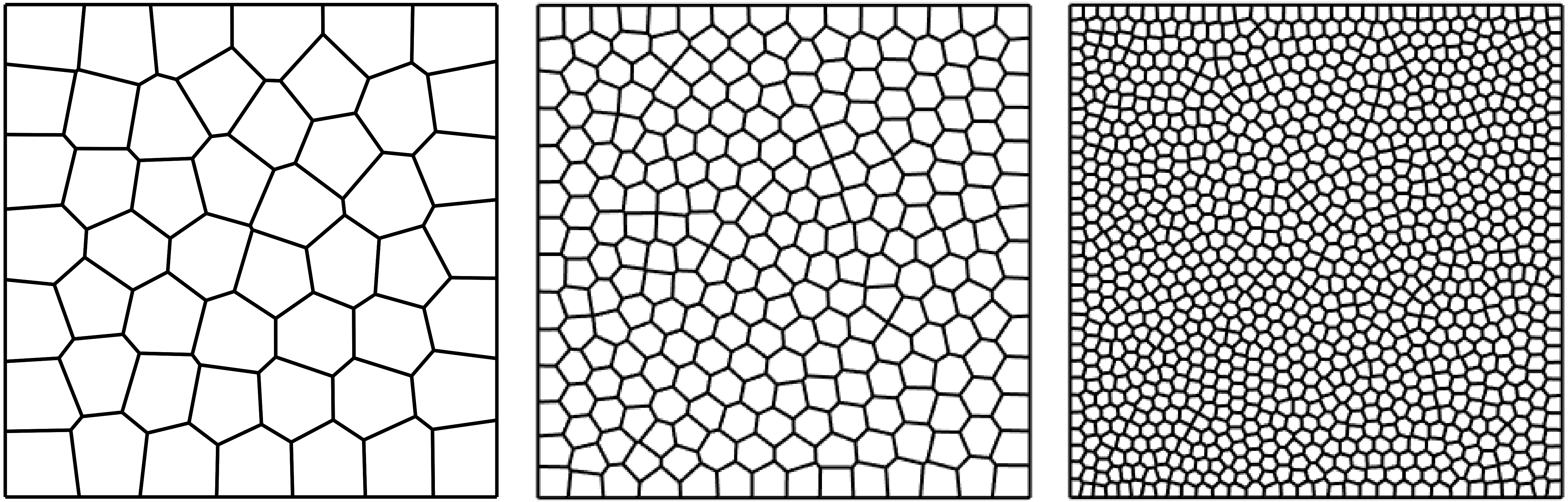
with $r_e \approx 2.81794 \times 10^{-15}\text{m}$ and $F(E, E', \cos\phi) = E' - \frac{E}{1+\frac{E}{511}(1-\cos\phi)}$.

- Finally, f and g_{D} are selected so that

$$u(\mathbf{x}, \boldsymbol{\mu}, E) = \mathrm{e}^{-(E\boldsymbol{\mu}\cdot\mathbf{x}/E_{max})^2}\,\mathrm{e}^{-(1-(E/E_{max})^2)^{-1}}.$$

Arthur Holly Compton; Peter Debye (1923)

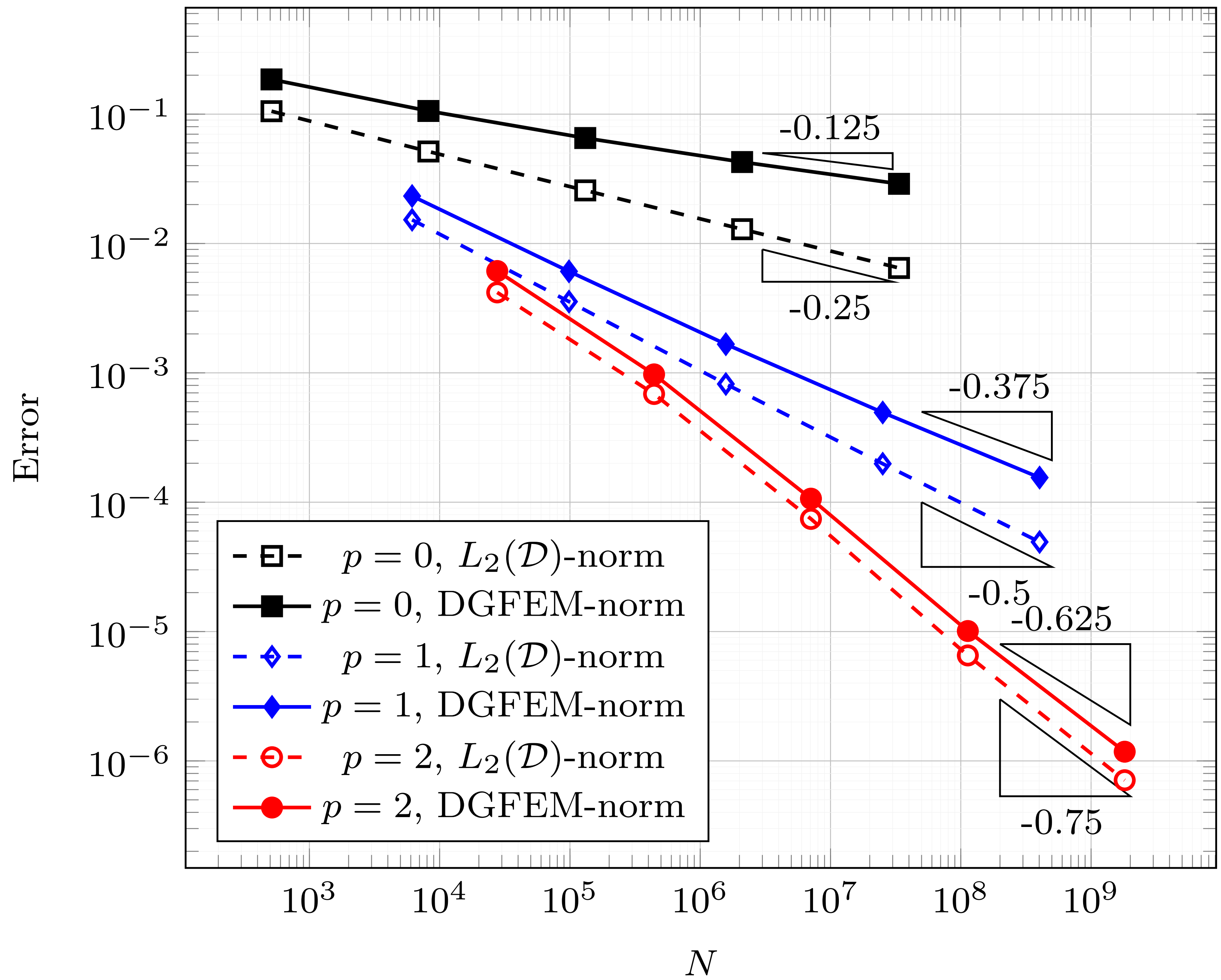
Example: Compton Scattering in Water



Polymesher; Talischi *et al.* 2012

Example: Compton Scattering in Water

[2 Spatial dimensions + 1 angular dimension + 1 energy dimension]



$[h \sim N^{-1/4}]$

Source Iteration vs GMRES (Fixed Tolerance per Energy Group)

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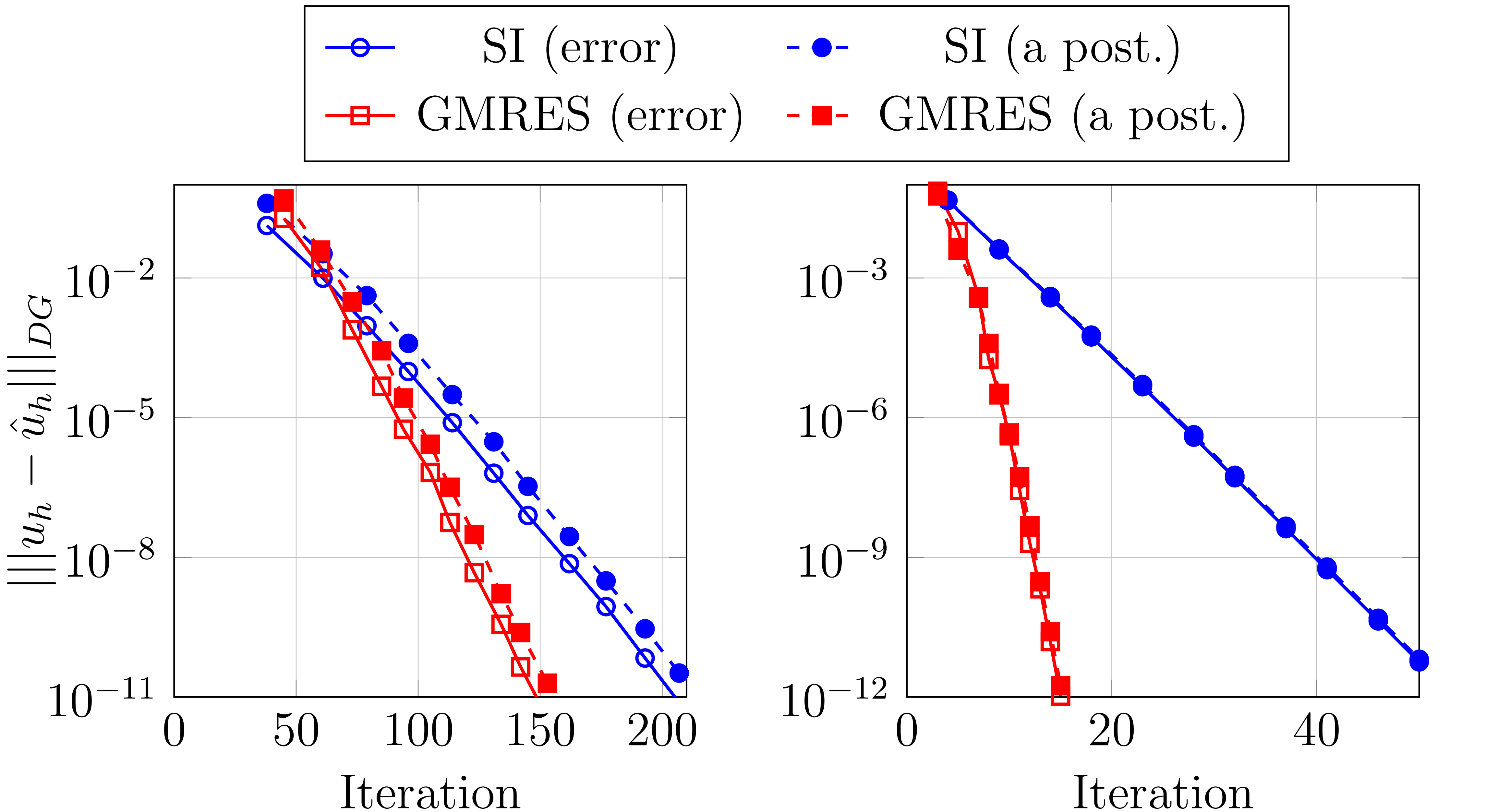
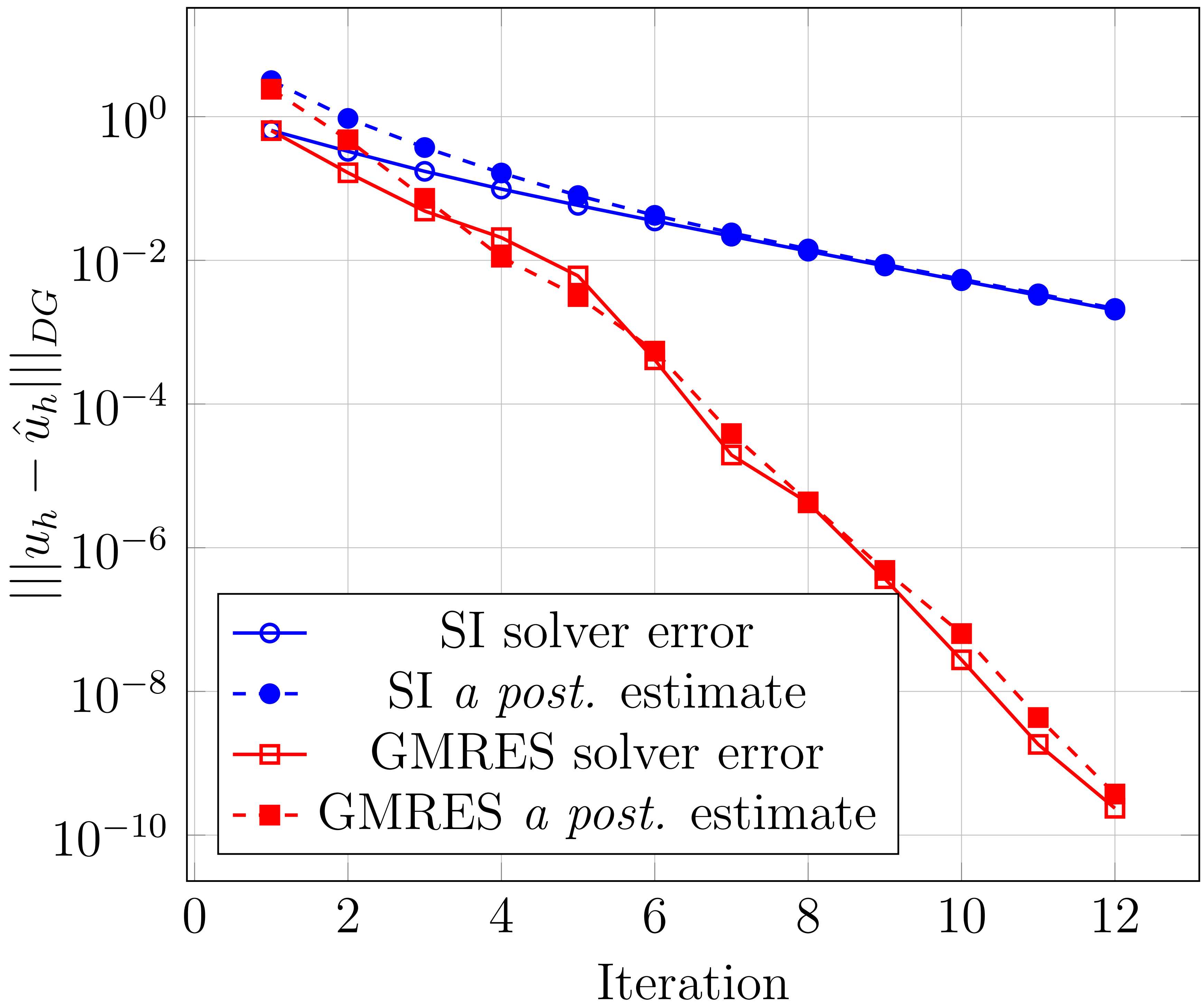


Full Energy Range

Lowest Energy Group

Source Iteration vs GMRES (Fixed No Itns per Energy Group)



Source Iteration vs GMRES (Mesh Dependence)

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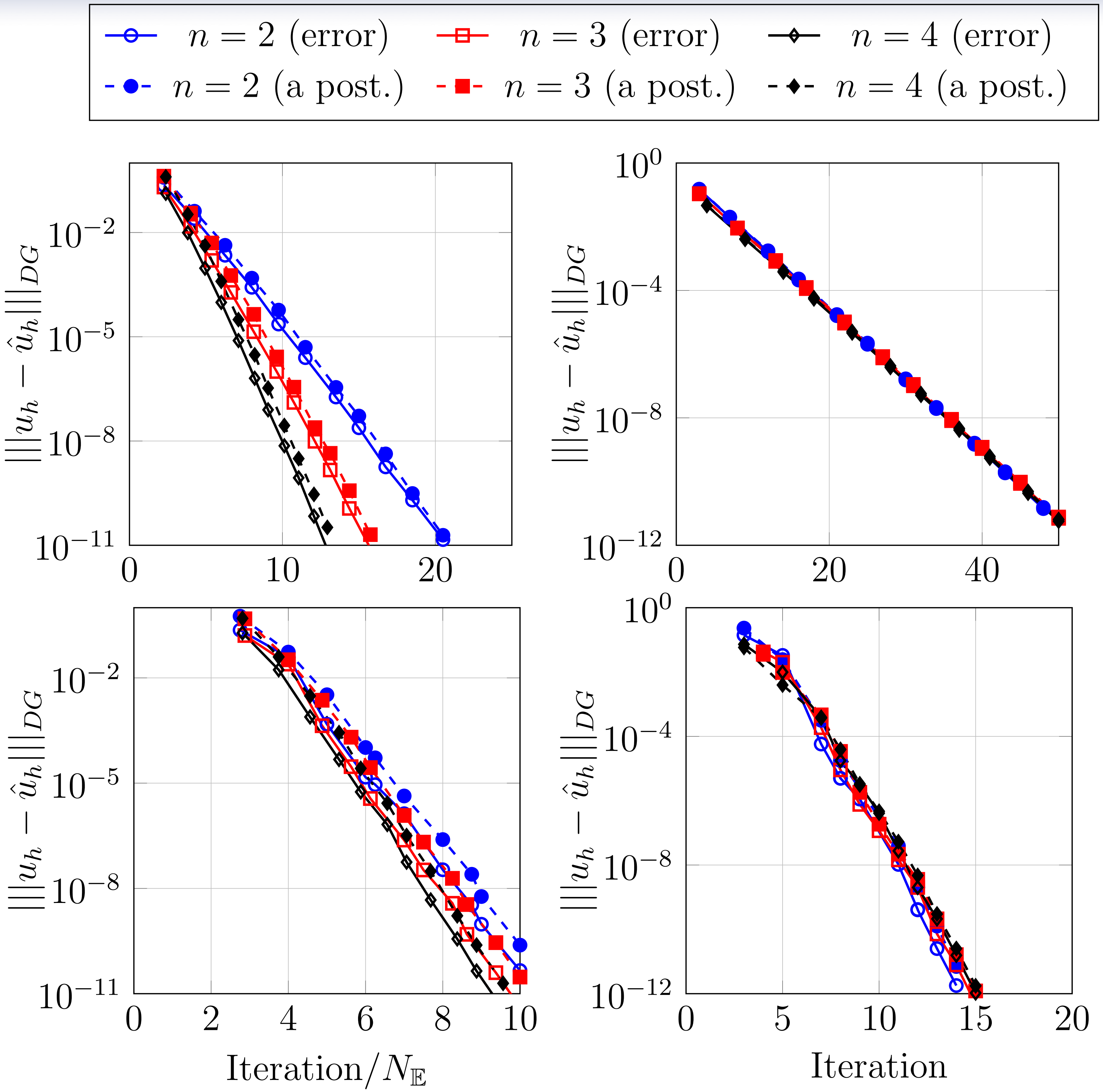
Source Iteration

GMRES



Full Energy Range **Lowest Energy Group**

Source Iteration vs GMRES (p-Dependence)

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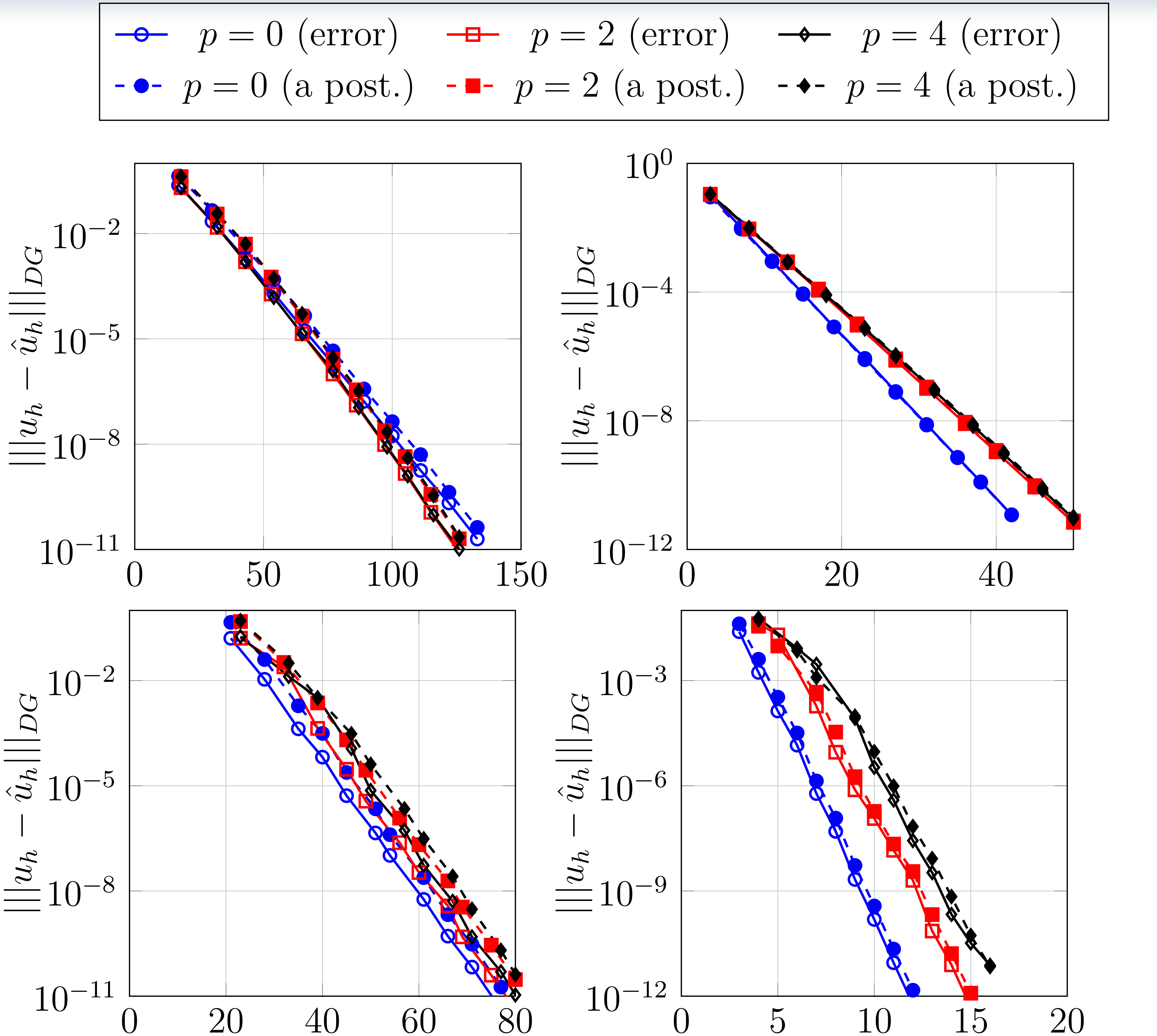


Source Iteration

GMRES

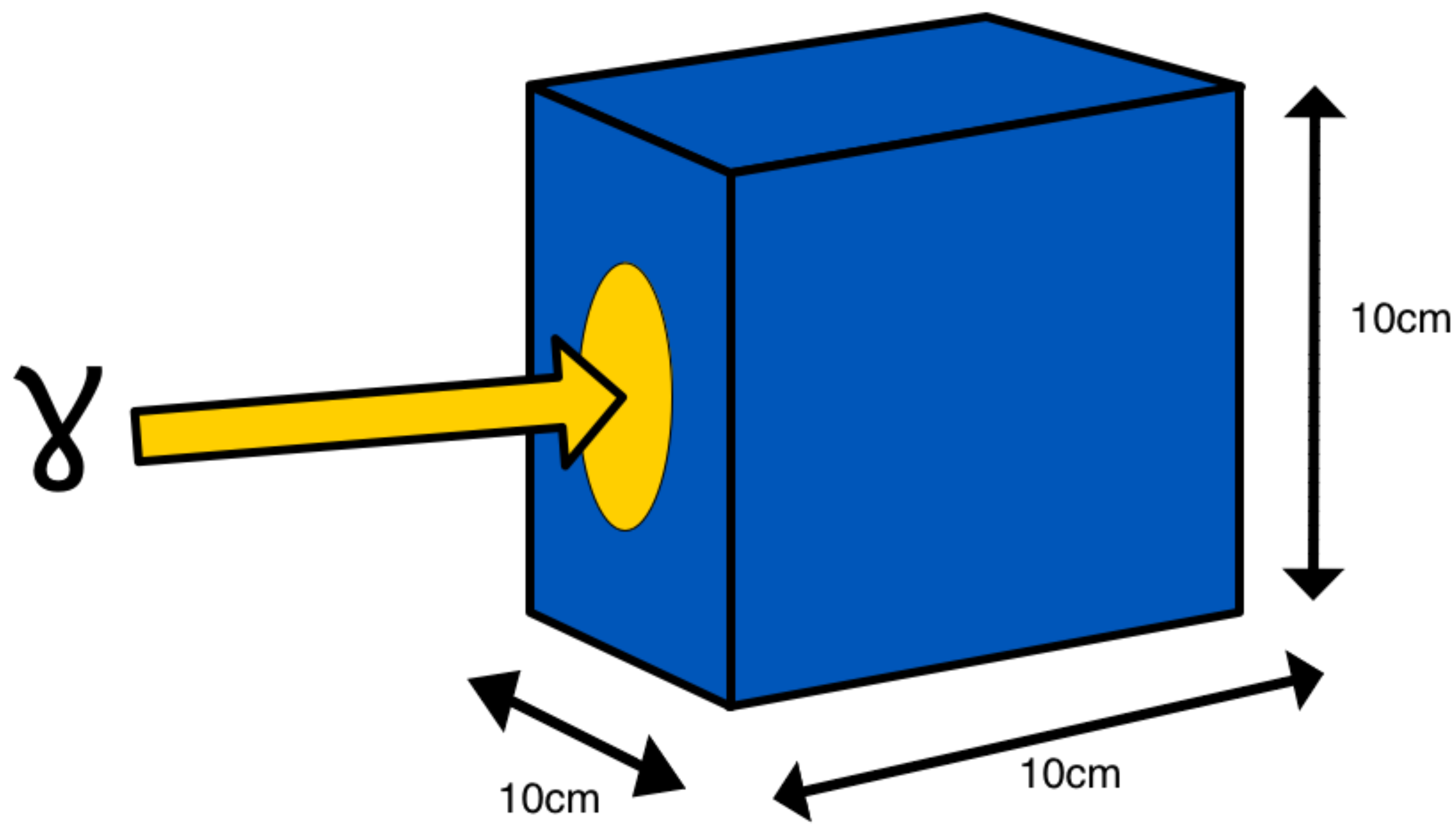
Full Energy Range

Lowest Energy Group

[3 Spatial dimensions + 2 angular dimensions + 1 energy dimension]

Radiation beam into 10cm x10cm x10cm cube of water

- 5cm circular cross section
- Gaussian energy profile (mean 800keV, fwhm 200keV)
- Gaussian(Von Mises-Fisher) angular distribution
- Compton scattering



Example: Physical Problem

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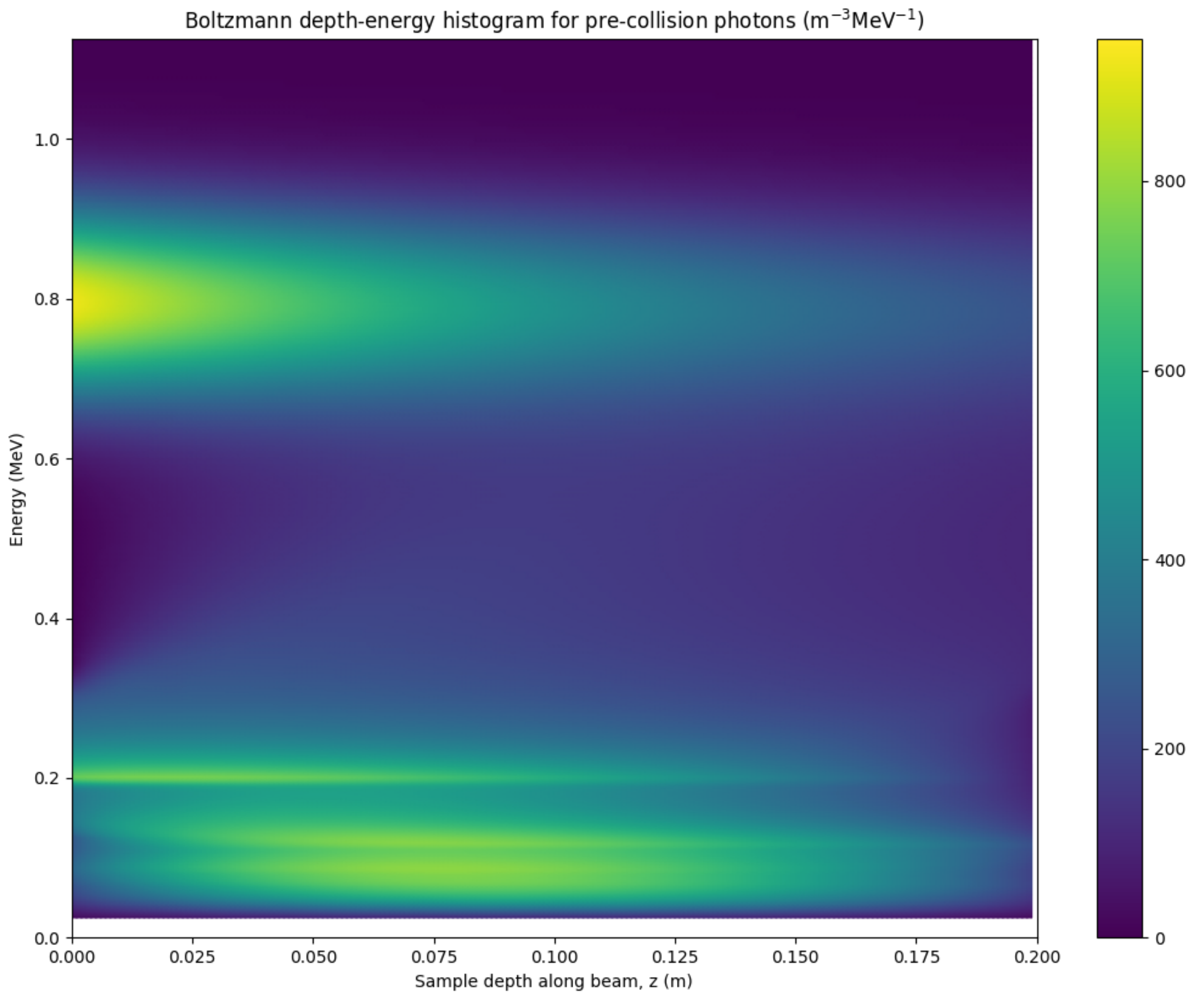
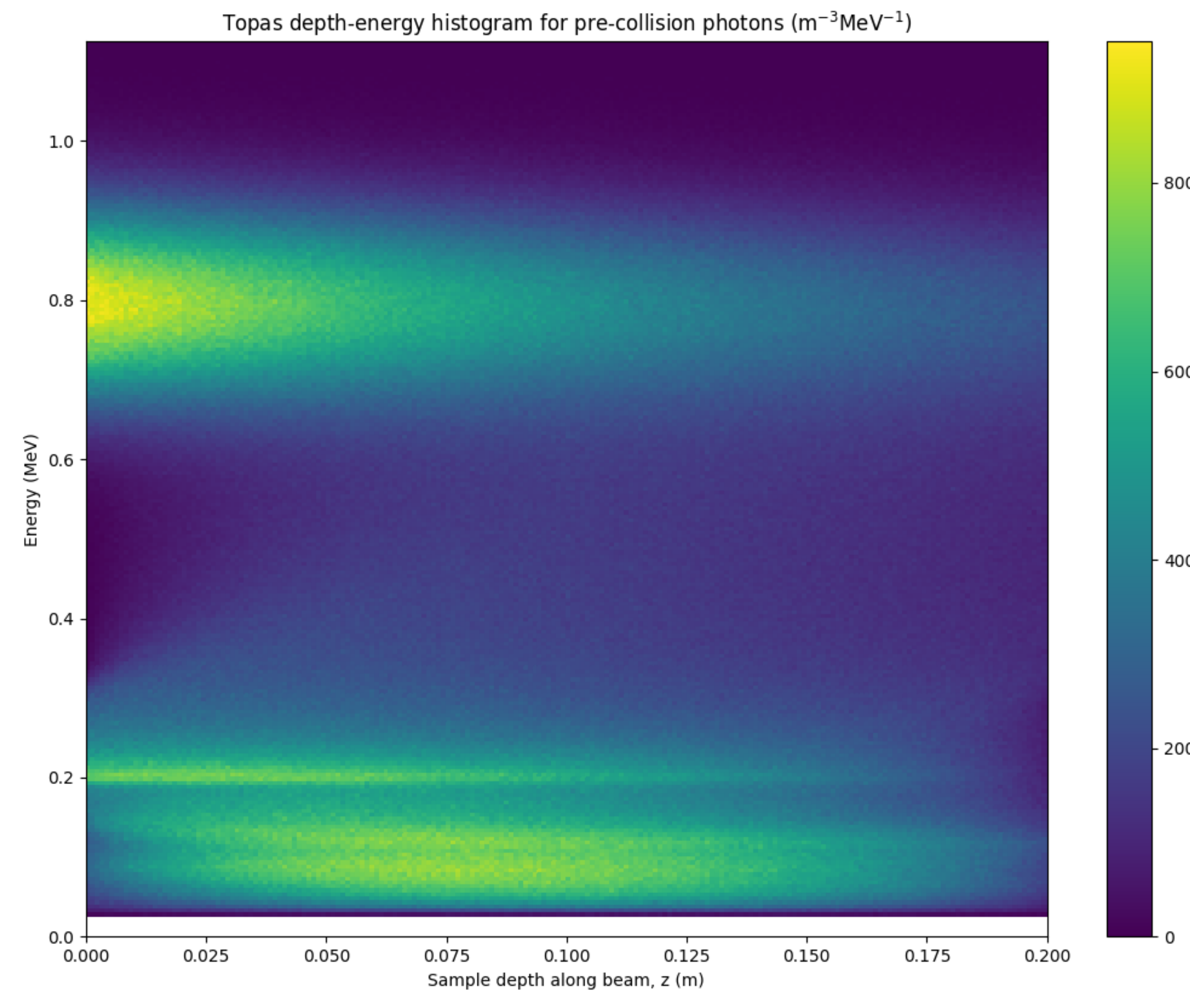
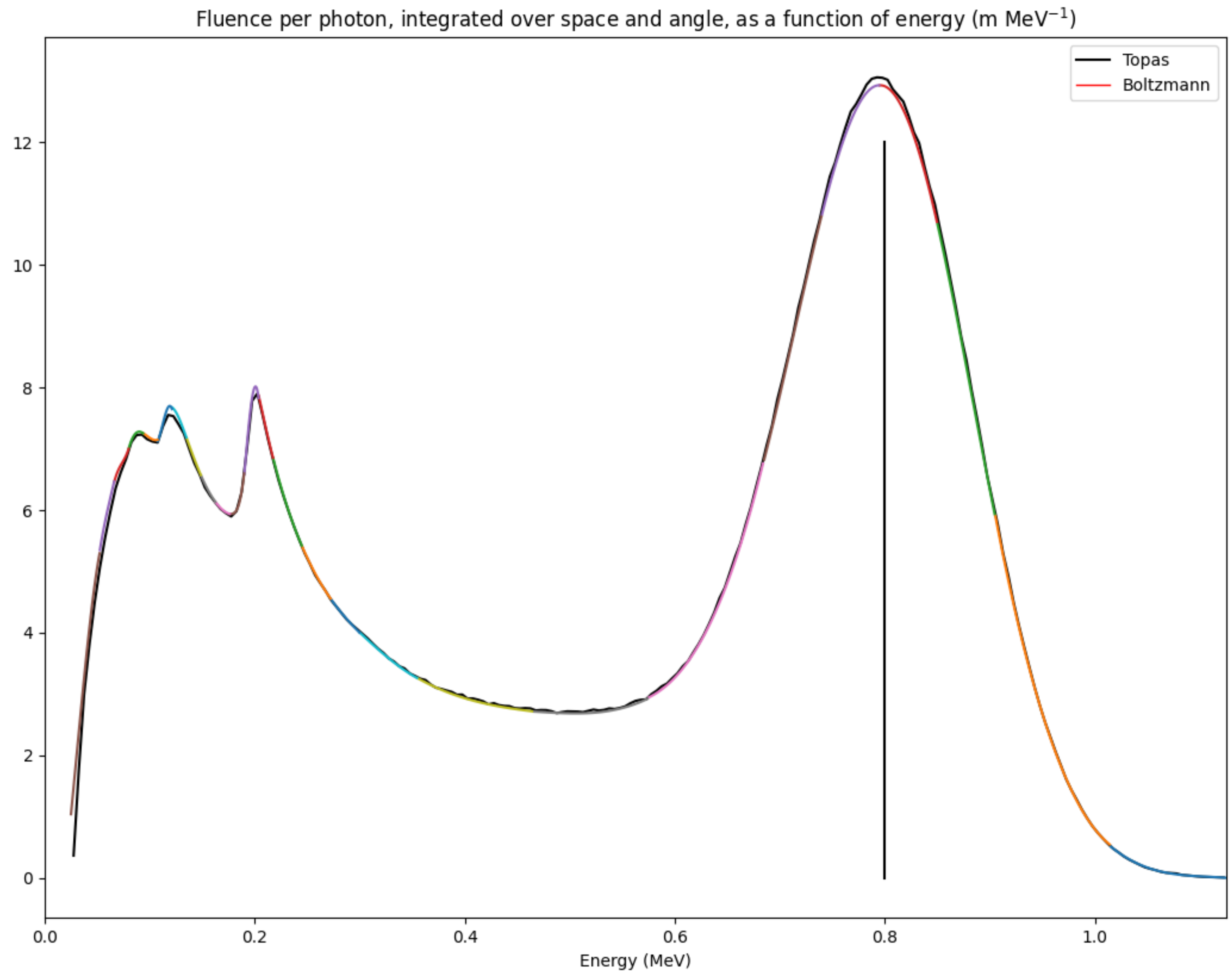


Boltzmann (DGFEM)



Monte Carlo (Topas MC)

Example: Physical Problem



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Summary and Outlook

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- Proposed DGFEM:
  - ☑ Generalization of existing schemes;
  - ☑ Handle complex geometric features in the spatial domain;
  - ☑ Method naturally admits high-order polynomial orders;
  - ☑ New stability and convergence results;
  - ☑ Simple algorithmic structure;
  - ☑ Source iteration convergent independent of the mesh parameters;
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- Extensions:
  - Incorporate additional radiotherapy physics (electrons);
  - Dosage calculations;
  - A posteriori error estimation and mesh adaptation;
  - Further validation against Monte Carlo schemes.

References

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