On accelerated iterative schemes for neutron transport using residual minimization

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NWO

Outline

Introduction

The transport equation and main theoretical result

Convergence analysis for a weak formulation

Numerical realization via Galerkin approximation

Numerical tests

Conclusions

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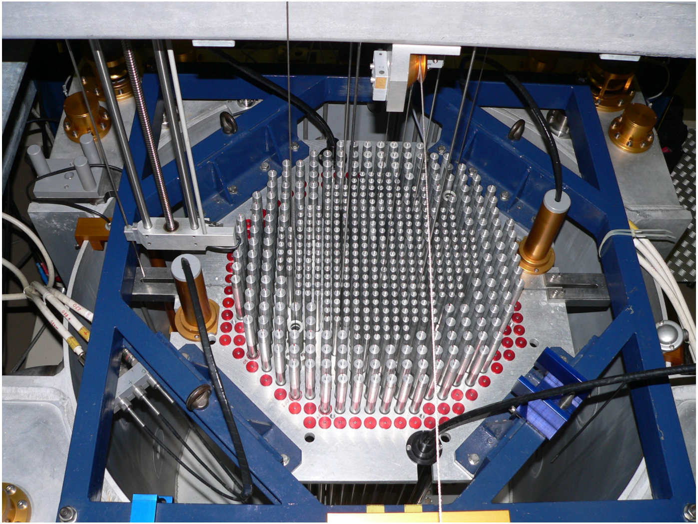
Motivating examples

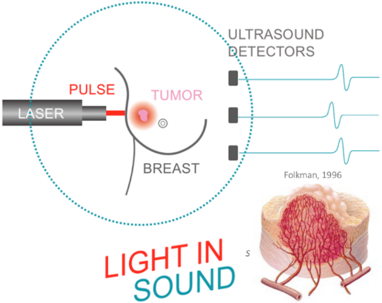
Nuclear reactors



Core of reactor CROCUS (EPFL); picture from wikipedia

Further applications

- biomedical imaging [Arridge et al 2009, Ntziachristos et al 2003]
- radiation therapy: [Swan et al 2020, St.Aubin et al 2016]
- climate simulation: [Thomas et al '99]
- ...



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The stationary radiative transfer equation (RTE)

a balance equation for streaming, absorption and scattering of a density

$$\hat{\mathbf{s}} \cdot \nabla u(\mathbf{r}, \hat{\mathbf{s}}) + \sigma_t(\mathbf{r}) u(\mathbf{r}, \hat{\mathbf{s}}) = \sigma_s(\mathbf{r}) (\Theta u)(\mathbf{r}, \hat{\mathbf{s}}) + q(\mathbf{r}, \hat{\mathbf{s}})$$

$$u = q_\partial \quad \text{on } \Gamma_- := \{(\mathbf{r}, \hat{\mathbf{s}}) \in \partial R \times S \text{ such that } \hat{\mathbf{s}} \cdot \hat{\mathbf{n}}(\mathbf{r}) < 0\}$$

$S \subset \mathbb{R}^{d-1}$ the unit sphere, $R \subset \mathbb{R}^d$ a Lipschitz domain

$u(\mathbf{r}, \hat{\mathbf{s}})$ directionally resolved density at $\mathbf{r} \in R$ in direction $\hat{\mathbf{s}} \in S$

$\sigma_a \geq 0$ absorption rate, $\sigma_s \geq 0$ scattering rate, $\sigma_t = \sigma_s + \sigma_a$

$$(\Theta u)(\mathbf{r}, \hat{\mathbf{s}}) = \int_S \theta(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') u(\mathbf{r}, \hat{\mathbf{s}}') d\hat{\mathbf{s}}'$$

scattering from $\hat{\mathbf{s}}' \to \hat{\mathbf{s}}$ with probability

$$\theta(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') = \frac{1}{4\pi} \frac{1 - g^2}{[1 - 2g(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') + g^2]^{3/2}}$$

q and q_∂ internal and boundary sources

[Chandrasekhar ('50)] [Case+Zweifel ('67)] [Ishimaru ('78)] ...

Well-posedness of the stationary RTE

$$\begin{aligned} \hat{\mathbf{s}} \cdot \nabla u + \sigma_t u &= \sigma_s \Theta u + q \quad &&\text{in } R \times S \\ u &= q_\partial &&\text{on } \Gamma_- \end{aligned}$$

Theorem. Let $\sigma_a, \sigma_s \geq 0$, $q \in L^2(R \times S)$, $q_\partial \in L^2(\Gamma_-; |\hat{\mathbf{s}} \cdot \hat{\mathbf{n}}|)$. Then the RTE has a unique solution $u \in L^2(R \times S)$ with

$$\begin{aligned} &\|\hat{\mathbf{s}} \cdot \nabla u\|_{L^2(R\times S)} + \|u\|_{L^2(R\times S)} + \|u\|_{L^2(\Gamma_+;|\hat{\mathbf{s}}\cdot\hat{\mathbf{n}}|)} \\ &\qquad \leq C\big(\|q\|_{L^2(R\times S)} + \|q_\partial\|_{L^2(\Gamma_-;|\hat{\mathbf{s}}\cdot\hat{\mathbf{n}}|)}\big). \end{aligned}$$

Proof (idea) Consider the mapping $T : L^2 \to L^2$, $u_k \mapsto u_{k+1}$, defined by

$$\begin{aligned} \hat{\mathbf{s}} \cdot \nabla u_{k+1} + \sigma_t u_{k+1} &= \sigma_s \Theta u_k + q \quad &&\text{in } R \times S \\ u_{k+1} &= q_\partial &&\text{on } \Gamma_-. \end{aligned}$$

Verify conditions of Banach's fixed-point theorem.

[Case Zweifel '63] [Dautray Lions '93] [Agoshkov '98] [Bal Jollivet 2008] [Egger S 2013]

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$$\begin{aligned} \|\hat{\mathbf{s}} \cdot \nabla u\|_{L^2(R\times S)} &+ \|u\|_{L^2(R\times S)} + \|u\|_{L^2(\Gamma_+;|\hat{\mathbf{s}}\cdot\hat{\mathbf{n}}|)} \\ &\leq C\big(\|q\|_{L^2(R\times S)} + \|q_\partial\|_{L^2(\Gamma_-;|\hat{\mathbf{s}}\cdot\hat{\mathbf{n}}|)}\big). \end{aligned}$$

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Verify conditions of Banach's fixed-point theorem.

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Remarks on convergence of source iteration

$$\hat{\mathbf{s}} \cdot \nabla u_{k+1} + \sigma_t u_{k+1} = \sigma_s \Theta u_k + q \text{ in } R \times S, \quad u_{k+1} = q_\delta \text{ on } \Gamma_-.$$

Convergence rate: $\rho = \|\sigma_s/\sigma_t\|_\infty \approx 1$ for optically thick problems*

Aim: Accelerate the scheme

- Anderson acceleration [Willert et al 2015] [Olivier et al 2022]
- preconditioning using diffusion problems [Adams Larsen 02]

$\hookrightarrow$ consistent discretization of diffusion problem (e.g., [Warsa et al 2018])

$\hookrightarrow$ subspace correction [Palii S, 2020, Dölz Palii S 2022, Bardin S 2025]

Focus here:

- anisotropic scattering and arbitrary dimension
- avoid inner-outer iterations
- higher-order diffusion (or ...)

[Adams Larsen 2002], see (*) [Egger S 2013] for convergence if $\rho = 1$.

Modified iteration and main theoretical results

Step 1. Source iteration: Given $u_k \in W$, compute $u_{k+\frac{1}{2}} \in W$ solution to

$$\hat{\mathbf{s}} \cdot \nabla u_{k+\frac{1}{2}} + \sigma_t u_{k+\frac{1}{2}} = \sigma_s \Theta u_k + q \text{ in } R \times S, \quad u_{k+\frac{1}{2}} = q_\partial \text{ on } \Gamma_-$$

Result 1: $\left\|\mathcal{R}(u_{k+\frac{1}{2}})\right\|_{\sigma_t} \leq \rho \|\mathcal{R}(u_k)\|_{\sigma_t}$ with $\mathcal{R}(u_k) = u_{k+\frac{1}{2}} - u_k$.

Step 2. Modify iterate using a correction

$$u_{k+1} := u_{k+\frac{1}{2}} + u^c_{k+\frac{1}{2}},$$

obtained by residual minimization over N-dimensional space $W_N \subset W$:

$$u^c_{k+\frac{1}{2}} := \operatorname*{argmin}_{v \in W_N} \left\|\mathcal{R}(u_{k+\frac{1}{2}} + v)\right\|_{\sigma_t}, \quad \text{with } \|v\|_{\sigma_t} := \|\sqrt{\sigma_t} v\|_{L^2(R\times S)}.$$

Result 2: $\|u - u_k\|_{\sigma_t} \leq \frac{\rho^k}{1-\rho} \|\mathcal{R}(u_0)\|_{\sigma_t}$ for $k \geq 0$ and any u_0.

Todos: Proof of results, choice of W_N, numerical realization.

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Even-odd splitting of the transport equation

Even-odd parities $u^{\pm}(\hat{\mathbf{s}}) = \frac{1}{2}(u(\hat{\mathbf{s}}) \pm u(-\hat{\mathbf{s}}))$

Observations

- $u = u^+ + u^-$ is an $L^2(S)$-orthogonal splitting
- Parity transformation

$$\hat{\mathbf{s}} \cdot \nabla u^+ \text{ is odd,} \qquad \Theta u^+ \text{ is even.}$$

Transport equation is equivalent to the system

$$\begin{aligned} \hat{\mathbf{s}} \cdot \nabla u^- + \sigma_t u^+ &= \sigma_s \Theta u^+ + q^+ \quad \text{in } R \times \mathcal{S} \\ \hat{\mathbf{s}} \cdot \nabla u^+ + \sigma_t u^- &= \sigma_s \Theta u^- + q^- \quad \text{in } R \times \mathcal{S} \\ u^+ + u^- &= q_\partial \quad \text{on } \Gamma_- \end{aligned}$$

[Vladimirov 91] [Egger S 2012]

Towards a weak formulation

Multiplying the first equation with smooth function v^+ yields

$$(\hat{\mathbf{s}}\cdot\nabla u^-, v^+)_{R\times\mathcal{S}} + (\sigma_t u^+, v^+)_{R\times\mathcal{S}} = (\sigma_s \Theta u^+, v^+)_{R\times\mathcal{S}} + (q^+, v^+)_{R\times\mathcal{S}}.$$

Apply divergence theorem to first term:

$$(\hat{\mathbf{s}}\cdot\nabla u^-, v^+)_{R\times\mathcal{S}} = -(u^-, \hat{\mathbf{s}}\cdot\nabla v^+)_{R\times\mathcal{S}} + (\hat{\mathbf{s}}\cdot\hat{\mathbf{n}} u^-, v^+)_{\partial R\times\mathcal{S}}$$

Observation: $\hat{\mathbf{s}} \mapsto \hat{\mathbf{s}}\cdot\hat{\mathbf{n}} u^- v^+$ is even. Since $u^+ + u^- = q_\partial$ on Γ_-:

$$(\hat{\mathbf{s}}\cdot\hat{\mathbf{n}} u^-, v^+)_{\partial R\times\mathcal{S}} = 2(u^-, v^+ \hat{\mathbf{s}}\cdot\hat{\mathbf{n}})_{\Gamma_-} = 2(q_\partial - u^+, v^+ \hat{\mathbf{s}}\cdot\hat{\mathbf{n}})_{\Gamma_-}.$$

Collecting all terms yields

$$\begin{aligned}(u^+, v^+|\hat{\mathbf{s}}\cdot\hat{\mathbf{n}}|)_\Gamma - (u^-, \hat{\mathbf{s}}\cdot\nabla v^+)_{R\times\mathcal{S}} + (\sigma_t u^+, v^+)_{R\times\mathcal{S}} \\ = (\sigma_s \Theta u^+, v^+)_{R\times\mathcal{S}} + (q^+, v^+)_{R\times\mathcal{S}} + 2(q_\partial, v^+ \hat{\mathbf{s}}\cdot\hat{\mathbf{n}})_{\Gamma_-}.\end{aligned}$$

Mixed variational framework

Find $u \in W$ such that for all $v \in W$

$$t(u, v) = s(u, v) + \ell(v),$$

with $t, s : W \times W \to \mathbb{R}$, and $\ell : W \to \mathbb{R}$ defined by

$$t(u, v) = (\sigma_t u, v) + (|\hat{\mathbf{s}} \cdot \hat{\mathbf{n}}|\, u^+, v^+)_\Gamma + \left(\hat{\mathbf{s}} \cdot \nabla u^+, v^-\right) - \left(u^-, \hat{\mathbf{s}} \cdot \nabla v^+\right)$$
$$s(u, v) = (\sigma_s \Theta u, v)$$
$$\ell(v) = (q, v) - 2(\hat{\mathbf{s}} \cdot \hat{\mathbf{n}}\, q_\partial, v^+)_{\Gamma_-}$$

- odd part $u^- \in L^2(R \times S)^- =: V^-$
- even part $u^+ \in W^+$ has more regularity: $\hat{\mathbf{s}} \cdot \nabla u^+ \in L^2$, regular trace
- mixed regularity space $W = W^+ \oplus V^-$.
- $\exists! u \in W$ solution, such that [Egger S 2012, Egger S 2014]

$$\|u\|_W \leq C(\inf \sigma_a, \|\sigma_t\|_\infty)(\|q\| + \|q_\partial\|_{L^2(\Gamma_-;|\hat{\mathbf{s}}\cdot\hat{\mathbf{n}}|)})$$

- boundary conditions are incorporated naturally

Convergence analysis

Proof of Result 1 (contraction of residuals). Step 1. Error reduction

Step 1 becomes: Given $u_k \in W$, compute $u_{k+\frac{1}{2}} \in W$ such that

$$t(u_{k+\frac{1}{2}}, v) = s(u_k, v) + \ell(v), \quad \forall v \in W.$$

Result (well-known) $\left\|u - u_{k+\frac{1}{2}}\right\|_{\sigma_t} \leq \rho \|u - u_k\|_{\sigma_t}$, with $\rho = \|\sigma_s/\sigma_t\|_\infty$.

Proof. For $e_{k+\frac{1}{2}} = u - u_{k+\frac{1}{2}}$ and $e_k = u - u_k$ we have that

$$t(e_{k+\frac{1}{2}}, v) = s(e_k, v), \quad \forall v \in W.$$

Setting $v = e_{k+\frac{1}{2}}$ and using the Cauchy-Schwarz inequality:

$$\left\|e_{k+\frac{1}{2}}\right\|_{\sigma_t}^2 = (\sigma_t e_{k+\frac{1}{2}}, e_{k+\frac{1}{2}}) \leq t(e_{k+\frac{1}{2}}, e_{k+\frac{1}{2}}) = s(e_k, e_{k+\frac{1}{2}})$$
$$\leq \rho \left\|e_{k+\frac{1}{2}}\right\|_{\sigma_t} \|e_k\|_{\sigma_t}.$$

Convergence analysis

Proof of Result 1 (contraction of residuals). Step 2. Residuals

Preconditioned residual operator $\mathcal{R} : W \to W$ defined by

$$t(\mathcal{R}(w), v) = \ell(v) - (t(w, v) - s(w, v)), \quad \forall v \in W.$$

Result 1: $\left\|\mathcal{R}(u_{k+\frac{1}{2}})\right\|_{\sigma_t} \leq \rho\|\mathcal{R}(u_k)\|_{\sigma_t}$ with $\|v\|_{\sigma_t} := \|\sqrt{\sigma_t}v\|_{L^2(R\times S)}$.

Convergence analysis

Proof of Result 1. Step 2. The actual proof

Claim: $\mathcal{R}(u_k) = u_{k+\frac{1}{2}} - u_k$.

$$
\begin{aligned}
t(\mathcal{R}(u_k), v) &= \ell(v) - (t(u_k, v) - s(u_k, v)) \\
&= t(e_k, v) - s(e_k, v) = t(e_k, v) - t(e_{k+\frac{1}{2}}, v) \\
&= t(u_{k+\frac{1}{2}} - u_k, v), \qquad \forall v \in W.
\end{aligned}
$$

Using the claim:

$$
\begin{aligned}
t(\mathcal{R}(u_{k+\frac{1}{2}}), v) &= \ell(v) - (t(u_{k+\frac{1}{2}}, v) - s(u_{k+\frac{1}{2}}, v)) \\
&= t(e_{k+\frac{1}{2}}, v) - s(e_{k+\frac{1}{2}}, v) = s(e_k, v) - s(e_{k+\frac{1}{2}}, v) \\
&= s(u_{k+\frac{1}{2}} - u_k, v) = s(\mathcal{R}(u_k), v).
\end{aligned}
$$

Hence, as in the proof of error reduction: $\left\|\mathcal{R}(u_{k+\frac{1}{2}})\right\|_{\sigma_t} \leq \rho \|\mathcal{R}(u_k)\|_{\sigma_t}$, which is *Result 1*.

Minimization problem

Let $W_N \subset W$ be a subspace of finite dimension N, compute

$$u^c_{k+\frac{1}{2}} := \operatorname*{argmin}_{w \in W_N} \left\| \mathcal{R}(u_{k+\frac{1}{2}} + w) \right\|_{\sigma_t}.$$

Lemma. The minimization problem has a unique solution $u^c_{k+\frac{1}{2}} \in W_N$.

The new iterate of the scheme is then defined as

$$u_{k+1} = u_{k+\frac{1}{2}} + u^c_{k+\frac{1}{2}}.$$

Corollary. $\|\mathcal{R}(u_{k+1})\|_{\sigma_t} \leq \rho \|\mathcal{R}(u_k)\|_{\sigma_t}$.

Remark. We do not know whether $\|u - u_{k+1}\|_{\sigma_t} \leq \rho \|u - u_k\|_{\sigma_t}$.

Proof of result 2

Error residual relationship and convergence

Result 2: $\|u - u_k\|_{\sigma_t} \leq \frac{\rho^k}{1-\rho}\|\mathcal{R}(u_0)\|_{\sigma_t}$ for $k \geq 0$ and any u_0.

Lemma. For the solution $u \in W$ it holds that

$$\|u - w\|_{\sigma_t} \leq \frac{1}{1-\rho}\|\mathcal{R}(w)\|_{\sigma_t} \qquad \forall w \in W.$$

Proof of Result 2: We have for $w = u_k$, using Result 1,

$$(1-\rho)\|u - u_k\|_{\sigma_t} \leq \|\mathcal{R}(u_k)\|_{\sigma_t} \leq \rho^k\|\mathcal{R}(u_0)\|_{\sigma_t}.$$

Remark. The 'art' here, is to show the error-residual relationship in an appropriate norm ($\|\cdot\|_{\sigma_t}$).

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Approximation space

- $\mathcal{T}_h^R$ shape regular, conforming triangulation of R
- $\mathcal{T}_h^S$ shape regular triangulation of S such that $-K^S \in \mathcal{T}_h^S$ for any $K^S \in \mathcal{T}_h^S$
- $S_h^{\pm} = S_h^{\pm}(\mathcal{T}_h^S)$ finite element spaces of even piecewise constant (+) and odd piecewise linear (–) functions
- $X_h^{\pm} = X_h^{\pm}(\mathcal{T}_h^R)$ finite element spaces of piecewise constant (–) and continuous piecewise linear (+) functions
- $W_h = S_h^+ \otimes X_h^+ + S_h^- \otimes X_h^-$

Galerkin approximation: Find $u_h \in W_h$ such that

$$t(u_h, v_h) = s(u_h, v_h) + \ell(v_h) \quad \forall v_h \in W_h.$$

Galerkin approximation is well-posed and quasi-optimal [Egger S, 2012],

$$\|u - u_h\|_W \leq C \inf_{v_h \in W_h} \|u - v_h\|_W.$$

Discrete scheme

Step 1: Given $u_{h,k} \in W_h$, compute $u_{h,k+\frac{1}{2}} \in W_h$ such that

$$t(u_{h,k+\frac{1}{2}}, v_h) = s(u_{h,k}, v_h) + \ell(v_h), \quad \forall v_h \in W_h.$$

Step 2.1: Preconditioned residual operator: $\mathcal{R}_h : W_h \to W_h$ defined via

$$t(\mathcal{R}_h(w_h), v_h) = \ell(v_h) - (t(w_h, v_h) - s(w_h, v_h)), \quad \forall v_h \in W_h,$$

Step 2.2: Minimization problem: Choose $W_{h,N} \subset W_h$, define

$$u^c_{h,k+\frac{1}{2}} := \operatorname*{argmin}_{w_h \in W_{h,N}} \left\| \mathcal{R}_h(u_{h,k+\frac{1}{2}} + w_h) \right\|_{\sigma_t}.$$

Step 2.3: Update

$$u_{h,k+1} = u_{h,k+\frac{1}{2}} + u^c_{h,k+\frac{1}{2}}.$$

Theorem. For any $u_{h,0} \in W_h$, the sequence $\{u_{h,k}\}$ defined above converges linearly to the discrete solution u_h, i.e.,

$$\|u_h - u_{h,k}\|_{\sigma_t} \leq \frac{\rho^k}{1-\rho} \|\mathcal{R}_h(u_{h,0})\|_{\sigma_t}.$$

Matrix formulation of mixed formulation

Coefficients $\mathbf{u}$ of discrete solution u_h are determined through

$$\mathbf{T}\mathbf{u} = \mathbf{S}\mathbf{u} + \mathbf{l}.$$

$$\mathbf{T} := \begin{bmatrix} \mathbf{B} + \mathbf{M}^+ & -\mathbf{A}^T \\ \mathbf{A} & \mathbf{M}^- \end{bmatrix}, \qquad \mathbf{S} := \begin{bmatrix} \mathbf{S}^+ & \\ & \mathbf{S}^- \end{bmatrix}, \qquad \mathbf{l} := \begin{bmatrix} \mathbf{l}^+ \\ \mathbf{l}^- \end{bmatrix}.$$

$$\mathbf{S}^+ := \mathbf{\Theta}^+ \otimes \mathbf{M}^+_{\sigma_s}, \qquad \mathbf{S}^- := \mathbf{\Theta}^- \otimes \mathbf{M}^-_{\sigma_s},$$

$$\mathbf{M}^+ := \mathbf{M} \otimes \mathbf{M}^+_{\sigma_t}, \qquad \mathbf{M}^- := \mathbf{M}^- \otimes \mathbf{M}^-_{\sigma_t},$$

$$\mathbf{A} := \sum_{i=1}^{d} \mathbf{A}_i \otimes \mathbf{D}_i, \qquad \mathbf{B} := \mathrm{blkdiag}(\mathbf{B}_1, \ldots, \mathbf{B}_{n_S^+}),$$

Remark. All matrices are sparse, except $\mathbf{\Theta}^+$ and $\mathbf{\Theta}^-$ (compression [Dölz Palii S, 2020]).

Matrix formulation of the iterative scheme

Step 1 becomes: given $\mathbf{u}_k$, compute $\mathbf{u}_{k+\frac{1}{2}}$

$$\mathbf{T}\mathbf{u}_{k+\frac{1}{2}} = \mathbf{S}\mathbf{u}_k + \mathbf{l},$$

Residual operator. Coordinate vector $\mathbf{R}(\mathbf{w})$ of $\mathcal{R}_h(w_h)$ is determined by

$$\mathbf{T}\,\mathbf{R}(\mathbf{w}) = \mathbf{l} - (\mathbf{T} - \mathbf{S})\mathbf{w}.$$

Additionally, define linear map $\mathbf{R}_0\mathbf{w} = \mathbf{R}(w) - \mathbf{R}(0)$.

Subspace. $\mathbf{W}_{h,N}$ is a matrix, corresponding to a basis for $W_{h,N}$.

Residuals of the subspace: $\mathbf{R}_0^N = \mathbf{R}_0\mathbf{W}_{h,N}$

Minimization $\quad (\mathbf{R}_0^N)^T\mathbf{M}\mathbf{R}_0^N w^* = -(\mathbf{R}_0^N)^T\mathbf{M}\,\mathbf{R}(\mathbf{u}_{k+\frac{1}{2}}),$

New iterate $\quad \mathbf{u}_{k+1} = \mathbf{u}_{k+\frac{d}{2}} + \mathbf{u}^c_{k+\frac{1}{2}}, \quad$ with $\mathbf{u}^c_{k+\frac{1}{2}} = \mathbf{W}_{h,N}w^*$

New residual $\quad \mathbf{R}(\mathbf{u}_{k+1}) = \mathbf{R}(\mathbf{u}_{k+\frac{1}{2}}) + \mathbf{R}_0^N w^*.$

Remarks on solving the linear systems

Solving for $\mathbf{u}_{k+\frac{1}{2}}$ can be done in two steps:

(i) Solve the symmetric positive definite system

$$(\mathbf{A}^T(\mathbf{M}^-)^{-1}\mathbf{A} + \mathbf{M}^+ + \mathbf{B})\mathbf{u}^+_{k+\frac{1}{2}} = \mathbf{S}^+\mathbf{u}^+_k + \mathbf{l}^+ + \mathbf{A}^T(\mathbf{M}^-)^{-1}(\mathbf{l}^- + \mathbf{S}^-\mathbf{u}^-_k).$$

Remark. Block diagonal system with n_S^+ many sparse blocks of size $n_R^+ \times n_R^+$ and can be solved in parallel, with straightforward parallelization over each element of $\mathcal{T}_h^S$.

(ii) Retrieve the odd part by solving the block-diagonal system

$$\mathbf{M}^-\mathbf{u}^-_{k+\frac{1}{2}} = \mathbf{S}^-\mathbf{u}^+_k - \mathbf{A}\mathbf{u}^+_{k+\frac{1}{2}} + \mathbf{l}^-.$$

Space for residual minimization

via Galerkin projection of correction equation

Recall:

$$t(u_h, v_h) = s(u_h, v_h) + \ell(v_h) \quad \forall v_h \in W_h,$$
$$t(u_{h,k+\frac{1}{2}}, v_h) = s(u_{h,k}, v_h) + \ell(v_h) \quad \forall v_h \in W_h.$$

Error equation:

$$t(u_h - u_{h,k+\frac{1}{2}}, v_h) = s(u_h - u_{h,k+\frac{1}{2}}, v_h) + s(u_{h,k+\frac{1}{2}} - u_{h,k}, v_h) \quad \forall v_h \in W_h.$$

Galerkin projection of error: onto space $Y_{h,K} \subset W_h$:

$$t(u^c_{h,k+\frac{1}{2}}, v_h) = s(u^c_{h,k+\frac{1}{2}}, v_h) + s(u_{h,k+\frac{1}{2}} - u_{h,k}, v_h) \quad \forall v_h \in Y_{h,K}.$$

Correction space for minimization: Define

$$W^c_{h,N} := \mathrm{span}\{u^c_{h,k+\frac{1}{2}}\} \subset W_h.$$

Choice of subspace for projected error equation

approximate spherical harmonics

Let $H^+_{h,k} \neq 0$ solve the generalized eigenvalue problem

$$(\Theta H^+_{h,k}, v^+_h) = \gamma_k (H^+_{h,k}, v^+_h)$$

for eigenvalues $\gamma_k \geq 0$ ordered non-increasingly.

Further define $H^-_{h,k,i} \in S^-_h$ by the relation

$$(H^-_{h,k,i}, \psi_l) = (\hat{\mathbf{s}}_i H^+_{h,k}, \psi_l) \quad \text{for all } l = 1, \ldots, n^-_S, \quad 1 \leq i \leq d.$$

Define the spaces

$$\begin{aligned} H^+_K &= \mathrm{span}\{H^+_{h,k} : 1 \leq k \leq K\} \\ H^-_K &= \mathrm{span}\{H^-_{h,k,i} : 1 \leq k \leq K,\ 1 \leq i \leq d\} \\ Y_{h,K} &= H^+_K \otimes X^+_h + H^-_K \otimes X^-_h \subset W_h. \end{aligned}$$

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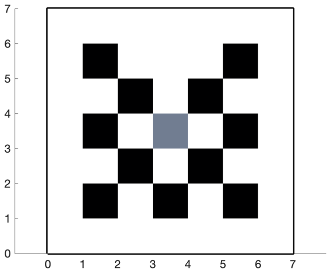
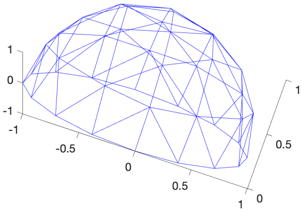
Setup of the lattice problem [Brunner (2005)]





$\sigma_s = 0$ and $\sigma_a = 1$ in the black regions

$\sigma_s = 10$ and $\sigma_a = 0.01$ else $\rightsquigarrow \rho \approx 0.999$

$q = 1$ in the grey region (middle) and $q = 0$ else

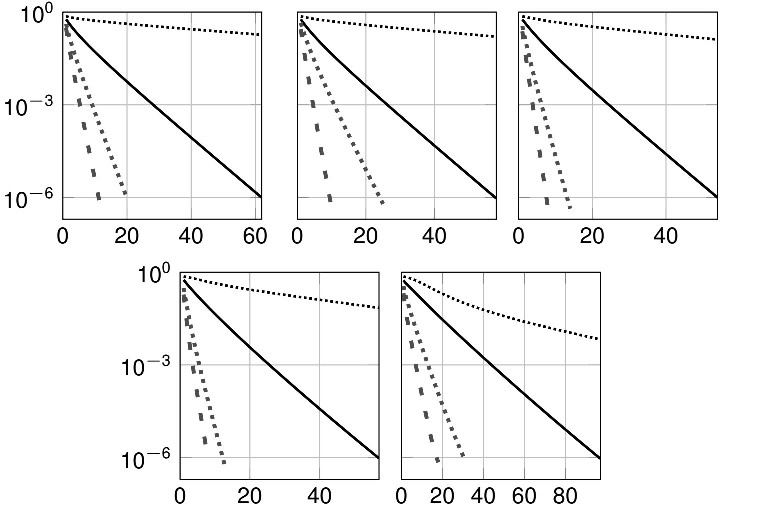
Iteration counts and contraction rates

Discretization parameters

- R is triangulated using 100 352 elements
- S is triangulated using 1 024 elements
- Number of dofs: 360 121 344
- dimension of $W_{h,N}^c$ in residual minimization: 1
- to compute basis of $W_{h,N}^c$, we use K functions $H_{h,k}^+$.
- stopping criterion $\|\mathcal{R}_h(u_k)\|_{\sigma_t} < 10^{-6}$

	g				
K	0.1	0.3	0.5	0.7	0.9
0	1018 (0.990)	863 (0.988)	701 (0.984)	531 (0.979)	358 (0.967)
1	62 (0.817)	58 (0.805)	54 (0.795)	57 (0.809)	97 (0.882)
6	20 (0.532)	25 (0.603)	14 (0.377)	13 (0.371)	31 (0.706)
15	12 (0.312)	10 (0.245)	8 (0.157)	8 (0.216)	18 (0.657)

Graphical visualization of residual convergence



From left to right, first row $g = 0.1,\ 0.3,\ 0.5$; second row, $g = 0.7,\ 0.9$ for $K = 0$ densely dotted; $K = 1$ solid; $K = 6$ dotted; $K = 15$ dashed.

Timings

Subspace correction with high-order discrete spherical harmonics pays off

Average time in seconds per iteration for different anisotropy parameters g and order K (total time in hours).

	g				
K	0.1	0.3	0.5	0.7	0.9
0	66 (18.72)	66 (15.93)	68 (13.32)	67 (9.98)	66 (6.63)
1	156 (2.70)	153 (2.48)	153 (2.30)	155 (2.46)	153 (4.14)
6	151 (0.84)	158 (1.10)	157 (0.61)	159 (0.57)	156 (1.35)
15	163 (0.54)	168 (0.47)	170 (0.38)	168 (0.37)	164 (0.82)

Grid dependency study

Iteration counts are robust upon mesh refinement

Parameters

- $g = 0.7$
- $K = 0$ (left) and $K = 6$ (right)
- n_R^+ vertices of triangulation of R
- n_S^+ elements of triangulation of S

$K = 0$	n_S^+			
n_R^+	16	64	256	1024
841	475	483	487	488
3 249	499	509	514	515
12 769	509	520	525	526
50 625	513	524	529	531

$K = 6$	n_S^+			
n_R^+	16	64	256	1024
841	8	8	9	9
3 249	8	9	10	10
12 769	8	10	11	11
50 625	9	11	12	13

Outline

Introduction

The transport equation and main theoretical result

Convergence analysis for a weak formulation

Numerical realization via Galerkin approximation

Numerical tests

Conclusions

Conclusions

Developed and analyzed an acceleration strategy for the source iteration

- provably convergent
- based on residual minimization over subspaces:
  - similarities to GMRES (if subspace consists of (all) previous iterates)
  - subspaces can be constructed using Galerkin projections
  - improved convergence rates, even for low dimensional correction spaces

Possible extensions and open questions

- Is it possible to quantify the error reduction observed numerically?
- Combine the outlined methodology with a multilevel scheme.
- Is there a better correction for $g \to 1$?

Riccardo Bardin, Matthias Schlottbom: On accelerated iterative schemes for anisotropic radiative transfer using residual minimization.
accepted at SISC, https://arxiv.org/abs/2407.13356

code: zenodo 14753969