On fast iterative methods for radiative transfer

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S18 Numerical methods of differential equations

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Outline

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The anisotropic radiative transfer equation (RTE)

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

$$s \cdot \nabla_r \phi(s,r) + \sigma_t(r)\phi(s,r) = \sigma_s(r) \int_S k(s \cdot s')\phi(s',r)ds' + q(s,r)$$

$$\phi = g \quad \text{on } \Gamma_- = \{(s,r) \in S \times \partial R \text{ such that } s \cdot n(r) < 0\}$$

$\phi(s,r)$ directionally resolved density at $r \in R$ in direction $s \in S$

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

scattering from $s' \to s$ with probability

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

q and g internal and boundary sources

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

Weak formulation

even-parity equations

Function space:

- $\mathbb{V} = \{w \in L^2(S \times R) : w(s,r) = w(-s,r)\}$
- $\mathbb{W} = \{w \in \mathbb{V} : s \cdot \nabla_r w \in L^2(S \times R),\ w_{|\Gamma_-} \in L^2(\Gamma_-; |s \cdot n|)\}$

Scattering operator: $\mathcal{K}u = \sigma_s \mathcal{S}u$, $\mathcal{S}u = \int_S k(s \cdot s')u(s')ds'$

Assumptions: $0 \leq \sigma_s, \sigma_t \in L^\infty(R)$ and $\|\sigma_s/\sigma_t\|_\infty < 1$.

Weak formulation: Find $u \in \mathbb{W}$: $(\mathcal{E} - \mathcal{K})u = f$ in $\mathbb{W}'$. $(\star)$

- $\langle \mathcal{E}u, w \rangle = ((\sigma_t \mathcal{I} - \mathcal{K})^{-1} s \cdot \nabla_r u, s \cdot \nabla_r w) + 2(u, w|s \cdot n|)_{\Gamma_-} + (\sigma_t u, w)$
- $f(w) = (q, w) + ((\sigma_t \mathcal{I} - \mathcal{K})^{-1} q, s \cdot \nabla_r w) + 2(g, w|s \cdot n|)_{\Gamma_-}$

Theorem [Egger+S (2012)] $\exists!$ weak solution $u \in \mathbb{W}$ of $(\star)$.

Preconditioned Richardson iteration for RTE

Step (i) Given $u_n \in \mathbb{W}$, $\mathcal{P}_\mathcal{E} : \mathbb{W}' \to \mathbb{W}$ sym. & pos., compute

$$u_{n+\frac{1}{2}} = u_n - \mathcal{P}_\mathcal{E}((\mathcal{E} - \mathcal{K})u_n - f).$$

Observation: Error $e_{n+1/2} = u - u_{n+1/2}$ satisfies

$$(\mathcal{E} - \mathcal{K})e_{n+\frac{1}{2}} = ((\mathcal{E} - \mathcal{K})\mathcal{P}_\mathcal{E} - \mathcal{I})((\mathcal{E} - \mathcal{K})u_n - f).$$

Step (ii) Compute a subspace correction $u_{c,n} \in \mathbb{W}_N \subset \mathbb{W}$:

$$\langle(\mathcal{E} - \mathcal{K})u_{c,n}, w\rangle = \langle((\mathcal{E} - \mathcal{K})\mathcal{P}_\mathcal{E} - \mathcal{I})((\mathcal{E} - \mathcal{K})u_n - f), w\rangle \quad \forall w \in \mathbb{W}_N$$

Update: $u_{n+1} = u_{n+\frac{1}{2}} + u_{c,n}$

Scheme: Given u_n, compute

$$u_{n+1} = u_n - \mathcal{P}((\mathcal{E} - \mathcal{K})u_n - f) \text{ with } \mathcal{P} = \mathcal{P}_\mathcal{E} + \mathcal{P}_G(\mathcal{I} - (\mathcal{E} - \mathcal{K})\mathcal{P}_\mathcal{E}).$$

Convergence analysis of preconditioned Richardson iteration

Generic choice: $\mathcal{P}_\mathcal{E} = \mathcal{E}^{-1}$

Error $e_n = u - u_n$ satisfies

$$\begin{aligned} \|e_{n+1}\|_{\mathcal{E}-\mathcal{K}} &= \inf_{w \in \mathbb{W}_N} \|e_{n+\frac{1}{2}} - w\|_{\mathcal{E}-\mathcal{K}} && \text{(projection)} \\ &\leq \|e_{n+\frac{1}{2}}\|_{\mathcal{E}-\mathcal{K}} && (w = 0) \\ &\leq \|\sigma_s/\sigma_t\|_\infty \|e_n\|_{\mathcal{E}-\mathcal{K}} && \text{(choice of } \mathcal{P}_\mathcal{E}) \end{aligned}$$

Since $\|\sigma_s/\sigma_t\|_\infty < 1$, convergence guaranteed.

Approximation properties of $\mathbb{W}_N$ can improve the error bound.

Motivation for effective subspaces for $\mathcal{P}_{\mathcal{E}} = \mathcal{E}^{-1}$

span $\mathbb{W}_N$ by low-order spherical harmonics

Error can be expanded in generalized eigenfunctions of

$$\mathcal{K}w = \delta \mathcal{E} w, \qquad \delta \in [0, \|\sigma_s/\sigma_t\|_\infty].$$

Slowly convergent modes are the ones with $\delta \approx 1$.

Spherical harmonics expansions of

$$w(s,r) = \sum_{l=0}^{\infty} \sum_{m=-2l}^{2l} w_m^{2l}(r) H_m^{2l}(s), \quad \mathcal{K}w = \sum_{l=0}^{\infty} g^{2l} \sum_{m=-2l}^{2l} \sigma_s(r) w_m^{2l}(r) H_m^{2l}(s)$$

Since $\mathcal{E} \geq \sigma_t \mathcal{I}$,

$$\sum_{l=0}^{\infty} (g^{2l} - \delta) \sum_{m=-2l}^{2l} \|\sqrt{\sigma_t} w_m^{2l}\|_{L^2(R)}^2 \geq 0$$

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Approximation spaces:

- $\mathbb{X}_h = \mathbb{P}_1^c(\mathcal{T}_h^R) = \mathrm{span}\{\varphi_i\}, \qquad n_R = \dim(\mathbb{X}_h)$
- $\mathbb{S}_h = \mathbb{P}_0(\mathcal{T}_h^S) \cap L^2(S)^+ = \mathrm{span}\{\chi_j\}, \quad n_S = \dim(\mathbb{S}_h)$
- $\mathbb{W}_h = \mathbb{S}_h \otimes \mathbb{X}_h \subset \mathbb{W}$

Galerkin approx: Find $u_h \in \mathbb{W}_h$: $\langle (\mathcal{E} - \mathcal{K})u_h, w_h \rangle = f(w_h)\ \forall w_h \in \mathbb{W}_h$.

Linear system: $(\mathbf{E} - \mathbf{K})\mathbf{u} = \mathbf{f}$

Richardson iteration: For $\mathbf{P} = \mathbf{P}_\mathbf{E} + \mathbf{P}_G(\mathbf{I} - (\mathbf{E} - \mathbf{K})\mathbf{P}_\mathbf{E})$

$$\mathbf{u}_{n+1} = \mathbf{u}_n - \mathbf{P}((\mathbf{E} - \mathbf{K})\mathbf{u}_n - \mathbf{f}).$$

Theorem [Dölz+Palii+S (2021)] $\mathbf{u}_n \to \mathbf{u}$ linearly with rate $\eta = \|(\mathbf{I} - \mathbf{P}_G)(\mathbf{I} - \mathbf{P}_\mathbf{E}(\mathbf{E} - \mathbf{K}))\|_{\mathbf{E}-\mathbf{K}} \le \|\sigma_s/\sigma_t\|_\infty$.

Application of $\mathbf{K}$ via $\mathcal{H}^2$-matrices in $\mathcal{O}(n_S n_R)$ [Hackbusch (2015)]

Complexity of applying $\mathbf{E} - \mathbf{K} = \mathcal{O}(n_S n_R/(1-cg)^{1/2})$.

Inexact preconditioning and subspace correction

Preconditioning $\mathbf{P}_{\mathbf{E}}^{\ell} \approx \mathbf{E}^{-1}$

Generic choice: $\mathbf{P}_{\mathbf{E}}^{\ell}\mathbf{r} = \mathbf{z}_\ell$, where

$$\mathbf{z}_0 = 0, \qquad \mathbf{z}_{k+1} = \mathbf{z}_k - \mathbf{E}_0^{-1}(\mathbf{E}\mathbf{z}_k - \mathbf{r}), \quad k < \ell$$

- $\mathbf{E}_0 \cong$ anisotropic elliptic problems ($\rightsquigarrow$ multigrid [Hemker ('84)])
- $\mathrm{cond}(\mathbf{P}_{\mathbf{E}}^{\ell}\mathbf{E}) = 1/(1-(cg)^\ell)$

Lemma **[Dölz+Palii+S (2021)]** Let $\ell \geq 1$ be fixed. The Richardson iteration with preconditioner $\mathbf{P}_{\mathbf{E}} = \mathbf{P}_{\mathbf{E}}^{\ell}$ converges linearly with rate $\eta \leq \|\sigma_s/\sigma_t\|_\infty$.

Subspace correction

Span correction space $\mathbb{W}_{h,N} \subset \mathbb{W}_h$ by discrete eigenfunctions of $\mathbf{S}$

Correction equations $\cong$ elliptic system ($\rightsquigarrow$ multigrid [Arridge+Egger+S (2013)])

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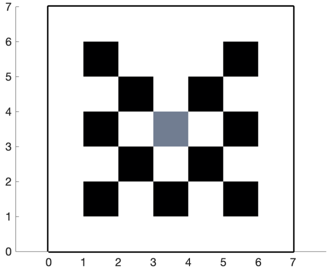
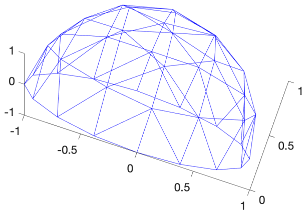
Setup of the lattice problem [Brunner (2005)]





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

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

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

Convergence rate $\eta = \|(\mathbf{I} - \mathbf{P}_G)(\mathbf{I} - \mathbf{P}_{\mathbf{E}}^{\ell}(\mathbf{E} - \mathbf{K}))\|$

for $n_R = 3\,249$, $n_S = 64$

$d_N := \dim \mathbb{W}_{h,N} = \#$ even spherical harmonics of degree $\leq N$

	$g = 0.1$			$g = 0.5$			$g = 0.9$		
ℓ $\quad d_N =$	1	6	15	1	6	15	1	6	15
1	0.432	0.247	0.161	0.553	0.499	0.499	—	—	0.899
2	0.429	0.237	0.141	0.489	0.301	0.255	0.808	0.808	0.808
3	0.429	0.237	0.141	0.482	0.260	0.175	0.775	0.758	0.727
4	0.429	0.237	0.141	0.480	0.254	0.159	0.773	0.757	0.653
5	0.429	0.237	0.141	0.480	0.253	0.156	0.772	0.757	0.587
6	0.429	0.237	0.141	0.480	0.253	0.156	0.772	0.757	0.528

For moderate ℓ and N, the contraction rate η is small

Iteration counts for solving the lattice problem

with $g = 0.5$, $\ell = 4$, $d_4 = 15$ eigenfunctions for the subspace correction

Expected contraction rate $\eta \approx 0.16$

Stopping criterion: $\|\mathbf{u}_n - \mathbf{u}_{n-1}\|_{\mathbf{E-K}} < 10^{-8} \|\mathbf{u}_1\|_{\mathbf{E-K}}$

Expectation: $\|\mathbf{u} - \mathbf{u}_n\|_{\mathbf{E-K}} < 10^{-8}$ for $n \approx 10$ iterations

Iteration index n (timings in sec.)

n_S	$n_R = 3\,249$	12 769	50 625
64	8 (50)	9 (236)	9 (1 470)
256	9 (114)	9 (499)	9 (2 476)
1 024	9 (300)	9 (1 107)	10 (6 580)
4 096	9 (1 017)	9 (4 983)	10 (34 029)

Conclusions

Richardson iteration: For $\mathbf{P} = \mathbf{P}_{\mathbf{E}}^{\ell} + \mathbf{P}_G(\mathbf{I} - (\mathbf{E} - \mathbf{K})\mathbf{P}_{\mathbf{E}}^{\ell})$

$$\mathbf{u}_{n+1} = \mathbf{u}_n - \mathbf{P}((\mathbf{E} - \mathbf{K})\mathbf{u}_n - \mathbf{f}).$$

- provably convergent for anisotropic radiative transfer
- mesh-independent convergence rates
- convergence is robust in optical parameters (heterogeneities, anisotropy, diffusive regime: $\sigma_s/\sigma_t \approx 1$)
- if $\mathbf{E}_0^{-1}$ can be applied in linear complexity, each iteration has linear computational complexity

local approximations in s: [Lewis+('84),Guermond+(2014),Dahmen+(2020),...]
survey on iterative methods: [Adams+(2002)]
schemes with consistent correction: [Warsa+(2002),Ragusa+(2010), Palii+S (2020)]

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