On classical and modern approximations for neutron transport in a unified framework

Matthias Schlottbom

October 26th, 2023

Mathematics for Nuclear Applications Seminar
Port-au-rocs, le Croisic October 23–27, 2023

UNIVERSITY OF TWENTE.

Outline

The neutron transfer equation (NTE)

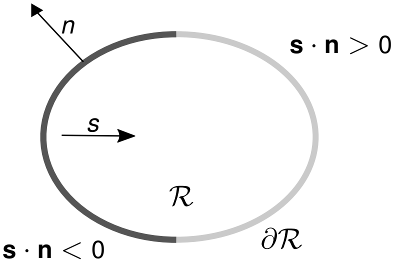
Perfectly matched layers for NTE

Discretization of PML formulation
- Variational formulation
- Galerkin approximation
- Numerical examples

Recall: NTE on bounded domains

Assumptions

- $\mathcal{R} \subset \mathbb{R}^3$ bounded convex domain
- $\mathrm{supp}(q) \subset \mathcal{R}$
- $\mathrm{supp}(\sigma) \subset \mathcal{R}$



Inflow boundary

$$\Gamma_- = \{(\mathbf{r}, \mathbf{s}) \in \partial\mathcal{R} \times \mathbb{S}^2 : \mathbf{s} \cdot \mathbf{n}(\mathbf{r}) < 0\}$$

$$\begin{aligned} \mathbf{s} \cdot \nabla_{\mathbf{r}}\phi + \sigma\phi &= \sigma_s K\phi + q && \text{in } \mathcal{R} \times \mathbb{S}^2 \\ \phi &= 0 && \text{on } \Gamma_- \end{aligned}$$

Half-space integrals

Recall the boundary functional of the variational formulation:

$$\langle|\mu|\phi^+, \psi^+\rangle_\Gamma = \int_{-1}^{1} \phi^+(z, \mu)\psi^+|\mu|d\mu.$$

For Legendre expansions $\phi^+(z, \mu) = \sum_{l=0}^{\infty} c_{2l}(z)P_{2l}(\mu)$ this led to a dense coupling, because

$$\int_{-1}^{1} P_{2l}(\mu)P_{2k}(\mu)|\mu|d\mu \neq 0 \quad \text{in general.}$$

Half-space integrals

Recall the boundary functional of the variational formulation:

$$\langle|\mu|\phi^+, \psi^+\rangle_\Gamma = \int_{-1}^{1} \phi^+(z,\mu)\psi^+|\mu|d\mu.$$

For Legendre expansions $\phi^+(z,\mu) = \sum_{l=0}^{\infty} c_{2l}(z)P_{2l}(\mu)$ this led to a dense coupling, because

$$\int_{-1}^{1} P_{2l}(\mu)P_{2k}(\mu)|\mu|d\mu \neq 0 \quad \text{in general.}$$

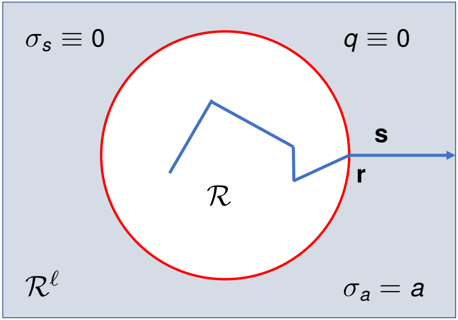
The same issue occurs in 3D for spherical harmonics Y_l^m expansions:

$$\int_{\Gamma_-} Y_l^m Y_k^n \mathbf{s}\cdot\mathbf{n}\, ds \neq 0 \quad \text{in general.}$$

Moreover, the integration over **s** depends on $\mathbf{n}(\mathbf{r})$, recall

$$\Gamma_- = \{(\mathbf{r},\mathbf{s}) \in \partial\mathcal{R}\times\mathbb{S}^2 : \mathbf{s}\cdot\mathbf{n}(\mathbf{r}) < 0\}.$$

Perfectly matched layers for NTE

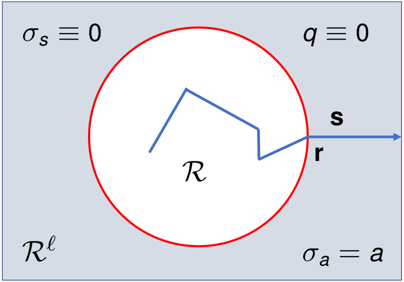


Beer-Lambert law: $\phi(\mathbf{r} + h\mathbf{s}, \mathbf{s}) = e^{-ha}\phi(\mathbf{r}, \mathbf{s}) \ll 1$ for $ha \gg 1$

Expectation: Modification of boundary conditions is a minor perturbation

cf. [Bérenger, 94] [Bécache Fauqueux Joly, 2003] [Appelö Hagstrom Kreiss, 2006]

Reflection boundary condition



$$\mathbf{s} \cdot \nabla_{\mathbf{r}} \phi_a + \sigma^a \phi_a = \sigma_s K \phi_a + q \quad \text{in } \mathcal{R}^\ell \times \mathbb{S}^2$$

$$\phi_a = R\phi_a \quad \text{on } \Gamma_-^\ell$$

Reflection operator $R\phi(\mathbf{r},\mathbf{s}) = \rho(\mathbf{r},\mathbf{s})\phi(\mathbf{r},\mathbf{s}) = \frac{|\mathbf{s}\cdot\mathbf{n}| - 1}{|\mathbf{s}\cdot\mathbf{n}| + 1}\phi(\mathbf{r},-\mathbf{s})$

Well-posedness of PML formulation

Theorem [Egger, S (2019)]: For $q \in L^2(\mathcal{R} \times \mathbb{S}^2)$, the PML problem has a unique solution $\phi_a \in L^2(\mathcal{R}^\ell \times \mathbb{S}^2)$ with $\mathbf{s} \cdot \nabla_{\mathbf{r}} \phi_a \in L^2(\mathcal{R}^\ell \times \mathbb{S}^2)$

$$\|\phi_a\|_{L^2(\Gamma^\ell)} \le C e^{-2a\ell} \|q\|_{L^2(\mathcal{R}^\ell \times \mathbb{S}^2)}.$$

Furthermore,

$$\|\mathbf{s} \cdot \nabla_{\mathbf{r}} (\phi_a - \phi)\|_{L^2(\mathcal{R} \times \mathbb{S}^2)} + \|\|\phi_a - \phi\|_{L^2(\mathcal{R} \times \mathbb{S}^2)} \le C e^{-2a\ell} \|q\|_{L^2(\mathcal{R} \times \mathbb{S}^2)}.$$

The neutron transfer equation (NTE)

Perfectly matched layers for NTE

Discretization of PML formulation

- Variational formulation
- Galerkin approximation
- Numerical examples

Recall: Even-odd splitting

Even-odd parities

$$\phi^{\pm}(\mathbf{r},\mathbf{s}) = \frac{1}{2}(\phi(\mathbf{r},\mathbf{s}) \pm \phi(\mathbf{r},-\mathbf{s}))$$

Observations

- $\phi = \phi^+ + \phi^-$ is an $L^2(\mathcal{R}^\ell \times \mathbb{S}^2)$-orthogonal splitting
- Parity transformation

$$\mathbf{s}\cdot\nabla_{\mathbf{r}}\phi^+ \text{ is odd,} \qquad K\phi^+ \text{ is even}$$

- Reflection boundary conditions

$$\phi_a^+ = \mathbf{s}\cdot\mathbf{n}\phi_a^- \quad \text{on } \Gamma_-^\ell$$

[Vladimirov ('61)]

Splitting of the NTE

NTE with reflection b.c. is equivalent to the system

$$\begin{aligned} \mathbf{s}\cdot\nabla_{\mathbf{r}}\phi_a^- + \mathcal{C}_a\phi_a^+ &= q^+ && \text{in } \mathcal{R}^\ell\times\mathbb{S}^2 \\ \mathbf{s}\cdot\nabla_{\mathbf{r}}\phi_a^+ + \mathcal{C}_a\phi_a^- &= q^- && \text{in } \mathcal{R}^\ell\times\mathbb{S}^2 \\ \phi_a^+ &= \mathbf{s}\cdot\mathbf{n}\phi_a^- && \text{on } \Gamma_-^\ell \end{aligned}$$

where $\mathcal{C}_a\phi_a = \sigma^a\phi_a - \sigma_s K\phi_a$.

Splitting of the NTE

NTE with reflection b.c. is equivalent to the system

$$\begin{aligned} \mathbf{s}\cdot\nabla_{\mathbf{r}}\phi_a^- + \mathcal{C}_a\phi_a^+ &= q^+ && \text{in } \mathcal{R}^\ell\times\mathbb{S}^2 \\ \mathbf{s}\cdot\nabla_{\mathbf{r}}\phi_a^+ + \mathcal{C}_a\phi_a^- &= q^- && \text{in } \mathcal{R}^\ell\times\mathbb{S}^2 \\ \phi_a^+ &= \mathbf{s}\cdot\mathbf{n}\phi_a^- && \text{on } \Gamma_-^\ell \end{aligned}$$

where $\mathcal{C}_a\phi_a = \sigma^a\phi_a - \sigma_s K\phi_a$.

Integration-by-parts:

$$(\mathbf{s}\cdot\nabla_{\mathbf{r}}\phi_a^-, \psi^+) = -(\phi_a^-, \mathbf{s}\cdot\nabla_{\mathbf{r}}\psi^+) + \langle \mathbf{s}\cdot\mathbf{n}\phi_a^-, \psi^+\rangle_{\partial\mathcal{R}^\ell\times\mathbb{S}^2}$$

Key observation: $s\mapsto \mathbf{s}\cdot\mathbf{n}\phi_a^-\psi^+$ is even

$$\langle \mathbf{s}\cdot\mathbf{n}\phi_a^-, \psi^+\rangle_{\partial\mathcal{R}^\ell\times\mathbb{S}^2} = 2\langle \mathbf{s}\cdot\mathbf{n}\phi_a^-, \psi^+\rangle_{\Gamma_-^\ell} = 2\langle \phi_a^+, \psi^+\rangle_{\Gamma_-^\ell} = \langle \phi_a^+, \psi^+\rangle_{\Gamma^\ell}$$

Mixed variational framework

Find $\phi_a = \phi_a^+ + \phi_a^-$ such that for all sufficiently smooth $\psi = \psi^+ + \psi^-$

$$\langle \phi_a^+, \psi^+ \rangle_{\Gamma^\ell} - (\phi_a^-, \mathbf{s} \cdot \nabla_\mathbf{r} \psi^+) + (\mathbf{s} \cdot \nabla_\mathbf{r} \phi_a^+, \psi^-) + (\mathcal{C}_a \phi_a, \psi) = (q, \psi)$$

Observations

- odd part $\phi_a^- \in \mathbb{V}^-$ with $\mathbb{V} := L^2(\mathcal{R}^\ell \times \mathbb{S}^2)$
- even part $\phi_a^+ \in \mathbb{W}^+ := \{\psi \in \mathbb{V}^+ : \mathbf{s} \cdot \nabla_\mathbf{r} \psi \in \mathbb{V},\ \psi|_{\Gamma^\ell} \in L^2(\Gamma^\ell)\}$
- boundary conditions are incorporated naturally
- boundary bilinear form has tensor product structure

Theorem [Egger, S (2018)]: For every $q \in L^2(\mathcal{R} \times \mathbb{S}^2)$ the mixed variational problem has a unique solution $\phi_a = \phi_a^+ + \phi_a^- \in \mathbb{W}^+ \oplus \mathbb{V}^-$.

Galerkin approximation

Let $\mathbb{W}_h^+ \subset \mathbb{W}^+$ and $\mathbb{V}_h^- \subset \mathbb{V}^-$ be finite dimensional spaces

Find $\phi_{a,h} \in \mathbb{W}_h^+ \oplus \mathbb{V}_h^-$ such that for all $\psi_h \in \mathbb{W}_h^+ \oplus \mathbb{V}_h^-$

$$\langle \phi_{a,h}^+, \psi_h^+ \rangle_{\Gamma^\ell} - (\phi_{a,h}^-, \mathbf{s}\cdot\nabla_{\mathbf{r}}\psi_h^+) + (\mathbf{s}\cdot\nabla_{\mathbf{r}}\phi_{a,h}^+, \psi_h^-) + (\mathcal{C}_a\phi_{a,h}, \psi_h) = (q, \psi_h)$$

Theorem [Egger & S (2019)]: If $\mathbf{s}\cdot\nabla_{\mathbf{r}}\mathbb{W}_h^+ \subset \mathbb{V}_h^-$ and $\mathcal{C}_a : \mathbb{V}^- \to \mathbb{V}^-$ is boundedly invertible, then the Galerkin problem is well-posed and

$$\|\phi - \phi_{a,h}\|_{\mathbb{W}^+\oplus\mathbb{V}^-} \leq C'(a) \underbrace{e^{-a\ell}\|q\|_{L^2(\mathcal{R}\times\mathbb{S}^2)}}_{\text{model error}} + C(a) \underbrace{\inf \|\phi_a - v_h\|_{\mathbb{W}^+\oplus\mathbb{V}^-}}_{\text{approx. error}},$$

where the infimum is taken over all $(v_h^+, v_h^-) \in \mathbb{W}_h^+ \times \mathbb{V}_h^-$.

P_N FEM

Even approximation space

- $\mathbb{X}_h^+ = P_1(T_h) \cap H^1(\mathcal{R}^\ell)$
- $\mathbb{S}_N^+ = \mathrm{span}\{H_{2l}^m : |m| \le l, 0 \le l \le (N-1)/2\}$ even spher. harm.
- *Approximation space* $\mathbb{W}_h^+ = \mathbb{S}_N^+ \otimes \mathbb{X}_h^+$, i.e.,

$$\phi_{a,h}^+(r,s) = \sum_{j=1}^{\dim \mathbb{X}_h^+} \sum_{l=0}^{(N-1)/2} \sum_{m=-l}^{l} p_{2l,m}^j \, \varphi_j(r) \, H_{2l}^m(s) \in \mathbb{S}_N^+ \otimes \mathbb{X}_h^+$$

Odd approximation space

- $\mathbb{X}_h^- = P_0(T_h) \subset L^2(\mathcal{R}^\ell)$
- $\mathbb{S}_N^- = \mathrm{span}\{H_{2l+1}^m : |m| \le l; 0 \le l \le (N-1)/2\}$ odd spher. harm.
- $\mathbb{V}_h^- = \mathbb{S}_N^- \otimes \mathbb{X}_h^-$, i.e.,

$$\phi_{a,h}^-(r,s) = \sum_{j=1}^{\dim \mathbb{X}_h^-} \sum_{l=0}^{(N-1)/2} \sum_{l=-m}^{m} p_{2l+1,m}^j \, \chi_j(r) \, H_{2l+1}^m(s) \in \mathbb{S}_N^- \otimes \mathbb{X}_h^-$$

P_N FEM: Properties

- If N is odd, then $\mathbf{s} \cdot \nabla_{\mathbf{r}} \mathbb{W}_h^+ \subset \mathbb{V}_h^-$
- Number of dofs $O(h^{-2}N^2)$
- Computational complexity for MatVec $O(h^{-2}N^2)$
- Galerkin approximation leads to linear system

$$\begin{pmatrix} \mathtt{M} + \mathtt{R} & -\mathtt{B}^\top \\ \mathtt{B} & \mathtt{C} \end{pmatrix} \begin{pmatrix} \mathtt{p}^+ \\ \mathtt{p}^- \end{pmatrix} = \begin{pmatrix} \mathtt{q}^+ \\ \mathtt{q}^- \end{pmatrix}$$

- Schur complement is symmetric positive definite

$$(\mathtt{B}^\top \mathtt{C}^{-1} \mathtt{B} + \mathtt{M} + \mathtt{R}) \mathtt{p}^+ = \mathtt{q}^+ + \mathtt{B}^\top \mathtt{C}^{-1} \mathtt{q}^-$$

- Numerical solution: Preconditioned CG
- Preconditioner: Spatial multigrid

Example 1: Constant coefficients

Setup

- Computational domain $\mathcal{R} = B_1(0) \subset \mathbb{R}^2$
- Model parameters: $k(\mathbf{r}, \mathbf{s}\cdot\mathbf{s}') = \frac{1}{4\pi}$, $\sigma_s = 10$, $\sigma_a = \frac{1}{10}$
- Isotropic source $q(\mathbf{r}, \mathbf{s}) = \exp(-5|\mathbf{r} - \mathbf{r}_0|^2)$, $\mathbf{r}_0 = (\frac{3}{4}, 0)$
- Extended domain $\mathcal{R}^\ell = B_{6/5}(0)$

Reference solution $\widetilde{\phi} = \phi_{a,h}$ computed for

- $N = 11$
- 177 761 vertices, i.e., $h = 0.005$
- $\dim \mathbb{W}_h^+ = 11\,732\,226$
- $\dim \mathbb{W}_h^+ + \dim \mathbb{W}_h^- = 39\,367\,938$

Error measure

$$e_h^2 = \|\widetilde{\phi} - \phi_{h,a}\|^2_{L^2(\mathcal{R}\times\mathbb{S}^2)} + \|\mathbf{s}\cdot\nabla_{\mathbf{r}}(\widetilde{\phi}^+ - \phi^+_{h,a})\|^2_{L^2(\mathcal{R}\times\mathbb{S}^2)}$$

Error table

	$N = 9$			$N = 11$		
$e^{-a\ell}$	$h = 0.02$	$h = 0.01$	$h = 0.005$	$h = 0.02$	$h = 0.01$	$h = 0.005$
$15/16$	0.085	0.072	0.068	0.082	0.068	0.0643
$7/8$	0.073	0.059	0.054	0.071	0.055	0.0500
$3/4$	0.061	0.042	0.035	0.059	0.038	0.0296
$2/3$	0.057	0.036	0.028	0.055	0.031	0.0204
$1/2$	**0.054**	0.031	0.021	**0.052**	0.025	0.0090
$1/4$	0.054	**0.029**	0.019	0.051	**0.023**	0.0023
$1/8$	0.054	0.029	**0.019**	0.051	0.023	0.0012
$1/16$	0.055	0.030	0.019	0.052	0.023	0.0005

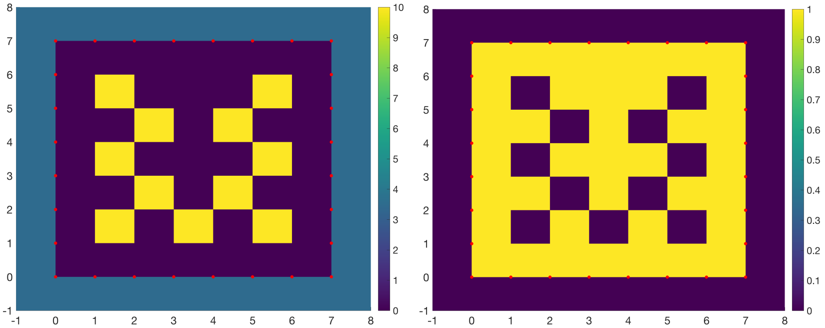
e_h for different h and a and N

Iteration counts and runtime

	$N = 9$			$N = 11$		
$e^{-a\ell}$	$h = 0.02$	$h = 0.01$	$h = 0.005$	$h = 0.02$	$h = 0.01$	$h = 0.005$
$15/16$	277 (104)	305 (518)	315 (2926)	316 (184)	350 (993)	364 (5214)
$7/8$	195 (75)	215 (394)	222 (2079)	220 (134)	246 (205)	256 (3611)
$3/4$	137 (51)	149 (259)	154 (1434)	153 (89)	172 (478)	179 (2475)
$2/3$	117 (44)	127 (224)	131 (1203)	132 (75)	146 (400)	152 (2087)
$1/2$	90 (35)	99 (178)	103 (947)	102 (62)	115 (324)	119 (1675)
$1/4$	68 (27)	73 (124)	75 (716)	76 (47)	85 (234)	87 (1231)
$1/8$	56 (23)	64 (116)	68 (647)	62 (39)	73 (210)	79 (1124)
$1/16$	57 (23)	70 (126)	77 (725)	63 (40)	78 (217)	88 (1248)
dofs	0.51M	2.01M	8.00M	0.74M	2.94M	11.73M

Iteration counts (runtime in sec) for different h and a and N

Example 2: Lattice problem



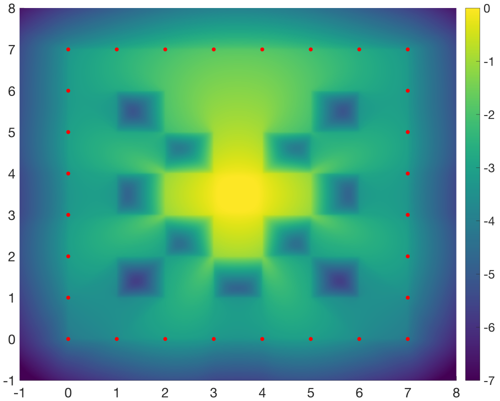
Left: Extended absorption coefficient. Right: Extended scattering coefficient

Reference solution $\widetilde{\phi} = \phi_{a,h}$ computed for

- $N = 31,332\,929$ vertices
- $\dim \mathbb{W}_h^+ = 165\,132\,784$
- $\dim \mathbb{W}_h^+ + \dim \mathbb{W}_h^- = 515\,488\,240$
- 4GB storage requirements for the reference solution

Results

$e^{-a\ell}$	$1/2$	$1/4$	$1/8$	$1/16$
$e_h \times 1000$	1.463	0.681	0.346	0.141



$\log_{10}$-plot of the angular average of the reference solution.

Conclusion

Analysis

- Developed perfectly matched layer approach for NTE
- Well-posedness and error analysis of the PML approach

Numerics

- Stable variational formulation with error bounds
- Variational framework that leads to sparse linear systems with Kronecker product structure

for details see [Egger & S (2019)]