Adaptive Source Term Iteration – A Stable Formulation for Radiative Transfer –

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(mono-energetic) Radiative Transfer Problem

We are looking for a particle density $u \in L_2(D \times S)$ satisfying $(\mathcal{T}_S - \mathcal{K}_S)u(x, s) = f(x, s) \quad \text{in } D \times S$ $u = g \quad \text{on } \Gamma_-$

with

$$\mathcal{T}_{\mathsf{S}} u(x, s) \coloneqq s \cdot \nabla u(x, s) + \sigma(x, s) u(x, s)$$
$$\mathcal{K}_{\mathsf{S}} u(x, s) \coloneqq \int_{\mathsf{S}} k(x, s', s) u(x, s') \, \mathrm{d}s'$$





Obstructions

- high dimensional (n = 2, 3 dimensional space + n 1 dimensional transport direction)
- global scattering kernel
- reliable error estimates?
 - a priori error estimates often require unrealistic regularity assumptions on the solution
- \rightarrow a posteriori estimates
 - error control of the solution
 - adaptive grid refinement





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$$u_0 = 0$$

 $u_{n+1} = \mathcal{T}_S^{-1}(\mathcal{K}_S u_n + f), \quad n = 0, 1, 2, \dots$





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- In the iterations:
 - Accuracy in solution of transport problems is dynamically increased across iterations

 → Need for tight error bounds to avoid adding unnecessary numerical effort ~→ DPG
 [Broersen et al., 2017]
 - Repeated application of \mathcal{K}_S with increased accuracy \rightsquigarrow Compression techniques.





We explain how to approximate

$$\mathcal{K}\mathbf{v}(\mathbf{x},\mathbf{s}) = \int_{\mathbf{S}} \mathbf{k}(\mathbf{s},\mathbf{s}')\mathbf{v}(\mathbf{x},\mathbf{s}') \,\mathrm{d}\mathbf{s}'$$

with the model kernel of Henyey and Greenstein [1941]

$$k(\boldsymbol{s}, \boldsymbol{s}') = k(\underbrace{\boldsymbol{s} \cdot \boldsymbol{s}'}_{=\cos \theta}) \coloneqq \frac{1}{2\pi} \frac{1 - \gamma^2}{1 + \gamma^2 - 2\gamma \boldsymbol{s} \cdot \boldsymbol{s}'}$$



where $\gamma \in (-1, 1)$.

The example illustrates the following issue:

- A naive approximation of $\mathcal{K}v$ with quadratures entails a quadratic cost in the number of directions.
- One can diminish this cost by exploiting sparsity.
- We illustrate how to achieve this depending on γ .

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Low-Rank Approximation of the Henyey–Greenstein Kernel





Singular values of Henyey–Greenstein kernel.





Wavelet Approximation of the Henyey–Greenstein Kernel



When $\gamma \to 1$, the matrix $(k_{\lambda,\lambda'})_{\lambda,\lambda'}$ becomes quasi-sparse and we can apply compression techniques to efficiently apply the kernel.





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When $\gamma \rightarrow 1$, the matrix $(k_{\lambda,\lambda'})_{\lambda,\lambda'}$ becomes quasi-sparse and we can apply compression techniques to efficiently apply the kernel.





$$\mathcal{T}_{s}u = s \cdot \nabla u + \sigma u = f.$$

To obtain reliable a posteriori error estimates, we solve this equation using a Discontinuous Petrov–Galerkin method.



Given a variational formulation:

Find $u \in \mathcal{U}$ such that

$$b(u, v) = \ell(v)$$
 for all $v \in \mathcal{V}$

for Hilbert spaces $(\mathcal{U}, \|\cdot\|_{\mathcal{U}}), (\mathcal{V}, \|\cdot\|_{\mathcal{V}})$, continuous bilinear form $b: \mathcal{U} \times \mathcal{V} \to \mathbb{R}$ and $\ell \in \mathcal{V}'$.

Goal: Stability



Given a variational formulation: Find $u_h \in \mathcal{U}_h$ such that

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Goal: Stability

• Discrete approximation yields a best approximation (up to a constant)

$$\|u - u_h\|_{\mathcal{U}} \leq \kappa_{\mathcal{U},\mathcal{V}'}(\mathcal{B}_h) \inf_{w_h \in \mathcal{U}_h} \|u - w_h\|_{\mathcal{U}}.$$



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Residual-based error bound

$$\|u-u_h\|_{\mathcal{U}}\simeq \|b(u_h,\cdot)-\ell\|_{\mathcal{V}'}$$
.



- For elliptic problems we can set $\mathcal{V}_{-}=\mathcal{U}$. Then coercivity

$$b(u, u) \geq c_B \|u\|_{\mathcal{U}}^2 \qquad \forall u \in \mathcal{U}$$

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- Without coercivity Banach–Nečas–Babuška guarantees stability when we choose the test space ${\cal V}\;$ in such a way that

$$\inf_{u \in \mathcal{U}} \sup_{v \in \mathcal{V}} \frac{b(u, v)}{\|u\|_{\mathcal{U}} \|v\|_{\mathcal{V}}} \geq c_B > 0.$$



• For elliptic problems we can set $\mathcal{V}_h = \mathcal{U}_h$. Then coercivity

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$$\inf_{\boldsymbol{u_h}\in\mathcal{U_h}}\sup_{\boldsymbol{v_h}\in\mathcal{V_h}}\frac{b(\boldsymbol{u_h},\boldsymbol{v_h})}{\|\boldsymbol{u_h}\|_{\mathcal{U_h}}\|\boldsymbol{v_h}\|_{\mathcal{V_h}}}\geq c_B>0.$$

This needs to be checked for the finite dimensional discretization, as it does not automatically carry over from the infinite dimensional setting!



Choose \mathcal{U}_h to Ensure Good Approximation Properties, Choose \mathcal{V}_h to Ensure Stability

How to choose \mathcal{V}_h for given \mathcal{U}_h ?



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Optimal test norm

$$\|\cdot\|_{\mathcal{V},opt}\coloneqq \sup_{u\in\mathcal{U}}rac{b(u,v)}{\|u\|_{\mathcal{U}}}$$



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$$\|\cdot\|_{\mathcal{V},opt} \coloneqq \sup_{u\in\mathcal{U}} \frac{b(u,v)}{\|u\|_{\mathcal{U}}}$$

Optimal test space V_h = B^{-*}R_UU_h, where R_U: U → U' is the Riesz isomorphism, that is V_h := T(U_h) where

$$\langle T(u_h), v \rangle_{\mathcal{V},opt} = b(u_h, v), \qquad \forall v \in \mathcal{V}$$



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- This yields
 - residual based error bound

$$\|u_h - u\|_{\mathcal{U}} = \|b(u_h, \cdot) - \ell\|_{\mathcal{V}', opt}$$

- best approximation property

$$\|u - u_h\|_{\mathcal{U}} = \inf_{w_h \in \mathcal{U}_h} \|u - w_h\|_{\mathcal{U}}$$



Computation of the Optimal Test Space

We have to compute \mathcal{V}_h by solving

$$\langle T(u_h), v \rangle_{\mathcal{V},opt} = b(u_h, v), \qquad \forall v \in \mathcal{V}$$

[see e.g. Demkowicz and Gopalakrishnan, 2015; Broersen et al., 2017]



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 - use an ultra-weak variational formulation

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We can compute an approximation for \mathcal{V}_h by solving

$$\langle \hat{T}(u_h), v
angle_{\mathcal{V},K} = b_K(u_h, v), \qquad \forall v \in \hat{\mathcal{V}} |_K,$$

where *K* is a single cell and $\langle \cdot, \cdot \rangle_{\mathcal{V},K}$ and $b_{\mathcal{K}}(\cdot, \cdot)$ denote restrictions to *K*.

[see e.g. Demkowicz and Gopalakrishnan, 2015; Broersen et al., 2017]





A Stable DPG Formulation of Linear Transport

In our ideal iteration, we need to solve transport problems of the type

 $\boldsymbol{s} \cdot \nabla \boldsymbol{u} + \sigma \boldsymbol{u} = \boldsymbol{f}.$





$$\int_{\mathsf{D}} \mathbf{s} \cdot \nabla u \mathbf{v} + \sigma u \mathbf{v} \, d\mathbf{x} = \int_{\mathsf{D}} \mathbf{f} \mathbf{v} \, d\mathbf{x}.$$

cell-wise integration by parts on a fixed grid D_h leads to

$$\int_{\mathsf{D}} \sigma u v - u s \cdot \nabla v \, dx + \int_{\partial \mathsf{D}_h} n \cdot s u \llbracket v \rrbracket \, dx = \int_{\mathsf{D}} f v \, dx.$$



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cell-wise integration by parts on a fixed grid D_h leads to

$$\int_{\mathsf{D}} \sigma u v - u s \cdot \nabla v \, dx + \int_{\partial \mathsf{D}_h} n \cdot s \theta \llbracket v \rrbracket \, dx = \int_{\mathsf{D}} f v \, dx.$$

Ultra-weak formulation with $u \in L_2(D)$.



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Ultra-weak formulation with $u \in L_2(D)$. Broken test space with broken norm

$$\|v\|_{H(s;D_h)} = \left(\sum_{T\in D_h} \|v\|_{H(s;K)}^2\right)^{1/2}$$







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Broersen et al. [2017]: Fullfills requirements of Banach-Nečas-Babuška.







Data of the checkerboard benchmark problem





To reach target accuracy η in a step of the Source Term Iteration, we have some freedom in distributing the discretization errors:

- $\kappa_1 \eta$: accuracy for kernel application
- $\kappa_2 \eta$: accuracy for evaluation of source term *f*
- $\kappa_3\eta$: accuracy for transport solver

To guarantee convergence, the following restriction holds:

 $C_{\mathcal{T}}\kappa_1 + C_{\mathcal{T}}\kappa_2 + 2\kappa_3 \leq 1.$









 $\kappa_1 = \theta / C_T, \kappa_2 = 0, \kappa_3 = (1 - \theta) / 2, \theta = 0.2$





 $\kappa_1 = \theta / C_T, \kappa_2 = 0, \kappa_3 = (1 - \theta) / 2, \theta = 0.02$





 $\kappa_1 = \theta / C_T, \, \kappa_2 = 0, \, \kappa_3 = (1 - \theta) / 2, \, \theta = 0.002$





 $\kappa_1 = \theta / C_T, \kappa_2 = 0, \kappa_3 = (1 - \theta) / 2, \theta = 0.0002$





Grids for two different transport solutions and the integrated solution.





- 0.1 - 0.09

- 0.08

0.07

- 0.06

- 0.05

- 0.04

- 0.03

- 0.02

- 0.01 - 0.0 Joint work with Angela Klewinghaus and Olga Mula [Gruber et al., 2017], based upon the Dune finite element library [Blatt et al., 2016] (https://dune-project.org/).

- Suitable for different types of problems, e.g.
 - radiative transport (O. Mula, F. Gruber)
 - convection-diffusion (A. Klewinghaus)
 - optimal control problems with transport constraints (A. Klewinghaus)
 - porous media (V. König)
- a posteriori estimation
- capable of adaptive *h* refinement
- free software (GPL 2 with runtime-exception) available at https://gitlab.dune-project.org/felix.gruber/dune-dpg



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