
The Discontinuous Petrov–Galerkin Method for Radiative Transfer Problems

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joint work with Wolfgang Dahmen and Olga Mula

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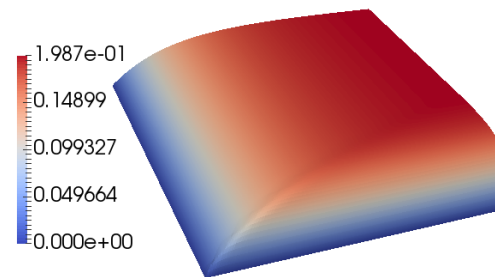
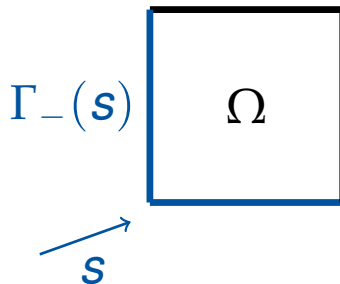
MathCCES Lunch Seminar, June 22, 2017

(mono-energetic) Radiative Transfer Problem

$$\begin{aligned} \mathcal{B}u(x, s) &:= (\mathcal{T}_S - \mathcal{K}_S)u(x, s) = f(x, s) && \text{in } \Omega \times S \\ u &= g && \text{on } \Gamma_- \end{aligned}$$

with

$$\begin{aligned} \mathcal{T}_S u(x, s) &:= s \cdot \nabla u(x, s) + \sigma(x, s)u(x, s) \\ \mathcal{K}_S u(x, s) &:= \int_S k(x, s', s)u(x, s') ds' \end{aligned}$$



(mono-energetic) Radiative Transfer Problem

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
 - a posteriori estimates
 - error control for “outer iteration”
 - adaptive grid refinement

Roadmap

- ideal iteration $u_{n+1} = u_n + \mathcal{P}(f - \mathcal{B}u_n)$, $n = 0, 1, 2, \dots$
 - in infinite dimensional setting
 - \mathcal{K}_S only needs to be evaluated
 - mapping property, norm equivalence
 - $\mathcal{P} = \mathcal{T}_S^{-1}$ for dominating transport, i. e. $\|\mathcal{T}_S^{-1}\mathcal{K}_S\|_{\mathcal{L}(L_2, L_2)} < 1$, otherwise use inner iteration for preconditioning
 - costs of last iteration dominate

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- numerical realization:
 - approximately solve inner iteration with prescribed accuracy; this accuracy has to be chosen to ensures convergence to the infinite dimensional solution
 - a posteriori error estimates for efficient transport solvers
 - adaptive grid refinement for non-smooth solutions
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 - convergence of ideal iteration
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- approximately applying \mathcal{K}_S
 - operator compression
 - low-rank approximation

Nested Iteration DPG

- Assuming $\|\mathcal{T}_S^{-1}\mathcal{K}_S\|_{\mathcal{L}(L_2,L_2)} = \rho < 1$, we choose $\mathcal{P} = \mathcal{T}_S^{-1}$ in the *ideal iteration* and obtain

$$\begin{aligned}u_0 &= 0 \\u_{n+1} &= u_n + \mathcal{T}_S^{-1}(f - \mathcal{B}u_n) \\&= \mathcal{T}_S^{-1}(\mathcal{K}_S u_n + f), \quad n = 0, 1, 2, \dots\end{aligned}$$

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- We need a numerical scheme to realize approximately the fixed point iterations while still guaranteeing contraction of the infinite dimensional iteration.
- 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 \rightsquigarrow DPG [Broersen et al., 2016]
 - Repeated application of \mathcal{K}_S with increased accuracy \rightsquigarrow Compression techniques.

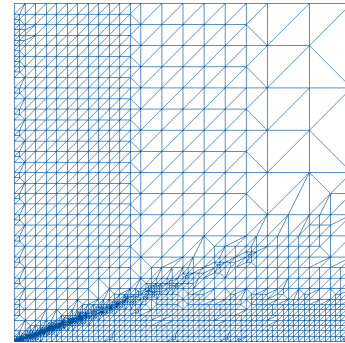
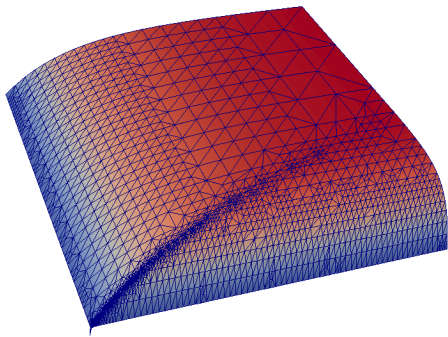
Nested Iteration DPG

Algorithm 1 NI-DPG [$\mathcal{T}_S, \mathcal{K}_S, f, \varepsilon$] $\rightarrow u_\varepsilon$

```
 $u \leftarrow 0$   
 $\text{err} \leftarrow \text{err}_0$   
while  $\text{err} > \varepsilon$  do  
    Approximatively compute  $w = \mathcal{K}_S u$ .  
    repeat  
        Solve  $\mathcal{T}_S u = f + w$  as a set of transport problems using DPG.  
        Refine grid.  
    until target accuracy is reached  
     $\text{err} \leftarrow$  combined error of computing  $w$  and  $u$   
    Increase target accuracy.  
end while  
 $u_\varepsilon \leftarrow u$ 
```

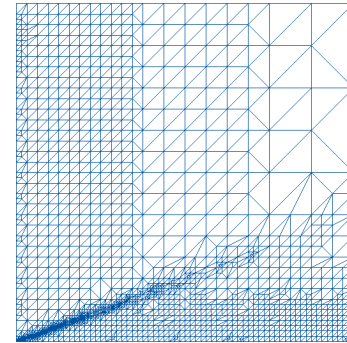
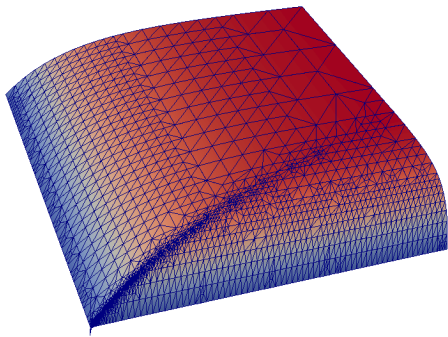
Adaptive Grid Refinement

Solutions to the transport problems are smooth in large parts → adaptive grid refinements keep the number of DoFs minimal.



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For the computation of the scattering integral, we need to merge the adaptively refined grids from the transport solutions.

But the more expensive task of computing transport solutions can be done on the smaller adaptively refined grids.

Stable Variational Formulations

Given a variational formulation:

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

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

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

Goal: Stability

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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

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

Stable Variational Formulations

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

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

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

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

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

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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

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

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

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

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

Choosing a Good Test Search Space

- δ -proximality (test search space $\hat{\mathcal{V}}$ close enough to optimal test space \mathcal{V}_h):

$$\forall 0 \neq v_h \in \mathcal{V}_h \exists \hat{v}_h \in \hat{\mathcal{V}} \text{ such that } \|v_h - \hat{v}_h\|_{\mathcal{V}} \leq \delta \|v_h\|_{\mathcal{V}}.$$

Dahmen et al. [2012]: This guarantees inf-sup constant $\geq (1 - \delta)$.

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- hard to verify
- for the transport problems that we solve, Broersen et al. [2016] show that $\hat{\mathcal{V}}$ can be chosen as a finite element space that has a slightly higher polynomial degree than the trial space and lives on a subgrid.

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

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

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Broken test space with broken norm

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

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Broersen et al. [2016]: Fullfills requirements of Banach–Nečas–Babuška.

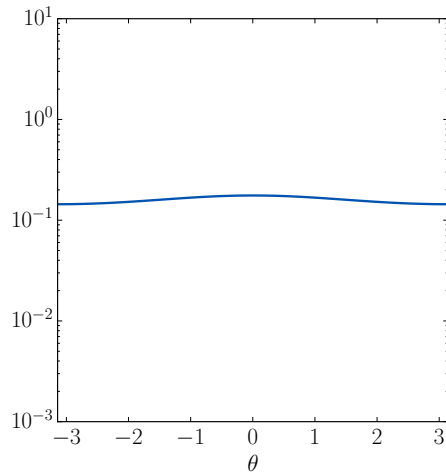
The Henyey–Greenstein Kernel

[Henyey and Greenstein, 1941]

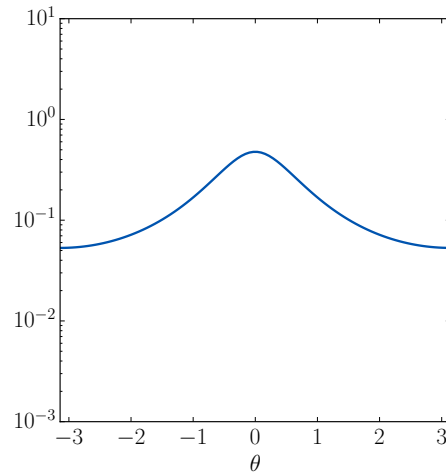
$$k(\mathbf{s}, \mathbf{s}') := \frac{1}{2\pi} \frac{1 - \gamma^2}{1 + \gamma^2 - 2\gamma \cos(\mathbf{s} - \mathbf{s}')} \quad \text{with } \gamma \in (-1, 1).$$

- When $\gamma \geq 0$, the scattering is forward peaked and K is positive semi-definite.
- Negative γ models backward scattering.
- Originally used to model light scattering in the milky way.
- Nowadays used in a wide variety of applications including nuclear physics [Sanchez and McCormick, 2004].

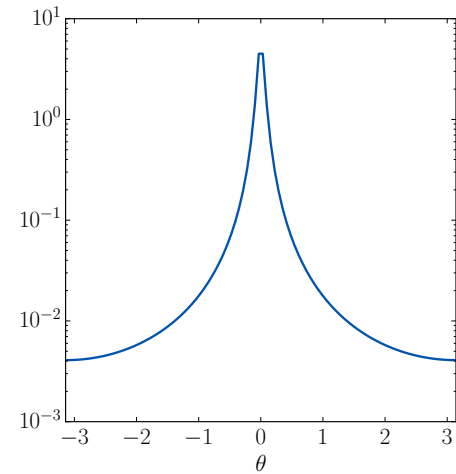
The Henyey–Greenstein Kernel



(a) $\gamma = 0.05$



(b) $\gamma = 0.5$

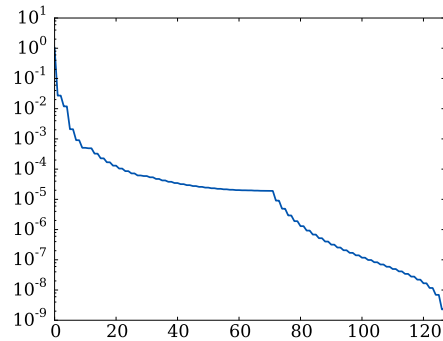


(c) $\gamma = 0.95$

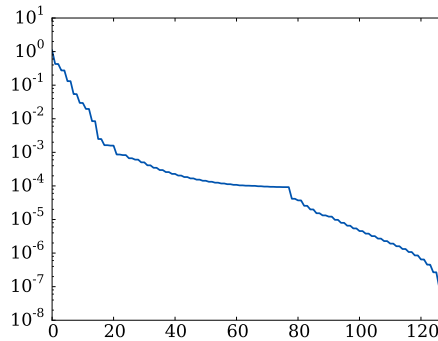
Figure: Henyey–Greenstein kernel as a function of $\theta = \angle(s, s')$

Larger γ leads to more concentrated forward-scattering.

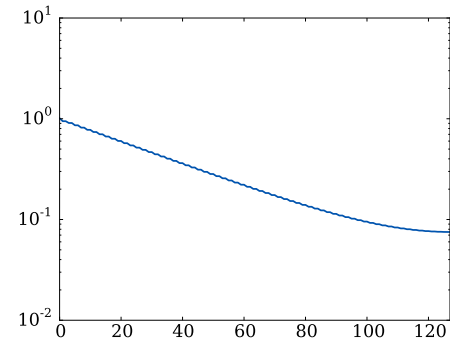
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(c) $\gamma = 0.95$

Figure: singular values of Henyey–Greenstein kernel

For small γ fast decay of singular values.

→ Kernel can be approximated by low rank matrix.

The Henyey–Greenstein Kernel

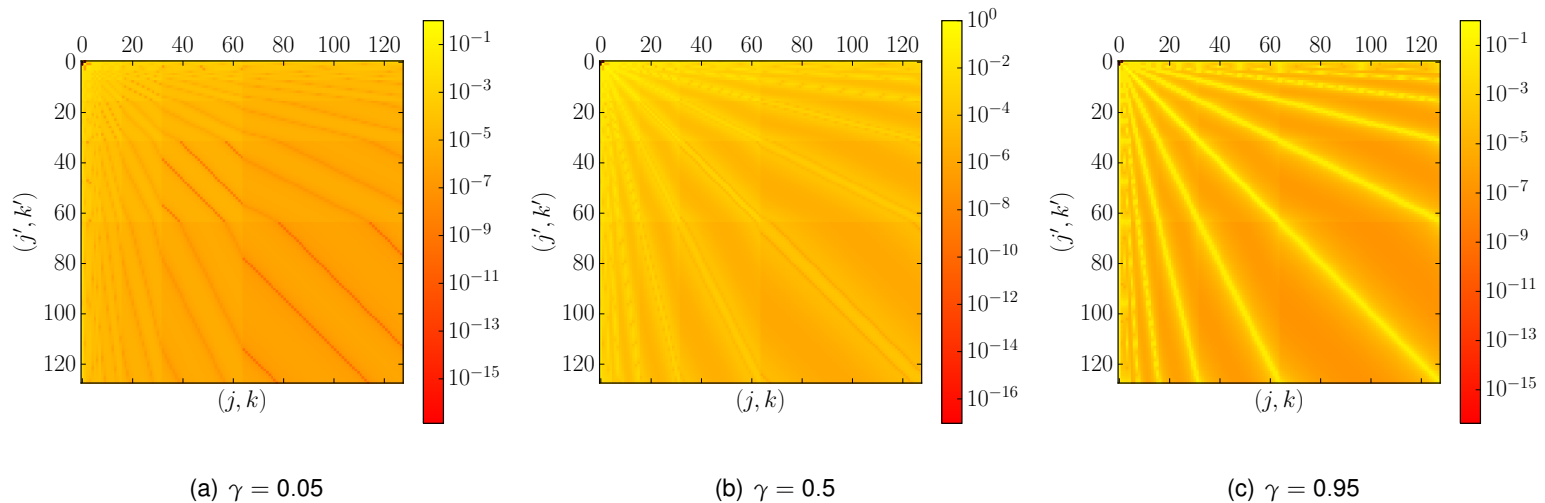


Figure: wavelet representation of Henyey–Greenstein kernel

- Behaviour similar to boundary integral problems.
- For γ close to 1 we can see the typical “finger” structure which hints at good wavelet-compressibility.

Numerical Results

Nested Iteration DPG for

$$\begin{aligned}(\mathcal{T}_S - \mathcal{K}_S)u(x, s) &= 1 \quad \text{in } \Omega \times S \\ u &= 0 \quad \text{on } \Gamma_-\end{aligned}$$

with

$$\mathcal{T}_S u(x, s) := s \cdot \nabla u(x, s) + 5u(x, s)$$

$$\mathcal{K}_S u(x, s) := \int_S k(x, s', s) u(x, s') ds'$$

where k is a Henyey–Greenstein scattering kernel with $\gamma = 0.9$.

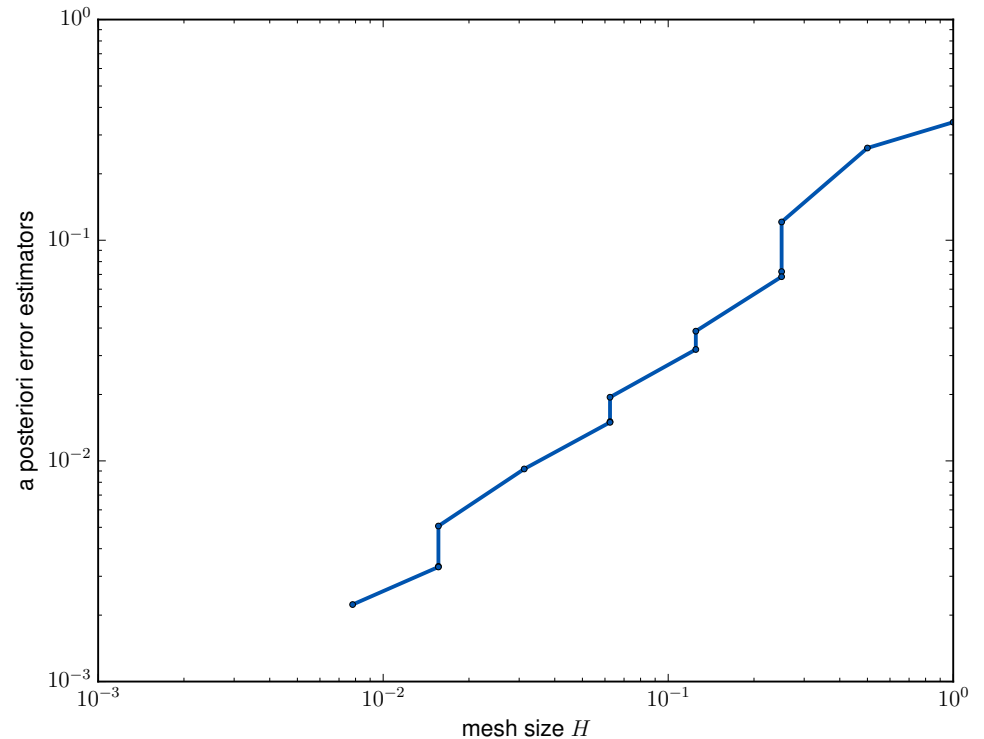


Figure: a posteriori errors of the adaptive sourceterm iteration

A Generic Library for DPG: dune-dpg

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)
 - soon: 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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