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Model reduction based on optimally stable variational formulations of parametrized transport equations

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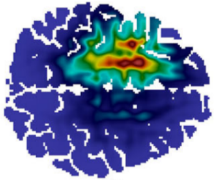
Motivation

- Project: **GlioMaTh** [1]
- Glioma invasion modeled by time-dependent kinetic transport equations



[Engwer et al. 2014]

This talk: (Parametrized) first-order transport equations

$$\partial_t u(\mu) + \vec{b}(\mu) \cdot \nabla u(\mu) + c(\mu) u(\mu) = f(\mu) \quad \text{with I.C., B.C.}$$

- Stable variational formulation
- Stable discretization
- Model order reduction $\Longrightarrow$ Reduced Basis Method

[1] Funded by German Federal Ministry of Education and Research

Existing works for similar equations

- Stable variational formulations and discretizations for transport equations: [Dahmen et al. 2012], DPG method, e.g. [Demkowicz, Gopalakrishnan 2010, 2011], [Broersen, Dahmen, Stevenson 2016], ...
- Model Reduction/RB for transport dominated problems: [Dahmen, Plesken, Welper 2014], [Zahm, Nouy 2016], [Abgrall, Amsallem, Crisovan 2016], [Billaud-Friess, Nouy, Zahm 2014], [Cagniart, Crisovan, Maday, Abgrall 2017], [Cagniart, Maday, Stamm 2016], [Carlberg 2015], [Gerbeau, Lombardi 2014], [Iollo, Lombardi 2014], [Ohlberger, Rave 2013], [Reiss et al. 2015], [Taddei, Perotto, Quarteroni 2013], [Welper 2017], ...

Non-parametric problem

First-order linear transport equation:

$$\begin{aligned} \vec{b}(x) \cdot \nabla u(x) + c(x)\, u(x) &= f(x) \quad && x \in \Omega \\ u(x) &= g(x) \quad && x \in \Gamma_{\text{in}} \end{aligned}$$

- $\Omega \subset \mathbb{R}^d$ spatial or space-time domain
- $\Gamma_{\text{in}} = \{x \in \partial\Omega : \vec{b}(x) \cdot \vec{n}(x) < 0\} \subset \partial\Omega$ inflow boundary
- Assume either

$$0 \neq \vec{b} \in C^1(\Omega, \mathbb{R}^d) \quad \text{or} \quad c - \frac{1}{2}\nabla \cdot \vec{b} \geq \kappa > 0 \quad \text{in } \Omega$$

(Optimal) variational formulation [Dahmen et al. 2012]

Bilinear form:

$$b(v,w) = \left(v, -\vec{b}\cdot\nabla w + w(c - \nabla\vec{b})\right)_{L_2(\Omega)} =: (v, B^* w)_{L_2(\Omega)}$$

- Define the space

$$C^1_{\mathrm{out}}(\Omega) = \{w \in C^1(\Omega) : w|_{\Gamma_{\mathrm{out}}} \equiv 0\}$$

- and the norm

$$\|w\|_{\mathcal{Y}} := \|B^* w\|_{L_2(\Omega)}$$

Trial space:

$$\mathcal{X} := L_2(\Omega)$$

Test space:

$$\mathcal{Y} := \mathrm{clos}_{\|\cdot\|_{\mathcal{Y}}} C^1_{\mathrm{out}}(\Omega) \subseteq L_2(\Omega)$$

(Optimal) variational formulation [Dahmen et al. 2012]

- Given $f \in \mathcal{Y}'$, there exists a unique $u \in L_2(\Omega)$ s.t.

$$b(u,v) = f(v) \quad \forall v \in \mathcal{Y}$$

- It holds

$$\gamma := \sup_{w \in L_2(\Omega)} \sup_{v \in \mathcal{Y}} \frac{b(w,v)}{\|w\|_{L_2(\Omega)} \|v\|_{\mathcal{Y}}} = 1$$

$$\beta := \inf_{w \in L_2(\Omega)} \sup_{v \in \mathcal{Y}} \frac{b(w,v)}{\|w\|_{L_2(\Omega)} \|v\|_{\mathcal{Y}}} = 1$$

Petrov-Galerkin methods

- Define finite dimensional trial and test spaces $\mathcal{X}_\delta \subset L_2(\Omega)$ and $\mathcal{Y}_\delta \subset \mathcal{Y}$.
- Petrov-Galerkin projection:

$$u_\delta \in \mathcal{X}_\delta : \qquad b(u_\delta, v_\delta) = f(v_\delta) \quad \forall v_\delta \in \mathcal{Y}_\delta.$$

- A unique solution u_δ exists iff

$$\beta_\delta := \inf_{w_\delta \in \mathcal{X}_\delta} \sup_{v_\delta \in \mathcal{Y}_\delta} \frac{b(w_\delta, v_\delta)}{\|w_\delta\|_{L_2(\Omega)} \|v_\delta\|_{\mathcal{Y}}} > 0.$$

$$\gamma_\delta := \sup_{w_\delta \in \mathcal{X}_\delta} \sup_{v_\delta \in \mathcal{Y}_\delta} \frac{b(w_\delta, v_\delta)}{\|w_\delta\|_{L_2(\Omega)} \|v_\delta\|_{\mathcal{Y}}} < \infty,$$

- Stability as $\delta \to 0$: $\beta_\delta \geq \tilde{\beta} > 0$, $\gamma_\delta \leq \tilde{\gamma} < \infty$, for all $\delta > 0$.

Error and residual

- Define the error e_δ and residual $r_\delta(w)$:

$$e_\delta := u - u_\delta, \qquad r_\delta(w) := f(w) - b(u_\delta, w) = b(e_\delta, w), \; w \in \mathcal{Y},$$

- Quasi-best approximation, [Xu, Zikatanov 2003]:

$$\|e_\delta\|_{L_2(\Omega)} = \|u - u_\delta\|_{L_2(\Omega)} \leq \frac{\gamma_\delta}{\beta_\delta} \inf_{v_\delta \in \mathcal{X}_\delta} \|u - v_\delta\|_{L_2(\Omega)}$$

- Error-residual relationship

$$\beta_\delta \, \|e_\delta\|_{L_2(\Omega)} \leq \|r_\delta\|_{\mathcal{Y}'} \leq \gamma_\delta \, \|e_\delta\|_{L_2(\Omega)}.$$

- Optimal case $\beta_\delta = \gamma_\delta = 1$:

$$\|e_\delta\|_{L_2(\Omega)} = \inf_{v_\delta \in \mathcal{X}_\delta} \|u - v_\delta\|_{L_2(\Omega)}$$

$$\|e_\delta\|_{L_2(\Omega)} = \|r_\delta\|_{\mathcal{Y}'}$$

Optimally stable discretization spaces

- Aim: Find discretization spaces $\mathcal{X}_\delta \subset L_2(\Omega)$, $\mathcal{Y}_\delta \subset \mathcal{Y}$ with β_δ (close to) optimal, i.e. $\beta_\delta \approx 1$
- [Dahmen et al. 2012]: Given trial space $\mathcal{X}_\delta \subset L_2(\Omega)$ the optimally stable test space is

$$\mathcal{Y}_\delta = B^{-*}\mathcal{X}_\delta \subset \mathcal{Y}$$

where $B^{-*} := (B^*)^{-1} : L_2(\Omega) \to \mathcal{Y}$.

- Challenge: Due to inverse operator B^{-*}, the *exact* space $\mathcal{Y}_\delta$ is not computable

[1] $B^* w = -\partial_t w - \vec{b} \cdot \nabla w + w(c - \nabla \vec{b})$

Existing works: Find near optimal test space

[Dahmen et al., 2012]

- Use large test search space $\mathcal{W}_\delta$ to compute approximate optimal test space $\tilde{\mathcal{Y}}_\delta \subset \mathcal{W}_\delta \subset \mathcal{Y}$
- Since computation of $\tilde{\mathcal{Y}}_\delta$ still numerically unfeasible, rewrite as *saddle point problem*

Other approach: [Broersen, Dahmen, Stevenson 2016], DPG scheme based on alternative (broken) bilinear form defined on DG-spaces

New idea: Find optimal trial space

- Ansatz: Given a test space $\mathcal{Y}_\delta$ the optimally stable trial space is

$$\mathcal{X}_\delta = B^* \mathcal{Y}_\delta \subset L_2(\Omega).$$

- (Differential) operator B^* instead of inverse B^{-*} has to be applied

$\Longrightarrow$ *exactly* and *easily* computable for many relevant operators and test spaces

$\Longrightarrow$ spaces $(\mathcal{X}_\delta, \mathcal{Y}_\delta)$ satisfying $\beta_\delta = 1$.

- Question: Does $\mathcal{X}_\delta$ have good approximation properties?

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[1] $B^* w = -\vec{b} \cdot \nabla w + w(c - \nabla \vec{b})$

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Numerical realization

Problem: Find $u_\delta \in \mathcal{X}_\delta$ such that

$$(u_\delta, B^* v_\delta)_{L_2(\Omega)} = f(v_\delta) \quad \forall v_\delta \in \mathcal{Y}_\delta$$

Solution process for optimal trial space $\mathcal{X}_\delta = B^* \mathcal{Y}_\delta$:

1. Find $w_\delta \in \mathcal{Y}_\delta$ such that

$$(B^* w_\delta, B^* v_\delta)_{L_2(\Omega)} = f(v_\delta) \quad \forall v_\delta \in \mathcal{Y}_\delta$$

2. Set $u_\delta := B^* w_\delta \in \mathcal{X}_\delta$

$\Longrightarrow$ *Note:* $w_\delta \in \mathcal{Y}_\delta$ is supremizer of the solution $u_\delta \in \mathcal{X}_\delta$, i.e.

$$\frac{b(u_\delta, w_\delta)}{\|u_\delta\|_{L_2(\Omega)} \|w_\delta\|_{\mathcal{Y}}} = \frac{(B^* w_\delta, B^* w_\delta)_{L_2(\Omega)}}{\|B^* w_\delta\|_{L_2(\Omega)} \|B^* w_\delta\|_{L_2(\Omega)}} = 1$$

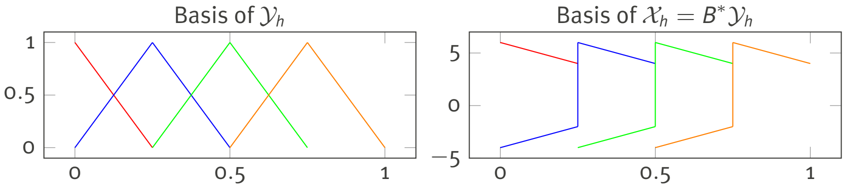
$\Longrightarrow$ Easy implementation of whole process

Example: 1D advection equation

- $\Omega := (0,1), \quad b(x) \equiv b > 0, \quad c(x) \equiv c$

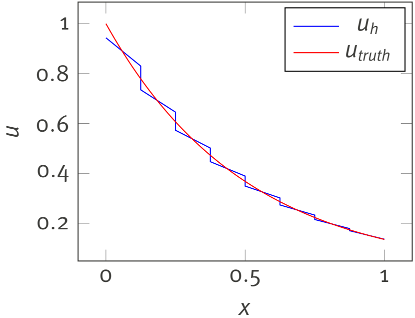
  $$Bu(x) := b\,u'(x) + c\,u(x),\ x \in \Omega, \qquad u(0) = g \quad (\Gamma_- = \{0\}).$$
- Adjoint operator: $B^*v(x) := -b\,v'(x) + c\,v(x)$
- Test space $\mathcal{Y}_h$: Standard piecewise linear Finite Elements with zero on right boundary $\Gamma_+ = \{1\}$

Basis functions for $h = \frac{1}{4}$, $b = 1$, $c = 2$:

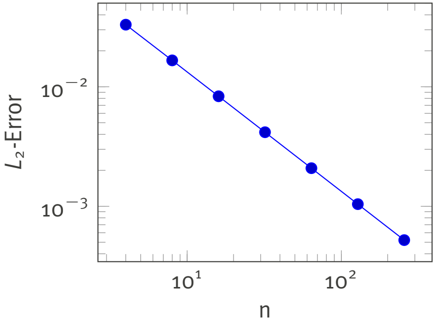


Example: 1D advection equation

True and approximate solution for $h = \frac{1}{8}$



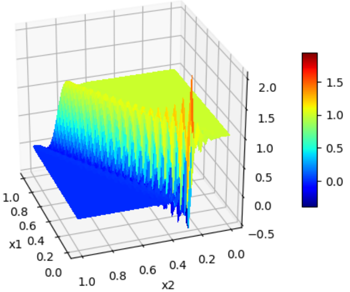
L_2-errors for varying grid sizes $n = h^{-1}$



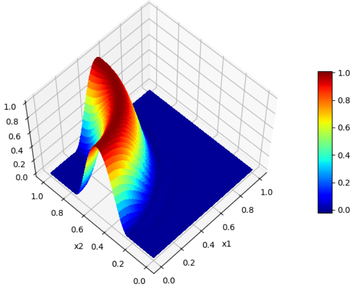
$\Longrightarrow$ Numerically observed first order convergence of the L_2-error

Example: 2D advection equation

Model problem: $\vec{b} \cdot \nabla u = 0$ in $\Omega = (0,1)^2$, $u = g$ on Γ_{in} .
Second order tensor product discrete spaces on rectangular grid



$\vec{b}$ constant, g p.w. constant
Observed L_2 convergence:
order $\approx 1/3$



$\vec{b} = (1-y, x)^T$, $g \in C^2(\Gamma_{in})$
Observed L_2 convergence:
order ≈ 1.65

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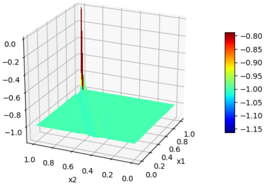
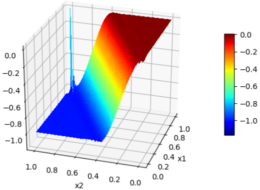
Example: 2D advection equation

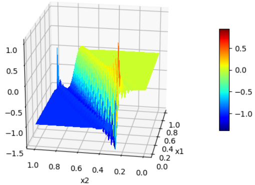
Drawback: Due to tensor product discrete spaces, unphysical restrictions of the trial space on the outflow boundary (in this example $u(1,1) = 0$)



$u \equiv -1$
Observed order ≈ 1



$g \in C^2(\Gamma_{\text{in}})$
Observed order ≈ 1



g p.w. constant
Observed order $\approx 1/3$

$\Longrightarrow$ Convergence order is limited to 1, no change of the order for less smooth problems

Parametrized problem

For each $\mu \in \mathcal{P}$ we want to solve

$$B_\mu u(\mu) = f_\mu$$

Optimal variational formulation for each μ:

Trial space:

$$\underbrace{\mathcal{X} := L_2(\Omega)}_{\text{Parameter independent}}$$

Test space:

$$\underbrace{\begin{aligned}\mathcal{Y}_\mu &:= \operatorname{clos}_{\|\cdot\|_{\mathcal{Y}_\mu}} C^1_{\mathrm{out},\mu}(\Omega) \subseteq L_2(\Omega) \\ \|w\|_{\mathcal{Y}_\mu} &:= \|B^*_\mu w\|_{L_2(\Omega)}\end{aligned}}_{\text{Parameter dependent}}$$

Reference test space: $\bar{\mathcal{Y}} := \bigcap_{\mu\in\mathcal{P}} \mathcal{Y}_\mu, \quad \|w\|_{\bar{\mathcal{Y}}} := \sup_{\mu\in\mathcal{P}} \|w\|_{\mathcal{Y}_\mu}$

Detailed discretization for the parametrized problem

- Test spaces:
  - Define discrete space $\bar{\mathcal{Y}}_\delta \subset \bar{\mathcal{Y}}$
  - Consider for each $\mu \in \mathcal{P}$ the space $\mathcal{Y}_{\delta,\mu} := (\bar{\mathcal{Y}}_\delta, \|\cdot\|_{\mathcal{Y}_\mu})$
- Optimal trial spaces:
  - Define for each $\mu \in \mathcal{P}$ the space $\mathcal{X}_{\delta,\mu} := B_\mu^* \mathcal{Y}_{\delta,\mu} \subset \mathcal{X}$

Parameter dependent pair of spaces:

$$
\begin{aligned}
\mathcal{X}_{\delta,\mu} &= \Big(\overbrace{B_\mu^* \bar{\mathcal{Y}}_\delta}^{\mu\text{-dependent}} , \overbrace{\|\cdot\|_{L_2(\Omega)}}^{\mu\text{-independent}} \Big) \\
\mathcal{Y}_{\delta,\mu} &= \Big(\underbrace{\bar{\mathcal{Y}}_\delta}_{\mu\text{-independent}} , \underbrace{\|B_\mu^* \cdot\|_{L_2(\Omega)}}_{\mu\text{-dependent}} \Big)
\end{aligned}
$$

$\Longrightarrow$ Optimal inf-sup constant $\beta_{\delta,\mu} = 1$ for each $\mu \in \mathcal{P}$

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Reduced discretization for the parametrized problem

- Test spaces:
  - Generate reduced space $\bar{\mathcal{Y}}_N \subset \bar{\mathcal{Y}}_\delta$
  - Consider for each $\mu \in \mathcal{P}$ the space $\mathcal{Y}_{N,\mu} := (\bar{\mathcal{Y}}_N, \|\cdot\|_{\mathcal{Y}_\mu})$
- Optimal trial spaces:
  - Define for each $\mu \in \mathcal{P}$ the space $\mathcal{X}_{N,\mu} := B^*_\mu \mathcal{Y}_{N,\mu} \subset \mathcal{X}_{\delta,\mu}$

Parameter dependent pair of spaces:

$$\mathcal{X}_{N,\mu} := \Big(\overbrace{B^*_\mu \bar{\mathcal{Y}}_N}^{\mu\text{-dependent}} , \overbrace{\|\cdot\|_{L_2(\Omega)}}^{\mu\text{-independent}} \Big) \subset \mathcal{X}_{\delta,\mu}$$

$$\mathcal{Y}_{N,\mu} := \Big(\underbrace{\bar{\mathcal{Y}}_N}_{\mu\text{-independent}} , \underbrace{\|B^*_\mu \cdot\|_{L_2(\Omega)}}_{\mu\text{-dependent}} \Big) \subset \mathcal{Y}_{\delta,\mu}$$

$\Longrightarrow$ Optimal inf-sup constant $\beta_{N,\mu} = 1$ for each $\mu \in \mathcal{P}$

Reduced discretization for the parametrized problem

- Reduced solution process for a given reduced test space $\mathcal{Y}_{N,\mu}$:
  1. Find $w_N(\mu) \in \mathcal{Y}_{N,\mu}$ such that
  $$(B_\mu^* w_N(\mu), B_\mu^* v_N)_{L_2(\Omega)} = f_\mu(v_N) \quad \forall v_N \in \mathcal{Y}_{N,\mu}$$
  2. Set $u_N(\mu) := B_\mu^* w_N(\mu)$
- Assumption: Affine parameter dependence:
$$B_\mu := \sum_{q=1}^{Q_B} \theta_b^q(\mu) B^q, \qquad f_\mu := \sum_{q=1}^{Q_f} \theta_f^q(\mu) f^q,$$

$\Longrightarrow$ Offline-/Online-Decomposition possible

Generation of reduced spaces

Generate reduced test space $\bar{\mathcal{Y}}_N \subset \bar{\mathcal{Y}}_\delta$

- Compute supremizer snapshots:
  First step of the detailed solution process: Find $w_\delta(\mu_i) \in \mathcal{Y}_{\delta,\mu_i}$ such that

$$(B^*_{\mu_i} w_\delta(\mu_i), B^*_{\mu_i} v_\delta)_{L_2(\Omega)} = f_{\mu_i}(v_\delta) \quad \forall v_\delta \in \mathcal{Y}_{\delta,\mu_i}$$

  $\Longrightarrow$ Supremizer of the solution $u_\delta(\mu_i) \in \mathcal{X}_{\delta,\mu_i}$
- Use (strong) Greedy algorithm to generate the reduced test space $\bar{\mathcal{Y}}_N \subset \mathrm{span}\{w_\delta(\mu_i), i \in I\}$
  $\Longrightarrow$ Optimal Trial Greedy algorithm

Existing works: Double Greedy algorithm

[Dahmen, Plesken, Welper, 2014]

$\Longrightarrow$ RB with near optimal test spaces

Double Greedy algorithm

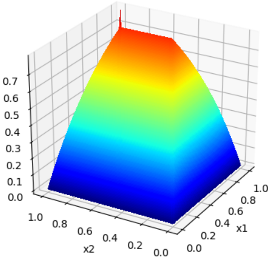
- Reduced discretization:
  - Fixed trial space X_N generated from snapshots
  - Test space Y_N with $\dim Y_N \geq \dim X_N$ (large enough to satisfy given stability threshold)
- Strategy:
  - Iteratively generate trial space with (“standard”) greedy search
  - With every new trial basis function:
    Stabilization of spaces by extending reduced test space until near optimal threshold for inf-sup constant is reached.

For better comparison: Use strong Double Greedy algorithm (without error indicators)

Parametrized 2D advection equation, constant data

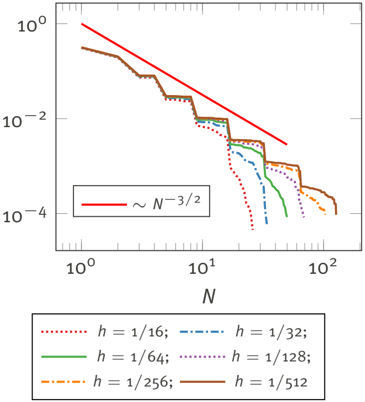
$$\begin{pmatrix}\cos \mu \\ \sin \mu\end{pmatrix} \cdot \nabla u(\mu) + u(\mu) = 1 \quad \text{in } \Omega$$
$$u(\mu) = 0 \quad \text{on } \Gamma_{in}$$

- $\mu \in \mathcal{P} := [0.2, \frac{\pi}{2} - 0.2]$



Full solution for $\mu = \pi/6$.

Optimal Trial Greedy



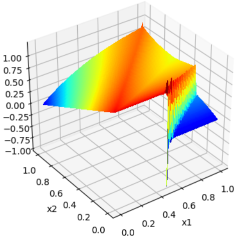
Param. 2D advection equation, non-regular data

$$\begin{pmatrix} \cos \mu \\ \sin \mu \end{pmatrix} \cdot \nabla u(\mu) + u(\mu) = f \quad \text{in } \Omega$$

$$u(\mu) = g \quad \text{on } \Gamma_{in}$$

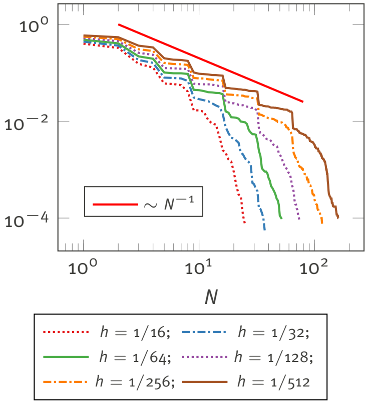
$$f = \begin{cases} 0.5, & x < y \\ 1, & x \geq y \end{cases}, \quad g = \begin{cases} 1 - y, & x \leq 0.5 \\ 0, & x \geq 0.5 \end{cases}$$

- $\mu \in \mathcal{P} := [0.2, \frac{\pi}{2} - 0.2]$



Full solution for $\mu = \pi/6$.

Optimal Trial Greedy



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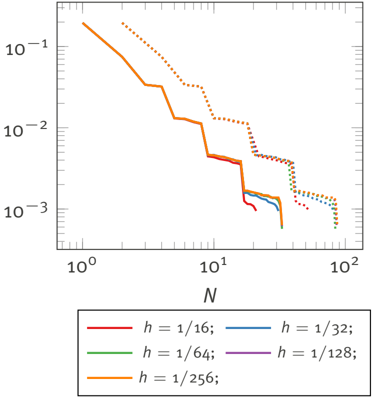
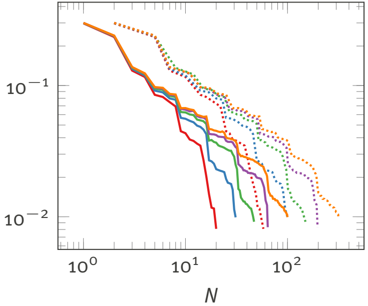
Results (strong) Double Greedy

Constant data, $\beta_N \geq 0.6$



Non-regular data, $\beta_N \geq 0.7$



Solid: Trial space dimension to error
Dotted: Test space dimension to error

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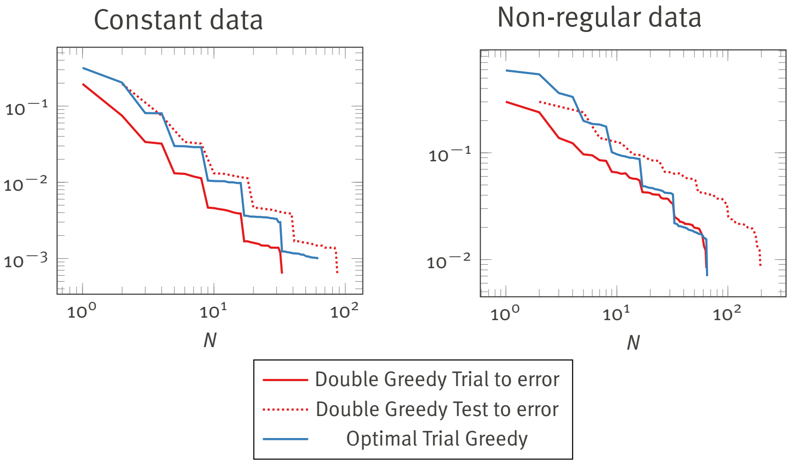
Comparison Opt. Trial Greedy / Double Greedy



Summary

- Optimally conditioned variational formulation for transport equations
- Computable optimally conditioned discrete spaces by
  - Choosing test space
  - Computing exact optimally stable trial space

$\Longrightarrow$ Best approximation property, tight error-residual relationship

- Application of the Reduced Basis method with
  - Generated test space
  - Parameter-dependent trial space
- Reduced discretization automatically optimally stable
- Good approximation properties in numerical experiments

Thank you for your attention!

J. Brunken, K. Smetana, and K. Urban.
(Parametrized) first order transport equations: realization of optimally stable Petrov-Galerkin methods.
https://arxiv.org/abs/1803.06925.

Code available: http://doi.org/10.5281/zenodo.1193260

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