Parametric Transport Problems

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Outline

The “Ideal Setting”

- $A_\mu u_\mu = f$, $A_\mu : \mathcal{H} \to \mathcal{H}'$, $\mu \in \mathcal{P}$, $\rightsquigarrow$ $\mathcal{S} := \{u_\mu : \mu \in \mathcal{P}\} \subset \mathcal{H}$
- Uniform “mapping property” $\|v\|_{\mathcal{H}} \sim \|A_\mu v\|_{\mathcal{H}'}$, $v \in \mathcal{H}$, $\mu \in \mathcal{P}$
- $S_n \subset \mathcal{H} \rightsquigarrow$ computable surrogates $R_n(u_\mu, \mu) \sim \|f - \Pi^\mu{}_n u_\mu\|_{\mathcal{H}'}$

$$c\, R_n(u_\mu) \le \mathrm{dist}_{\mathcal{H}}(u_\mu, S_n) = \|u_\mu - P_{S_n} u_\mu\|_{\mathcal{H}} \le C\, R_n(u_\mu)$$

- Greedy construction of S_n: given $u_j = u_{\mu_j}, j = 0, \dots, n-1$, $S_n = \mathrm{span}\,\{u_j : j = 0, \dots, n-1\}$

$$u_n := \mathrm{argmax}_{\mu \in \mathcal{P}} R_n(u_\mu), \quad \Rightarrow \quad \|u_n - P_{S_n} u_n\|_{\mathcal{H}} \ge \frac{c}{C} \mathrm{dist}_{\mathcal{H}}(\mathcal{S}, S_n)$$

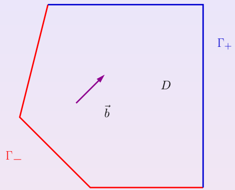
- Convergence [Binev/Cohen/D/DeVore/Petrova/Wojtasczyk]:

$$\inf_{\dim Y_n = n} \mathrm{dist}_{\mathcal{H}}(\mathcal{S}, Y_n) = O(n^{-\alpha}) \quad \Longrightarrow \quad \mathrm{dist}_{\mathcal{H}}(\mathcal{S}, S_n) = O(n^{-\alpha})$$

  $\mu \mapsto u_\mu$ smooth $\rightsquigarrow$ n small...
- What about transport dominated problems?

A Model Problem: Transport Equation

$$\vec{b} \cdot \nabla u + cu = f_\circ \quad \text{in } D$$
$$u = g \quad \text{on } \Gamma_-$$



$$\Gamma_- = \{x \in \partial D : \vec{b}(x) \cdot \vec{n}(x) < 0\} \quad \text{inflow boundary}$$
$$\Gamma_+ = \{x \in \partial D : \vec{b}(x) \cdot \vec{n}(x) > 0\} \quad \text{outflow boundary}$$
$$\Gamma_0 = \{x \in \partial D : \vec{b}(x) \cdot \vec{n}(x) = 0\} \quad \text{characteristic boundary}$$

Parameters:
- Inflow boundary data,
- parameter dependent velocity field $\vec{b}(\mu)$

Variational Formulation

$$\int_D f_\circ \, v \, dx = \int_D (\vec{b}\cdot\nabla u + cu)\, v\, dx = \underbrace{\int_D u(-\vec{b}\cdot\nabla v + v(c - \nabla\cdot\vec{b}))\, dx}_{=:(u,A^* v)}$$

$$+ \int_{\Gamma_-} uv(\vec{b}\cdot\vec{n})\, ds + \int_{\Gamma_+} uv(\vec{b}\cdot\vec{n})\, ds \quad u, v \in C^1(D)\cap C(\overline{D})$$

Natural test space: $Y := \mathrm{clos}_{\|A^*\cdot\|_{L_2(D)}}\{v \in C^1(D)\cap C(\overline{D}),\ v\,|_{\Gamma_+} = 0\}$

THEOREM:

Given $f_\circ \in Y'$, $g \in L_2(\Gamma_-,\omega)$, the problem: find $u \in L_2(D)$, s.t.

$$a(u,v) := (u, A^* v) = \int_D f_\circ v dx + \int_{\Gamma_-} |\vec{b}\cdot\vec{n}| g\gamma_-(v) ds =: f(v), \quad \forall\ v \in Y$$

has a unique solution satisfying $\|u\|_{L_2(D)} \lesssim \|f\|_{Y'}$.

If $u \in C^1(D)\cap C(\bar{D})$ then $\vec{b}\cdot\nabla u + cu = f_\circ$ in D, and $u|_{\Gamma_-} = g$.

A Simple Mechanism...

...how to choose the "energy space"

Mapping Properties:

Assume dense embeddings $X \subseteq L_2(D) \subseteq X'$ such that

$$A^* : D(A^*) \to X' \text{ injective}$$

- set $|||v||| := \|A^* v\|_{X'}$, $Y := \mathrm{clos}_{|||\cdot|||} D(A^*)$, $\|v\|_Y = \|A^* v\|_{X'}$
- then $\|Av\|_{Y'} = \|v\|_X$ and $1 = \|A^*\|_{Y \to X'} = \|A\|_{X \to Y'} = \|A^{-1}\|_{Y' \to X}$

In particular: $X = X' = L_2(D)$

$$\rightsquigarrow \|v\|_Y = \|A^* v\|_{L_2(D)}, \quad \langle v, w \rangle_Y = (A^* v, A^* w)$$

and

$$a(u, v) = (u, A^* v) = {}_{Y'}\langle Au, v \rangle_Y = {}_{Y'}\langle f, v \rangle_Y, \quad v \in Y$$

is perfectly well conditioned

"Ideal" Discretizations

PROPOSITION:

For any $X_h \subset L_2(D)$ one has

- $\|u - v_h\|_{L_2(D)} = \|A(u - v_h)\|_{Y'} = \|f - Av_h\|_{Y'}, \quad \forall\, v_h \in X_h$
- $u_h = \mathrm{argmin}_{v_h \in X_h} \|u - v_h\|_{L_2(D)} \quad \Leftrightarrow \quad u_h = \mathrm{argmin}_{v_h \in X_h} \|Av_h - f\|_{Y'}$
- $u_h = \mathrm{argmin}_{v_h \in X_h} \|u - v_h\|_{L_2(D)} \quad \Leftrightarrow$

  $a(u_h, y_h) := (u_h, A^* y_h) = {}_{Y'}\langle f, y_h \rangle_Y \quad \forall\, y_h \in Y_h := A^{-*} X_h$

BUT: ideal test space Y_h is not computable

... perhaps a perturbed version suffices...

A Stability Condition

δ-Proximal Subspaces

$\delta \in (0,1)$: $Y_h^\delta \subset Y$ is called δ-proximal for $X_h \subset L_2(D)$ if

$$\forall\ y_h \in Y_h := A^{-*}X_h \ \ \exists\ \ \tilde{y}_h \in Y_h^\delta \text{ such that } \|y_h - \tilde{y}_h\|_Y \le \delta \|y_h\|_Y$$

THEOREM:

Let $a(v,z) := (u, A^* z)$. If Y_h^δ is δ-proximal for X_h, one has

$$\inf_{v_h \in X_h} \sup_{z_h \in Y_h^\delta} \frac{a(v_h, z_h)}{\|v_h\|_{L_2(D)} \|z_h\|_Y} \ge \frac{1-\delta}{1+\delta}$$

Moreover, $u_{h,\delta} \in X_h$, defined by $a(u_{h,\delta}, v_h) = \ell(v_h) \quad \forall v_h \in Y_h^\delta$, satisfies

$$\|u - u_{h,\delta}\|_{L_2(D)} \le \frac{2}{1-\delta} \inf_{v_h \in X_h} \|u - v_h\|_{L_2(D)}$$

How to Realize δ-Proximity? – Y-Projections

For X_h pick $Z_h \subset Y$ "somewhat larger" $\dim Z_h > \dim Y_h = \dim X_h$

$$Y_h^\delta := P_{Y,h}(A^{-*}X_h), \quad \langle P_{Y,h}y, z_h\rangle_Y = \langle y, z_h\rangle_Y \quad \forall\, z_h \in Z_h$$

Note: for $y_h = A^{-*}v_h \in Y_h$, $v_h \in X_h$, $\tilde{y}_h = P_h y_h$ is given by

$$(A^*\tilde{y}_h, A^*z_h) = (v_h, A^*z_h), \quad \forall\, z_h \in Z_h$$

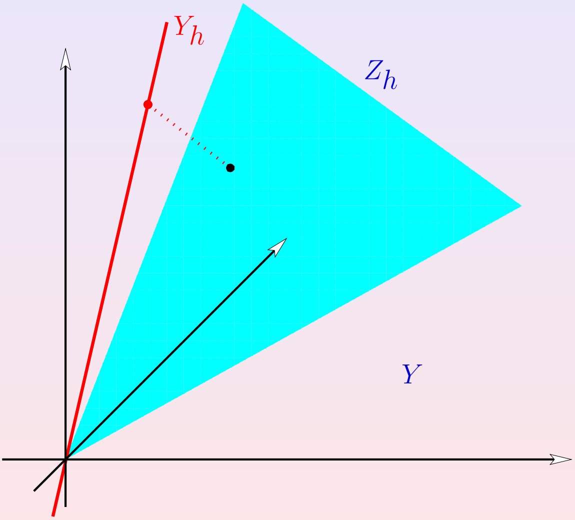
Note:

- δ-proximity relies on choice of auxiliary spaces Z_h
- In simple cases

$$X_h = \mathbb{P}_{p,\mathcal{T}_h} \subset L_2(D) \;\rightsquigarrow\; Z_h = \mathbb{P}_{p+q,\mathcal{T}_{2^{-r}h}} \cap C(D) \subset Y$$

Numerical experiments: $q = 1, r = 1$ or $q = 0, r = 2$ suffice

Illustration



Motivation: $u = u + A^{-1}(f - Au)$

$$
\begin{aligned}
\Leftrightarrow (u,v) &= (u,v) + (A^{-1}(f-Au), v) && \text{for all} \quad v \in L_2(D)\\
\Leftrightarrow (u,v) &= (u,v) + {}_{Y'}\langle f - Au, A^{-*}v\rangle_Y && \text{for all} \quad v \in L_2(D)\\
\Leftrightarrow (u,v) &= (u,v) + {}_{Y'}\langle f - Au, (AA^*)^{-1}Av\rangle_Y && \text{for all} \quad v \in L_2(D)\\
\Leftrightarrow (u,v) &= (u,v) + {}_{Y}\langle (AA^*)^{-1}(f - Au), Av\rangle_{Y'} && \text{for all} \quad v \in L_2(D)\\
\rightsquigarrow (u^{k+1},v) &= (u^k,v) + {}_{Y}\langle \underbrace{(AA^*)^{-1}(f - Au^k)}_{=:\hat{r}^k}, Av\rangle_{Y'} && \text{for all} \quad v \in L_2(D)
\end{aligned}
$$

$$
\Longleftrightarrow \left\{ \begin{array}{rcll} (A^*\hat{r}^k, A^*z) &=& {}_{Y'}\langle f - Au^k, z\rangle_Y & \text{for all} \quad z \in Y \\ (u^{k+1}, v) &=& (u^k, v) + (A^*\hat{r}^k, v) & \text{for all} \quad v \in L_2(D) \end{array} \right\}
$$

$\rightsquigarrow$ numerical scheme:

$$
\begin{array}{rcll} (A^*\hat{r}_h^k, A^*z_h) &=& {}_{Y'}\langle f - Au_h^k, z\rangle_Y & \text{for all} \quad z_h \in Z_h \subset Y \\ (u_h^{k+1}, v_h) &=& (u_h^k, v_h) + (A^*\hat{r}_h^k, v_h) & \text{for all} \quad v_h \in X_h \end{array}
$$

Properties of the Iterative Scheme

THEOREM:

$$a(u_{h,\delta}, \tilde{y}_h) = {}_{Y'}\langle f, \tilde{y}_h \rangle_Y, \quad \tilde{y}_h \in P_{Y,h}(A^{-*} X_h) \quad \rightsquigarrow$$

$$\|u_{h,\delta} - u_h^{k+1}\|_{L_2} \leq \delta \|u_{h,\delta} - u_h^k\|_{L_2}, \ k \in \mathbb{N}_0$$

$\rightsquigarrow$ stable Petrov-Galerkin solution without computing test basis!

PROPOSITION:

$(A^* \hat{r}_h, A^* z_h) = {}_{Y'}\langle \tilde{f}_h - Av_h, z_h \rangle_Y$ for all $z_h \in Z_h$
(Stab-OSC) $\rightsquigarrow$

$$(1-\delta)\|\tilde{f}_h - Av_h\|_{Y'} \leq \|\hat{r}_h\|_Y = \|A^* \hat{r}_h\|_{L_2(D)} \leq \|\tilde{f}_h - Av_h\|_{Y'}$$

Can be used to formulate an adaptive refinement scheme with optimal convergence

Radiative transfer:

$$
\begin{aligned}
A_\circ u(x,\mu) = \mu \cdot \nabla u(x,\mu) + \kappa(x) u(x,\mu) &= f_\circ(x), \quad x \in D \subset \mathbb{R}^d, \\
u(x,\mu) &= g(x,\mu),\ x \in \Gamma_-(\mu),
\end{aligned}
$$

where

$$
\Gamma_\pm(\mu) := \{x \in \partial D : \mp \mu \cdot \mathbf{n}(x) < 0\}, \qquad \mu \in \mathcal{S}\ .
$$

- For $D \subset \mathbb{R}^3$, $\mathcal{S} = S^2$, the unit $2-$sphere

  $\rightsquigarrow$ high dimensional problems
- Weak formulation in $X = L_2(D \times \mathcal{S})$ or even $X = L_2(D \times \mathcal{S}) \times [0, T]$
- Reduced basis method

Exploit the Mapping Property

$$\int_D (\mu\cdot\nabla u+\kappa u)v dx = \int_D u \underbrace{(-\mu\cdot\nabla v+\kappa v)}_{=:A(\mu)^* v} dx + \int_{\Gamma(\mu)_-} uv(\mu\cdot\mathbf{n}(x))d\Gamma, \quad v|_{\Gamma(\mu)_+} = 0$$

Given $X_n = \mathrm{span}\,\{\phi_0,\ldots,\phi_{n-1}\} \subset L_2(D)$, $\tilde{Y}_n(\mu) = P_{Y(\mu),Z_m}(A(\mu)^{-*}X_n)$

$$\begin{aligned}
\max_{\mu\in\mathcal{S}} \|u(\cdot,\mu) - P_{X_n}u(\cdot,\mu)\|_{L_2(D)} &\sim \|u(\cdot,\mu) - u_{n,\delta}(\cdot,\mu)\|_{L_2(D)} \\
&= \|f - Au_{n,\delta}(\cdot,\mu)\|_{Y(\mu)'} \\
&\sim \|f - Au_n^k(\cdot,\mu)\|_{Y(\mu)'} \\
&\sim \max_{\mu\in\mathcal{S}} \|A(\mu)^*\hat{r}_{n,\mu}(u_n^k)\|_{L_2(D)}
\end{aligned}$$

where $(A(\mu)^*\hat{r}_{n,\mu}(v), A(\mu)^*z) = {}_{Y(\mu)'}\langle f - Av, z\rangle_{Y(\mu)}$, $z \in Z_m$

Idea: along with X_n build a somewhat larger space $Z_m \subset \bigcap_{\mu\in\mathcal{S}} Y(\mu)$ so that $P_{Y(\mu),Z_m}$- projections realize δ-proximality uniformly in μ

A "Double" Greedy Scheme

X_h, Z_h "large" FE spaces, so that $P_{Y(\mu),Z_h}(A(\mu)^{-*}X_h)$ is δ-proximal for $\mu \in \mathcal{S}$

(0) Initialize: $\phi_0 = u_h(\cdot,\mu_0) \in X_h$, $\theta_0 := P_{Y(\mu_0),Z_h}(A(\mu)^{-*}\phi_0)$

(1) Given $X_n := \mathrm{span}\,\{\phi_0,\dots,\phi_{n-1}\}$, $Z_m := \mathrm{span}\,\{\theta_0,\dots,\theta_{m-1}\}$, compute

$$d_{n,m} := \max_{\mu\in\mathcal{S}} \max_{v\in X_n:\|v\|_{L_2}=1} \min_{z\in Z_m} \|A(\mu)^* z - v\|_{L_2}$$

if $d_{n,m} \le \delta$, goto (2); else, extend Z_m:

$$\bar{u}_h(\cdot,\mu) = \mathrm{argmax}_{v\in X_n:\|v\|_{L_2}=1} \min_{z\in Z_m} \|A(\mu)^* z - v\|_{L_2}$$

$$\bar{\mu} = \mathrm{argmax}_{\mu\in\mathcal{S}}\Big(\min_{z\in Z_m} \|A(\mu)^* z - \bar{u}_h(\cdot,\mu)\|_{L_2}\Big),\ \theta_m := P_{Y(\bar{\mu}),Z_h}(A(\bar{\mu})^{-*}\bar{u}_h(\cdot,\bar{\mu}))$$

(2) extend X_n: $\mu_n := \mathrm{argmax}_{\mu\in\mathcal{S}}\|A(\mu)^*\hat{r}_{n,\mu}(u_n^k)\|_{L_2}$, $\quad \phi_n := u_{h,\delta}(\cdot,\mu_n) \in X_h$

Computational Tasks

Set: $\mathbf{A}(\mu) := \big((A(\mu)^*\theta_i, \phi_j)\big)_{i,j}^{m,n}$, $\mathbf{B}(\mu) := \big((A(\mu)^*\theta_i, A(\mu)^*\theta_j)\big)_{i,j}^{m}$

$v = \sum_{i=0}^{n-1} v_i\phi_i, \quad z = \sum_{j=0}^{m-1} z_j\theta_j, \ \rightsquigarrow$

$$\max_{v\in X_n:\|v\|_{L_2}=1} \min_{z\in Z_m} \|A(\mu)^*z - v\|_{L_2}^2 = \max_{\mathbf{v}\in\mathbb{R}^n} \frac{\mathbf{v}^T\big(\mathbf{I} - \mathbf{A}(\mu)^T\mathbf{B}(\mu)^{-1}\mathbf{A}(\mu)\big)\mathbf{v}}{\mathbf{v}^T\mathbf{v}}$$

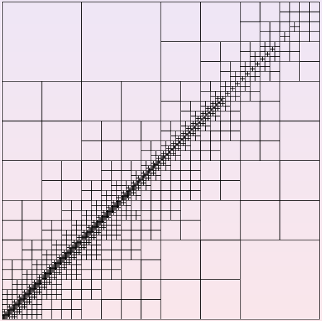
$(A(\mu)^*\hat{r}_{n,\mu}(v), A(\mu)^*z) = {}_{Y(\mu)'}\langle f - Av, z\rangle_{Y(\mu)}, \ z \in Z_m \rightsquigarrow$

$$\mathbf{r}_{n,\mu}(\mathbf{v}) = \mathbf{B}(\mu)^{-1}(\mathbf{f} - \mathbf{A}(\mu)\mathbf{v}), \quad \mathbf{f} = {}_{Y(\mu)'}\langle f, \theta_j\rangle_{Y(\mu)}, \ \hat{r}_{n,\mu}(v) = \sum_{j=0}^{m-1}(\mathbf{r}_{n,\mu}(v))_j\theta_j$$

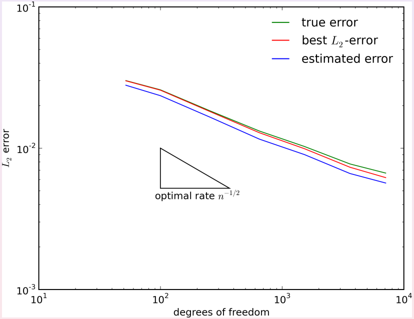
$$\mathbf{u}_n^{k+1}(\mu) = \mathbf{u}_n^k(\mu) + \mathbf{A}(\mu)^T\mathbf{r}_{n,\mu}^k, \quad \|A(\mu)^*\hat{r}_{n,s}(u_n^k)\|_{L_2}^2 = (\mathbf{r}_{n,\mu}^k)^T\mathbf{B}(\mu)\mathbf{r}_{n,\mu}^k \ \to \max_\mu$$

Adaptive Solution ($(p = 2, r = 2)$) for Fixed Velocity

$$\mu = (1,1), \quad c = 1, \quad f = \begin{cases} 1, & x > y \\ 0.5, & x \le y. \end{cases}$$

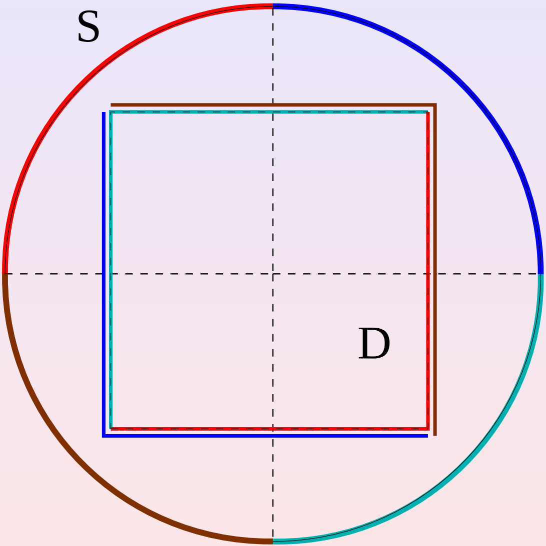


(a) Corresponding adaptive refinement grid of (b) in Figure 2.



(b) Convergence rate

First RB-Experiments



angles/estimated errors:

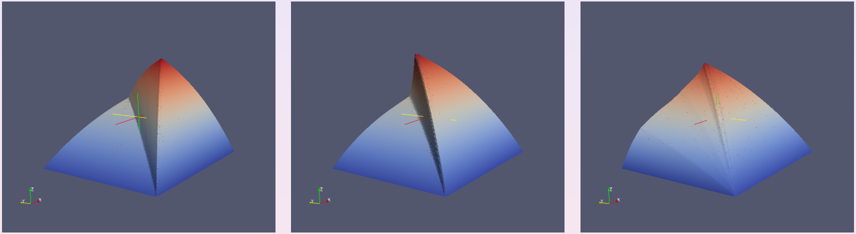


Figure: 0.567/0.000471, 0.85/0.000474, 1.255/0.00103

Error Decay: very preliminary