Space-time finite elements for the optimal control of parabolic equations

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Model problem

Given desired states $y_d \in L^2(Q)$, $y_{d,T} \in L^2(\Omega)$, Find controls $u \in L^2(Q)$, $u_0 \in L^2(\Omega)$ s.t.

$$\min \alpha \|y - y_d\|_Q^2 + \beta \|y(T) - y_{d,T}\|_\Omega^2 + \lambda \|u\|_Q^2 + \lambda_0 \|u_0\|_\Omega^2$$

subject to

$$\begin{aligned} \partial_t y - \Delta_x y &= f + u && \text{in } Q = (0,T) \times \Omega, \\ y &= 0 && \text{on } (0,T) \times \partial\Omega, \\ y(0) &= y_0 + u_0 && \text{in } \Omega. \end{aligned}$$

- $f \in L^2(Q)$, $y_0 \in L^2(\Omega)$
- $\alpha, \beta \geq 0$, $\alpha + \beta > 0$
- $\lambda, \lambda_0 \geq 0$, $\lambda + \lambda_0 > 0$

Building block: fem and time stepping for heat eq.

- Backward Euler with time-step k: $u^0 \approx u_0$, and

$$u^{n+1} - k\Delta u^{n+1} = kf + u^n.$$

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Observation:

- Optimal control of parabolic equation: Advantage 1 vanishes!

First-order formulation of heat equation

$$\begin{aligned} \partial_t y - \operatorname{div}_x \boldsymbol{\sigma} &= f, \\ \nabla_x y - \boldsymbol{\sigma} &= 0, \\ y(0) &= y_0, \\ y|_{\partial\Omega} &= 0 \end{aligned}$$

Unique solution $(y, \boldsymbol{\sigma})$ minimizes

$$J(y, \boldsymbol{\sigma}) = \|\partial_t y - \operatorname{div}_x \boldsymbol{\sigma} - f\|_Q^2 + \|\nabla_x y - \boldsymbol{\sigma}\|_Q^2 + \|y(0) - y_0\|_\Omega^2$$

Führer, K. '21, Gantner, Stevenson '21

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What is the “right” setting?

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What is the “right” setting?

A priori: $y \in L^2(H_0^1(\Omega)) \cap H^1(H^{-1}(\Omega))$, $\boldsymbol{\sigma} \in L^2(Q)$.

Observation: If $f \in L^2(Q)$ then $\operatorname{div}(y, -\boldsymbol{\sigma}) \in L^2(Q)$

Führer, K. ’21, Gantner, Stevenson ’21

Least-squares FEM 1/2

Space

$$Y = \big\{(y, \boldsymbol{\sigma}) \in L^2(H_0^1(\Omega)) \times L^2(Q)^d \,:\, \partial_t y - \operatorname{div}_x \boldsymbol{\sigma} \in L^2(Q)\big\}$$

Norm (graph)

$$\|(y, \boldsymbol{\sigma})\|_Y^2 = \|\nabla_x y\|_Q^2 + \|\boldsymbol{\sigma}\|_Q^2 + \|\partial_t y - \operatorname{div}_x \boldsymbol{\sigma}\|_Q^2$$

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Least-squares operator: $\mathcal{L}\colon Y \to L^2(Q)^{1+d} \times L^2(\Omega)$

$$\mathcal{L}(y, \boldsymbol{\sigma}) = (\partial_t y - \operatorname{div}_x \boldsymbol{\sigma}, \nabla_x y - \boldsymbol{\sigma}, y(0))$$

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Proposition (Gantner & Stevenson '21)

Y is Hilbert space and $\mathcal{L}$ is isomorphism

Minimization problem

$$\min_{(y,\boldsymbol{\sigma}) \in Y} \|\partial_t y - \operatorname{div}_x \boldsymbol{\sigma} - f\|_Q^2 + \|\nabla_x y - \boldsymbol{\sigma}\|_Q^2 + \|y(0) - y_0\|_\Omega^2$$

Least-squares FEM 2/2

Euler–Lagrange, $b((y,\boldsymbol{\sigma}),(z,\boldsymbol{\tau})) = (\mathcal{L}(y,\boldsymbol{\sigma})\,,\mathcal{L}(z,\boldsymbol{\tau}))$

$$(y,\boldsymbol{\sigma}) \in Y :\ b((y,\boldsymbol{\sigma}),(z,\boldsymbol{\tau})) = (f\,,\partial_t z - \operatorname{div}_x \boldsymbol{\tau}) + (y_0\,, z(0))_\Omega \quad \forall (z,\boldsymbol{\tau}) \in Y.$$

Least-squares FEM: Replace Y by $Y_h \subseteq Y$ (closed)

$$\min_{(y_h,\boldsymbol{\sigma}_h)\in Y_h} \|\partial_t y_h - \operatorname{div}_x \boldsymbol{\sigma}_h - f\|_Q^2 + \|\nabla_x y_h - \boldsymbol{\sigma}_h\|_Q^2 + \|y_h(0) - y_0\|_\Omega^2$$

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Theorem (Führer, K. '21, Gantner & Stevenson '21)

BLF $b(\cdot,\cdot) : Y \times Y \to \mathbb{R}$ symmetric, coercive.
Thus, unique solutions that are quasi-optimal

$$\|(y,\boldsymbol{\sigma}) - (y_h,\boldsymbol{\sigma}_h)\|_Y \lesssim \min_{(z,\boldsymbol{\tau})\in Y_h} \|(y,\boldsymbol{\sigma}) - (z,\boldsymbol{\tau})\|_Y$$

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- Discrete system of equations leads to SPD matrix
- Any(!) choice of discrete spaces is allowed, particularly, space-time adapted meshes!
  Unconditionally $\inf\text{–}\sup$ stability
- Control of "natural" norm:

$$\|\nabla_x y\|_Q + \|\partial_t y\|_{L^2(H^{-1}(\Omega))} \lesssim \|(y, \boldsymbol{\sigma})\|_Y$$

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- Built-in a posteriori error estimator (efficient+reliable)

$$\|(y, \boldsymbol{\sigma}) - (y_h, \boldsymbol{\sigma}_h)\|_Y^2 \\ \eqsim \|\partial_t y_h - \operatorname{div}_x \boldsymbol{\sigma}_h - f\|_Q^2 + \|\nabla_x y_h - \boldsymbol{\sigma}_h\|_Q^2 + \|y_h(0) - y_0\|_\Omega^2$$

Overview on some literature

Recent space-time FEMs

- FEM: Steinbach '15
- MINRES: Andreev '13, Stevenson & Westerdiep '20
- Least-squares: Gantner & Stevenson '21, '22, Führer K. '21
- D(iscontinuous)P(etrov)G(alerkin): Diening & Storn '21

Space-time methods for optimal control problems

- Meidner & Vexler '07, '08
- Gong, Hinze, Zhou '12
- Langer, Steinbach, Tröltzsch, Yang '21
- Langer, Steinbach, Yang '22
- Gantner & Stevenson '22+

There are many ways . . .

Table 11.1 from Bochev & Gunzberger '09

Property↓	Method 0	1	2	3	4	5	6
Discrete inf–sup not required	–	√	–	√	√	√	√
Locking impossible	√	√	√	–	√	√	–
Optimal error estimate	√	√	√	–	√	√	–
Symmetric matrix system	√	√	√	√	√	√	√
Reduced number of unknowns	–	–	√	√	–	√	√
Positive definite matrix system	–	√	√	√	–	√	√

For the first formulation we follow Method 4
For the second formulation we follow (more or less) Method 1

Optimality system 1/2

First-order optimality condition (with $\lambda_0 = 0$, $\alpha = \beta = 1$):
find $(u, y, \boldsymbol{\sigma}) \in L^2(Q) \times Y$ s.t.

$$\lambda(u\,, v)_Q + (y\,, z)_Q + (y(T)\,, z(T))_\Omega = (y_d\,, z)_Q + (y_{d,T}\,, z(T))_\Omega,$$
$$\mathcal{L}(y, \boldsymbol{\sigma}) - (u, 0, 0) = (0, 0, y_0),$$

for $v \in L^2(Q)$ where $z \in L^2(H_0^1(\Omega)) \cap H^1(H^{-1}(\Omega))$ solves

$$\begin{aligned} \partial_t z - \Delta_x z &= v, \\ z(0) &= 0, \\ z\big|_{(0,T)\times\partial\Omega} &= 0. \end{aligned}$$

Optimality system 2/2

Introducing space-time LS formulation and Lagrangian multiplier: find $(u, y, \boldsymbol{\sigma}, w, \boldsymbol{\chi}) \in L^2(Q) \times Y \times Y$ s.t.

$$
\begin{aligned}
a(u, y, \boldsymbol{\sigma}; v, z, \boldsymbol{\tau}) + \widetilde{b}(v, z, \boldsymbol{\tau}; w, \boldsymbol{\chi}) &= (y_d\,, z)_Q + (y_{d,T}\,, z(T))_\Omega, \\
\widetilde{b}(u, y, \boldsymbol{\sigma}; r, \boldsymbol{\rho}) &= (y_0\,, r(0))_\Omega
\end{aligned}
$$

for all $(v, z, \boldsymbol{\tau}, r, \boldsymbol{\rho}) \in L^2(Q) \times Y \times Y$, with BLFs

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Discretization: Subspaces $Y_h \subseteq Y$, $U_h \subseteq L^2(Q)$:
Find $(u_h, y_h, \boldsymbol{\sigma}_h, w, \boldsymbol{\chi}) \in U_h \times Y_h \times Y_h$ s.t.

$$
\begin{aligned}
a(u_h, y_h, \boldsymbol{\sigma}_h; v, z, \boldsymbol{\tau}) + \widetilde{b}(v, z, \boldsymbol{\tau}; w_h, \boldsymbol{\chi}_h) &= (y_d\,, z)_Q + (y_{d,T}\,, z(T))_\Omega, \\
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Analysis

Theorem (Führer, K. '22+)

Continuous and discrete formulations admit unique solutions and satisfy quasi-optimality

$$\begin{aligned}\|u-u_h\|_Q + \|(y-y_h,\boldsymbol{\sigma}-\boldsymbol{\sigma}_h)\|_Y + \|(w-w_h,\boldsymbol{\chi}-\boldsymbol{\chi}_h)\|_Y \\ \lesssim \|u-v_h\|_Q + \|(y-z_h,\boldsymbol{\sigma}-\boldsymbol{\tau}_h)\|_Y + \|(w-r_h,\boldsymbol{\chi}-\boldsymbol{\rho}_h)\|_Y\end{aligned}$$

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Although indefinite system
the Babuška–Brezzi conditions for discrete system are automatically satisfied

A posteriori estimator 1/2

Need to characterize Lagrangian multiplier $(w, \boldsymbol{\chi})$

Lemma (Adjoint state ↔ Lagrangian multiplier)

Adjoint state $p = -\lambda u$ solves "backward" heat equation

$$
\begin{aligned}
-\partial_t p - \Delta_x p &= y - y_d, \\
p(T) &= y(T) - y_{d,T}, \\
p|_{(0,T)\times\partial\Omega} &= 0.
\end{aligned}
$$

Characterization of $(w, \boldsymbol{\chi})$:

$$
\begin{aligned}
\partial_t w - \Delta_x w &= -p + \Delta_x p, \\
w(0) &= -p(0), \\
w|_{(0,T)\times\partial\Omega} &= 0, \\
\boldsymbol{\chi} &= \nabla_x w + \nabla_x p.
\end{aligned}
$$

A posteriori estimator 2/2

Estimator

$$\begin{aligned}\eta^2 = {} & \|\partial_t y_h - \operatorname{div}_x \boldsymbol{\sigma}_h - u_h\|_Q^2 + \|\nabla_x y_h - \boldsymbol{\sigma}_h\|_Q^2 + \|y_h(0) - y_0\|_\Omega^2 \\ & + \|\lambda^{-1}(\partial_t w_h - \operatorname{div}_x \boldsymbol{\chi}_h) - u_h\|_Q^2 + \|\boldsymbol{\chi}_h - \nabla_x w_h - \boldsymbol{\psi}_h\|_Q^2 + \|\partial_t w_h - \operatorname{div}_x \boldsymbol{\chi}_h + p_h\|_Q^2 \\ & + \|y_h - y_d + \partial_t p_h + \operatorname{div}_x \boldsymbol{\psi}_h\|_Q^2 + \|\nabla p_h - \boldsymbol{\psi}_h\|_Q^2 + \|p_h(T) - (y_h(T) - y_{d,T})\|_\Omega^2\end{aligned}$$

A posteriori estimator 2/2

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Pair $(p_h, \boldsymbol{\psi}_h) \in Y_h^\star \subseteq Y^\star = \{(v, \boldsymbol{\tau}) \in L^2(H_0^1(\Omega)) \times L^2(Q) \,:\, \mathrm{div}(v, \boldsymbol{\tau}) \in L^2(Q)\}$ solves adjoint state problem with discrete data

$$\min_{(p_h, \boldsymbol{\psi}_h) \in Y_h^\star} \|y_h - y_d + \partial_t p_h + \mathrm{div}_x\, \boldsymbol{\psi}_h\|_Q^2 + \|\nabla p_h - \boldsymbol{\psi}_h\|_Q^2 + \|p_h(T) - (y_h(T) - y_{d,T})\|_\Omega^2$$

A posteriori estimator 2/2

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$$\eta^2 = \|\partial_t y_h - \operatorname{div}_x \boldsymbol{\sigma}_h - u_h\|_Q^2 + \|\nabla_x y_h - \boldsymbol{\sigma}_h\|_Q^2 + \|y_h(0) - y_0\|_\Omega^2$$
$$+ \|\lambda^{-1}(\partial_t w_h - \operatorname{div}_x \boldsymbol{\chi}_h) - u_h\|_Q^2 + \|\boldsymbol{\chi}_h - \nabla_x w_h - \boldsymbol{\psi}_h\|_Q^2 + \|\partial_t w_h - \operatorname{div}_x \boldsymbol{\chi}_h + p_h\|_Q^2$$
$$+ \|y_h - y_d + \partial_t p_h + \operatorname{div}_x \boldsymbol{\psi}_h\|_Q^2 + \|\nabla p_h - \boldsymbol{\psi}_h\|_Q^2 + \|p_h(T) - (y_h(T) - y_{d,T})\|_\Omega^2$$

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Theorem (Führer, K. '22+)

The estimator η is reliable + efficient,

$$\eta^2 \eqsim \|\boldsymbol{u} - \boldsymbol{u}_h\|^2$$

where $\boldsymbol{u} = (u, y, \boldsymbol{\sigma}, w, \boldsymbol{\chi}, p, \boldsymbol{\psi})$.

Experiment 1

$Q = (0,1) \times (0,1)$, $y_0 = 0$, $\alpha = 0$, $\beta = 1$, $\lambda = 1$, $\lambda_0 = 0$

$$y_{d,T}(x) = \sin(\pi x)$$

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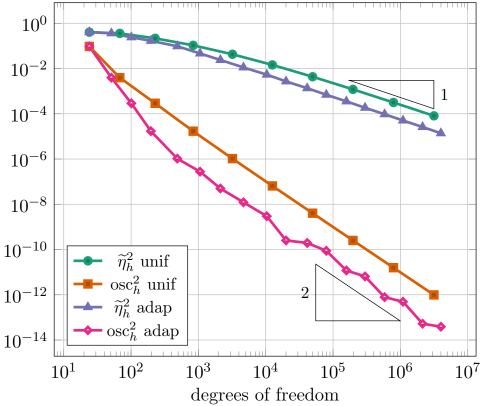

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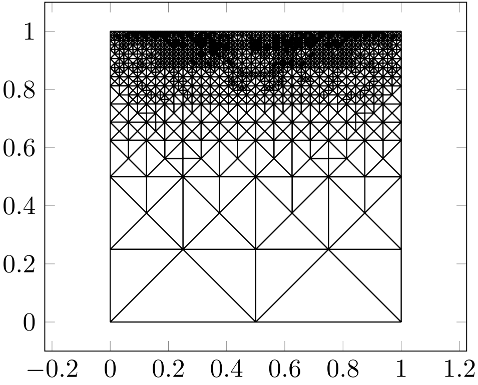

Experiment 2

$Q = (0,1) \times (0,1)$, $y_0 = 0$, $\alpha = 1$, $\beta = 0$, $\lambda = 1$, $\lambda_0 = 0$

$$u_d(t,x) = \begin{cases} 1 & 0.5 \le t \text{ and } 0.2 \le x \le 0.8, \\ 0 & \text{else.} \end{cases}$$

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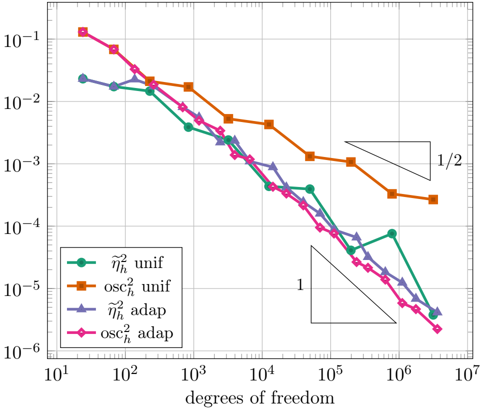

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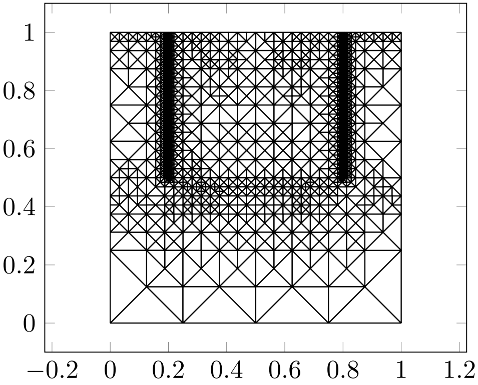

Idea

Solve state and adjoint state equations simultaneously:

$$
\begin{aligned}
\partial_t y - \Delta_x y &= u, \\
y(0) &= y_0, \\
-\partial_t p - \Delta_x p &= y - y_d, \\
p(T) &= y(T) - y_{d,T}, \\
(p + \lambda u\,, v - u) &\geq 0 \quad \forall v \in X_{\mathrm{ad}}
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with admissible controls $X_{\mathrm{ad}} = \left\{ v \in L^2(Q) \,:\, a \leq v \leq b \right\}$.

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\mathcal{L}\boldsymbol{y} &= (\partial_t y - \operatorname{div}_x \boldsymbol{\sigma}, \nabla_x y - \boldsymbol{\sigma}, y(0)) \\
\mathcal{L}^\star \boldsymbol{p} &= (-\partial_t p - \operatorname{div}_x \boldsymbol{\psi}, \nabla_x p - \boldsymbol{\psi}, p(T))
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2nd Method

Nitsche-type coupling BLF

$$\begin{aligned} a(u,\boldsymbol{y},\boldsymbol{p};v,\boldsymbol{z},\boldsymbol{q}) &= (\mathcal{L}\boldsymbol{y}-(u,0,0)\,,\mathcal{L}\boldsymbol{z}-(v,0,0)) \\ &\quad + (\mathcal{L}^\star\boldsymbol{p}-(y,0,0)\,,\mathcal{L}^\star\boldsymbol{q}-(z,0,0)) + \gamma(p+\lambda u\,,v) \\ \ell(v,\boldsymbol{z},\boldsymbol{q}) &= ((0,0,y_0)\,,\mathcal{L}\boldsymbol{z}) + ((-y_d,0,-y_{d,T})\,,\mathcal{L}^\star\boldsymbol{q}) \end{aligned}$$

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Variational inequality (VI): Find $(u, \boldsymbol{y}, \boldsymbol{p}) \in U = X_{\mathrm{ad}} \times Y \times Y^\star$

$$
a(u, \boldsymbol{y}, \boldsymbol{p}; v - u, \boldsymbol{z} - \boldsymbol{y}, \boldsymbol{q} - \boldsymbol{p}) \geq \ell(v - u, \boldsymbol{z} - \boldsymbol{y}, \boldsymbol{q} - \boldsymbol{p}) \quad \forall (v, \boldsymbol{z}, \boldsymbol{q}) \in U
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Theorem (Führer, K. '22+)

For $0<\gamma\leq\gamma_0$ BLF a is coercive.
Consequently, VI and any discretization admits unique solution

Error estimator

Variational inequality

$$(p + \lambda u \, , v - u) \geq 0 \quad \forall v \in X_{\text{ad}} = \left\{ w \in L^2(Q) \, : \, a \leq w \leq b \right\}$$

gives metric projection $u = \Pi_{\text{ad}}(-\lambda^{-1} p)$

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$$\eta^2 = \|\mathcal{L}\boldsymbol{y}_h - (u_h, 0, 0)\|^2 + \|\mathcal{L}^\star \boldsymbol{p}_h - (y_h - y_d, 0, y_h(T) - y_{d,T})\|^2 + \|u_h - \widetilde{u}_h\|_Q^2$$

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Theorem (Führer., K. '22+)

Estimator is reliable and efficient, i.e.,

$$\eta^2 \eqsim \|u - u_h\|_Q^2 + \|\boldsymbol{y} - \boldsymbol{y}_h\|_Y^2 + \|\boldsymbol{p} - \boldsymbol{p}_h\|_{Y^\star}^2$$

Unconstrained problem

If $X_{\mathrm{ad}} = L^2(Q)$, then $(p + \lambda u\,, v - u) \geq 0$ implies

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Theorem (Führer, K. '22+)

Minimization problem admits unique solution $(\boldsymbol{y}_h, \boldsymbol{p}_h)$ *over any closed* $Y_h \times Y_h^\star \subseteq Y \times Y^\star$ *Particularly,*

$$\|\mathcal{L}\boldsymbol{y}_h - (-\lambda^{-1} p_h, 0, 0)\|^2 + \|\mathcal{L}^\star \boldsymbol{p}_h - (y_h - y_d, 0, y_h(T) - y_{d,T})\|^2 \\ \eqsim \|\boldsymbol{y} - \boldsymbol{y}_h\|_Y^2 + \|\boldsymbol{p} - \boldsymbol{p}_h\|_{Y^\star}^2$$

Experiment

$\lambda = 10^{-1} = \lambda_0$, manufactured solution

$$y(x,t) = t\sin(\pi x), \quad p(x,t) = (1-t)x(1-x)$$

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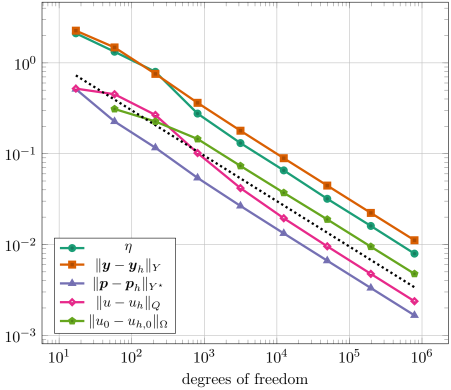

Conclusion

Space-time least-squares FEM

- SPD matrices
- $\inf\text{–}\sup$ stability for any conforming discretization
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First approach for optimal control (Lagrangian multiplier)

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Second approach for optimal control (Variational ineq.)

- Coercive formulation, but non-symmetric
- $\inf$–$\sup$ stability for any conforming discretization
- Fully computable error estimator for constrained problems
- Reduces to pure least-squares FEM for unconstrained problems

Thank you for your attention!

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