Model reduction of PPDEs – Advances, trends and challenges

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Trends in Math. Sciences, Erlangen, June 2024

Introduction - I

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  - system-theoretic model reduction (Numerical Linear Algebra)
  - ➢ partial differential equations (PDEs) depending on parameters: PPDEs

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  - the coefficients of a PDE (e.g. the porosity or conductivity of a material)
  - the geometry of the domain (e.g. the size, shape, etc.)

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- different application frameworks
  - solve for *many* values of the parameter: *multi-query*
  - *realtime*

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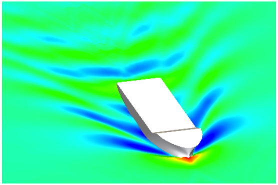
- different application frameworks
  - solve for *many* values of the parameter: *multi-query*
  - *realtime*
  - embedded systems: *cold computing*

(T. Patera, MIT)

Introduction - II

- assume: highly efficient numerical solvers for PPDEs available
  - used for a *fixed value* of the parameter
  - often (even optimal) schemes are known
  - complexity is too high: $\mathcal{N}$
  - up to any accuracy: “truth”

Optimal steering



Optimal shape

Optimal control

Offline training – online reduced simulation

Basic idea:

- offline training
  - select parameter samples $\mu^{(1)}, ..., \mu^{(N)} \in \mathcal{P}$
  - compute *snapshots* $u^{\mathcal{N}}(\mu^{(i)}) \approx u(\mu^{(i)})$ by "truth" numerical simulation: $\mathcal{N}$
  - determine reduced model (small dimension $N \ll \mathcal{N}$)
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  - precompute and store parameter-independent terms
- online
  - given new parameter values (optimization loop, control, measurements, data,...)
  - setup and solve reduced system (small dimension N)
  - compute error bound (certification)

Some mathematical questions

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- comparison with (simple) interpolation w.r.t. parameters?
- how to combine with data?
- ...

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  - example (strong form)

$$B(\mu)u(x) = \nabla \cdot (\underline{\boldsymbol{\alpha}}_\mu(x)\, \nabla u(x)) + \boldsymbol{\beta}_\mu(x) \cdot \nabla u(x) + \gamma_\mu(x)\, u(x)$$

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- given a right-hand side $f(\mu) : \Omega \to \mathbb{R}$:

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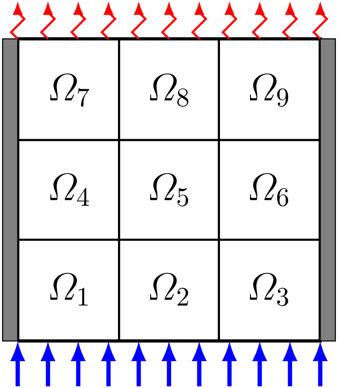
- ensure well-posedness (i.e., existence, uniqueness and stability): $B(\mu)$ should be an isomorphism (bijective, bounded, inverse bounded)
- denote unique solution by $u(\mu)$

The thermal block – our "fruit fly"

- $\mathbb{R}^d \supset \Omega = \bigcup_{p=1}^{P} \Omega_p$, $\boldsymbol{\mu} = (\mu_1, ..., \mu_P)^T$

$(P = 9)$



$$B(\mu)\, u := -\sum_{p=1}^{P} \nabla \cdot (\mu_p\, \chi_{\Omega_p}\, \nabla u) = f,$$

$$\mu_p > 0, p = 1, ..., P,$$

$$u_{|\partial\Omega} = 0,$$

$f : \Omega \to \mathbb{R}$ external force

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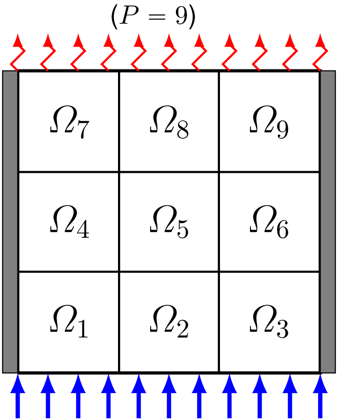

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$$f : \Omega \to \mathbb{R} \quad \text{external force}$$

- variational form: $u(\mu) \in H_0^1(\Omega)$:

$$b(u(\mu), v; \mu) := \sum_{p=1}^{P} \mu_p \int_{\Omega_p} \nabla u \cdot \nabla v\, dx$$

$$= (f, v)_{L_2(\Omega)} \qquad \forall v \in H_0^1(\Omega)$$

Variational formulation of PPDE - I

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- bilinear form $b(\mu) \equiv b(\cdot, \cdot; \mu) : \mathcal{U} \times \mathcal{V} \to \mathbb{R}$ induced by $B(\mu)$:

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Definition 1.1 (Continuity / inf-sup)

(a) $b(\mu)$ is *continuous* (or *bounded*) if $\exists C_\mu > 0$ (*continuity constant*):

$$|b(u, v; \mu)| \leqslant C_\mu \, \|u\|_{\mathcal{U}} \, \|v\|_{\mathcal{V}} \qquad \forall u \in \mathcal{U}, v \in \mathcal{V}.$$

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(b) $b(\mu)$ satisfies an *inf-sup condition* if $\exists \beta_\mu > 0$ (*inf-sup constant*):

$$\sup_{v \in \mathcal{V}} \frac{b(u, v; \mu)}{\|v\|_{\mathcal{V}}} \geqslant \beta_\mu \, \|u\|_{\mathcal{U}} \ \forall u \in \mathcal{U} \quad \Longleftrightarrow \quad \inf_{u \in \mathcal{U}} \sup_{v \in \mathcal{V}} \frac{b(u, v; \mu)}{\|u\|_{\mathcal{U}} \, \|v\|_{\mathcal{V}}} \geqslant \beta_\mu. \tag{1.1}$$

Variational formulation of PPDE - II

Theorem 1.2 (Banach–Nečas theorem)

Let $\mu \in \mathcal{P}$; $b(\mu) : \mathcal{U} \times \mathcal{V} \to \mathbb{R}$ be a continuous bilinear form.
Then, the following statements are equivalent:

(i) $\forall f(\mu) \in \mathcal{V}' \;\; \exists!\, u(\mu) \in \mathcal{U}$ *(with continuous dependency on the data)*:

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(ii) *(a) inf-sup condition* (1.1) *holds, and*
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Theorem 1.3 (Lax–Milgram theorem)

Let $\mu \in \mathcal{P}$*;* $b(\mu) : \mathcal{U} \times \mathcal{U} \to \mathbb{R}$ *symmetric, continuous, coercive BLF.*
Then: $\forall f(\mu) \in \mathcal{U}' \;\; \exists!\, u(\mu) \in \mathcal{U}$ *s.t.* $b(u(\mu), v; \mu) = f(v; \mu) \;\; \forall v \in \mathcal{U}.$

The “truth”: Petrov-Galerkin - I

- assume: *detailed simulation* method available (“truth”)
  - approximate $u(\mu)$ with any desired accuracy for a given (fixed) parameter
  - might be computationally costly: $\mathcal{N}$
  - “truth” approximation: $u^{\mathcal{N}}(\mu)$

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- Petrov-Galerkin: finite-dimensional subspaces

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Lemma 2.1 (error / residual relation)

- Let conditions of Banach-Nečas and inf-sup for $\beta_\mu > 0$ hold.

Then, for the *residual* $r^{\mathcal{N}}(\mu) := f(\mu) - B(\mu)\, u^{\mathcal{N}}(\mu)$

$$\|u(\mu) - u^{\mathcal{N}}(\mu)\|_{\mathcal{U}} \leqslant \frac{1}{\beta_\mu} \|r^{\mathcal{N}}(\mu)\|_{\mathcal{V}'}.$$

The "truth": Petrov-Galerkin - II (stability)

Definition 2.2 (Ladyshenskaya–Babuška–Brezzi (LBB) condition)

$\mathcal{U}^{\mathcal{N}} \subset \mathcal{U}$ and $\mathcal{V}^{\mathcal{N}} \subset \mathcal{V}$ satisfy LBB w.r.t. $b(\mu) : \mathcal{U} \times \mathcal{V} \to \mathbb{R}$, $\mu \in \mathcal{P}$,
if $\exists \beta_\mu^\circ > 0$ such that

$$\inf_{u^{\mathcal{N}} \in \mathcal{U}^{\mathcal{N}}} \sup_{v^{\mathcal{N}} \in \mathcal{V}^{\mathcal{N}}} \frac{b(u^{\mathcal{N}}, v^{\mathcal{N}}; \mu)}{\|u^{\mathcal{N}}\|_{\mathcal{U}} \, \|v^{\mathcal{N}}\|_{\mathcal{V}}} \geqslant \beta_\mu^\circ \quad \text{for all } \mathcal{N} \tag{2.2}$$

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Theorem 2.3 (Best approximation[a])

[a] Xu and Zikatanov 2003.

Continuity (C_μ: continuity constant) and LBB $\rightsquigarrow$

$$\|u(\mu) - u^{\mathcal{N}}(\mu)\|_{\mathcal{U}} \leqslant \frac{C_\mu}{\beta_\mu^\circ} \inf_{w^{\mathcal{N}} \in \mathcal{U}^{\mathcal{N}}} \|u(\mu) - w^{\mathcal{N}}\|_{\mathcal{U}}. \tag{2.3}$$

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  notation $\mu^{(n)}$: each $\mu^{(n)} = (\mu_1^{(n)}, ..., \mu_P^{(n)})^T \in \mathcal{P} \subset \mathbb{R}^P$

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  - $\rightsquigarrow$ perform "truth" approximation $N \ll \mathcal{N}$ times offline

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  $\rightsquigarrow$ approximation

$$\sigma_{\mathcal{U}}(u(\mu), U_N) := \inf_{w_N \in U_N} \|u(\mu) - w_N\|_{\mathcal{U}}.$$

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- determine test space $V_N(\mu)$ for stability ($\rightsquigarrow$ size of C_μ and β_μ°)

Online reduced approximation - I

- given new parameter μ
- reduced approximation: seek $u_N(\mu) \in U_N$ such that

$$b(u_N(\mu), v_N; \mu) = \langle f(\mu), v_N \rangle \quad \forall v_N \in V_N(\mu) \tag{3.1}$$

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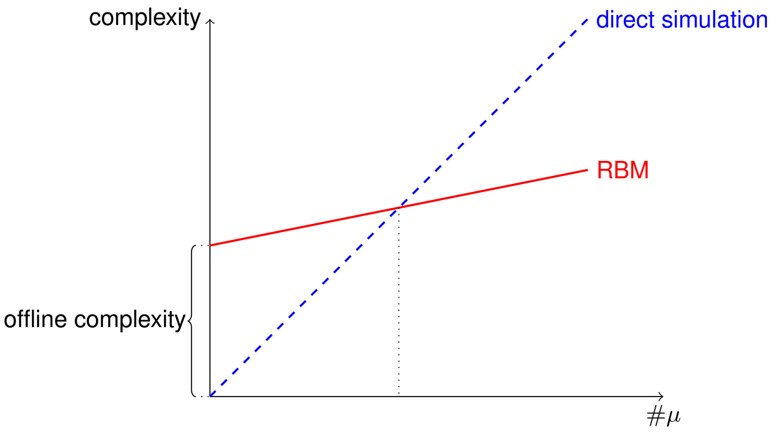
- we cannot hope to solve (3.1) in linear complexity
- assume complexity is $\mathcal{O}(N^\bullet)$ ("$\bullet$" some power, typically $\bullet = 3$)
- meaningful if $N^\bullet \ll \mathcal{N}$ and $N^\bullet$ independent of $\mathcal{N}$: *online-efficient*

Online reduced approximation - II



Why should that work at all? – Affine decomposition

Definition 4.1 (affine decomposition)

(a) $b(\mu)$ is called *affine (in the parameter)*
if $\exists Q^b \in \mathbb{N}$, $\vartheta_q^b : \mathcal{P} \to \mathbb{R}$ & continuous BLFs $b_q : \mathcal{U} \times \mathcal{V} \to \mathbb{R}$, $1 \leqslant q \leqslant Q^b$:

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(b) similar for $f(\mu)$

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(b) similar for $f(\mu)$

(c) The parametric problem (1.2) is called *affine (in the parameter)*
if both $b(\mu)$ and $f(\mu)$ are affine in the parameter. (Otherwise: approximate by EIM[a])

[a] Barrault, Maday, Nguyen, and Patera 2004.

Why should that work at all? – Affine decomposition

Definition 4.1 (affine decomposition)

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Lemma 4.2 (Reduced residual is affine)

Let (1.2) be affine, then $r_N(\mu) := f(\mu) - B(\mu) \; u_N(\mu)$ is affine.

What is the benchmark? - I

- $\mathcal{F} := \{u^{\mathcal{N}}(\mu) : \mu \in \mathcal{P}\}$ "solution manifold"

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$$d_N(\mathcal{F}) := \inf_{w_N \in U_N} \|u^{\mathcal{N}}(\mu) - w_N\|_{\mathcal{U}} \tag{5.1}$$

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$$d_N(\mathcal{F}) := \inf_{\substack{U_N \subset X \\ \dim(U_N) = N}} \sup_{\mu \in \mathcal{P}} \inf_{w_N \in U_N} \|u^{\mathcal{N}}(\mu) - w_N\|_{\mathcal{U}} \tag{5.1}$$

What is the benchmark? - II

Theorem 5.1 (Kolmogorov N-width[a])

[a] Ohlberger and Rave 2016; KU 2023.

Let

- $b(\cdot,\cdot;\mu)$ *be bounded, inf-sup stable and affine (with* Q^b *terms)*
- U_N, V_N *are LBB-stable,*

then $\exists 0 < c, C < \infty$:

$$d_N(\mathcal{F}) \leqslant C \exp(-c\, N^{1/Q^b}) \qquad (2.2.2)$$

What is the benchmark? - III

Theorem 5.2 (Transport equation[a])

[a] Ohlberger and Rave 2016.

For $u_t + \mu u_x = 0$, $u(0,x) = 0$, $u(t,0) = 1$, *it holds*

$$d_N(\mathcal{F}) \geqslant \frac{1}{2} N^{-1/2}.$$

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Theorem 5.3 (Wave equation[a])

[a] Greif and KU 2019.

For $\ddot{u} - \mu u_{xx} = 0$, $\dot{u}(0,x) = 0$ *and*

$$u(0,x) := \begin{cases} 1 & x \leqslant 0, \\ -1 & x \geqslant 0, \end{cases}$$

it holds

$$\frac{1}{4} N^{-1/2} \leqslant d_N(\mathcal{F}) \leqslant \frac{1}{2} (N-1)^{-1/2}.$$

Offline-online decomposition

- goal: compute the reduced (linear) approximation

$$u_N(\mu) = \sum_{n=1}^{N} \alpha_n(\mu)\, \xi_n, \qquad \alpha_n(\mu) \in \mathbb{R} \text{ coefficients}$$

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- by linear system $\boldsymbol{B}_N(\mu)\, \boldsymbol{\alpha}_N(\mu) = \mathbf{f}_N(\mu)$

$$\boldsymbol{B}_N(\mu) = \cdots = \sum_{q,q'=1}^{Q^b} \vartheta_q^b(\mu)\, \vartheta_{q'}^b(\mu)\, \mathbb{B}_{N,q,q'}, \qquad \mathbb{B}_{N,q,q'} \in \mathbb{R}^{N\times N}$$

A posteriori error estimation

- aim: *a posteriori error estimator* $\|u(\mu) - u_N(\mu)\|_{\mathcal{U}} \leqslant \Delta_N(\mu)$
  - for selection of the sample set S_N
  - for the certification of the reduced approximation

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- fast computation
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  - Riesz representation offline and affine decomposition for $\|r_N(\mu)\|_{\mathcal{V}'}$

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  - Riesz representation offline and affine decomposition for $\|r_N(\mu)\|_{\mathcal{V}'}$
- $\Delta_N(\mu)$ is even a *surrogate* for the error w.r.t. the truth

$$\|u^{\mathcal{N}}(\mu) - u_N(\mu)\|_{\mathcal{U}} \leqslant \Delta_N(\mu) \leqslant \frac{C_\mu}{\beta_\mu^\circ}\|u^{\mathcal{N}}(\mu) - u_N(\mu)\|_{\mathcal{U}} \qquad (5.2)$$

[1]Huynh, Rozza, Sen, and Patera 2007

Greedy selection of the reduced basis

Algorithm 5.4 (Weak greedy method)

input: training sample $\mathcal{P}_{\text{train}} \subseteq \mathcal{P}$, parameter $\gamma \in (0,1]$, tolerance $\varepsilon > 0$

chose $\mu^{(1)} \in \mathcal{P}_{\text{train}}$

Initialize $S_1 \leftarrow \{\mu^{(1)}\}$, $U_1 := \text{span}\{\xi_1\}$, $N := 1$

while `true` **do**

  if $\max_{\mu \in \mathcal{P}_{\text{train}}} \Delta_N(\mu) \leqslant \varepsilon$ **then return**

$$\mu^{(N+1)} \leftarrow \arg \max_{\mu \in \mathcal{P}_{\text{train}}} \Delta_N(\mu)$$

  compute snapshot $\xi_{N+1} := u^{\mathcal{N}}(\mu^{(N+1)})$

  compute supremizers $\eta_{N,q}$, $q = 1, ..., Q^f$

  $S_{N+1} \leftarrow S_N \cup \{\mu^{(N+1)}\}$, $U_{N+1} := \text{span}\{U_N, \xi_{N+1}\}$

  $N \leftarrow N + 1$

end while

output: sample set S_N, reduced trial space U_N, supremizers

Weak-Greedy convergence

Can we reach the benchmark? Yes, we can! – by (weak) greedy!

Theorem 5.5 (Weak-Greedy convergence[a])

[a] Binev, Cohen, Dahmen, DeVore, Petrova, and Wojtaszczyk 2011; KU 2023.

Let $0 < \gamma \leqslant 1$, $d_0(\mathcal{F}) \leqslant M$, *then*

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Let $0 < \gamma \leqslant 1$, $d_0(\mathcal{F}) \leqslant M$, *then*

- *if* $d_N(\mathcal{F}) \leqslant M\, N^{-\alpha}$, $N > 0$, $\alpha > 0$, $C := q^{1/2}(4q)^{\alpha}$, $q := \lceil 2^{\alpha+1}\gamma^{-1}\rceil^2$

$$\max_{\mu\in\mathcal{P}} \|u^{\mathcal{N}}(\mu) - u_N(\mu)\|_X \leqslant C\, M\, N^{-\alpha}$$

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$$\max_{\mu\in\mathcal{P}} \|u^{\mathcal{N}}(\mu) - u_N(\mu)\|_X \leqslant C\, M\, N^{-\alpha}$$

- *if* $d_N(\mathcal{F}) \leqslant M\, e^{-aN^{\alpha}}$, $N \geqslant 0$, $M, a, \alpha > 0$, *then*

$$\max_{\mu\in\mathcal{P}} \|u^{\mathcal{N}}(\mu) - u_N(\mu)\|_X \leqslant C\, M\, \exp(-cN^{\beta})$$

where $\beta := \frac{\alpha}{\alpha+1}$, $0 \leqslant \theta < 1$, $c := \min\{|\log\theta|, (4q)^{-\alpha}a\}$,
$C := \max\{e^{cN_0^{\beta}}, q^{1/2}\}$, $q := \lceil 2\gamma^{-1}\theta^{-1}\rceil^2$, $N_0 := \lceil (8q)^{\alpha+1}\rceil$.

The thermal block

- $\mathcal{U} = \mathcal{V} = H_0^1(\Omega)$ and $b(u, v; \mu) = \sum_{p=1}^{P} \mu_p \int_{\Omega_p} \nabla u(x) \cdot \nabla v(x)\, dx$

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- N-width decays exponentially!

Time-dependent problems - I

- parameterized parabolic problem ($A(\mu)$ elliptic)

$$u_t + A(\mu)u = f(t;\mu), \quad t \in (0,T) =: I, \qquad u(0) = u_0 \tag{5.3}$$

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- usually $\rightsquigarrow$ error bound grows (exponentially) over time $\lightning$

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Space/Time-variational formulation

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- treat time as variational variable[3] (not via semigroup theory)

[3] Dautray and Lions 1992; Schwab and Stevenson 2009; KU and Patera 2012; KU and Patera 2014

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Space/Time-variational formulation

- treat time as variational variable[3] (not via semigroup theory)
  - ⇝ Lebesgue-Bochner spaces for in time and space ($X = H_0^1(\Omega)$)

$$\mathcal{V} = L_2(I;X) := \left\{ v : I \to X \,:\, \|v\|^2_{L_2(I;X)} := \int_I \|v(t)\|^2_X \, dt < \infty \right\}$$

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- truth: tensor-product system in $d+1$ dimensions $\rightsquigarrow$ uniform LBB

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Parameterized parabolic problem

		Rational Krylov Space Method				Crank Nicolson	
N_h	N_t	Its	μ_{mem}	rank	Time (s)	Direct	Iterative
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	500	13	14	9	30.46	143.71	78.01
	700	13	14	9	28.17	153.38	93.03
347361	300	14	15	9	820.17	14705.10	792.42
	500	14	15	9	828.34	15215.47	1041.47
	700	14	15	7	826.93	15917.52	1212.57

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- use in industrial problems
- ...