
MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG
CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY
Low-rank tensor methods
for PDE-constrained optimization
under uncertainty
Peter Benner
Joint work with
Sergey Dolgov (U Bath)
Martin Stoll (TU Chemnitz)
Akwum Onwunta (U Maryland)
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The Max Planck Institute (MPI) in Magdeburg

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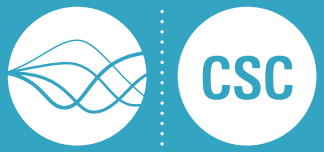
- operates 84 institutes — 79 in Germany, 2 in Italy (Rome, Florence), 1 each in The Netherlands, Luxembourg, US;
- has $\sim$ 23,000 employees;
- had 18 Nobel Laureates since 1948.

"The first MPI in engineering. . ."

- founded 1998
- 4 departments (directors)
- 10 research groups
- budget $\sim$ 15 Mio. EUR
- $\sim$ 230 employees
- $\sim$ 160 scientific staff,
- doing research in
  - biotechnology
  - chemical engineering
  - process engineering
  - energy conversion
  - applied math
  - HPC



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A (big) data problem in flow simulation

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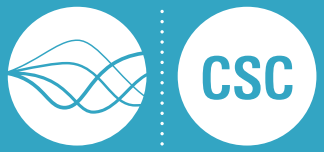

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- Why not starting with a compressed data format from the very beginning, and computing all trajectories all-at-once?
- This is the idea we pursue in this talk, where we store the data in a compressed (low-rank) $1 + 10 + 1(3)$–way tensor! (Above example $\rightsquigarrow$ terabyte-range.)

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- data are unpredictable, e.g, wind shear.

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- The rank of $[AV_k \quad V_k] \in \mathbb{R}^{n,2r}$, $[W_k \quad AW_k] \in \mathbb{R}^{n_t,2r}$ increases but can be controlled using truncation. $\rightsquigarrow$ Low-rank Krylov subspace solvers. [Kressner/Tobler, B/Breiten, Savostyanov/Dolgov, ...].

PDE-constrained Optimization under Uncertainty

We consider the problem:

$$\min_{y \in \mathcal{Y}, u \in \mathcal{U}} \mathcal{J}(y, u) \quad \text{subject to} \quad c(y, u) = 0,$$

where

- $c(y, u) = 0$ represents a (linear or nonlinear) PDE (system) with uncertain coefficient(s).
- The state y and control u are random fields.
- The cost functional $\mathcal{J}$ is a real-valued Fréchet-differentiable functional on $\mathcal{Y} \times \mathcal{U}$.

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and go one step further applying low-rank tensor (instead of matrix) techniques.

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Using low-rank tensor techniques, we need $\approx 7 \cdot 10^7$ **bytes** $= 70$ **GB** to solve the KKT system in MATLAB in less than one hour!

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Unsteady Heat Equation

Consider the optimization problem

$$\mathcal{J}(t,y,u) = \frac{1}{2}||y-\bar{y}||^2_{L^2(0,T;\mathcal{D})\otimes L^2(\Omega)} + \frac{\alpha}{2}||\mathrm{std}(y)||^2_{L^2(0,T;\mathcal{D})} + \frac{\beta}{2}||u||^2_{L^2(0,T;\mathcal{D})\otimes L^2(\Omega)}$$

subject, $\mathbb{P}$-almost surely, to

$$\begin{cases} \dfrac{\partial y(t,\mathbf{x},\omega)}{\partial t} - \nabla\cdot(a(\mathbf{x},\omega)\nabla y(t,\mathbf{x},\omega)) = u(t,\mathbf{x},\omega), \quad \text{in } (0,T]\times\mathcal{D}\times\Omega, \\ y(t,\mathbf{x},\omega) = 0, \quad \text{on } (0,T]\times\partial\mathcal{D}\times\Omega, \\ y(0,\mathbf{x},\omega) = y_0, \quad \text{in } \mathcal{D}\times\Omega, \end{cases}$$

where

- for any $z : \mathcal{D}\times\Omega\to\mathbb{R}$, $z(\mathbf{x},\cdot)$ is a random variable defined on the complete probability space $(\Omega,\mathcal{F},\mathbb{P})$ for each $\mathbf{x}\in\mathcal{D}$,
- $\exists\ 0 < a_{\min} < a_{\max} < \infty$ s.t. $\mathbb{P}(\omega\in\Omega : a(x,\omega)\in[a_{\min},a_{\max}]\ \forall\, x\in\mathcal{D}) = 1$.

Discretization

We discretize and then optimize the stochastic control problem.

- Under finite noise assumption we can use N-term (truncated) **Karhunen-Loève expansion (KLE)**

$$a \equiv a(\mathbf{x}, \omega) \approx a_N(\mathbf{x}, \xi(\omega)) \equiv a_N(\mathbf{x}, \xi_1(\omega), \xi_2(\omega), \ldots, \xi_N(\omega)).$$

- Assuming a known continuous covariance $C_a(\mathbf{x}, \mathbf{y})$, we get the KLE

$$a_N(\mathbf{x}, \xi(\omega)) = \mathbb{E}[a](\mathbf{x}) + \sigma_a \sum_{i=1}^{N} \sqrt{\lambda_i} \varphi_i(\mathbf{x}) \xi_i(\omega),$$

  where (λ_i, φ_i) are the dominant eigenpairs of C_a.

- Doob-Dynkin Lemma allows same parametrization for solution y.
- Use linear finite elements for the spatial discretization and implicit Euler in time.

This is used within a **stochastic Galerkin FEM (SGFEM)** approach.

Stochastic Galerkin Finite Element Method

Weak formulation of the random PDE

Seek $y \in H^1\left(0, T; H_0^1(\mathcal{D}) \otimes L^2(\Omega)\right)$ such that, $\mathbb{P}$-almost surely,

$$\langle y_t, v\rangle + \mathcal{B}(y, v) = \ell(u, v) \quad \forall\, v \in H_0^1(\mathcal{D}) \otimes L^2(\Omega),$$

with the coercive (as $\mathbb{P}(a(\mathbf{x}, \omega) \geq a_{\min} > 0) = 1$) bilinear form

$$\mathcal{B}(y, v) := \int_\Omega \int_{\mathcal{D}} a(\mathbf{x}, \omega) \nabla y(\mathbf{x}, \omega) \cdot \nabla v(\mathbf{x}, \omega) d\mathbf{x}\, d\mathbb{P}(\omega), \quad v, y \in H_0^1(\mathcal{D}) \otimes L^2(\Omega),$$

and

$$\begin{aligned} \ell(u, v) &= \langle u(\mathbf{x}, \omega), v(\mathbf{x}, \omega)\rangle \\ &=: \int_\Omega \int_{\mathcal{D}} u(\mathbf{x}, \omega) v(\mathbf{x}, \omega) d\mathbf{x}\, d\mathbb{P}(\omega), \quad u, v \in H_0^1(\mathcal{D}) \otimes L^2(\Omega). \end{aligned}$$

Coercivity and boundedness of $\mathcal{B}$ + Lax-Milgram $\Longrightarrow$ unique solution exists.

[Deb/Babuška/Oden '01, Xiu/Karniadakis '03, Babuška/Tempone/Zouraris '04, Rosseel/Wells '12, Gunzburger/Webster/Zhang '14]

Weak formulation of the optimality system

Theorem [Chen/Quarteroni '14, B./Onwunta/Stoll '18]

Under appropriate regularity assumptions, there exists a unique adjoint state p and optimal solution (y, u, p) to the optimal control problem for the random unsteady heat equation, satisfying the stochastic optimality conditions (KKT system) for $t \in (0, T]$ $\mathbb{P}$-almost surely

$$\begin{aligned}
\langle y_t, v\rangle + \mathcal{B}(y, v) &= \ell(u, v), && \forall\, v \in H_0^1(\mathcal{D}) \otimes L^2(\Omega),\\
\langle p_t, w\rangle - \mathcal{B}^*(p, w) &= \ell\left((y - \bar{y}) + \frac{\alpha}{2}\mathcal{S}(y), w\right), && \forall\, w \in H_0^1(\mathcal{D}) \otimes L^2(\Omega),\\
\ell(\beta u - p, \tilde{w}) &= 0, && \forall\, \tilde{w} \in L^2(\mathcal{D}) \otimes L^2(\Omega),
\end{aligned}$$

where

- $\mathcal{S}(y)$ is the Fréchet derivative of $\|\mathrm{std}(y)\|^2_{L^2(0,T;\mathcal{D})}$;
- $\mathcal{B}^*$ is the adjoint operator of $\mathcal{B}$.

Stochastic Galerkin Finite Element Method

Discretization of the random PDE

- y, p, u are approximated using standard Galerkin ansatz, yielding approximations of the form

$$z(t, \mathbf{x}, \omega) = \sum_{k=0}^{P-1} \sum_{j=1}^{J} z_{jk}(t)\phi_j(\mathbf{x})\psi_k(\xi) = \sum_{k=0}^{P-1} z_k(t, \mathbf{x})\psi_k(\xi).$$

- Here,
  - $\{\phi_j\}_{j=1}^{J}$ are linear finite elements;
  - $\{\psi_k\}_{k=0}^{P-1}$ are the $P = \frac{(N+n)!}{N!n!}$ multivariate Legendre polynomials of degree $\leq n$.
  - Implicit Euler/dG(0) used for temporal discretization with constant time step τ.

The Fully Discretized Optimal Control Problem

Discrete first order optimality conditions/KKT system

$$\begin{bmatrix} \tau\mathcal{M}_1 & 0 & -\mathcal{K}_t^T \\ 0 & \beta\tau\mathcal{M}_2 & \tau\mathcal{N}^T \\ -\mathcal{K}_t & \tau\mathcal{N} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \tau\mathcal{M}_\alpha\bar{\mathbf{y}} \\ \mathbf{0} \\ \mathbf{d} \end{bmatrix},$$

where

- $\mathcal{M}_1 = D \otimes G_\alpha \otimes M =: D \otimes \mathcal{M}_\alpha, \quad \mathcal{M}_2 = D \otimes G_0 \otimes M,$
- $\mathcal{K}_t = I_{n_t} \otimes \left[\sum_{i=0}^N G_i \otimes \hat{K}_i\right] + (C \otimes G_0 \otimes M),$
- $\mathcal{N} = I_{n_t} \otimes G_0 \otimes M,$

and

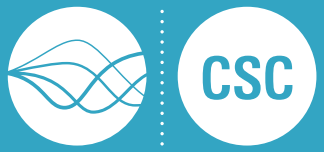
- $G_0 = \operatorname{diag}\left(\left\langle\psi_0^2\right\rangle, \left\langle\psi_1^2\right\rangle, \ldots, \left\langle\psi_{P-1}^2\right\rangle\right), \quad G_i(j,k) = \left\langle\xi_i\psi_j\psi_k\right\rangle, \quad i = 1, \ldots, N,$
- $G_\alpha = G_0 + \alpha \operatorname{diag}\left(0, \left\langle\psi_1^2\right\rangle, \ldots, \left\langle\psi_{P-1}^2\right\rangle\right)$ (with first moments $\langle\,.\,\rangle$ w.r.t. $\mathbb{P}$),
- $\hat{K}_0 = M + \tau K_0, \quad \hat{K}_i = \tau K_i, \quad i = 1, \ldots, N,$
- $M, K_i \in \mathbb{R}^{J\times J}$ are the mass and stiffness matrices w.r.t. the spatial discretization, where K_i corresponds to the contributions of the ith KLE term to the stiffness,
- $C = -\operatorname{diag}(\mathtt{ones}, -1), \quad D = \operatorname{diag}\left(\frac{1}{2}, 1, \ldots, 1, \frac{1}{2}\right) \in \mathbb{R}^{n_t\times n_t}.$

The Fully Discretized Optimal Control Problem

Discrete first order optimality conditions/KKT system

$$\begin{bmatrix} \tau\mathcal{M}_1 & 0 & -\mathcal{K}_t^T \\ 0 & \beta\tau\mathcal{M}_2 & \tau\mathcal{N}^T \\ -\mathcal{K}_t & \tau\mathcal{N} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \tau\mathcal{M}_\alpha\bar{\mathbf{y}} \\ \mathbf{0} \\ \mathbf{d} \end{bmatrix},$$

Linear system with $3JPn_t$ unknowns!

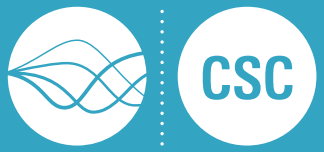


Solving the KKT System

Optimality system leads to saddle point problem

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix}.$$

- Very large scale setting, (block-)structured sparsity $\rightsquigarrow$ iterative solution.



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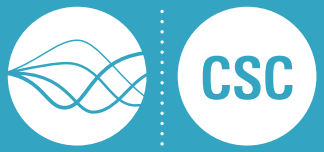

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MINRES finds the exact solution in at most three steps.

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- Here, $A \sim$ mass matrices $\rightsquigarrow$ application of A^{-1} is approximated using a small number of Chebyshev semi-iterations.

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Theorem [B./Onwunta/Stoll '16]

Let $\alpha \in [0, +\infty)$, $\gamma = \sqrt{(1+\alpha)/\beta}$, $\mathcal{K} = \sum_{i=0}^{N} G_i \otimes K_i$, and

$$\tilde{S} = \frac{1}{\tau} (\mathcal{K} + \tau\gamma\mathcal{N}) \mathcal{M}_1^{-1} (\mathcal{K} + \tau\gamma\mathcal{N})^T.$$

Then the eigenvalues of $\tilde{S}^{-1}S$ satisfy

$$\lambda(\tilde{S}^{-1}S) \subset \left[\frac{1}{2(1+\alpha)}, 1 \right), \quad \forall \alpha < \left(\frac{\sqrt{\kappa(\mathcal{K})}+1}{\sqrt{\kappa(\mathcal{K})}-1} \right)^2 - 1.$$

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Corollary [B./Onwunta/Stoll '16]

Let $\mathcal{A}$ be the KKT matrix from the stochastic Galerkin approach, and $\mathcal{P}$ the preconditioner using the Schur complement approximation $\tilde{S}$ (and exact A). Then

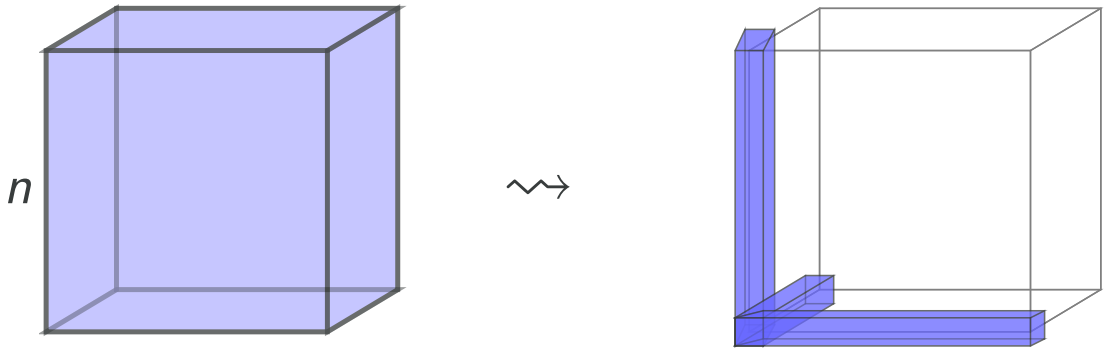
$$\lambda(\mathcal{P}^{-1}\mathcal{A}) \subset \{1\} \cup \mathcal{I}^+ \cup \mathcal{I}^-,$$

where

$$\mathcal{I}^{\pm} = \frac{1}{2}\left(1 \pm \left[\sqrt{1+\frac{2}{1+\alpha}}, \sqrt{5}\right]\right).$$

Tensor Techniques

Separation of variables and low-rank approximation



- Approximate: $\underbrace{\mathbf{x}(i_1, \ldots, i_d)}_{\text{tensor}} \approx \underbrace{\sum_{\alpha} \mathbf{x}_{\alpha}^{(1)}(i_1)\mathbf{x}_{\alpha}^{(2)}(i_2) \cdots \mathbf{x}_{\alpha}^{(d)}(i_d)}_{\text{tensor product decomposition}}.$

Goals:

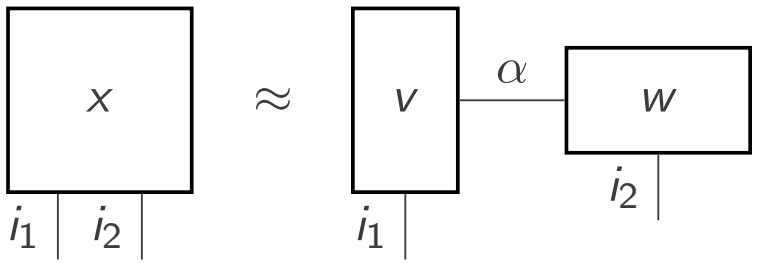
- Store and manipulate x — $\mathcal{O}(dn)$ cost *instead of* $\mathcal{O}(n^d)$.
- Solve equations $Ax = b$ — $\mathcal{O}(dn^2)$ cost *instead of* $\mathcal{O}(n^{2d})$.

Data Compression in 2D: Low-Rank Matrices

- Discrete *separation of variables*:

$$\begin{bmatrix} x_{1,1} & \cdots & x_{1,n} \\ \vdots & & \vdots \\ x_{n,1} & \cdots & x_{n,n} \end{bmatrix} = \sum_{\alpha=1}^{r} \begin{bmatrix} v_{1,\alpha} \\ \vdots \\ v_{n,\alpha} \end{bmatrix} \begin{bmatrix} w_{\alpha,1} & \cdots & w_{\alpha,n} \end{bmatrix} + \mathcal{O}(\varepsilon).$$

- Diagrams:



- *Rank* $r \ll n$.
- $\mathtt{mem}(v) + \mathtt{mem}(w) = 2nr \ll n^2 = \mathtt{mem}(x)$.
- *Singular Value Decomposition (SVD)*
  $\Longrightarrow$ $\varepsilon(r)$ optimal w.r.t. spectral/Frobenius norm.

Data Compression in Higher Dimensions

Tensor Trains/Matrix Product States

[Wilson '75, White '93, Verstraete '04, Oseledets '09/'11]

For indices

$$\overline{i_p \dots i_q} = (i_p - 1)n_{p+1} \cdots n_q + (i_{p+1} - 1)n_{p+2} \cdots n_q + \cdots + (i_{q-1} - 1)n_q + i_q,$$

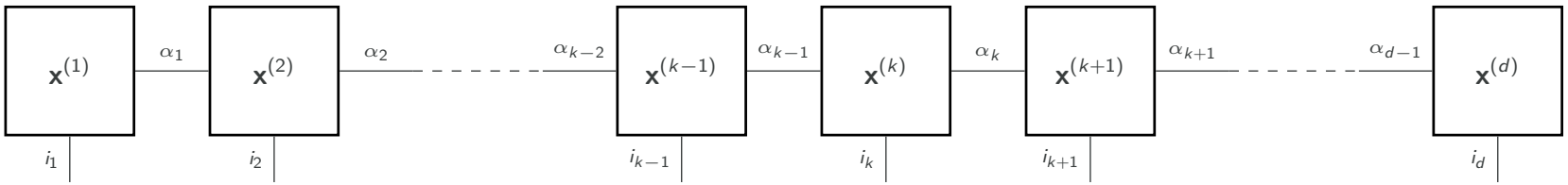
the TT format can be expressed as

$$x(\overline{i_1 \dots i_d}) = \sum_{\boldsymbol{\alpha}=\mathbf{1}}^{\mathbf{r}} \mathbf{x}^{(1)}_{\alpha_1}(i_1) \cdot \mathbf{x}^{(2)}_{\alpha_1,\alpha_2}(i_2) \cdot \mathbf{x}^{(3)}_{\alpha_2,\alpha_3}(i_3) \cdots \mathbf{x}^{(d)}_{\alpha_{d-1},\alpha_d}(i_d)$$

or

$$x(\overline{i_1 \dots i_d}) = \mathbf{x}^{(1)}(i_1) \cdots \mathbf{x}^{(d)}(i_d), \quad \mathbf{x}^{(k)}(i_k) \in \mathbb{R}^{r_{k-1} \times r_k} \text{ w/ } r_0, r_d = 1,$$

or



Storage: $\mathcal{O}(dnr^2)$ instead of $\mathcal{O}(n^d)$.

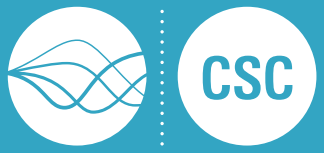
Overloading Tensor Operations

Always work with *factors* $\mathbf{x}^{(k)} \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ instead of full tensors.

- Sum $z = x + y \quad \rightsquigarrow \quad$ increase of tensor rank $\quad r_z = r_x + r_y$.
- TT format for a high-dimensional operator

$$A(\overline{i_1 \dots i_d}, \overline{j_1 \dots j_d}) = \mathbf{A}^{(1)}(i_1, j_1) \cdots \mathbf{A}^{(d)}(i_d, j_d)$$

- *Matrix-vector* multiplication $y = Ax$; $\quad \rightsquigarrow$ tensor rank $r_y = r_A \cdot r_x$.
- Additions and multiplications *increase* TT ranks.
- *Decrease* ranks quasi-optimally via QR and SVD.



Solving KKT System using TT Format

The dimensionality of the saddle point system is vast $\Rightarrow$ use tensor structure and low tensor ranks.

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Use tensor train format to approximate the solution as

$$\mathbf{y}(i_1,\ldots,i_d) \approx \sum_{\alpha_1\ldots\alpha_{d-1}=1}^{r_1\ldots r_{d-1}} \mathbf{y}^{(1)}_{\alpha_1}(i_1)\mathbf{y}^{(2)}_{\alpha_1,\alpha_2}(i_2)\cdots\mathbf{y}^{(d-1)}_{\alpha_{d-2},\alpha_{d-1}}(i_{d-1})\mathbf{y}^{(d)}_{\alpha_{d-1}}(i_d),$$

and represent the coefficient matrix as

$$\mathcal{A}(i_1\cdots i_d, j_1\cdots j_d) \approx \sum_{\beta_1\ldots\beta_{d-1}=1}^{R_1\ldots R_{d-1}} \mathbf{A}^{(1)}_{\beta_1}(i_1,j_1)\mathbf{A}^{(2)}_{\beta_1,\beta_2}(i_2,j_2)\cdots\mathbf{A}^{(d)}_{\beta_{d-1}}(i_d,j_d),$$

where the multi-index $\mathbf{i} = (i_1,\ldots,i_d)$ is implied by the parametrization of the approximate solutions of the form

$$\mathbf{z}(t,\xi_1,\ldots,\xi_N,\mathbf{x}), \quad \mathbf{z} = \mathbf{y},\mathbf{u},\mathbf{p},$$

i.e., solution vectors are represented by d-way tensor with $d = N+2$.

Numerical Results

Mean-Based Preconditioned TT-MinRes

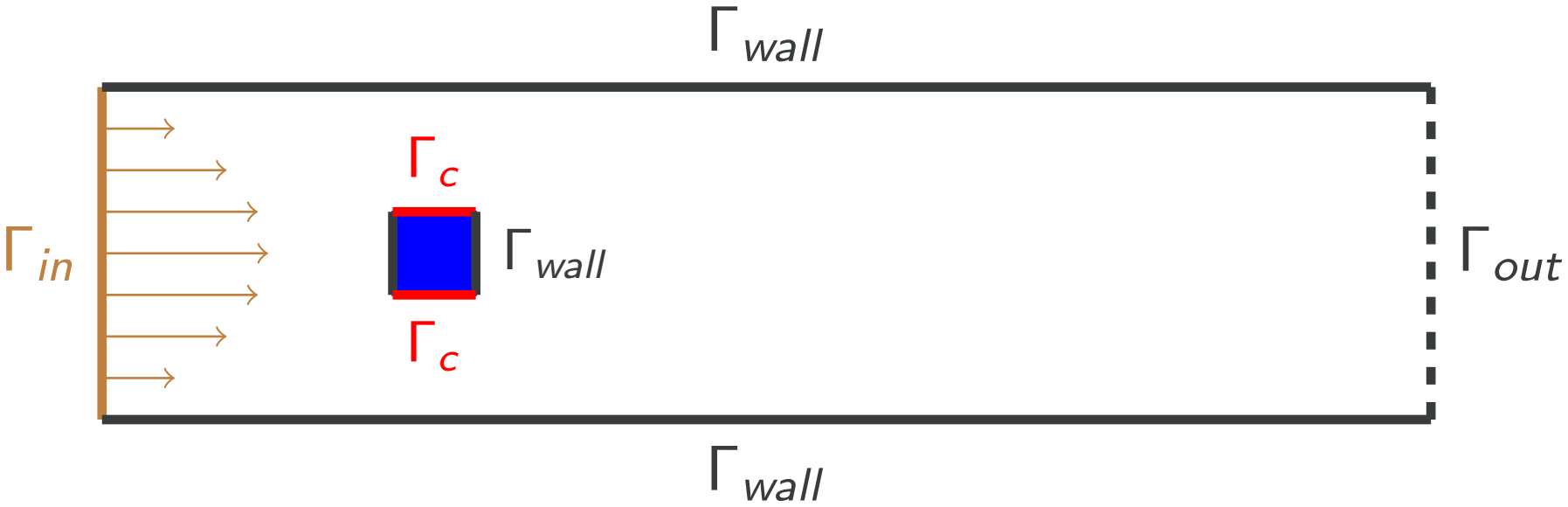
TT-MINRES	# iter (t)	# iter (t)	# iter (t)
n_t	2^5	2^6	2^8
$\dim(\mathcal{A}) = 3JPn_t$	$10,671,360$	$21,342,720$	$85,370,880$
$\alpha = 1,\ \text{tol} = 10^{-3}$			
$\beta = 10^{-5}$	6 (285.5)	6 (300.0)	8 (372.2)
$\beta = 10^{-6}$	4 (77.6)	4 (130.9)	4 (126.7)
$\beta = 10^{-8}$	4 (56.7)	4 (59.4)	4 (64.9)
$\alpha = 0,\ \text{tol} = 10^{-3}$			
$\beta = 10^{-5}$	4 (207.3)	6 (366.5)	6 (229.5)
$\beta = 10^{-6}$	4 (153.9)	4 (158.3)	4 (172.0)
$\beta = 10^{-8}$	2 (35.2)	2 (37.8)	2 (40.0)

Outline

Unsteady Navier-Stokes Equations

Model Problem: 'Uncertain' flow past a rectangular obstacle domain

▸ to Numerical Experiments



- We model this as a boundary control problem.
- Our constraint $c(y, u) = 0$ is given by the unsteady incompressible Navier-Stokes equations with uncertain viscosity $\nu := \nu(\omega)$.

Model Problem

Minimize:

$$\mathcal{J}(v,u) = \frac{1}{2}\|\mathrm{curl} v\|^2_{L^2(0,T;\mathcal{D})\otimes L^2(\Omega)} + \frac{\beta}{2}\|u\|^2_{L^2(0,T;\mathcal{D})\otimes L^2(\Omega)} \tag{1}$$

subject to

$$\begin{aligned}
\frac{\partial v}{\partial t} - \nu\Delta v + (v\cdot\nabla)v + \nabla p &= 0, \quad \text{in} \quad \mathcal{D},\\
-\nabla\cdot v &= 0, \quad \text{in} \quad \mathcal{D},\\
v &= \theta, \quad \text{on} \quad \Gamma_{in},\\
v &= 0, \quad \text{on} \quad \Gamma_{wall},\\
\frac{\partial v}{\partial n} &= u, \quad \text{on} \quad \Gamma_c,\\
\frac{\partial v}{\partial n} &= 0, \quad \text{on} \quad \Gamma_{out},\\
v(\cdot,0,\cdot) &= v_0, \quad \text{in} \quad \mathcal{D}.
\end{aligned} \tag{2}$$

Model Problem Set-up (cf. [Powell/Silvester '12])

We assume

- $\nu(\omega) = \nu_0 + \nu_1 \xi(\omega), \quad \nu_0, \nu_1 \in \mathbb{R}^+, \quad \xi \sim \mathcal{U}(-1, 1).$
- $\mathbb{P}\left(\omega \in \Omega : \nu(\omega) \in [\nu_{\min}, \nu_{\max}]\right) = 1$, for some $0 < \nu_{\min} < \nu_{\max} < +\infty$.
- $\Rightarrow$ velocity v, control u and pressure p are random fields on $L^2(\Omega)$.
- $L^2(\Omega) := L^2(\Omega, \mathcal{F}, \mathbb{P})$ is a complete probability space.
- $L^2(0, T; \mathcal{D}) := L^2(\mathcal{D}) \times L^2(\mathcal{T})$.

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Computational challenges

- Nonlinearity (due to the nonlinear convection term $(v \cdot \nabla)v$) .
- Uncertainty (due to random $\nu(\omega)$).
- High dimensionality (of the resulting linear/optimality systems).

OTD Strategy and Picard (Oseen) Iteration $\rightsquigarrow$

state equation

$$v_t - \nu\Delta v + (\bar{v}\cdot\nabla)\, v + \bigtriangledown p = 0$$
$$\nabla \cdot v = 0 + \text{ boundary conditions}$$

adjoint equation

$$-\chi_t - \Delta\chi - (\bar{v}\cdot\nabla)\,\chi + (\nabla\bar{v})^T\,\chi + \bigtriangledown\mu = -\mathrm{curl}^2 v$$
$$\nabla\cdot\chi = 0$$
$$\text{on} \quad \Gamma_{wall}\cup\Gamma_{in}: \qquad \chi = 0$$
$$\text{on} \quad \Gamma_{out}\cup\Gamma_c: \qquad \frac{\partial\chi}{\partial n} = 0$$
$$\chi(\cdot, T, \cdot) = 0$$

gradient equation

$$\beta u + \chi|_{\Gamma_c} = 0.$$

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- $\bar{v}$ denotes the velocity from the previous Oseen iteration.
- Having solved this system, we update $\bar{v} = v$ until convergence.

Stochastic Galerkin Finite Element Method

- Velocity v and control u are of the form

$$z(t,x,\omega) = \sum_{k=0}^{P-1} \sum_{j=1}^{J_v} z_{jk}(t)\phi_j(x)\psi_k(\xi) = \sum_{k=0}^{P-1} z_k(t,x)\psi_k(\xi).$$

- Pressure p is of the form

$$p(t,x,\omega) = \sum_{k=0}^{P-1} \sum_{j=1}^{J_p} p_{jk}(t)\tilde{\phi}_j(x)\psi_k(\xi) = \sum_{k=0}^{P-1} p_k(t,x)\psi_k(\xi).$$

- Here,
  - $\{\phi_j\}_{j=1}^{J_v}$ and $\{\tilde{\phi}_j\}_{j=1}^{J_p}$ are Q2–Q1 finite elements (inf-sup stable);
  - $\{\psi_k\}_{k=0}^{P-1}$ are Legendre polynomials.
- Implicit Euler/dG(0) used for temporal discretization.

Discrete Stochastic Control Problem

Linearization and SGFEM discretization yields the following saddle point system

$$\underbrace{\begin{bmatrix} M_y & 0 & L^* \\ 0 & M_u & N^\top \\ L & N & 0 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} y \\ u \\ \lambda \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} f \\ 0 \\ g \end{bmatrix}}_{b}.$$

Each of the block matrices in A is of the form

$$\sum_{\alpha=1}^{R} X_\alpha \otimes Y_\alpha \otimes Z_\alpha,$$

corresponding to temporal, stochastic, and spatial discretizations.

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Size: $\sim 3 n_t P (J_v + J_p)$, e.g., for $P = 10$, $n_t = 2^{10}$, $J \approx 10^5$ $\rightsquigarrow \approx 10^9$ unknowns!

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Central Question

How to solve $Ax = b$ if Krylov solvers become too expensive?

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Data are given in TT format:

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- $b(i) = \mathbf{b}^{(1)}(i_1) \cdots \mathbf{b}^{(d)}(i_d)$.

Seek the solution in the same format:

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Use a new block-variant of *Alternating Least Squares* in a new block TT format to overcome difficulties with indefiniteness of KKT system matrix.

Alternating Least Squares Method [Kroonenberg '80, De Lathauwer '00, Schneider '12]

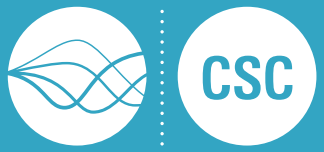
- If $A = A^\top > 0$: minimize $J(x) = x^\top A x - 2x^\top b$.

Alternating Least Squares (ALS):

- replace $\min_x J(x)$ by iteration — size n^d
- `for` $k = 1, \ldots, d$, — size $r^2 n$
  solve $\min_{\mathbf{x}^{(k)}} J\left(\mathbf{x}^{(1)}(i_1) \cdots \mathbf{x}^{(k)}(i_k) \cdots \mathbf{x}^{(d)}(i_d)\right)$.
  (all other blocks are fixed)

ALS for $d = 3$

1. $\hat{\mathbf{x}}^{(1)} = \arg\min_{\mathbf{x}^{(1)}} J\left(\mathbf{x}^{(1)}(i_1)\mathbf{x}^{(2)}(i_2)\mathbf{x}^{(3)}(i_3)\right)$



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ALS for $d = 3$

1. $\hat{\mathbf{x}}^{(1)} = \arg\min_{\mathbf{x}^{(1)}} J\left(\mathbf{x}^{(1)}(i_1)\mathbf{x}^{(2)}(i_2)\mathbf{x}^{(3)}(i_3)\right)$
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5. repeat 1.–4. until convergence

ALS = Projection method

If we differentiate J w.r.t. TT blocks, we see that...

- ...each step means solving a *Galerkin linear system*

$$\left(X_{\neq k}^\top A X_{\neq k}\right) \hat{x}^{(k)} = \left(X_{\neq k}^\top b\right) \in \mathbb{R}^{nr^2}.$$

- $X_{\neq k} = \underbrace{\mathrm{TT}\left(\hat{\mathbf{x}}^{(1)} \dots \hat{\mathbf{x}}^{(k-1)}\right)}_{n^{k-1} \times r_{k-1}} \otimes \underbrace{I}_{n \times n} \otimes \underbrace{\mathrm{TT}\left(\mathbf{x}^{(k+1)} \dots \mathbf{x}^{(d)}\right)}_{n^{d-k} \times r_k}.$

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Properties of ALS include:

- \+ Effectively 1D complexity in a prescribed format.
- − Tensor format (ranks) is fixed and cannot be adapted.
- − Convergence may be very slow, stagnation is likely.

ALS: Getting rid of "–"

- Density Matrix Renormalization Group (DMRG) [White '92]
  – updates *two* blocks $\mathbf{x}^{(k)}\mathbf{x}^{(k+1)}$ *simultaneously*.
- Alternating Minimal Energy (AMEn) [Dolgov/Savostyanov '13]
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But..., what about saddle point systems A?

- Recall our KKT system:

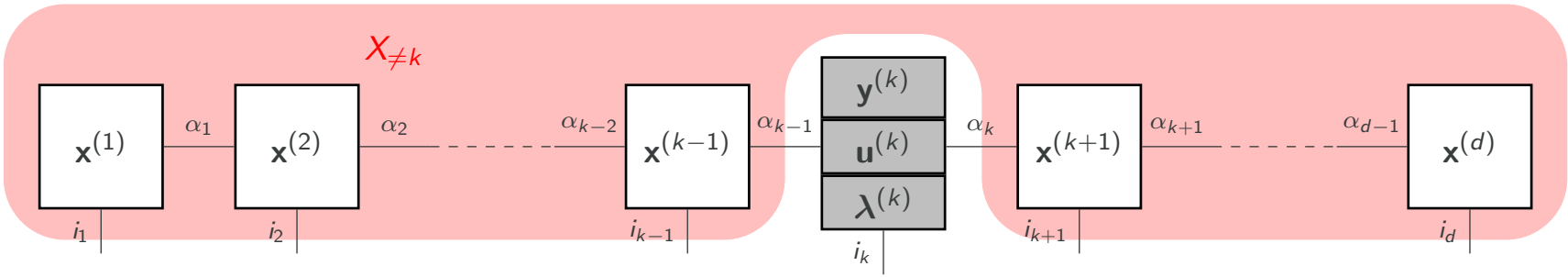
$$\underbrace{\begin{bmatrix} M_y & 0 & L^* \\ 0 & M_u & N^\top \\ L & N & 0 \end{bmatrix}}_{A} \begin{bmatrix} y \\ u \\ \lambda \end{bmatrix} = \begin{bmatrix} f \\ 0 \\ g \end{bmatrix}.$$

- The whole matrix is indefinite $\Rightarrow$ $X_{\neq k}^\top A X_{\neq k}$ can be degenerate.

Block ALS [B./Dolgov/Onwunta/Stoll 2016, 2017]

- Work-around: Block TT representation

$$\begin{bmatrix} y \\ u \\ \lambda \end{bmatrix} = \mathbf{x}^{(1)}_{\alpha_1} \otimes \cdots \otimes \begin{bmatrix} \mathbf{y}^{(k)}_{\alpha_{k-1},\alpha_k} \\ \mathbf{u}^{(k)}_{\alpha_{k-1},\alpha_k} \\ \boldsymbol{\lambda}^{(k)}_{\alpha_{k-1},\alpha_k} \end{bmatrix} \otimes \cdots \otimes \mathbf{x}^{(d)}_{\alpha_{d-1}}.$$



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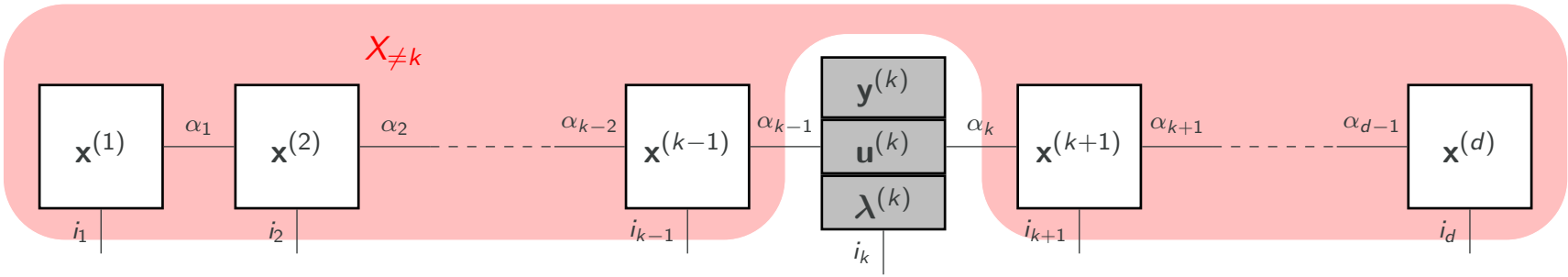


- $X_{\neq k}$ is the *same* for y, u, λ.
- Project each *submatrix*:

$$\begin{bmatrix} \hat{M}_y & 0 & \hat{L}^* \\ 0 & \hat{M}_u & \hat{N}^\top \\ \hat{L} & \hat{N} & 0 \end{bmatrix} \begin{bmatrix} y^{(k)} \\ u^{(k)} \\ \lambda^{(k)} \end{bmatrix} = \begin{bmatrix} \hat{f} \\ 0 \\ \hat{g} \end{bmatrix}, \qquad \widehat{(\cdot)} = X_{\neq k}^\top (\cdot) X_{\neq k}$$

Numerical Experiments

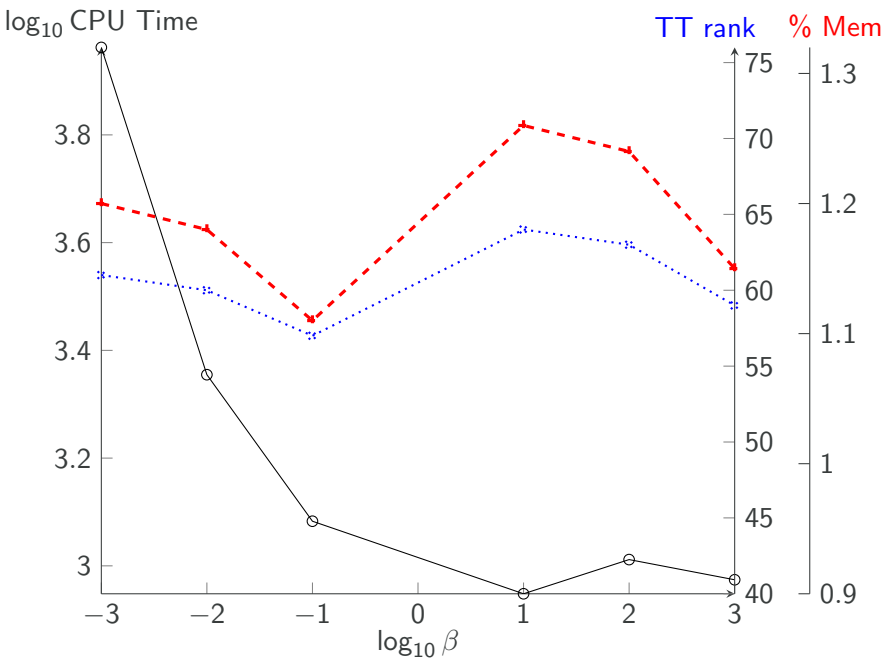
◂ Kármán vortex street

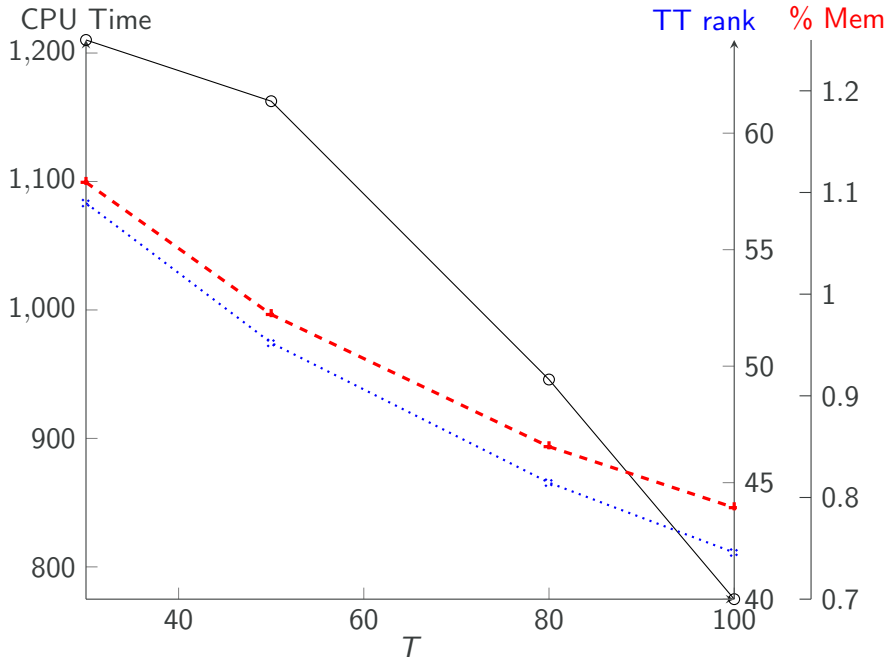
Vary one of the default parameters:

- TT truncation tolerance $\varepsilon = 10^{-4}$,
- mean viscosity $\nu_0 = 1/20$,
- uncertainty $\nu_1 = 1/80$,
- regularization/penalty parameter $\beta = 10^{-1}$,
- number of time steps: $n_t = 2^{10}$,
- time horizon $T = 30$,
- spatial grid size $h = 1/4 \rightsquigarrow J = 2488$,
- max. degree of Legendre polynomials: $P = 8$.

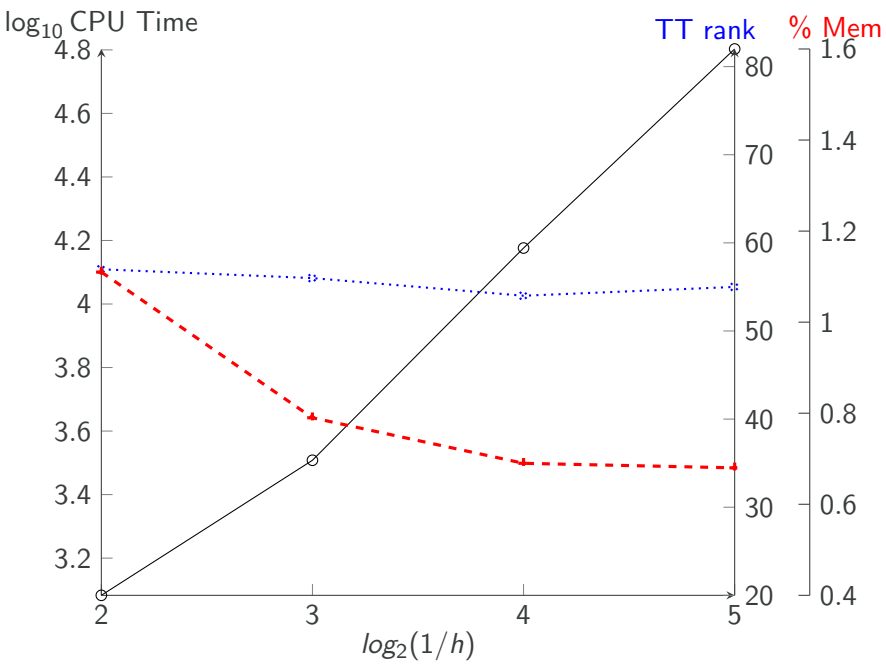
Solve projected linear systems using block-preconditioned GMRES using efficient approximation of Schur complement [B/Onwunta/Stoll 2016].

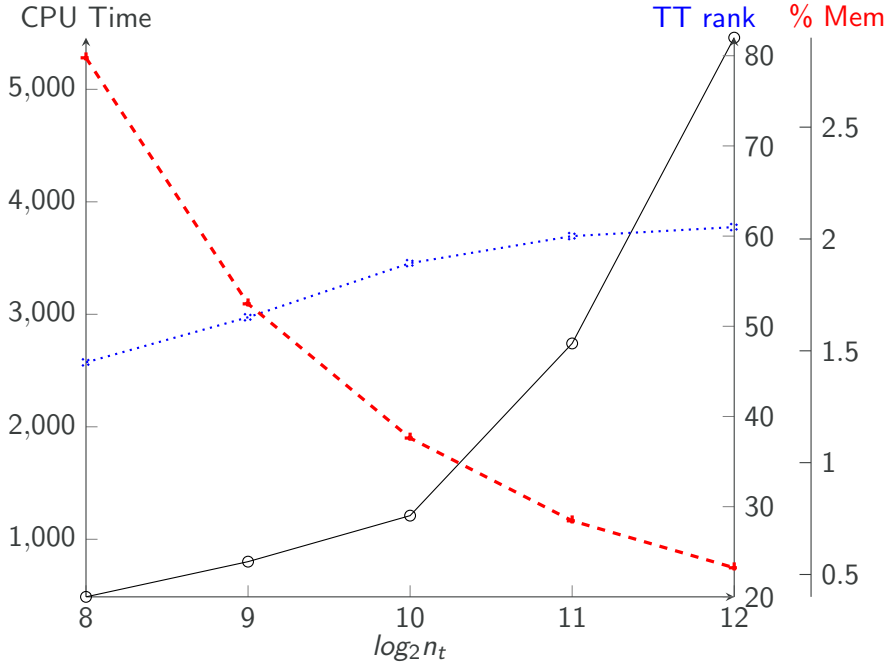
Varying regularization β (left) and time T (right)





Varying Spatial h (left) / Temporal n_t (right) Mesh





Varying the Viscosity

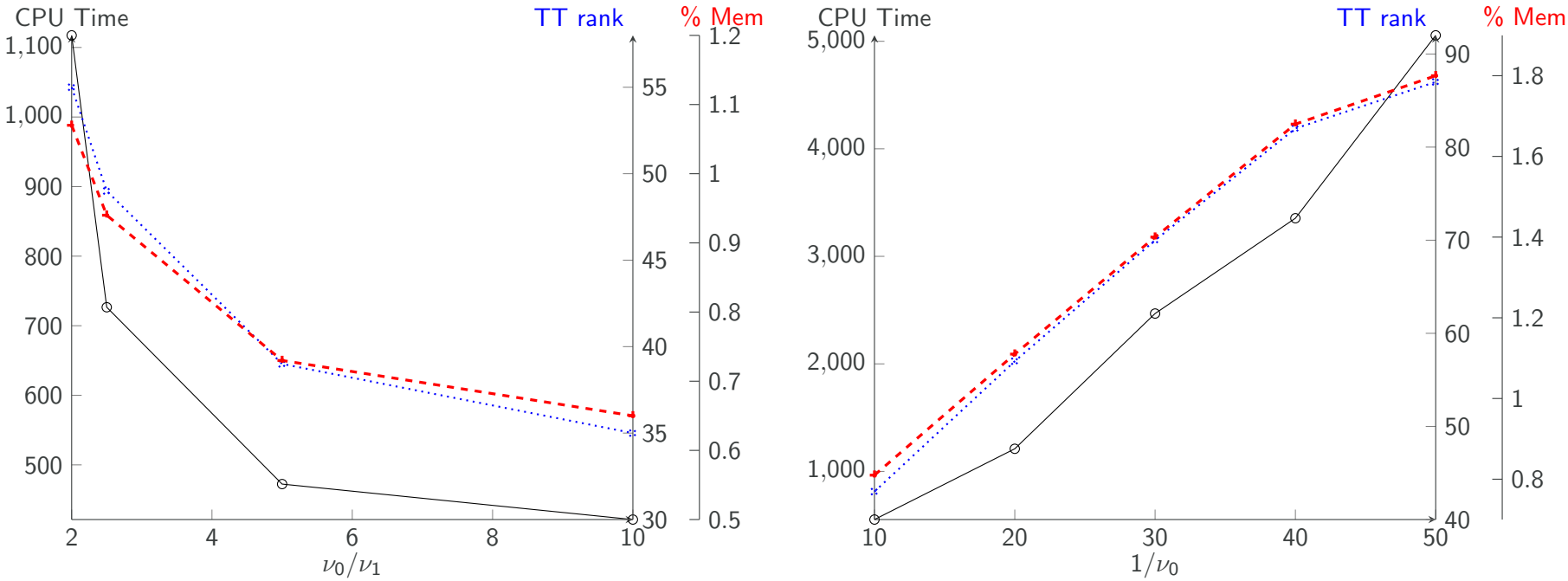
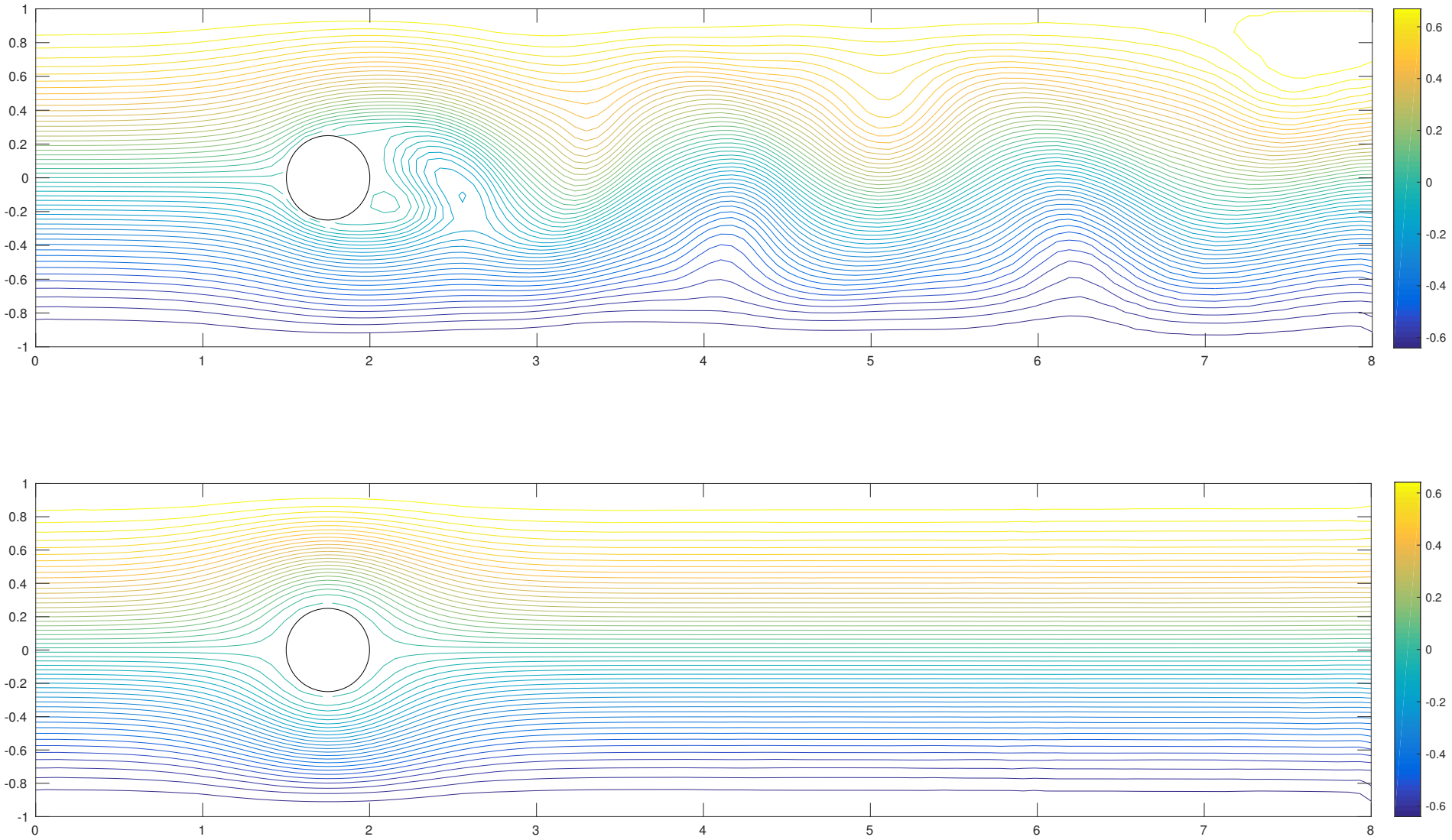


Figure: Left: $\nu_0 = 1/10$, ν_1 is varied. Right: ν_1 and ν_0 are varied together as $\nu_1 = 0.25\nu_0$

Controlled von Kármán Vortex Street



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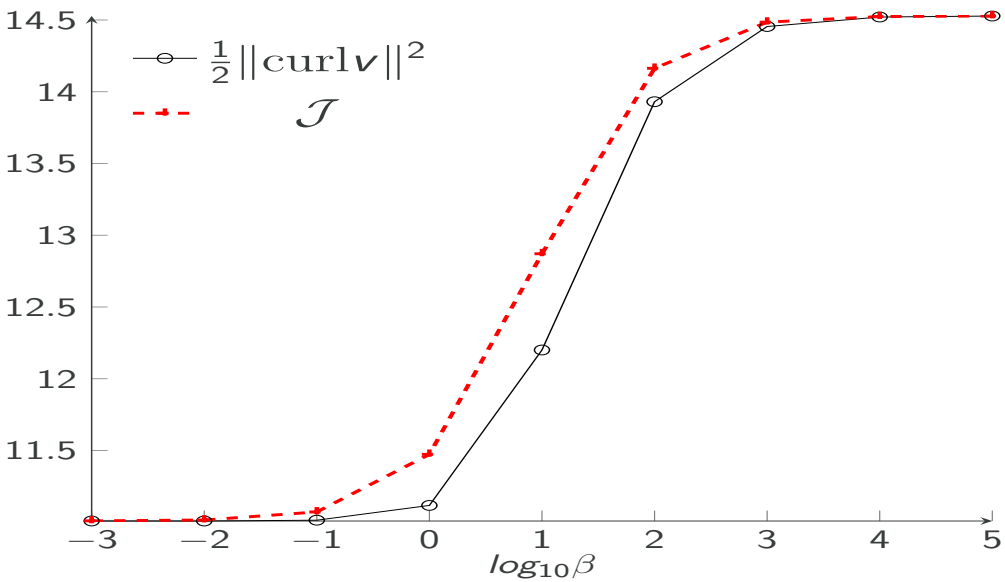
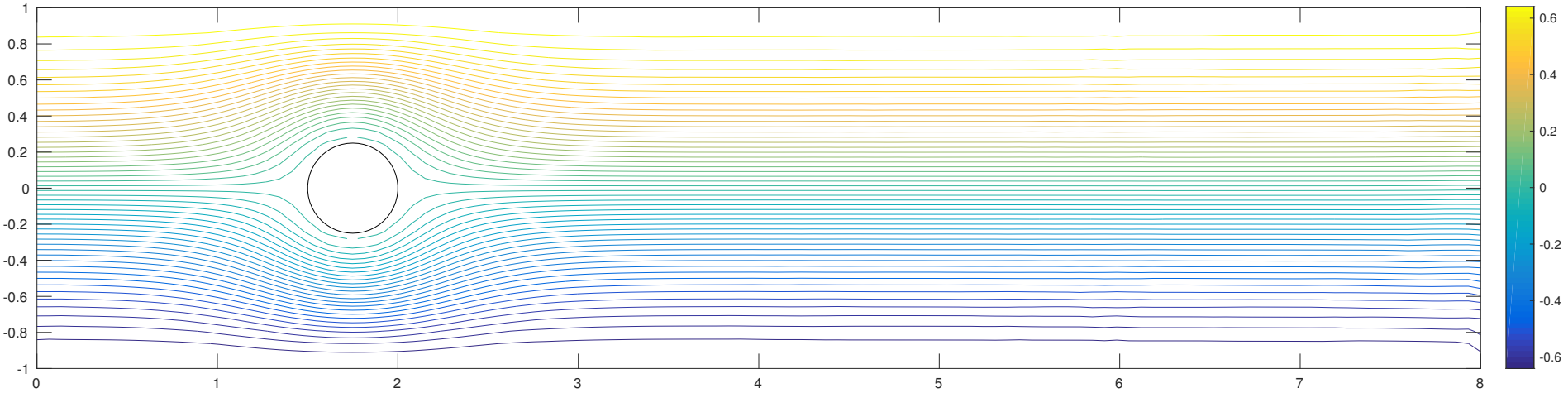


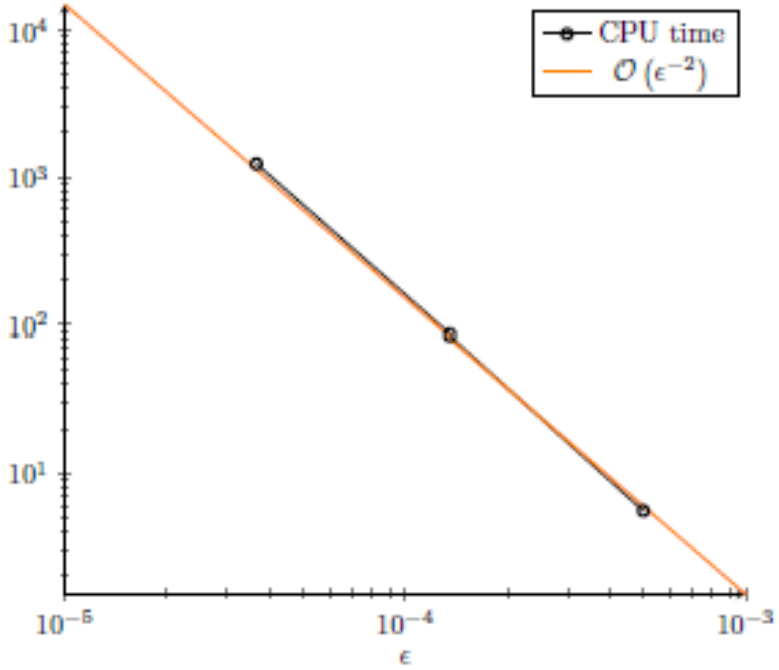


Emprical Complexity Study

Balance all errors w.r.t.

- time, spatial, and stochastic discretization;
- TT truncation.

Call the balanced error ε.



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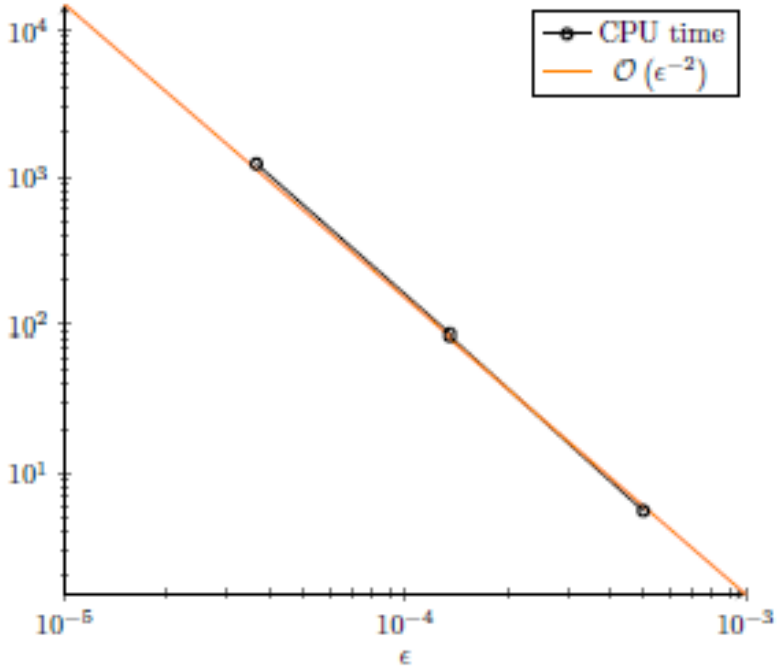

This indicates asymptotic complexity ε^{-2}, asymptotically equal complexity as for deterministic problem.

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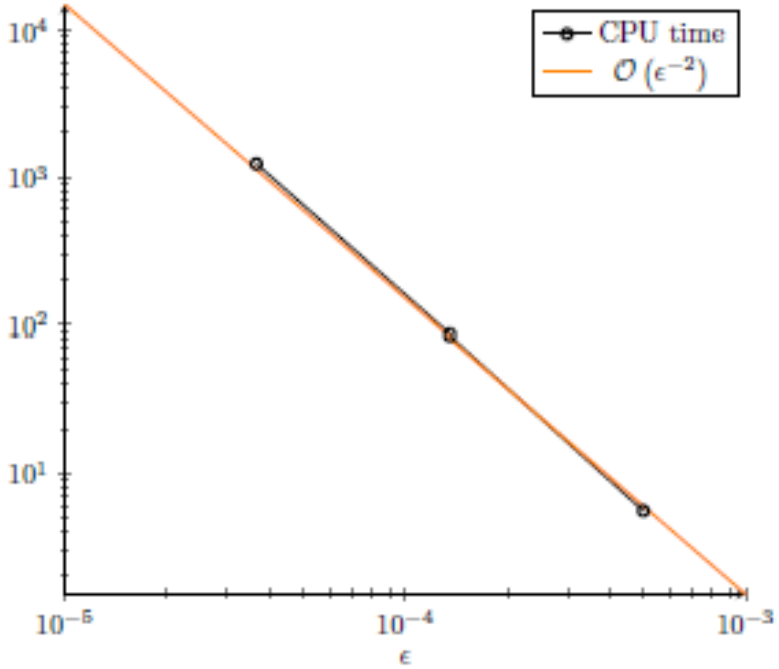

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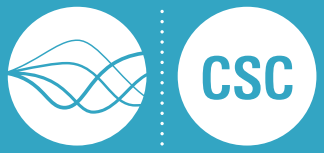
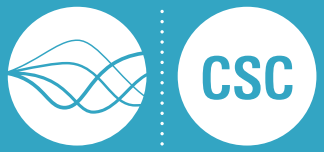
This compares favorably to

- Monte-Carlo $\mathcal{O}(\varepsilon^{-4})$,
- quasi Monte-Carlo / stochastic collocation $\mathcal{O}(\varepsilon^{-3})$.



Outline



Conclusions & Outlook

- Low-rank tensor solver for unsteady heat and Navier-Stokes equations with uncertain viscosity.
- Similar techniques already used for ▸ 3D Stokes(-Brinkman) optimal control problems.
- With 1 stochastic parameter, the scheme reduces complexity by up to 2–3 orders of magnitude.
- To consider next:

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- Low-rank tensor solver for unsteady heat and Navier-Stokes equations with uncertain viscosity.
- Similar techniques already used for ▸ 3D Stokes(-Brinkman) optimal control problems.
- With 1 stochastic parameter, the scheme reduces complexity by up to 2–3 orders of magnitude.
- To consider next:
  - many parameters coming from uncertain geometry or Karhunen-Loève expansion of random fields;
    Basic observation: the more parameters, the more significant is the complexity reduction w.r.t. memory — up to a factor of 10^9 for the control problem for a backward facing step set-up.
  - HPC implementation of AMEn-like solver to deal with even larger problems.

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P. Benner, S. Dolgov, A. Onwunta, and M. Stoll.
Low-rank solvers for unsteady Stokes-Brinkman optimal control problem with random data.
Computer Methods in Applied Mechanics and Engineering, 304:26–54, 2016.

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Low rank solution of unsteady diffusion equations with stochastic coefficients.
SIAM/ASA Journal on Uncertainty Quantification, 3(1):622–649, 2015.

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SIAM Journal on Matrix Analysis and Applications, 37(2):491–518, 2016.

P. Benner, S. Dolgov, A. Onwunta, and M. Stoll.
Solving optimal control problems governed by random Navier-Stokes equations using low-rank methods. arXiv:1703.06097, March 2017.

P. Benner, A. Onwunta, and M. Stoll.
On the existence and uniqueness of the solution of parabolic optimal control problems with uncertain inputs. Submitted, September 2018.

Outline

Low-rank Techniques in Other Areas

Low-rank techniques in stochastic eigenvalue problems

Consider eigenproblem depending on uncertain parameter(s), e.g., uncertainty in Young's modulus in elasticity problems,

$$\begin{aligned} \mathcal{A}(\omega)\varphi(\omega) &= \lambda(\omega)\varphi(\omega), \quad \omega \in \Omega, \\ \varphi(\omega)^T\varphi(\omega) &= 1. \end{aligned}$$

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Parametrization of uncertain parameter, (generalized) polynomial chaos expansion and stochastic Galerkin ansatz $\rightsquigarrow$ multi-parametric eigenvalue problem

$$\left[G_0 \otimes A_0 + \sum_{k=1}^{m} G_k \otimes A_k\right] \Phi = \left[\sum_{k=0}^{N_\xi - 1} \lambda_k (H_k \otimes I_{N_x})\right] \Phi,$$

where $(\lambda_0, \ldots, \lambda_{N_\xi - 1})$ represents the parametrization of a single stochastic eigenvalue $\lambda(\omega)$, and $\Phi = (\Phi) = \operatorname{vec}\left(\left[\varphi_0, \varphi_1, \ldots, \varphi_{N_\xi - 1}\right]\right) \in \mathbb{R}^{N_x N_\xi}$ parameterizes the corresponding stochastic eigenvector $\varphi(\omega)$.

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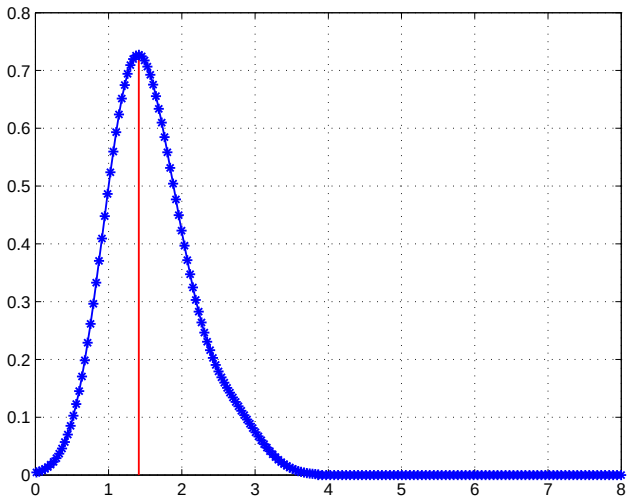
$$\begin{aligned} \mathcal{A}(\omega)\varphi(\omega) &= \lambda(\omega)\varphi(\omega), \quad \omega \in \Omega, \\ \varphi(\omega)^T\varphi(\omega) &= 1. \end{aligned}$$

Developed an inexact Krylov-Newton solver for the multi-parametric eigenvalue problem, using again low-rank techniques.

Example: Probability density of $\lambda_2(\omega)$, $\langle\lambda_2\rangle = 1.412$, for uncertain linear elasticity problem, $\sigma_a = 0.1$.



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P. Benner, A. Onwunta, and M. Stoll.

A low-rank inexact Newton-Krylov method for stochastic eigenvalue problems.

Computational Methods in Applied Mathematics (CMAM), 2018 (online).

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Low-rank techniques in Bayesian inverse problems

Bayesian inference problem: determine unknown parameters U from observations y_{obs}, assuming additive noise:

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Bayesian inference problem: determine unknown parameters U from observations y_{obs}, assuming additive noise:

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Want posterior probability density function π_{post}, apply Bayes' theorem ... $\rightsquigarrow$

$$\pi_{\text{post}} \propto \pi_{\text{prior}}(u)\pi_{\text{noise}}(y_{\text{obs}} - f(u))$$

Want (diagonal of) posterior covariance matrix Γ_{post}:

$$\Gamma_{\text{post}} = \left(A^T \Gamma_{\text{noise}}^{-1} A + \Gamma_{\text{prior}}^{-1}\right)^{-1}.$$

For a discretized partial differential operator A, this formula is numerically infeasible.

[Lieberman/Willcox/Ghattas '10, Flath et al '11, Bui-Thanh et al '13]

Low-rank Techniques in Other Areas

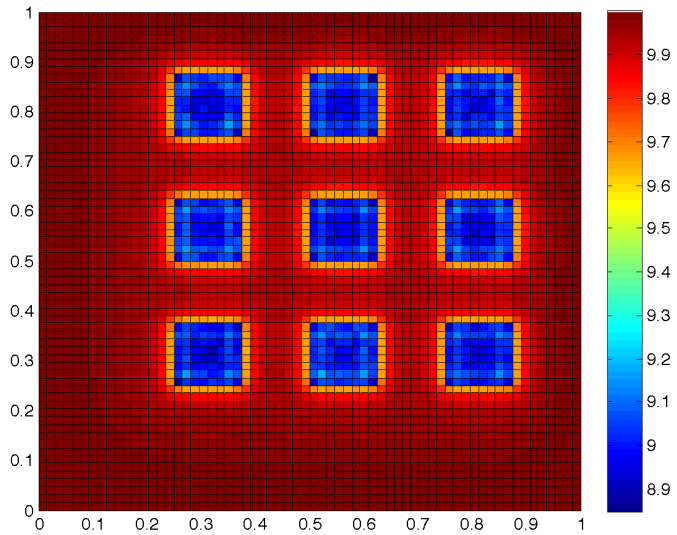
Low-rank techniques in Bayesian inverse problems

Bayesian inference problem: determine unknown parameters U from observations y_{obs}, assuming additive noise:

$$Y = f(U) + E.$$

Developed a low-rank (TT format) Lanczos technique to compute dominant eigenvectors, and to obtain low-rank approximation to Γ_{post}.

Example: determine initial condition for heat flow problem, 9 sensors distributed in the domain, 64×64 mesh.



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P. Benner, Y. Qiu, and M. Stoll.

Low-rank eigenvector compression of posterior covariance matrices for linear Gaussian inverse problems.

SIAM/ASA Journal on Uncertainty Quantification, 6(2):965–989, 2018.

Save the dates!

- 28–30 August 2019, Graz, Austria:

  4th Workshop on
  Model Reduction of Complex Dynamical Systems

  MODRED 2019

  https://imsc.uni-graz.at/modred2019/

- 6–8 November 2019, Magdeburg, Germany:

  8th Workshop on Matrix Equations and Tensor Techniques

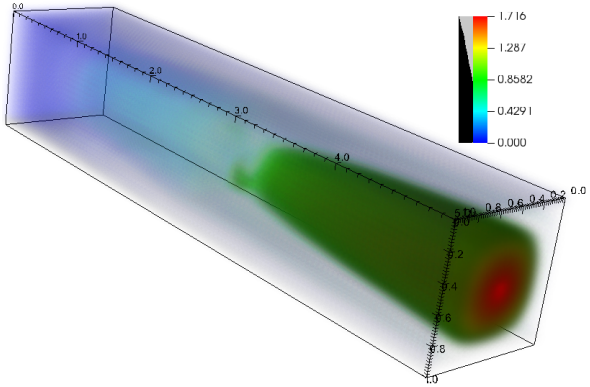
  METT-VIII

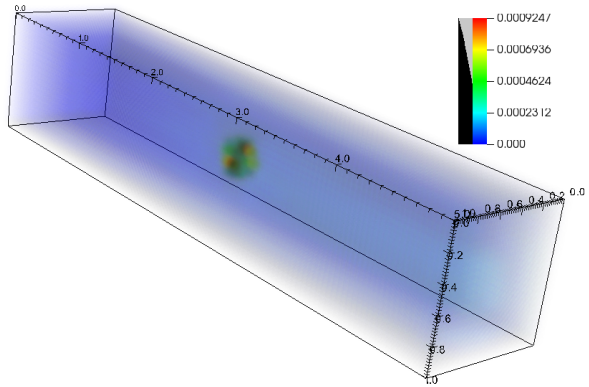
3D Stokes-Brinkman control problem

Mean

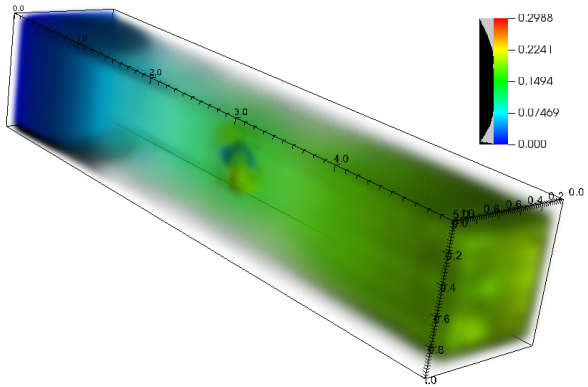
Standard deviation

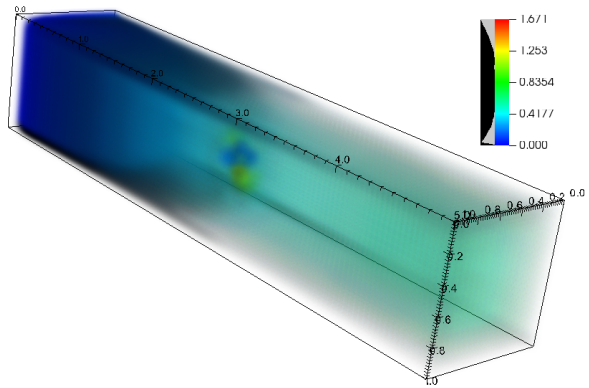
State





Control





- Full size: $n_{\mathbf{x}} n_\xi n_t \approx 3 \cdot 10^9$. Reduction: $\dfrac{\mathtt{mem}(TT)}{\mathtt{mem}(full)} = 0.002.$

return