MAX PLANCK INSTITUTE FOR DYNAMICS OF COMPLEX TECHNICAL SYSTEMS MAGDEBURG

CSC COMPUTATIONAL METHODS IN SYSTEMS AND CONTROL THEORY

Low-rank Tensor Methods for Optimal Control of Uncertain Flow Problems

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Joint work with
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MS PDE-constrained optimization under uncertainty
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CDS Forschungszentrum Dynamische Systeme

Outline

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$$10^{10} \cdot 10^3 \cdot 10^6 \cdot 4 \cdot 4 = 1.6 \cdot 10^{20} \text{bytes} \approx 160 \text{ exabytes of memory!}$$

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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) $1 + 10 + 1(4)$–way tensor! (Above example $\rightsquigarrow$ terabyte-range.)

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- data are predictable, but difficult to measure, e.g., porosity above oil reservoirs ("aleatoric uncertainty");
- data are unpredictable, e.g, wind shear ("epistemic uncertainty").

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Increase in matrix size of discretized differential operator for $h \to \frac{h}{2}$ by factor 2^d.

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$$(I \otimes A + A \otimes I)\, x =: \mathcal{A}x = b \qquad \Longleftrightarrow \qquad AX + XA^T = B$$

with $x = \mathrm{vec}(X)$ and $b = \mathrm{vec}(B)$ with low-rank right hand side $B \approx b_1 b_2^T$.

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- Hence, $\mathcal{A}\mathrm{vec}(X_k) = \mathcal{A}\mathrm{vec}(V_k W_k^T) = \mathrm{vec}\left([\,AV_k,\ V_k\,][\,W_k,\ AW_k\,]^T\right)$

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- Hence, $\mathcal{A}\operatorname{vec}(X_k) = \mathcal{A}\operatorname{vec}\left(V_k W_k^T\right) = \operatorname{vec}\left(\left[\, AV_k,\ V_k \,\right]\left[\, W_k,\ AW_k \,\right]^T\right)$
- 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, ...].

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 we assume that

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

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PDE-constrained optimization problems under uncertainty,

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

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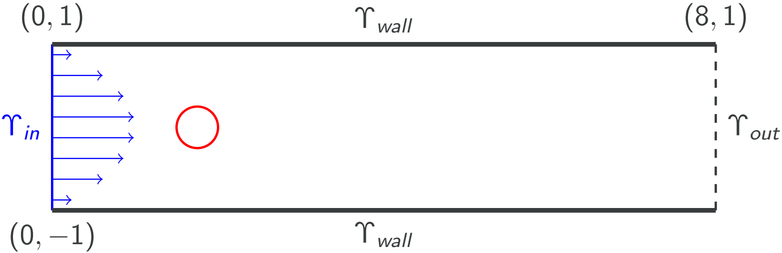
Using low-rank tensor techniques, we need $\approx 7 \cdot 10^7$ **bytes** $= 70$ **GB** to solve the KKT system in MATLAB in less than one hour!

Outline

Model Problem 1: uncertain flow past a circular obstacle

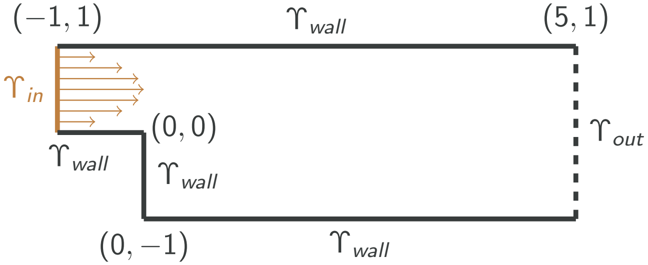
to Numerical Experiments



- 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 $\nu := \nu(\omega)$/ inflow condition $\theta_2(t, x, \omega) = 0$ and

$$\theta_1(t, x, \omega) = \left((1 + x_2)(1 - x_2) + \sum_{k=1}^{m} k^{-\gamma-1/2} \cdot \sin(\pi k x_2) \cdot \xi_k(\omega) \right) (1 - \mathrm{e}^{-t}).$$

Model Problem 2: uncertain flow in a backward facing step domain



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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

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

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

We assume

- $\nu(\omega) = \nu_0 + \nu_1\xi(\omega), \ \ \nu_0, \nu_1 \in \mathbb{R}^+, \ \ \xi \sim \mathcal{U}(-1, 1).$
- $\mathbb{P}\,(\omega \in \Omega : \nu(\omega) \in [\nu_{\min}, \nu_{\max}]) = 1$, 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 $\nu(\omega)$ and $\sigma(t, x, \omega)$).
- High dimensionality (of the resulting linear/optimality systems).

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

state equation

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

adjoint equation

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

gradient equation

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

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gradient equation

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

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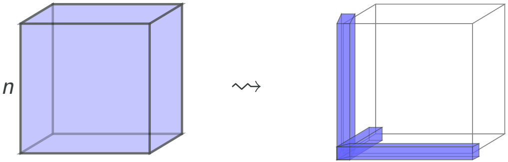
Size: $\sim 3n_t P(J_v + J_p)$, e.g., for $P = 10$, $n_t = 2^{10}$, $J \approx 10^5 \rightsquigarrow \approx 10^9$ unknowns!

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:

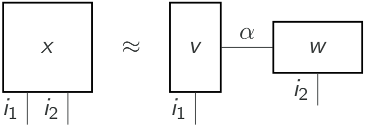
- Store and manipulate x — $\mathcal{O}(dn)$ cost *instead of* $\mathcal{O}(n^d)$.
- Solve equations $Ax = b$ — $\mathcal{O}(dn^2)$ cost *instead of* $\mathcal{O}(n^{2d})$.

Data Compression in 2D: Low-Rank Matrices

- Discrete *separation of variables*:

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

- Diagrams:



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

Tensor Trains/Matrix Product States

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

For indices

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

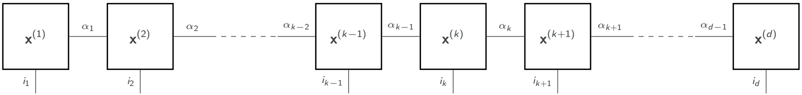
the TT format can be expressed as

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

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 $d=N+2$.

Linear Systems in TT Format

Central Question

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

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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.

- 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 $d = 3$

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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?

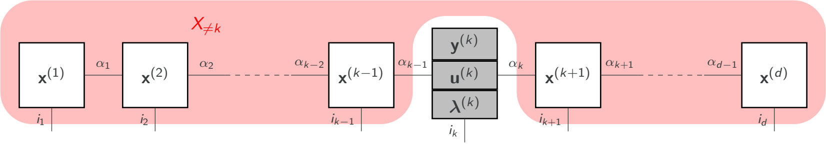
- Recall our KKT system:

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

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

- 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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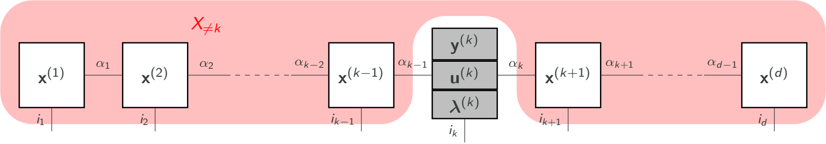


- $X_{\neq k}$ is the *same* for y, u, λ.
- Project each *submatrix*:

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

Numerical Experiments

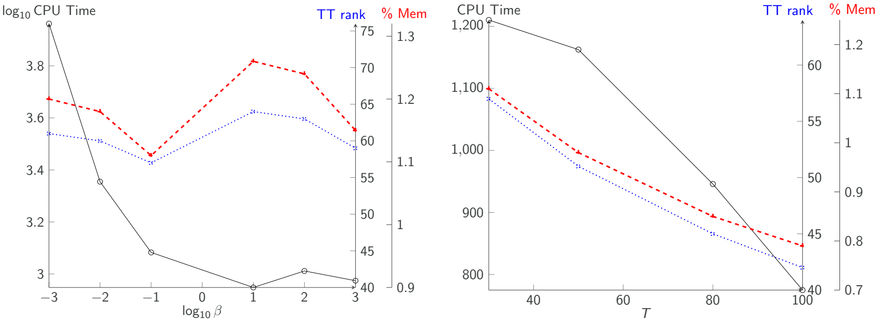
◂ Kármán vortex street

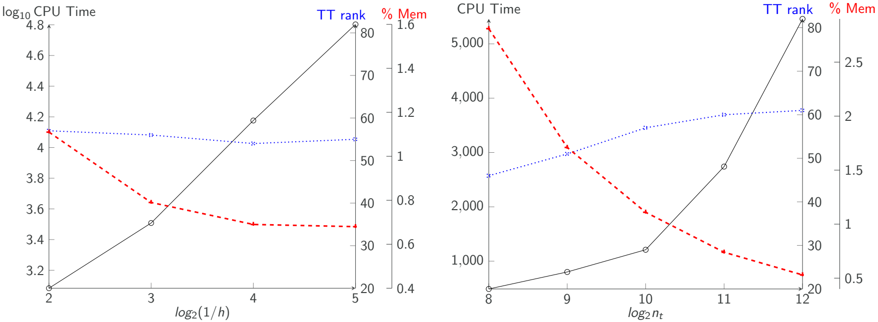
Vary one of the default parameters:

- 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)




log10 CPU Time
TT rank
% Mem
log2(1/h)
CPU Time
TT rank
% Mem
log2 n_t

Varying the Viscosity

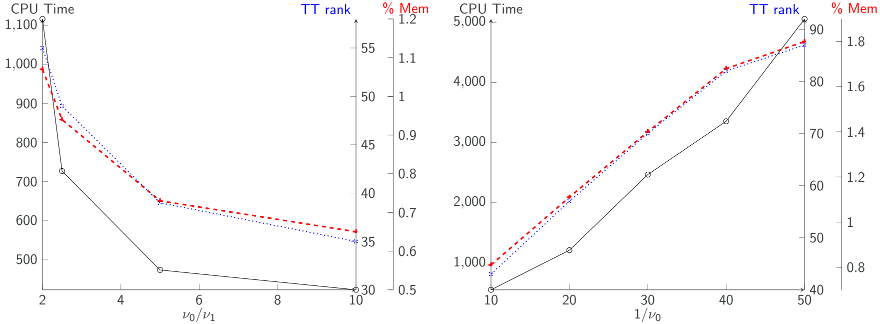
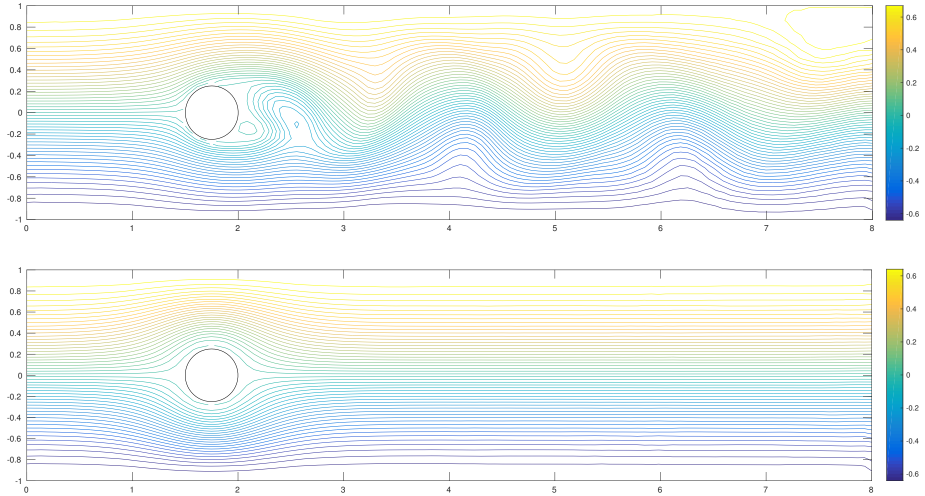


Figure: Left: $\nu_0 = 1/10$, ν_1 is varied. Right: ν_1 and ν_0 are varied together as $\nu_1 = 0.25\nu_0$

Controlled von Kármán Vortex Street



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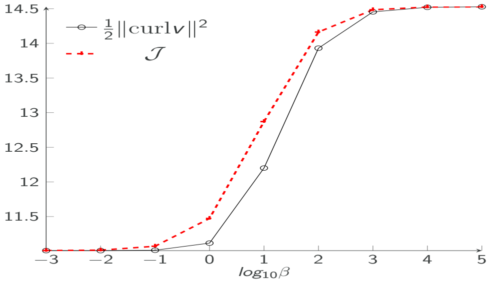
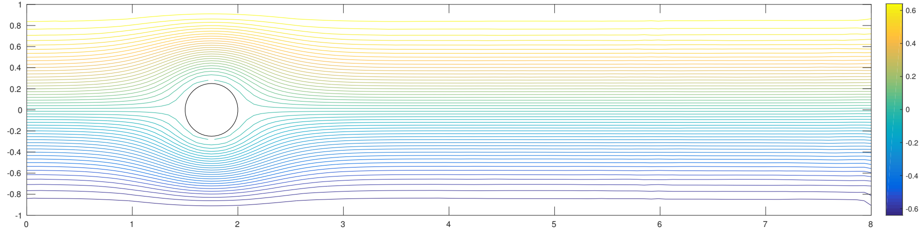


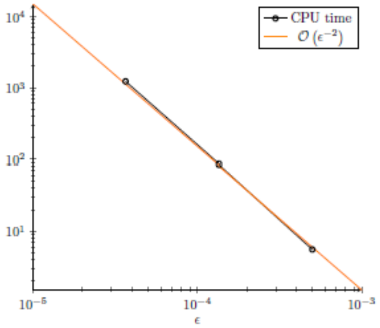


Emprical Complexity Study

Balance all errors w.r.t.

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

Call the balanced error ε.



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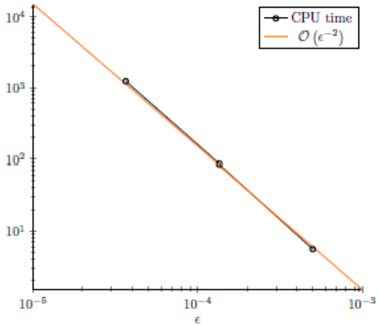

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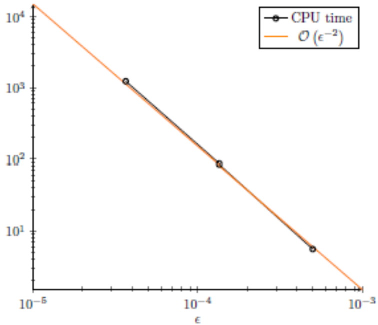

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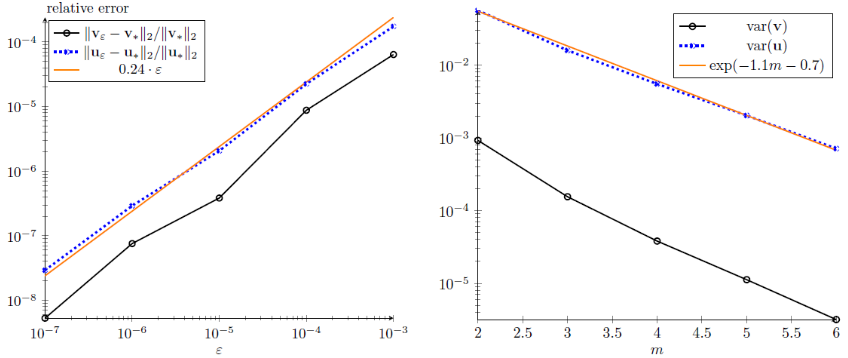
This compares favorably to

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

Relative errors for different TT approximation thresholds (left) and varying m (right)

Parameters:

viscosity $\nu \equiv \nu_0 = 10^{-3}$, final time $T = 20$, regularization parameter $\beta = 10^{-2}$, KL decay rate $\gamma = 2.5$ for inflow condition.



Results for Backward Facing Step

Total CPU time (left) and TT rank (right) versus total approximation error.

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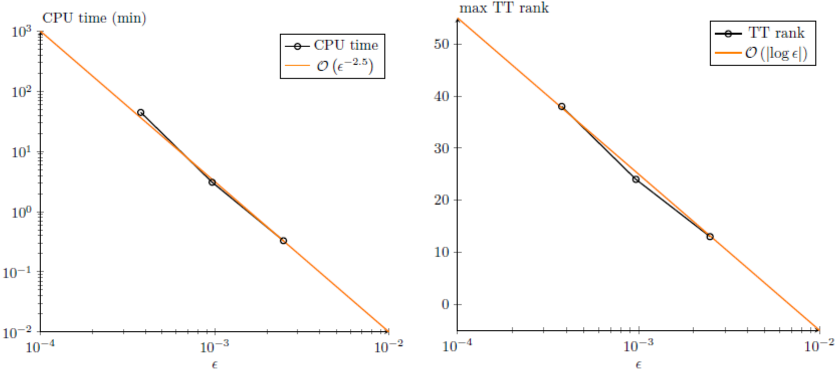

Outline

1. Introduction
2. Optimal Control of Unsteady Navier-Stokes Equations under Uncertainty
3. Conclusions

Conclusions & Outlook

- Low-rank tensor solver for unsteady heat and Navier-Stokes equations with uncertain viscosity.
- Similar techniques already used for Stokes(-Brinkman) optimal control problems.
- Adapted AMEn (TT) solver to saddle point systems.
- With 1 stochastic parameter, the scheme reduces complexity by up to 2–3 orders of magnitude.
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- 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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