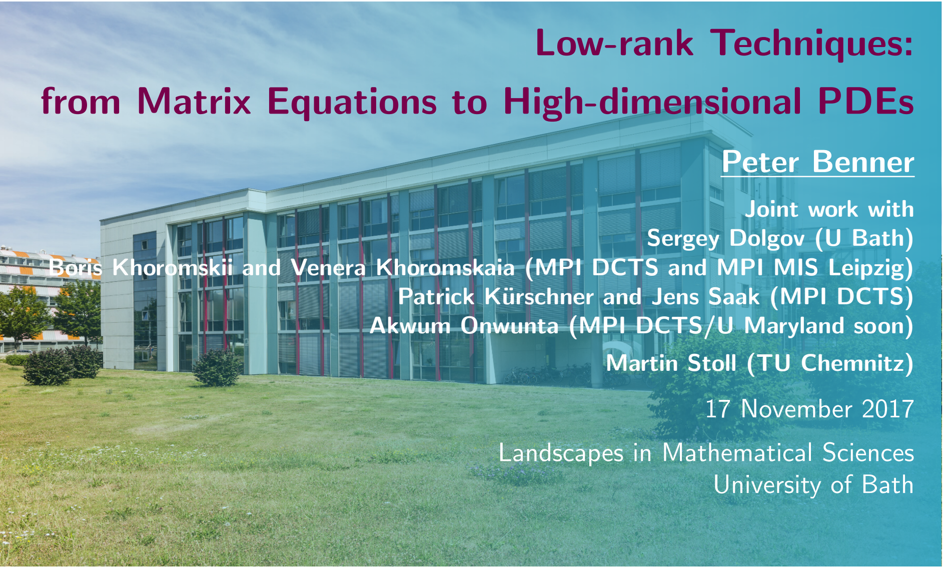
MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC COMPUTATIONAL METHODS IN SYSTEMS AND CONTROL THEORY



Low-rank Techniques: from Matrix Equations to High-dimensional PDEs

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Joint work with
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Landscapes in Mathematical Sciences
University of Bath

The Max Planck Institute (MPI) in Magdeburg

The Max Planck **Society**

- operates 84 institutes — 79 in Germany, 2 in Italy, 1 each in The Netherlands, Luxembourg, and the USA;
- has $\sim$ 23,000 employees;
- had 18 Nobel Laureates since 1948.

"The first MPI in engineering. . . "

MPI Magdeburg

- founded 1998
- 4 departments (directors)
- 9 research groups
- budget $\sim$ 15 Mio. EUR
- $\sim$ 230 employees
- 130 scientists,
- doing research in
  - biotechnology
  - chemical engineering
  - process engineering
  - energy conversion
  - applied math

Outline

1. Motivation
2. Solving Large-Scale Sylvester and Lyapunov Equations
   - Some Basics
   - The Low-Rank Structure
   - LR-ADI Method
   - The New LR-ADI Applied to Lyapunov Equations
3. From Matrix Equations to PDEs in d Dimensions
   - The Curse of Dimensionality
   - Tensor Techniques
   - Numerical Examples

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1. Motivation
2. Solving Large-Scale Sylvester and Lyapunov Equations
3. From Matrix Equations to PDEs in d Dimensions

Model Reduction in Frequency Domain

Approximate the linear control system

$$\begin{aligned} \dot{x} &= Ax + Bu, \qquad A \in \mathbb{R}^{n\times n},\ B \in \mathbb{R}^{n\times m}, \\ y &= Cx + Du, \qquad C \in \mathbb{R}^{q\times n},\ D \in \mathbb{R}^{q\times m}, \end{aligned}$$

by reduced-order system

$$\begin{aligned} \dot{\hat{x}} &= \hat{A}\hat{x} + \hat{B}u, \quad \hat{A} \in \mathbb{R}^{r\times r},\ \hat{B} \in \mathbb{R}^{r\times m}, \\ \hat{y} &= \hat{C}\hat{x} + \hat{D}u, \quad \hat{C} \in \mathbb{R}^{q\times r},\ \hat{D} \in \mathbb{R}^{q\times m} \end{aligned}$$

of order $r \ll n$, such that

$$\| y - \hat{y} \| = \| Gu - \hat{G}u \| \leq \| G - \hat{G} \| \cdot \| u \| < \text{tolerance} \cdot \| u \|,$$

where

$$G(s) = C(sI_n - A)^{-1}B + D, \quad \hat{G}(s) = \hat{C}(sI_r - \hat{A})^{-1}\hat{B} + \hat{D}$$

are the associated transfer functions of the system.

Balanced Truncation [Moore '81]

- System $\Sigma : \begin{cases} \dot{x}(t) = Ax(t) + Bu(t), \\ y(t) = Cx(t), \end{cases}$ with A stable, i.e., $\Lambda(A) \subset \mathbb{C}^-$,

  is balanced, if system Gramians = solutions P, Q of Lyapunov equations

  $$AP + PA^T + BB^T = 0, \qquad A^T Q + QA + C^T C = 0,$$

  satisfy: $P = Q = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n > 0$.

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- $\{\sigma_1, \ldots, \sigma_n\}$ are the Hankel singular values (HSVs) of Σ.
- Compute balanced realization of Σ via state-space transformation

$$\begin{aligned} \mathcal{T} : (A, B, C) \quad &\mapsto \quad (TAT^{-1}, TB, CT^{-1}) \\ &= \quad \left(\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \begin{bmatrix} C_1 & C_2 \end{bmatrix} \right). \end{aligned}$$

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- Truncation $\rightsquigarrow (\hat{A}, \hat{B}, \hat{C}) = (A_{11}, B_1, C_1)$.

Prelude — 20 years of working in low-rank methods

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. . . is one of the greatest model reduction techniques for linear systems since

- the reduced-order model is stable with HSVs $\sigma_1, \ldots, \sigma_r$;
- it allows adaptive choice of r via computable error bound (there is a free lunch!):

$$\| y - \hat{y} \|_2 \leq \| G - \hat{G} \|_{\mathcal{H}_\infty} \| u \|_2 \leq \left(2 \sum\nolimits_{k=r+1}^{n} \sigma_k \right) \| u \|_2 .$$

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But: as suggested in [Moore '81], it is an $\mathcal{O}(n^3)$ **method!**
(Bottleneck: solution of the Lyapunov equations, followed by SVD of their Cholesky factors to determine necessary parts of T and T^{-1}.)

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In **1997**, we derived a method to compute **low-rank factors** $S, R \in \mathbb{R}^{n\times\ell}$, $\ell \ll n$, such that $P \approx SS^T$, $Q \approx RR^T$ [1] and then showed that the truncation could be obtained via cheap $\ell_S \times \ell_R$ SVD of $S^T R$ [2]!

(Some similar ideas: low-rank Lyapunov solver [Saad '90, Jaimoukha/Kasenally '94], small-scale SVD in BT [Penzl '98, Li/White '99].)

P. Benner and E.S. Quintana-Ortí. Solving stable generalized Lyapunov equations with the matrix sign function. Numerical Algorithms, 20(1):75–100, 1999. (Preprint SFB393 97–23)

P. Benner, E.S. Quintana-Ortí, and G. Quintana-Ortí. Balanced truncation model reduction of large-scale dense systems on parallel computers. Mathematical and Computer Modeling of Dynamical Systems, 6(4):383–405, 2000.

Outline

Sylvester equation

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Lyapunov equation

Alexander Michailowitsch Ljapunow
(June 6, 1857 – November 3, 1918)

$$AX + XA^T = C, \quad C = C^T.$$

Generalizations of Sylvester $(AX + XB = C)$ and Lyapunov $(AX + XA^T = C)$ Equations

Generalized Sylvester equation:

$$AXD + EXB = C.$$

Generalized Lyapunov equation:

$$AXE^T + EXA^T = C, \quad C = C^T.$$

Stein equation:

$$X - AXB = C.$$

(Generalized) discrete Lyapunov/Stein equation:

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Note:

- Consider only regular cases, having a unique solution!
- Solutions of symmetric cases are symmetric, $X = X^T \in \mathbb{R}^{n \times n}$; otherwise, $X \in \mathbb{R}^{n \times \ell}$ with $n \neq \ell$ in general.

Applications

- Gramian-based model order reduction
- Linear stability analysis
- Continuation algorithms for detecting Hopf bifurcations
- Determining metastable equilibrium points of stochastic differential equations
- Block-triangularization of matrices and matrix pencils
- Computing covariance matrices, e.g., in biochemical reaction networks
- Numerical solution of fractional partial differential equations
- Solving algebraic Riccati equations via Newton's method
- . . .

Exemplarily, consider the generalized Sylvester equation

$$AXD + EXB = C. \tag{1}$$

Existence of Solutions of Linear Matrix Equations

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Vectorization (using Kronecker product) $\rightsquigarrow$ representation as linear system:

$$\big(\underbrace{D^T \otimes A + B^T \otimes E}_{=:\mathcal{A}}\big)\underbrace{\mathrm{vec}(X)}_{=:x} = \underbrace{\mathrm{vec}(C)}_{=:c} \qquad \Longleftrightarrow \qquad \mathcal{A}x = c.$$

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Lemma

$$\Lambda(\mathcal{A}) = \{\alpha_j + \beta_k \mid \alpha_j \in \Lambda(A, E),\ \beta_k \in \Lambda(B, D)\}.$$

Hence, (1) has unique solution $\Longleftrightarrow \Lambda(A, E) \cap -\Lambda(B, D) = \emptyset$.

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Example: Lyapunov equation $AX + XA^T = C$ has unique solution

$$\Longleftrightarrow \nexists\, \mu \in \mathbb{C}\ :\ \pm\mu \in \Lambda(A).$$

The Low-Rank Structure

Sylvester Equations

Find $X \in \mathbb{R}^{n\times m}$ solving

$$AX - XB = FG^T,$$

where $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{m\times m}$, $F \in \mathbb{R}^{n\times r}$, $G \in \mathbb{R}^{m\times r}$.

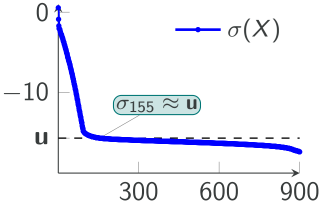
If n, m large, but $r \ll n, m$

$\rightsquigarrow$ X has a small numerical rank.

[Penzl 1999, Grasedyck 2004, Antoulas/Sorensen/Zhou 2002]

$$\operatorname{rank}(X, \tau) = f \ll \min(n, m)$$

singular values of 1600×900 example



$\rightsquigarrow$ Compute low-rank solution factors $Z \in \mathbb{R}^{n\times f}$, $Y \in \mathbb{R}^{m\times f}$, $D \in \mathbb{R}^{f\times f}$, such that $X \approx ZDY^T$ with $f \ll \min(n, m)$.

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Lyapunov Equations

Find $X \in \mathbb{R}^{n \times n}$ solving

$$AX + XA^T = -FF^T,$$

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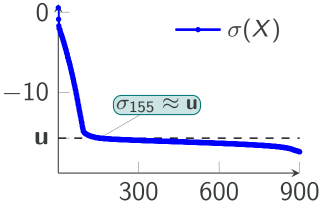

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Theoretical Foundation of the Low-rank Structure

Lyapunov case: [Grasedyck '04]

$$AX + XA^T + BB^T = 0 \iff \underbrace{(I_n \otimes A + A \otimes I_n)}_{=:\mathcal{A}} \operatorname{vec}(X) = -\operatorname{vec}(BB^T).$$

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For stable M, i.e., $\Lambda(M) \subset \mathbb{C}^-$, apply

$$M^{-1} = -\int_0^\infty \exp(tM)\mathrm{d}t$$

to $\mathcal{A}$ and approximate the integral via (sinc) quadrature $\Rightarrow$

$$\mathcal{A}^{-1} \approx -\sum_{i=-k}^{k} \omega_i \exp(t_k \mathcal{A}),$$

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Now observe that

$$\exp(t_i \mathcal{A}) = \exp\left(t_i(I_n \otimes A + A \otimes I_n)\right) \equiv \exp(t_i A) \otimes \exp(t_i A).$$

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Hence,

$$\begin{aligned} \operatorname{vec}(X_k) &= \sum_{i=-k}^{k} \omega_i \left(\exp(t_i A) \otimes \exp(t_i A)\right) \operatorname{vec}(BB^T) \\ \Longrightarrow \quad X_k &= \sum_{i=-k}^{k} \omega_i \exp(t_i A) B B^T \exp(t_i A^T) \equiv \sum_{i=-k}^{k} \omega_i B_i B_i^T, \end{aligned}$$

so that $\operatorname{rank}(X_k) \leq (2k+1)m$ with

$$\|X - X_k\|_2 \lesssim \exp(-\sqrt{k}) \qquad (\exp(-k) \text{ for } A = A^T)!$$

Extended to $AX + XA^T + \sum_{j=1}^m N_j X N_j^T + BB^T = 0.$ [B./Breiten 2012]

Exploiting the Low-Rank Structure I

For simplicity, consider again the Lyapunov equation $AX + XA^T + BB^T = 0$.

Definition

The matrix sign function of $M \in \mathbb{R}^{n \times n}$ with no purely imaginary eigenvalues is

$$\operatorname{sign}(M) = \operatorname{sign}\left(T \begin{bmatrix} J_- & 0 \\ 0 & J_+ \end{bmatrix} T^{-1} \right) = T \begin{bmatrix} -I & 0 \\ 0 & I \end{bmatrix} T^{-1}$$

with $J_\pm$ containing all Jordan blocks of M corresponding to eigenvalues with positive/negative real parts.

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Observations

1. $\operatorname{sign}\left(\begin{bmatrix} A & BB^T \\ 0 & -A^T \end{bmatrix} \right) = \begin{bmatrix} -I & 2X \\ 0 & I \end{bmatrix}$.
2. $\operatorname{sign}(M) = \lim_{k\to\infty} M_k$ with $M_{k+1} = \frac{1}{2}(M_k + M_k^{-1})$ if $M_0 = M$.

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Sign function iteration for solving Lyapunov equations

$M_0 = \begin{bmatrix} A & BB^T \\ 0 & -A^T \end{bmatrix}$, and inversion formula for block-triangular matrices:

$$\begin{aligned} A_{k+1} &\leftarrow \frac{1}{2}(A_k + A_k^{-1}) \\ B_{k+1}B_{k+1} &\leftarrow \frac{1}{2}(B_k B_k^T + A_k^{-1} B_k B_k^T A_k^{-T}) \end{aligned}$$

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so that $B_k \to \frac{1}{\sqrt{2}}Z$ with $X = ZZ^T$.

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Factored sign function iteration for Lyapunov equations [B./Quintana-Ortí 1997/99]

$$\begin{aligned} A_{k+1} &\leftarrow \frac{1}{2}(A_k + A_k^{-1}) \\ B_{k+1} &\leftarrow \frac{1}{\sqrt{2}}[\,B_k,\ A_k^{-1}B_k\,] \end{aligned}$$

Problem: number of columns in B_k doubles each iteration!

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Factored sign function iteration for Lyapunov equations [B./Quintana-Ortí 1997/99]

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Problem: number of columns in B_k doubles each iteration!

Cure: **truncation operator** $B_{k+1} \leftarrow \mathcal{T}_\varepsilon\left(\frac{1}{\sqrt{2}}[\,B_k,\ A_k^{-1}B_k\,]\right)$ with, e.g., $\mathcal{T}_\varepsilon$ returning the scaled left singular vectors of the truncated SVD w.r.t. the numerical rank tolerance ε.

Exploiting the Low-rank Structure for Large and **Sparse** Coefficients

Sylvester equation $AX - XB = FG^T$ is equivalent to linear system of equations

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Possible solvers:

- Standard Krylov subspace solvers in operator from [Hochbruck, Starke, Reichel, ...]
- Block-Tensor-Krylov subspace methods with truncation [Kressner/Tobler, Bollhöfer/Eppler, B./Breiten, ...]
- Galerkin-type methods based on (extended, rational) Krylov subspace methods [Jaimoukha, Kasenally, Jbilou, Simoncini, Druskin, Knizhermann,...]
- Doubling-type methods [Smith, Chu et al., B./Sadkane/El Khoury, ...]
- ADI methods [Wachspress, Reichel, Li, Penzl, B., Saak, Kürschner, Opmeer/Reis, ...]

LR-ADI Method

Sylvester and Stein equations

Let $\alpha \neq \beta$ with $\alpha \notin \Lambda(B)$, $\beta \notin \Lambda(A)$, then

$$\underbrace{AX - XB = FG^T}_{\text{Sylvester equation}} \quad \Leftrightarrow \quad \underbrace{X = \mathcal{A} X \mathcal{B} + (\beta - \alpha)\mathcal{F}\mathcal{G}^H}_{\text{Stein equation}}$$

with the Cayley-like (Möbius) transformations

$$\mathcal{A} := (A - \beta I_n)^{-1}(A - \alpha I_n), \qquad \mathcal{B} := (B - \alpha I_m)^{-1}(B - \beta I_m),$$
$$\mathcal{F} := (A - \beta I_n)^{-1}F, \qquad \mathcal{G} := (B - \alpha I_m)^{-H}G.$$

$\rightsquigarrow$ fix point iteration

$$X_k = \mathcal{A} X_{k-1} \mathcal{B} + (\beta - \alpha)\mathcal{F}\mathcal{G}^H$$

for $k \geq 1$, $X_0 \in \mathbb{R}^{n \times m}$.

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$$\mathcal{A}_\mathbf{k} := (A - \beta_\mathbf{k} I_n)^{-1}(A - \alpha_\mathbf{k} I_n), \qquad \mathcal{B}_\mathbf{k} := (B - \alpha_\mathbf{k} I_m)^{-1}(B - \beta_\mathbf{k} I_m),$$

$$\mathcal{F}_\mathbf{k} := (A - \beta_\mathbf{k} I_n)^{-1} F, \qquad \mathcal{G}_\mathbf{k} := (B - \alpha_\mathbf{k} I_m)^{-H} G.$$

$\rightsquigarrow$ **alternating directions implicit (ADI)** iteration

$$X_k = \mathcal{A}_\mathbf{k} X_{k-1} \mathcal{B}_\mathbf{k} + (\beta_\mathbf{k} - \alpha_\mathbf{k}) \mathcal{F}_\mathbf{k} {\mathcal{G}_\mathbf{k}}^H$$

for $k \geq 1$, $X_0 \in \mathbb{R}^{n \times m}$. [Wachspress 1988]

LR-ADI Method

Sylvester ADI iteration [Wachspress 1988]

$$\begin{aligned}
X_k &= \mathcal{A}_k X_{k-1} \mathcal{B}_k + (\beta_k - \alpha_k)\mathcal{F}_k \mathcal{G}_k^H, \\
\mathcal{A}_k &:= (A - \beta_k I_n)^{-1}(A - \alpha_k I_n), \quad \mathcal{B}_k := (B - \alpha_k I_m)^{-1}(B - \beta_k I_m), \\
\mathcal{F}_k &:= (A - \beta_k I_n)^{-1} F \in \mathbb{R}^{n \times r}, \quad \mathcal{G}_k := (B - \alpha_k I_m)^{-H} G \in \mathbb{C}^{m \times r}.
\end{aligned}$$

Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$X_1 = \mathcal{A}_1 X_0 \mathcal{B}_1 + (\beta_1 - \alpha_1)\mathcal{F}_1 \mathcal{G}_1^H$$

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Sylvester ADI iteration [Wachspress 1988]

$$X_k = \mathcal{A}_k X_{k-1} \mathcal{B}_k + (\beta_k - \alpha_k)\mathcal{F}_k \mathcal{G}_k^H,$$
$$\mathcal{A}_k := (A - \beta_k I_n)^{-1}(A - \alpha_k I_n), \quad \mathcal{B}_k := (B - \alpha_k I_m)^{-1}(B - \beta_k I_m),$$
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Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$X_1 = (\beta_1 - \alpha_1)(A - \beta_1 I_n)^{-1} F G^T (B - \alpha_1 I_m)^{-1}$$
$$\Rightarrow V_1 := Z_1 = (A - \beta_1 I_n)^{-1} F \in \mathbb{R}^{n\times r},$$
$$D_1 = (\beta_1 - \alpha_1) I_r \in \mathbb{R}^{r\times r},$$
$$W_1 := Y_1 = (B - \alpha_1 I_m)^{-H} G \in \mathbb{C}^{m\times r}.$$

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Sylvester ADI iteration [Wachspress 1988]

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Now set $X_0 = 0$ and find factorization $X_k = Z_k D_k Y_k^H$

$$\begin{aligned}
X_2 &= \mathcal{A}_2 X_1 \mathcal{B}_2 + (\beta_2 - \alpha_2)\mathcal{F}_2 \mathcal{G}_2^H \\
V_2 &= V_1 + (\beta_2 - \alpha_1)(A + \beta_2 I)^{-1} V_1 \in \mathbb{R}^{n \times r}, \\
W_2 &= W_1 + \overline{(\alpha_2 - \beta_1)}(B + \alpha_2 I)^{-H} W_1 \in \mathbb{R}^{m \times r}, \\
Z_2 &= [Z_1, \ V_2], \\
D_2 &= \operatorname{diag}(D_1, (\beta_2 - \alpha_2) I_r), \\
Y_2 &= [Y_1, \ W_2].
\end{aligned}$$

LR-ADI Algorithm [B. 2005, Li/Truhar 2008, B./Li/Truhar 2009]

Algorithm 1: Low-rank Sylvester ADI / factored ADI (fADI)

Input : Matrices defining $AX - XB = FG^T$ and shift parameters $\{\alpha_1, \ldots, \alpha_{k_{\max}}\}$, $\{\beta_1, \ldots, \beta_{k_{\max}}\}$.

Output: Z, D, Y such that $ZDY^H \approx X$.

$Z_1 = V_1 = (A - \beta_1 I_n)^{-1} F$,

$Y_1 = W_1 = (B - \alpha_1 I_m)^{-H} G$.

$D_1 = (\beta_1 - \alpha_1) I_r$

for $k = 2, \ldots, k_{\max}$ **do**

  $V_k = V_{k-1} + (\beta_k - \alpha_{k-1})(A - \beta_k I_n)^{-1} V_{k-1}$.

  $W_k = W_{k-1} + \overline{(\alpha_k - \beta_{k-1})}(B - \alpha_k I_n)^{-H} W_{k-1}$.

  Update solution factors

$$Z_k = [Z_{k-1}, V_k], \quad Y_k = [Y_{k-1}, W_k], \quad D_k = \operatorname{diag}\left(D_{k-1}, (\beta_k - \alpha_k) I_r\right).$$

Disadvantages of Low-Rank ADI as of 2012:

1. No efficient stopping criteria:
   - Difference in iterates $\rightsquigarrow$ norm of added columns/step: not reliable, stops often too late.
   - Residual is a full dense matrix, can not be calculated as such.
2. Requires complex arithmetic for real coefficients when complex shifts are used.
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Key observation: residual is low-rank matrix, with rank less than or equal to that of right-hand side!

$\Longrightarrow$ **speed-ups old vs. new LR-ADI can be up to 20!**

Other Low-rank Lyapunov Solvers...

...for Lyapunov equation $0 = AX + XA^T + BB^T$

Projection-based methods for Lyapunov equations with $A + A^T < 0$:

1. Compute orthonormal basis $\mathrm{range}(Z)$, $Z \in \mathbb{R}^{n\times r}$, for subspace $\mathcal{Z} \subset \mathbb{R}^n$, $\dim \mathcal{Z} = r$.
2. Set $\hat{A} := Z^T AZ$, $\hat{B} := Z^T B$.
3. Solve small-size Lyapunov equation $\hat{A}\hat{X} + \hat{X}\hat{A}^T + \hat{B}\hat{B}^T = 0$.
4. Use $X \approx Z\hat{X}Z^T$.

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Examples:

- Krylov subspace methods, i.e., for $m = 1$:

$$\mathcal{Z} = \mathcal{K}(A, B, r) = \mathrm{span}\{B, AB, A^2B, \ldots, A^{r-1}B\}$$

  [Saad 1990, Jaimoukha/Kasenally 1994, Jbilou 2002–2008].

- Extended Krylov subspace method (EKSM) [Simoncini 2007],

$$\mathcal{Z} = \mathcal{K}(A, B, r) \cup \mathcal{K}(A^{-1}, B, r).$$

- Rational Krylov subspace methods (RKSM) [Druskin/Simoncini 2011].

The New LR-ADI Applied to Lyapunov Equations

Example: an ocean circulation problem [Van Gijzen et al. 1998]

- FEM discretization of a simple 3D ocean circulation model (barotropic, constant depth) $\rightsquigarrow$ stiffness matrix $-A$ with $n = 42,249$, choose artificial constant term $B = \texttt{rand(n,5)}$.

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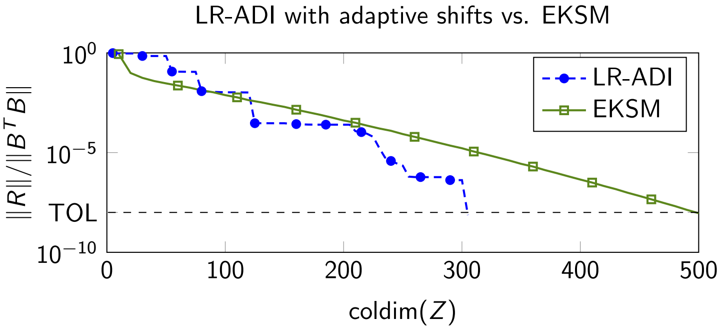

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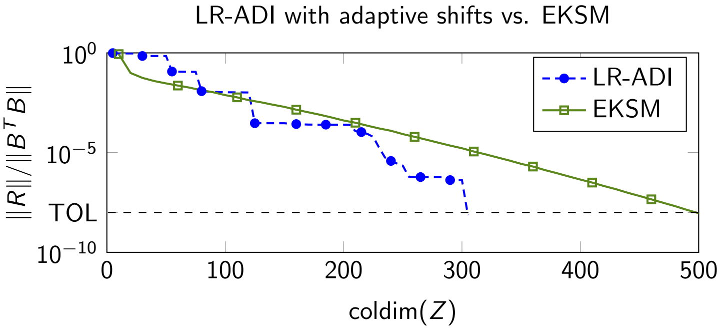

- CPU times: LR-ADI $\approx$ 110 sec, EKSM $\approx$ 135 sec.

Summary & Outlook (Matrix Equations)

- Numerical enhancements of low-rank ADI for large Sylvester/Lyapunov equations:
  1. low-rank residuals, reformulated implementation,
  2. compute real low-rank factors in the presence of complex shifts,
  3. self-generating shift strategies (quantification in progress).

For diffusion-convection-reaction example:
332.02 sec. down to **17.24 sec.** $\rightsquigarrow$ acceleration by factor almost **20**.

- Generalized version enables derivation of low-rank solvers for various generalized Sylvester equations.
- Ongoing work:
  - Apply LR-ADI in Newton methods for algebraic Riccati equations

$$\mathcal{R}(X) = AX + XA^T + GG^T - XSS^TX = 0,$$

$$\mathcal{D}(X) = AXA^T - EXE^T + GG^T + A^TXF(I_r + F^TXF)^{-1}F^TXA = 0.$$

For nonlinear AREs see

P. Benner, P. Kürschner, J. Saak. *Low-rank Newton-ADI methods for large nonsymmetric algebraic Riccati equations.* J. Franklin Inst., 2015.

Outline

1. Motivation

2. Solving Large-Scale Sylvester and Lyapunov Equations

3. From Matrix Equations to PDEs in d Dimensions
   - The Curse of Dimensionality
   - Tensor Techniques
   - Numerical Examples

The Curse of Dimensionality [Bellman 1957]

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

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- Ideas correspond to **separation of variables** in continuous-time: $b(x, y) \approx b_1(x) b_2(y)$.

From Matrix Equations to PDEs in d Dimensions

Ideas extend to $d \geq 3$: let $A_j \in \mathbb{R}^{n_j \times n_j}$, $j = 1, \ldots, d$, be 1d-discretization matrices corresponding to "grid points" $x_j^{(1)}, x_j^{(2)}, \ldots, x_j^{(n_j)}$, then under certain assumptions, the Laplace operator (w/ homogeneous boundary conditions) can be discretized as

$$\mathcal{A} = A_1 \otimes I \otimes \cdots \otimes I + I \otimes A_2 \otimes I \otimes \cdots \otimes I + \ldots + I \otimes \cdots \otimes I \otimes A_d.$$

Note: if $n_j = n \, \forall \, j$, then $\mathcal{A} \in \mathbb{R}^{n^d \times n^d}$!

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If source term can be written as $f(x_1, x_2, \ldots, x_d) = f_1(x_1) f_2(x_2) \cdots f_d(x_d)$, discretized right-hand side becomes

$$b = b_1 \otimes b_2 \otimes \cdots \otimes b_d \in \mathbb{R}^{n^d} \quad \text{with} \quad b_j = [\, f_j(x_j^{(1)}), \ldots, f_j(x_j^{(n)}) \,].$$

From Matrix Equations to PDEs in d Dimensions

Ideas extend to $d \geq 3$: let $A_j \in \mathbb{R}^{n_j \times n_j}$, $j = 1, \ldots, d$, be 1d-discretization matrices corresponding to "grid points" $x_j^{(1)}, x_j^{(2)}, \ldots, x_j^{(n_j)}$, then under certain assumptions, the Laplace operator (w/ homogeneous boundary conditions) can be discretized as

$$\mathcal{A} = A_1 \otimes I \otimes \cdots \otimes I + I \otimes A_2 \otimes I \otimes \cdots \otimes I + \ldots + I \otimes \cdots \otimes I \otimes A_d.$$

Note: if $n_j = n \; \forall \, j$, then $\mathcal{A} \in \mathbb{R}^{n^d \times n^d}$!

If source term can be written as $f(x_1, x_2, \ldots, x_d) = f_1(x_1) f_2(x_2) \cdots f_d(x_d)$, discretized right-hand side becomes

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Now if the solution x of $\mathcal{A}x = b$

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then we could hope to reduce the storage and computational complexity from n^d to dn!

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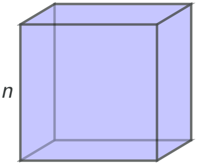
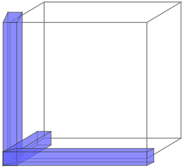
then we could hope to reduce the storage and computational complexity from n^d to dn! This requires **low-rank tensor techniques.**

(Note: for x we will need a more complex representation as 1. does not hold in general!)

Separation of Variables and Low-rank Approximation



$\rightsquigarrow$



- 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:

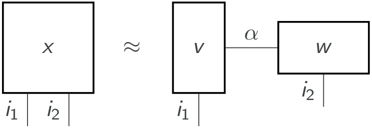
- Store and manipulate x — $\mathcal{O}(dn)$ cost *instead of* $\mathcal{O}(n^d)$.
- Solve equations $Ax = b$ — $\mathcal{O}(dn^2)$ cost *instead of* $\mathcal{O}(n^{2d})$.

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)*
  $\Longrightarrow \quad \varepsilon(r)$ optimal w.r.t. spectral/Frobenius norm.

Tensor Trains

- Matrix Product States/Tensor Train (TT) format
  [Wilson '75, White '93, Verstraete '04, Oseledets '09/'11]:

  For indices

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

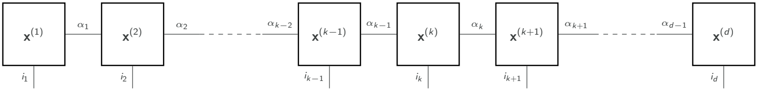
  the TT format can be expressed as

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

  or

  $$x(\overline{i_1 \ldots i_d}) = \mathbf{x}^{(1)}(i_1) \cdots \mathbf{x}^{(d)}(i_d), \qquad \mathbf{x}^{(k)}(i_k) \in \mathbb{R}^{r_{k-1} \times r_k}.$$

  or



- Storage: $\mathcal{O}(dnr^2)$.

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

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

- *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 truncation operator $\mathcal{T}_\varepsilon$ using SVD (or QR).
- Iterative linear solvers (and preconditioners) can be implemented in TT format; we use, e.g., TT-GMRES.

Numerical Examples

Our work

Apply low-rank iterative solvers in TT format to discrete optimality systems resulting from

PDE-constrained optimization problems under uncertainty,

discretized by **stochastic Galerkin method**, i.e., applying Galerkin projection to weak formulation using

- implicit Euler (discontinuous Galerkin, dG(0)) in time,
- classical finite element methods (FEM) in physical space,
- generalized polynomial chaos in N-dimensional parameter space (resulting from parameterizing uncertain parameters).

This yields naturally a $(1 + 2(3) + N)$-way tensor representation of solution, which we approximate in low-rank TT format.

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Biggest problem solved so far has $n = 1.29 \cdot 10^{15}$ unknowns (optimality system for unsteady incompressible Navier-Stokes control problem with uncertain viscosity).

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

Optimal Control of 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

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

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. $\mathbb{P}(\omega\in\Omega : a(x,\omega)\in[a_{\min},a_{\max}]\ \forall x\in\mathcal{D}) = 1$.

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[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.

[1] due to the positivity assumption on $a(\mathbf{x}, \omega)$

Weak formulation of the optimality system

Theorem [Chen/Quarteroni 2014, B./Onwunta/Stoll 2016]

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

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

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 $\mathcal{B}$.

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 w/ 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

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

and

- $G_0 = \operatorname{diag}\left(\langle\psi_0^2\rangle, \langle\psi_1^2\rangle, \ldots, \left\langle\psi_{P-1}^2\right\rangle\right), \quad G_i(j,k) = \langle\xi_i\psi_j\psi_k\rangle, \quad i = 1,\ldots,N,$
- $G_\alpha = G_0 + \alpha \operatorname{diag}\left(0, \langle\psi_1^2\rangle, \ldots, \left\langle\psi_{P-1}^2\right\rangle\right)$ (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,
- $C = -\operatorname{diag}(\text{ones}, -1), \quad D = \operatorname{diag}\left(\frac{1}{2}, 1, \ldots, 1, \frac{1}{2}\right) \in \mathbb{R}^{n_t\times n_t}.$

Discrete first order optimality conditions/KKT system

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Linear system with $3JPn_t$ unknowns!

Solving the Optimality 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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  $$\mathcal{P} := \begin{bmatrix} A & 0 \\ 0 & -S \end{bmatrix} \qquad \text{with the Schur complement} \quad S := -BA^{-1}B^T,$$

  MINRES finds the exact solution in at most three steps.

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  $$\begin{bmatrix} \hat{A} & 0 \\ 0 & \hat{S} \end{bmatrix}.$$
- Implemented in TT format $\rightsquigarrow$ TT-MINRES.

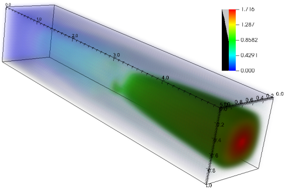
Mean-Based Preconditioned TT-MINRES

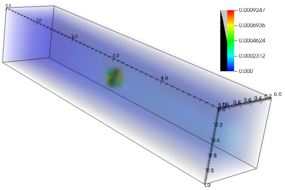
TT-MINRES	# iter (t)	# iter (t)	# iter (t)
n_t	2^5	2^6	2^8
$\dim(\mathcal{A}) = 3JPn_t$	$10,671,360$	$21,342,720$	$85,370,880$
$\alpha = 1,\ \mathrm{tol} = 10^{-3}$			
$\beta = 10^{-5}$	6 (285.5)	6 (300.0)	8 (372.2)
$\beta = 10^{-6}$	4 (77.6)	4 (130.9)	4 (126.7)
$\beta = 10^{-8}$	4 (56.7)	4 (59.4)	4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

Optimal Control 3D Stokes-Brinkman w/ Uncertain Viscosity

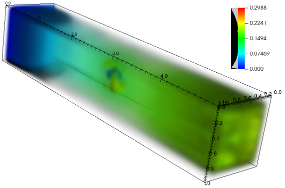
Mean | Standard deviation

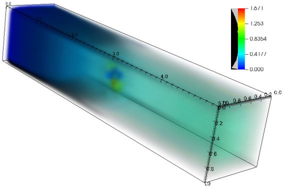
State





Control





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

Conclusions (High-dimensional PDEs)

- Low-rank tensor solver for unsteady heat **and Navier-Stokes equations** with uncertain viscosity.
- Similar techniques used for Stokes(-Brinkman) optimal control problems.
- Adapted AMEn (TT) solver to saddle point systems.
- To consider next:

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- To consider next:
  - Navier-Stokes: many parameters coming from uncertain geometry or Karhunen-Loève expansion of random fields;
    Initial results: 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.
  - exploit multicore technology (need efficient parallelization of AMEn).

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