MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

LOW-RANK METHODS FOR PDE-CONSTRAINED OPTIMIZATION UNDER UNCERTAINTY

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Joint work with Sergey Dolgov (U Bath), Martin Stoll (TU Chemnitz) and Akwum Onwunta (MPI DCTS Magdeburg, moving to U Maryland)

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Overview

PDEs with stochastic coefficients for UQ

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- data are predictable, but difficult to measure, e.g., porosity above oil reservoirs;
- data are unpredictable, e.g, wind shear.

Motivation I: Low-Rank Solvers

Curse of Dimensionality [Bellman '57]

Increase matrix size of discretized differential operator for $h \rightarrow \frac{h}{2}$ 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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- 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

- $c(y,u)=0$ 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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PDE-constrained optimization problems under uncertainty,

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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!

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

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

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

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.

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 '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 $\mathcal{B}$.

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

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

and

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

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

  MINRES finds the exact solution in at most three steps.

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- 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 $\alpha \in [0, +\infty)$ and

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

where $\gamma = \sqrt{(1+\alpha)/\beta}$ and $\mathcal{K} = \sum_{i=0}^{N} G_i \otimes K_i$.
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]

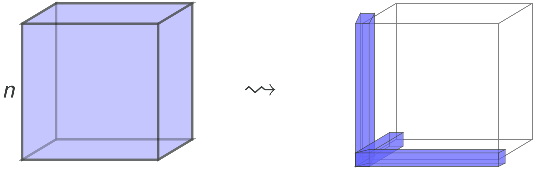
Let $\mathcal{A}$ be the KKT matrix from the stochastic Galerkin approach, and $\mathcal{P}$ the preconditioner using the Schur complement approximation $\tilde{S}$ (and exact A). Then

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

where

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

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:

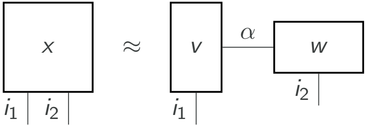
- Store and manipulate x — $\mathcal{O}(dn)$ cost *instead of* $\mathcal{O}(n^d)$.
- Solve equations $Ax = b$ — $\mathcal{O}(dn^2)$ cost *instead of* $\mathcal{O}(n^{2d})$.

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)*

  $\Longrightarrow \quad \varepsilon(r)$ 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

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

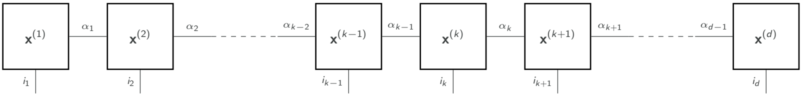
the TT format can be expressed as

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

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

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

- *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 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 $d=N+2$.

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)

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.
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- To consider next:
  - 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 in efficient parallelization.

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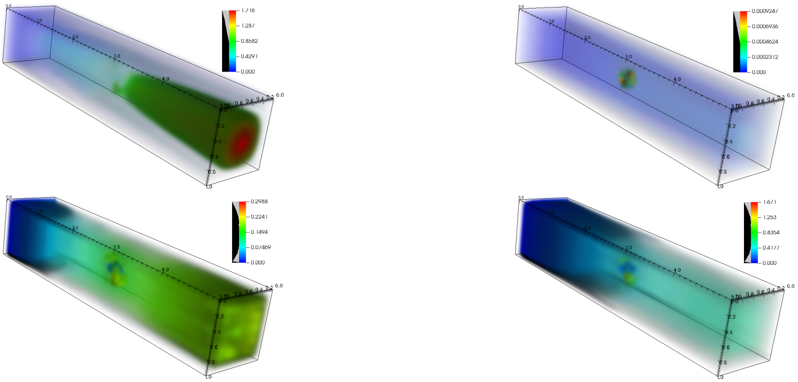
Mean | Standard deviation

State

Control



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

return