

Computational methods for large-scale matrix equations and application to PDEs

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Eigenvalue pbs and tracking, Control, MOR, Assignment pbs, Riccati eqn

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Control, (Stochastic) PDEs, ... Survey article: V.Simoncini, SIAM Review 2016.

• Systems of linear matrix equations:

$$A_2 \mathbf{X} + \mathbf{X} A_1 + B^T \mathbf{P} = F_1$$
$$A_1 \mathbf{Y} + \mathbf{Y} A_2 + \mathbf{P} B = F_2$$
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• Riccati equation: Find $\mathbf{X} \in \mathbb{R}^{n imes n}$ such that

$$A\mathbf{X} + \mathbf{X}A^{\top} - \mathbf{X}BB^{\top}\mathbf{X} + C^{\top}C = 0$$

workhorse in Control Theory

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Focus: All or some of the matrices are large (and possibly sparse)

Solving the Lyapunov equation. The problem Approximate ${\bf X}$ in:

 $A\mathbf{X} + \mathbf{X}A^{\top} + BB^{\top} = 0$ $A \in \mathbb{R}^{n \times n} \text{ neg.real} \qquad B \in \mathbb{R}^{n \times p}, \qquad 1 \le p \ll n$

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Time-invariant linear system:

$$\mathbf{x}'(t) = A\mathbf{x}(t) + B\mathbf{u}(t), \qquad \mathbf{x}(0) = x_0$$

Closed form solution:

$$\mathbf{X} = \int_0^\infty e^{-tA} B B^\top e^{-tA^\top} dt$$

 \Rightarrow X symmetric semidef.

see, e.g., Antoulas '05, Benner '06

Linear systems vs linear matrix equations

Large linear systems:

$$Ax = b, \quad A \in \mathbb{R}^{n \times n}$$

- Krylov subspace methods (CG, MINRES, GMRES, BiCGSTAB, etc.)
- \bullet Preconditioners: find P such that

$$AP^{-1}\widetilde{x} = b$$
 $x = P^{-1}\widetilde{x}$

is easier and fast to solve

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Large linear matrix equations:

$$A\mathbf{X} + \mathbf{X}A^{\top} + BB^{\top} = 0$$

- No preconditioning to preserve symmetry
- ${\bf X}$ is a large, dense matrix \Rightarrow low rank approximation

$$\mathbf{X} \approx \widetilde{X} = Z Z^{\top}, \quad Z \text{ tall}$$

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Large linear matrix equations:

$$A\mathbf{X} + \mathbf{X}A^{\top} + BB^{\top} = 0$$

Kronecker formulation:

$$(A \otimes I + I \otimes A)x = b$$
 $x = \operatorname{vec}(\mathbf{X})$

Given an low dimensional approximation space \mathcal{K} ,

 $\mathbf{X} \approx X_m \qquad \operatorname{col}(X_m) \in \mathcal{K}$

Galerkin condition: $R := AX_m + X_m A^\top + BB^\top \perp \mathcal{K}$

$$V_m^{\top} R V_m = 0 \qquad \qquad \mathcal{K} = \operatorname{Range}(V_m)$$

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Assume $V_m^{\top}V_m = I_m$ and let $X_m := V_m Y_m V_m^{\top}$. Projected Lyapunov equation:

$$V_m^{\top} (A V_m Y_m V_m^{\top} + V_m Y_m V_m^{\top} A^{\top} + B B^{\top}) V_m = 0$$

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Early contributions: Saad '90, Jaimoukha & Kasenally '94, for $\mathcal{K} = \mathcal{K}_m(A, B) = \text{Range}([B, AB, \dots, A^{m-1}B])$ More recent options as approximation space

Enrich space to decrease space dimension

• Extended Krylov subspace

$$\mathcal{K} = \mathbb{E}\mathbb{K} := \mathcal{K}_m(A, B) + \mathcal{K}_m(A^{-1}, A^{-1}B),$$

that is, $\mathcal{K} = \text{Range}([B, A^{-1}B, AB, A^{-2}B, A^2B, A^{-3}B, \dots,])$ (Druskin & Knizhnerman '98, Simoncini '07) More recent options as approximation space

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• Rational Krylov subspace

$$\mathcal{K} = \mathbb{K} := \operatorname{Range}([B, (A - s_1 I)^{-1} B, \dots, (A - s_m I)^{-1} B])$$

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usually, $\{s_1, \ldots, s_m\} \subset \mathbb{C}^+$ chosen either a-priori or dynamically In both cases, for $\text{Range}(V_m) = \mathcal{K}$, projected Lyapunov equation:

$$(V_m^{\top}AV_m)Y_m + Y_m(V_m^{\top}A^{\top}V_m) + V_m^{\top}BB^{\top}V_m = 0$$

 $X_m = V_m Y_m V_m^\top$

Multiterm linear matrix equation

$$A_1 \mathbf{X} B_1 + A_2 \mathbf{X} B_2 + \ldots + A_\ell \mathbf{X} B_\ell = C$$

Applications:

- Control
- (Stochastic) PDEs
- Matrix least squares
- ...

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Main device: Kronecker formulation

$$(B_1^{\top} \otimes A_1 + \ldots + B_{\ell}^{\top} \otimes A_{\ell}) x = c$$

Iterative methods: matrix-matrix multiplications and rank truncation (Benner, Breiten, Bouhamidi, Chehab, Damm, Grasedyck, Jbilou, Kressner, Matthies, Onwunta, Raydan, Stoll, Tobler, Zander, and many others...)

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Alternative approaches:

- Projection onto rich approximation space
- Compression to two-term matrix equation
- Splitting strategy towards two-term matrix equation
- ...

PDEs on uniform grids and separable coeffs

 $-\varepsilon\Delta u + \phi_1(x)\psi_1(y)u_x + \phi_2(x)\psi_2(y)u_y + \gamma_1(x)\gamma_2(y)u = f \quad (x,y) \in \Omega$

 $\phi_i, \psi_i, \gamma_i, i = 1, 2$ sufficiently regular functions + b.c.

Problem discretization by means of a tensor basis

Multiterm linear equation:

 $-\varepsilon T_1 \mathbf{U} - \varepsilon \mathbf{U} T_2 + \Phi_1 B_1 \mathbf{U} \Psi_1 + \Phi_2 \mathbf{U} B_2^\top \Psi_2 + \Gamma_1 \mathbf{U} \Gamma_2 = F$

Finite Diff.: $U_{i,j} = U(x_i, y_j)$ approximate solution at the nodes

PDEs with random inputs

Stochastic steady-state diffusion eqn: Find $u: D \times \Omega \rightarrow \mathbb{R} \ s.t. \ \mathbb{P}$ -a.s.,

$$\begin{cases} -\nabla \cdot (a(\mathbf{x}, \omega) \nabla u(\mathbf{x}, \omega)) = f(\mathbf{x}) & in D \\ u(\mathbf{x}, \omega) = 0 & on \partial D \end{cases}$$

- *f*: deterministic;
- a: random field, linear function of finite no. of real-valued random variables $\xi_r: \Omega \to \Gamma_r \subset \mathbb{R}$

Common choice: truncated Karhunen–Loève (KL) expansion,

$$a(\mathbf{x},\omega) = \mu(\mathbf{x}) + \sigma \sum_{r=1}^{m} \sqrt{\lambda_r} \phi_r(\mathbf{x}) \xi_r(\omega),$$

 $\mu(\mathbf{x}): \text{ expected value of diffusion coef.} \qquad \sigma: \text{ std dev.}$ $(\lambda_r, \phi_r(\mathbf{x})) \text{ eigs of the integral operator } \mathcal{V} \text{ wrto } V(\mathbf{x}, \mathbf{x}') = \frac{1}{\sigma^2} C(\mathbf{x}, \mathbf{x}')$ $(\lambda_r \searrow \qquad C: D \times D \to \mathbb{R} \text{ covariance fun.})$

Discretization by stochastic Galerkin

Approx with space in tensor product form^a $\mathcal{X}_h \times S_p$

$$\mathcal{A}\mathbf{x} = \mathbf{b}, \qquad \mathcal{A} = G_0 \otimes K_0 + \sum_{r=1}^m G_r \otimes K_r, \quad \mathbf{b} = \mathbf{g}_0 \otimes \mathbf{f}_0,$$

x: expansion coef. of approx to u in the tensor product basis $\{\varphi_i \psi_k\}$ $K_r \in \mathbb{R}^{n_x \times n_x}$, FE matrices (sym) $G_r \in \mathbb{R}^{n_\xi \times n_\xi}$, $r = 0, 1, \ldots, m$ Galerkin matrices associated w/ S_p (sym.) g_0: first column of G_0

$$\mathbf{f}_0$$
: FE rhs of deterministic PDE

$$n_{\xi} = \dim(S_p) = \frac{(m+p)!}{m!p!} \implies \boxed{n_x \cdot n_{\xi}}$$
huge

 ${}^{\mathrm{a}}S_p$ set of multivariate polyn of total degree $\leq p$

The matrix equation formulation

 $(G_0 \otimes K_0 + G_1 \otimes K_1 + \ldots + G_m \otimes K_m) \mathbf{x} = \mathbf{g}_0 \otimes \mathbf{f}_0$ transforms into

 $K_0 \mathbf{X} G_0 + K_1 \mathbf{X} G_1 + \ldots + K_m \mathbf{X} G_m = F, \qquad F = \mathbf{f}_0 \mathbf{g}_0^\top$ $(G_0 = I)$

Solution strategy. Conjecture:

• $\{K_r\}$ from trunc'd Karhunen–Loève (KL) expansion

$$\label{eq:X} \begin{split} & \Downarrow \\ \mathbf{X} \approx \widetilde{X} \text{ low rank, } \widetilde{X} = X_1 X_2^T \end{split}$$

(Possibly extending results of Grasedyck, 2004)

Matrix Galerkin approximation of the deterministic part. 1

Approximation space \mathcal{K}_k and basis matrix V_k : $\mathbf{X} \approx X_k = V_k Y$

$$V_k^{\top} R_k = 0, \qquad R_k := K_0 X_k + K_1 X_k G_1 + \ldots + K_m X_k G_m - \mathbf{f}_0 \mathbf{g}_0^{\top}$$

Computational challenges:

- Generation of \mathcal{K}_k involved m+1 different matrices $\{K_r\}$!
- Matrices K_r have different spectral properties
- n_x, n_{ξ} so large that X_k, R_k should not be formed !

(Powell & Silvester & Simoncini, SISC 2017)

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Systems of linear matrix equations

Find $\mathbf{X} \in \mathbb{R}^{n_1 \times n_2}$ and $\mathbf{P} \in \mathbb{R}^{m \times n_2}$ such that

$$A_1 \mathbf{X} + \mathbf{X} A_2 + B^T \mathbf{P} = F_1$$
$$B \mathbf{X} = F_2$$

with $A_i \in \mathbb{R}^{n_i \times n_i}$, $B \in \mathbb{R}^{m \times n_1}$, $F_1 \in \mathbb{R}^{n_1 \times n_2}$, $F_2 \in \mathbb{R}^{m \times n_2}$, $m \le n_1$

Emerging matrix formulation of different application problems

- Constraint control
- Mixed formulations of stochastic diffusion problems
- Discretized deterministic/stochastic (Navier-)Stokes equations
- ...

An example. Mixed FE formulation of stochastic Galerkin diffusion pb

$$c^{-1}\vec{u} - \nabla p = 0,$$

$$-\nabla \cdot \vec{u} = f,$$

Assume that $c^{-1} = c_0 + \sum_{r=1}^{\ell} \sqrt{\lambda_r} c_r(\vec{x}) \xi_r(\omega)$ and that an appropriate class of finite elements is used for the discretization of the problem (see, e.g., the derivation in Elman & Furnival & Powell, 2010) After discretization the problem reads:

$$\begin{bmatrix} G_0 \otimes K_0 + \sum_{r=1}^{\ell} \sqrt{\lambda} G_r \otimes K_r & G_0^T \otimes B_0^T \\ G_0 \otimes B_0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} 0 \\ f \end{bmatrix}$$

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For $\ell = 1$ we obtain

$$K_0 \mathbf{X} G_0 + K_1 \mathbf{X} G_1 + B_0^T \mathbf{P} G_0 = 0,$$
$$B_0 \mathbf{X} G_0 = F$$

Computational strategies for systems of matrix equations

$$A_1 \mathbf{X} + \mathbf{X} A_2 + B^T \mathbf{P} = F_1$$
$$B \mathbf{X} = F_2$$

Kronecker formulation (monolithic):

$$\begin{bmatrix} \mathcal{A} & \mathcal{B}^T \\ \mathcal{B} & \mathcal{O} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, \quad \mathcal{A} = I \otimes A_1 + A_2^T \otimes I, \quad \mathcal{B} = B \otimes I$$

with $\mathbf{x} = \operatorname{vec}(\mathbf{X})$, $\mathbf{p} = \operatorname{vec}(\mathbf{P})$, $f_1 = \operatorname{vec}(F_1)$ and $f_2 = \operatorname{vec}(F_2)$

Extremely rich literature from saddle point algebraic linear systems

Problem: Coefficient matrix has size $(n_1n_2 + mn_2) \times (n_1n_2 + mn_2)$

Computational strategies for systems of matrix equations. Cont'd

$$A_1 \mathbf{X} + \mathbf{X} A_2 + B^T \mathbf{P} = F_1$$
$$B \mathbf{X} = F_2$$

* Derive numerical strategies that directly work with the matrix equations:

- Small scale: Null space method
- Small and medium scale: Schur complement method (also directly applicable to trilinear case)
- Large scale: Iterative method for low rank F_i , i = 1, 2

"Small and medium scale" actually means "Large scale" for the Kronecker form!

V.Simoncini, 2018, to appear in IMA J. Numer. Analysis

Large scale problem. Iterative method. 1/3

$$A_1 \mathbf{X} + \mathbf{X} A_2 + B^T \mathbf{P} = F_1$$
$$B \mathbf{X} = F_2$$

Rewrite as

$$\begin{bmatrix} A_1 & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} + \begin{bmatrix} I_{n_1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} A_2 = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix}, \quad \Leftrightarrow \quad \mathcal{M}\mathbf{Z} + \mathcal{D}_0\mathbf{Z}A_2 = F$$

with

$$\mathcal{M}, \mathcal{D}_0 \in \mathbb{R}^{(n_1+m) \times (n_1+m)}$$

 $A_2 \in \mathbb{R}^{n_2 \times n_2}$ nonsingular

 \mathcal{D}_0 highly singular

If F low rank, exploit projection-type strategies for Sylvester equations

Large scale problem. Iterative method. 2/3

$$\begin{bmatrix} A_1 & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} + \begin{bmatrix} I_{n_1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} A_2 = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} \quad \Leftrightarrow \quad \mathcal{M}\mathbf{Z} + \mathcal{D}_0\mathbf{Z}A_2 = F$$

with F low rank. We rewrite the matrix equation as a Sylvester equation:

$$\mathbf{Z}A_2^{-1} + \mathcal{M}^{-1}\mathcal{D}_0\mathbf{Z} = \widehat{F}$$

with $\widehat{F} = \mathcal{M}^{-1}FA_2^{-1}$ of low rank if F is of low rank, $\widehat{F} = \widehat{F}_{\ell}\widehat{F}_r^T$

$$\Rightarrow \qquad \mathbf{Z} \approx \widetilde{\mathbf{Z}}_k = V_k \mathcal{Z}_k W_k^T$$

with $\operatorname{Range}(V_k)$, $\operatorname{Range}(W_k)$ appropriate approximation spaces of small dimensions

Large scale problem. Iterative method. 3/3 Galerkin-Projection method

$$\mathbf{Z}A_2^{-1} + \mathcal{M}^{-1}\mathcal{D}_0\mathbf{Z} = \widehat{F}_l\widehat{F}_r^T \quad \Rightarrow \quad \mathbf{Z}\approx \widetilde{\mathbf{Z}}_k = V_k\mathcal{Z}_kW_k^T$$

Choice of V_k , W_k . A possible strategy:

- $W_k = \mathbb{E}\mathbb{K}_k(A_2^{-T}, \widehat{F}_r)$, Extended Krylov subspace
- $V_k = K_k(\mathcal{M}^{-1}\mathcal{D}_0, \widehat{F}_l) \cup K_k((\mathcal{M}^{-1}\mathcal{D}_0 + \sigma I)^{-1}, \widehat{F}_l)$ Augmented Krylov subspace, $\sigma \in \mathbb{R}$ (see, e.g., Shank & Simoncini, 2013)

Note:
$$\mathcal{M}$$
 has size $(n_1 + m) \times (n_1 + m)$
(Compare with $(n_1n_2 + mn_2) \times (n_1n_2 + mn_2)$ of the Kronecker form)

Numerical experiments

$$A_1 \mathbf{X} - \mathbf{X} A_2 + B^T \mathbf{P} = 0, \quad \text{vs} \quad \mathcal{A} \mathbf{z} = f$$

 $B \mathbf{X} = F_2$

$$\begin{split} A_1 &\to \mathcal{L}_1 = -u_{xx} - u_{yy}, & F_2 \text{ rank-1} \\ A_2 &\to \mathcal{L}_1 = -(e^{-10xy}u_x)_x - (e^{10xy}u_y)_y + 10(x+y)u_x \\ B &= \text{bidiag}(-1,\underline{1}) \in \mathbb{R}^{(n_2 - n_1) \times n_2}, & \text{params: tol} = 10^{-6}, \ \sigma = 10^{-2} \end{split}$$

n_1	n_2	$size(\mathcal{A})$	Monolithic	Matrix eqns
			Elapsed Time	Elapsed Time
400	100	79,000	6.9769e-02	3.1523e-02 (4)
900	225	401,625	3.4808e-01	5.0447e-02 (4)
1600	400	1272,000	1.1319e+00	7.8018e-02 (4)
2500	625	3109,375	3.1212e+00	1.5282e-01 (5)
3600	900	6453,000	1.0210e+01	2.8053e-01 (5)
4900	1225	11,962,125	3.7699e+01	1.4754e+00 (5)

Monolithic: direct solver (iterative not competitive)

Numerical experiments. 1D stochastic Stokes problem.

$$\begin{bmatrix} \mathcal{H} & \mathcal{B}^T \\ \mathcal{B} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, \qquad \mathcal{H} = (\nu_0 G_0 + \nu_1 G_1) \otimes A_x, \quad \mathcal{B} = G_0 \otimes B_x$$

where $\nu = \nu_0 + \nu_1 \xi(\omega)$ uncertain viscosity, ξ random variable

Then

$$A_x \mathbf{X} G_0 \nu_0 + A_x \mathbf{X} G_1 \nu_1 + B_x^T \mathbf{P} G_0 = F_1, \quad B_x \mathbf{X} = F_2$$

with $G_0 = I$. This corresponds to

$$\begin{bmatrix} \nu_0 A_x & B_x^T \\ B_x & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} + \begin{bmatrix} \nu_1 A_x \\ 0 \end{bmatrix} \begin{bmatrix} \mathbf{X} \\ \mathbf{P} \end{bmatrix} G_1 = \begin{bmatrix} F1 \\ F2 \end{bmatrix}$$

that is

$$\mathcal{M}\mathbf{Z} + \mathcal{D}_0\mathbf{Z}G_1 = F$$

Numerical experiments. 1D stochastic Stokes problem.

 $\mathcal{M}\mathbf{Z} + \mathcal{D}_0\mathbf{Z}G_1 = F \qquad \text{vs} \qquad \mathcal{A}\mathbf{z} = f$

Element Time

 $\nu_0 = 1/10, \nu_1 = 3\nu_0/10$ Powell & Silvester, 2012

			⊏іар	sed Time		
n_1	n_2	n_B	$size(\mathcal{A})$	Monolithic	Monolithic	Iterative
				direct	MINRES	$\mathbb{EK}(\sigma)$
1256	4	389	6,580	0.1852	0.146 (11)	0.19 (2)
3526	4	990	18,064	0.9063	0.275 (11)	0.52 (2)
9812	4	2615	49,708	4.6418	0.981 (10)	2.09 (2)
n_1	n_2	n_B	$size(\mathcal{A})$	Monolithic	Monolithic	Iterative
				direct	MINRES	$\mathbb{EK}(\sigma)$
1256	165	389	271,425	2.91	1.53 (11)	0.20 (2)
3526	165	990	745,140	12.16	7.43 (11)	0.45 (2)
9812	165	2615	2050,455	-	-	1.87 (2)

• n_2 could be much larger, $n_2 = O(10^3)$

• Memory requirements are limited, $\widetilde{\mathbf{Z}} = Z_1 Z_2^T$ of very low rank

Numerical experiments. 2D stochastic Stokes problem

$\begin{bmatrix} \mathcal{B}^T \\ 0 \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{p} \end{bmatrix}$	$\begin{bmatrix} \mathbf{x} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, \mathcal{H} = \text{blkdiag}((\nu_0 G_0 + \nu_1 G_1) \otimes A_x, (\nu_0 G_0 - \mathcal{H}_1) \otimes A_y) \\ \mathcal{H} = [G_0 \otimes B_x, G_0 \otimes B_y]$				
	\mathcal{N}	$1\mathbf{Z} + \mathcal{D}_0\mathbf{Z}G$	$t_1 = F$ vs	$\mathcal{A}\mathbf{z} = f$	
n_1	n_2	$size(\mathcal{A})$	Monolithic	Monolithic	Iterative
			direct	MINRES	$\mathbb{EK}(\sigma)$
2512	4	11,604	0.55	0.12 (12)	0.28 (2)
7052	4	32,168	3.73	0.36 (12)	1.22 (2)
19624	4	88,956	11.93	1.51 (12)	4.37 (2)
n_1	n_2	$size(\mathcal{A})$	Monolithic	Monolithic	Iterative
			direct	MINRES	$\mathbb{EK}(\sigma)$
2512	165	478 665	7.60	3.16 (17)	0.33 (2)
7052	165	1 326 930	34.08	15.52 (18)	1.32 (2)
19624	165	3 669 435	_	_	5.69 (3)

 $\nu_0 = 1/10, \nu_1 = 3\nu_0/10$ Powell-Silvester (2012)

Not discussed but in this category

• Sylvester-like linear matrix equations

$$AX + f(X)B = C$$

typically (but not only!): $f(X) = \overline{X}, f(X) = X^{\top}, \text{ or } f(X) = X^*$ (Bevis, Braden, Byers, Chiang, De Terán, Dopico, Duan, Feng, Gonzalez, Guillery, Hall, Hartwig, Ikramov, Kressner, Montealegre, Reyes, Schröder, Vorntsov, Watkins, Wu, ...)

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• Linear systems with complex tensor structure

$$\mathcal{A}\mathbf{x} = b$$
 with $\mathcal{A} = \sum_{j=1}^{k} I_{n_1} \otimes \cdots \otimes I_{n_{j-1}} \otimes A_j \otimes I_{n_{j+1}} \cdots \otimes I_{n_k}.$

Dolgov, Grasedyck, Khoromskij, Kressner, Oseledets, Tobler, Tyrtyshnikov, and many more...

Conclusions

Large-scale (Multiterm) linear equations are a new computational tool

- Great advances in solving really large linear matrix equations
- Second order (matrix) challenges rely on strength and maturity of linear system solvers
- Low-rank tensor formats is the new generation of approximations

Reference for linear matrix equations:

 \star V. Simoncini,

Computational methods for linear matrix equations,

SIAM Review, Sept. 2016.