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

## V. Simoncini

Dipartimento di Matematica
Alma Mater Studiorum - Università di Bologna valeria.simoncini@unibo.it

Some matrix equations

- Sylvester matrix equation

$$
A \mathbf{X}+\mathbf{X} B+D=0
$$

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

Some matrix equations

- Sylvester matrix equation

$$
A \mathbf{X}+\mathbf{X} B+D=0
$$

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

- Lyapunov matrix equation

$$
A \mathbf{X}+\mathbf{X} A^{\top}+D=0, \quad D=D^{\top}
$$

Stability analysis in Control and Dynamical systems, Signal processing, eigenvalue computations

Some matrix equations

- Sylvester matrix equation

$$
A \mathbf{X}+\mathbf{X} B+D=0
$$

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

- Lyapunov matrix equation

$$
A \mathbf{X}+\mathbf{X} A^{\top}+D=0, \quad D=D^{\top}
$$

Stability analysis in Control and Dynamical systems, Signal processing, eigenvalue computations

- Multiterm matrix equation

$$
A_{1} \mathbf{X} B_{1}+A_{2} \mathbf{X} B_{2}+\ldots+A_{\ell} \mathbf{X} B_{\ell}=C
$$

Control, (Stochastic) PDEs, ...

Some matrix equations

- Sylvester matrix equation

$$
A \mathbf{X}+\mathbf{X} B+D=0
$$

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

- Lyapunov matrix equation

$$
A \mathbf{X}+\mathbf{X} A^{\top}+D=0, \quad D=D^{\top}
$$

Stability analysis in Control and Dynamical systems, Signal processing, eigenvalue computations

- Multiterm matrix equation

$$
A_{1} \mathbf{X} B_{1}+A_{2} \mathbf{X} B_{2}+\ldots+A_{\ell} \mathbf{X} B_{\ell}=C
$$

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

More matrix equations

- Systems of linear matrix equations:

$$
\begin{aligned}
A_{2} \mathbf{X}+\mathbf{X} A_{1}+B^{T} \mathbf{P} & =F_{1} \\
A_{1} \mathbf{Y}+\mathbf{Y} A_{2}+\mathbf{P} B & =F_{2} \\
B \mathbf{X}+\mathbf{Y} B^{T} & =F_{3}
\end{aligned}
$$

More matrix equations

- Systems of linear matrix equations:

$$
\begin{aligned}
A_{2} \mathbf{X}+\mathbf{X} A_{1}+B^{T} \mathbf{P} & =F_{1} \\
A_{1} \mathbf{Y}+\mathbf{Y} A_{2}+\mathbf{P} B & =F_{2} \\
B \mathbf{X}+\mathbf{Y} B^{T} & =F_{3}
\end{aligned}
$$

- Riccati equation: Find $\mathbf{X} \in \mathbb{R}^{n \times n}$ such that

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

workhorse in Control Theory

More matrix equations

- Systems of linear matrix equations:

$$
\begin{aligned}
A_{2} \mathbf{X}+\mathbf{X} A_{1}+B^{T} \mathbf{P} & =F_{1} \\
A_{1} \mathbf{Y}+\mathbf{Y} A_{2}+\mathbf{P} B & =F_{2} \\
B \mathbf{X}+\mathbf{Y} B^{T} & =F_{3}
\end{aligned}
$$

- Riccati equation: Find $\mathbf{X} \in \mathbb{R}^{n \times n}$ such that

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

workhorse in Control Theory
Focus: All or some of the matrices are large (and possibly sparse)

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

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

$A \in \mathbb{R}^{n \times n}$ neg.real $\quad B \in \mathbb{R}^{n \times p}, \quad 1 \leq p \ll n$

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

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

$A \in \mathbb{R}^{n \times n}$ neg.real $\quad B \in \mathbb{R}^{n \times p}, \quad 1 \leq p \ll n$

Time-invariant linear system:

$$
\mathbf{x}^{\prime}(t)=A \mathbf{x}(t)+B \mathbf{u}(t), \quad \mathbf{x}(0)=x_{0}
$$

Closed form solution:

$$
\mathbf{X}=\int_{0}^{\infty} e^{-t A} B B^{\top} e^{-t A^{\top}} d t
$$

$\Rightarrow \quad \mathrm{X}$ symmetric semidef.
see, e.g., Antoulas '05, Benner '06

Linear systems vs linear matrix equations
Large linear systems:

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

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

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

is easier and fast to solve

Linear systems vs linear matrix equations
Large linear systems:

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

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

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

is easier and fast to solve
Large linear matrix equations:

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

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

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

Linear systems vs linear matrix equations
Large linear systems:

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

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

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

is easier and fast to solve
Large linear matrix equations:

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

Kronecker formulation:

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

## Projection-type methods

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

$$
\mathbf{X} \approx X_{m} \quad \operatorname{col}\left(X_{m}\right) \in \mathcal{K}
$$

Galerkin condition: $\quad R:=A X_{m}+X_{m} A^{\top}+B B^{\top} \perp \mathcal{K}$

$$
V_{m}^{\top} R V_{m}=0 \quad \mathcal{K}=\operatorname{Range}\left(V_{m}\right)
$$

## Projection-type methods

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

$$
\mathbf{X} \approx X_{m} \quad \operatorname{col}\left(X_{m}\right) \in \mathcal{K}
$$

Galerkin condition: $\quad R:=A X_{m}+X_{m} A^{\top}+B B^{\top} \perp \quad \mathcal{K}$

$$
V_{m}^{\top} R V_{m}=0 \quad \mathcal{K}=\operatorname{Range}\left(V_{m}\right)
$$

Assume $V_{m}^{\top} V_{m}=I_{m}$ and let $X_{m}:=V_{m} Y_{m} V_{m}^{\top}$.
Projected Lyapunov equation:

$$
V_{m}^{\top}\left(A V_{m} Y_{m} V_{m}^{\top}+V_{m} Y_{m} V_{m}^{\top} A^{\top}+B B^{\top}\right) V_{m}=0
$$

## Projection-type methods

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

$$
\mathbf{X} \approx X_{m} \quad \operatorname{col}\left(X_{m}\right) \in \mathcal{K}
$$

Galerkin condition: $\quad R:=A X_{m}+X_{m} A^{\top}+B B^{\top} \perp \quad \mathcal{K}$

$$
V_{m}^{\top} R V_{m}=0 \quad \mathcal{K}=\operatorname{Range}\left(V_{m}\right)
$$

Assume $V_{m}^{\top} V_{m}=I_{m}$ and let $X_{m}:=V_{m} Y_{m} V_{m}^{\top}$.
Projected Lyapunov equation:

$$
\begin{aligned}
V_{m}^{\top}\left(A V_{m} Y_{m} V_{m}^{\top}+V_{m} Y_{m} V_{m}^{\top} A^{\top}+B B^{\top}\right) V_{m} & =0 \\
\left(V_{m}^{\top} A V_{m}\right) Y_{m}+Y_{m}\left(V_{m}^{\top} A^{\top} V_{m}\right)+V_{m}^{\top} B B^{\top} V_{m} & =0
\end{aligned}
$$

## Projection-type methods

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

$$
\mathbf{X} \approx X_{m} \quad \operatorname{col}\left(X_{m}\right) \in \mathcal{K}
$$

Galerkin condition: $\quad R:=A X_{m}+X_{m} A^{\top}+B B^{\top} \perp \quad \mathcal{K}$

$$
V_{m}^{\top} R V_{m}=0 \quad \mathcal{K}=\operatorname{Range}\left(V_{m}\right)
$$

Assume $V_{m}^{\top} V_{m}=I_{m}$ and let $X_{m}:=V_{m} Y_{m} V_{m}^{\top}$.
Projected Lyapunov equation:

$$
\begin{aligned}
V_{m}^{\top}\left(A V_{m} Y_{m} V_{m}^{\top}+V_{m} Y_{m} V_{m}^{\top} A^{\top}+B B^{\top}\right) V_{m} & =0 \\
\left(V_{m}^{\top} A V_{m}\right) Y_{m}+Y_{m}\left(V_{m}^{\top} A^{\top} V_{m}\right)+V_{m}^{\top} B B^{\top} V_{m} & =0
\end{aligned}
$$

Early contributions: Saad '90, Jaimoukha \& Kasenally '94, for
$\mathcal{K}=\mathcal{K}_{m}(A, B)=\operatorname{Range}\left(\left[B, A B, \ldots, A^{m-1} B\right]\right)$

More recent options as approximation space
Enrich space to decrease space dimension

- Extended Krylov subspace

$$
\mathcal{K}=\mathbb{E} \mathbb{K}:=\mathcal{K}_{m}(A, B)+\mathcal{K}_{m}\left(A^{-1}, A^{-1} B\right)
$$

that is, $\mathcal{K}=\operatorname{Range}\left(\left[B, A^{-1} B, A B, A^{-2} B, A^{2} B, A^{-3} B, \ldots,\right]\right)$
(Druskin \& Knizhnerman '98, Simoncini '07)

More recent options as approximation space
Enrich space to decrease space dimension

- Extended Krylov subspace

$$
\mathcal{K}=\mathbb{E} \mathbb{K}:=\mathcal{K}_{m}(A, B)+\mathcal{K}_{m}\left(A^{-1}, A^{-1} B\right)
$$

that is, $\mathcal{K}=\operatorname{Range}\left(\left[B, A^{-1} B, A B, A^{-2} B, A^{2} B, A^{-3} B, \ldots,\right]\right)$
(Druskin \& Knizhnerman '98, Simoncini '07)

- Rational Krylov subspace

$$
\mathcal{K}=\mathbb{K}:=\operatorname{Range}\left(\left[B,\left(A-s_{1} I\right)^{-1} B, \ldots,\left(A-s_{m} I\right)^{-1} B\right]\right)
$$

usually, $\left\{s_{1}, \ldots, s_{m}\right\} \subset \mathbb{C}^{+}$chosen either a-priori or dynamically

More recent options as approximation space
Enrich space to decrease space dimension

- Extended Krylov subspace

$$
\mathcal{K}=\mathbb{E} \mathbb{K}:=\mathcal{K}_{m}(A, B)+\mathcal{K}_{m}\left(A^{-1}, A^{-1} B\right)
$$

that is, $\mathcal{K}=\operatorname{Range}\left(\left[B, A^{-1} B, A B, A^{-2} B, A^{2} B, A^{-3} B, \ldots,\right]\right)$
(Druskin \& Knizhnerman '98, Simoncini '07)

- Rational Krylov subspace

$$
\mathcal{K}=\mathbb{K}:=\operatorname{Range}\left(\left[B,\left(A-s_{1} I\right)^{-1} B, \ldots,\left(A-s_{m} I\right)^{-1} B\right]\right)
$$

usually, $\left\{s_{1}, \ldots, s_{m}\right\} \subset \mathbb{C}^{+}$chosen either a-priori or dynamically In both cases, for Range $\left(V_{m}\right)=\mathcal{K}$, projected Lyapunov equation:

$$
\begin{aligned}
& \left(V_{m}^{\top} A V_{m}\right) Y_{m}+Y_{m}\left(V_{m}^{\top} A^{\top} V_{m}\right)+V_{m}^{\top} B B^{\top} V_{m}=0 \\
X_{m}= & V_{m} Y_{m} V_{m}^{\top}
\end{aligned}
$$

$$
\begin{aligned}
& \text { Multiterm linear matrix equation } \\
& A_{1} \mathbf{X} B_{1}+A_{2} \mathbf{X} B_{2}+\ldots+A_{\ell} \mathbf{X} B_{\ell}=C
\end{aligned}
$$

Applications:

- Control
- (Stochastic) PDEs
- Matrix least squares

$$
\begin{aligned}
& \text { Multiterm linear matrix equation } \\
& A_{1} \mathbf{X} B_{1}+A_{2} \mathbf{X} B_{2}+\ldots+A_{\ell} \mathbf{X} B_{\ell}=C
\end{aligned}
$$

Applications:

- Control
- (Stochastic) PDEs
- Matrix least squares

Main device: Kronecker formulation

$$
\left(B_{1}^{\top} \otimes A_{1}+\ldots+B_{\ell}^{\top} \otimes A_{\ell}\right) x=c
$$

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...)

$$
\begin{aligned}
& \text { Multiterm linear matrix equation } \\
& A_{1} \mathbf{X} B_{1}+A_{2} \mathbf{X} B_{2}+\ldots+A_{\ell} \mathbf{X} B_{\ell}=C
\end{aligned}
$$

Applications:

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

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.: $\mathbf{U}_{i, j}=\mathbf{U}\left(x_{i}, y_{j}\right)$ 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.,

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

$f$ : deterministic;
$a$ : random field, linear function of finite no. of real-valued random variables $\xi_{r}: \Omega \rightarrow \Gamma_{r} \subset \mathbb{R}$
Common choice: truncated Karhunen-Loève (KL) expansion,

$$
a(\mathbf{x}, \omega)=\mu(\mathbf{x})+\sigma \sum_{r=1}^{m} \sqrt{\lambda_{r}} \phi_{r}(\mathbf{x}) \xi_{r}(\omega),
$$

$\mu(\mathbf{x})$ : expected value of diffusion coef. $\sigma$ : std dev.
$\left(\lambda_{r}, \phi_{r}(\mathbf{x})\right)$ eigs of the integral operator $\mathcal{V}$ wrto $V\left(\mathbf{x}, \mathbf{x}^{\prime}\right)=\frac{1}{\sigma^{2}} C\left(\mathbf{x}, \mathbf{x}^{\prime}\right)$
$\left(\lambda_{r} \searrow \quad C: D \times D \rightarrow \mathbb{R}\right.$ covariance fun. )

## Discretization by stochastic Galerkin

Approx with space in tensor product form ${ }^{\text {a }} \mathcal{X}_{h} \times S_{p}$

$$
\mathcal{A} \mathbf{x}=\mathbf{b}, \quad \mathcal{A}=G_{0} \otimes K_{0}+\sum_{r=1}^{m} G_{r} \otimes K_{r}, \quad \mathbf{b}=\mathbf{g}_{0} \otimes \mathbf{f}_{0}
$$

$\mathbf{x}$ : expansion coef. of approx to $u$ in the tensor product basis $\left\{\varphi_{i} \psi_{k}\right\}$
$K_{r} \in \mathbb{R}^{n_{x} \times n_{x}}$, 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.)
$\mathrm{g}_{0}$ : first column of $G_{0}$
$f_{0}$ : FE rhs of deterministic PDE

$$
n_{\xi}=\operatorname{dim}\left(S_{p}\right)=\frac{(m+p)!}{m!p!} \quad \Rightarrow n_{x} \cdot n_{\xi} \text { huge }
$$

[^0]The matrix equation formulation

$$
\left(G_{0} \otimes K_{0}+G_{1} \otimes K_{1}+\ldots+G_{m} \otimes K_{m}\right) \mathbf{x}=\mathbf{g}_{0} \otimes \mathbf{f}_{0}
$$

transforms into

$$
\begin{aligned}
& \quad K_{0} \mathbf{X} G_{0}+K_{1} \mathbf{X} G_{1}+\ldots+K_{m} \mathbf{X} G_{m}=F, \quad F=\mathbf{f}_{0} \mathbf{g}_{0}^{\top} \\
& \left(G_{0}=I\right)
\end{aligned}
$$

Solution strategy. Conjecture:

- $\left\{K_{r}\right\}$ from trunc'd Karhunen-Loève (KL) expansion
$\Downarrow$

$$
\mathbf{X} \approx \widetilde{X} \text { low rank, } \widetilde{X}=X_{1} X_{2}^{T}
$$

(Possibly extending results of Grasedyck, 2004)

Matrix Galerkin approximation of the deterministic part. 1
Approximation space $\mathcal{K}_{k}$ and basis matrix $V_{k}: \quad \mathbf{X} \approx X_{k}=V_{k} Y$

$$
V_{k}^{\top} R_{k}=0, \quad R_{k}:=K_{0} X_{k}+K_{1} X_{k} G_{1}+\ldots+K_{m} X_{k} G_{m}-\mathbf{f}_{0} \mathbf{g}_{0}^{\top}
$$

Computational challenges:

- Generation of $\mathcal{K}_{k}$ involved $m+1$ different matrices $\left\{K_{r}\right\}$ !
- Matrices $K_{r}$ have different spectral properties
- $n_{x}, n_{\xi}$ so large that $X_{k}, R_{k}$ should not be formed !
(Powell \& Silvester \& Simoncini, SISC 2017)

Matrix Galerkin approximation of the deterministic part. 1
Approximation space $\mathcal{K}_{k}$ and basis matrix $V_{k}: \quad \mathbf{X} \approx X_{k}=V_{k} Y$

$$
V_{k}^{\top} R_{k}=0, \quad R_{k}:=K_{0} X_{k}+K_{1} X_{k} G_{1}+\ldots+K_{m} X_{k} G_{m}-\mathbf{f}_{0} \mathbf{g}_{0}^{\top}
$$

Computational challenges:

- Generation of $\mathcal{K}_{k}$ involved $m+1$ different matrices $\left\{K_{r}\right\}$ !
- Matrices $K_{r}$ have different spectral properties
- $n_{x}, n_{\xi}$ so large that $X_{k}, R_{k}$ should not be formed !
(Powell \& Silvester \& Simoncini, SISC 2017)


## 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

$$
\begin{aligned}
A_{1} \mathbf{X}+\mathbf{X} A_{2}+B^{T} \mathbf{P} & =F_{1} \\
B \mathbf{X} & =F_{2}
\end{aligned}
$$

with $A_{i} \in \mathbb{R}^{n_{i} \times n_{i}}, B \in \mathbb{R}^{m \times n_{1}}, F_{1} \in \mathbb{R}^{n_{1} \times n_{2}}, F_{2} \in \mathbb{R}^{m \times n_{2}}, m \leq n_{1}$

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

$$
\begin{aligned}
c^{-1} \vec{u}-\nabla p & =0 \\
-\nabla \cdot \vec{u} & =f
\end{aligned}
$$

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:

$$
\left[\begin{array}{cc}
G_{0} \otimes K_{0}+\sum_{r=1}^{\ell} \sqrt{\lambda} G_{r} \otimes K_{r} & G_{0}^{T} \otimes B_{0}^{T} \\
G_{0} \otimes B_{0}
\end{array}\right]\left[\begin{array}{l}
u \\
p
\end{array}\right]=\left[\begin{array}{l}
0 \\
f
\end{array}\right]
$$

An example. Mixed FE formulation of stochastic Galerkin diffusion pb

$$
\begin{aligned}
c^{-1} \vec{u}-\nabla p & =0 \\
-\nabla \cdot \vec{u} & =f
\end{aligned}
$$

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:

$$
\left[\begin{array}{cc}
G_{0} \otimes K_{0}+\sum_{r=1}^{\ell} \sqrt{\lambda} G_{r} \otimes K_{r} & G_{0}^{T} \otimes B_{0}^{T} \\
G_{0} \otimes B_{0}
\end{array}\right]\left[\begin{array}{l}
u \\
p
\end{array}\right]=\left[\begin{array}{l}
0 \\
f
\end{array}\right]
$$

For $\ell=1$ we obtain

$$
\begin{aligned}
K_{0} \mathbf{X} G_{0}+K_{1} \mathbf{X} G_{1}+B_{0}^{T} \mathbf{P} G_{0} & =0 \\
B_{0} \mathbf{X} G_{0} & =F
\end{aligned}
$$

Computational strategies for systems of matrix equations

$$
\begin{array}{ll}
A_{1} \mathbf{X}+\mathbf{X} A_{2}+B^{T} \mathbf{P} & =F_{1} \\
B \mathbf{X} & =F_{2}
\end{array}
$$

Kronecker formulation (monolithic):

$$
\left[\begin{array}{cc}
\mathcal{A} & \mathcal{B}^{T} \\
\mathcal{B} & \mathcal{O}
\end{array}\right]\left[\begin{array}{l}
\mathbf{x} \\
\mathbf{p}
\end{array}\right]=\left[\begin{array}{l}
f_{1} \\
f_{2}
\end{array}\right], \quad \mathcal{A}=I \otimes A_{1}+A_{2}^{T} \otimes I, \quad \mathcal{B}=B \otimes I
$$

with $\mathbf{x}=\operatorname{vec}(\mathbf{X}), \mathbf{p}=\operatorname{vec}(\mathbf{P}), f_{1}=\operatorname{vec}\left(F_{1}\right)$ and $f_{2}=\operatorname{vec}\left(F_{2}\right)$

Extremely rich literature from saddle point algebraic linear systems

Problem: Coefficient matrix has size $\left(n_{1} n_{2}+m n_{2}\right) \times\left(n_{1} n_{2}+m n_{2}\right)$

Computational strategies for systems of matrix equations. Cont'd

$$
\begin{array}{ll}
A_{1} \mathbf{X}+\mathbf{X} A_{2}+B^{T} \mathbf{P} & =F_{1} \\
B \mathbf{X} & =F_{2}
\end{array}
$$

* 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. $1 / 3$

$$
\begin{aligned}
A_{1} \mathbf{X}+\mathbf{X} A_{2}+B^{T} \mathbf{P} & =F_{1} \\
B \mathbf{X} & =F_{2}
\end{aligned}
$$

Rewrite as

$$
\left[\begin{array}{cc}
A_{1} & B^{T} \\
B & 0
\end{array}\right]\left[\begin{array}{l}
\mathbf{X} \\
\mathbf{P}
\end{array}\right]+\left[\begin{array}{cc}
I_{n_{1}} & 0 \\
0 & 0
\end{array}\right]\left[\begin{array}{l}
\mathbf{X} \\
\mathbf{P}
\end{array}\right] A_{2}=\left[\begin{array}{l}
F_{1} \\
F_{2}
\end{array}\right], \quad \Leftrightarrow \quad \mathcal{M} \mathbf{Z}+\mathcal{D}_{0} \mathbf{Z} A_{2}=F
$$

with
$\mathcal{M}, \mathcal{D}_{0} \in \mathbb{R}^{\left(n_{1}+m\right) \times\left(n_{1}+m\right)}$
$A_{2} \in \mathbb{R}^{n_{2} \times n_{2}}$ nonsingular
$\mathcal{D}_{0}$ highly singular

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

Large scale problem. Iterative method. 2/3

$$
\left[\begin{array}{cc}
A_{1} & B^{T} \\
B & 0
\end{array}\right]\left[\begin{array}{l}
\mathbf{X} \\
\mathbf{P}
\end{array}\right]+\left[\begin{array}{cc}
I_{n_{1}} & 0 \\
0 & 0
\end{array}\right]\left[\begin{array}{l}
\mathbf{X} \\
\mathbf{P}
\end{array}\right] A_{2}=\left[\begin{array}{l}
F_{1} \\
F_{2}
\end{array}\right] \Leftrightarrow \quad \mathcal{M} \mathbf{Z}+\mathcal{D}_{0} \mathbf{Z} A_{2}=F
$$

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 $\widehat{F}=\mathcal{M}^{-1} F A_{2}^{-1}$ of low rank if $F$ is of low rank, $\quad \widehat{F}=\widehat{F}_{\ell} \widehat{F}_{r}^{T}$

$$
\Rightarrow \quad \mathbf{Z} \approx \widetilde{\mathbf{Z}}_{k}=V_{k} \mathcal{Z}_{k} W_{k}^{T}
$$

with Range $\left(V_{k}\right)$, Range $\left(W_{k}\right)$ appropriate approximation spaces of small dimensions

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

$$
\mathbf{Z} A_{2}^{-1}+\mathcal{M}^{-1} \mathcal{D}_{0} \mathbf{Z}=\widehat{F}_{l} \widehat{F}_{r}^{T} \quad \Rightarrow \quad \mathbf{Z} \approx \widetilde{\mathbf{Z}}_{k}=V_{k} \mathcal{Z}_{k} W_{k}^{T}
$$

Choice of $V_{k}, W_{k}$. A possible strategy:

- $W_{k}=\mathbb{E} \mathbb{K}_{k}\left(A_{2}^{-T}, \widehat{F}_{r}\right), \quad$ Extended Krylov subspace
- $V_{k}=K_{k}\left(\mathcal{M}^{-1} \mathcal{D}_{0}, \widehat{F}_{l}\right) \cup K_{k}\left(\left(\mathcal{M}^{-1} \mathcal{D}_{0}+\sigma I\right)^{-1}, \widehat{F}_{l}\right)$

Augmented Krylov subspace, $\sigma \in \mathbb{R}$ (see, e.g., Shank \& Simoncini, 2013)

Note: $\mathcal{M}$ has size $\left(n_{1}+m\right) \times\left(n_{1}+m\right)$
(Compare with $\left(n_{1} n_{2}+m n_{2}\right) \times\left(n_{1} n_{2}+m n_{2}\right)$ of the Kronecker form)

## Numerical experiments

$$
\begin{aligned}
A_{1} \mathbf{X}-\mathbf{X} A_{2}+B^{T} \mathbf{P} & =0, \quad \text { vs } \quad \mathcal{A} \mathbf{z}=f \\
B \mathbf{X} & =F_{2}
\end{aligned}
$$

$$
\begin{aligned}
& A_{1} \rightarrow \mathcal{L}_{1}=-u_{x x}-u_{y y}, \quad F_{2} \text { rank-1 } \\
& A_{2} \rightarrow \mathcal{L}_{1}=-\left(e^{-10 x y} u_{x}\right)_{x}-\left(e^{10 x y} u_{y}\right)_{y}+10(x+y) u_{x} \\
& B=\operatorname{bidiag}(-1, \underline{1}) \in \mathbb{R}^{\left(n_{2}-n_{1}\right) \times n_{2}}, \quad \text { params: tol }=10^{-6}, \sigma=10^{-2}
\end{aligned}
$$

Monolithic: direct solver (iterative not competitive)

Numerical experiments. 1D stochastic Stokes problem.

$$
\left[\begin{array}{cc}
\mathcal{H} & \mathcal{B}^{T} \\
\mathcal{B} & 0
\end{array}\right]\left[\begin{array}{l}
\mathbf{x} \\
\mathbf{p}
\end{array}\right]=\left[\begin{array}{l}
f_{1} \\
f_{2}
\end{array}\right], \quad \mathcal{H}=\left(\nu_{0} G_{0}+\nu_{1} G_{1}\right) \otimes A_{x}, \quad \mathcal{B}=G_{0} \otimes B_{x}
$$

where $\nu=\nu_{0}+\nu_{1} \xi(\omega)$ uncertain viscosity, $\xi$ 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

$$
\left[\begin{array}{cc}
\nu_{0} A_{x} & B_{x}^{T} \\
B_{x} & 0
\end{array}\right]\left[\begin{array}{l}
\mathbf{X} \\
\mathbf{P}
\end{array}\right]+\left[\begin{array}{ll}
\nu_{1} A_{x} & \\
& 0
\end{array}\right]\left[\begin{array}{l}
\mathbf{X} \\
\mathbf{P}
\end{array}\right] G_{1}=\left[\begin{array}{l}
F 1 \\
F 2
\end{array}\right]
$$

that is

$$
\mathcal{M} \mathbf{Z}+\mathcal{D}_{0} \mathbf{Z} G_{1}=F
$$

Numerical experiments. 1D stochastic Stokes problem.

$$
\mathcal{M} \mathbf{Z}+\mathcal{D}_{0} \mathbf{Z} G_{1}=F \quad \text { vs } \quad \mathcal{A} \mathbf{z}=f
$$

$\nu_{0}=1 / 10, \nu_{1}=3 \nu_{0} / 10 \quad$ Powell \& Silvester, 2012
Elapsed Time

| $n_{1}$ | $n_{2}$ | $n_{B}$ | $\operatorname{size}(\mathcal{A})$ | Monolithic <br> direct | Monolithic <br> MINRES | Iterative <br> $\mathbb{E K}(\sigma)$ |
| :---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 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 | $0.981(10)$ | $2.09(2)$ |
| $n_{1}$ | $n_{2}$ | $n_{B}$ | $\operatorname{size}(\mathcal{A})$ | Monolithic | Monolithic | Iterative |
|  |  |  |  | direct | MINRES | $\mathbb{E K K}(\sigma)$ |
| 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, $n_{2}=O\left(10^{3}\right)$
- Memory requirements are limited, $\widetilde{\mathbf{Z}}=Z_{1} Z_{2}^{T}$ of very low rank

Numerical experiments. 2D stochastic Stokes problem

$$
\begin{aligned}
& {\left[\begin{array}{cc}
\mathcal{H} & \mathcal{B}^{T} \\
\mathcal{B} & 0
\end{array}\right]\left[\begin{array}{l}
\mathbf{x} \\
\mathbf{p}
\end{array}\right]=\left[\begin{array}{l}
f_{1} \\
f_{2}
\end{array}\right], \quad \begin{array}{l}
\mathcal{H}=\operatorname{blkdiag}\left(\left(\nu_{0} \mathrm{G}_{0}+\nu_{1} \mathrm{G}_{1}\right) \otimes \mathrm{A}_{\mathbf{x}},\left(\nu_{0} \mathrm{G}_{0}+\nu_{1} \mathrm{G}_{1}\right) \otimes \mathrm{A}_{\mathbf{y}}\right) \\
\left.\mathcal{B} 0 B_{x}, G_{0} \otimes B_{y}\right]
\end{array}} \\
& \mathcal{M} \mathbf{Z}+\mathcal{D}_{0} \mathbf{Z} G_{1}=F \quad \text { vs } \quad \mathcal{A} \mathbf{z}=f
\end{aligned}
$$

| $n_{1}$ | $n_{2}$ | $\operatorname{size}(\mathcal{A})$ | Monolithic <br> direct | Monolithic <br> MINRES | Iterative <br> $\mathbb{E K}(\sigma)$ |
| :---: | :---: | ---: | ---: | ---: | ---: |
| 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 | $1.51(12)$ | $4.37(2)$ |
| $n_{1}$ | $n_{2}$ | $\operatorname{size}(\mathcal{A})$ | Monolithic | Monolithic | Iterative |


|  |  |  | direct | MINRES | $\mathbb{E K}(\sigma)$ |
| ---: | ---: | ---: | ---: | ---: | ---: |
| 2512 | 165 | 478665 | 7.60 | $3.16(17)$ | $0.33(2)$ |
| 7052 | 165 | 1326930 | 34.08 | $15.52(18)$ | $1.32(2)$ |
| 19624 | 165 | 3669435 | - | - | $5.69(3)$ |

$\nu_{0}=1 / 10, \nu_{1}=3 \nu_{0} / 10 \quad$ Powell-Silvester (2012)

## Not discussed but in this category

- Sylvester-like linear matrix equations

[^1]
## Not discussed but in this category

- Sylvester-like linear matrix equations

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

typically (but not only!): $\quad f(X)=\bar{X}, f(X)=X^{\top}$, 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, ...)

- Linear systems with complex tensor structure

$$
\mathcal{A} \mathbf{x}=b \quad \text { with } \quad \mathcal{A}=\sum_{j=1}^{k} I_{n_{1}} \otimes \cdots \otimes I_{n_{j-1}} \otimes A_{j} \otimes I_{n_{j+1}} \cdots \otimes I_{n_{k}} .
$$

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:

* V. Simoncini,

Computational methods for linear matrix equations, SIAM Review, Sept. 2016.


[^0]:    ${ }^{\mathrm{a}} S_{p}$ set of multivariate polyn of total degree $\leq p$

[^1]:    $$
    A X+f(X) B=C
    $$

    typically (but not only!): $\quad f(X)=\bar{X}, f(X)=X^{\top}$, 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, ...)

