

Solving multiterm linear matrix equations

order reduction strategies and applications

Valeria Simoncini

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

The matrix equation problem

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

$A_i \in \mathbb{R}^{n \times n}$, $B_i \in \mathbb{R}^{m \times m}$, \mathbf{X} unknown matrix

Possibly large dimensions, structured coefficient matrices

The problem in its full generality is far from tractable, although the transformation to a matrix-vector equation [...] allows us to use the considerable arsenal of numerical weapons currently available for the solution of such problems.

Peter Lancaster, SIAM Rev. 1970

The matrix equation problem

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

$A_i \in \mathbb{R}^{n \times n}$, $B_i \in \mathbb{R}^{m \times m}$, \mathbf{X} unknown matrix

Possibly large dimensions, structured coefficient matrices

The problem in its full generality is far from tractable, although the transformation to a matrix-vector equation [...] allows us to use the considerable arsenal of numerical weapons currently available for the solution of such problems.

Peter Lancaster, SIAM Rev. 1970

Multiterm linear matrix equation. Classical device

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

Kronecker formulation

$$(B_1^\top \otimes A_1 + \dots + B_\ell^\top \otimes A_\ell) \mathbf{x} = c \quad \Leftrightarrow \quad \mathcal{A} \mathbf{x} = c$$

Iterative methods: matrix-matrix multiplications and rank truncation

(Benner, Breiten, Bouhamidi, Chehab, Damm, Grasedyck, Jbilou, Kressner, Matthies, Nagy, Onwunta, Raydan, Stoll, Tobler, Wedderburn, Zander, ...)

$$\text{Kronecker product : } M \otimes P = \begin{bmatrix} m_{11}P & \dots & m_{1n}P \\ \vdots & \ddots & \vdots \\ m_{n1}P & \dots & m_{nn}P \end{bmatrix} \quad \text{and } \text{vec}(AXB) = (B^\top \otimes A)\text{vec}(X)$$

Applications:

Control

Deterministic and stochastic, and time dependent PDEs

Inverse problems and optimization

Multiterm linear matrix equation. Classical device

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

Kronecker formulation

$$(B_1^\top \otimes A_1 + \dots + B_\ell^\top \otimes A_\ell) \mathbf{x} = c \quad \Leftrightarrow \quad \mathcal{A} \mathbf{x} = c$$

Iterative methods: matrix-matrix multiplications and rank truncation

(Benner, Breiten, Bouhamidi, Chehab, Damm, Grasedyck, Jbilou, Kressner, Matthies, Nagy, Onwunta, Raydan, Stoll, Tobler, Wedderburn, Zander, ...)

$$\text{Kronecker product : } M \otimes P = \begin{bmatrix} m_{11}P & \dots & m_{1n}P \\ \vdots & \ddots & \vdots \\ m_{n1}P & \dots & m_{nn}P \end{bmatrix} \quad \text{and } \text{vec}(AXB) = (B^\top \otimes A)\text{vec}(X)$$

Applications:

Control

Deterministic and stochastic, and time dependent PDEs

Inverse problems and optimization

Multiterm linear matrix equation

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

Alternative approaches to the Kronecker form:

- ▶ Fixed point iterations (an “evergreen” ...)
- ▶ Projection-type methods \Rightarrow low rank approximation
- ▶ Ad-hoc problem-dependent procedures
- ▶ etc.

A sample of these methodologies on different problems:

- ♣ Stochastic PDE
- ♣ PDEs on polygonal domains
- ♣ All-at-once PDE-constrained optimization problem
- ♣ Bilinear control problems
- ♣

Multiterm linear matrix equation

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

Alternative approaches to the Kronecker form:

- ▶ Fixed point iterations (an “evergreen” ...)
- ▶ Projection-type methods \Rightarrow low rank approximation
- ▶ Ad-hoc problem-dependent procedures
- ▶ etc.

A sample of these methodologies on different problems:

- ♣ Stochastic PDE
- ♣ PDEs on polygonal domains
- ♣ All-at-once PDE-constrained optimization problem
- ♣ Bilinear control problems
- ♣

PDEs with random inputs

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

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

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,

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

$\mu(\mathbf{x})$: expected value of diffusion coef.

σ : std dev.

$(\lambda_r, \phi_r(\mathbf{x}))$ eigs of the integral operator \mathcal{V} wrto $V(\mathbf{x}, \mathbf{x}') = \frac{1}{\sigma^2} C(\mathbf{x}, \mathbf{x}')$

($\lambda \searrow$ $C : D \times D \rightarrow \mathbb{R}$ covariance fun.)

PDEs with random inputs

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

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

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,

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

$\mu(\mathbf{x})$: expected value of diffusion coef.

σ : std dev.

$(\lambda_r, \phi_r(\mathbf{x}))$ eigs of the integral operator \mathcal{V} wrto $V(\mathbf{x}, \mathbf{x}') = \frac{1}{\sigma^2} C(\mathbf{x}, \mathbf{x}')$

($\lambda \searrow$ $C : D \times D \rightarrow \mathbb{R}$ covariance fun.)

Stochastic Galerkin discretization. The SPDE-practitioner approach.

Approx with space in tensor product form¹ $\mathcal{X}_h \times S_p$

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

\mathbf{x} : expansion coef. of approx to u in the tensor product basis $\{\varphi_i \psi_k\}$

$K_r \in \mathbb{R}^{n_x \times n_x}$, FE matrices (sym)

$G_r \in \mathbb{R}^{n_\xi \times n_\xi}$, $r = 0, 1, \dots, m$ Galerkin matrices associated w/ S_p (sym.)

\mathbf{g}_0 : first column of G_0

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

$$n_\xi = \dim(S_p) = \frac{(\ell + p)!}{\ell! p!} \Rightarrow \boxed{n_x \cdot n_\xi} \text{ huge}$$

¹ S_p set of multivariate polyn of total degree $\leq p$

The matrix equation formulation

$$(G_0 \otimes K_0 + G_1 \otimes K_1 + \dots + G_\ell \otimes K_\ell) \mathbf{x} = \mathbf{g}_0 \otimes \mathbf{f}_0$$

transforms into

$$K_0 \mathbf{X} G_0 + K_1 \mathbf{X} G_1 + \dots + K_\ell \mathbf{X} G_\ell = F, \quad F = \mathbf{f}_0 \mathbf{g}_0^\top$$

$$(G_0 = I)$$

Solution strategy. Conjecture:

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

⇓

$$\mathbf{X} \approx \tilde{\mathbf{X}} \text{ low rank, } \tilde{\mathbf{X}} = X_1 X_2^\top$$

Matrix Galerkin approximation of the deterministic part

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

$$V_k^\top R_k = 0, \quad R_k := K_0 X_k + K_1 X_k G_1 + \dots + K_\ell X_k G_\ell - \mathbf{f}_0 \mathbf{g}_0^\top$$

Computational challenges:

- ▶ Generation of \mathcal{K}_k involved $\ell + 1$ 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 2017)

Example. $-\nabla \cdot (a\nabla u) = 1$, $D = (-1, 1)^2$. KL expansion

$\mu = 1$, $\xi_r \sim U(-\sqrt{3}, \sqrt{3})$ and $C(\vec{x}_1, \vec{x}_2) = \sigma^2 \exp\left(-\frac{\|\vec{x}_1 - \vec{x}_2\|_1}{2}\right)$, $n_x = 65,025$, $\sigma = 0.3$

ℓ	p	n_ξ	k	inner its	n_k \mathcal{K}_k	rank $\tilde{\mathbf{X}}$	time secs	CG	
								time	(its)
8 87%	2	45	17	9.8	128	45	32.1	13.4	(8)
	3	165	21	12.2	160	129	41.4	56.6	(10)
	4	495	24	14.5	183	178	51.1	197.0	(12)
	5	1,287	27	16.9	207	207	64.0	553.0	(13)
12 89%	2	91	15	9.9	165	89	47.8	30.0	(8)
	3	455	18	12.2	201	196	61.6	175.0	(10)
	4	1,820	21	15.0	236	236	86.4	821.0	(12)
	5	6,188	25	18.6	281	281	188.0	3070.0	(13)
20 93%	2	231	16	9.4	281	206	111.0	94.7	(8)
	3	1,771	23	12.3	399	399	197.0	845.0	(10)
	4	10,626	26	15.4	454	454	556.0	Out of Mem	

% of variance integral of a

Linear matrix equations for convection-diffusion PDEs

$$-\alpha_1 u_{xx} - \alpha_2 u_{yy} + \mathbf{w} \cdot \nabla u + \beta u = f, \quad (x, y) \in \Omega,$$

$\Omega \subset \mathbb{R}^2$ sufficiently regular domains, e.g., polygons, not necessarily convex

Standard procedures giving $\mathcal{A}u = f$:

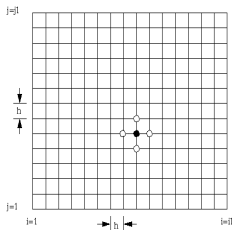
- ▶ Large class of finite element methods
- ▶ Spectral (element) methods
- ▶ Isogeometric Analysis
- ▶ Mimetic FD or Virtual element methods
- ▶ Classical Finite differences
- ▶ ...

Proof of concept:

Explore venues leading to linear matrix equations

The Poisson equation in a square

$$-u_{xx} - u_{yy} = f, \quad \text{in } \Omega = (0, 1)^2 \quad (+\text{hom. Dirb.c.})$$



Usual lexicographic ordering $\Rightarrow \quad Au = b$

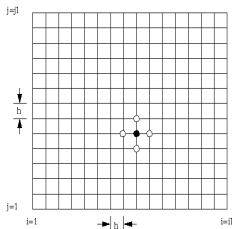
Discretization: $U_{i,j} \approx u_{x_i, y_j}$, with (x_i, y_j) interior nodes, so that

$$u_{xx}(x_i, y_j) \approx \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2} = \frac{1}{h^2} [1, -2, 1] \begin{bmatrix} U_{i-1,j} \\ U_{i,j} \\ U_{i+1,j} \end{bmatrix}$$

$$u_{yy}(x_i, y_j) \approx \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{h^2} = \frac{1}{h^2} [U_{i,j-1}, U_{i,j}, U_{i,j+1}] \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

The Poisson equation in a square

$$-u_{xx} - u_{yy} = f, \quad \text{in } \Omega = (0, 1)^2 \quad (+hom.Dirb.c.)$$



Usual lexicographic ordering $\Rightarrow \quad Au = b$

Discretization: $U_{i,j} \approx u_{x_i, y_j}$, with (x_i, y_j) interior nodes, so that

$$u_{xx}(x_i, y_j) \approx \frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2} = \frac{1}{h^2} [1, -2, 1] \begin{bmatrix} U_{i-1,j} \\ U_{i,j} \\ U_{i+1,j} \end{bmatrix}$$

$$u_{yy}(x_i, y_j) \approx \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{h^2} = \frac{1}{h^2} [U_{i,j-1}, U_{i,j}, U_{i,j+1}] \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

The Poisson equation - matrix formulation

Let $T = \frac{1}{h^2} \text{tridiag}(-1, 2, -1)$

$$u_{xx}(x_i, y_j) \approx \frac{1}{h^2} [1, -2, 1] \begin{bmatrix} U_{i-1,j} \\ U_{i,j} \\ U_{i+1,j} \end{bmatrix} \quad u_{yy}(x_i, y_j) \approx \frac{1}{h^2} [U_{i,j-1}, U_{i,j}, U_{i,j+1}] \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

Collecting all nodes together,

$$-u_{xx} \approx TU, \quad -u_{yy} \approx UT$$

Therefore, directly from the grid,

$$-u_{xx} - u_{yy} = f \quad \Rightarrow \quad TU + UT = F, \quad F_{ij} = f(x_i, y_j)$$

Convection-diffusion eqns in a rectangle (with D. Palitta)

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

$(x, y) \in \Omega \subset \mathbb{R}^2$, ϕ_i, ψ_i, γ_i , $i = 1, 2$ sufficiently regular func's + b.c.

Problem discretization by means of a tensor basis

Multiterm linear matrix equation:

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

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

but also Isogeometric Analysis (IGA), certain spectral methods, etc.

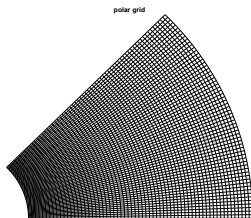
... A classical approach, Bickley & McNamee, 1960, Wachspress, 1963
(Early literature on difference equations)

Discretization of more complex domains (with Y. Hao)

$$-u_{xx} - u_{yy} = f, \quad \text{in } \Omega$$

$$(x, y) \in \Omega, \quad x = r \cos \theta, \quad y = r \sin \theta$$

$$(r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$



♣ Transformed equation in polar coordinates:

$$-r^2 \tilde{u}_{rr} - r \tilde{u}_r - \tilde{u}_{\theta\theta} = \tilde{f}, \quad (r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$

Matrix equation after mapping to the rectangle:

$$\Phi^2 T \tilde{U} + \tilde{U} T - \Phi B \tilde{U} = \tilde{F}$$

♣ Transformed equation in log-polar coordinates ($r = e^\rho$):

$$-\hat{u}_{\rho\rho} - \hat{u}_{\theta\theta} = \hat{f}, \quad (r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$

Matrix equation after mapping to the rectangle:

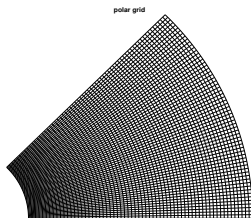
$$T \hat{U} + \hat{U} T = \hat{F}$$

Discretization of more complex domains (with Y. Hao)

$$-u_{xx} - u_{yy} = f, \quad \text{in } \Omega$$

$$(x, y) \in \Omega, \quad x = r \cos \theta, \quad y = r \sin \theta$$

$$(r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$



♣ Transformed equation in polar coordinates:

$$-r^2 \tilde{u}_{rr} - r \tilde{u}_r - \tilde{u}_{\theta\theta} = \tilde{f}, \quad (r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$

Matrix equation after mapping to the rectangle:

$$\Phi^2 T \tilde{U} + \tilde{U} T - \Phi B \tilde{U} = \tilde{F}$$

♣ Transformed equation in log-polar coordinates ($r = e^\rho$):

$$-\hat{u}_{\rho\rho} - \hat{u}_{\theta\theta} = \hat{f}, \quad (r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$

Matrix equation after mapping to the rectangle:

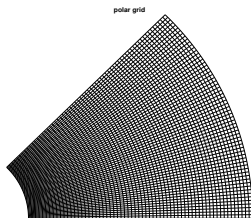
$$T \hat{U} + \hat{U} T = \hat{F}$$

Discretization of more complex domains (with Y. Hao)

$$-u_{xx} - u_{yy} = f, \quad \text{in } \Omega$$

$$(x, y) \in \Omega, \quad x = r \cos \theta, \quad y = r \sin \theta$$

$$(r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$



♣ Transformed equation in polar coordinates:

$$-r^2 \tilde{u}_{rr} - r \tilde{u}_r - \tilde{u}_{\theta\theta} = \tilde{f}, \quad (r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$

Matrix equation after mapping to the rectangle:

$$\Phi^2 T \tilde{U} + \tilde{U} T - \Phi B \tilde{U} = \tilde{F}$$

♣ Transformed equation in log-polar coordinates ($r = e^\rho$):

$$-\hat{u}_{\rho\rho} - \hat{u}_{\theta\theta} = \hat{f}, \quad (r, \theta) \in [r_0, r_1] \times [0, \frac{\pi}{4}]$$

Matrix equation after mapping to the rectangle:

$$T \hat{U} + \hat{U} T = \hat{F}$$

Discretization of polygons with > 4 edges (with Y. Hao)

We need an automatic procedure to map a polygon into a rectangle

Schwarz-Christoffel conformal mappings

$\{z_1, \dots, z_n\}$: polygon vertices $\{\phi_1\pi, \dots, \phi_n\pi\}$: vertices interior angles
Pre-images of the vertices (or pre-vertices): $\omega_1, \dots, \omega_n \in \mathbb{R}$, with

$$\omega_1 < \omega_2 < \dots < \omega_n = \infty.$$

Schwarz-Christoffel (SC) map g :
$$g(\omega) = g(\omega_0) + c \int_{\omega_0}^{\omega} \prod_{j=1}^{n-1} (\zeta - \omega_j)^{\phi_j - 1} d\zeta \quad (*)$$

Practical problems associated with Schwarz-Christoffel maps:

- ▶ *SC parameter problem*: determining the pre-vertices ω_j in closed form;
- ▶ *quadrature formulas*: Integrating the rhs of (*)

Schwarz-Christoffel Toolbox for Matlab, T. Driscoll, 1996, 2005

Discretization of polygons with > 4 edges (with Y. Hao)

We need an automatic procedure to map a polygon into a rectangle

Schwarz-Christoffel conformal mappings

$\{z_1, \dots, z_n\}$: polygon vertices $\{\phi_1\pi, \dots, \phi_n\pi\}$: vertices interior angles
Pre-images of the vertices (or pre-vertices): $\omega_1, \dots, \omega_n \in \mathbb{R}$, with

$$\omega_1 < \omega_2 < \dots < \omega_n = \infty.$$

Schwarz-Christoffel (SC) map g :
$$g(\omega) = g(\omega_0) + c \int_{\omega_0}^{\omega} \prod_{j=1}^{n-1} (\zeta - \omega_j)^{\phi_j - 1} d\zeta \quad (*)$$

Practical problems associated with Schwarz-Christoffel maps:

- ▶ *SC parameter problem*: determining the pre-vertices ω_j in closed form;
- ▶ *quadrature formulas*: Integrating the rhs of (*)

Schwarz-Christoffel Toolbox for Matlab, T. Driscoll, 1996, 2005

Discretization of polygons with > 4 edges (with Y. Hao)

We need an automatic procedure to map a polygon into a rectangle

Schwarz-Christoffel conformal mappings

$\{z_1, \dots, z_n\}$: polygon vertices $\{\phi_1\pi, \dots, \phi_n\pi\}$: vertices interior angles
Pre-images of the vertices (or pre-vertices): $\omega_1, \dots, \omega_n \in \mathbb{R}$, with

$$\omega_1 < \omega_2 < \dots < \omega_n = \infty.$$

Schwarz-Christoffel (SC) map g :
$$g(\omega) = g(\omega_0) + c \int_{\omega_0}^{\omega} \prod_{j=1}^{n-1} (\zeta - \omega_j)^{\phi_j - 1} d\zeta \quad (*)$$

Practical problems associated with Schwarz-Christoffel maps:

- ▶ *SC parameter problem*: determining the pre-vertices ω_j in closed form;
- ▶ *quadrature formulas*: Integrating the rhs of (*)

Schwarz-Christoffel Toolbox for Matlab, T. Driscoll, 1996, 2005

Discretization of polygons with > 4 edges (with Y. Hao)

We need an automatic procedure to map a polygon into a rectangle

Schwarz-Christoffel conformal mappings

$\{z_1, \dots, z_n\}$: polygon vertices $\{\phi_1\pi, \dots, \phi_n\pi\}$: vertices interior angles
Pre-images of the vertices (or pre-vertices): $\omega_1, \dots, \omega_n \in \mathbb{R}$, with

$$\omega_1 < \omega_2 < \dots < \omega_n = \infty.$$

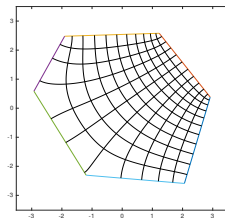
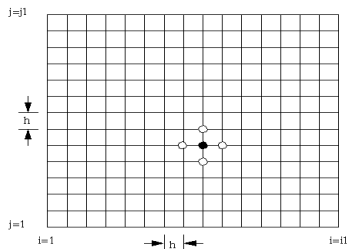
Schwarz-Christoffel (SC) map g :
$$g(\omega) = g(\omega_0) + c \int_{\omega_0}^{\omega} \prod_{j=1}^{n-1} (\zeta - \omega_j)^{\phi_j - 1} d\zeta \quad (*)$$

Practical problems associated with Schwarz-Christoffel maps:

- ▶ *SC parameter problem*: determining the pre-vertices ω_j in closed form;
- ▶ *quadrature formulas*: Integrating the rhs of (*)

Schwarz-Christoffel Toolbox for Matlab, T. Driscoll, 1996, 2005

Computing with Schwarz-Christoffel maps (with Y. Hao)



Canonical rectangular domain $\Pi \rightarrow z = g(\xi, \eta) \rightarrow$ (Convex) physical domain Ω

$$z = g(\omega) = g(\xi + i\eta) = x(\xi, \eta) + iy(\xi, \eta)$$

Jacobian matrix of the conformal map g :

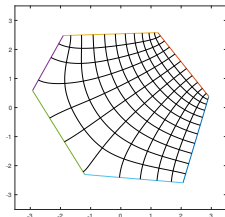
$$\mathcal{J} = \begin{bmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{bmatrix} \quad \mathcal{J} = \mathcal{J}(\xi, \eta) = \det(\mathcal{J}) = x_\xi y_\eta - x_\eta y_\xi = x_\xi^2 + x_\eta^2 > 0$$

and $\tilde{u}_\xi = u_x x_\xi + u_y y_\xi$, $\tilde{u}_\eta = u_x x_\eta + u_y y_\eta$

Poisson equation in a polygon (with Y. Hao)

$$-u_{xx} - u_{yy} = f, \quad (x, y) \in \Omega$$

$$-\tilde{u}_{\xi\xi} - \tilde{u}_{\eta\eta} = \mathcal{J}\tilde{f}, \quad (\xi, \eta) \in \Pi$$



With finite diff. discretization:

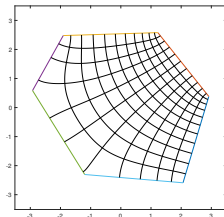
$$\boxed{T_1 U + U T_2 = F}, \quad \tilde{F} + b.c., \quad \text{and} \quad \tilde{F}_{i,j} = (\mathcal{J}\tilde{f})(\xi_i, \eta_j), \quad 1 \leq i \leq n_1, \quad 1 \leq j \leq n_2$$

Poisson equation is the ideal setting for SC mappings!

Poisson equation in a polygon (with Y. Hao)

$$-u_{xx} - u_{yy} = f, \quad (x, y) \in \Omega$$

$$-\tilde{u}_{\xi\xi} - \tilde{u}_{\eta\eta} = \mathcal{J}\tilde{f}, \quad (\xi, \eta) \in \Pi$$



With finite diff. discretization:

$$\boxed{T_1 U + U T_2 = F}, \quad \tilde{F} + b.c., \quad \text{and} \quad \tilde{F}_{i,j} = (\mathcal{J}\tilde{f})(\xi_i, \eta_j), \quad 1 \leq i \leq n_1, \quad 1 \leq j \leq n_2$$

Poisson equation is the ideal setting for SC mappings!

Adding a reaction term

$$-\Delta u + \beta u = f, \quad (x, y) \in \Omega, \quad u = 0 \quad \text{on } \partial\Omega.$$

In the canonical (reference) domain Π :

$$-\tilde{u}_{\xi\xi} - \tilde{u}_{\eta\eta} + (\mathcal{J}\tilde{\beta})\tilde{u} = \mathcal{J}\tilde{f}, \quad (\xi, \eta) \in \Pi, \quad \tilde{u} = 0, \quad (\xi, \eta) \in \partial\Pi.$$

thus giving the following matrix equation:

$$\boxed{T_1 U + U T_2 + G \circ U = F}$$

(\circ denotes the (element-wise) Hadamard product)

with $G(i, j) := (\mathcal{J}\tilde{\beta})(\xi_i, \eta_j)$, with $1 \leq i \leq n_1$ and $1 \leq j \leq n_2$

Adding a reaction term

$$-\Delta u + \beta u = f, \quad (x, y) \in \Omega, \quad u = 0 \quad \text{on } \partial\Omega.$$

In the canonical (reference) domain Π :

$$-\tilde{u}_{\xi\xi} - \tilde{u}_{\eta\eta} + (\mathcal{J}\tilde{\beta})\tilde{u} = \mathcal{J}\tilde{f}, \quad (\xi, \eta) \in \Pi, \quad \tilde{u} = 0, \quad (\xi, \eta) \in \partial\Pi.$$

thus giving the following matrix equation:

$$\boxed{T_1 U + U T_2 + G \circ U = F}$$

(\circ denotes the (element-wise) Hadamard product)

with $G(i, j) := (\mathcal{J}\tilde{\beta})(\xi_i, \eta_j)$, with $1 \leq i \leq n_1$ and $1 \leq j \leq n_2$

A simple convection-diffusion problem

$$-u_{xx} - u_{yy} + \mathbf{w} \cdot \nabla u = f, \quad (x, y) \in \Omega$$

Transformed SC-mapped problem:

$$-\varepsilon(\tilde{u}_{\xi\xi} + \tilde{u}_{\eta\eta}) + x_\xi \tilde{u}_\xi + x_\eta \tilde{u}_\eta = \mathcal{J} \tilde{f}, \quad (\xi, \eta) \in \Pi, \tilde{u} = 0, \quad (\xi, \eta) \in \partial\Pi,$$

where we used $\mathbf{w} = (1, 0)$.

This yields the matrix equation

$$\varepsilon T_1 U + \varepsilon U T_2 + X_\xi \circ (B_1 U) + X_\eta \circ (U B_2) = F,$$

where $(X_\xi)_{i,j} = x_\xi(\xi_i, \eta_j)$, $(X_\eta)_{i,j} = x_\eta(\xi_i, \eta_j)$, $i = 1, \dots, n_1$, $j = 1, \dots, n_2$

Conclusions. 1

- ▶ Linear matrix equations can be obtained for general domains with different discretization procedures (IGA, FD, conformal mappings, ...)
- ▶ Structural properties should be exploited (different from Kronecker formulations)
- ▶ 3D case leads to linear **tensor** equations: a new research area

Solution strategies: Projection-type methods. 1

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

Given approximation spaces $\mathcal{K}_A, \mathcal{K}_B$,

$$\mathbf{X} \approx X_m \quad \text{with} \quad \text{vec}(X_m) \in \mathcal{K}_B \otimes \mathcal{K}_A$$

X is approximated by a low rank matrix !

Galerkin condition: $R := A_1 X_m B_1 + A_2 X_m B_2 + \dots + A_\ell X_m B_\ell - C \perp \mathcal{K}_B \otimes \mathcal{K}_A$

$$V_m^T R W_m = 0 \quad \mathcal{K}_A = \text{Range}(V_m), \mathcal{K}_B = \text{Range}(W_m)$$

Let $X_m := V_m Y_m W_m^T$.

Projected matrix equation:

$$\begin{aligned} V_m^T (A_1 X_m B_1 + \dots + A_\ell X_m B_\ell - C) W_m &= 0 \\ (V_m^T A_1 V_m) Y (W_m^T B_1 W_m) + \dots + (V_m^T A_\ell V_m) Y (W_m^T B_\ell W_m) - V_m^T C W_m &= 0 \end{aligned}$$

Solution strategies: Projection-type methods. 1

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

Given approximation spaces $\mathcal{K}_A, \mathcal{K}_B$,

$$\mathbf{X} \approx X_m \quad \text{with} \quad \text{vec}(X_m) \in \mathcal{K}_B \otimes \mathcal{K}_A$$

\mathbf{X} is approximated by a low rank matrix !

Galerkin condition: $R := A_1 X_m B_1 + A_2 X_m B_2 + \dots + A_\ell X_m B_\ell - C \perp \mathcal{K}_B \otimes \mathcal{K}_A$

$$V_m^T R W_m = 0 \quad \mathcal{K}_A = \text{Range}(V_m), \mathcal{K}_B = \text{Range}(W_m)$$

Let $X_m := V_m Y_m W_m^T$.

Projected matrix equation:

$$\begin{aligned} V_m^T (A_1 X_m B_1 + \dots + A_\ell X_m B_\ell - C) W_m &= 0 \\ (V_m^T A_1 V_m) Y (W_m^T B_1 W_m) + \dots + (V_m^T A_\ell V_m) Y (W_m^T B_\ell W_m) - V_m^T C W_m &= 0 \end{aligned}$$

Solution strategies: Projection-type methods. 1

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

Given approximation spaces $\mathcal{K}_A, \mathcal{K}_B$,

$$\mathbf{X} \approx X_m \quad \text{with} \quad \text{vec}(X_m) \in \mathcal{K}_B \otimes \mathcal{K}_A$$

\mathbf{X} is approximated by a low rank matrix !

Galerkin condition: $R := A_1 X_m B_1 + A_2 X_m B_2 + \dots + A_\ell X_m B_\ell - C \perp \mathcal{K}_B \otimes \mathcal{K}_A$

$$V_m^\top R W_m = 0 \quad \mathcal{K}_A = \text{Range}(V_m), \mathcal{K}_B = \text{Range}(W_m)$$

Let $X_m := V_m Y_m W_m^\top$.

Projected matrix equation:

$$\begin{aligned} V_m^\top (A_1 X_m B_1 + \dots + A_\ell X_m B_\ell - C) W_m &= 0 \\ (V_m^\top A_1 V_m) \mathbf{Y} (W_m^\top B_1 W_m) + \dots + (V_m^\top A_\ell V_m) \mathbf{Y} (W_m^\top B_\ell W_m) - V_m^\top C W_m &= 0 \end{aligned}$$

Solution strategies: Projection-type methods. 2

Solve for \mathbf{Y} :

$$(V_m^\top A_1 V_m) \mathbf{Y} (W_m^\top B_1 W_m) + \dots + (V_m^\top A_\ell V_m) \mathbf{Y} (W_m^\top B_\ell W_m) - V_m^\top C W_m = 0$$

Then, implicitly generate $X_m := V_m Y_m W_m^\top$

Procedure generalizes the case $\ell = 2$, using the classical *Galerkin projection* methodology

Crucial issues for effectiveness:

- ▶ Choice of spaces $\mathcal{K}_A, \mathcal{K}_B$
- ▶ Generation of the two spaces $\mathcal{K}_A, \mathcal{K}_B$. Ideally,

$$\text{range}(V_m) \subseteq \text{range}(V_{m+1}), \quad \text{range}(W_m) \subseteq \text{range}(W_{m+1})$$

- ▶ Solution of the reduced multiterm equation

Solution strategies: Projection-type methods. 2

Solve for \mathbf{Y} :

$$(V_m^\top A_1 V_m) \mathbf{Y} (W_m^\top B_1 W_m) + \dots + (V_m^\top A_\ell V_m) \mathbf{Y} (W_m^\top B_\ell W_m) - V_m^\top C W_m = 0$$

Then, implicitly generate $X_m := V_m Y_m W_m^\top$

Procedure generalizes the case $\ell = 2$, using the classical *Galerkin projection* methodology

Crucial issues for effectiveness:

- ▶ Choice of spaces $\mathcal{K}_A, \mathcal{K}_B$
- ▶ Generation of the two spaces $\mathcal{K}_A, \mathcal{K}_B$. Ideally,

$$\text{range}(V_m) \subseteq \text{range}(V_{m+1}), \quad \text{range}(W_m) \subseteq \text{range}(W_{m+1})$$

- ▶ Solution of the reduced multiterm equation

Computational methods for certain structured problems

A particular case²:

$$A\mathbf{X} + \mathbf{X}A^T + M_1\mathbf{X}M_1 + \dots + M_\ell\mathbf{X}M_\ell = F,$$

with $A \in \mathbb{R}^{n \times n}$, and the M_i s having very low rank s_i , $M_i = U_i V_i^T$

Using the Kronecker form ($\ell = 1$):

$$(A \otimes I + I \otimes A + (U_1 \otimes U_1)(V_1 \otimes V_1)^T)\mathbf{x} = f$$

that is

$$(A + UV^T)\mathbf{x} = f$$

with $U = U_1 \otimes U_1$, $V = V_1 \otimes V_1$ again of low rank s_1^2

Solution method: Sherman-Morrison-Woodbury formula

$$\mathbf{x} = (A + UV^T)^{-1}f = A^{-1}f - A^{-1}U(I + V^T A^{-1}U)^{-1}V^T A^{-1}f$$

²In fact, terms in the form $M_i\mathbf{X}N_i$ can also be treated

Computational methods for certain structured problems

A particular case²:

$$\mathbf{A}\mathbf{X} + \mathbf{X}\mathbf{A}^T + M_1\mathbf{X}M_1 + \dots + M_\ell\mathbf{X}M_\ell = F,$$

with $A \in \mathbb{R}^{n \times n}$, and the M_i s having very low rank s_i , $M_i = U_i V_i^T$

Using the Kronecker form ($\ell = 1$):

$$(\mathbf{A} \otimes \mathbf{I} + \mathbf{I} \otimes \mathbf{A} + (\mathbf{U}_1 \otimes \mathbf{U}_1)(\mathbf{V}_1 \otimes \mathbf{V}_1)^T)\mathbf{x} = f$$

that is

$$(\mathcal{A} + \mathcal{U}\mathcal{V}^T)\mathbf{x} = f$$

with $\mathcal{U} = U_1 \otimes U_1$, $\mathcal{V} = V_1 \otimes V_1$ again of low rank s_1^2

Solution method: Sherman-Morrison-Woodbury formula

$$\mathbf{x} = (\mathbf{A} + \mathcal{U}\mathcal{V}^T)^{-1}f = \mathbf{A}^{-1}f - \mathbf{A}^{-1}\mathcal{U}(\mathbf{I} + \mathcal{V}^T\mathbf{A}^{-1}\mathcal{U})^{-1}\mathcal{V}^T\mathbf{A}^{-1}f$$

²In fact, terms in the form $M_i\mathbf{X}N_i$ can also be treated

Computational methods for certain structured problems

A particular case²:

$$A\mathbf{X} + \mathbf{X}A^T + M_1\mathbf{X}M_1 + \dots + M_\ell\mathbf{X}M_\ell = F,$$

with $A \in \mathbb{R}^{n \times n}$, and the M_i s having very low rank s_i , $M_i = U_i V_i^T$

Using the Kronecker form ($\ell = 1$):

$$(A \otimes I + I \otimes A + (U_1 \otimes U_1)(V_1 \otimes V_1)^T)\mathbf{x} = f$$

that is

$$(A + UV^T)\mathbf{x} = f$$

with $U = U_1 \otimes U_1$, $V = V_1 \otimes V_1$ again of low rank s_1^2

Solution method: Sherman-Morrison-Woodbury formula

$$\mathbf{x} = (A + UV^T)^{-1}f = A^{-1}f - A^{-1}U(I + V^T A^{-1}U)^{-1}V^T A^{-1}f$$

²In fact, terms in the form $M_i\mathbf{X}N_i$ can also be treated

Matrix-oriented Sherman-Morrison-Woodbury formula

$$\mathbf{x} = \mathcal{A}^{-1}\mathbf{f} - \mathcal{A}^{-1}\mathcal{U}(\mathbf{I} + \mathcal{V}^T\mathcal{A}^{-1}\mathcal{U})^{-1}\mathcal{V}^T\mathcal{A}^{-1}\mathbf{f}$$

1. Solve $\mathcal{A}w = f$
2. Solve $\mathcal{A}p_j = u_j$ where $\mathcal{U} = [u_1, \dots, u_{s^2}]$ to give $\mathcal{P} = [p_1, \dots, p_{s^2}]$;
3. Compute $H = \mathbf{I} + \mathcal{V}^T\mathcal{P} \in \mathbb{R}^{s^2 \times s^2}$
4. Solve $Hg = \mathcal{V}^T w$
5. Compute $x = w - \mathcal{P}g$.

Steps 1. and 2.:

$$w = \mathcal{A}^{-1}f \quad \Leftrightarrow \quad AW + WA^T = F, \quad f = \text{vec}(F)$$

Analogously for each $p_j = \text{vec}(P_j)$ in step 2

$AW + WA^T = P_j$ Lyapunov equations, with the same A - cheap “direct” solution

Step 3.

$$v_j^T \mathcal{A}^{-1}u_t = v_i^T P_t v_k, \quad j = (k-1)s + i$$

Analogously for $\mathcal{V}^T w$ in step 4

Matrix-oriented Sherman-Morrison-Woodbury formula

$$\mathbf{x} = \mathcal{A}^{-1}\mathbf{f} - \mathcal{A}^{-1}\mathcal{U}(\mathbf{I} + \mathcal{V}^T\mathcal{A}^{-1}\mathcal{U})^{-1}\mathcal{V}^T\mathcal{A}^{-1}\mathbf{f}$$

1. Solve $\mathcal{A}\mathbf{w} = \mathbf{f}$
2. Solve $\mathcal{A}\mathbf{p}_j = \mathbf{u}_j$ where $\mathcal{U} = [\mathbf{u}_1, \dots, \mathbf{u}_{s^2}]$ to give $\mathcal{P} = [\mathbf{p}_1, \dots, \mathbf{p}_{s^2}]$;
3. Compute $\mathbf{H} = \mathbf{I} + \mathcal{V}^T\mathcal{P} \in \mathbb{R}^{s^2 \times s^2}$
4. Solve $\mathbf{H}\mathbf{g} = \mathcal{V}^T\mathbf{w}$
5. Compute $\mathbf{x} = \mathbf{w} - \mathcal{P}\mathbf{g}$.

Steps 1. and 2.:

$$\mathbf{w} = \mathcal{A}^{-1}\mathbf{f} \quad \Leftrightarrow \quad \mathbf{A}\mathbf{W} + \mathbf{W}\mathbf{A}^T = \mathbf{F}, \quad \mathbf{f} = \text{vec}(\mathbf{F})$$

Analogously for each $\mathbf{p}_j = \text{vec}(\mathbf{P}_j)$ in step 2

$\mathbf{A}\mathbf{W} + \mathbf{W}\mathbf{A}^T = \mathbf{P}_j$ Lyapunov equations, with the same \mathbf{A} - cheap “direct” solution

Step 3.

$$\mathbf{v}_j^T \mathcal{A}^{-1} \mathbf{u}_t = \mathbf{v}_i^T \mathbf{P}_t \mathbf{v}_k, \quad j = (k-1)s + i$$

Analogously for $\mathcal{V}^T\mathbf{w}$ in step 4

Matrix-oriented Sherman-Morrison-Woodbury formula

$$\mathbf{x} = \mathcal{A}^{-1}\mathbf{f} - \mathcal{A}^{-1}\mathcal{U}(\mathbf{I} + \mathcal{V}^T\mathcal{A}^{-1}\mathcal{U})^{-1}\mathcal{V}^T\mathcal{A}^{-1}\mathbf{f}$$

1. Solve $\mathcal{A}w = \mathbf{f}$
2. Solve $\mathcal{A}p_j = \mathbf{u}_j$ where $\mathcal{U} = [\mathbf{u}_1, \dots, \mathbf{u}_{s^2}]$ to give $\mathcal{P} = [p_1, \dots, p_{s^2}]$;
3. Compute $H = \mathbf{I} + \mathcal{V}^T\mathcal{P} \in \mathbb{R}^{s^2 \times s^2}$
4. Solve $Hg = \mathcal{V}^T w$
5. Compute $\mathbf{x} = w - \mathcal{P}g$.

Steps 1. and 2.:

$$w = \mathcal{A}^{-1}\mathbf{f} \quad \Leftrightarrow \quad AW + WA^T = F, \quad \mathbf{f} = \text{vec}(F)$$

Analogously for each $p_j = \text{vec}(P_j)$ in step 2

$AW + WA^T = P_j$ Lyapunov equations, with the same A - cheap “direct” solution

Step 3.

$$\mathbf{v}_j^T \mathcal{A}^{-1}\mathbf{u}_t = \mathbf{v}_i^T P_t \mathbf{v}_k, \quad j = (k-1)s + i$$

Analogously for $\mathcal{V}^T w$ in step 4

Numerical examples. 1

Let X_* be a ref. soln (uniformly distr.random), and rhs computed explicitly

We monitor: $Err := \frac{\|X - X_*\|_F}{\|X_*\|_F}$

n	s_1/s_2	Matrix form		Vector Form	
		CPU time	Err	CPU time	Err
40	3/5	0.013	3.817934e-11	0.195	2.292375e-10
	6/10	0.017	9.051326e-10	0.657	4.987161e-10
	12/20	0.035	5.259884e-09	2.333	1.357709e-08
80	3/5	0.022	2.152743e-10	5.283	1.228423e-09
	6/10	0.033	8.380606e-09	15.408	1.849484e-08
	12/20	0.074	2.502003e-08	56.347	3.467476e-08
160	3/5	0.043	1.291839e-09	129.957	6.891372e-09
	6/10	0.070	1.102578e-08	281.946	2.691323e-08
	12/20	0.220	2.907566e-07	1030.242	1.202511e-06

Table: Symmetric and dense matrix A and U_1, U_2 ($\ell = 2$) for various ranks s_1, s_2

Numerical examples. 2

n	Matrix form		Vector Form	
	CPU time	Err	CPU time	Err
40	0.012	6.452267e-10	0.037	7.231068e-10
80	0.013	2.750854e-10	0.124	2.012480e-09
160	0.024	3.253562e-09	0.581	7.208432e-09
320	0.056	4.615180e-08	2.763	1.710614e-07

Table: Numerical results for symmetric and tridiagonal banded matrix A and U_1, U_2 random with $s_1 = 3, s_2 = 5$ columns, resp.

n	Matrix form		Vector Form	
	CPU time	Err	CPU time	Err
40	0.063	6.582486e-11	0.361	1.410898e-10
80	0.093	1.184547e-08	6.116	1.867875e-08
160	0.430	2.691697e-07	278.895	1.301593e-06

Table: Numerical results for nonsymmetric and full matrix A , with $s_1 = 3, s_2 = 5$ columns, resp.

Conclusions. 2

- ▶ First examples where structure can be exploited

(Not reported) This approach can be used for solving linear *tensor* equations

- ▶ Devise more general “direct” solvers, to be used in the projection phase!

Visit: www.dm.unibo.it/~simoncin

Email address: valeria.simoncini@unibo.it

REFERENCES

1. Yue Hao and V. S., *Matrix equation solving of PDEs on regular domains* April 2020. HAL archive: hal-02902456
2. Yue Hao and V. S., *The Sherman-Morrison-Woodbury formula for generalized linear matrix equations and applications*, July 2020. HAL archive hal-02902455.
3. Catherine E. Powell, David Silvester and V. S., *An efficient reduced basis solver for stochastic Galerkin matrix equations*, SIAM J. Scientific Computing, 39 (1), (2017).
4. Davide Palitta and V. S., *Matrix-equation-based strategies for convection-diffusion equations*, BIT Numerical Mathematics, 56-2, (2016).
5. V. S., *Computational methods for linear matrix equations*, SIAM Review, 58-3, (2016), pp. 377-441.

Conclusions. 2

- ▶ First examples where structure can be exploited

(Not reported) This approach can be used for solving linear *tensor* equations

- ▶ Devise more general “direct” solvers, to be used in the projection phase!

Visit: www.dm.unibo.it/~simoncin

Email address: valeria.simoncini@unibo.it

REFERENCES

1. Yue Hao and V. S., *Matrix equation solving of PDEs on regular domains* April 2020. HAL archive: hal-02902456
2. Yue Hao and V. S., *The Sherman-Morrison-Woodbury formula for generalized linear matrix equations and applications*, July 2020. HAL archive hal-02902455.
3. Catherine E. Powell, David Silvester and V. S., *An efficient reduced basis solver for stochastic Galerkin matrix equations*, SIAM J. Scientific Computing, 39 (1), (2017).
4. Davide Palitta and V. S., *Matrix-equation-based strategies for convection-diffusion equations*, BIT Numerical Mathematics, 56-2, (2016).
5. V. S., *Computational methods for linear matrix equations*, SIAM Review, 58-3, (2016), pp. 377-441.

Conclusions. 2

- ▶ First examples where structure can be exploited

(Not reported) This approach can be used for solving linear *tensor* equations

- ▶ Devise more general “direct” solvers, to be used in the projection phase!

Visit: www.dm.unibo.it/~simoncin

Email address: valeria.simoncini@unibo.it

REFERENCES

1. Yue Hao and V. S., *Matrix equation solving of PDEs on regular domains* April 2020. HAL archive: hal-02902456
2. Yue Hao and V. S., *The Sherman-Morrison-Woodbury formula for generalized linear matrix equations and applications*, July 2020. HAL archive hal-02902455.
3. Catherine E. Powell, David Silvester and V. S., *An efficient reduced basis solver for stochastic Galerkin matrix equations*, SIAM J. Scientific Computing, 39 (1), (2017).
4. Davide Palitta and V. S., *Matrix-equation-based strategies for convection-diffusion equations*, BIT Numerical Mathematics, 56-2, (2016).
5. V. S., *Computational methods for linear matrix equations*, SIAM Review, 58-3, (2016), pp. 377-441.