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Recent advances in low-rank matrix equation solvers

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Some matrix equations

- Sylvester matrix equation $\quad A\mathbf{X} + \mathbf{X}B + D = 0$

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

- Lyapunov matrix equation $\quad A\mathbf{X} + \mathbf{X}A^\top + D = 0, \qquad D = D^\top$

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

- Multiterm matrix equation

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

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Survey article: V.S., SIAM Review 2016.

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More matrix equations

- Systems of linear matrix equations:

$$\begin{aligned} A_2\boldsymbol{X} + \boldsymbol{X}A_1 + B^\top \boldsymbol{P} &= F_1 \\ A_1\boldsymbol{Y} + \boldsymbol{Y}A_2 + \boldsymbol{P}B &= F_2 \\ B\boldsymbol{X} + \boldsymbol{Y}B^\top &= F_3 \end{aligned}$$

(V.S., 2019)

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

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

workhorse in Control Theory

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

$$(H \otimes M \otimes A + M \otimes A \otimes H + A \otimes H \otimes M)\mathbf{x} + c = 0 \quad \mathbf{x} = \mathrm{vec}(\mathbf{X})$$

Discretization of (parameter-dependent) PDEs

(Kronecker product, $(M \otimes N) = (M_{i,j}N)$)

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which linear equation | which matrix structure | which size

- key property: tensor product space approximation to the continuous problem

  - Finite differences, e.g., Bickley & McNamee, 1960, Wachspress, 1963
  - Certain spectral methods, e.g., Canuto, Hussaini, Quarteroni and Zang, 1980s
  - Isogeometric Analysis (IGA)
  - Space-parameter, Space-time and Parallel-in-Time (PinT) discretizations
  - ...

- Symmetry, sparsity, etc., and also low-rank properties of data and solution

- Matrix equation size

  Tiny   Small   Large

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What do we expect from this ?

Pros:

- ✓ Smaller dimensional matrices
- ✓ Preserve continuous problem's properties
- ✓ Exploit structure (e.g., symmetry)
- ✓ Reach more complex problems

Cons:

- ✗ Extra effort to go beyond vectors
- ✗ Need to leave "comfort zone" of established NLA
- ✗ Different interpretation of your NLA data

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The Poisson equation

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

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

$$T_1 \mathbf{U} + \mathbf{U} T_1^\top = F, \quad F_{ij} = f(x_i, y_j), \quad T_1 = -\frac{1}{h^2}\text{tridiag}(1, -2, 1)$$

Lexicographic ordering: $\mathbf{U} \to \mathbf{u} = [\mathbf{U}_{11}, \mathbf{U}_{n,1}, \mathbf{U}_{1,2}, \ldots, \mathbf{U}_{n,2}, \ldots]^\top$

$$A\mathbf{u} = f \qquad A = I \otimes T_1 + T_1 \otimes I, \;\; f = \text{vec}(F),$$

More generally, w/separable coefficients (and convection-diffusion)

$$\phi(x,y)u_{xx} + \psi(x,y)u_{yy} = f \qquad \Rightarrow \qquad A_1 \boldsymbol{U} M_1 + M_2 \boldsymbol{U} A_2 = F$$

$$(M_2^{-1} A_1)\boldsymbol{U} + \boldsymbol{U}(A_2 M_1^{-1}) = \widehat{F}$$

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Numerical solution of the Sylvester equation

$$AU + UB = F$$

Various settings:

- Tiny A and B: Kron will do!
- Small A and B: Bartels-Stewart algorithm (Computes the Schur form of A and B)
- Large A and B: Iterative solution (F low rank)
  - Projection methods
  - ADI (Alternating Direction Iteration)
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All-at-once heat equation

$$u_t + \ell(u) = f \qquad u(0) = 0 \quad \text{(for convenience)}$$

Variational formulation

$$\text{find } u \in U : \quad b(u,v) = \langle f, v\rangle \quad \text{for all } v \in V$$

where $U := H^1_{(0)}(\mathcal{I}; X') \cap L_2(\mathcal{I}, X),\ X := H^1_0(\Omega),\ V := L_2(\mathcal{I}; X)$

$b(u,v) := \int_0^{\tau} \int_\Omega u_t(t,x)\, v(t,x)\, dx\, dt + \int_0^{\tau} a(u(t), v(t))\, dt$

$\langle f, v\rangle := \int_0^{\tau} \int_\Omega f(t,x)\, v(t,x)\, dx\, dt.$

Discretization: Petrov-Galerkin method with trial and test spaces $U_\delta \subset U$, $V_\delta \subset V$

$$\text{find } u_\delta \in U_\delta : \quad b(u_\delta, v_\delta) = \langle f, v_\delta\rangle \quad \text{for all } v_\delta \in V_\delta$$

with $U_\delta := S_{\Delta t} \otimes X_h$, $V_\delta = Q_{\Delta t} \otimes X_h$ where

$S_{\Delta t}$: piecewise linear FE on $\mathcal{I}$
$Q_{\Delta t}$: piecewise constant FE on $\mathcal{I}$

X_h : any conformal space, e.g., p.w. linear FE

♣ Well-posedness (discrete inf-sup cond) depends on the choice of U_δ, V_δ

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The final linear system

$$B_\delta^\top u_\delta = f_\delta$$

where

$$[B_\delta]_{(k,i),(\ell,j)} = (\dot\sigma^k, \tau^\ell)_{L_2(\mathcal{I})}\,(\phi_i,\phi_j)_{L_2(\Omega)} + (\sigma^k,\tau^\ell)_{L_2(\mathcal{I})}\,a(\phi_i,\phi_j),$$
$$[f_\delta]_{(\ell,j)} = (f, \tau^\ell \otimes \phi_j)_{L_2(\mathcal{I};H)}$$

that is, $B_\delta = D_{\Delta t} \otimes M_h + C_{\Delta t} \otimes K_h$

Remark: We approximate f_δ to achieve full tensor-product structure

Resulting generalized Sylvester equation:

$$M_h \mathbf{U}_\delta D_{\Delta t} + K_h \mathbf{U}_\delta C_{\Delta t} = F_\delta, \qquad \text{with} \quad F_\delta = [g_1,\ldots,g_P][h_1,\ldots,h_P]^\top$$

F_δ matrix of low rank $\Rightarrow$ $\mathbf{U}_\delta$ approx by low rank matrix $\widetilde{\mathbf{U}}_\delta$

(Julian Henning, Davide Palitta, V. S., Karsten Urban, 2021)

A simple example

$\Omega = (-1,1)^3$, with homogeneous Dirichlet boundary conditions
$\mathcal{I} = (0,10)$ and initial conditions $u(0,x,y,z) \equiv 0$
$f(t,x,y,z) := 10\sin(t)t\cos(\frac{\pi}{2}x)\cos(\frac{\pi}{2}y)\cos(\frac{\pi}{2}z)$ (F_δ is thus low rank)

		RKSM				CN Time(s)	
N_h	N_t	Its	μ_{mem}	rank($\widetilde{U}_\delta$)	Time(s)	Direct	Iterative
41 300	300	13	14	9	25.96	123.43	59.10
	500	13	14	9	30.46	143.71	78.01
	700	13	14	9	28.17	153.38	93.03
347 361	300	14	15	9	820.17	14705.10	792.42
	500	14	15	9	828.34	15215.47	1041.47
	700	14	15	7	826.93	15917.52	1212.57

♣ Memory allocations in CN are for full problem
♣ Sylvester-oriented method: overall Space and Time independence

The multiterm matrix equation problem

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

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

- Kronecker form and back on track
- 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 PDEs
- PDEs on polygonal domains, IGA, spectral methods, etc
- Space-time PDEs
- All-at-once PDE-constrained optimization problem
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"Ultraweak" variational formulations of the wave equation

$$\ddot{u}(t) + A\,u(t) = f(t) \text{ in } V',\ \ t \in I \text{ a.e.}, \qquad u(0) = u_0 \in H,\ \dot{u}(0) = u_1 \in V'.$$

initial state in, say, $L_2(\Omega)$, initial velocity in, say, $H^{-1}(\Omega)$ (very low regularity)
$\Rightarrow$ weakly smooth solution

$$b(u_\delta, v_\delta) = g(v_\delta) \quad \forall v_\delta \in \mathbb{V}_\delta$$

with

$$b(u_\delta, v_\delta) := (u_\delta, \ddot{v}_\delta + Av_\delta)_{\mathcal{H}}, \qquad g(v_\delta) := (f_\delta, v_\delta)_{\mathcal{H}} + \langle u_1, v_\delta(0)\rangle - (u_0, \dot{v}(0))_H,$$

* Test space $\mathbb{V}_\delta$: proper piecewise quadratic splines in time and conformal (e.g. piecewise quadratic) finite elements in space,

* Trial space $\mathbb{U}_\delta$: adjoint operator $B^* = \partial_{tt} + A$ applied to test basis functions

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The resulting linear system

In the optimal inf-sup case, $\mathbb{B}_\delta = \boldsymbol{Q}_{\Delta t} \otimes \boldsymbol{M}_h + \boldsymbol{N}_{\Delta t} \otimes \boldsymbol{N}_h^\top + \boldsymbol{N}_{\Delta t}^\top \otimes \boldsymbol{N}_h + \boldsymbol{M}_{\Delta t} \otimes \boldsymbol{Q}_h$,

$$\mathbb{B}_\delta \boldsymbol{u}_\delta = \boldsymbol{g}_\delta \qquad \mathbb{B}_\delta \text{ spd for } A = -\Delta$$

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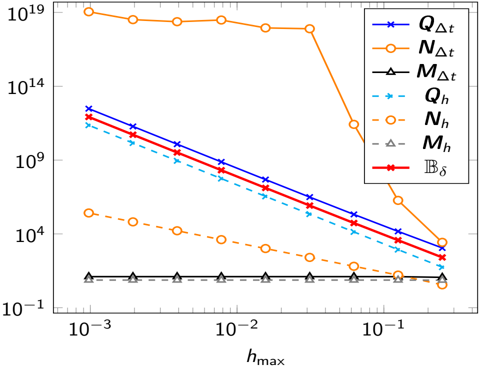

The resulting linear system

For $\mathbb{B}_\delta = \boldsymbol{Q}_{\Delta t} \otimes \boldsymbol{M}_h + (\boldsymbol{N}_{\Delta t} + \boldsymbol{N}_{\Delta t}^\top) \otimes \boldsymbol{N}_h^\top + \boldsymbol{M}_{\Delta t} \otimes \boldsymbol{Q}_h$,

$$\mathbb{B}_\delta \boldsymbol{u}_\delta = \boldsymbol{g}_\delta \qquad (*)$$

- Structure-aware Preconditioned "matrix-oriented" Conjugate gradients
  - Robust preconditioning $\mathbb{K}_\delta^\top \mathbb{M}_\delta^{-1} \mathbb{K}_\delta$ ($\mathbb{M}_\delta := \boldsymbol{M}_{\Delta t} \otimes \boldsymbol{M}_h$ and $\mathbb{K}_\delta := \boldsymbol{N}_{\Delta t} \otimes \boldsymbol{M}_h + \boldsymbol{M}_{\Delta t} \otimes \boldsymbol{N}_h$)
  - (cheaper) Sylvester preconditioning $\mathbb{P} = \boldsymbol{Q}_{\Delta t} \otimes \boldsymbol{M}_h + \boldsymbol{M}_{\Delta t} \otimes \boldsymbol{Q}_h$

- Galerkin method

  Transform $(*)$ into linear multiterm matrix equation:

$$\boldsymbol{M}_h \boldsymbol{U} \boldsymbol{Q}_{\Delta t}^\top + \boldsymbol{N}_h^\top \boldsymbol{U}(\boldsymbol{N}_{\Delta t}^\top + \boldsymbol{N}_{\Delta t}) + \boldsymbol{Q}_h \boldsymbol{U} \boldsymbol{M}_{\Delta t} = \boldsymbol{G}, \qquad \boldsymbol{G} = \boldsymbol{G}_1 \boldsymbol{G}_2^\top$$

  Approximate $\boldsymbol{U}$ as $\boldsymbol{U}_k = \boldsymbol{V}_k \boldsymbol{Y}_k \boldsymbol{W}_k^\top$ of low rank:

  i) Properly chose $\boldsymbol{V}_k, \boldsymbol{W}_k$

  ii) Impose Galerkin orthogonality of residual wrto $\boldsymbol{W}_k \otimes \boldsymbol{V}_k$

  This gives

$$(\boldsymbol{V}_k^\top \boldsymbol{M}_h \boldsymbol{V}_k)\boldsymbol{Y}_k(\boldsymbol{W}_k^\top \boldsymbol{Q}_{\Delta t}^\top \boldsymbol{W}_k) + (\boldsymbol{V}_k^\top \boldsymbol{N}_h^\top \boldsymbol{V}_k)\boldsymbol{Y}_k(\boldsymbol{W}_k^\top(\boldsymbol{N}_{\Delta t}^\top + \boldsymbol{N}_{\Delta t})\boldsymbol{W}_k) + (\boldsymbol{V}_k^\top \boldsymbol{Q}_h \boldsymbol{V}_k)\boldsymbol{Y}_k(\boldsymbol{W}_k^\top \boldsymbol{M}_{\Delta t} \boldsymbol{W}_k) = (\boldsymbol{V}_k^\top \boldsymbol{G}_1)(\boldsymbol{G}_2^\top \boldsymbol{W}_k).$$

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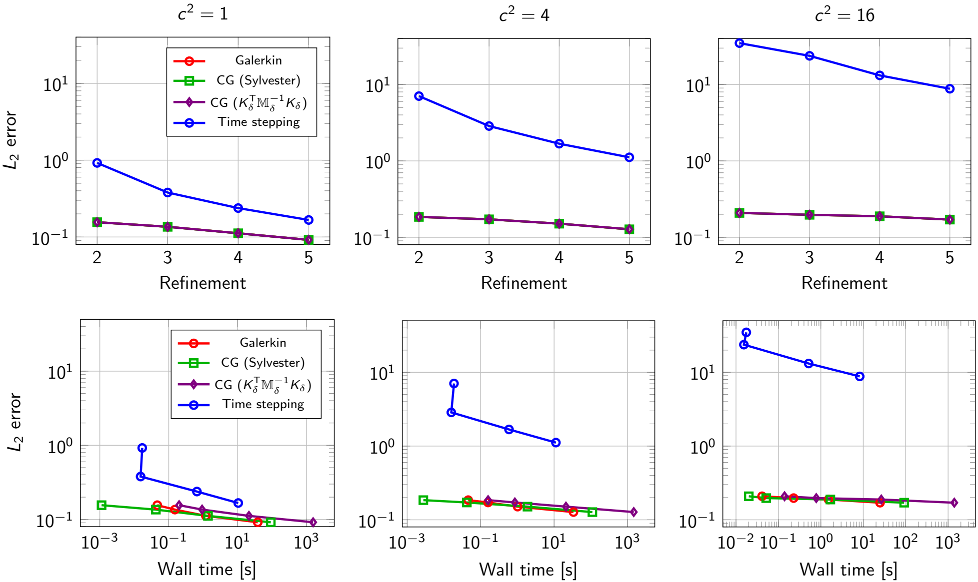
A numerical example. Discontinuous solution.

$A = -c^2\Delta$ (c wave speed), $H = L_2(\Omega)$, $\Omega = (0,1)^3$, $V = H_0^1(\Omega)$
$u_0 = \mathbf{1}_{r<\sqrt{2}/5}$



PDE-Constrained optimization problems

Functional to be minimized:

$$J(y,u) = \frac{1}{2}\int_0^T \int_{\Omega_1} (y-\hat{y})^2 \mathrm{dxdt} + \frac{\beta}{2}\int_0^T \int_{\Omega_u} u^2 \mathrm{dxdt}$$

⋆ y: is the state, $\hat{y}$ is the desired state given on a subset Ω_1 of Ω,
⋆ u is the control on a subset Ω_u of Ω,

(regularized by the control cost parameter β)

PDE constraining the functional $J(y,u)$ (Dirichlet b.c.): for instance,

$$\begin{aligned} \dot{y} - \Delta y &= u \quad \text{in} \quad \Omega_u, \\ \dot{y} - \Delta y &= 0 \quad \text{in} \quad \Omega \setminus \Omega_u, \\ y &= 0 \quad \text{on} \quad \partial\Omega. \end{aligned}$$

♣ All-at-once strategy (space, time, multipliers)

♣ Resulting matrix equation efficiently solved by using a tailored low-rank Galerkin method

(Alexandra Bünger, V.S., and Martin Stoll, 2021)

Further considerations

- More structure yields improved algorithmic design. For instance,

$$A\boldsymbol{X} + \boldsymbol{X}B + M_1\boldsymbol{X}M_2 = C$$

  with M_1, M_2 low rank
- *Truncated* versions of matrix-oriented Krylov methods have better chances
- 3D case leads to linear **tensor** equations: a new research area
- Matrix-oriented discretization methods for reaction-diffusion PDEs

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