

Matrix-oriented numerical methods for semilinear PDEs

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Joint works with

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The differential problem

We are interested in solving

$$u_t = \ell(u) + f(u, t), \quad u = u(x, y, t) \quad \text{with } (x, y) \in \Omega \subset \mathbb{R}^2, t \in \mathcal{T}$$

with given initial conditions $u(x, y, 0) = u_0(x, y)$ and proper b.c.

- ▶ ℓ linear in u (typically 2nd order diff operator in space, w/separable coeffs)
- ▶ f nonlinear function in u

Discretization: use tensor bases
(finite differences, conformal mappings, IGA, spectral methods, etc.)

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The matrix differential problem. 1

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Linear operator:

$$\boxed{\ell(u) = \Delta u}$$

Standard (vector) discretization in space, $n_x \times n_y$ grid:

- ▶ $\Delta u \Rightarrow \mathcal{A}u \quad \mathcal{A} \in \mathbb{R}^{n_x n_y \times n_x n_y}$
- ▶ $f(u, t) \Rightarrow \mathbf{f}(u, t) \quad (n_x n_y \text{ components, evaluated component-wise})$

with lexicographic ordering of the rectangle nodes

Matrix-oriented discretization in space:

- ▶ $\Delta u \Rightarrow AU + UB, \quad A \in \mathbb{R}^{n_x \times n_x}, B \in \mathbb{R}^{n_y \times n_y}, (U)_{ij} \approx u(x_i, y_j)$
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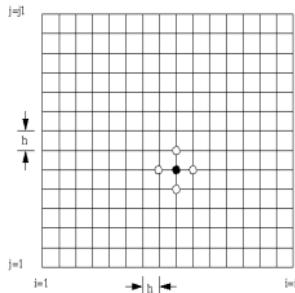
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Matrix-oriented discretization in space:

- ▶ $\Delta u \Rightarrow A\mathbf{U} + \mathbf{U}B, \quad A \in \mathbb{R}^{n_y \times n_x}, B \in \mathbb{R}^{n_y \times n_y}, (\mathbf{U})_{ij} \approx u(x_i, y_j)$
- ▶ $f(u, t) \Rightarrow \mathcal{F}(\mathbf{U}, t) \quad (n_x \times n_y, \text{ evaluated component-wise})$

Reminder: matrix formulation of tensor discretization



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

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

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

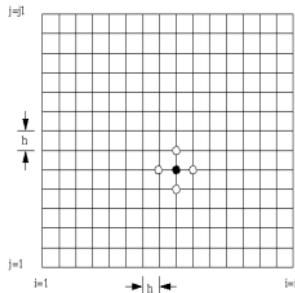
Let $T = \frac{1}{h^2}\text{tridiag}(-1, 2, -1)$. Collecting all nodes together,

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

Therefore, directly from the grid,

$$-u_{xx} - u_{yy} \quad \Rightarrow \quad TU + UT + b.c.$$

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The matrix differential equation

$$\dot{\boldsymbol{U}}(t) = \boldsymbol{A}\boldsymbol{U}(t) + \boldsymbol{U}(t)\boldsymbol{B} + \mathcal{F}(\boldsymbol{U}, t), \quad \boldsymbol{U}(0) = \boldsymbol{U}_0$$

Computational strategies. Time stepping methods:

- ▶ **Small scale:** matrix-oriented IMEX methods, exponential integrators
- ▶ **Large scale:** In sequence:
 1. Order reduction procedure (\Rightarrow POD-type)
 2. Feasible handling of nonlinear term $\mathcal{F}(\boldsymbol{U}, t)$ (\Rightarrow matrix DEIM)
 3. Time stepping of reduced problem

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- ▶ Problem is **stiff**
 - ▶ Use appropriate time discretizations
 - ▶ Time stepping constraints
- ▶ Possibly long time period (e.g., for pattern detection), with occurrence of transient unstable phase
- ▶ Phenomenon sets in only if domain is well represented

$$\dot{\mathbf{U}}(t) = A\mathbf{U}(t) + \mathbf{U}(t)B + \mathcal{F}(\mathbf{U}, t), \quad \mathbf{U}(0) = \mathbf{U}_0$$

Time stepping Matrix-oriented methods

IMEX methods

1. First order Euler: $\mathbf{u}_{n+1} - \mathbf{u}_n = h_t(\mathcal{A}\mathbf{u}_{n+1} + f(\mathbf{u}_n))$ so that

$$(I - h_t\mathcal{A})\mathbf{u}_{n+1} = \mathbf{u}_n + h_t f(\mathbf{u}_n), \quad n = 0, \dots, N_t - 1$$

Matrix-oriented form: $U_{n+1} - U_n = h_t(AU_{n+1} + U_{n+1}B) + h_tF(U_n)$,
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$$3\mathbf{u}_{n+2} - 4\mathbf{u}_{n+1} + \mathbf{u}_n = 2h_t\mathcal{A}\mathbf{u}_{n+2} + 2h_t(2f(\mathbf{u}_{n+1}) - f(\mathbf{u}_n)), \quad n = 0, 1, \dots, N_t$$

Matrix-oriented form: for $n = 0, \dots, N_t - 2$,

$$(3I - 2h_t\mathcal{A})U_{n+2} + U_{n+2}(-2h_t B) = 4U_{n+1} - U_n + 2h_t(2F(U_{n+1}) - F(U_n))$$

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Exponential integrator

Exponential first order Euler method:

$$\boxed{\mathbf{u}_{n+1} = e^{h_t \mathcal{A}} \mathbf{u}_n + h_t \varphi_1(h_t \mathcal{A}) f(\mathbf{u}_n)}$$

$e^{h_t \mathcal{A}}$: matrix exponential, $\varphi_1(z) = (e^z - 1)/z$ first “phi” function

That is,

$$\mathbf{u}_{n+1} = e^{h_t \mathcal{A}} \mathbf{u}_n + h_t \mathbf{v}_n, \quad \text{where } \mathcal{A} \mathbf{v}_n = e^{h_t \mathcal{A}} f(\mathbf{u}_n) - f(\mathbf{u}_n) \quad n = 0, \dots, N_t - 1.$$

Matrix-oriented form: since $e^{h_t \mathcal{A}} \mathbf{u} = \left(e^{h_t B^\top} \otimes e^{h_t A} \right) \mathbf{u} = \text{vec}(e^{h_t A} \mathbf{U} e^{h_t B})$

1. Compute $E_1 = e^{h_t A}$, $E_2 = e^{h_t B^\top}$

2. For each n

Solve $A \mathbf{V}_n + \mathbf{V}_n B = E_1 F(\mathbf{U}_n) E_2^\top - F(\mathbf{U}_n)$

Compute $\mathbf{U}_{n+1} = E_1 \mathbf{U}_n E_2^\top + h_t \mathbf{V}_n$

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Time stepping Matrix-oriented methods

Computational issues:

- ▶ Dimensions of A, B very modest
 - ▶ A, B quasi-symmetric (non-symmetry due to bc's)
 - ▶ A, B do not depend on time step
- ♣ Matrix-oriented form all in spectral space (after eigenvector transformation)

Numerical properties:

Structural properties are preserved

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A numerical example of system of RD-PDEs

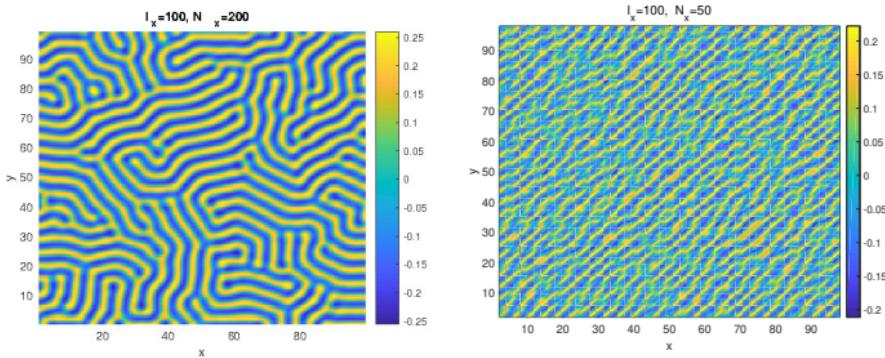
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Model describing an electrodeposition process for metal growth

$$f_1(u, v) = \rho (A_1(1 - v)u - A_2 u^3 - B(v - \alpha))$$

$$f_2(u, v) = \rho (C(1 + k_2 u)(1 - v)[1 - \gamma(1 - v)] - Dv(1 + k_3 u)(1 + \gamma v)))$$

Turing pattern



Joint work with M.C. D'Autilia & I. Sgura, Università di Lecce

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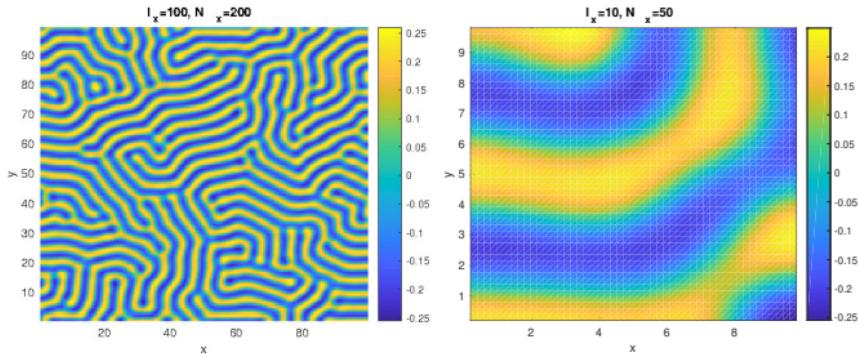
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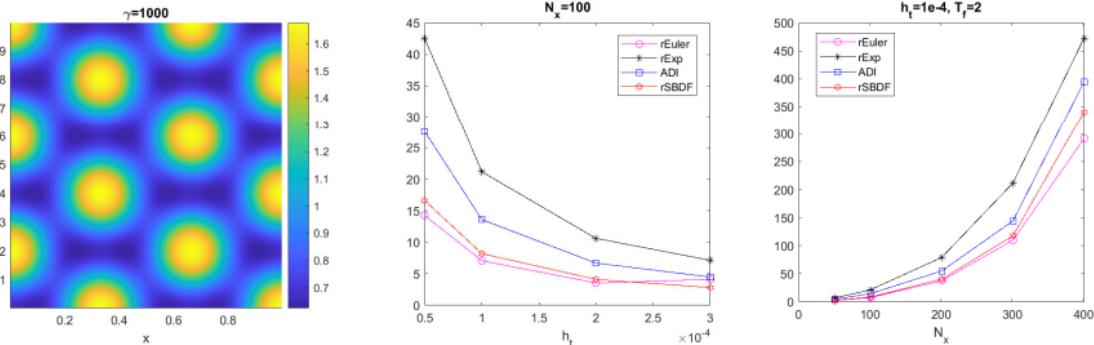
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Schnackenberg model

$$f_1(u, v) = \gamma(a - u + u^2v), \quad f_2(u, v) = \gamma(b - u^2v)$$



Left plot: Turing pattern solution for $\gamma = 1000$ ($N_x = 400$)

Center plot: CPU times (sec), $N_x = 100$ variation of h_t

Right plot: CPU times (sec), $h_t = 10^{-4}$, increasing values of $N_x = 50, 100, 200, 300, 400$

Large scale time stepping

$$\dot{\mathbf{U}}(t) = A\mathbf{U}(t) + \mathbf{U}(t)B + \mathcal{F}(\mathbf{U}, t), \quad \mathbf{U}(0) = \mathbf{U}_0$$

Approximation strategy: $\mathbf{U} \in \mathbb{R}^{n_x \times n_y}$,

$$\mathbf{U} \approx \mathbf{V}_{\ell,U} \mathbf{Y}_k(t) \mathbf{W}_{r,U}^\top = \boxed{} \quad \boxed{} \quad \boxed{}, \quad t \in [0, T_f]$$

♣ $\mathbf{V}_{\ell,U} \in \mathbb{R}^{n_x \times k_1}$, $\mathbf{W}_{r,U} \in \mathbb{R}^{n_y \times k_2}$ matrices¹ to be determined, independent of time

♣ Function $\mathbf{Y}_k(t)$ numerical solution to *reduced* semilinear problem:

$$\begin{aligned}\dot{\mathbf{Y}}_k(t) &= A_k \mathbf{Y}_k(t) + \mathbf{Y}_k(t) B_k + \widehat{\mathcal{F}_k}(\mathbf{Y}_k, t) \\ \mathbf{Y}_k(0) &= \mathbf{Y}_k^{(0)} := \mathbf{V}_{\ell,U}^\top \mathbf{U}_0 \mathbf{W}_{r,U}\end{aligned}$$

with $A_k = \mathbf{V}_{\ell,U}^\top A \mathbf{V}_{\ell,U}$, $B_k = \mathbf{W}_{r,U}^\top B \mathbf{W}_{r,U}$,

♣ $\widehat{\mathcal{F}_k}(\mathbf{Y}_k, t)$ is a matrix-oriented DEIM approximation to

$$\mathcal{F}_k(\mathbf{Y}_k, t) = \mathbf{V}_{\ell,U}^\top \mathcal{F}(\mathbf{V}_{\ell,U} \mathbf{Y}_k \mathbf{W}_{r,U}^\top, t) \mathbf{W}_{r,U}.$$

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Large scale time stepping: computational steps

- ▶ Determine $\mathbf{V}_{\ell,U} \in \mathbb{R}^{n_x \times k_1}$, $\mathbf{W}_{r,U} \in \mathbb{R}^{n_y \times k_2}$ via new two-sided matrix POD
(literature: parameter-based affine formulations/approximations (MDEIM, Manzoni et al), Jacobian approximation (Stefanescu et al 2017),...)
- ▶ Determine $\widehat{\mathcal{F}_k(\mathbf{Y}_k, t)}$ via new matrix-oriented DEIM
- ▶ Matrix-oriented time stepping for $\mathbf{Y}_k(t)$ (small scale)

for general vector treatment, Benner, Gugercin, Willcox, SIREV 2015

- ♣ Matrix formulation preserves structure, e.g., symmetry

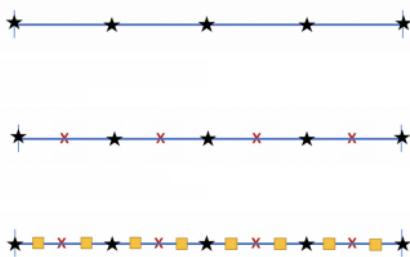
Two-sided matrix POD

POD: select an approximation basis using solution “snapshots” $\{\mathbf{U}(t_i)\}_{i=1}^{n_{\max}}$

Matrix-oriented POD: select **two** bases

Snapshot dynamic selection procedure

Refinements \mathcal{I}_j , $j = 1, \dots, 3$ of time interval



♣ In fact: Snapshots computed on the fly (SI Euler) while the time interval is spanned

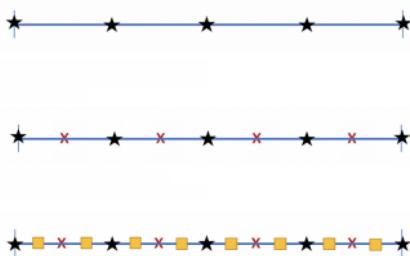
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Two-sided matrix POD

Given snapshots $\{\mathbf{U}(t_i)\}_{i=1}^{n_{\max}}$ and three refinements \mathcal{I}_j , $j = 1, \dots, 3$ of time interval

for each $j = 1, \dots, 3$,

for each $t_i \in \mathcal{I}_j$ such that \mathbf{U}_i is to be included

- Compute $[\mathbf{V}_i, \Sigma_i, \mathbf{W}_i] = \text{svds}(\mathbf{U}_i, \kappa)$
- Append $\tilde{\mathbf{V}}_i \leftarrow (\tilde{\mathbf{V}}_{i-1}, \mathbf{V}_i)$, $\tilde{\mathbf{W}}_i \leftarrow (\tilde{\mathbf{W}}_{i-1}, \mathbf{W}_i)$, $\tilde{\Sigma}_i \leftarrow \text{blkdiag}(\tilde{\Sigma}_{i-1}, \Sigma_i)$
- Decreasingly order the entries of (diagonal) $\tilde{\Sigma}_i$ and keep the first κ
- Order $\tilde{\mathbf{V}}_i$ and $\tilde{\mathbf{W}}_i$ accordingly and keep the first κ vectors of each

Check if next refinement is needed

Matrix-oriented DEIM approximation of nonlinear function

Matrix-oriented POD: Given snapshots $\{\mathcal{F}(t_j)\}_{j=1}^{n_s}$ use dynamic selection to generate $\mathbf{V}_{\ell,\mathcal{F}} \in \mathbb{R}^{n \times p_1}$ such that

$$\mathcal{F}(t) \approx \mathbf{V}_{\ell,\mathcal{F}} \mathbf{C}(t) \mathbf{W}_{r,\mathcal{F}}^\top$$

with $\mathbf{C}(t)$ to be determined.

DEIM strategy, in a two-sided context (2S-DEIM):

$$\mathbf{V}_{\ell,\mathcal{F}} \mathbf{C}(t) \mathbf{W}_{r,\mathcal{F}}^\top = \mathcal{F}(t)$$

1. Select independent rows of $\mathbf{V}_{\ell,\mathcal{F}}$ and $\mathbf{W}_{r,\mathcal{F}}$ (via reduction indices)

$$\mathbf{P}_{\ell,\mathcal{F}}^\top \mathbf{V}_{\ell,\mathcal{F}} \mathbf{C}(t) \mathbf{W}_{r,\mathcal{F}}^\top \mathbf{P}_{r,\mathcal{F}} = \mathbf{P}_{\ell,\mathcal{F}}^\top \mathcal{F}(t) \mathbf{P}_{r,\mathcal{F}},$$

Solve for $\mathbf{C}(t)$

2. Project onto U -spaces: (element-wise eval of \mathcal{F})

$$\begin{aligned}\mathcal{F}_k(\mathbf{Y}_k, t) &\approx \mathbf{V}_{\ell,U}^\top \mathbf{V}_{\ell,\mathcal{F}} (\mathbf{P}_{\ell,\mathcal{F}}^\top \mathbf{V}_{\ell,\mathcal{F}})^{-1} \mathbf{P}_{\ell,\mathcal{F}}^\top \mathcal{F}(\mathbf{V}_{\ell,U} \mathbf{Y}_k(t) \mathbf{W}_{r,U}^\top, t) \mathbf{P}_{r,\mathcal{F}} (\mathbf{W}_{r,\mathcal{F}}^\top \mathbf{P}_{r,\mathcal{F}})^{-1} \mathbf{W}_{r,\mathcal{F}}^\top \mathbf{W}_{r,U} \\ &= \mathbf{V}_{\ell,U}^\top \mathbf{V}_{\ell,\mathcal{F}} (\mathbf{P}_{\ell,\mathcal{F}}^\top \mathbf{V}_{\ell,\mathcal{F}})^{-1} \mathcal{F}(\mathbf{P}_{\ell,\mathcal{F}}^\top \mathbf{V}_{\ell,U} \mathbf{Y}_k(t) \mathbf{W}_{r,U}^\top \mathbf{P}_{r,\mathcal{F}}, t) (\mathbf{W}_{r,\mathcal{F}}^\top \mathbf{P}_{r,\mathcal{F}})^{-1} \mathbf{W}_{r,\mathcal{F}}^\top \mathbf{W}_{r,U} \\ &=: \widehat{\mathcal{F}_k(\mathbf{Y}_k, t)}\end{aligned}$$

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Algorithm 2S-POD-DEIM

INPUT: n_{max} , κ , and τ , n_t , $\{t_i\}$, $i = 0, \dots, n_t$

OUTPUT: $V_{\ell,U}$, $W_{r,U}$ and $Y_k^{(i)}$, $i = 0, \dots, n_t$ (for $V_{\ell,U} Y_k^{(i)} W_{r,U}^\top \approx U(t_i)$)

Offline:

1. Determine $V_{\ell,U}$, $W_{r,U}$ for $\{U\}_{i=1}^{n_{max}}$ and $V_{\ell,\mathcal{F}}$, $W_{r,\mathcal{F}}$ for $\{\mathcal{F}\}_{i=1}^{n_{max}}$ via dynamic procedure
2. Compute $Y_k^{(0)} = V_{\ell,U}^\top U_0 W_{r,U}$, $A_k = V_{\ell,U}^\top A V_{\ell,U}$, $B_k = W_{r,U}^\top B W_{r,U}$
3. Determine $P_{\ell,\mathcal{F}}$, $P_{r,\mathcal{F}}$ using 2S-DEIM
4. Compute $V_{\ell,U}^\top V_{\ell,\mathcal{F}} (P_{\ell,\mathcal{F}}^\top V_{\ell,\mathcal{F}})^{-1}$, $(W_{r,\mathcal{F}}^\top P_{r,\mathcal{F}})^{-1} W_{r,\mathcal{F}}^\top W_{r,U}$, $P_{\ell,\mathcal{F}}^\top V_{\ell,U}$ and $W_{r,U}^\top P_{r,\mathcal{F}}$

Online:

For each $i = 1, \dots, n_t$

- (i) Evaluate $f(Y_k^{(i-1)}) := \overbrace{\mathcal{F}_k(Y_k^{(i-1)}, t_{i-1})}^{\text{Matrix exponential integrator}}$
- (ii) Matrix exponential integrator: solve the matrix equation

$$A_k \Phi + \Phi B_k = e^{hA_k} f(Y_k^{(i-1)}) e^{hB_k} - f(Y_k^{(i-1)})$$

and compute

$$Y_k^{(i)} = e^{hA_k} Y_k^{(i-1)} e^{hB_k} + h \Phi^{(i-1)}$$

A numerical example, the 2D Allen-Cahn equation

$$u_t = \epsilon_1 \Delta u - \frac{1}{\epsilon_2^2} (u^3 - u), \quad \Omega = [a, b] \times [a, b], \quad t \in [0, T_f], \quad u(x, y, 0) = u_0$$

EXAMPLE AC1

([Song, Jian, Li, 2016])

$$\epsilon_1 = 10^{-2}, \quad \epsilon_2 = 1, \quad a = 0, \quad b = 2\pi, \quad T_f = 5$$

$u_0 = 0.05 \sin x \cos y$ and zero Dirichlet b.c.

EXAMPLE AC2

([Evans, Spruck, 1991, Ju, Zhang, Zhu, Du, 2015])

$$\epsilon_1 = 1, \quad \epsilon_2 \in \{0.01, 0.02, 0.04\}, \quad a = -0.5, \quad b = 0.5, \quad T_f = 0.075$$

$u_0 = \tanh \left(\frac{0.4 - \sqrt{x^2 + y^2}}{\sqrt{2}\epsilon_2} \right)$ and periodic b.c.

Problem dimension: $n_x = n_y \equiv n = 1000$

Numerical results. 1

PB.	n_{\max}/κ	Ξ	ALGORITHM	\mathcal{I}	REFIN	n_s	ν_ℓ/ν_r
AC 1	40/50	\mathcal{U}	DYNAMIC	1	8	9/2	
			VECTOR	2	9	9	
		\mathcal{F}	DYNAMIC	1	7	10/3	
			VECTOR	2	9	9	
AC 2 $\epsilon_2 = 0.04$	400/50	\mathcal{U}	DYNAMIC	1	2	15/15	
			VECTOR	2	25	25	
		\mathcal{F}	DYNAMIC	1	3	27/27	
			VECTOR	2	40	40	
AC 2 $\epsilon_2 = 0.02$	1200/70	\mathcal{U}	DYNAMIC	1	3	30/30	
			VECTOR	1	28	28	
		\mathcal{F}	DYNAMIC	1	4	39/39	
			VECTOR	2	53	53	
AC 2 $\epsilon_2 = 0.01$	5000/150	\mathcal{U}	DYNAMIC	1	3	62/62	
			VECTOR	1	43	43	
		\mathcal{F}	DYNAMIC	1	5	73/73	
			VECTOR	2	92	92	

n_{\max} : max # snapshots κ : max allowed POD dim

n_s : employed # snapshots ν_ℓ, ν_r : dim two POD bases

Numerical results. 2

PB.	METHOD	OFFLINE			ONLINE		REL. ERROR
		BASIS TIME	DEIM TIME	MEMORY	TIME (n_t)	MEMORY	
AC 1	DYNAMIC	1.8	0.001	$200n$	0.009 (300)	$24n$	$1 \cdot 10^{-4}$
	VECTOR	0.6	0.228	$18n^2$	0.010 (300)	$18n^2$	$1 \cdot 10^{-4}$
AC 2 0.04	DYNAMIC	0.8	0.005	$200n$	0.010 (300)	$84n$	$3 \cdot 10^{-4}$
	VECTOR	8.4	3.745	$65n^2$	0.020 (300)	$65n^2$	$2 \cdot 10^{-4}$
AC 2 0.02	DYNAMIC	1.8	0.004	$280n$	0.140 (1000)	$138n$	$2 \cdot 10^{-4}$
	VECTOR	14.6	5.273	$81n^2$	0.120 (1000)	$81n^2$	$3 \cdot 10^{-5}$
AC 2 0.01	DYNAMIC	5.3	0.008	$600n$	0.820 (2000)	$270n$	$5 \cdot 10^{-4}$
	VECTOR	46.2	13.820	$135n^2$	0.420 (2000)	$135n^2$	$2 \cdot 10^{-4}$

Conclusions and outlook

- ▶ Two-sided matrix-oriented approximation $\mathbf{V}_{\ell,U} \mathbf{Y}_k(t) \mathbf{W}_{r,U}^\top$ is a feasible and effective technique (memory and CPU time saving, structure aware)
- ▶ Matrix approach enables combining POD-DEIM with robust exponential integrators
- ▶ 3D (tensor) version already available (G. Kirsten, arXiv 2103.04343 (2021))
- ▶ Multiparameter version can be foreseen

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- Gerhard Kirsten and V. Simoncini
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