Treatment of numerical instabilities due to advection-dominance in POD solution to advection-diffusion-reaction equations

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OUTLINE

1. Mathematical formulation of a stabilized **POD-ROM**: approximation of an IBVP for the *advection-diffusion-reaction equations*.
   - POD methodology + Streamline Derivative projection-based stabilization (**SD-POD-ROM**).
2. **A posteriori offline/online stabilization** for **POD-ROM** on *strongly advection-dominated problems*.
3. Application to numerical simulation of relevant test cases on relatively coarse grids:
   - *2D Rotating cylinder* ($\nu = 10^{-20}$);
   - *2D Traveling wave* ($\nu = 10^{-8}$).

Mathematical and variational formulation

- $\Omega \subset \mathbb{R}^d =$ bounded domain $(d = 2, 3)$.
- $\Gamma = \partial\Omega =$ Lipschitz boundary.

ADR Equations with homogeneous Dirichlet BCs:

Find $u : \Omega \times (0, T) \longrightarrow \mathbb{R}^d$ *s.t.:*

$$\left\{ \begin{array}{rcll} \partial_t u + \mathbf{b} \cdot \nabla u - \nu \Delta u + gu & = & f & \text{in } \Omega \times (0, T), \\ u & = & 0 & \text{on } \Gamma \times (0, T), \\ u(\mathbf{x}, 0) & = & u_0(\mathbf{x}) & \text{in } \Omega, \end{array} \right. \qquad (1)$$

- $X = H^1_0(\Omega)$ (Continuous solution space).

Variational Formulation: *Find* $u : (0, T) \longrightarrow X$ *s.t.*

$$\frac{d}{dt}(u, v) + (\mathbf{b} \cdot \nabla u, v) + \nu(\nabla u, \nabla v) + (g\, u, v) = (f, v) \quad \forall v \in X. \qquad (2)$$

Full Order Model (LPS-FEM)

FE approximation:

$$X_h \subset X \text{ suitable FE space.}$$

Standard Galerkin FEM: *Find* $u_h : (0,T) \longrightarrow X_h$ *s.t.*

$$\frac{d}{dt}(u_h, v_h) + (\mathbf{b}\cdot\nabla u_h, v_h) + \nu(\nabla u_h, \nabla v_h) + (g\, u_h, v_h) = (f, v_h) \quad \forall v_h \in X_h. \quad (3)$$

- Low diffusion coefficient: $\nu << 1$.
- **Standard Galerkin FEM** generally unstable.
- **Offline LPS by interpolation procedure**: offline control on the high frequencies component of the advection derivative.

T. Chacón et al., *A high order term-by-term stabilization solver for incompressible flow problems*, **IMAJNA**, (2013).

LPS by interpolation FEM

FE space:

$$X_h = P_m \cap X, \quad m \geq 2.$$

Definition [τ-scalar product and norm]

$$(\cdot,\cdot)_\tau : L^2(\Omega) \times L^2(\Omega) \to \mathbb{R}, \quad (v,w)_\tau = \sum_{K \in \mathcal{T}_h} \tau_K (v,w)_K,$$

$$\|v\|_\tau = (v,v)_\tau^{1/2}.$$

LPS by interpolation FEM: *Find $u_h : (0,T) \longrightarrow X_h$ s.t.*

$$\left\{ \begin{array}{l} \dfrac{d}{dt}(u_h, v_h) + (\mathbf{b}\cdot\nabla u_h, v_h) + (\pi_h'(\mathbf{b}\cdot\nabla u_h), \pi_h'(\mathbf{b}\cdot\nabla v_h))_\tau \\ + \quad \nu(\nabla u_h, \nabla v_h) + (g\, u_h, v_h) = (f, v_h) \quad \forall v_h \in X_h, \end{array} \right. \tag{4}$$

$\pi_h' = Id - \pi_h, \quad \pi_h : L^2(\Omega) \to D_h = P_{m-1} =$ Continuous "buffer" FE space.

- $\pi_h \equiv$ *Scott-Zhang-like interpolation operator*.

Reduced Order Model (SD-POD-ROM)

POD space:

$$X_r = \text{span}\{\varphi_1, \ldots, \varphi_r\} \subset X_h.$$

Standard Galerkin POD-ROM: *Find* $u_r(\mathbf{x}, t) = \sum_{i=1}^{r} a_i(t)\varphi_i(\mathbf{x})$ *s.t.*

$$\frac{d}{dt}(u_r, \varphi) + (\mathbf{b} \cdot \nabla u_r, \varphi) + \nu(\nabla u_r, \nabla \varphi) + (g\, u_r, \varphi) = (f, \varphi) \quad \forall \varphi \in X_r. \quad (5)$$

- Low diffusion coefficient: $\nu << 1$.
- **Standard Galerkin POD-ROM** generally unstable.
- **Online SD projection-based procedure**: online control on the high frequencies component of the advection derivative.

S. Rubino, *A streamline derivative POD-ROM for advection-diffusion-reaction equations*, **ESAIM: ProcS**, (2018).

SD projection-based POD-ROM

POD projection space:

$$\widehat{X}_r = \text{span}\left\{\widehat{\varphi}_1, \ldots, \widehat{\varphi}_r\right\},$$

$\{\widehat{\varphi}_i\}_{i=1}^r :=$ POD modes associated to $\widehat{K} =$ **Advection correlation matrix** s.t.

$$\widehat{K}_{mn} = \frac{1}{N+1}\left(\mathbf{b}\cdot\nabla u_h(t_n), \mathbf{b}\cdot\nabla u_h(t_m)\right), \quad \text{for } m,n = 0,\ldots,N. \tag{6}$$

Definition [L^2-orthogonal projection on $\widehat{X}_r$]

$$P_r : L^2(\Omega) \longrightarrow \widehat{X}_r \text{ s.t. } (u - P_r u, \widehat{\varphi}) = 0 \quad \forall \widehat{\varphi} \in \widehat{X}_r. \tag{7}$$

$P_r' = Id - P_r =$ "fluctuation" operator.

SD-POD-ROM: *Find $u_r \in X_r$ s.t.*

$$\left\{\begin{array}{rl} & \dfrac{d}{dt}(u_r,\varphi) + (\mathbf{b}\cdot\nabla u_r,\varphi) + (P_r'(\mathbf{b}\cdot\nabla u_r), P_r'(\mathbf{b}\cdot\nabla\varphi))_\tau \\ + & \nu(\nabla u_r,\nabla\varphi) + (g\, u_r,\varphi) = (f,\varphi) \quad \forall\varphi\in X_r. \end{array}\right. \tag{8}$$

A posteriori stabilization

General framework:

(i) Elliptic variational problem:

$$\text{Find } x \in X \text{ s.t. } b(x, w) = l(w) = \langle f, w \rangle \quad \forall w \in X. \tag{9}$$

(ii) Galerkin method:

$$\text{Find } x_i \in X_i \text{ s.t. } b(x_i, w_i) = l(w_i) \quad \forall w_i \in X_i \subset X, \quad i \in \mathcal{I}. \tag{10}$$

(iii) Space/solution decomposition: $X_i = Y_i \oplus Z_i \Rightarrow x_i = y_i + z_i$.

(iv) Static "condensation" operator: $\mathcal{R}_i : X' \mapsto Z_i$ s.t.

$$b(\mathcal{R}_i(\varphi), w_i) = \langle \varphi, w_i \rangle \quad \forall w_i \in Z_i.$$

(v) "Condensed" variational formulation:

$$\underline{\text{Find } y_i \in Y_i \text{ s.t. } b_c(y_i, v_i) = l_c(v_i) \quad \forall v_i \in Y_i}, \tag{11}$$

$$b_c(y, v) = b(y, v) - b(\mathcal{R}_i(\mathcal{A}^* v), \mathcal{R}_i(\mathcal{A} y)), \quad l_c(v) = l(v) - b(\mathcal{R}_i(\mathcal{A}^* v), \mathcal{R}_i(f)),$$
$$\mathcal{A} : X \mapsto X' \text{ s.t. } \langle \mathcal{A} v, w \rangle = b(v, w) \quad \forall w \in X.$$

A posteriori stabilization

Definition [Saturation property]

The family of finite-dimensional spaces $\{(Y_i, Z_i)\}_{i\in\mathcal{I}}$ is called to satisfy the **saturation property** if there exists a constant $\alpha > 0$ s.t.

$$\|y_i\|_X + \|z_i\|_X \leq \alpha \|x_i + y_i\|_X \quad \forall y_i \in Y_i,\ z_i \in Z_i, \quad \forall i \in \mathcal{I}.$$

Remark [cf. Chacón&Domínguez, **CMAME**, (2000)]

The **saturation property** is equivalent to the existence of a constant $\beta > 0$ s.t.

$$|(y_i, z_i)_X| \leq (1-\beta)\,\|y_i\|_X \|z_i\|_X, \quad \forall y_i \in Y_i,\ z_i \in Z_i. \quad \left[\beta = \frac{2}{\alpha^2}\right] \qquad (12)$$

$\Rightarrow$ The angle

$$\arccos\left(\sup_{y_i\in Y_i\setminus\{0\},\, z_i\in Z_i\setminus\{0\}} \frac{(y_i, z_i)_X}{\|y_i\|_X \|z_i\|_X}\right)$$

between spaces Y_i and Z_i is uniformly bounded from below by a positive angle.

A posteriori stabilization

Theorem [cf. Chacón&Domínguez, CMAME, (2000)]

Assume that the spaces Y_i and Z_i satisfy $Y_i \cap Z_i = \{0\}$. Then:

1. Let $x_i = y_i + z_i$ be the ! decomposition that x_i admits with $y_i \in Y_i$ and $z_i \in Z_i$. Then, x_i is the solution of the Galerkin method (10) *iff* y_i is the solution of the "condensed" variational formulation (11), and $z_i = \mathcal{R}_i(l - \mathcal{A}(y_i))$.
2. Assume, in addition, that the family of pairs of spaces $\{(Y_i, Z_i)\}_{i\in\mathcal{I}}$ satisfies the saturation property. Then, $\exists$ a constant $C > 0$ s.t.

$$\|y_i\|_X + \|z_i\|_X \leq C\,\|l\|_{X'}, \quad \|c_i\|_X \leq C\,\|l\|_{X'}, \tag{13}$$

where $c_i = \mathcal{R}_i(\mathcal{A}(y_i))$.

- Y_i: **Large scales (low frequency)** components of X_i;
- Z_i: **Small scales (high frequency)** components of X_i.

OFF-FE framework: $X_i \equiv X_h \Rightarrow Y_i \equiv X_{2h} \subset X_h$.

ON-POD framework: $X_i \equiv X_r \Rightarrow Y_i \equiv X_{r-R} \subset X_r$.

Space/time discretization and implementation

Space discretization: P_2 FE on realtively coarse uniform grids.

- $h >$ width internal layers.

OFF-ON Time discretization: backward Euler time stepping.

- $\Delta t = 10^{-3}$.

Stabilization coefficients:

Working expression [Asymptotic scaling arguments]

$$\tau_K = \left[c_1 \frac{\nu}{h_K^2} + c_2 \frac{\|\mathbf{b}\|_\infty}{h_K} + c_3 g \right]^{-1}.$$

Implementation:

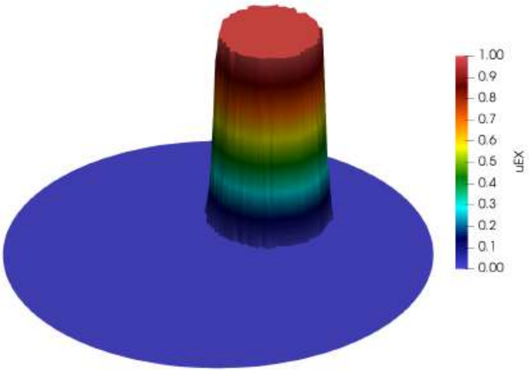
- **FreeFEM** - https://freefem.org/.

M. Azaïez et al., *A cure for instabilities due to advection-dominance in POD solution to advection-diffusion-reaction equations*, **JCP**, (2021).

2D Rotating cylinder

- Computational spatial domain: $\Omega = \{(x, y) \in \mathbb{R}^2 : x^2 + y^2 < 1\}$.
- Data: $\mathbf{b} = (-y, x)^{\mathrm{T}}$, $g = 0$, $f = 0$, $\nu = 10^{-20}$,

$$u_0 = 0.5 \left[\tanh \left(\frac{e^{-10[(x-0.3)^2+(y-0.3)^2-0.5]}}{10^{-3}} \right) + 1 \right].$$



2D Rotating cylinder

- **Initial condition**: Sharp internal layer of width $= 10^{-3}$;
- **Mesh size**: $h = 4.26 \cdot 10^{-2}$ (Under-resolved internal layer);
- **Diffusion coefficient**: Strongly advection-dominated problem $\nu = 10^{-20} \Rightarrow$ Offline/Online stabilization procedure.

Offline phase: **LPS by interpolation FEM** with or without *Offline* stabilizing post-processing.
Online phase: **SD POD-ROM** with or without *Online* stabilizing post-processing.

- **Quantity of interest**: *Measure for under- and overshoots*

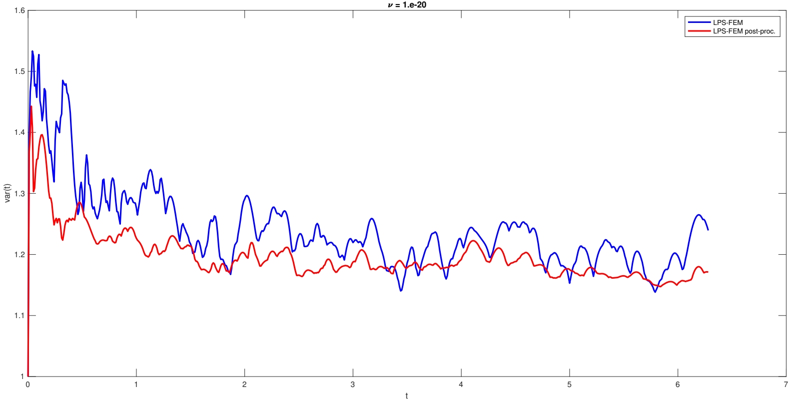
$$var(t) = \max_{(x,y)\in\Omega} u(x,y,t) - \min_{(x,y)\in\Omega} u(x,y,t). \quad [\text{opt} = 1]$$

2D Rotating cylinder - Short time behavior

Offline phase

- Time interval: $[0, T] = [0, 2\pi]$.

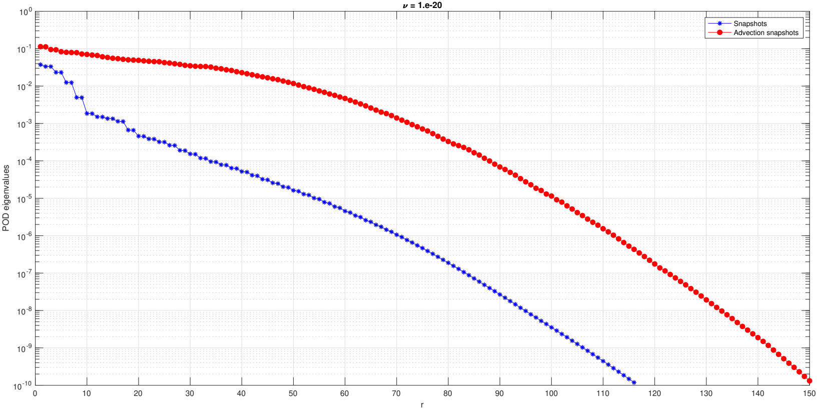
$$var_h(t) = \max_{(x,y)\in\Omega} u_h(x,y,t) - \min_{(x,y)\in\Omega} u_h(x,y,t).$$



2D Rotating cylinder - Short time behavior

Online phase

- Snapshots: Every 10^{th} LPS-FEM post-proc. sol. in $[0, T]$;
- POD modes generation: Method of snapshots in L^2.



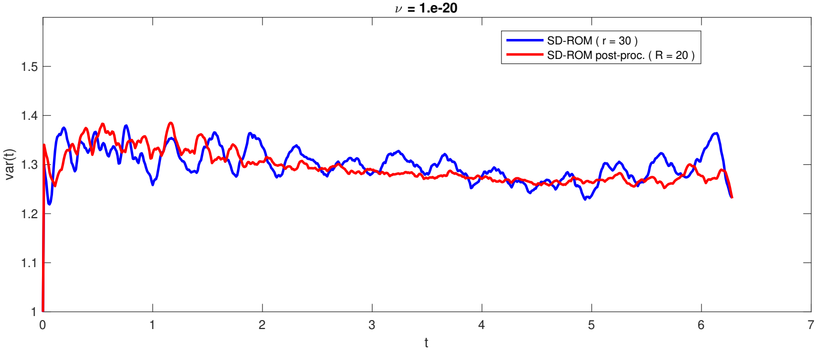
2D Rotating cylinder - Short time behavior

Online phase

- Time interval: $[0,\ T] = [0, 2\pi]$.

$$var_r(t) = \max_{(x,y)\in\Omega} u_r(x,y,t) - \min_{(x,y)\in\Omega} u_r(x,y,t).$$

Captured system's kinetic energy: $E_{kin} = 99.35\%$. $[r = 30]$



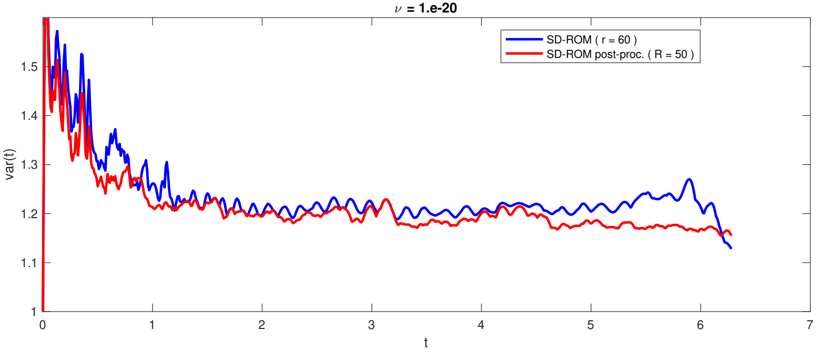
2D Rotating cylinder - Short time behavior

Online phase

- Time interval: $[0,\ T] = [0, 2\pi]$.

$$var_r(t) = \max_{(x,y)\in\Omega} u_r(x,y,t) - \min_{(x,y)\in\Omega} u_r(x,y,t).$$

Captured system's kinetic energy: $E_{kin} = 99.99\%$. $[r = 60]$



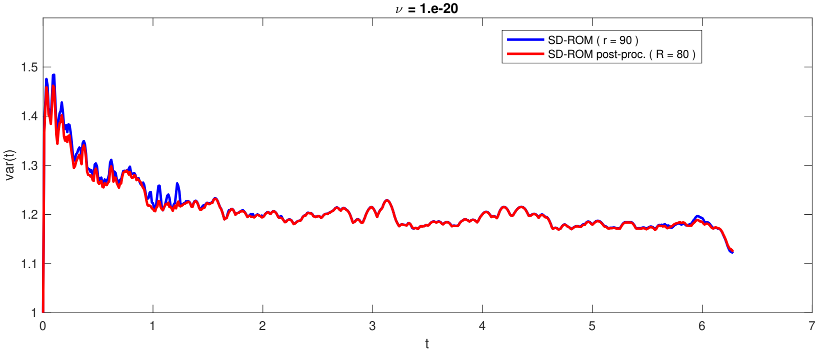
2D Rotating cylinder - Short time behavior

Online phase

- Time interval: $[0, T] = [0, 2\pi]$.

$$var_r(t) = \max_{(x,y)\in\Omega} u_r(x,y,t) - \min_{(x,y)\in\Omega} u_r(x,y,t).$$

Captured system's kinetic energy: $E_{kin} > 99.99\%$. $[r = 90]$



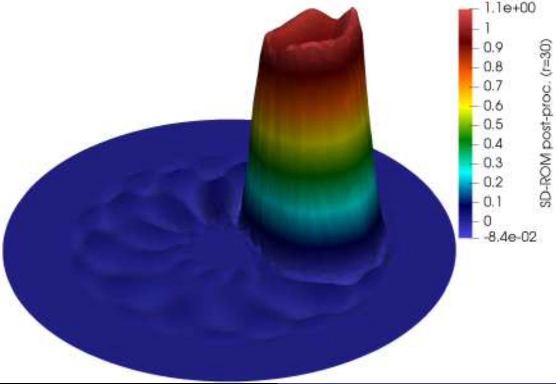
2D Rotating cylinder - Short time behavior

Online phase

- Time interval: $[0, T] = [0, 2\pi]$.

$u_r(t = T)$, **SD POD-ROM** with *Online* stabilizing post-processing.

Captured system's kinetic energy: $E_{kin} = 99.35\%$. $[r = 30]$



2D Rotating cylinder - Short time behavior

Online phase

- Time interval: $[0, T] = [0, 2\pi]$.

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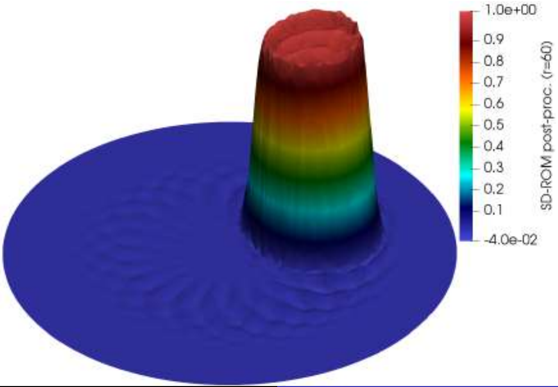


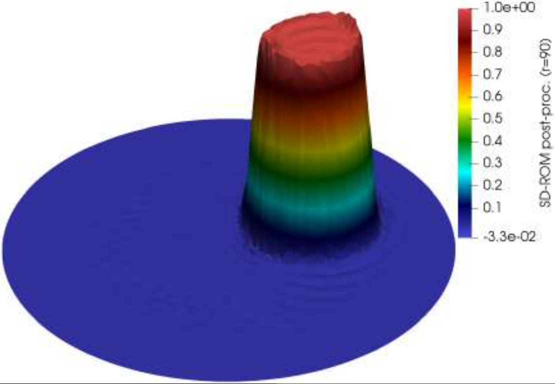
2D Rotating cylinder - Short time behavior

Online phase

- Time interval: $[0, T] = [0, 2\pi]$.

$u_r(t = T)$, **SD POD-ROM** with *Online* stabilizing post-processing.

Captured system's kinetic energy: $E_{kin} > 99.99\%$. $[r = 90]$

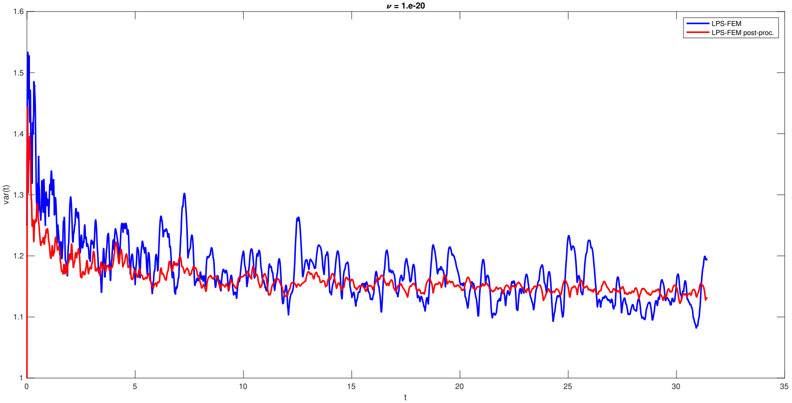


2D Rotating cylinder - Long time behavior

Offline phase

- Time interval: $[0, T] = [0, 10\pi]$.

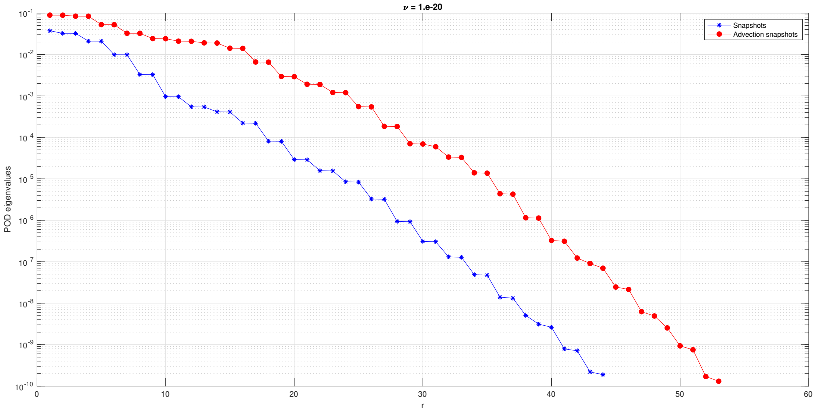
$$var_h(t) = \max_{(x,y)\in\Omega} u_h(x,y,t) - \min_{(x,y)\in\Omega} u_h(x,y,t).$$



2D Rotating cylinder - Long time behavior

Online phase

- Snapshots: Every 10^{th} LPS-FEM post-proc. sol. in $[4T/5, T]$;
- POD modes generation: Method of snapshots in L^2.



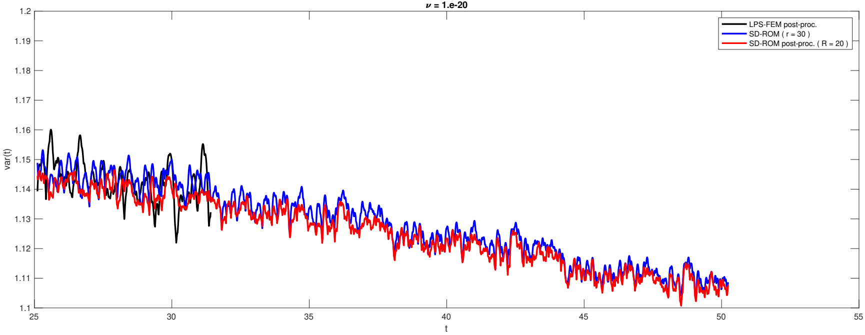
2D Rotating cylinder - Long time behavior

Online phase

- Time interval: $[8\pi, 16\pi]$ = 4 x POD basis time window.

$$var_r(t) = \max_{(x,y)\in\Omega} u_r(x,y,t) - \min_{(x,y)\in\Omega} u_r(x,y,t).$$

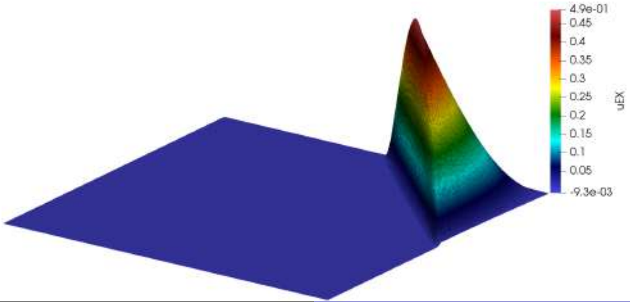
Captured system's kinetic energy: $E_{kin} > 99.99\%$. $[r = 30]$



2D Traveling wave

- Computational spatial domain: $\Omega = (0,1)^2$.
- Computational time interval: $[0, T] = [0, 1]$.
- Data: $\mathbf{b} = \left(\cos\frac{\pi}{3}, \sin\frac{\pi}{3}\right)^{\mathrm{T}}$, $g = 1$, $\nu = 10^{-8}$.
- Exact solution:

$$u(x,y,t) = 0.5\sin(\pi x)\sin(\pi y)\left[\tanh\left(\frac{x+y-t-0.5}{4\sqrt{\nu}}\right)+1\right].$$



2D Traveling wave

- **Exact solution**: Sharp internal layer of width $= \mathcal{O}(\sqrt{\nu})$;
- **Mesh size**: $h \approx 10^{-2}$ (Under-resolved internal layer);
- **Diffusion coefficient**: Strongly advection-dominated problem $\nu = 10^{-8} \Rightarrow$ Offline/Online stabilization procedure.

Offline phase: **LPS by interpolation FEM** with or without *Offline* stabilizing post-processing.

Online phase: **SD POD-ROM** with or without *Online* stabilizing post-processing.

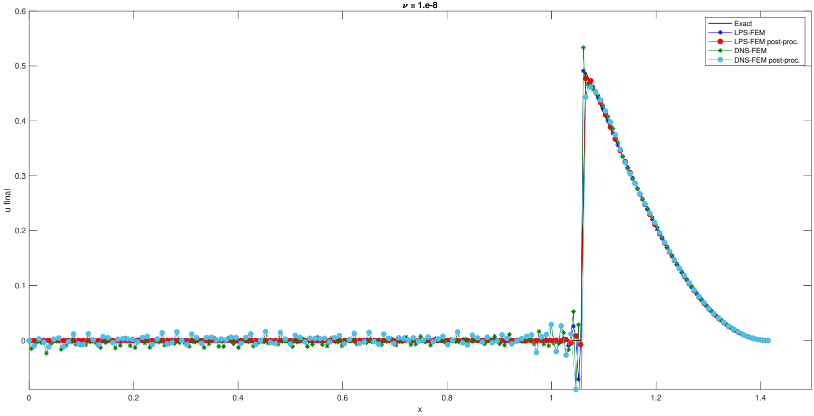
- **Quantity of interest**:
  Deviation for the final solution profile along the mean diagonal

$$e_0^{FOM/ROM} = \left[\frac{\int_0^{\sqrt{2}} \left| u_{ex}^{fin} - u_{h/r}^{fin} \right|^2}{\int_0^{\sqrt{2}} \left| u_{ex}^{fin} \right|^2} \right]^{1/2}.$$

2D Traveling wave

Offline phase

- Mesh size: $h = 9.43 \cdot 10^{-3}$;
- Time interval: $[0, T] = [0, 1]$.



2D Traveling wave

Offline phase

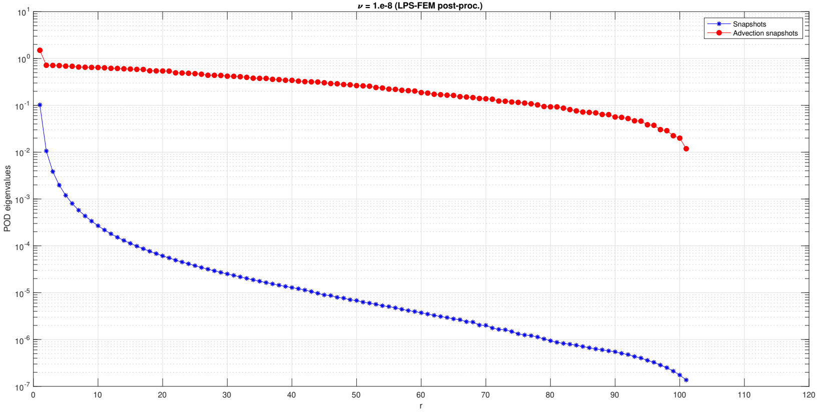
- Mesh size: $h = 9.43 \cdot 10^{-3}$;
- Time interval: $[0, T] = [0, 1]$.

Offline methods	e_0^{FOM}, $\nu = 10^{-8}$
DNS-FEM	0.1816
DNS-FEM post-proc.	0.1345
LPS-FEM	0.1247
LPS-FEM post-proc.	0.0393

2D Traveling wave

Online phase

- Snapshots: Every 10^{th} LPS-FEM post-proc. sol. in $[0, T]$;
- POD modes generation: Method of snapshots in L^2.

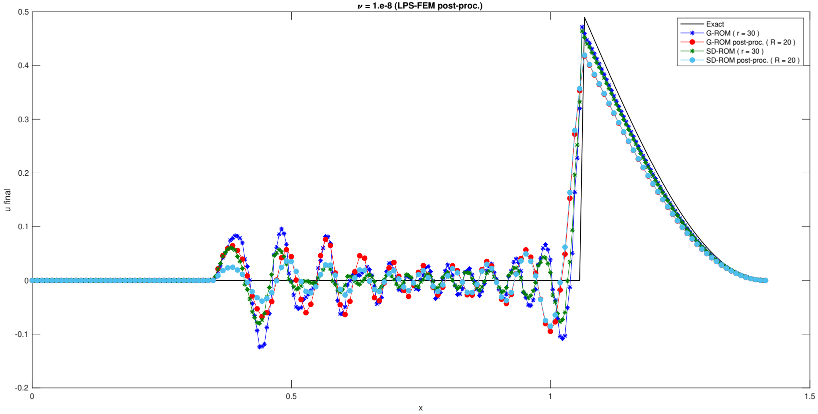


2D Traveling wave

Online phase

- Time interval: $[0, T] = [0, 1]$.

Captured system's kinetic energy: $E_{kin} = 99.71\%$. $[r = 30]$

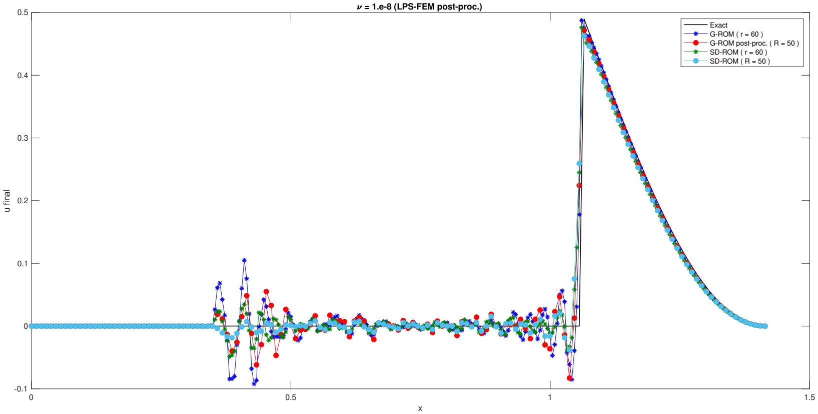


2D Traveling wave

Online phase

- Time interval: $[0, T] = [0, 1]$.

Captured system's kinetic energy: $E_{kin} = 99.96\%$. $[r = 60]$

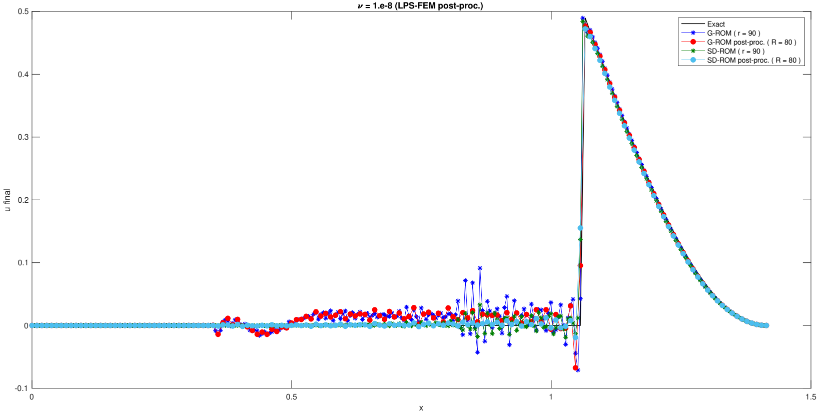


2D Traveling wave

Online phase

- Time interval: $[0, T] = [0, 1]$.

Captured system's kinetic energy: $E_{kin} > 99.99\%$. $[r = 90]$



2D Traveling wave

Online phase

- Time interval: $[0, T] = [0, 1]$.

$\nu = 10^{-8}$	$r = 30$	$r = 60$	$r = 90$
Captured system's $E_{kin}(\%)$	99.71	99.96	> 99.99

$\nu = 10^{-8}$	e_0^{ROM}		
Online methods	$r = 30$	$r = 60$	$r = 90$
G-ROM	0.3733	0.1676	0.1224
G-ROM post-proc.	0.3086	0.1493	0.0884
SD-ROM	0.3417	0.1463	0.0675
SD-ROM post-proc.	0.2596	0.1449	0.0589

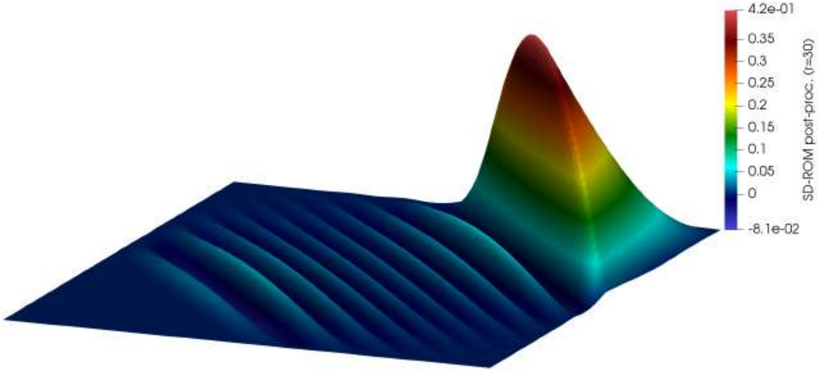
2D Traveling wave

Online phase

- Time interval: $[0, T] = [0, 1]$.

$u_r(t = T)$, **SD POD-ROM** with *Online* stabilizing post-processing.

Captured system's kinetic energy: $E_{kin} = 99.71\%$. $[r = 30]$



2D Traveling wave

Online phase

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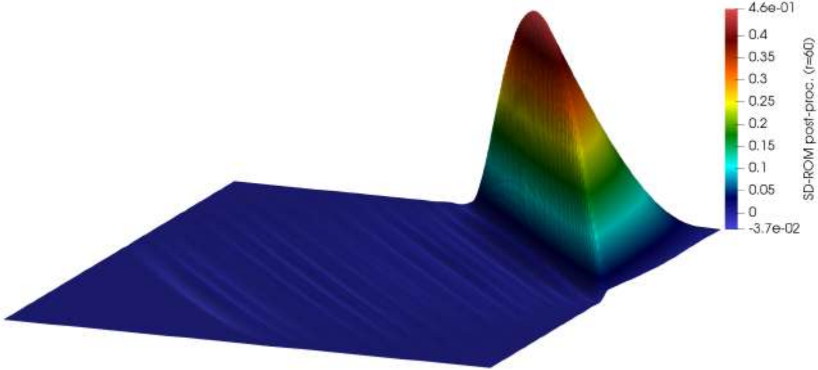


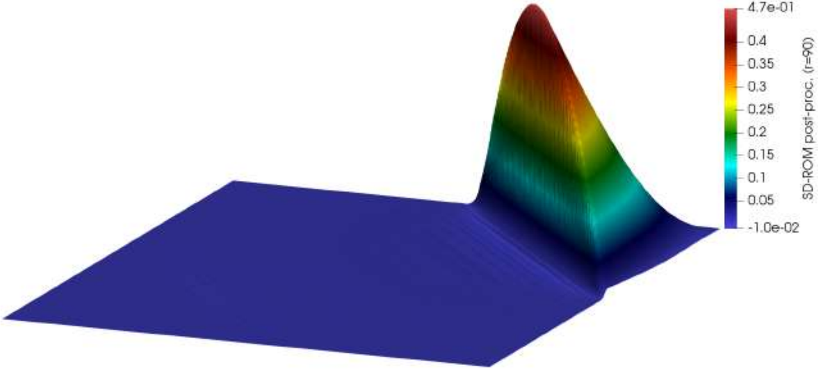
2D TRAVELING WAVE

Online phase

- Time interval: $[0, T] = [0, 1]$.

$u_r(t = T)$, **SD POD-ROM** with *Online* stabilizing post-processing.

Captured system's kinetic energy: $E_{kin} > 99.99\%$. $[r = 90]$



Conclusions

Stabilizing Post-Processing Stategy:

1. Accurate/Efficient for strongly advection-dominated regime.
2. Robust for long time integrations on quasi periodic systems.
3. Offline phase: Limit the influence of POD noisy modes online.
4. Online phase: Compute more stable and accurate solutions.

Work in Progress & Future Research Lines:

- Shock or discontinuity capturing method: Adaptation to **POD-ROM** framework?
- Similar numerical investigation for **NSE**. (*convection-dominated and turbulent flows*)

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Thank you for your kind attention!

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