



POD-DEIM based model order reduction for speed-up of flow parametric studies

M. Isoz^a

^a Institute of Thermomechanics of the Czech Academy of Sciences

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Introduction

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Original system

$$\dot{y} = Ay + f(t, y), \quad y(t) \in \mathbb{R}^m, \quad y(0) = y_0, \quad t \in [0, T],$$

$$\text{system matrix} \quad \dots \quad A \in \mathbb{R}^{m \times m},$$

$$\text{nonlinearities} \quad \dots \quad f(t, y) \in \mathbb{R}^m$$

Reduced-order system

$$\dot{\eta}^\ell = A^\ell \eta^\ell + f^\ell(t, \eta^\ell), \quad \eta^\ell(t) \in \mathbb{R}^\ell, \quad \eta^\ell(0) = \eta_0^\ell, \quad t \in [0, T],$$

$$\text{system matrix} \quad \dots \quad A^\ell \in \mathbb{R}^{\ell \times \ell},$$

$$\text{nonlinearities} \quad \dots \quad f^\ell(t, \eta^\ell) \in \mathbb{R}^\ell$$

$$\text{gain} \quad \dots \quad \ell \ll m$$



Proper orthogonal decomposition & Discrete empirical interpolation method

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Introduce the Galerkin ansatz and Fourier modes

- Prerequisites:

$$\dot{y} = Ay + f(t, y), \quad y(t) \in \mathbb{R}^m, \quad y(0) = y_0, \quad t \in [0, T]$$

$$y(t) \in V = \text{span}\{\psi_j\}_{j=1}^d \quad \forall t \in [0, T]$$

$\Psi = \{\psi_j\}_{j=1}^d$... orthonormal basis

$$y(t) = \sum_{j=1}^d \langle y(t), \psi_j \rangle_W \psi_j, \quad \forall t \in [0, T], \quad W \dots \text{appropriate weights}$$

- Ansatz for Galerkin projection, $\ell < d$

$$y^\ell(t) := \sum_{j=1}^{\ell} \langle y^\ell(t), \psi_j \rangle_W \psi_j, \quad \forall t \in [0, T], \quad \eta_j^\ell(t) := \langle y^\ell(t), \psi_j \rangle_W$$

- Put the above together, !! $\psi_j \in \mathbb{R}^m$, $j = 1, \dots, \ell$, $m > \ell$!!

$$\begin{aligned} \sum_{j=1}^{\ell} \dot{\eta}_j^\ell \psi_j &= \sum_{j=1}^{\ell} \eta_j^\ell A \psi_j + f(t, y^\ell(t)), \quad t \in (0, T) \\ y_0 &= \sum_{j=1}^{\ell} \eta_j^\ell(0) \psi_j \end{aligned}$$



Introduce the reduced-order model

- Assume, that the above holds after projection on $V^\ell = \text{span}\{\psi_j\}_{j=1}^\ell$, remember that $\langle \psi_j, \psi_i \rangle_W = \delta_{ij}$ and write,

$$\dot{\eta}_i^\ell = \sum_{j=1}^{\ell} \eta_j^\ell \langle A\psi_j, \psi_i \rangle_W + \langle f(t, y^\ell), \psi_i \rangle_W, \quad 1 \leq i \leq \ell \text{ and } t \in (0, T]$$

- Define the matrix $A^\ell = (a_{ij}^\ell) \in \mathbb{R}^{\ell \times \ell}$ with $a_{ij}^\ell = \langle A\psi_j, \psi_i \rangle_W$
- Define the vector valued mapping $\eta^\ell = (\eta_1^\ell, \dots, \eta_\ell^\ell)^\top : [0, T] \rightarrow \mathbb{R}^\ell$
- Define the non-linearity $f^\ell = (f_1^\ell, \dots, f_\ell^\ell)^\top : [0, T] \rightarrow \mathbb{R}^\ell$, where

$$f_i^\ell(t, \eta) = \left\langle f \left(t, \sum_{j=1}^{\ell} \eta_j \psi_j \right), \psi_i \right\rangle_W$$

- Introduce the IC, $\eta^\ell(0) = \eta_0^\ell = (\langle y_0, \psi_1 \rangle_W, \dots, \langle y_0, \psi_\ell \rangle_W)^\top$
- Write the ROM, $\dot{\eta}^\ell = A^\ell \eta^\ell + f^\ell(t, \eta^\ell)$, for $t \in (0, T]$, $\eta^\ell(0) = \eta_0^\ell$

Where to get a suitable base $\{\psi_j\}_{j=1}^d$?

Discrete version of Proper orthogonal decomposition



Original system

$$\dot{y} = Ay + f(t, y), \quad y(t) \in \mathbb{R}^m, \quad y(0) = y_0, \quad t \in [0, T],$$

Solution snapshots ← Approximation obtained from FOM

$$S = \left\{ \mathbf{y}_j = \mathbf{y}(t_j) = e^{At_j} \mathbf{y}_0 + \int_0^{t_j} e^{A(t_j-s)} \mathbf{b}(s, \mathbf{y}(s)) \, ds \right\}_{j=1}^n \approx \tilde{S} \leftarrow \text{FOM}$$

Matrix of snapshots (tildes denoting approximate solutions are omitted)

$$Y = [\mathbf{y}_1, \dots, \mathbf{y}_n] \in \mathbb{R}^{m \times n}, \quad \text{rank}(Y) = d \leq \min\{m, n\},$$

Where to get a suitable base $\{\psi_j\}_{j=1}^d$?

Discrete version of Proper orthogonal decomposition



Goal

Approximate all the spatial coordinate vectors \mathbf{y}_j of Y simultaneously by $\ell \leq d$ normalized vectors as well as possible.

(P)

$$\max_{\tilde{\psi}_1, \dots, \tilde{\psi}_\ell \in \mathbb{R}^m} \sum_{i=1}^{\ell} \sum_{j=1}^n \left| \langle \mathbf{y}_j, \tilde{\psi}_i \rangle_{\mathbb{R}^m} \right|^2$$

subject to

$$\langle \tilde{\psi}_i, \tilde{\psi}_j \rangle_{\mathbb{R}^m} = \delta_{ij} \quad \text{for } 1 \leq i, j \leq \ell,$$

Where to get a suitable base $\{\psi_j\}_{j=1}^d$?

Discrete version of Proper orthogonal decomposition



Fundamental theorem of Proper orthogonal decomposition

Let Y be a given matrix of snapshots. Also, let $Y = \Psi \Sigma \Phi^T$ be the singular value decomposition of Y , where $\Psi = [\psi_1, \dots, \psi_m] \in \mathbb{R}^{m \times m}$ and $\Phi = [\phi_1, \dots, \phi_n] \in \mathbb{R}^{n \times n}$ are orthogonal matrices and the matrix Σ has the structure of

$$\Sigma = \begin{bmatrix} \text{diag}(\sigma_1, \dots, \sigma_d) & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{m \times n},$$

where $\sigma_1, \dots, \sigma_d$ are the singular values of the matrix Y . Then, for any $\ell \in \{1, \dots, d\}$ the solution to problem **(P)** is given by the singular vectors $\{\psi_i\}_{i=1}^\ell$, i.e. by the first ℓ columns of Ψ . Moreover,

$$\text{argmax}(\mathbf{P}) = \sum_{i=1}^{\ell} \sigma_i^2.$$

Proof

- Obtained via Lagrange framework
- Rather long and technical, can be found in literature (e.g. [**VolkweinBook**])



Deal with the non-linearities I

- Identify the problem,

$$f_i^\ell(t, \eta) = \left\langle f \left(t, \sum_{j=1}^{\ell} \eta_j \psi_j \right), \psi_i \right\rangle_W \dots \sum_{j=1}^{\ell} \eta_j \psi_j \in \mathbb{R}^m \leftarrow \text{FO}$$

- Approximate the non-linearities via the POD basis, Φ ,

$$b(t) := f(t, \Psi \eta^\ell) \approx \sum_{k=1}^p \phi_k c_k(t) = \Phi c(t) \dots \text{Galerkin ansatz}$$

- Approximate $f^\ell(t, \eta^\ell)$ through Ψ, W, Φ ,

$$f^\ell(t, \eta^\ell) = \Psi^T W f(t, \Psi \eta^\ell) = \Psi^T W b(t) \approx \Psi^T W \Phi c(t), \quad c(t) \in \mathbb{R}^p$$

- Select (**greedy**) only p rows to make system consistent, introduce \vec{i}

$$P := [e_{i_1}, \dots, e_{i_p}] \in \mathbb{R}^{m \times p}, \quad e_{i_k} = (0, \dots, 0, 1, 0, \dots, 0)^T \in \mathbb{R}^m$$



Deal with the non-linearities II (yes, almost done)

- Plug in the matrix P ,

$$P^T \Phi c(t) \approx P^T b(t), \quad c(t) \in \mathbb{R}^p, \Phi \in \mathbb{R}^{m \times p}, b(t) \in \mathbb{R}^m$$

$$\det(P^T \Phi) \neq 0 \implies c(t) \approx (P^T \Phi)^{-1} P^T b(t) = (P^T \Phi)^{-1} P^T f(t, \Psi \eta^\ell)$$

- If $f(t, \Psi \eta^\ell)$ is pointwise evaluable,

$$(P^T \Phi)^{-1} P^T f(t, \Psi \eta^\ell) = (P^T \Phi)^{-1} f(t, P^T \Psi \eta^\ell), \quad P^T \Psi \eta^\ell \in \mathbb{R}^p$$

- Write the final ROM

$$\dot{\eta}^\ell = A^\ell \eta^\ell + f^\ell(t, \eta^\ell), \quad \text{for } t \in (0, T], \quad \eta^\ell(0) = \eta_0^\ell,$$

where

$$f^\ell(t, \eta^\ell) = \Psi^T W \Phi (P^T \Phi)^{-1} f(t, P^T \Psi \eta^\ell)$$



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Rewrite OpenFOAM discretization as above studied problem

OpenFOAM - FVM based solver for CFD applications, pressure-linked NS equations

FVM semi-discretized PDR

$$\Delta\Omega^h \dot{y} + \mathcal{L}^h(t, y) = 0 \implies \dot{y} = -(\Delta\Omega^h)^{-1} \mathcal{L}^h(t, y),$$

$\mathcal{L}^h = -\tilde{A}(t)y - \tilde{b}(t, y)$... FVM spatial discretization operator in OpenFOAM

After some operations

$$\dot{y} = A(\textcolor{red}{t})y + b(t, y), \quad A(t) = (\Delta\Omega^h)^{-1} \tilde{A}(t), \quad b(t, y) = (\Delta\Omega^h)^{-1} \tilde{b}(t, y)$$



Needed snapshots

$$\mathcal{S} = \{\mathbf{y}_j, \mathbf{A}_i, b_i\}_{i=1}^n, \quad \mathbf{A}_i \in \mathbb{R}^{m \times m}$$

\mathbf{A}_i ... sparse, $\sim 7m$ non-zero elements $\implies \sim 7m$ floats and $\sim 8m$ integers to be stored

Linear interpolation between the stored matrices

$$\varpi(t) = \frac{t - t_{i-1}}{t_i - t_{i-1}}, \quad \hat{\mathbf{A}}(t) = \varpi(t)\mathbf{A}_{i-1} + (1 - \varpi(t))\mathbf{A}_i$$

$$\begin{aligned} \hat{\mathbf{A}}^\ell(t) &= \Psi^T W \hat{\mathbf{A}}(t) \Psi = \Psi^T W (\varpi(t)\mathbf{A}_{i-1} + (1 - \varpi(t))\mathbf{A}_i) \Psi = \\ &= \varpi(t)\Psi^T W \mathbf{A}_{i-1} \Psi + (1 - \varpi(t))\Psi^T W \mathbf{A}_i \Psi = \varpi(t)\mathbf{A}_{i-1}^\ell + (1 - \varpi(t))\mathbf{A}_i^\ell \end{aligned}$$

Construction of ROM for Navier-Stokes equations

Start with steady state, proceed to dynamics



Parameter dependent steady state, $\mu \in \mathbb{R}$

$$\begin{aligned} \mathcal{M}_x := \nabla \cdot (u \otimes u) - \nabla \cdot (\nu \nabla u) &= -\nabla \tilde{p} + \tilde{f} \\ \nabla \cdot u &= 0 \end{aligned} \quad \rightsquigarrow \quad \begin{aligned} BD^{-1}B^T \tilde{p} &= BD^{-1}(f - (L + U)u^*) \\ u &= D^{-1}(f - (L + U)u^*) - D^{-1}B^T p \end{aligned}$$

$$0 = A(\mu)p + b(\mu, p), \quad A(\mu) := BD^{-1}B^T, \quad b(\mu, p) := -BD^{-1}(f - (L + U)u^*)$$

Transient case

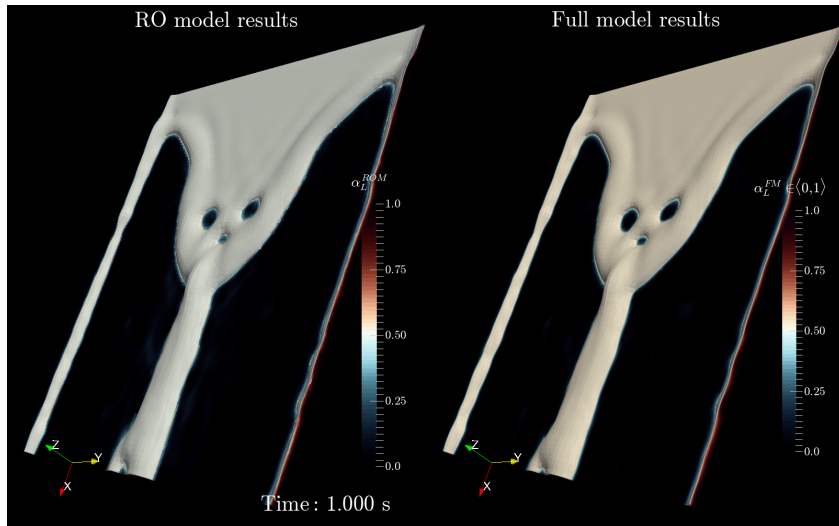
$$\mathcal{M}_t := u_t, \quad \mathcal{M}_t + \mathcal{M}_x = -\nabla \tilde{p} + \tilde{f}$$

use only \mathcal{M}_x to construct the pressure equation

$${}''\dot{p}'' = A(t)p + b(t, p), \quad A(t) := BD^{-1}B^T, \quad b(t, p) := -BD^{-1}(f - (L + U)u^*)$$

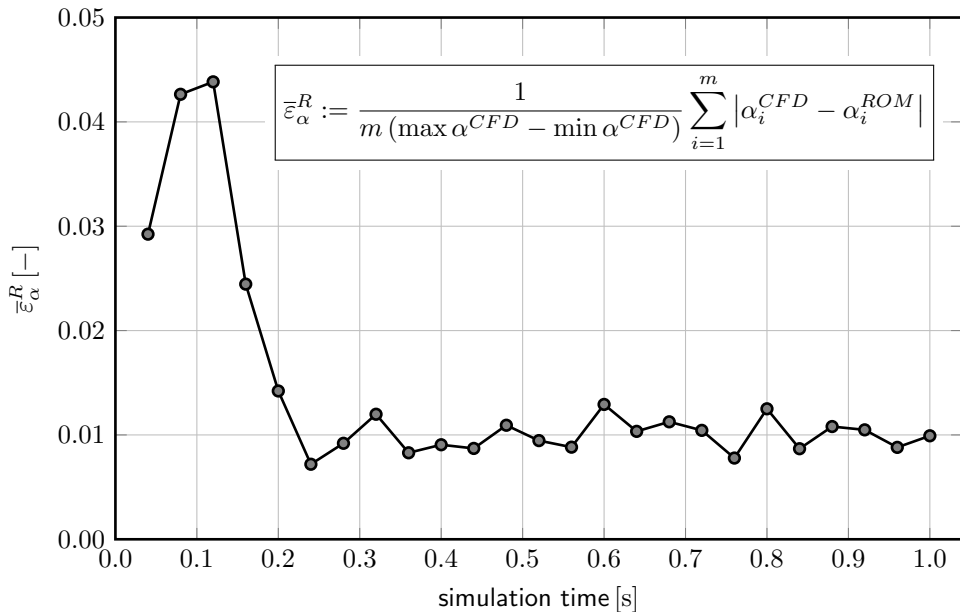
Example 1 – Passive scalar advection

Numerical results



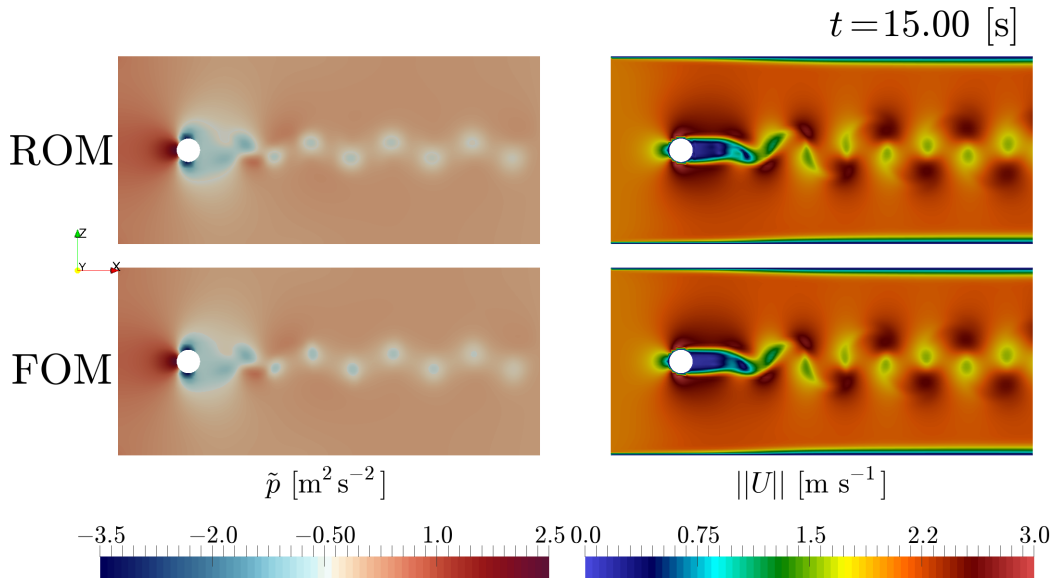
Example 1 – Passive scalar advection

Numerical results



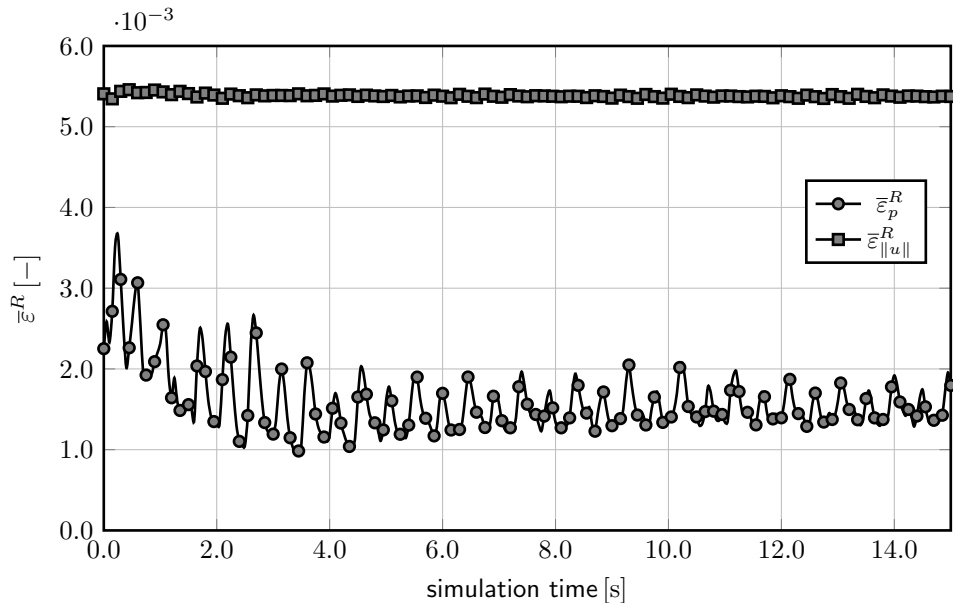
Example 2 – Von Karman vortex street

Validation of the approach – incompressible single phase flow



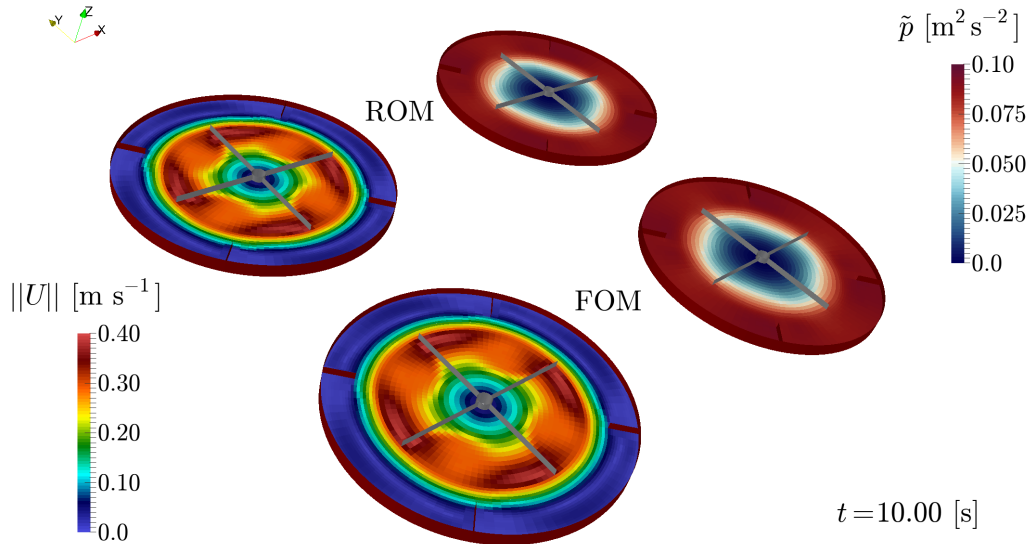
Example 2 – Von Karman vortex street

Validation of the approach – incompressible single phase flow



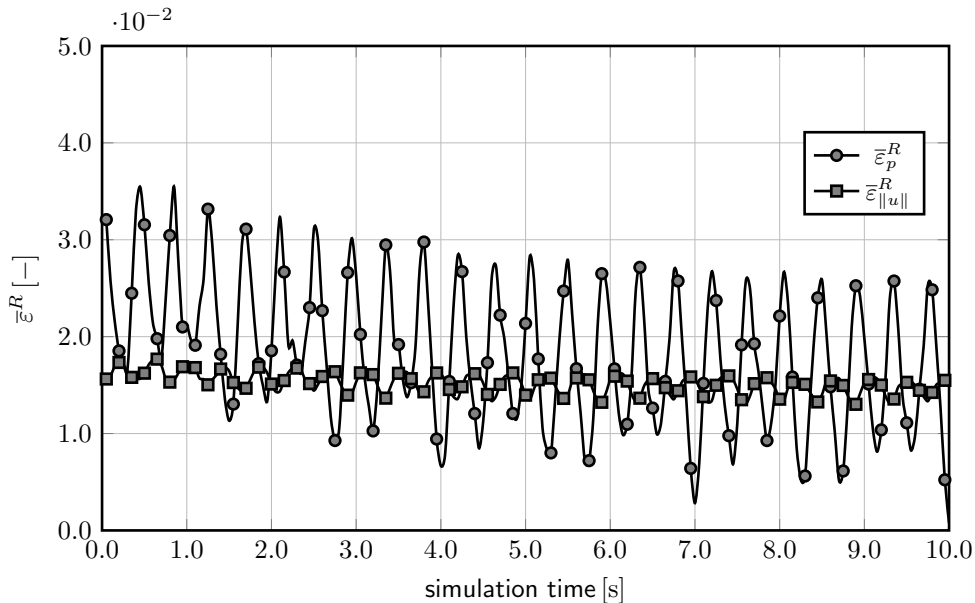
Example 3 – 2D mixer

Validation of the approach – arbitrary mesh interface



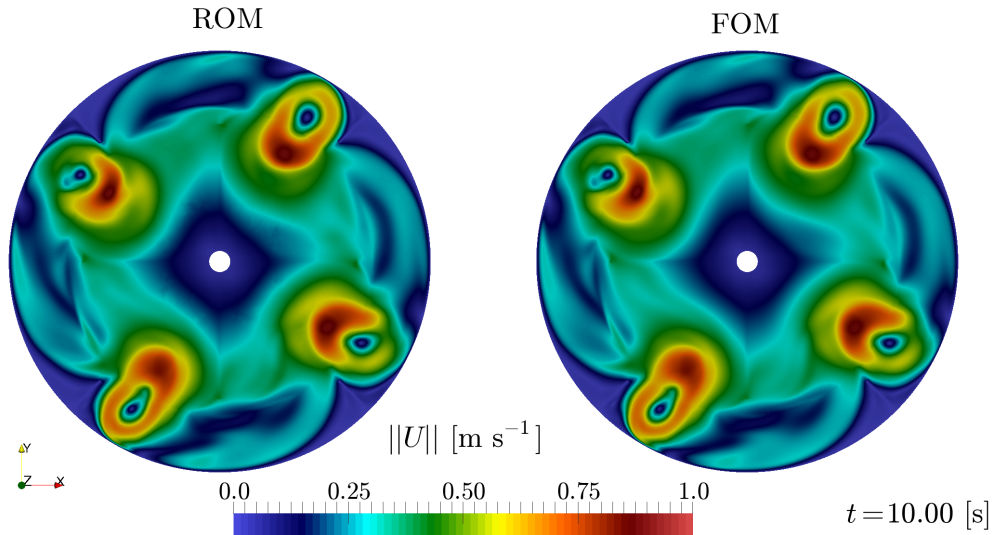
Example 3 – 2D mixer

Validation of the approach – arbitrary mesh interface



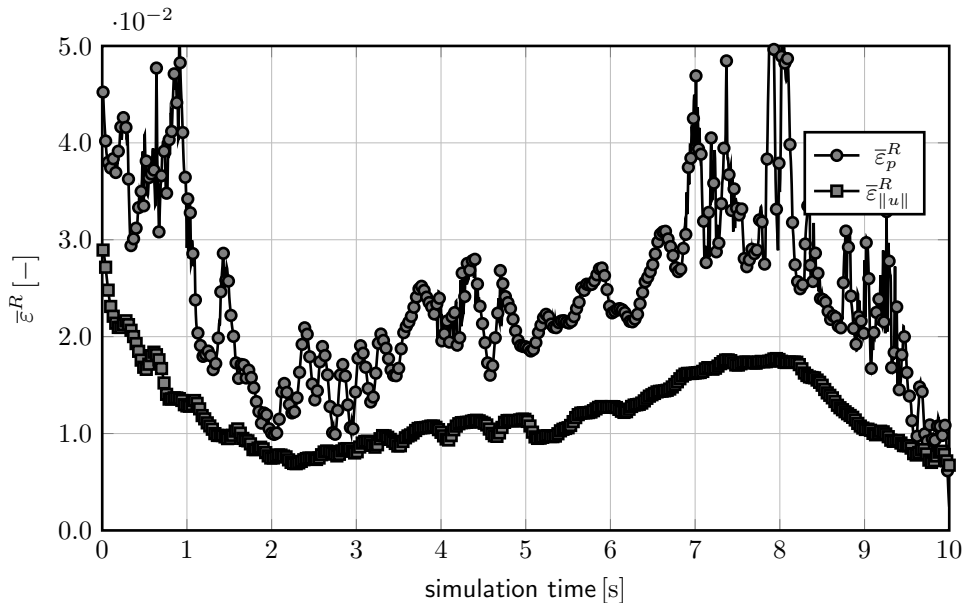
Example 4 – 2D mixer

Validation of the approach – multiple reference frames



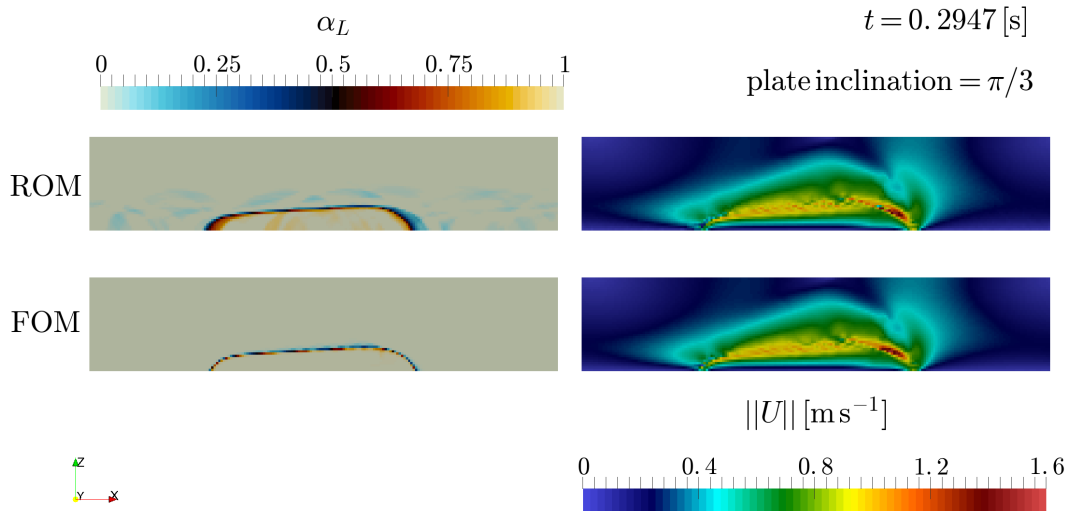
Example 4 – 2D mixer

Validation of the approach – multiple reference frames



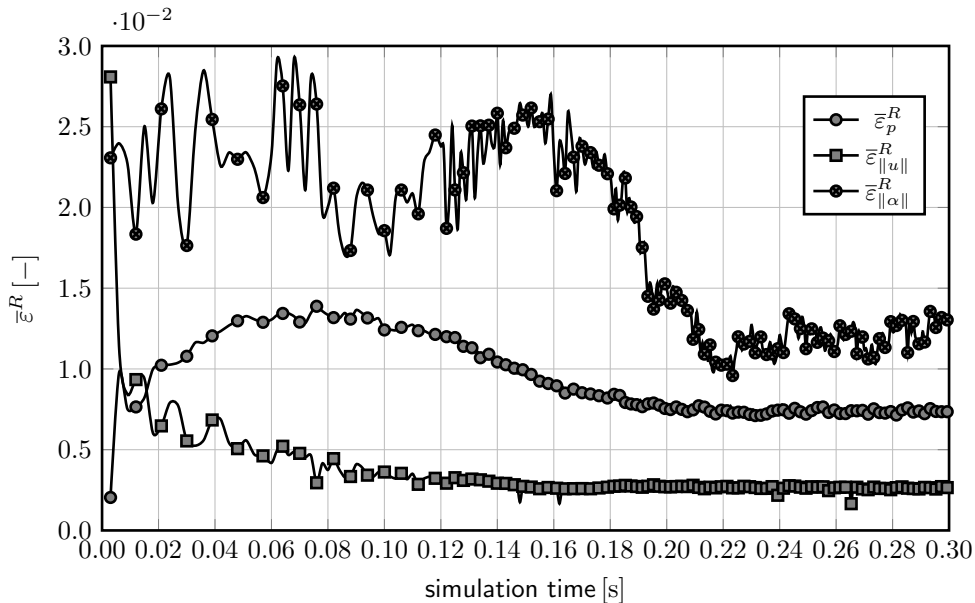
Example 5 – Sliding drop

Validation of the approach – multiphase flow



Example 5 – Sliding drop

Validation of the approach – multiphase flow





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Use ROM to speed up parametric studies

Sample parameter space and predict initial guesses for SIMPLE



Suitable snapshot selection: Leverage the continuity equation

Define cost function for snapshot selection

$$S_{\text{cont}} = \sum_{\Omega_P^h \in \Omega^h} \left| \sum_{f \in \{f\}_P} \Phi_f^V \right|, \quad S_{\text{cont}}^{\text{nn}} = d_{\text{nn}}^q S_{\text{cont}}$$

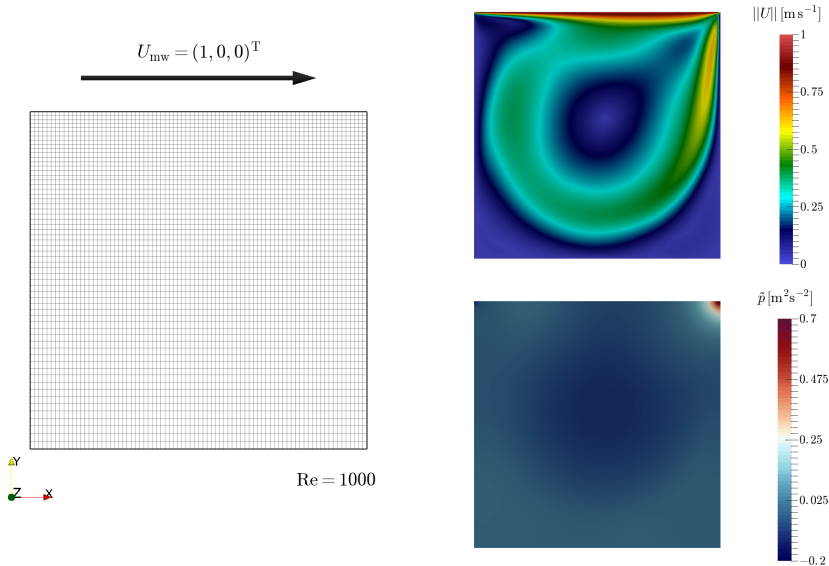
Identify snapshot to include into the basis

$(\mathbf{P}_{\tilde{\mu}}^{\text{nn}})$

$$\tilde{\mu} := \operatorname{argmax}_{\mu \in D \setminus \mu_u} S_{\text{cont}}^{\text{nn}}(\mu)$$

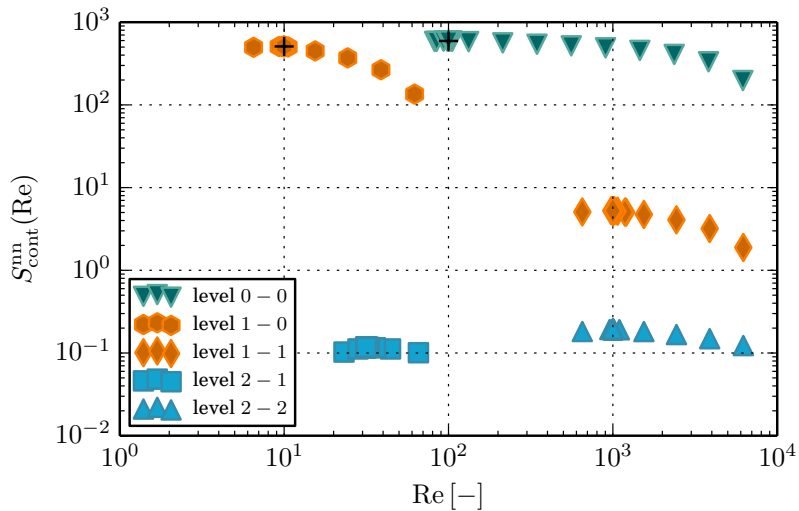
Use ROM to speed up parametric studies

Sample parameter space and predict initial guesses for SIMPLE



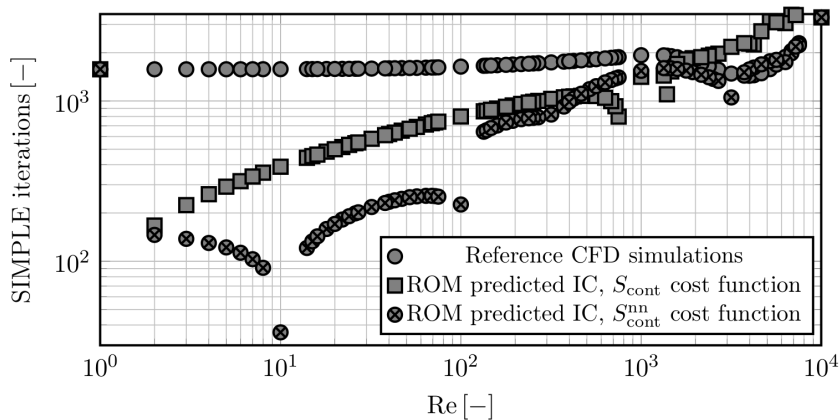
Use ROM to speed up parametric studies

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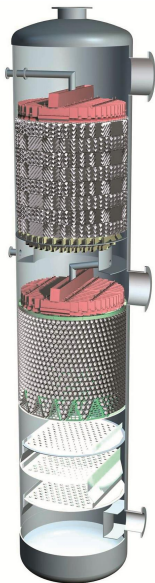
Use ROM to speed up parametric studies

Sample parameter space and predict initial guesses for SIMPLE



Real-life applications

ROM is a tremendous tool for parametric studies or repeated model evaluations



[Sulzer ChemTech]

Importance

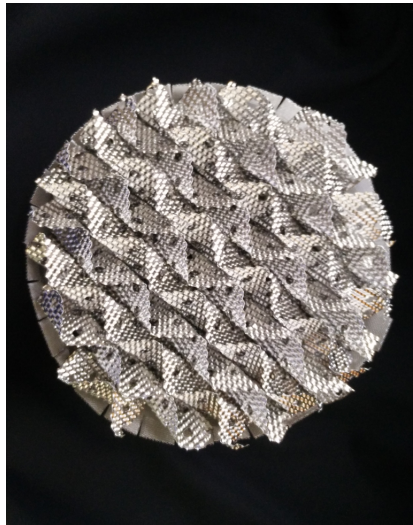
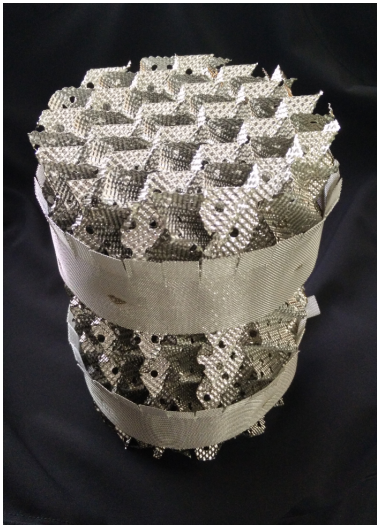
- Chemical industry creates mixtures but sells "pure species" (e.g. oil)
- 2014, 3% of energy consumption of the USA was due to the separation columns

Challenges

- Multiphase flow \rightarrow non-steady process
- Complex geometry
- Simultaneous heat and mass transfer

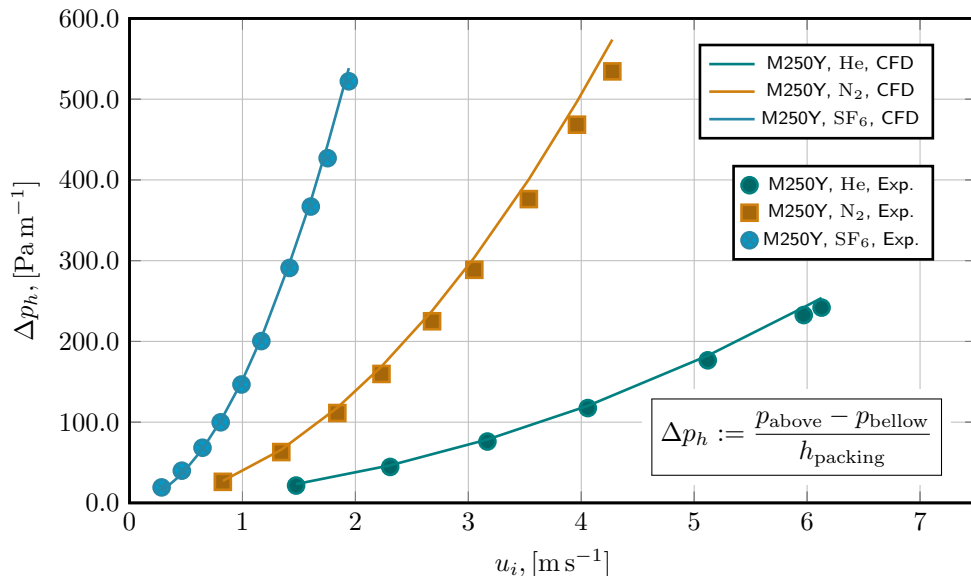


Challenge: Geometry of structured packing



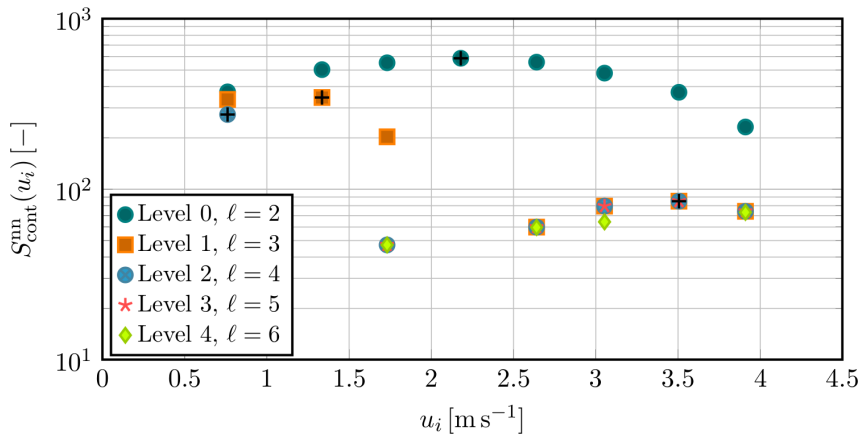


Comparison with experimental data: [Haidl, J. UCT Prague]



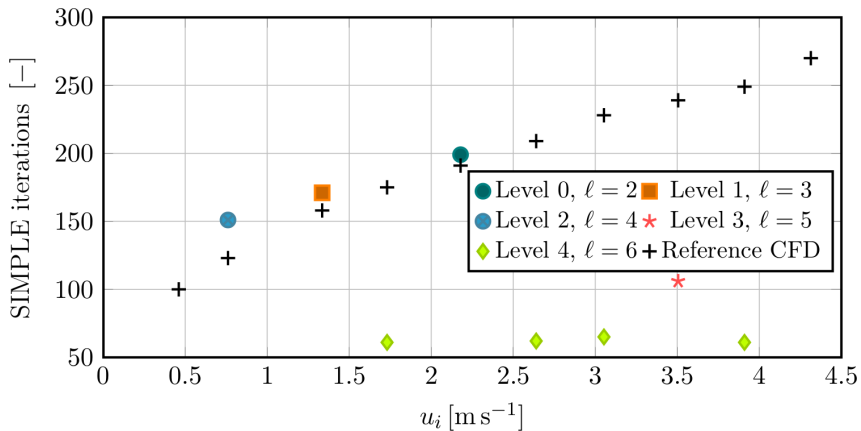


Snapshot selection:



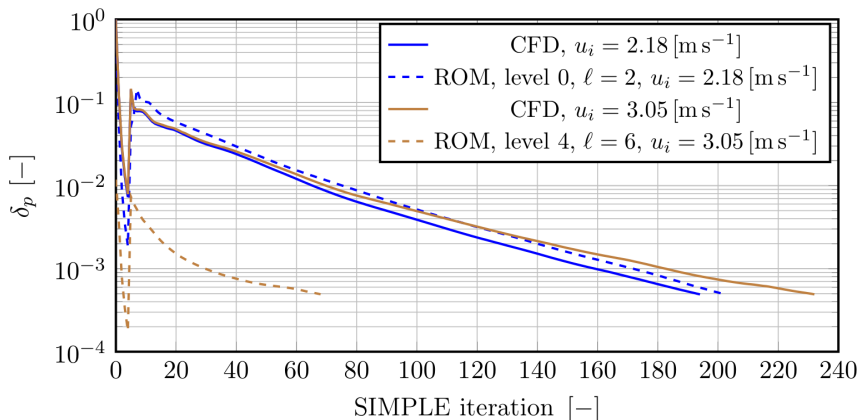


SIMPLE iterations:





Residuals evolution:

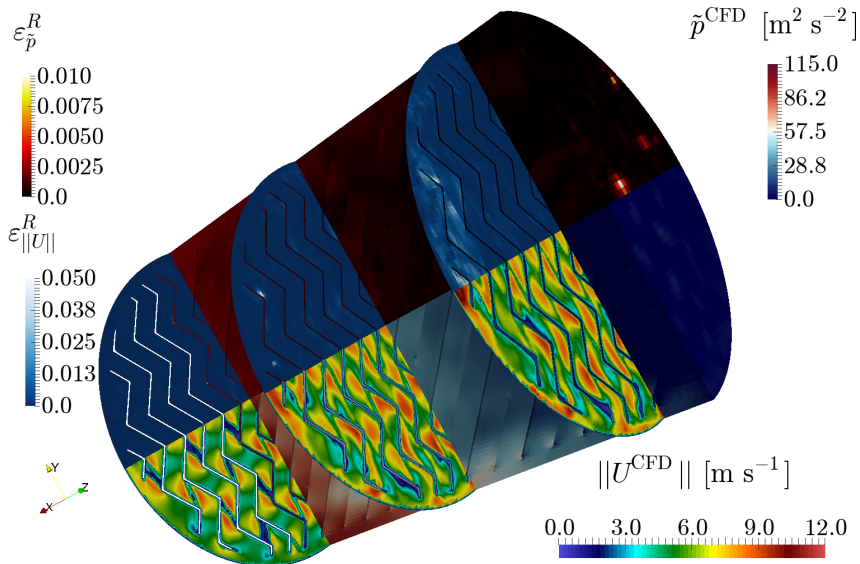


Semi-industrial scale application

ROM based initial guess prediction for full NS solver (simpleFoam)

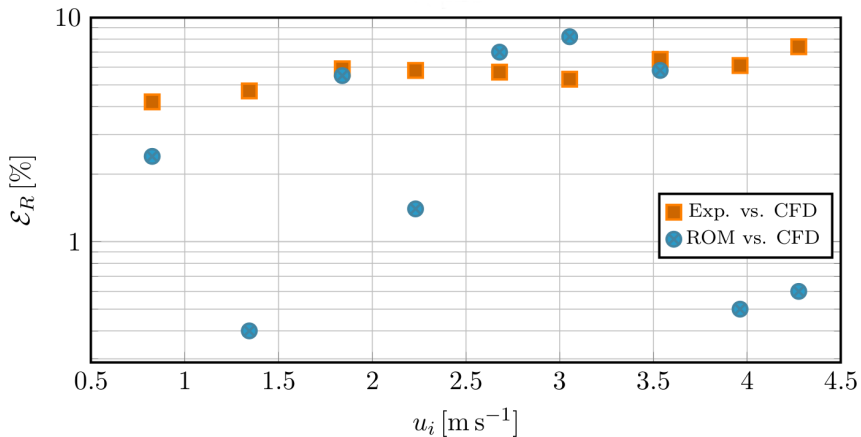


Full case: Predicted vs. converged solution, $\ell = 6 \text{ N}_2$ gas





Comparison with experimental data: $\ell = 6$, N_2 gas





Cost function: Single phase, toy problem

$$F(u_0) = \frac{\Delta\tilde{p} - \Delta\tilde{p}_{Max}}{\Delta\tilde{p}_{Max}} + K \frac{Q^2 - 2Q_{Max}Q + Q_{Min}(2Q_{Max} - Q_{Min})}{(Q_{Max} - Q_{Min})^2},$$

$$\Delta\tilde{p} = \Delta\tilde{p}(u_0), \quad Q = Q(u_0), \quad U_0 = (-u_0, 0, 0),$$

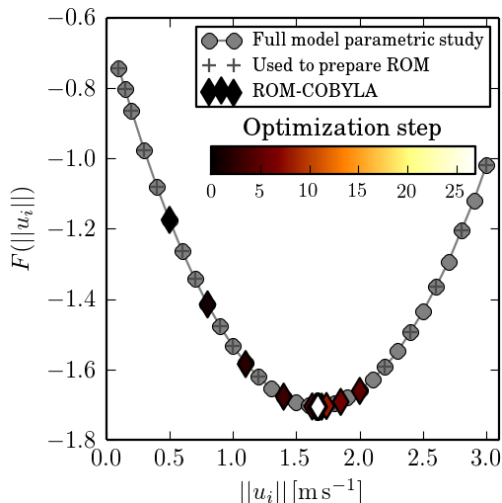
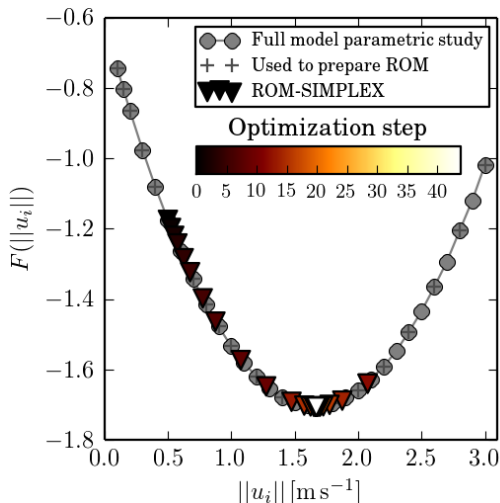
$\Delta\tilde{p}_{Max}$ maximal allowable pressure loss

$Q_{Max}, (Q_{Min})$ maximal, (minimal) allowable gas flow rate

K relative importance of the two terms



Cost function minimization: Results of SIMPLEX and COBYLA algorithms





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Currently available

- Extended snapshot preparation for `simpleFoam`, `pimpleFoam` and `interFoam`
- Python module for ROM creation based on prepared outputs from OpenFOAM
- ROM preparation in OpenFOAM - **Steady-state parametric studies**
- OpenFOAM is well prepared for algebraic manipulations necessary for ROM construction.

Advantages

- All connected to ROM is done in postprocessing - **simulations can be ran in parallel**
- **All the OpenFOAM capabilities are accessible** (including e.g. MRF or turbulence modeling)

Disadvantages

- Extended snapshots have to be stored - **a lot of data**
- Creation of A_i^ℓ , $i = 1, \dots, n$ is time consuming



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- [2] Volkwein, S.: Proper Orthogonal Decomposition: Applications in Optimization and Control
- [3] Chaturantabut, S. Sorensen, D. C.: Nonlinear Model Reduction Via Discrete Empirical Interpolation, *SIAM J. Sci. Comput.*, vol. 32, (2010) pp. 2737–2764.
- [4] Chaturantabut, S. Sorensen, D. C.: Application of POD and DEIM on Dimension Reduction of Nonlinear Miscible Viscous Fingering in Porous Media, *Math. Comput. Model. Dyn. Syst.*, (Technical Report: CAAM), Rice University, TR09-25
- [5] Alla, A. Kutz, J. N.: Nonlinear Model Order Reduction Via Dynamic Mode Decomposition, *preprint*



Thank you for your attention



Algorithm 1 POD basis of rank ℓ with weighted inner product

Require: Snapshots $\{y_j\}_{j=1}^n$, POD rank $\ell \leq d$, symmetric positive-definite matrix of weights $W \in \mathbb{R}^{m \times m}$

- 1: Set $Y = [y_1, \dots, y_n] \in \mathbb{R}^{m \times n}$;
 - 2: Determine $\bar{Y} = W^{1/2}Y \in \mathbb{R}^{m \times n}$;
 - 3: Compute SVD, $[\bar{\Psi}, \Sigma, \bar{\Phi}] = \text{svd}(\bar{Y})$;
 - 4: Set $\sigma = \text{diag}(\Sigma)$;
 - 5: Compute $\varepsilon(\ell) = \sum_{i=1}^{\ell} \sigma_i / \sum_{i=1}^d \sigma_i$;
 - 6: Truncate $\bar{\Psi} \leftarrow [\psi_1, \dots, \psi_\ell] \in \mathbb{R}^{m \times \ell}$;
 - 7: Compute $\Psi = W^{-1/2}\bar{\Psi} \in \mathbb{R}^{m \times \ell}$;
 - 8: **return** POD basis, Ψ , and ratio $\varepsilon(\ell)$
-

Notes:

- All the operations on W have to be cheap, including its inversion.
- Do not perform the full SVD, $\Sigma \in \mathbb{R}^{d \times d}$, $d = \text{rank}(\bar{Y})$.



Algorithm 2 DEIM

Require: p and matrix $F = [f(t_1, y_1), \dots, f(t_1, y_1)] \in \mathbb{R}^{m \times n}$

- 1: Compute POD basis $\Phi = [\phi_1, \dots, \phi_p]$ for F
 - 2: $\text{idx} \leftarrow \arg \max_{j=1, \dots, m} |(\phi_1)_{\{j\}}|;$
 - 3: $U = [\phi_1]$ and $\vec{i} = \text{idx};$
 - 4: **for** $i = 2$ **to** p **do**
 - 5: $u \leftarrow \phi_i;$
 - 6: Solve $U_{\vec{i}}^T c = u_{\vec{i}};$
 - 7: $r \leftarrow u - U c;$
 - 8: $\text{idx} \leftarrow \arg \max_{j=1, \dots, m} |(r)_{\{j\}}|;$
 - 9: $U \leftarrow [U, u]$ and $\vec{i} \leftarrow [\vec{i}, \text{idx}];$
 - 10: **end for**
 - 11: **return** $\Phi \in \mathbb{R}^{m \times p}$ and index vector, $\vec{i} \in \mathbb{R}^p$
-

Notes:

- Most of the computational cost is hidden on line 6.



- Let us have rather nice functions defined on a nice domain,

$$\varphi, \tilde{\varphi} \in L^2(\Omega), \quad \Omega \subset \mathbb{R}^3 \dots \text{bounded, connected, } \dots$$

- A brief reminder,

$$\langle \varphi, \tilde{\varphi} \rangle_{L^2(\Omega)} = \int_{\Omega} \varphi \tilde{\varphi} \, dx, \quad \|\varphi\|_{L^2(\Omega)} = \sqrt{\langle \varphi, \varphi \rangle_{L^2(\Omega)}}$$

- Denote Ω^h a FVM discretization of Ω and $\delta\Omega_i^h$ the volume of the i -th cell,

$$\Omega \approx \Omega^h = \bigcup_{i=1}^{\text{nCells}} \Omega_i^h, \quad V(\Omega) \approx V(\Omega^h) = \sum_{i=1}^{\text{nCells}} \delta\Omega_i^h$$

- Introduce a discrete inner product, $\langle \varphi, \tilde{\varphi} \rangle_{L_h^2}$,

$$\langle \varphi, \tilde{\varphi} \rangle_{L^2(\Omega)} = \int_{\Omega} \varphi \tilde{\varphi} \, dx \approx \sum_{i=1}^{\text{nCells}} \int_{\Omega_i^h} \varphi \tilde{\varphi} \, dx = \sum_{i=1}^{\text{nCells}} \varphi_i^h \tilde{\varphi}_i^h \delta\Omega_i^h = \langle \varphi, \tilde{\varphi} \rangle_{L_h^2}$$

- Denote $W = \text{diag}(\delta\Omega_1^h, \dots, \delta\Omega_{\text{nCells}}^h)$. Hence, $\langle \varphi, \tilde{\varphi} \rangle_{L_h^2} = (\varphi^h)^T W \varphi^h$.