Proper orthogonal decomposition and discrete empirical interpolation in CFD applications

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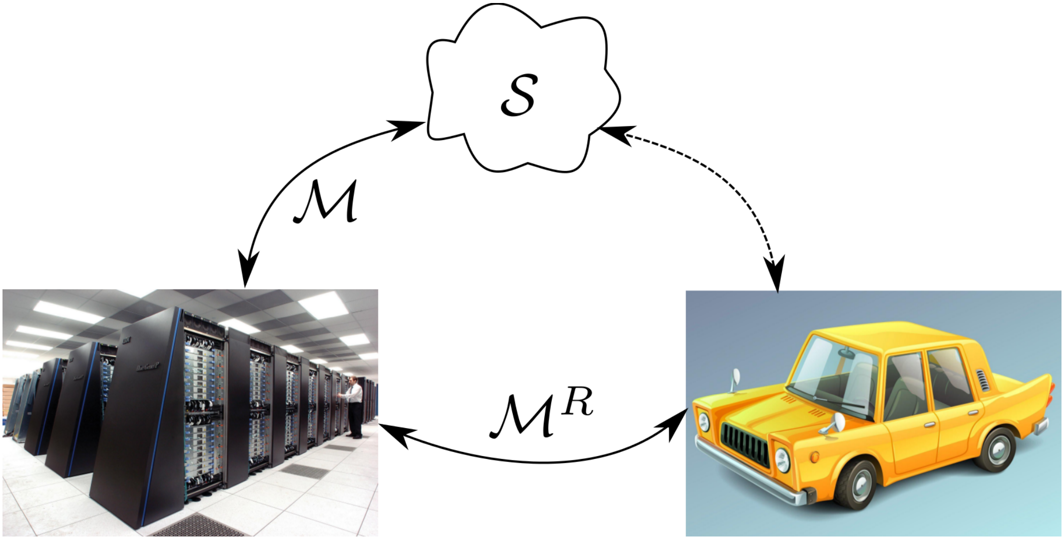
Introduction

Research motivation

Reducing the computational cost of modeling of complex systems



Original system

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

system matrix ... $A \in \mathbb{R}^{m \times m}$,

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

Reduced-order system

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

system matrix ... $A^\ell \in \mathbb{R}^{\ell \times \ell}$,

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

gain ... $\ell \ll m$

Proper orthogonal decomposition & Discrete empirical interpolation method

Introduce the Galerking ansatz and Fourier modes

- Prerequisities:

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

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

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

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

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

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

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

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

Introduce the reduced-order model

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

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

- Define the matrix $A^\ell = (a_{ij}^\ell) \in \mathbb{R}^{l \times l}$ with $a_{ij}^\ell = \langle A\psi_j, \psi_i \rangle_W$
- Define the vector valued mapping $\eta^\ell = (\eta_1^\ell, \dots, \eta_l^\ell)^{\mathrm{T}} : [0, T] \to \mathbb{R}^\ell$
- Define the non-linearity $f^\ell = (f_1^\ell, \dots, f_l^\ell)^{\mathrm{T}} : [0, T] \to \mathbb{R}^\ell$, 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, $\eta^\ell(0) = \eta_0^\ell = (\langle y_0, \psi_1 \rangle_W, \dots, \langle y_0, \psi_1 \rangle_W)^{\mathrm{T}}$
- Write the ROM, $\dot{\eta}^\ell = A^\ell \eta^\ell + f^\ell(t, \eta^\ell)$, for $t \in (0, T]$, $\eta^\ell(0) = \eta_0^\ell$

Original system

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

Solution snapshots←Approximation obtained from FOM

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

Matrix of snapshots (tildes denoting approximate solutions are omitted)

$$Y = [\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n] \in \mathbb{R}^{m \times n}, \quad \mathrm{rank}(Y) = d \le \min\{m, n\}\,,$$

Goal

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

(P)

$$\boxed{\begin{gathered}\max_{\tilde{\boldsymbol{\psi}}_1,\ldots,\tilde{\boldsymbol{\psi}}_\ell \in \mathbb{R}^m} \sum_{i=1}^{\ell} \sum_{j=1}^{n} \left| \langle \boldsymbol{y}_j, \tilde{\boldsymbol{\psi}}_i \rangle_{\mathbb{R}^m} \right|^2 \\ \text{subject to} \\ \langle \tilde{\boldsymbol{\psi}}_i, \tilde{\boldsymbol{\psi}}_j \rangle_{\mathbb{R}^m} = \delta_{ij} \quad \text{for} \quad 1 \leq i, j \leq \ell\,,\end{gathered}}$$

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 $\Psi = [\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_m] \in \mathbb{R}^{m\times m}$ and $\Phi = [\boldsymbol{\phi}_1, \ldots, \boldsymbol{\phi}_n] \in \mathbb{R}^{n\times n}$ are orthogonal matrices and the matrix Σ has the structure of

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

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

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

Proof

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

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 $Y = [y_1, \ldots, y_n] \in \mathbb{R}^{m\times n}$;
2: Determine $\bar{Y} = W^{1/2} Y \in \mathbb{R}^{m\times n}$;
3: Compute SVD, $[\bar{\Psi}, \Sigma, \bar{\Phi}] = \mathrm{svd}(\bar{Y})$;
4: Set $\sigma = \mathrm{diag}(\Sigma)$;
5: Compute $\varepsilon(\ell) = \sum_{i=1}^{\ell} \sigma_i / \sum_{i=1}^{d} \sigma_i$;
6: Truncate $\bar{\Psi} \leftarrow [\bar{\psi}_1, \ldots, \bar{\psi}_l] \in \mathbb{R}^{m\times\ell}$;
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, $\Sigma \in \mathbb{R}^{d\times d}$, $d = \mathrm{rank}(\bar{Y})$.

Deal with the non-linearities I

- Identify the problem,

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

- 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,

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

- Plug-in the last output of the DEIM algorithm, $\vec{i}$

$$P := [e_{\vec{i}1}, \dots, e_{\vec{i}p}] \in \mathbb{R}^{m\times p},\ e_{\vec{i}k} = (0,\dots,0,1,0,\dots,0)^{\mathrm{T}} \in \mathbb{R}^m$$

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

- Plug in the matrix P,

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

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

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

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

- Write the final ROM

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

where

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

Discrete Empirical Interpolation Method

POD & Greedy algorithm based method for handling non-linearities

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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: $\mathrm{idx} \leftarrow \arg\max_{j=1,\dots,m} |(\phi_1)_{\{j\}}|$;

3: $U = [\phi_1]$ and $\vec{i} = \mathrm{idx}$;

4: **for** $i = 2$ **to** p **do**

5:     $u \leftarrow \phi_i$;

6:     Solve $U_{\vec{i}}c = u_{\vec{i}}$;

7:     $r \leftarrow u - Uc$;

8:     $\mathrm{idx} \leftarrow \arg\max_{j=1,\dots,m} |(r)_{\{j\}}|$;

9:     $U \leftarrow [U, u]$ and $\vec{i} \leftarrow [\vec{i}, \mathrm{idx}]$;

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.

Link with OpenFOAM

Rewrite OpenFOAM discretization as above studied problem

- With $\Delta\Omega^h := \mathrm{diag}(\delta\Omega_i^h) \in \mathbb{R}^{m\times m}$ a FVM semi-discretized problem can be written as,

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

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

- It is possible to formally write (almost) the same system as before,

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

- The time dependence of A is a result of the linearization process. E.g. $\nabla\cdot(u^k \otimes u^k) \approx \nabla\cdot(u^{k-1}\otimes u^k)$
- The POD-DEIM approach to ROM creation will have to be slightly modified

Address the risen difficulties

- Needed snapshots, $\{(y_i, A_i, b_i)\}_{i=1}^{n}$, $A_i \in \mathbb{R}^{m\times m}$, $i = 1, \ldots, m$ but A_i are sparse matrices, with $\sim 5m$ non-zero elements $\implies \sim 5m$ floats and $\sim 8m$ integers will be stored.
- A way for ROM evaluation between the stored snapshots is needed $\implies$ I need to interpolate between A_{i-1} and A_i and b_{i-1} and b_i, $i = 2, n$
- Simplest case: linear interpolation,

$$\varpi(t) = \frac{t - t_{i-1}}{t_i - t_{i-1}},\ \hat{A}(t) = \varpi(t)A_{i-1} + (1 - \varpi(t))A_i$$

$$\hat{A}^\ell(t) = \Psi^{\mathrm{T}} W \hat{A}(t)\Psi = \Psi^{\mathrm{T}} W \left(\varpi(t)A_{i-1} + (1 - \varpi(t))A_i\right)\Psi =$$

$$= \varpi(t)\Psi^{\mathrm{T}} W A_{i-1}\Psi + (1 - \varpi(t))\Psi^{\mathrm{T}} W A_i\Psi = \varpi(t)A^\ell_{i-1} + (1 - \varpi(t))A^\ell_i$$

- Same trick can be done for $b(t, y)$ and after the ROM creation, I do not need to store the full data.

interFoam – Volume-of-Fluid model for multiphase flow

$$\alpha_t + \nabla \cdot (u\alpha) + \nabla \cdot (u_r \alpha(1-\alpha)) = 0$$

$$\alpha_t + \mathcal{L}^h_\alpha(t,\alpha) = 0 \to \alpha_t = A_\alpha(t)\alpha + b_\alpha(t,\alpha) \to \dot{\eta}^\ell_\alpha = \hat{A}^\ell_\alpha(t)\eta^\ell_\alpha + \hat{b}^\ell_\alpha(t,\eta^\ell_\alpha)$$

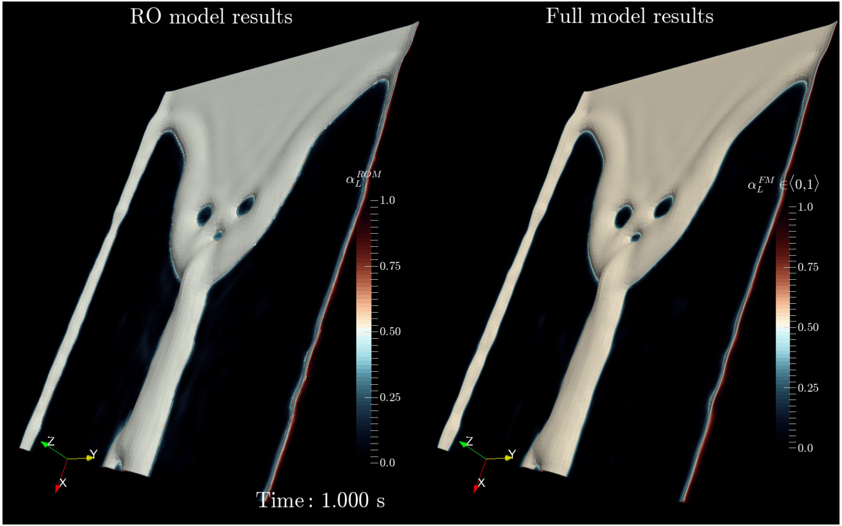
Wanted: $\dot{y}_\alpha = A_\alpha(t) y_\alpha + b_\alpha(t,y)$

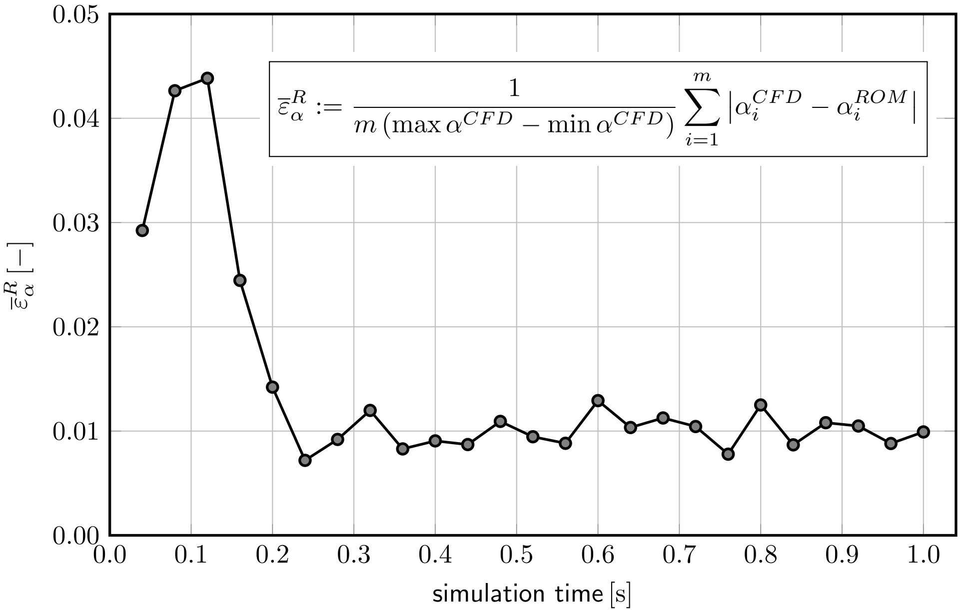
Example of implementation in OpenFOAM

```
    fvm::div( phi, alpha1, alphaScheme )
  + fvc::div(
        -fvc::flux(
            -phir, scalar(1)-alpha1, alpharScheme
        ),
        alpha1, alpharScheme
    ) == 0
```

Link: $\texttt{fvm} \to A_\alpha(t)$, $\texttt{fvc} \to b_\alpha(t,y)$

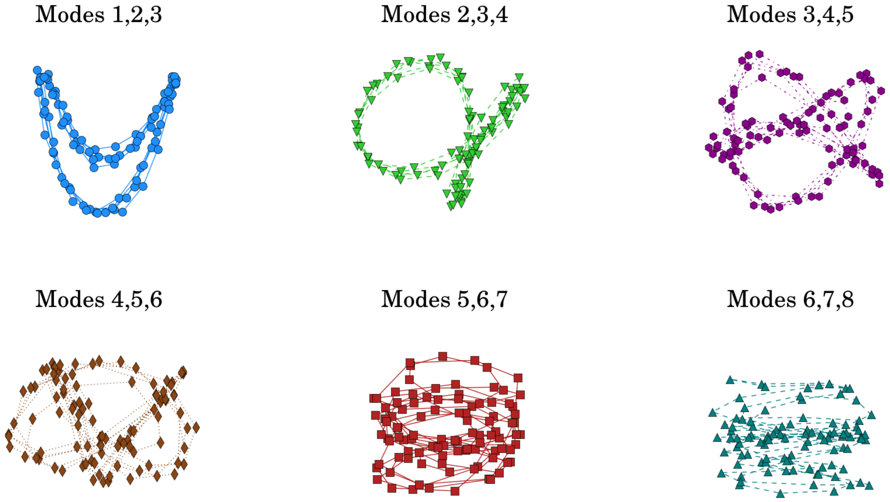
Example 1 – Passive scalar advection
Numerical results




$\overline{\varepsilon}_\alpha^R := \frac{1}{m\left(\max \alpha^{CFD} - \min \alpha^{CFD}\right)} \sum_{i=1}^{m} \left|\alpha_i^{CFD} - \alpha_i^{ROM}\right|$
0.05
0.04
0.03
0.02
0.01
0.00
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
$\overline{\varepsilon}_\alpha^R\,[-]$
simulation time $[\mathrm{s}]$

Example 1 – Passive scalar advection

Numerical results



Saddle-point problem

$$\begin{aligned} u_t + \nabla\cdot(u\otimes u) - \nabla\cdot(\nu\nabla u) &= -\nabla\tilde{p} + \tilde{f} \\ \nabla\cdot u &= 0 \end{aligned} \rightsquigarrow \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix}\begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

Jacobi iterations with Schur-complement based p-U coupling

$$u^* \leftarrow Au^* = f - B^{\mathrm{T}}p^{k-1}$$

$$p^k \leftarrow BD^{-1}B^{\mathrm{T}}p^k = BD^{-1}\left(f - (L+U)u^*\right)$$

$$u^k \leftarrow D^{-1}\left(f - (L+U)u^* - B^{\mathrm{T}}p^k\right)$$

At convergence

$$BD^{-1}B^{\mathrm{T}}p^k = BD^{-1}\left(f - (L+U)u^*\right) \approx BA^{-1}B^{\mathrm{T}}p = BA^{-1}f$$

$$u = D^{-1}\left(f - (L+U)u^*\right) - D^{-1}B^{\mathrm{T}}p$$

Outcome for ROM

- "Natural" is to construct ROM for p
- For the velocity, I can choose between computational cost and consistency and accuracy

Notation

$D^{-1} \to \mathtt{rAU}$ and $D^{-1}(f - (L+U)u^*) \to \mathtt{HbyA}$ (in oF, $*\mathtt{Eqn.A()} \to D$)

Implementation of pressure eqauation in OpenFOAM

```
fvm::laplacian(rAU, p) == fvc::div(HbyA)
```

Wanted: $\dot{y}_p = A_p(t) y_p + b_p(t, y_p)$

Implicit definition of time derivative for pressure

$$\begin{aligned} \nabla \cdot (u \otimes u) - \nabla \cdot (\nu \nabla u) &= -\nabla \tilde{p} + \tilde{f} \\ \nabla \cdot u &= 0 \end{aligned} \quad \rightsquigarrow \quad \begin{array}{c} \mathtt{UEqnMORE} \\ D_h^{-1} \to \mathtt{rAUMORE} \\ D_h^{-1}(f_h - (L_h + U_h)u_h *) \to \\ \to \mathtt{HMOREbyAMORE} \end{array}$$

```
fvm::laplacian(rAUMORE, p) == fvc::div(HMOREbyAMORE)
```

Link: $\mathtt{fvm} \to A_p(t)$, $\mathtt{fvc} \to b_p(t, y_p)$

Expansion of snapshots for pressure

Standard approach snapshots: $\mathcal{S} = \{(y_{k,i}, A_{k,i}, b_{k,i}\}_{i=1}^{n}, k = p, U$

Expanded snapshots for pressure:

$$\mathcal{S}^e = \{(y_{p,i}, A_{p,i}, b_{p,i}, \mathtt{rAUMORE}_i, \mathtt{HMOREbyAMORE}_i\}_{i=1}^{n}$$

Storage

$\mathcal{S}$ $\ldots n\left[(1+3)m + (5+5)m + (1+3)m\right] \approx 15nm$ values

$\mathcal{S}^e$ $\ldots n(m + 5m + m + 1m + 3m) \approx 11nm$ values

Computational cost

$\mathcal{S}$ $\ldots \sim 4n$ calculations of $\Psi^{\mathrm{T}} W A(t) \Psi$, evaluation of ~ 4 ROMs

$\mathcal{S}^e$ $\ldots$

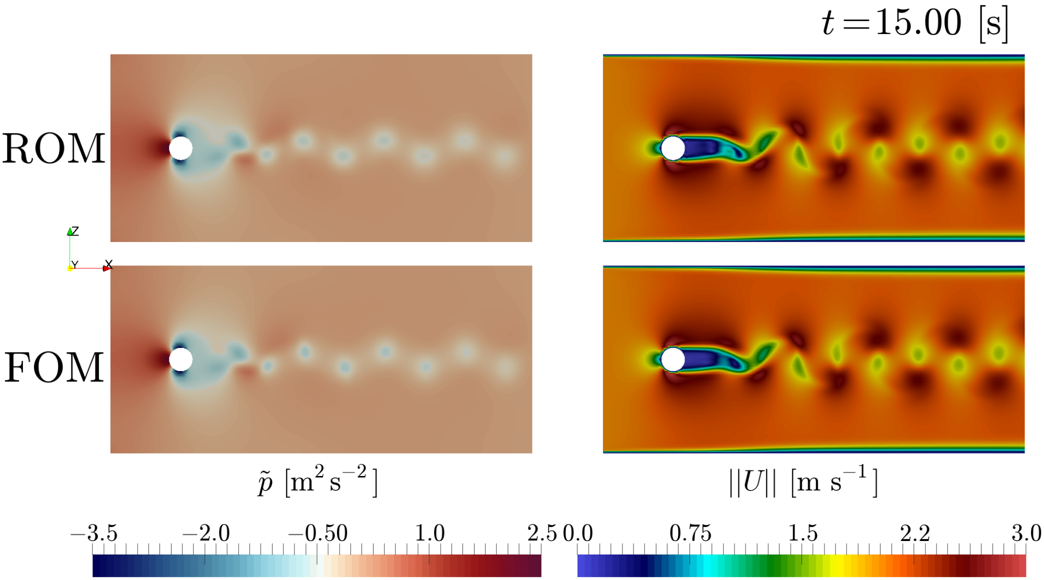
$\sim n$ calculations of $\Psi^{\mathrm{T}} W A(t) \Psi$,

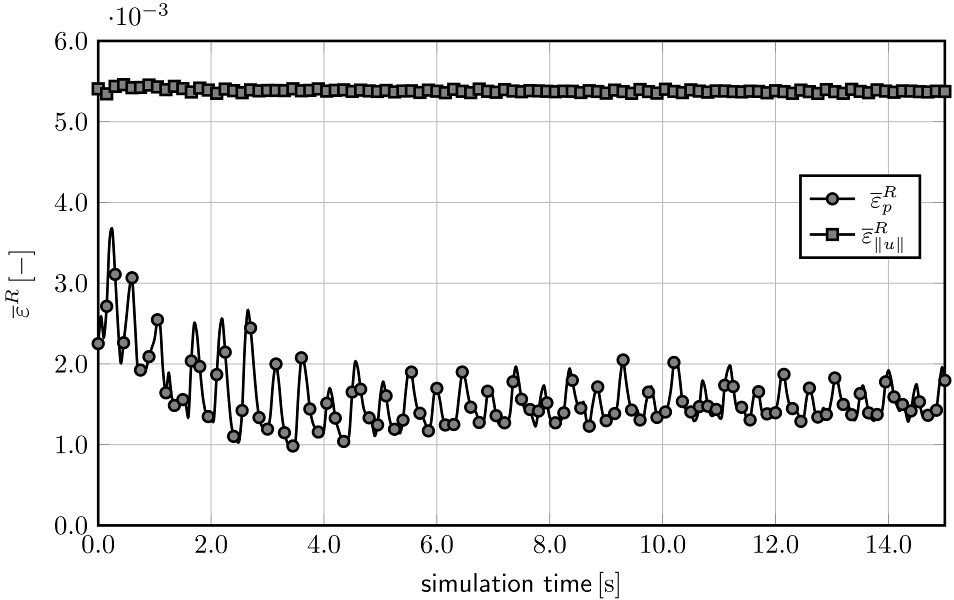
$\sim n$ calculations of $\Psi^{\mathrm{T}} W \mathtt{rAUMORE}_i \Psi$,

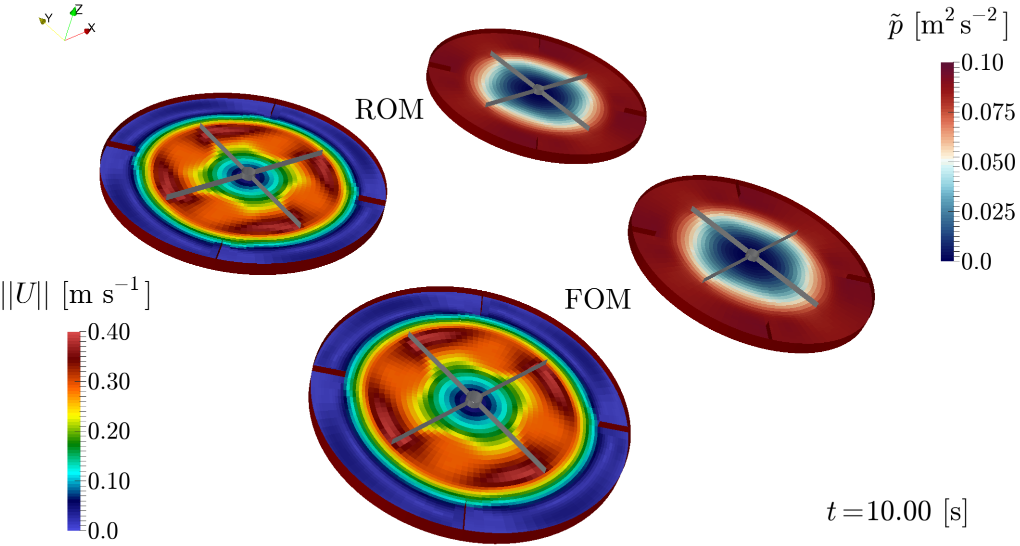
$\sim n$ calculations of $\Psi^{\mathrm{T}} W \mathtt{HMOREbyAMORE}_i \Psi$,

evaluation of 1 ROM + interpolation between $\mathtt{rAUMORE}_i{}^{ROM}$ and between $\mathtt{HMOREbyAMORE}_i{}^{ROM}$

$$U_i \approx \mathtt{HMOREbyAMORE}^{ROM} + \mathtt{rAUMORE}^{ROM} \nabla p^{ROM}$$

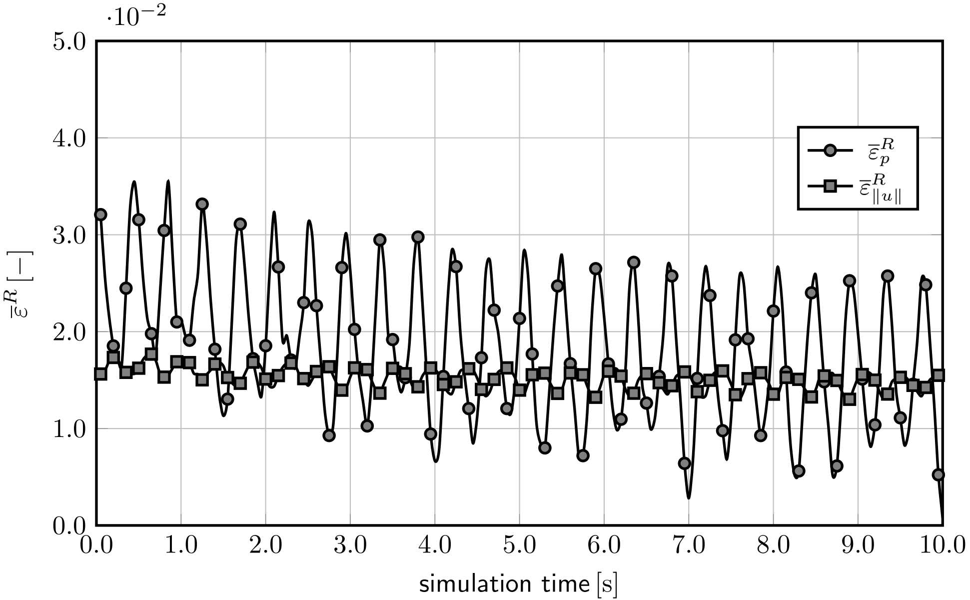

$t = 15.00$ [s]
ROM
FOM
Z
Y
X
$\tilde{p}$ [$m^2 s^{-2}$]
$||U||$ [$m\ s^{-1}$]
−3.5
−2.0
−0.50
1.0
2.5
0.0
0.75
1.5
2.2
3.0


$\cdot 10^{-3}$
6.0
5.0
4.0
3.0
2.0
1.0
0.0
$\overline{\varepsilon}^R$ $[-]$
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
simulation time $[\mathrm{s}]$
$\overline{\varepsilon}_p^R$
$\overline{\varepsilon}_{\|u\|}^R$

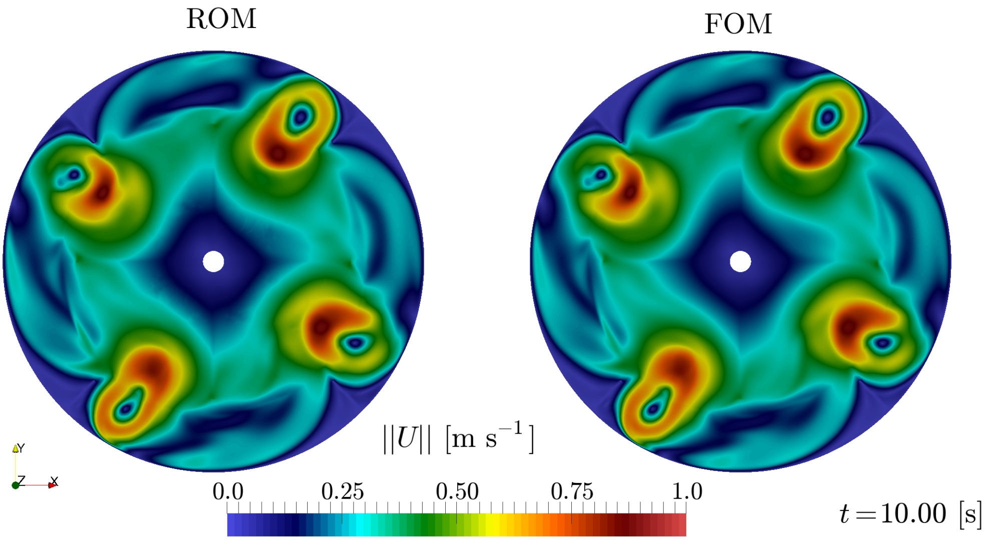

Y
Z
X
ROM
FOM
$\tilde{p}$ [m^2 s^{-2}]
0.10
0.075
0.050
0.025
0.0
$||U||$ [m s^{-1}]
0.40
0.30
0.20
0.10
0.0
$t = 10.00$ [s]

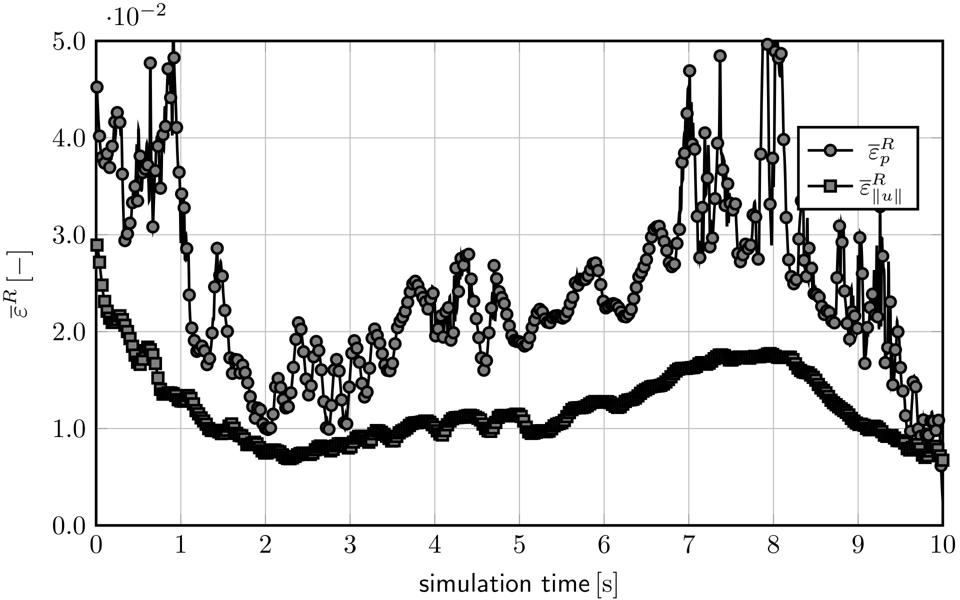
Example 3 – 2D mixer

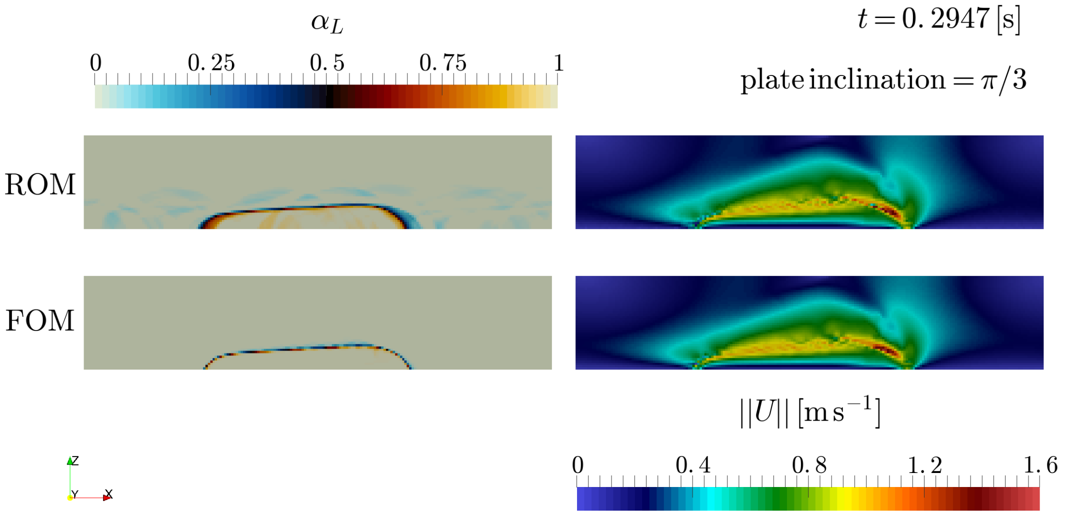
Validation of the approach – arbitrary mesh interface



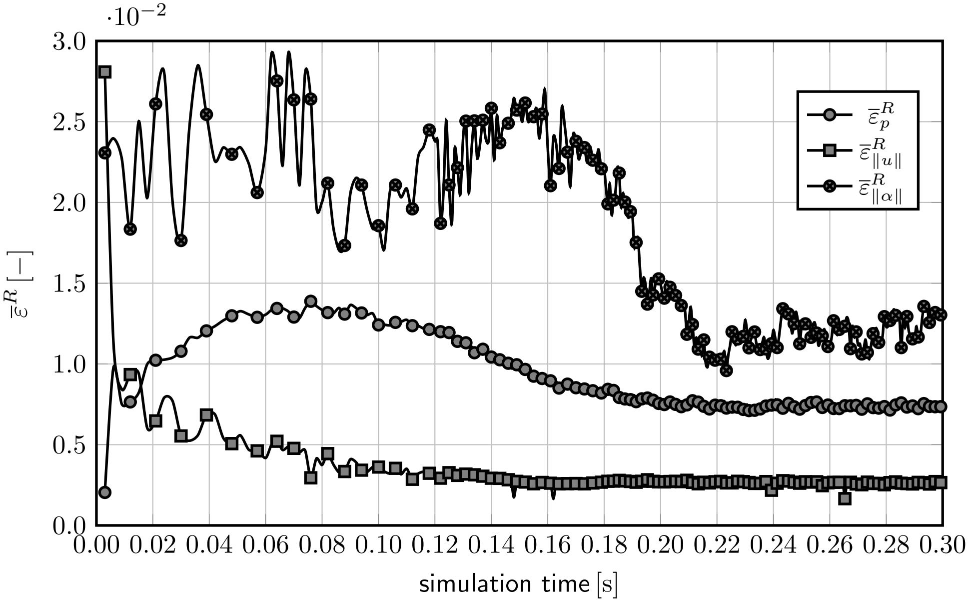
Validation of the approach – multiple reference frames




$\cdot 10^{-2}$
5.0
4.0
3.0
2.0
1.0
0.0
0
1
2
3
4
5
6
7
8
9
10
$\overline{\varepsilon}^R\,[-]$
simulation time $[\mathrm{s}]$
$\overline{\varepsilon}_p^R$
$\overline{\varepsilon}_{\|u\|}^R$



α_L
0
0.25
0.5
0.75
1
$t = 0.2947$ [s]
plate inclination $= \pi/3$
ROM
FOM
$||U||$ [m s^{-1}]
0
0.4
0.8
1.2
1.6
Z
Y
X

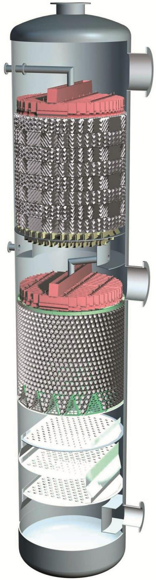


$\cdot 10^{-2}$
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.00 0.02 0.04 0.06 0.08 0.10 0.12 0.14 0.16 0.18 0.20 0.22 0.24 0.26 0.28 0.30
simulation time [s]
$\overline{\varepsilon}^R$ [−]
$\overline{\varepsilon}_p^R$
$\overline{\varepsilon}_{\|u\|}^R$
$\overline{\varepsilon}_{\|\alpha\|}^R$

Applications

Real-life applications

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



[Sulzer ChemTech]

Importance

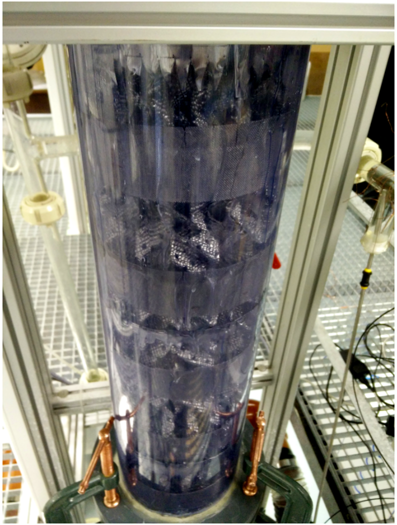
- Chemical industry creates mixtures but sells "pure species" (e.g. oil)
- 2014, 3% of energy consumption of the USA was due to the separation columns

Challenges

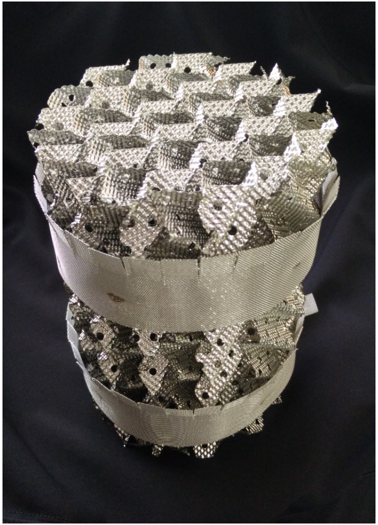
- Multiphase flow $\rightarrow$ non-steady process
- Complex geometry
- Simultaneous heat and mass transfer

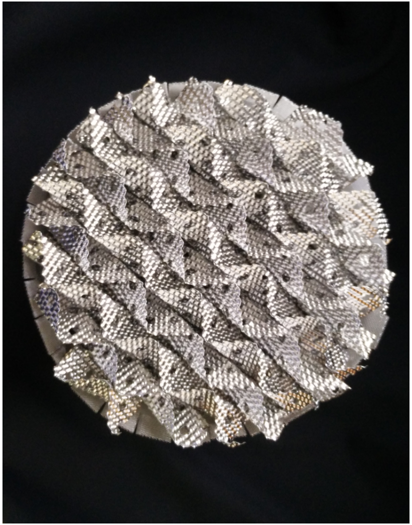
Packed column

Complex multiphase flow

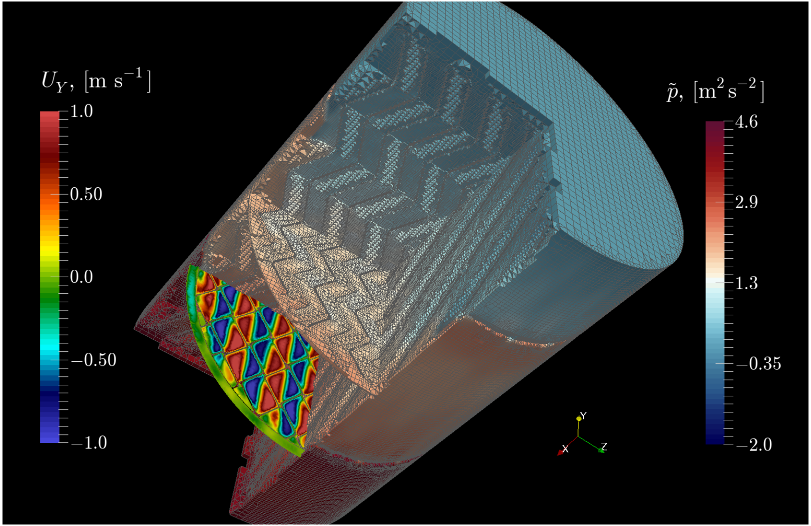


Challenge: Geometry of structured packing

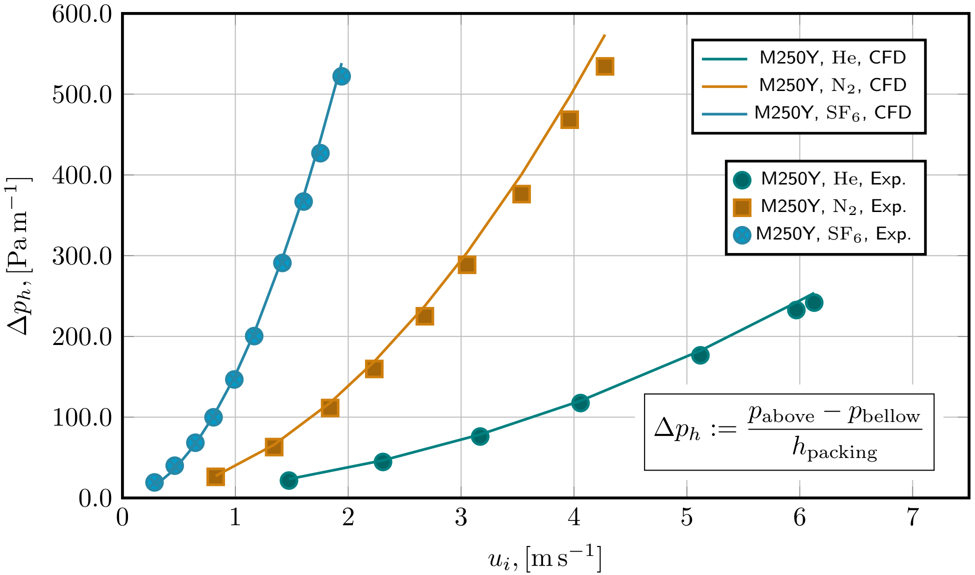




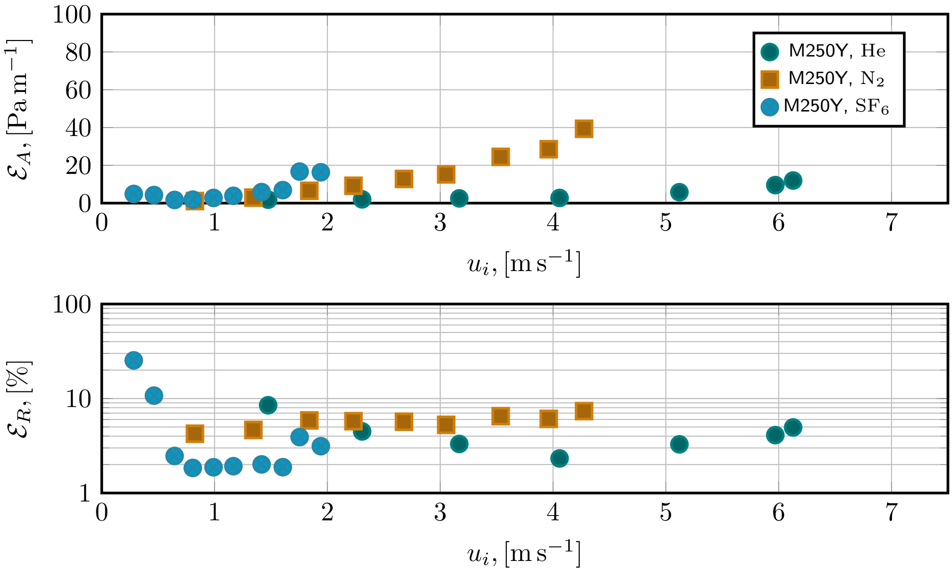
Gas flow simulation: Incompressible steady state RANS simulation



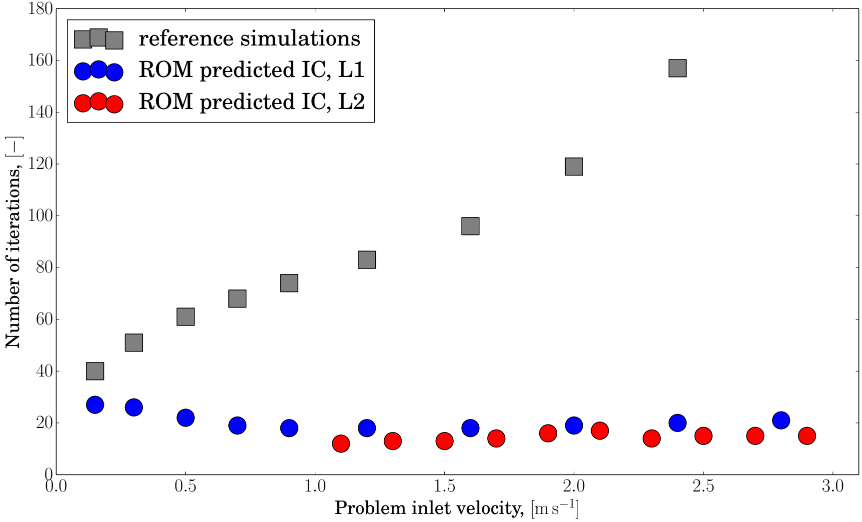
Comparison with experimental data: [Haidl, J. UCT Prague]



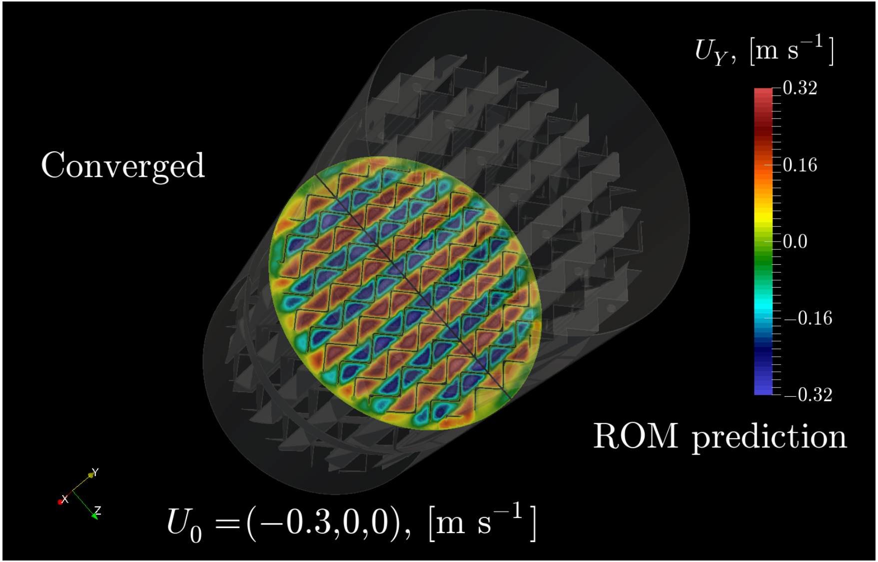
Comparison with experimental data: [Haidl, J. UCT Prague]



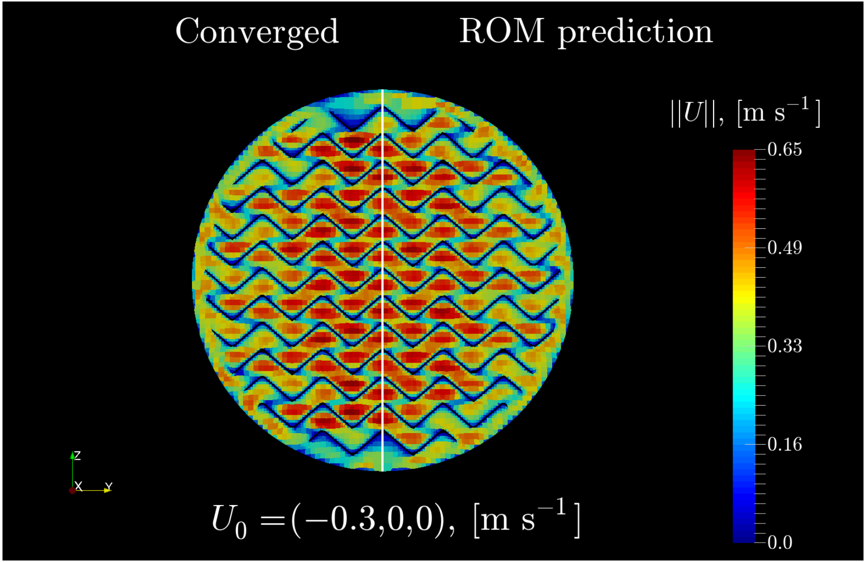
Full case: Flow through the Mellapak 250.X packing



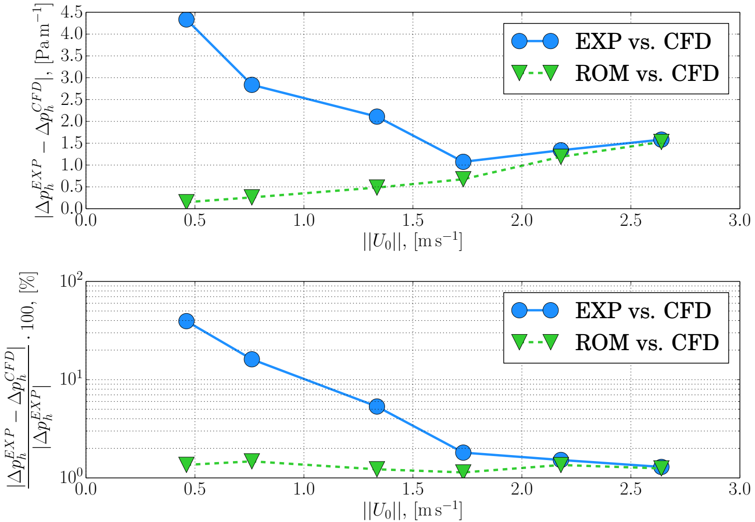
Full case: Predicted vs. converged solution in L1



Full case: Predicted vs. converged solution in L1



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



Cost function: Single phase, toy problem

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

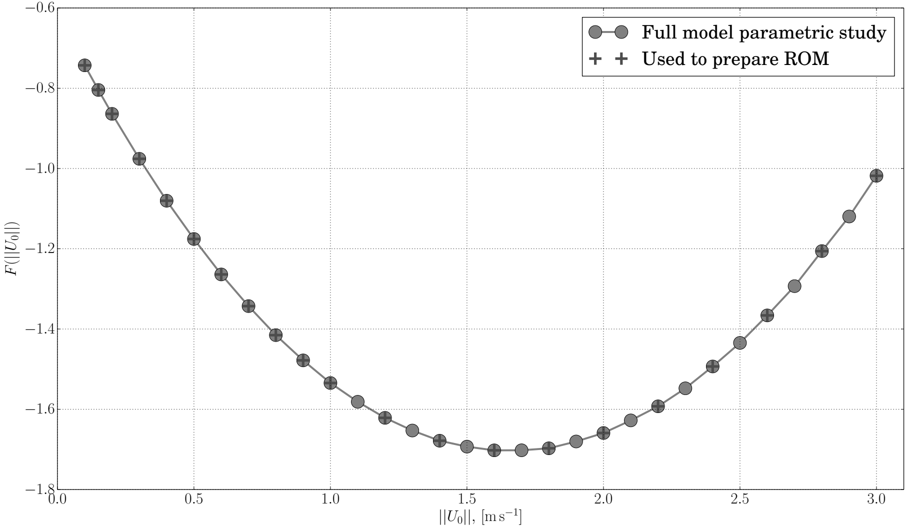
$$\Delta\tilde{p} = \Delta\tilde{p}(u_0), \quad Q = Q(u_0), \quad U_0 = (-u_0, 0, 0),$$

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

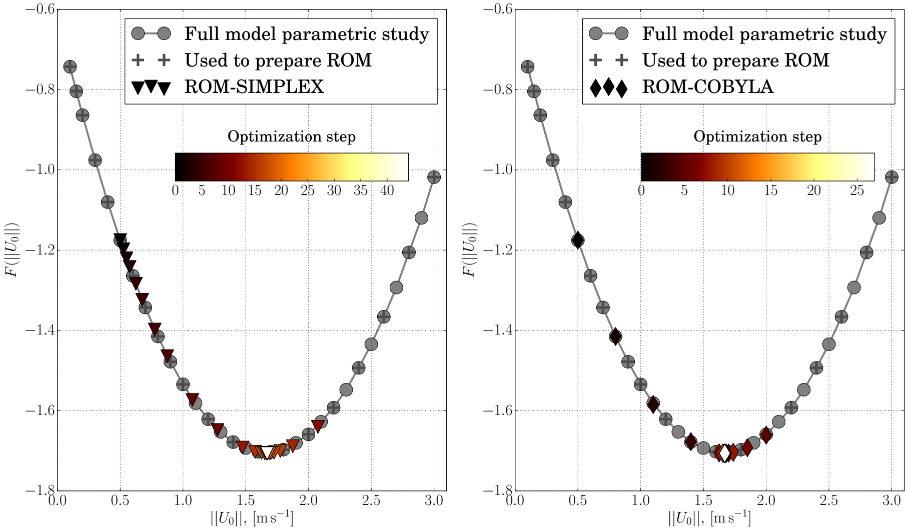
Q_{Max}, (Q_{Min}) .... maximal, (minimal) allowable gas flow rate

K .... relative importance of the two terms

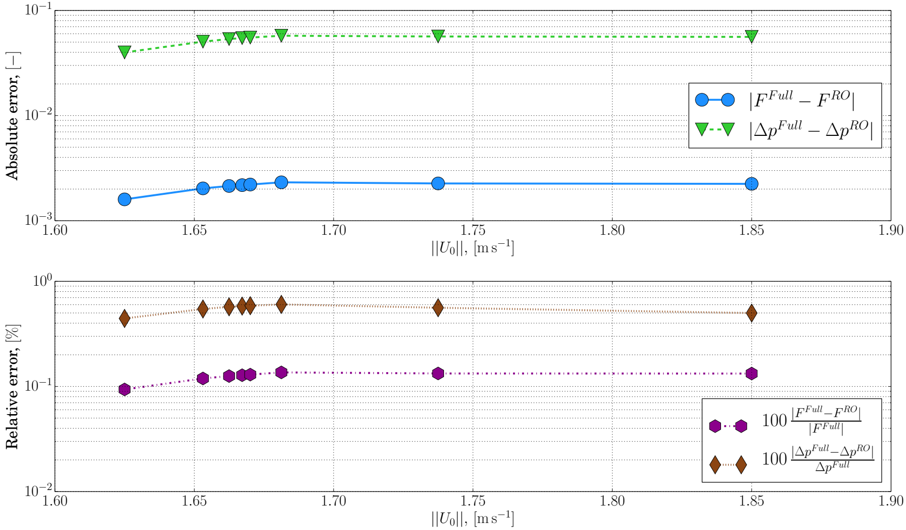
Available data: Cost function curve, $F(u_0)$, $u_0 \in \langle 0.1, 3.0 \rangle$



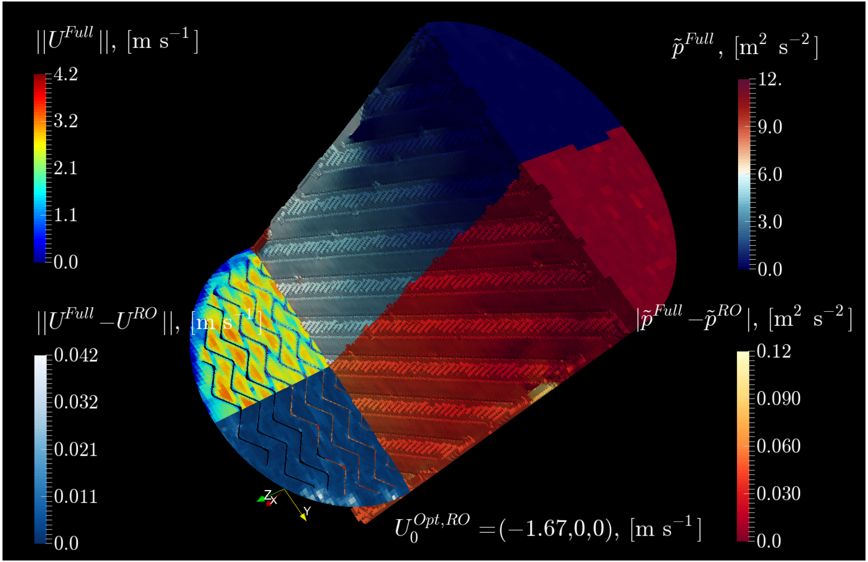
Cost function minimization: Results of SIMPLEX and COBYLA algorithms



Solution quality: Comparison of ROM results with reference simulations (COBYLA)



Solution quality: Comparison of RO and Full models results



Conclusions

Currently available

- Extended snapshot preparation for `simpleFoam`, `pimpleFoam` and `interFoam`
- Python module for ROM creation based on prepared outputs from OpenFOAM

Advantages

- Snaphots are created during postprocessing - simulations can be ran in parallel
- All the OpenFOAM capabilities are accessible (including e.g. MRF or turbulence modeling)

Disadvantages

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

Acknowledgments

The work of M. Isoz was supported by the Centre of Excellence for nonlinear dynamic behaviour of advanced materials in engineering CZ.02.1.01/0.0/0.0/15_003/0000493 (Excellent Research Teams) in the framework of Operational Programme Research, Development and Education.

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References

[1] Volkwein, S.: Proper Orthogonal Decomposition: Theory and Reduced-Order Modelling. *LN*, University of Konstanz, 2013.

[2] Volkwein, S.: Proper Orthogonal Decomposition: Applications in Optimization and Control

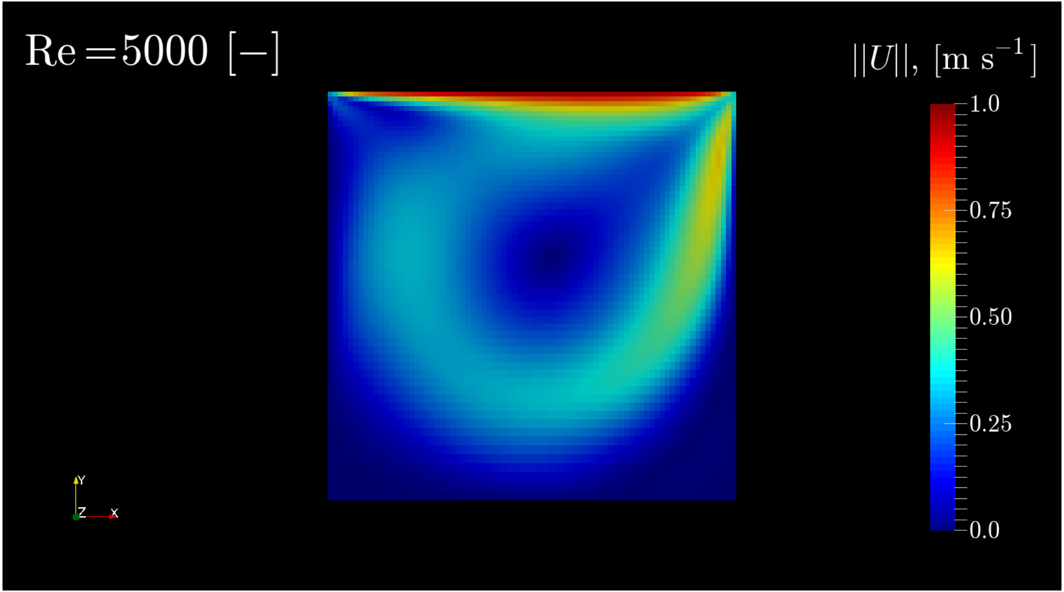
[3] Chaturantabut, S. Sorensen, D. C.: Nonlinear Model Reduction Via Discrete Empirical Interpolation, *SIAM J. Sci. Comput.*, vol. 32, (2010) pp. 2737–2764.

[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

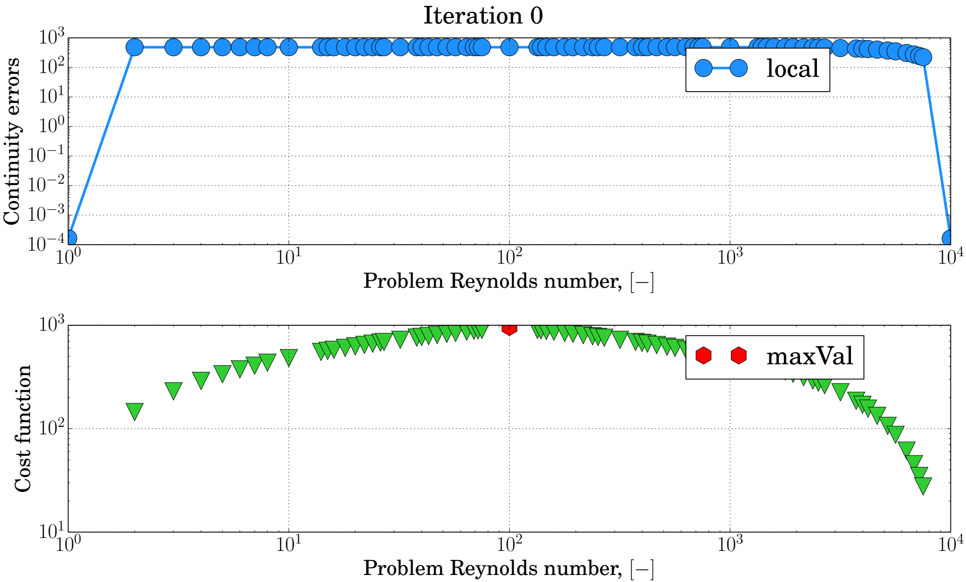
[5] Alla, A. Kutz, J. N.: Nonlinear Model Order Reduction Via Dynamic Mode Decomposition, *preprint*

Thank you for your attention

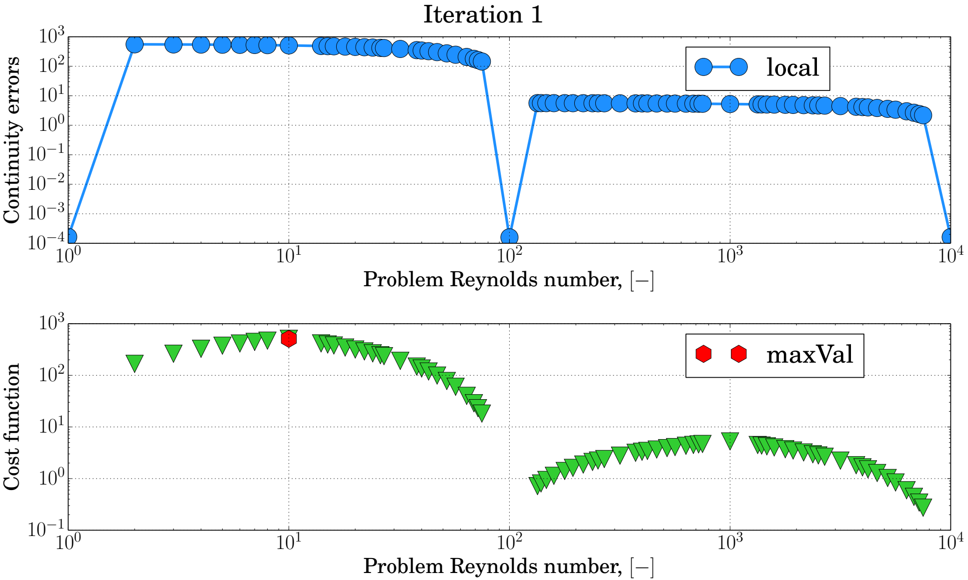
ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm



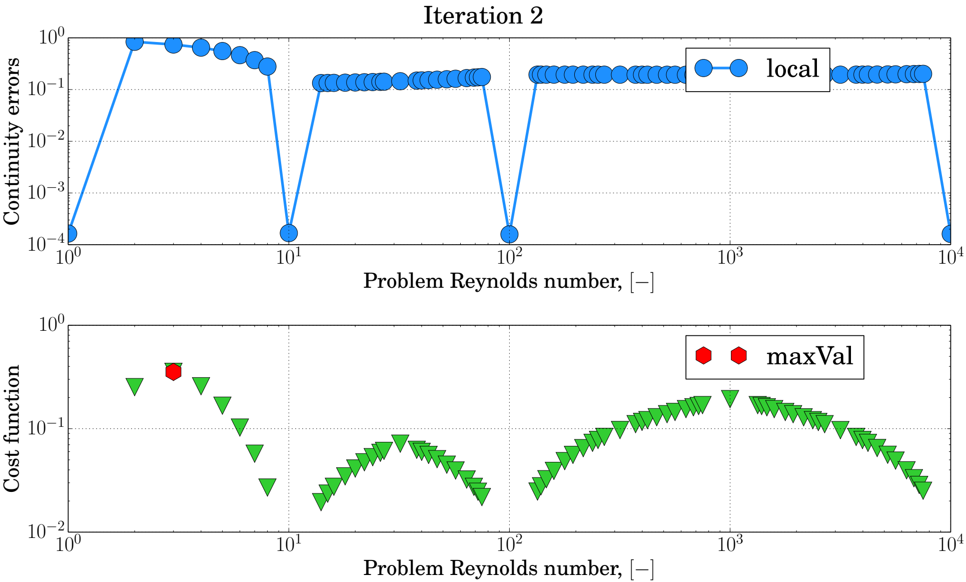
ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm



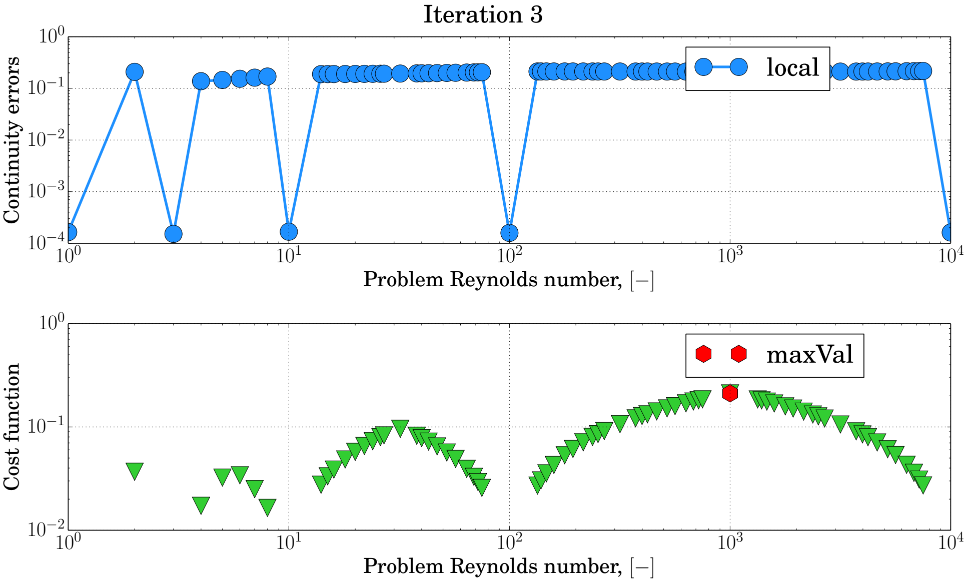
ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm



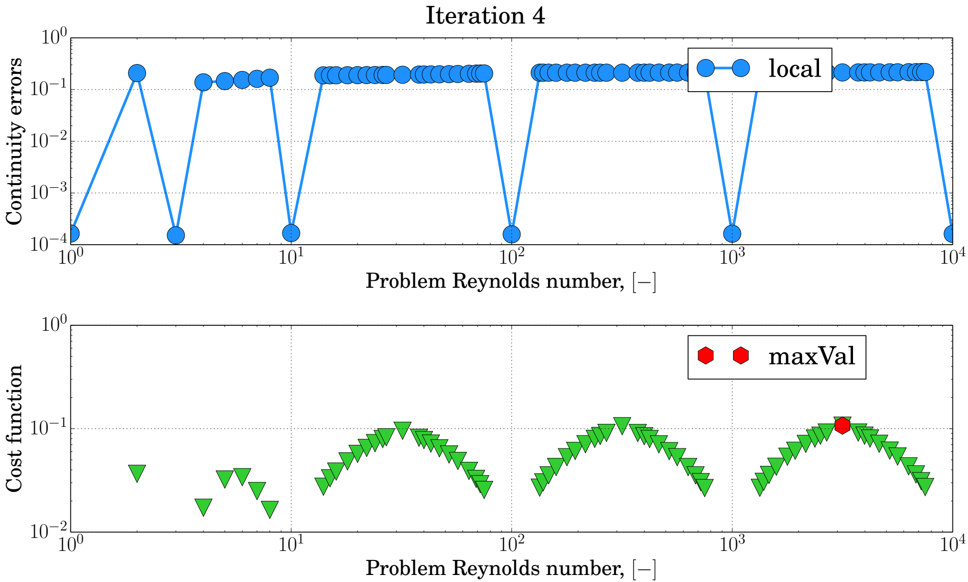
ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm



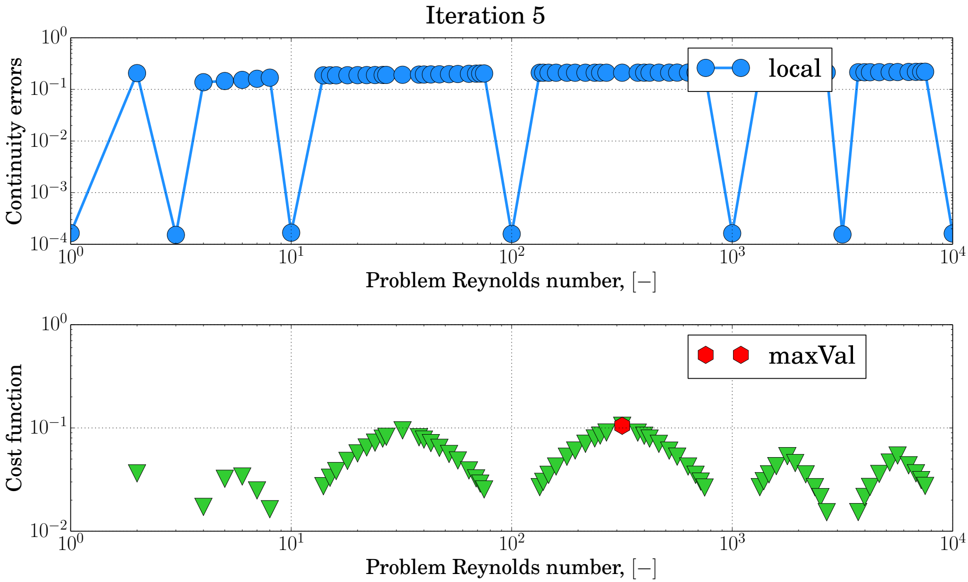
ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm



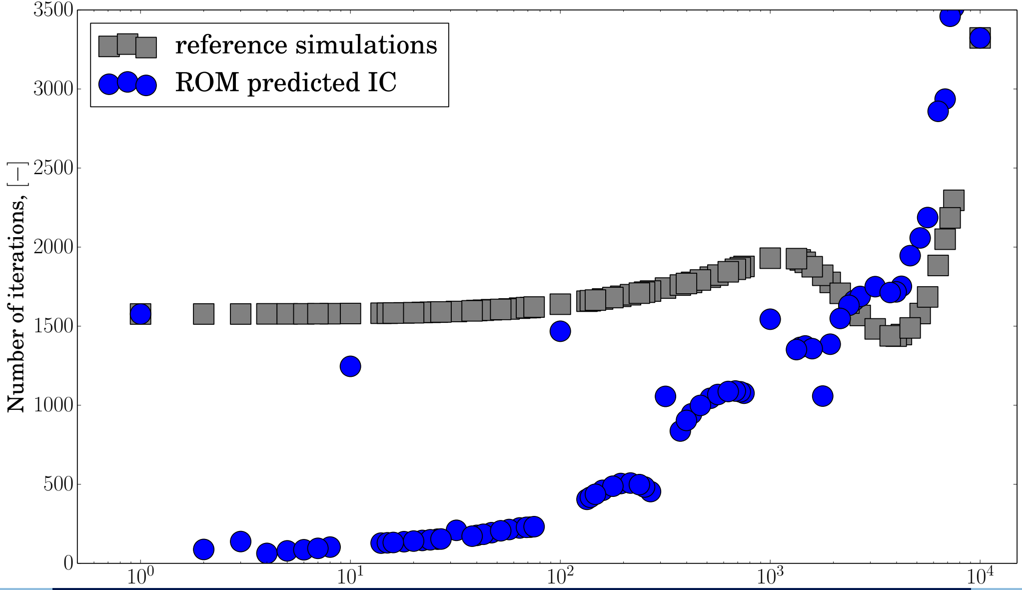
ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm



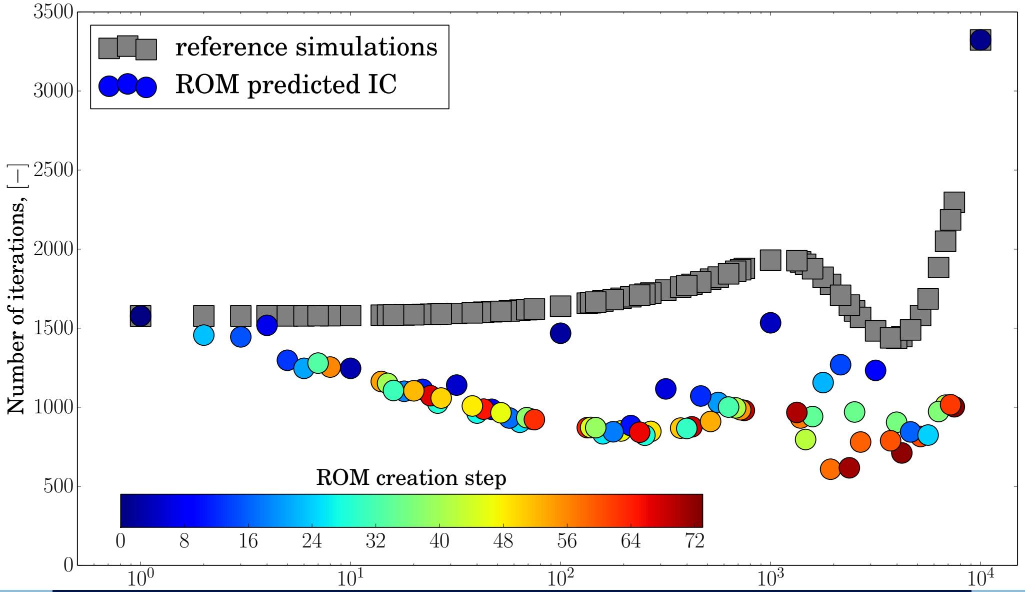
ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm

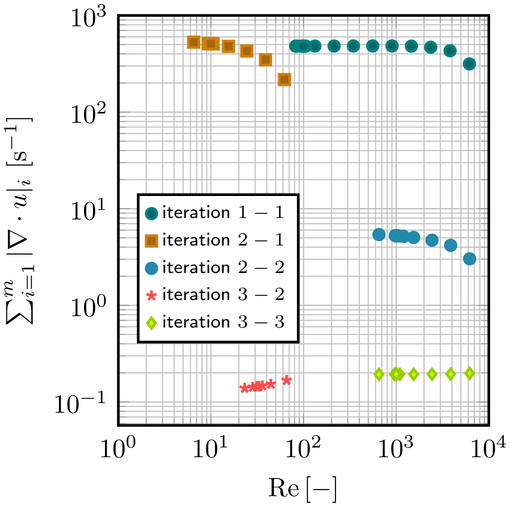


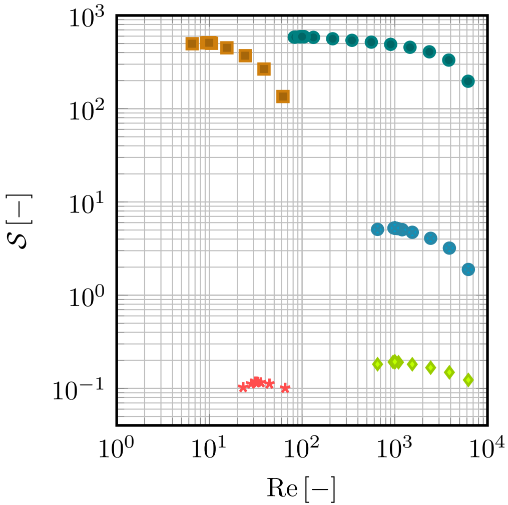
ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm



ROM size reduction: $\mathcal{S}^e$ selection based on greedy algorithm




10^3
10^2
10^1
10^0
10^{-1}
$\sum_{i=1}^{m} |\nabla \cdot u|_i \, [s^{-1}]$
iteration 1 — 1
iteration 2 — 1
iteration 2 — 2
iteration 3 — 2
iteration 3 — 3
10^0 10^1 10^2 10^3 10^4
Re [−]


10^3
10^2
10^1
10^0
10^{-1}
S [−]
10^0 10^1 10^2 10^3 10^4
Re [−]

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

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

- A brief reminder,

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

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

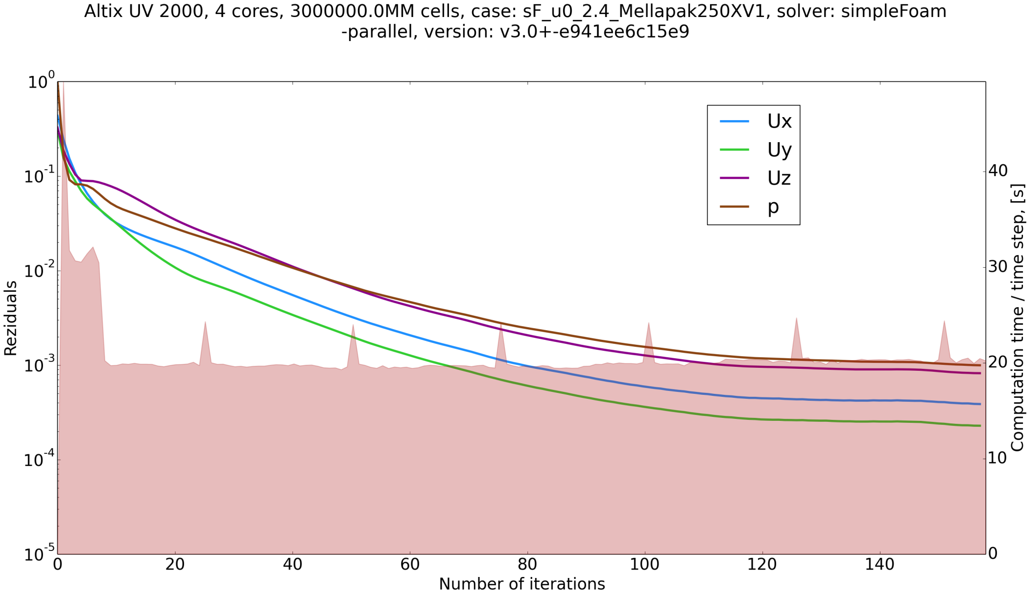
$$\Omega \approx \Omega^h = \bigcup_{i=1}^{\texttt{nCells}} \Omega_i^h, \quad V(\Omega) \approx V(\Omega^h) = \sum_{i=1}^{\texttt{nCells}} \delta\Omega_i^h$$

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

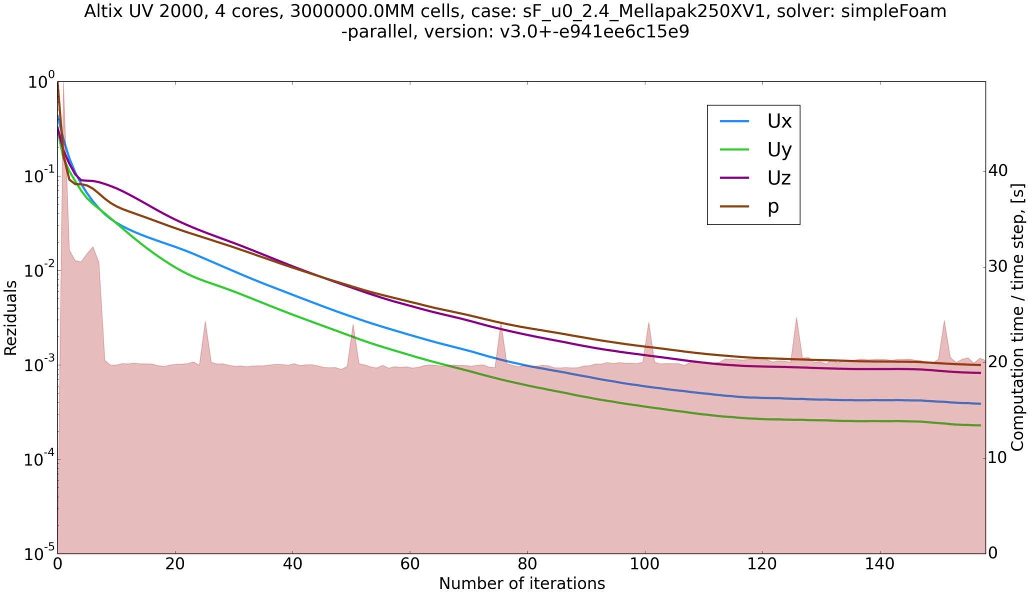
$$\langle \varphi, \tilde{\varphi} \rangle_{L^2(\Omega)} = \int_\Omega \varphi \tilde{\varphi} \, \mathrm{d}x \approx \sum_{i=1}^{\texttt{nCells}} \int_{\Omega_i^h} \varphi \tilde{\varphi} \, \mathrm{d}x = \sum_{i=1}^{\texttt{nCells}} \varphi_i^h \tilde{\varphi}_i^h \delta\Omega_i^h = \langle \varphi,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

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

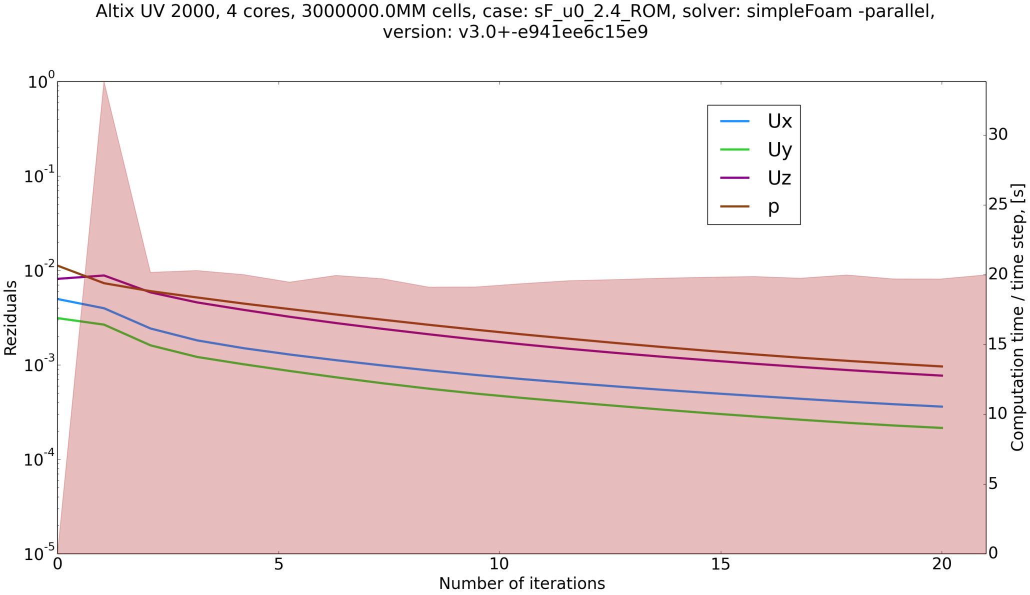
Full case: Residuals evolution, from potentialFoam initialized fields



Full case: Residuals evolution, from potentialFoam initialized fields



Full case: Residuals evolution, from ROM predicted fields, L1



Full case: Residuals evolution, from ROM predicted fields, L2