

POD-DEIM based ROMs for CFD applications



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MORE seminar,
Prague November 7 2016



① Introduction

② POD & DEIM

- Problem setting
- POD
- DEIM
- ROM

③ Link with OpenFOAM

- oF basics
- NS and p-U coupling

④ Applications

- Initial guess estimation for S.-S. simulations
- Full scale application example
- ROM based optimization

⑤ Conclusions



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Introduction

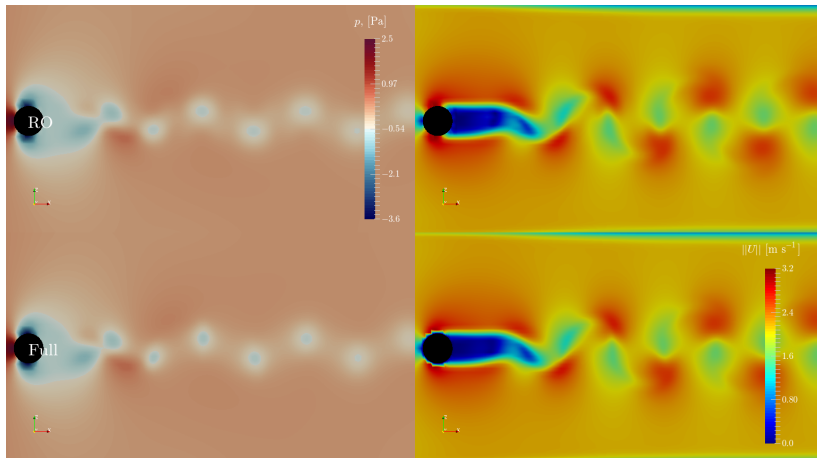


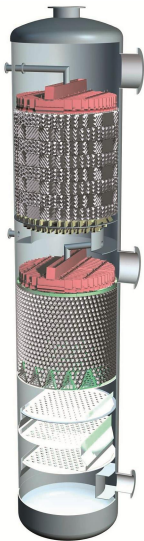
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Research motivation

Reducing the computational cost of modeling of complex systems





[Sulzer ChemTech]

Importance

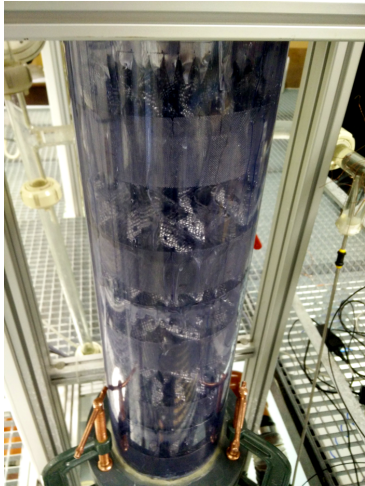
- Chemical industry creates mixtures but sells "pure species" (e.g. oil)
- 2014, 3% of energy consumption of the USA was due to the separation columns

Challenges

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

Packed column

Complex multiphase flow





Momentum and continuity equations, N phases

$$\rho_i \frac{\partial}{\partial t}(u_i) + \nabla \cdot (\rho_i u_i \otimes u_i) = \nabla \cdot \tau + F_i, \quad i = 1, \dots, N$$

$$\rho_i = \rho(c_i, T_i), \quad \nabla \cdot (u_i) = S_i^\rho = \sum_{j=1}^M \hat{R}_{i,j}^c$$

Mass transfer (no reaction), M species

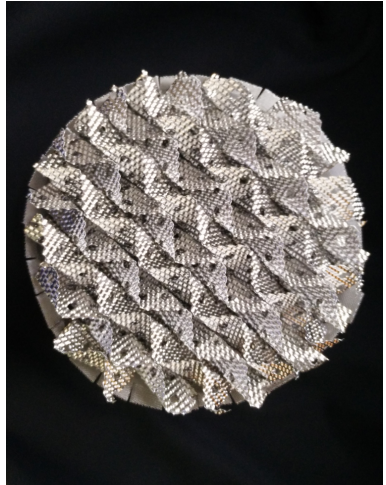
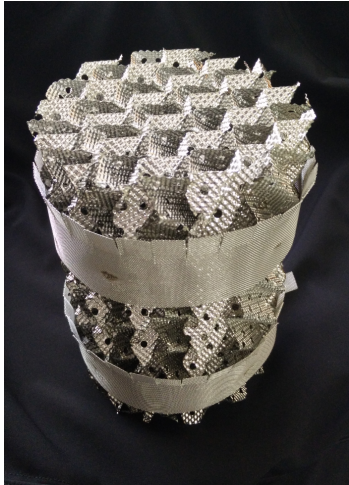
$$\frac{\partial}{\partial t} c_{i,j} + \nabla \cdot (u_i c_{i,j}) = \nabla \cdot (\Gamma_{i,j}^c \nabla c_{i,j}) + S_{i,j}^c, \quad j = 1, \dots, M$$

Heat transfer (no reaction), N phases

$$\frac{\partial}{\partial t} T_i + \nabla \cdot (u_i T_i) = \nabla \cdot (\Gamma_i^T \nabla T_i) + S_i^T, \quad i = 1, \dots, N$$

Structured packing

Curled, textured, perforated plate





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POD & DEIM



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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

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

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

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

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



Algorithm 1 POD basis of rank l with weighted inner product

Require: Snapshots $\{y_j\}_{j=1}^n$, POD rank $l \leq d$, 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, $[\bar{\Psi}, \Sigma, \bar{V}] = \text{svd}(\bar{Y})$;
 - 4: Set $\sigma = \text{diag}(\Sigma)$;
 - 5: Compute $\varepsilon(l) = \sum_{i=1}^l \sigma_i / \sum_{i=1}^d \sigma_i$;
 - 6: Truncate $\bar{\Psi} \leftarrow [\bar{\psi}_1, \dots, \bar{\psi}_l] \in \mathbb{R}^{m \times l}$;
 - 7: Compute $\Psi = W^{-1/2}\bar{\Psi} \in \mathbb{R}^{m \times l}$;
 - 8: **return** POD basis, Ψ , and ratio $\varepsilon(l)$
-

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 $U_{\vec{i}} c = u_{\vec{i}};$
 - 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.



Introduce the Galerkin ansatz and Fourier modes

- Prerequisites: $\Psi \in \mathbb{R}^{m \times l}$, $\Phi \in \mathbb{R}^{m \times p}$, $W \in \mathbb{R}^{m \times m}$, $\vec{i} \in \mathbb{R}^p$
- Quick note,

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

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

- Ansatz for Galerkin projection, $l < d$

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

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

$$\sum_{j=1}^l \dot{\eta}_j^l \psi_j = \sum_{j=1}^l \eta_j^l A \psi_j + f(t, y^l(t)), \quad t \in (0, T)$$

$$y_0 = \sum_{j=1}^l \eta_j^l(0) \psi_j$$



Introduce the reduced-order model

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

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

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

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

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



Deal with the non-linearities I

- Identify the problem,

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

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

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

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

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

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

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



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

- Plug in the matrix P ,

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

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

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

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

- Write the final ROM

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

where

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



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Link with OpenFOAM



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Rewrite OpenFOAM discretization as above studied problem

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

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

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

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

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

- 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, $\{(y_i, A_i, b_i)\}_{i=1}^n$, $A_i \in \mathbb{R}^{m \times m}$, $i = 1, \dots, n$
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,

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

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

$$= \varpi(t)\Psi^T W A_{i-1} \Psi + (1 - \varpi(t))\Psi^T W A_i \Psi = \varpi(t)A_{i-1}^l + (1 - \varpi(t))A_i^l$$

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

Example 1 – Passive scalar advection

Phase-volume fraction advection in multiphase flow



interFoam – Volume-of-Fluid model for multiphase flow

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

$$\alpha_t + \mathcal{L}_\alpha^h(t, \alpha) = 0 \rightarrow \alpha_t = A_\alpha(t)\alpha + b_\alpha(t, \alpha) \rightarrow \dot{\eta}_\alpha^l = \hat{A}_\alpha^l(t)\eta_\alpha^l + \hat{b}_\alpha^l(t, \eta_\alpha^l)$$

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

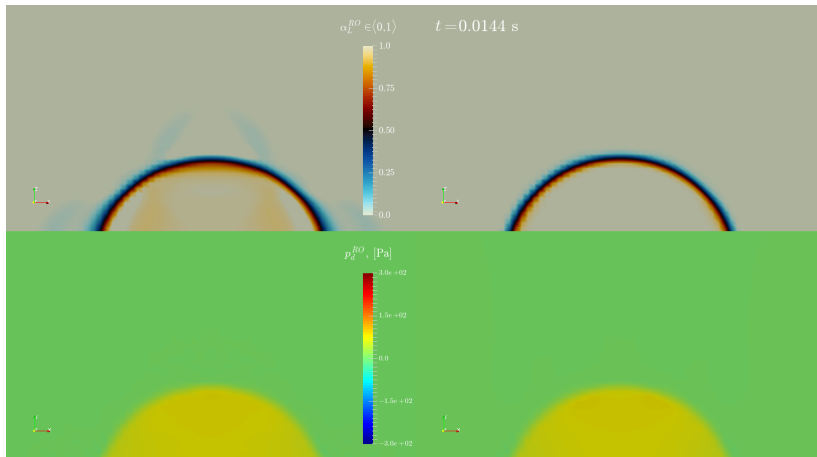
Example of implementation in OpenFOAM

```
fvm::div( phi, alphas, alphaScheme )
+ fvc::div(
    -fvc::flux(
        -phir, scalar(1)-alpha, alphasScheme
    ),
    alphas, alphasScheme
) == 0
```

Link: $fvm \rightarrow A_\alpha(t)$, $fvc \rightarrow b_\alpha(t, y)$

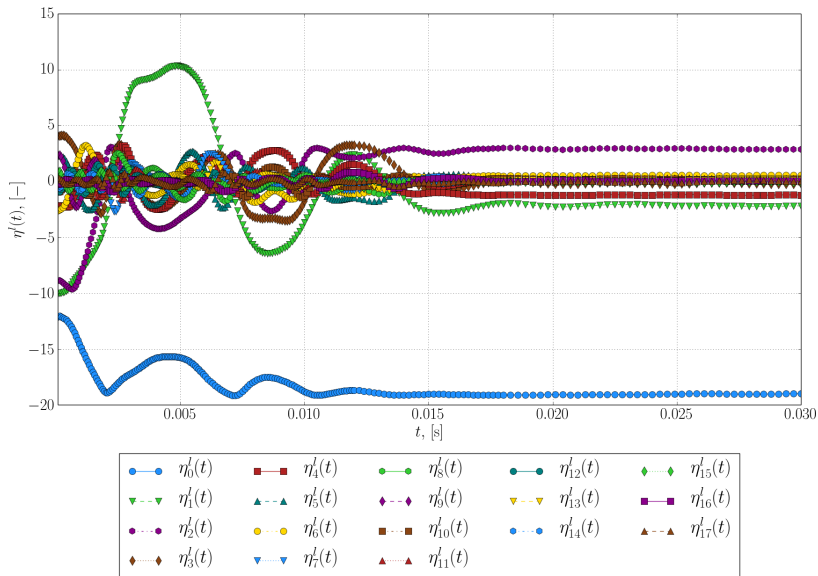
Example 1 – Passive scalar advection

Numerical results



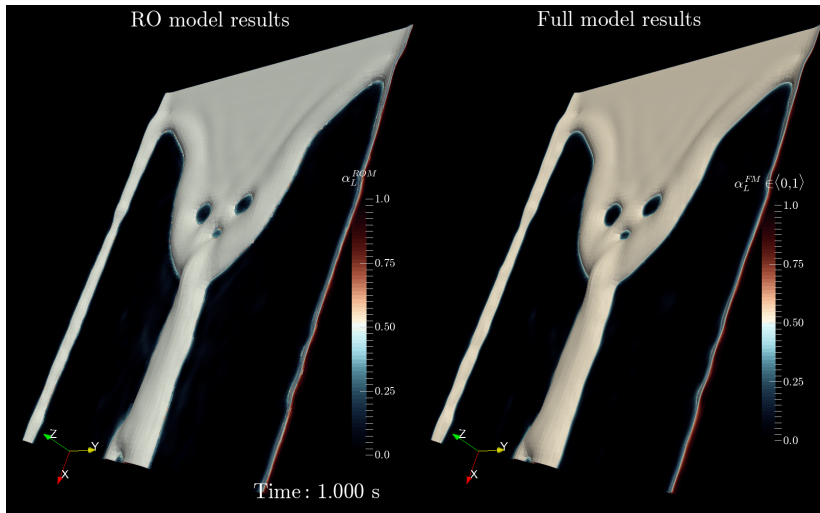
Example 1 – Passive scalar advection

Numerical results



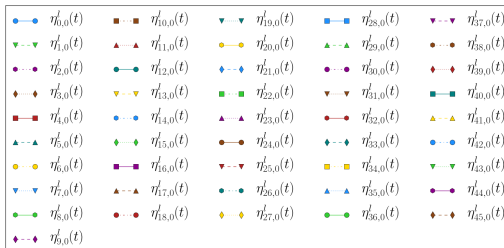
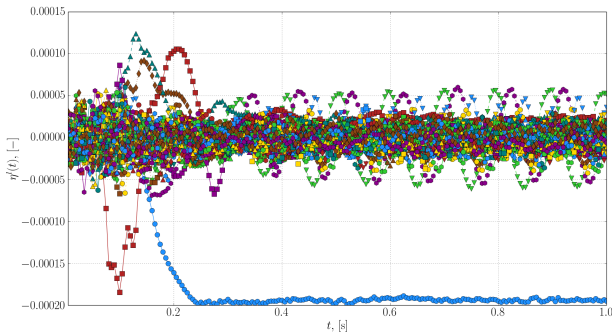
Example 1 – Passive scalar advection

Numerical results



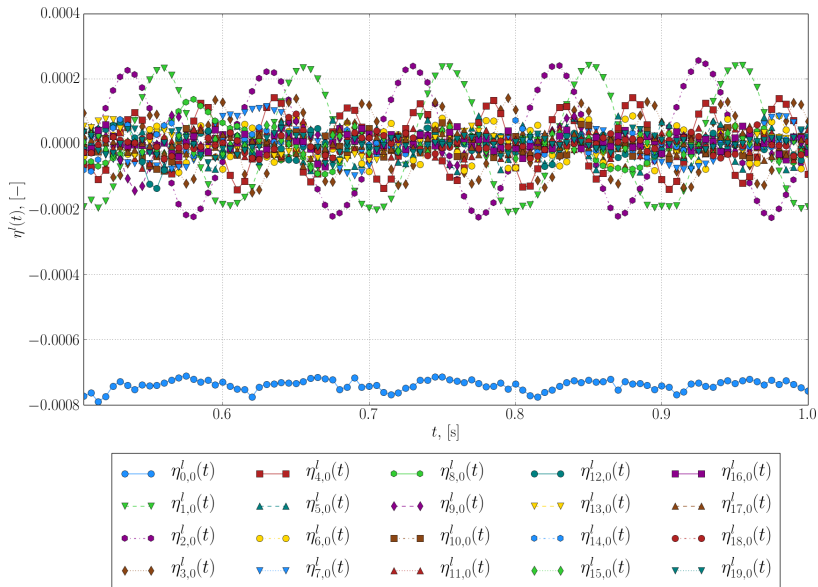
Example 1 – Passive scalar advection

Numerical results



Example 1 – Passive scalar advection

Numerical results

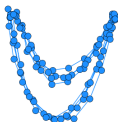


Example 1 – Passive scalar advection

Numerical results



Modes 1,2,3



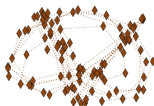
Modes 2,3,4



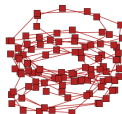
Modes 3,4,5



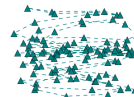
Modes 4,5,6



Modes 5,6,7



Modes 6,7,8





Navier-Stokes equations for incompressible fluids

$$u_t + \nabla \cdot (u \otimes u) - \nabla \cdot (\nu \nabla u) = -\nabla \tilde{p} + \tilde{f}$$

$$\nabla \cdot u = 0$$

$$u = G(u), p = H(p) \quad \forall (t, x) \in I \times \partial\Omega$$

$$u = u_0, p = p_0 \quad \forall (0, x) \in \Omega$$

Wanted: $\dot{y}_u = A_u(t)y_u + b_u(t, y_u)$

Example of implementation in OpenFOAM

```
fvm::div(phi, U)
+ turbulence->divDevReff(U)
==
-fvc::grad(p) + fvOptions(U)
```

Link: $\text{fvm} \rightarrow A_u(t), \text{fvc} \rightarrow b_u(t, y_u), \text{turbulence} \rightarrow A_u(t), b_u(t, y_u)$



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

$$\begin{aligned} u^* &\leftarrow Au^* = f - B^T p^{k-1} \\ p^k &\leftarrow BD^{-1} B^T p^k = BD^{-1} (f - (L + U)u^*) \\ u^k &\leftarrow D^{-1} (f - (L + U)u^* - B^T p^k) \end{aligned}$$

At convergence

$$\begin{aligned} BD^{-1} B^T p^k &= BD^{-1} (f - (L + U)u^*) \approx BA^{-1} B^T p = BA^{-1} f \\ u &= D^{-1} (f - (L + U)u^*) - D^{-1} B^T p \end{aligned}$$

Outcome for ROM

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

Construction of ROM for p

Implementation of pressure equation in OpenFOAM and construction of ROM based on it



Notation

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

Implementation of pressure equation 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

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

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

Link: $\mathbf{fvm} \rightarrow A_p(t), \mathbf{fvc} \rightarrow b_p(t, y_p)$



Expansion of snapshots for pressure

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

Expanded snapshots for pressure:

$$\mathcal{S}^e = \{(y_{p,i}, A_{p,i}, b_{p,i}, \textcolor{blue}{rAUMORE}_i, \textcolor{blue}{HMOREbyAUMORE}_i)_{i=1}^n\}$$

Storage

$\mathcal{S} \dots n [(1 + \textcolor{red}{3})m + (5 + \textcolor{red}{5})m + (1 + \textcolor{red}{3})m] \approx 15nm$ values

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

Computational cost

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

$\mathcal{S}^e \dots$

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

$\sim n$ calculations of $\Psi^T W \textcolor{blue}{rAUMORE}_i \Psi$,

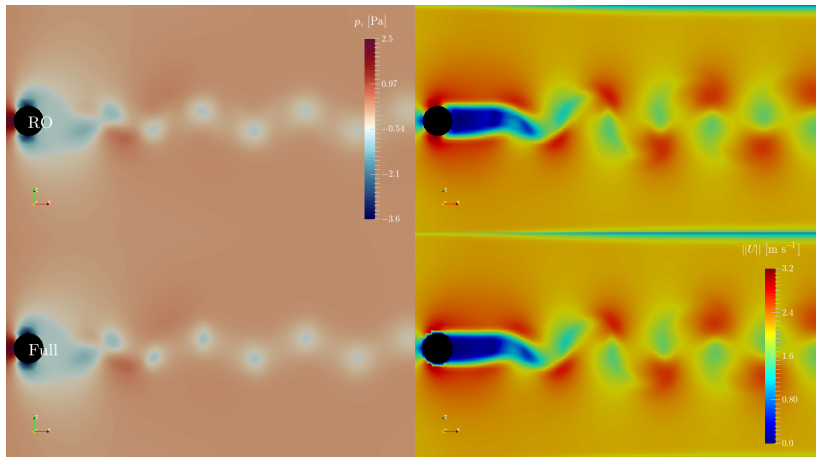
$\sim n$ calculations of $\Psi^T W \textcolor{blue}{HMOREbyAUMORE}_i \Psi$,

evaluation of 1 ROM + interpolation between $\textcolor{blue}{rAUMORE}_i^{\textcolor{brown}{ROM}}$ and between $\textcolor{blue}{HMOREbyAUMORE}_i^{\textcolor{brown}{ROM}}$

$$U_i \approx \textcolor{blue}{HMOREbyAUMORE}^{\textcolor{brown}{ROM}} + \textcolor{blue}{rAUMORE}^{\textcolor{brown}{ROM}} \nabla p^{\textcolor{brown}{ROM}}$$

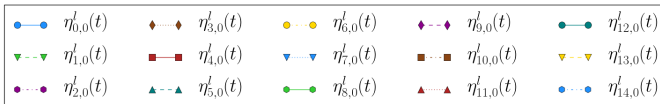
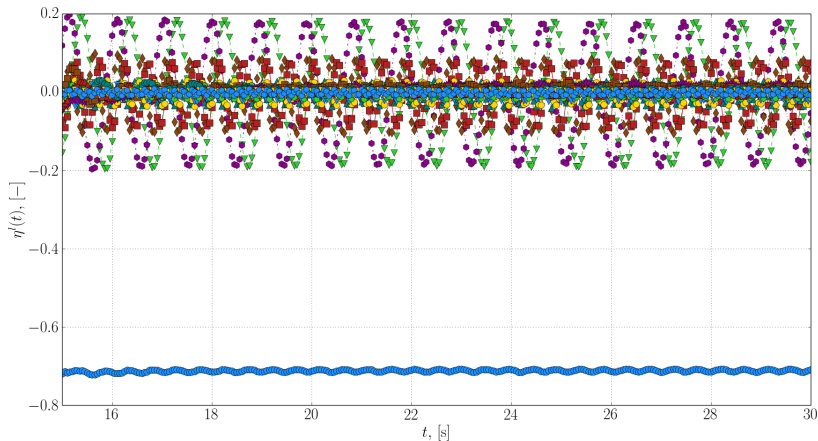
Example 2 – Von Karman vortex row

Validation of the approach



Example 2 – Von Karman vortex row

Validation of the approach

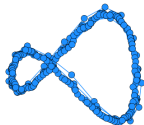


Example 2 – Von Karman vortex row

Validation of the approach



Modes 1,2,3



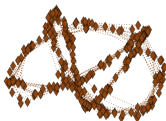
Modes 2,3,4



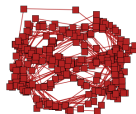
Modes 3,4,5



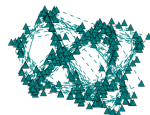
Modes 4,5,6



Modes 5,6,7



Modes 6,7,8





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Applications

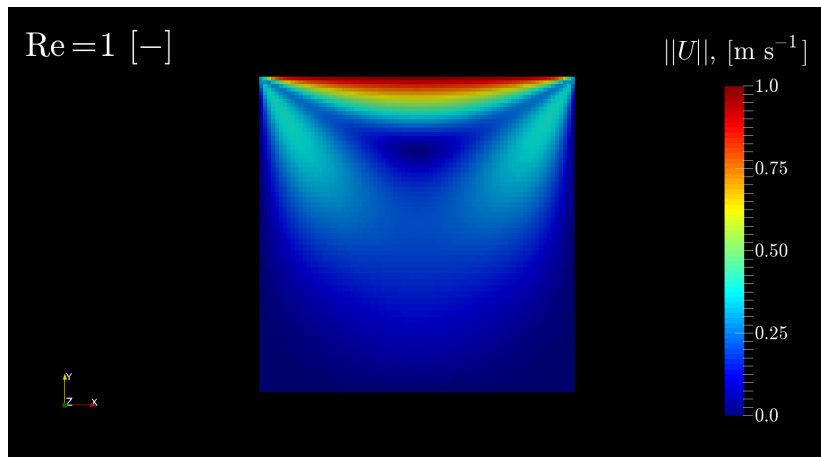


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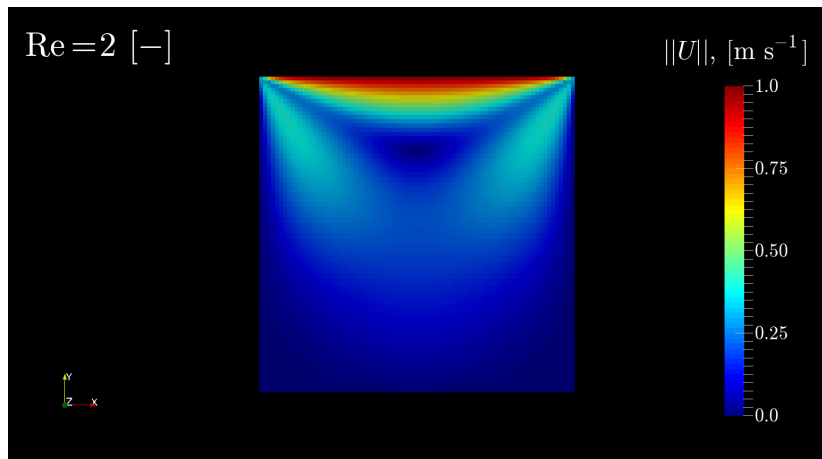


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



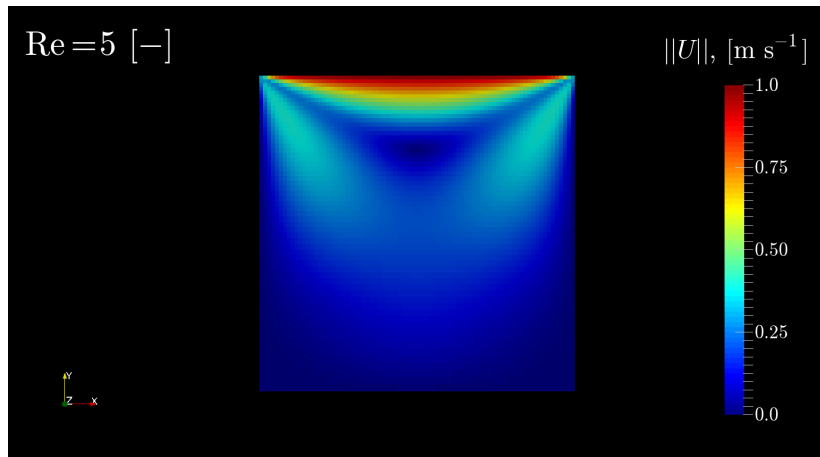


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



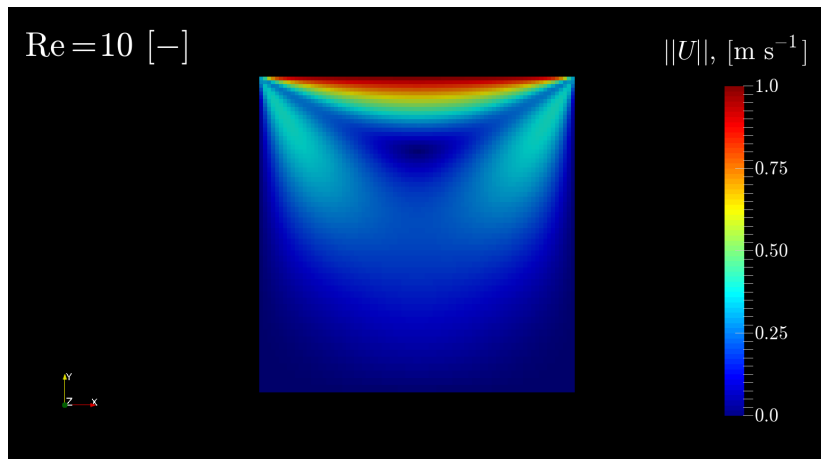


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



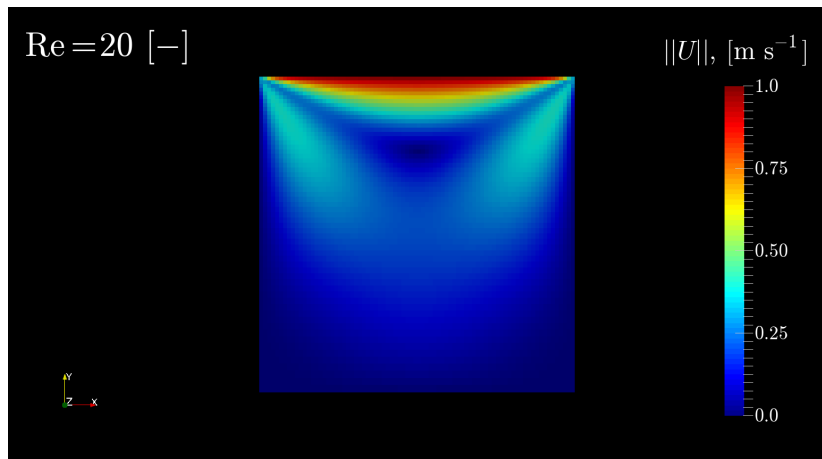


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



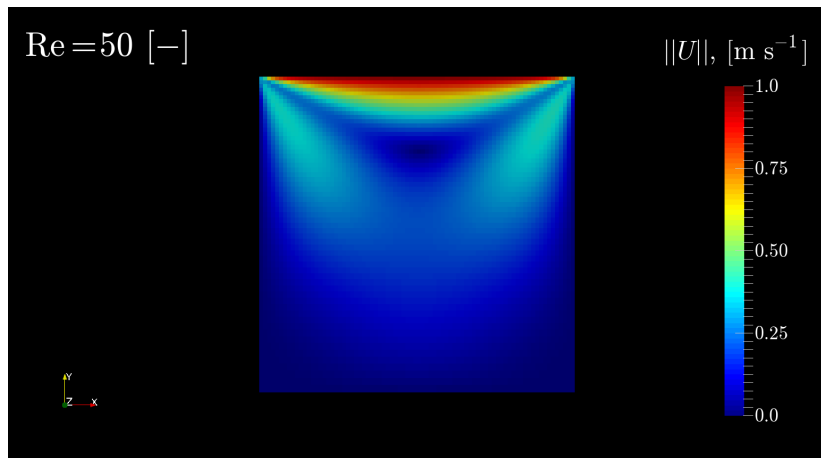


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



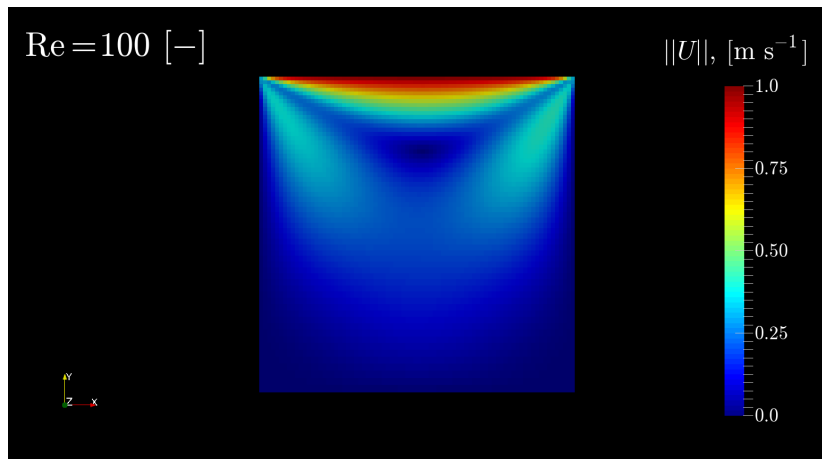


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



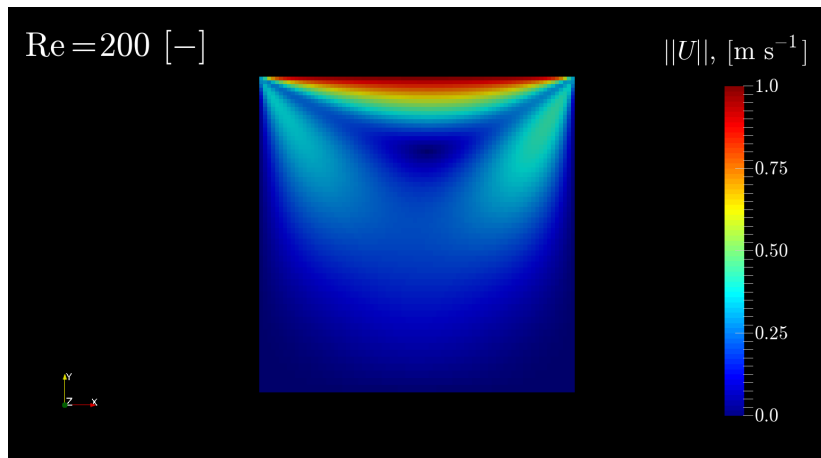


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



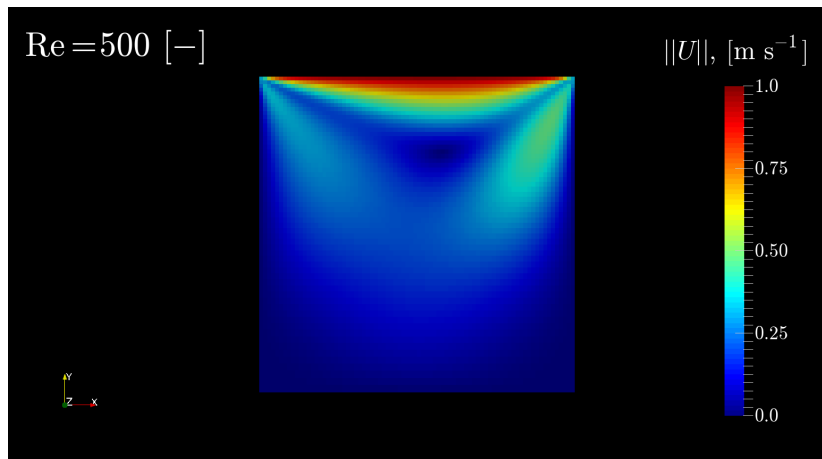


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



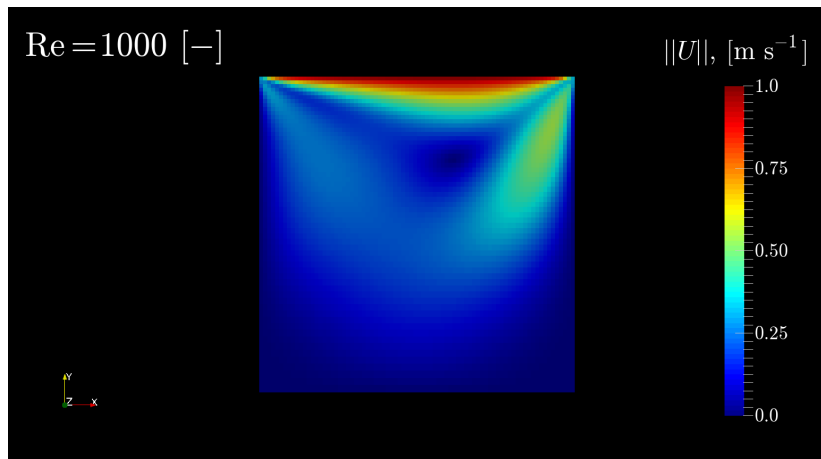


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



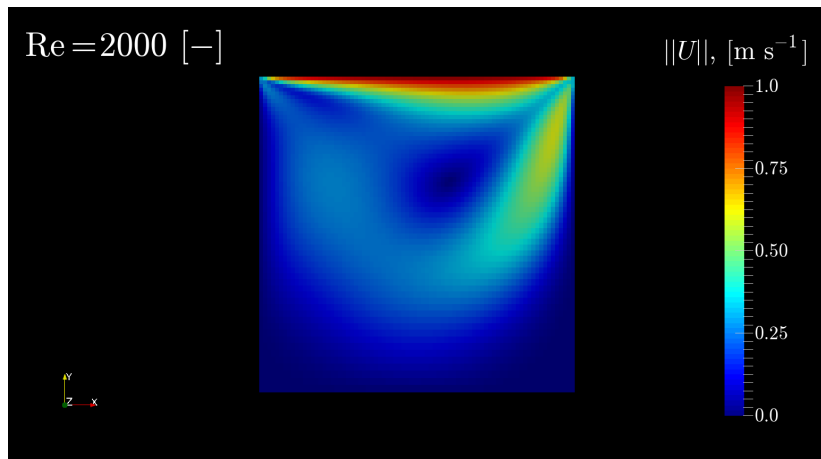


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



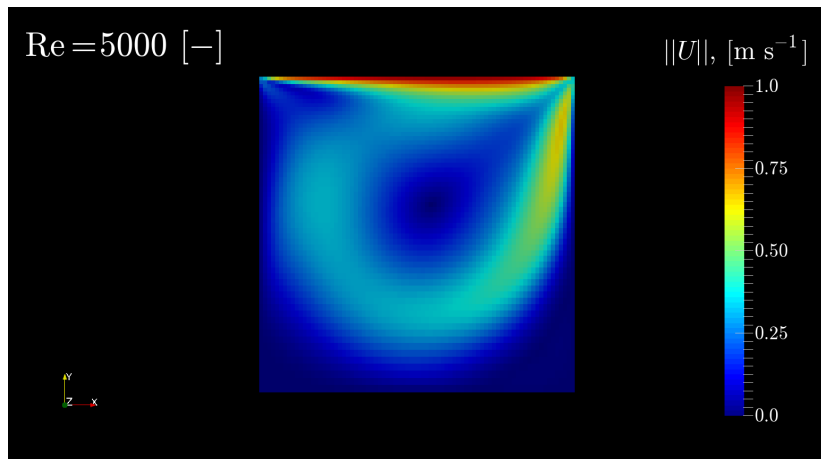


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



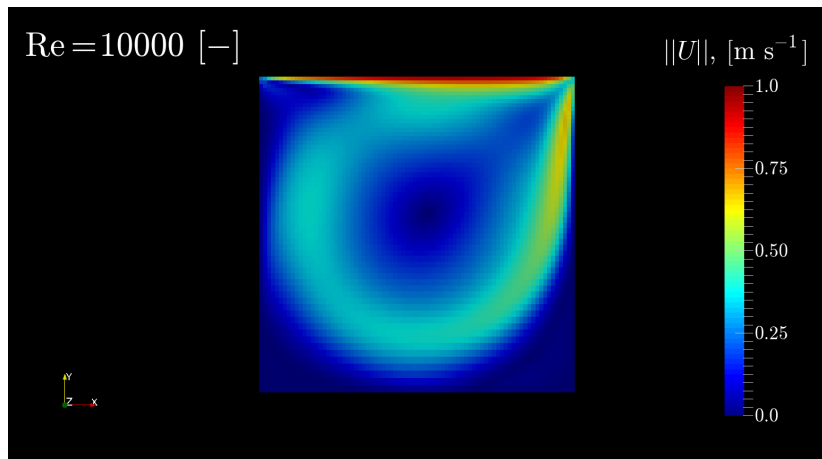


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



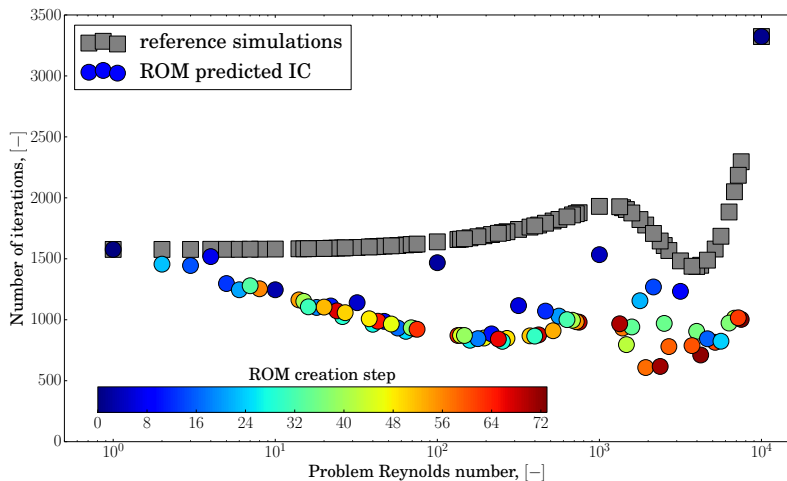


Test case: Standard OpenFOAM cavity case, variable $Re = LU/\nu$



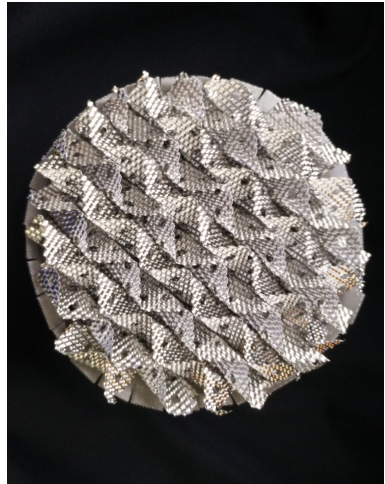
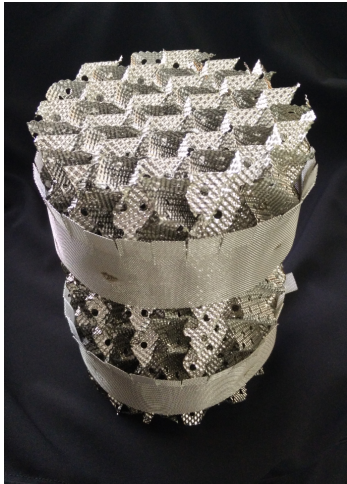


Test case: Iteration save-up for simpleFoam (serial run)



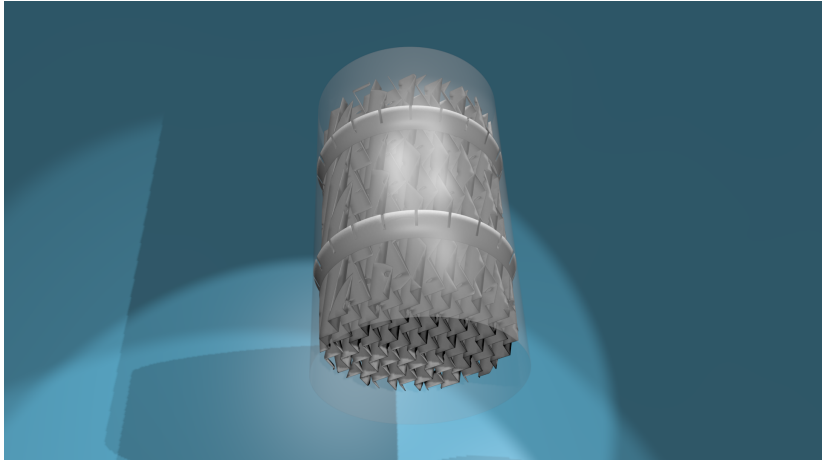


Remainder: Geometry of structured packing



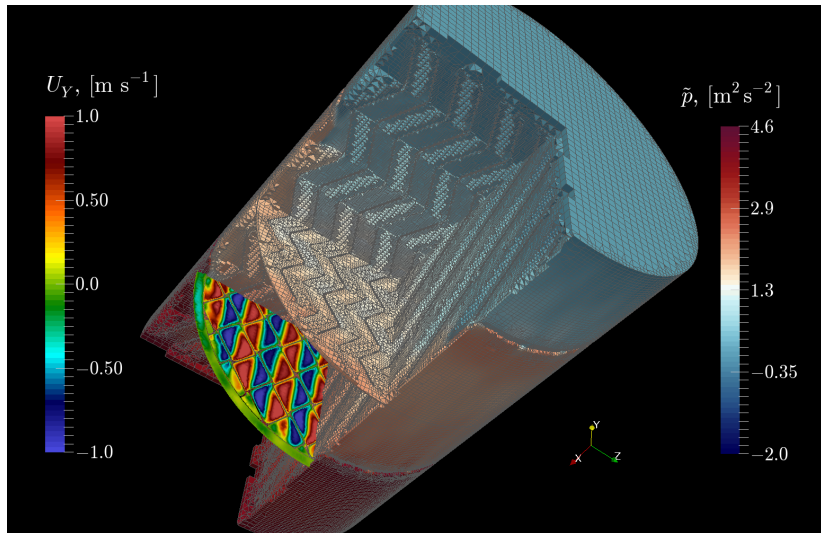


Geometry: Mellapak 250.X structured packing



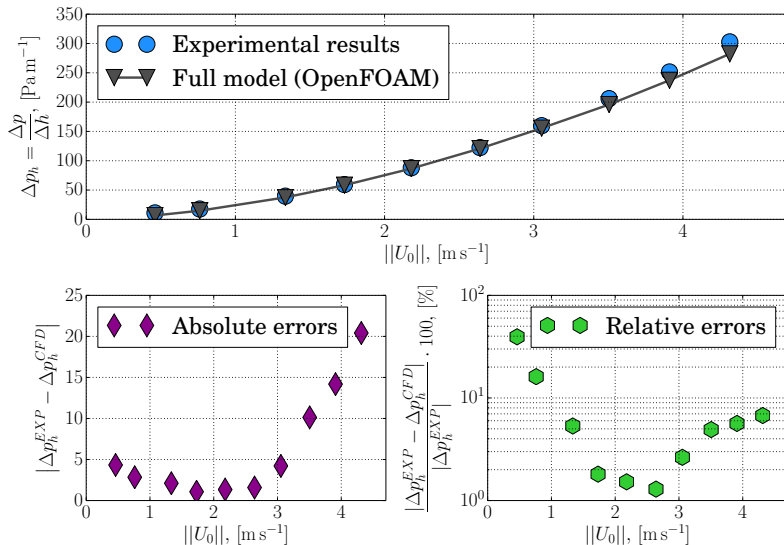


Gas flow simulation: Incompressible steady state RANS simulation



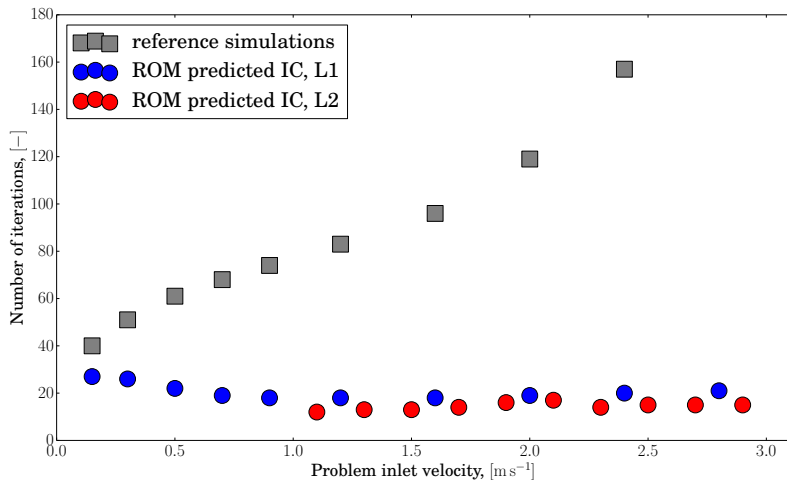


Comparison with experimental data: [Haidl, J. UCT Prague]





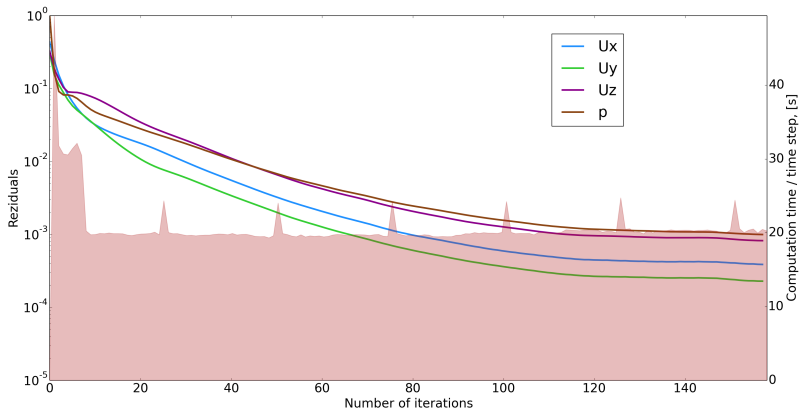
Full case: Flow through the Mellapak 250.X packing





Full case: Residuals evolution, from potentialFoam initialized fields

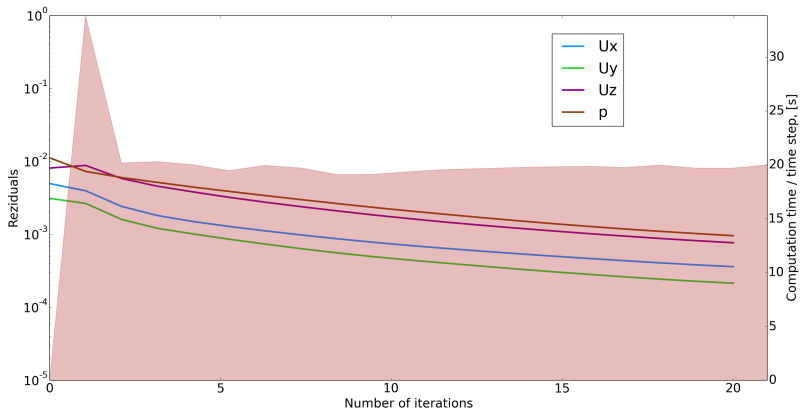
Altix UV 2000, 4 cores, 3000000.0MM cells, case: sF_u0_2.4_Mellapak250XV1, solver: simpleFoam
-parallel, version: v3.0+-e941ee6c15e9





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

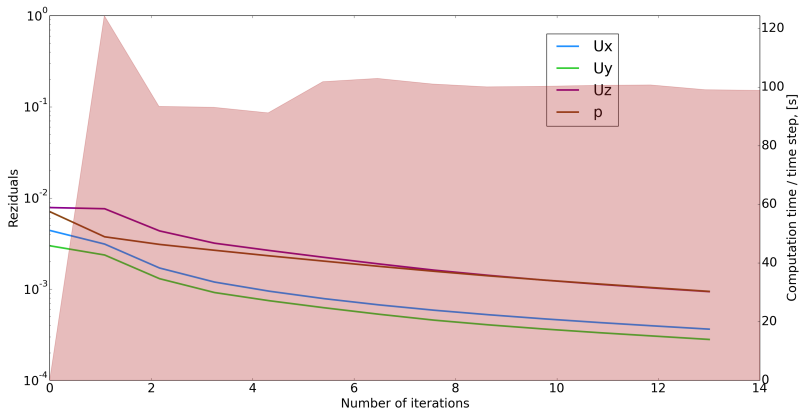
Altix UV 2000, 4 cores, 3000000.0MM cells, case: sF_u0_2.4_ROM, solver: simpleFoam -parallel,
version: v3.0+-e941ee6c15e9





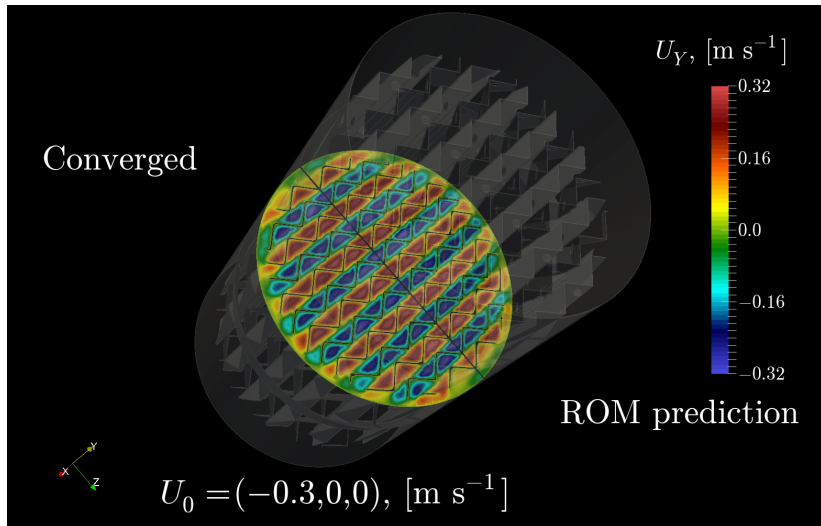
Full case: Residuals evolution, from ROM predicted fields, L2

Intel(R) Core(TM) i5-5200U CPU @ 2.20GHz, 4 cores, 3000000.0MM cells, case: sF_u0_1.5_ROM2, solver: simpleFoam -parallel, version: v3.0+-e941ee6c15e9



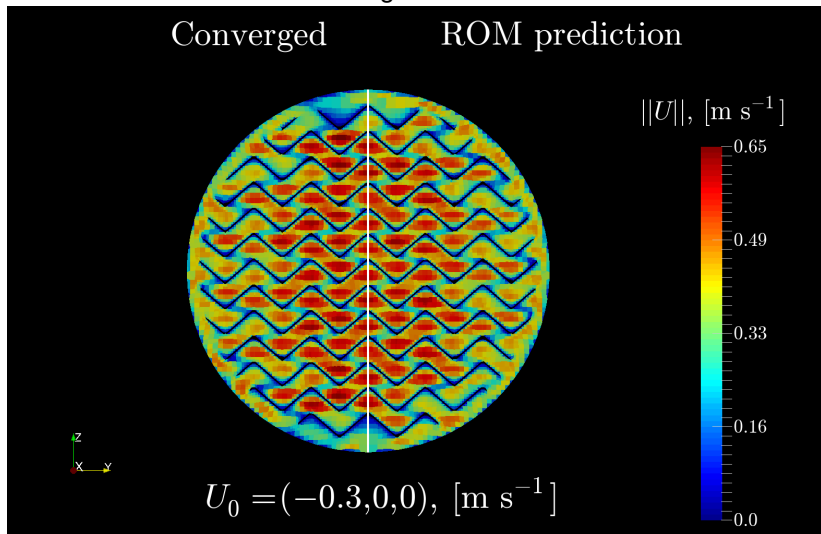


Full case: Predicted vs. converged solution in L1



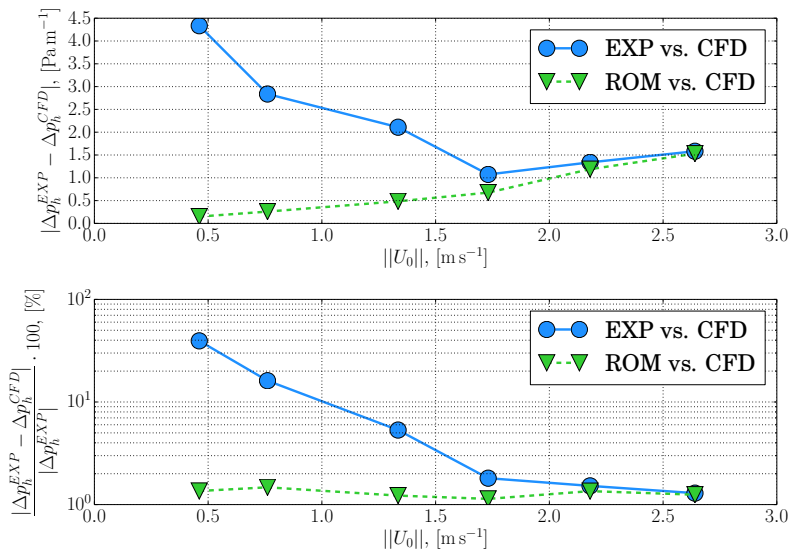


Full case: Predicted vs. converged solution in L1





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





Cost function: Single phase, toy problem

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

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

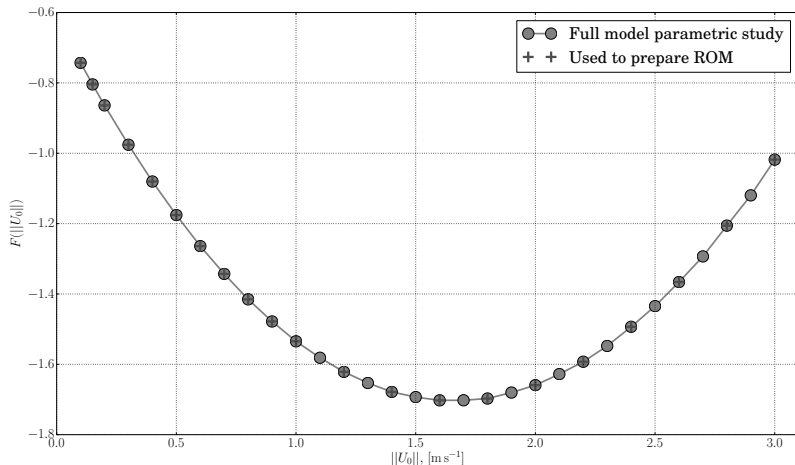
$\Delta\tilde{p}_{Max}$ maximal allowable pressure loss

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

K relative importance of the two terms

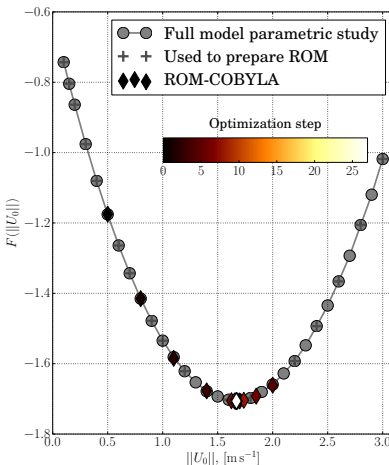
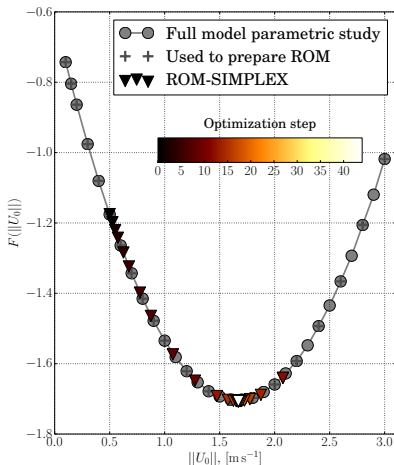


Available data: Cost function curve, $F(u_0)$, $u_0 \in \langle 0.1, 3.0 \rangle$



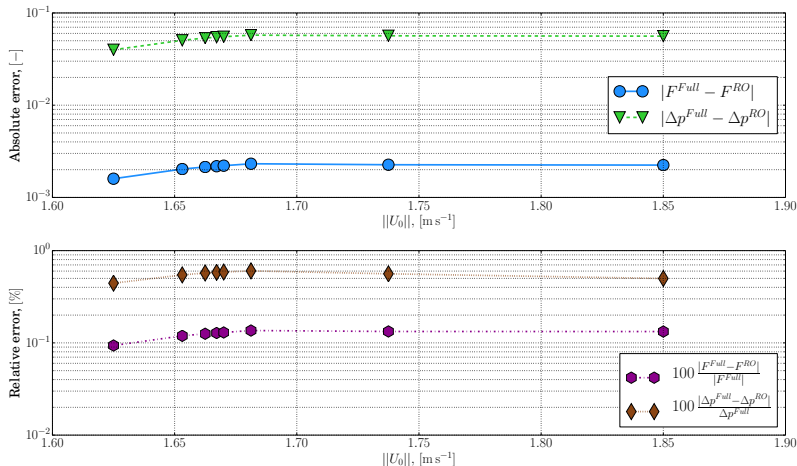


Cost function minimization: Results of SIMPLEX and COBYLA algorithms



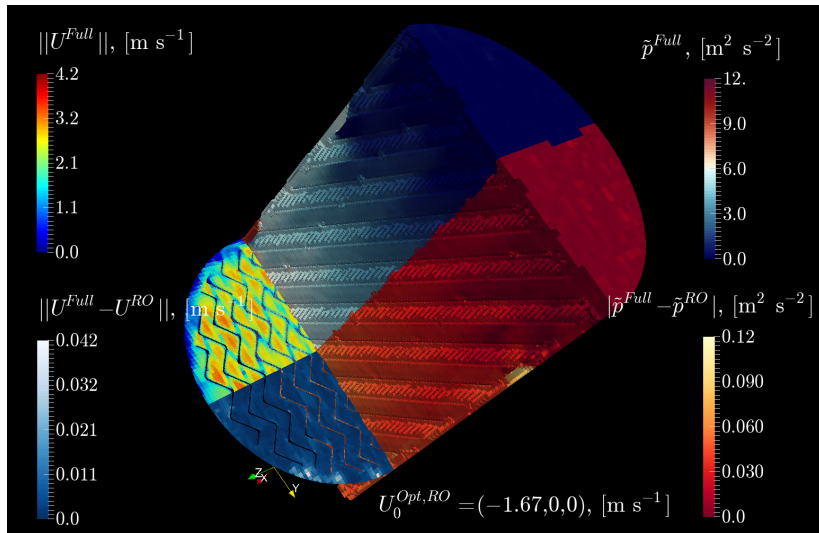


Solution quality: Comparison of ROM results with reference simulations (COBYLA)





Solution quality: Comparison of RO and Full models results





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Conclusions



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Currently available

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

Advantages

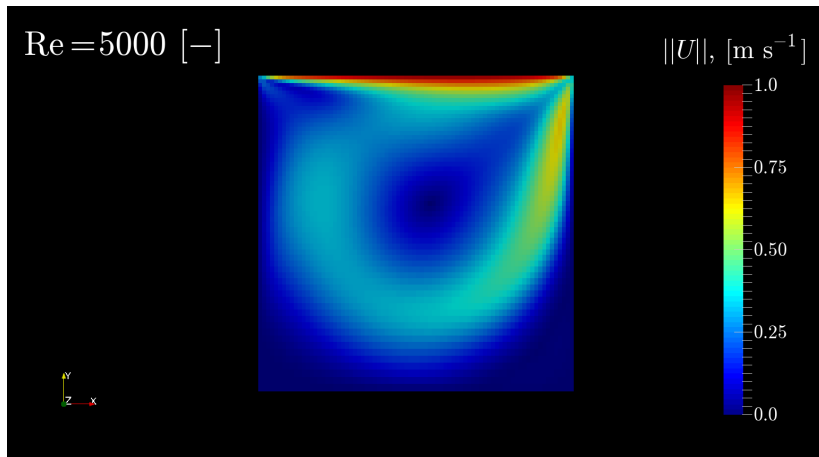
- Snapshots are created during postprocessing - **simulations can be ran in parallel**
- **All the OpenFOAM capabilities are accessible** (including e.g. MRF or turbulence modeling)

Disadvantages

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

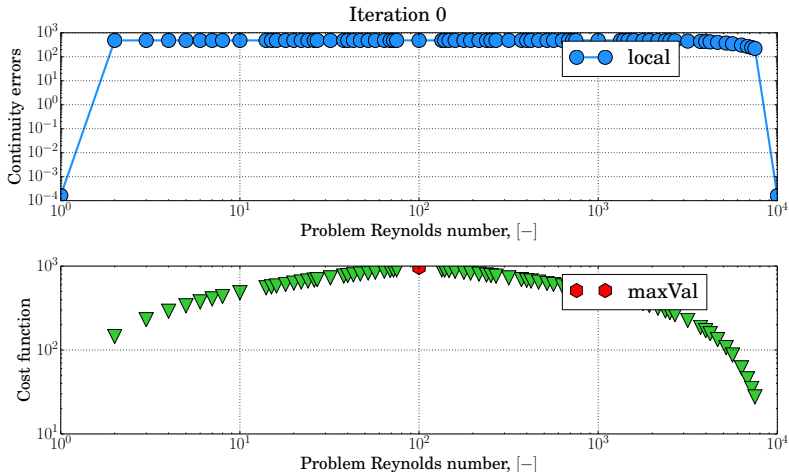


ROM size reduction: \mathcal{S}^e selection based on greedy algorithm



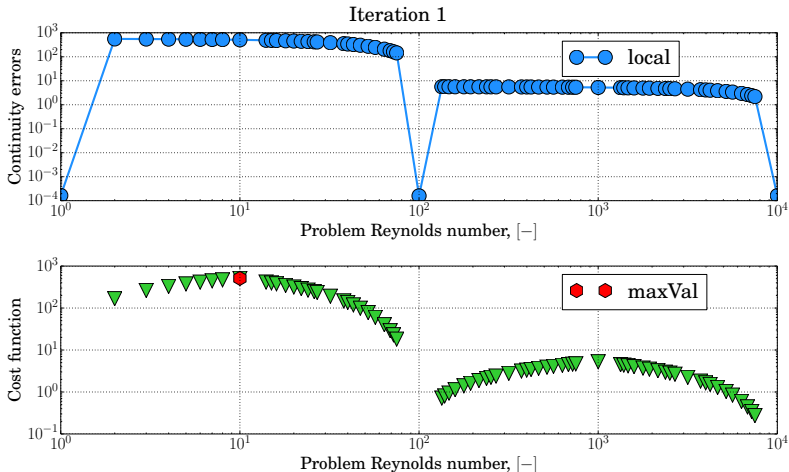


ROM size reduction: \mathcal{S}^e selection based on greedy algorithm

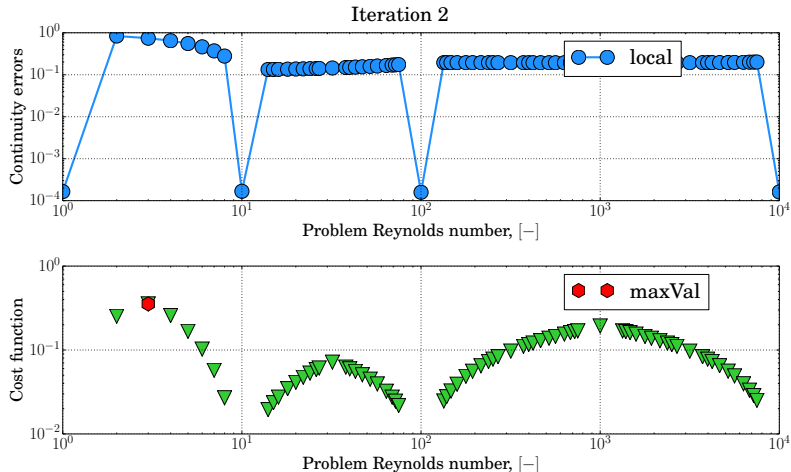




ROM size reduction: \mathcal{S}^e selection based on greedy algorithm

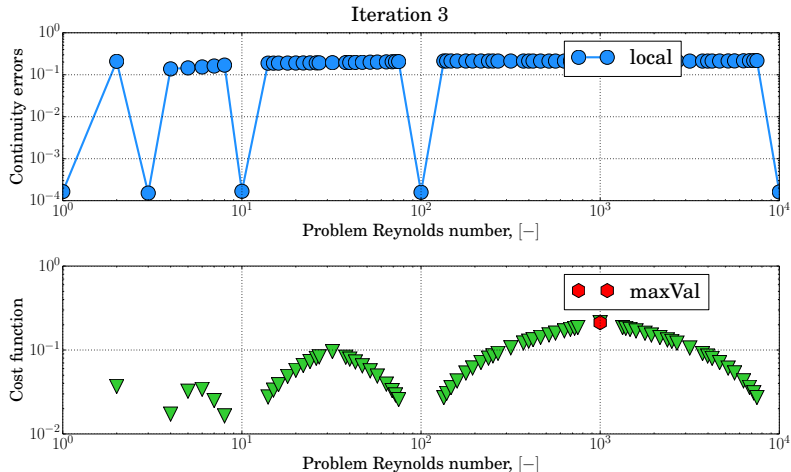


ROM size reduction: \mathcal{S}^e selection based on greedy algorithm



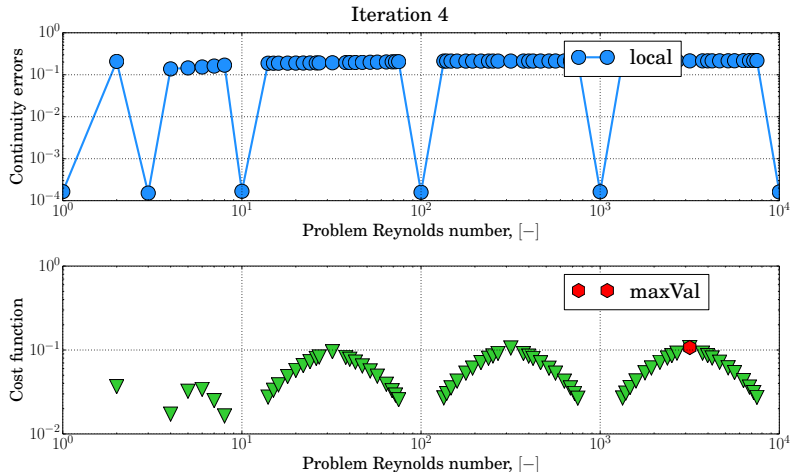


ROM size reduction: \mathcal{S}^e selection based on greedy algorithm



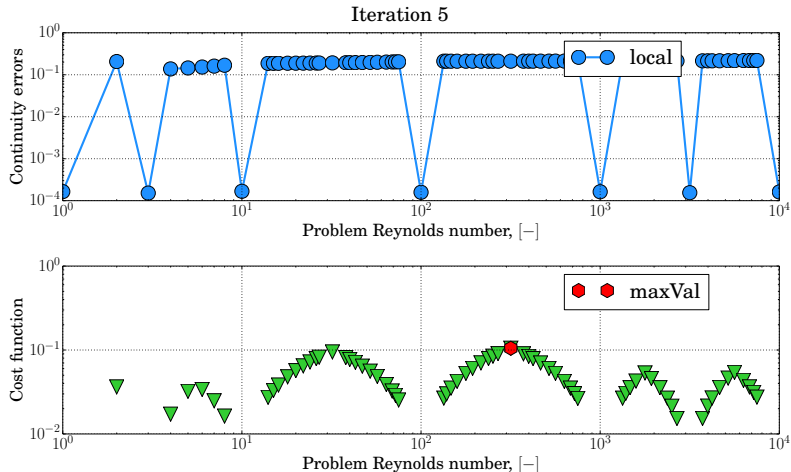


ROM size reduction: \mathcal{S}^e selection based on greedy algorithm

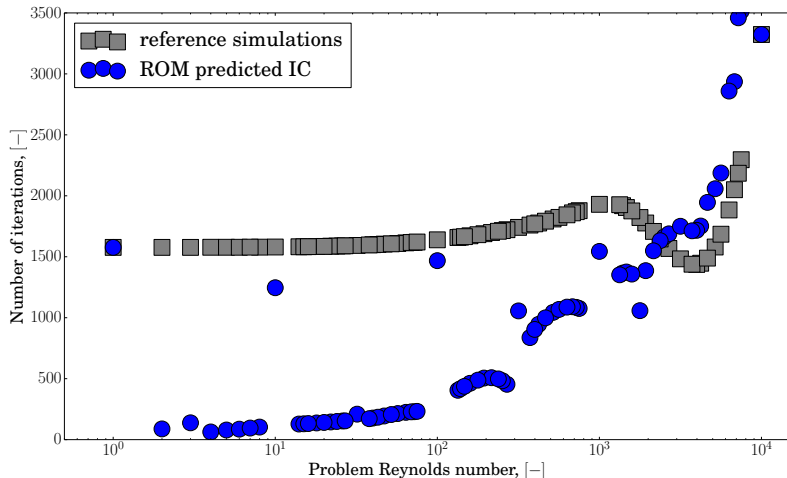




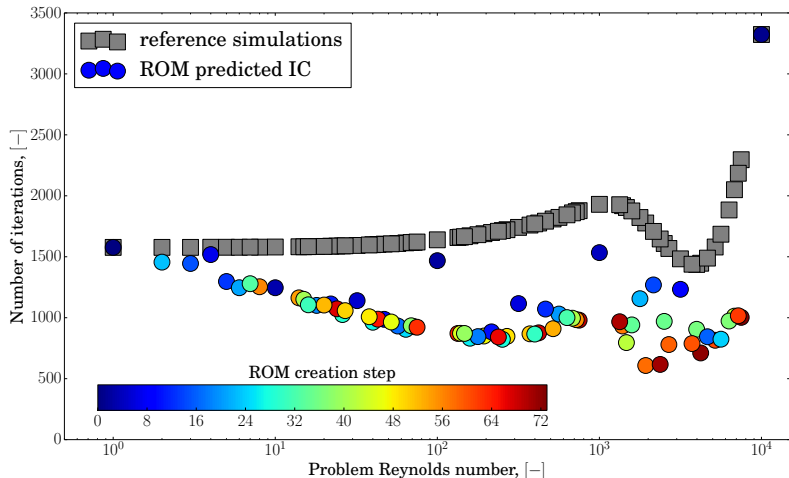
ROM size reduction: \mathcal{S}^e selection based on greedy algorithm



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



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





- [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, *SIAM J. Sci. Comput.*, vol. 32, (2010) pp. 2737–2764.
- [5] Alla, A. Kutz, J. N.: Nonlinear Model Order Reduction Via Dynamic Mode Decomposition, *preprint*



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Thank you for your
attention



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- 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, $\langle \varphi, \tilde{\varphi} \rangle_{L_h^2} = (\varphi^h)^T W \varphi^h$.