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# Reduced-Order subscales for POD models in fluid mechanics

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Model problem (convection-diffusion-reaction equation):

$$\begin{aligned} \mathcal{L}u := -k\Delta u + \boldsymbol{a}\cdot\nabla u + su = f \qquad & \text{in } \Omega \\ u = 0 \qquad & \text{on } \partial\Omega \end{aligned}$$

Variational formulation:

$$B(u,v) = \langle f, v\rangle \quad \forall v \in V$$

$$B(u,v) = k(\nabla u, \nabla v) + (\boldsymbol{a}\cdot\nabla u, v) + s(u,v)$$

Galerkin finite element approximation:

$$B(u_h,v_h) = \langle f, v_h\rangle \quad \forall v_h \in V_h$$

Essential idea of the VMS method (Hughes, 1995):

$$V = V_h \oplus \tilde{V}$$

After splinting unknown and test function into finite element and subgrid-scale (or subscale) component:

$$B(u_h, v_h) + B(\tilde{u}, v_h) = \langle f, v_h \rangle \quad \forall v_h \in V_h$$
$$B(u_h, \tilde{v}) + B(\tilde{u}, \tilde{v}) = \langle f, \tilde{v} \rangle \quad \forall \tilde{v} \in \tilde{V}$$

Formally:

$$B(u_h, v_h) + \langle \tilde{u}, \mathcal{L}^* v_h \rangle = \langle f, v_h \rangle \quad \forall v_h \in V_h$$
$$\langle \mathcal{L} u_h, \tilde{v} \rangle + \langle \mathcal{L} \tilde{u}, \tilde{v} \rangle = \langle f, \tilde{v} \rangle \quad \forall \tilde{v} \in \tilde{V}$$

First approximation: neglecting the subscale flux jumps (can be relaxed!)

$$\langle \mathcal{L} v_h, \tilde{v} \rangle \approx \sum_K (\mathcal{L} v_h, \tilde{v})_K \equiv (\mathcal{L} v_h, \tilde{v})_h$$

Key approximation: lumping of the differential operator applied to the subscales

$$\langle \mathcal{L} \tilde{u}, \tilde{v} \rangle \approx \tau^{-1} (\tilde{u}, \tilde{v}) \quad \text{where} \quad \tau^{-1} = c_1 \frac{k}{h^2} + c_2 \frac{|a|}{h} + c_3 s$$

Resulting problem:

$$B(u_h, v_h) + (\tilde{u}, \mathcal{L}^* v_h)_h = \langle f, v_h \rangle \quad \forall v_h \in V_h$$
$$(\mathcal{L} u_h, \tilde{v})_h + \tau^{-1} (\tilde{u}, \tilde{v}) = \langle f, \tilde{v} \rangle \quad \forall \tilde{v} \in \tilde{V}$$

The subscales are given by:

$$\tilde{u} = \tau \tilde{P} (f - \mathcal{L} u_h)$$

**When inserted into the FEM equation, leads to a problem for the FEM solution**

Options for the subscale space:

$$\tilde{V} \subset \mathcal{L}V_h + \operatorname{span}\{f\} \iff \tilde{u} = \tau(f - \mathcal{L}u_h)$$

$$\tilde{V} = V_h^{\perp} \iff \tilde{u} = \tau P_h^{\perp}(f - \mathcal{L}u_h)$$

Using for example the first option, the problem for the FEM solution is:

$$B(u_h, v_h) + \tau(\mathcal{L}u_h, -\mathcal{L}^* v_h)_h = \langle f, v_h \rangle + \tau(f, -\mathcal{L}^* v_h)_h$$

This problem has enhanced stability properties with respect to the Galerkin Method, both in

- Singularly perturbed problems
- Mixed problems

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# POD for a general problem

$$\boldsymbol{F}(\boldsymbol{U}_{n+1}, \boldsymbol{U}_n, \boldsymbol{U}_{n-1}, ..) :=$$

$$\boldsymbol{A}(\boldsymbol{U}_{n+1})\boldsymbol{U}_{n+1} - \boldsymbol{B}_n(\boldsymbol{U}_n)\boldsymbol{U}_n - \boldsymbol{B}_{n-1}(\boldsymbol{U}_{n-1})\boldsymbol{U}_{n-1} - ... - \boldsymbol{C} = \boldsymbol{0}.$$

- System dimension:

$$\boldsymbol{U}_{n+1}, \boldsymbol{U}_n, ..., \boldsymbol{F}, \boldsymbol{C} \in \mathbb{R}^M$$

$$\boldsymbol{A}, \boldsymbol{B}_n, \boldsymbol{B}_{n-1}, ... \in \mathbb{R}^{M \times M}$$

- Matrices might have a non-linear dependence on *U*

Grouping terms:

$$\boldsymbol{R}(\boldsymbol{U}_n, \boldsymbol{U}_{n-1}, ...) := \boldsymbol{B}_n(\boldsymbol{U}_n)\boldsymbol{U}_n + \boldsymbol{B}_{n-1}(\boldsymbol{U}_{n-1})\boldsymbol{U}_{n-1} + ... + \boldsymbol{C}.$$

Final system:

$$\boldsymbol{A}(\boldsymbol{U}^{n+1})\boldsymbol{U}^{n+1} = \boldsymbol{R}(\boldsymbol{U}^n, \boldsymbol{U}^{n-1}, ...),$$

# POD for a general problem

Projection onto a low dimensional subspace $\mathcal{V}_\Phi \subset \mathbb{R}^M$

$$\boldsymbol{U} \approx \boldsymbol{\Phi}\boldsymbol{U}_\Phi + \overline{\boldsymbol{U}} \qquad \boldsymbol{\Phi} \in \mathbb{R}^{M\times m} \qquad \boldsymbol{U}_\Phi \in \mathbb{R}^m \qquad m << M$$

Obtention of the reduced basis by means of a proper orthogonal decomposition (POD) procedure:

- Solve a Full-Order problem (FOM)
- Collect snapshots during the solution procedure
- Perform a singular value decomposition (SVD) of the snapshot collection
- Keep the *m* first SVD basis functions to form the POD basis

# Additional definitions

Constant value mean vector: $\boldsymbol{U} \approx \boldsymbol{\Phi} \boldsymbol{U}_{\Phi} + \overline{\boldsymbol{U}}.$

Restriction operator: $\mathcal{R}_{\Phi} : \mathbb{R}^M \rightarrow \mathbb{R}^m$ $\mathcal{R}_{\Phi}\left(\boldsymbol{U}\right) = \boldsymbol{\Phi}^T \left(\boldsymbol{U} - \overline{\boldsymbol{U}}\right) \in \mathbb{R}^m$

Extension operator: $\mathcal{E} : \mathbb{R}^m \rightarrow \mathbb{R}^M$ $\mathcal{E}\left(\boldsymbol{U}_{\Phi}\right) = \boldsymbol{\Phi} \boldsymbol{U}_{\Phi} + \overline{\boldsymbol{U}} \in \mathbb{R}^M$

Projection operator: $\mathcal{V}_{\Phi}, \Pi_{\Phi} : \mathbb{R}^M \rightarrow \mathbb{R}^M$ $\Pi_{\Phi}\left(\boldsymbol{U}\right) = \mathcal{E}\left(\mathcal{R}_{\Phi}\left(\boldsymbol{U}\right)\right)$

# Additional Definitions

Some notation:

$$\begin{aligned} \boldsymbol{A}_\Phi &:= \boldsymbol{\Phi}^T \boldsymbol{A} \boldsymbol{\Phi} & \in \mathbb{R}^{m\times m}, \\ \boldsymbol{R}_\Phi &:= \boldsymbol{\Phi}^T \left( \boldsymbol{R} - \boldsymbol{A}\overline{\boldsymbol{U}} \right) & \in \mathbb{R}^{m}, \end{aligned}$$

Reduced-Order System (Galerkin projection):

$$\boldsymbol{A}_\Phi \boldsymbol{U}_\Phi^{n+1} = \boldsymbol{R}_\Phi$$

For non-symmetric problems it will be convenient to use a Petrov-Galerkin projection, but we do the development using the Galerkin projection.

# Construction of the Reduced-Order Basis

The reduced-order basis is built through a Singular Value Decomposition.

Let us define the snapshots matrix:

$$\mathcal{U} \in \mathbb{R}^{M \times N}$$

where N is the number of snapshots. The jth snapshot is denoted as:

$$\mathcal{U}_{(:,j)}$$

We define the general **one matrix** as a matrix full of ones:

$$\mathbf{1}^{k \times l} \in \mathbb{R}^{k \times l} \quad | \quad \mathbf{1}^{k \times l}_{ij} = 1 \quad \forall i, j.$$

and then we can define the mean value of the snapshots as:

$$\overline{U} = \frac{\mathcal{U}\mathbf{1}^{N \times 1}}{N} \in \mathbb{R}^{M \times 1}$$

# Construction of the Reduced-Order Basis

The snapshots' mean matrix is:

$$\overline{\mathcal{U}} = \overline{U}\mathbf{1}^{1\times N} \in \mathbb{R}^{M\times N}$$

And finally the singular value decomposition can be written as:

$$\mathcal{U} = \overline{\mathcal{U}} + \mathbf{\Phi}_0\mathbf{\Sigma}_0\mathbf{\Psi}_0^T.$$

If we keep only the group of most relevant snapshots:

$$\mathcal{U} - \overline{\mathcal{U}} \approx \mathbf{\Phi\Sigma\Psi}^T$$

where $\mathbf{\Phi}$ and $\mathbf{\Psi}^T$ are orthogonal matrices.

We can now define the restriction of the snapshots onto the reduced-order subspace:

$$\mathcal{U}_\Phi = \mathcal{R}_\Phi\left(\mathcal{U}\right) := \mathbf{\Phi}^T\left(\mathcal{U} - \overline{\mathcal{U}}\right)$$

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# Preliminaries

We aim at taking into account the effect of the discarded modes in our POD model. Let us consider the solution to the full-order problem:

$$\boldsymbol{U}^{n+1} = \boldsymbol{A}^{-1}\boldsymbol{R},$$

Our starting assumption is that the best possible approximation to $\boldsymbol{U}^{n+1}$ in the reduced-order subspace is the projection (or restriction when expressed in the reduced-order basis):

$$\Pi_\Phi\left(\boldsymbol{U}^{n+1}\right) \qquad \mathcal{R}_\Phi\left(\boldsymbol{U}^{n+1}\right)$$

We can now split the unknown into its best possible approximation in the reduced-order subspace, and the **part which cannot be captured by the reduced-order model, the subscales:**

$$\boldsymbol{U}^{n+1} = \Pi_\Phi\left(\boldsymbol{U}^{n+1}\right) + \tilde{\boldsymbol{U}}^{n+1}$$

This introduces the subscales subspace, which must be the orthogonal complementary to the reduced-order subspace:

$$\mathcal{V} = \mathcal{V}_\Phi \oplus \mathcal{V}_\Phi^\perp,$$

$$\mathcal{V}_\Phi^\perp = \left\{\boldsymbol{X} \in \mathcal{V} : \quad \boldsymbol{X}^T\boldsymbol{Y} = 0 \quad \forall \boldsymbol{Y} \in \mathcal{V}_\Phi\right\}$$

# Preliminaries

The new reduced-order system taking into account the subscales is:

$$\boldsymbol{A}_\Phi \mathcal{R}_\Phi \left(\boldsymbol{U}^{n+1}\right) + \boxed{\boldsymbol{\Phi}^T \boldsymbol{A} \tilde{\boldsymbol{U}}^{n+1}} = \boldsymbol{R}_\Phi,$$

In general $\boldsymbol{\Phi}^T \boldsymbol{A} \tilde{\boldsymbol{U}}^{n+1} \neq \mathbf{0}$ and this affects the accuracy of the reduced-order model.

We propose an approximation to the neglected terms of the form:

$$\boldsymbol{A}_\Phi \boldsymbol{S}_\Phi^{n+1} \approx \boldsymbol{\Phi}^T \boldsymbol{A} \tilde{\boldsymbol{U}}^{n+1}$$

where $\boldsymbol{S}_\Phi^{n+1} \in \mathbb{R}^m$ are the reduced-order subscales. The reduced-order system now becomes:

$$\boldsymbol{A}_\Phi \left(\boldsymbol{U}_\Phi^{n+1} + \boldsymbol{S}_\Phi^{n+1}\right) = \boldsymbol{R}_\Phi$$

# A Least-Squares Model for the subscales

We propose to model the subscales through a linear model of the form:

$$\boldsymbol{S}_{\Phi}^{n+1} = \boldsymbol{C}_s \boldsymbol{U}_{\Phi}^{n+1} + \boldsymbol{D}_S.$$

With $\boldsymbol{C}_S \in \mathbb{R}^{m \times m}$ and $\boldsymbol{D}_S \in \mathbb{R}^m$

The model for the subscales will be built a posteriori using the information of the snapshot set.

For each snapshot, we project the exact system of equations onto the reduced-order subspace:

$$\begin{aligned}
\boldsymbol{A}_{\Phi\Pi} &= \boldsymbol{\Phi}^T \boldsymbol{A}\left(\Pi_{\Phi}\left(\boldsymbol{U}^{n+1}\right)\right) \boldsymbol{\Phi}, \\
\boldsymbol{R}_{\Phi\Pi} &= \boldsymbol{\Phi}^T \left(\boldsymbol{R}\left(\Pi_{\Phi}\left(\boldsymbol{U}^{n}\right)\right) - \boldsymbol{A}\left(\Pi_{\Phi}\left(\boldsymbol{U}^{n+1}\right)\right) \overline{\boldsymbol{U}}\right),
\end{aligned}$$

The predicted reduced-order solution, **without** the subscales is:

$$\boldsymbol{A}_{\Phi\Pi} \boldsymbol{U}_{\Phi,\mathrm{pred}}^{n+1} = \boldsymbol{R}_{\Phi\Pi}$$

# A Least-Squares Model for the subscales

The exact subscales for each snapshot can be computed as:

$$\boldsymbol{S}_{\Phi,\text{pred}}^{n+1} = \boldsymbol{U}_{\Phi,\text{pred}}^{n+1} - \mathcal{R}_{\Phi}\left(\boldsymbol{U}^{n+1}\right).$$

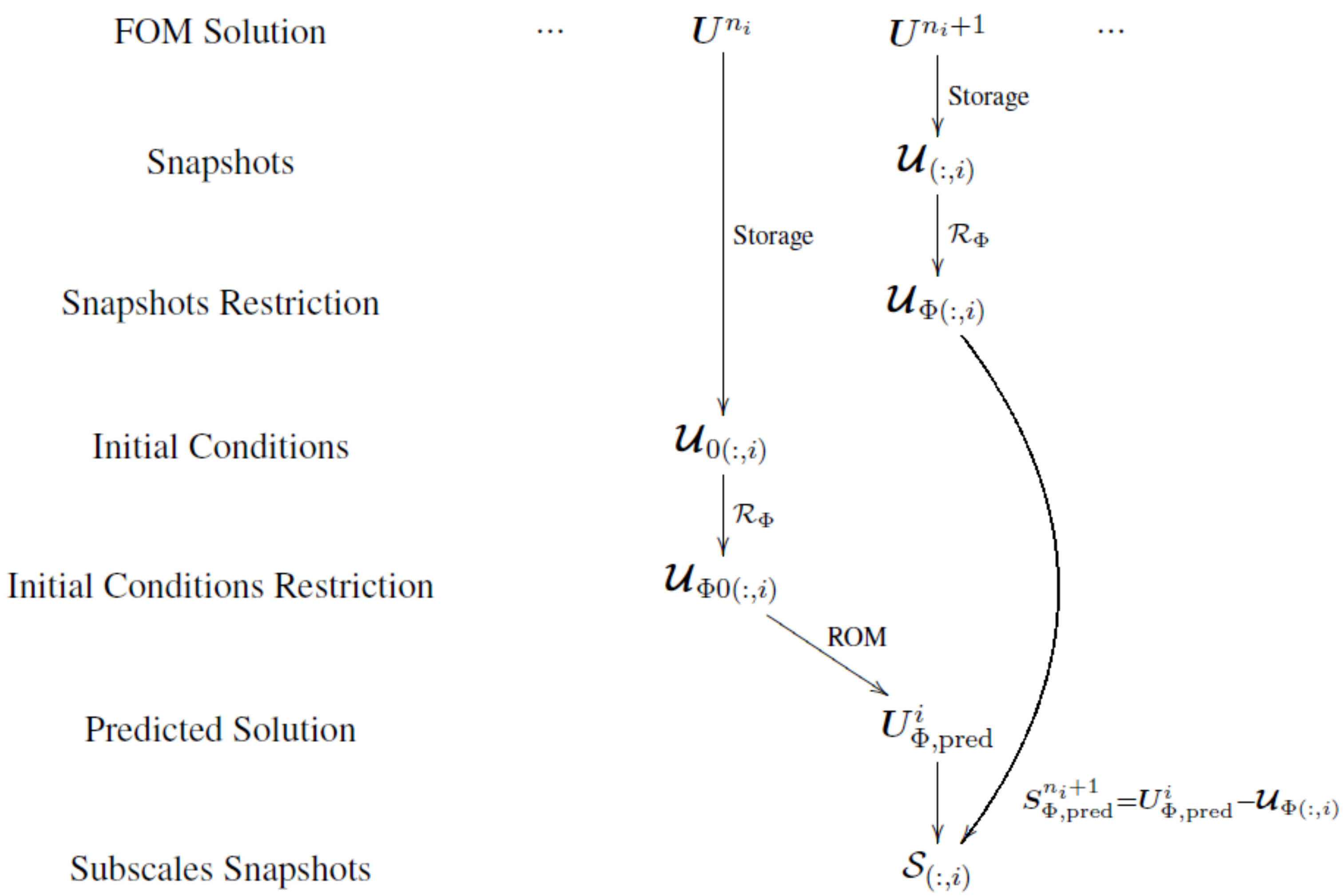
From here, we can easily compute the coefficients for the model for the subscales as the optimum (from a least-squares point of view) amongst all possible coefficients:

$$\boldsymbol{C}_S, \boldsymbol{D}_S = \arg \min_{\boldsymbol{a}\in\mathbb{R}^{m\times m}, \boldsymbol{b}\in\mathbb{R}^m} \sum_{i=1}^{N} ||\boldsymbol{\mathcal{S}}_{\Phi,(:,i)} - \boldsymbol{a}\boldsymbol{\mathcal{U}}_{\Phi(:,i)} - \boldsymbol{b}||^2$$

Final reduced-order system taking into account the subscales:

$$\boxed{\boldsymbol{A}_{\Phi}\left(\boldsymbol{I}_{\Phi} + \boldsymbol{C}_S\right)\boldsymbol{U}_{\Phi}^{n+1} = \boldsymbol{R}_{\Phi} - \boldsymbol{A}_{\Phi}\boldsymbol{D}_S},$$

# A Least-Squares Model for the subscales



# A Least-Squares Model for the subscales

$$\boldsymbol{C}_S, \boldsymbol{D}_S = \arg \min_{a \in \mathbb{R}^{m \times m}, b \in \mathbb{R}^m} \sum_{i=1}^{N} ||\boldsymbol{\mathcal{S}}_{\Phi,(:,i)} - \boldsymbol{a}\boldsymbol{\mathcal{U}}_{\Phi(:,i)} - \boldsymbol{b}||^2$$

$$\boxed{\boldsymbol{A}_\Phi \left(\boldsymbol{I}_\Phi + \boldsymbol{C}_S\right) \boldsymbol{U}_\Phi^{n+1} = \boldsymbol{R}_\Phi - \boldsymbol{A}_\Phi \boldsymbol{D}_S},$$

Interesting properties:

$$\boxed{\boldsymbol{C}_S^T = \mathrm{var}_{\mathcal{U}}^{-1} \mathrm{cov}_{\mathcal{U}S}}$$

The variance matrix is diagonal due to the properties of the SVD, **each coefficient of the coefficients matrix can be computed independently**

$$\boxed{\boldsymbol{D}_S^T = \overline{\boldsymbol{\mathcal{S}}_\Phi^T} - \overline{\boldsymbol{\mathcal{U}}_\Phi^T} \boldsymbol{C}_S^T}$$

# Final adjustments to the subscales model

Dropping the components of the model with a negligible contribution:

The diagonal variance matrix:

$$\begin{aligned} \mathrm{var}_{\mathcal{S}} &\in \mathbb{R}^{m\times m} \\ \mathrm{var}_{\mathcal{S},ij} &= \delta_{ij}\left[\overline{\boldsymbol{\mathcal{S}}_{\Phi}^{T}\boldsymbol{\mathcal{S}}_{\Phi}} - \overline{\boldsymbol{\mathcal{S}}_{\Phi}^{T}}\,\overline{\boldsymbol{\mathcal{S}}_{\Phi}}\right]_{ij} \end{aligned}$$

Pearson's correlation coefficient ranges from -1 to 1, it measures the correlation between variables:

$$\boldsymbol{P}_{\mathcal{S}}^{T} = \mathrm{var}_{\mathcal{U}}^{-1/2}\mathrm{cov}_{\mathcal{U}\mathcal{S}}\mathrm{var}_{\mathcal{S}}^{-1/2}$$

In our model, we drop the coefficients with a low contribution (correlation) to the model:

If $P_{\mathcal{S},ij} < \mathrm{tol}_{\mathrm{Pearson}}$ then we fix $C_{\mathcal{S},ij} = 0$

This allows to reduce the computational cost in case a large number of degrees of freedom is required.

# Final adjustments to the subscales model

Discarding the components of the model with large error:

We define the relative error associated to the ith reduced-order component as:

$$e_i = \frac{||\boldsymbol{\mathcal{S}}_{\Phi(i,:)}||}{||\boldsymbol{\mathcal{U}}_{\Phi(i,:)}||}$$

We don't want the model for the subscales to predict the subscales using components of the reduced-order model with a large error, so we fix a tolerance and we discard the corresponding components:

$$\boldsymbol{C}_{S(:,j)} = \boldsymbol{0}^{m\times 1} \quad \text{if } e_j > \text{tol}_{\text{error}}$$

However, we try to improve the performance of the discarded variable for the subscales model, that is:

$$\boldsymbol{C}_{S(j,:)} \neq \boldsymbol{0}^{1\times m}$$

**Algorithm 1** Algorithm for the calculation of the subscales model.

1. Collect the high-fidelity solution snapshots $\boldsymbol{\mathcal{U}}, \boldsymbol{\mathcal{U}}_0$ .
2. Perform the singular value decomposition of $\boldsymbol{\mathcal{U}}$, compute the restrictions $\mathcal{R}_\Phi(\boldsymbol{\mathcal{U}}), \mathcal{R}_\Phi(\boldsymbol{\mathcal{U}}_0)$.
3. For all the snapshots initial conditions $\mathcal{R}_\Phi(\boldsymbol{\mathcal{U}}_0)$, solve the reduced-order model problem and obtain the subscales snapshots matrix $\boldsymbol{\mathcal{S}}_\Phi$ by comparing the reduced-order solution with $\mathcal{R}_\Phi(\boldsymbol{\mathcal{U}})$.
4. Compute the variance of the snapshots expressed in the reduced-order basis $\mathrm{var}_{\mathcal{U}}$.
5. Compute the variance of the subscales expressed in the reduced-order basis $\mathrm{var}_{\mathcal{S}}$.
6. Compute the covariance of the snapshots against the subscales $\mathrm{cov}_{\mathcal{US}}$.
7. Compute $\boldsymbol{C}_{\mathcal{S}}^T = \mathrm{var}_{\mathcal{U}}^{-1}\mathrm{cov}_{\mathcal{US}}$ .
8. Compute the Pearson's correlation coefficient matrix $\boldsymbol{P}_{\mathcal{S}}$ .
9. Modify $\boldsymbol{C}_{\mathcal{S}}$ by dropping the coefficients $C_{\mathcal{S},ij}$ for which $P_{ij} < \mathrm{tol}_{\mathrm{Pearson}}$.
10. Compute the relative error associated to each degree of freedom.
11. Modify $\boldsymbol{C}_{\mathcal{S}}$ by dropping the columns $C_{\mathcal{S}(:,j)}$ for which $e_j > \mathrm{tol}_{\mathrm{error}}$.
12. Compute $\boldsymbol{D}_{\mathcal{S}}^T = \overline{\mathcal{S}_\Phi^T} - \overline{\boldsymbol{\mathcal{U}}_\Phi^T}\boldsymbol{C}_{\mathcal{S}}^T$.

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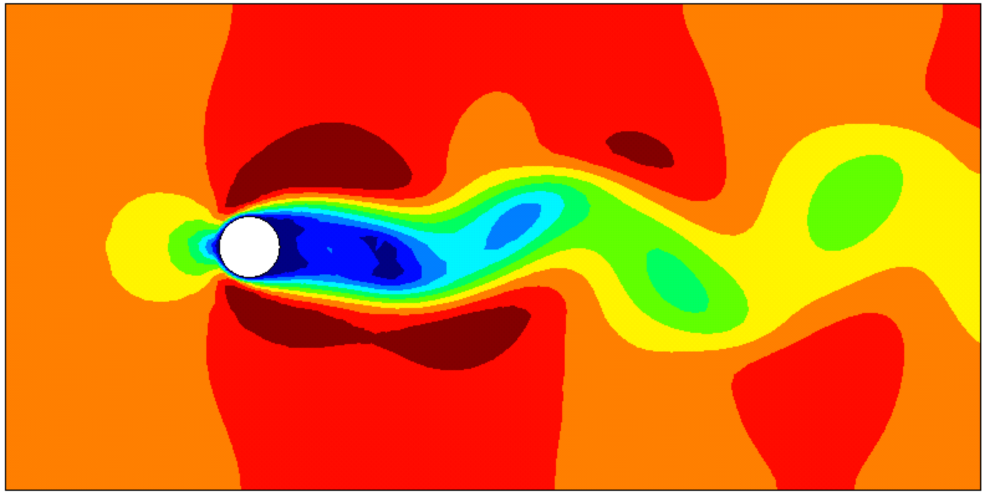
# Improving the performance of the ROM

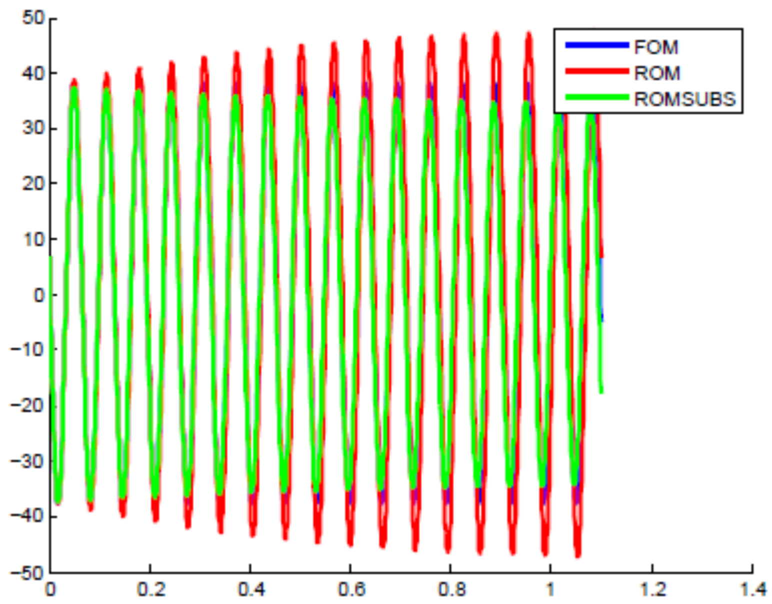
Incompressible flow past a cylinder:

$$\begin{aligned} \partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} - \nu \Delta \boldsymbol{u} + \nabla p &= \boldsymbol{f}, \\ \nabla \cdot \boldsymbol{u} &= 0. \end{aligned}$$



# Improving the performance of the ROM

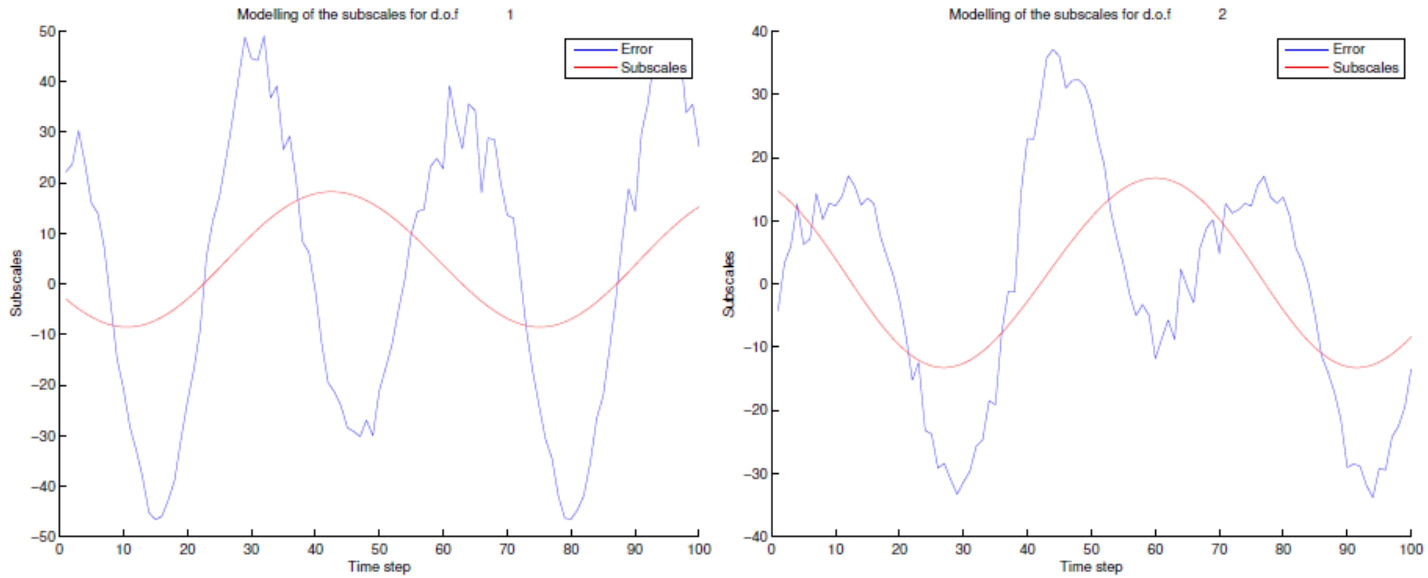
Comparison of the full-order results, reduced-order results (2 degrees of freedom) and reduced-order results with subscales (2 degrees of freedom)




FOM amplitude: 38 ROM amplitude: 48 ROM with subs amplitude: 35

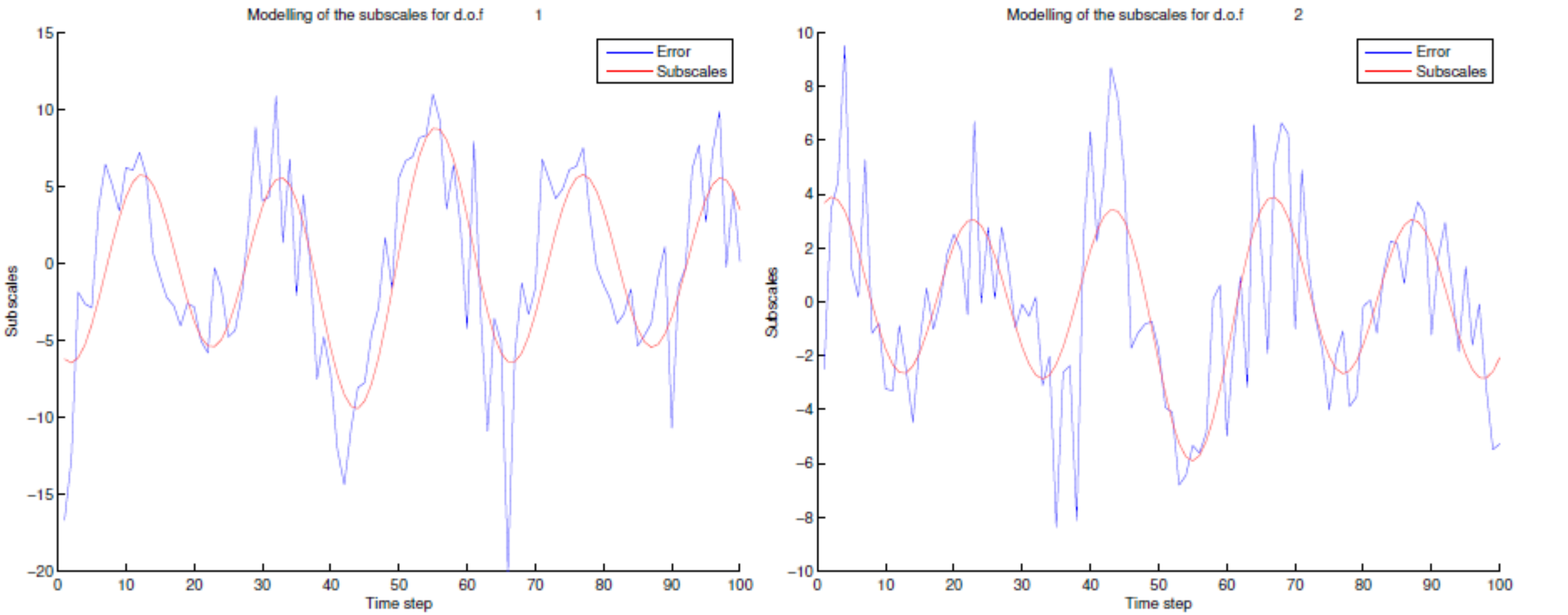
# Improving the performance of the ROM

Real subscales versus modelled subscales for the 2 degrees of freedom reduced-order model.



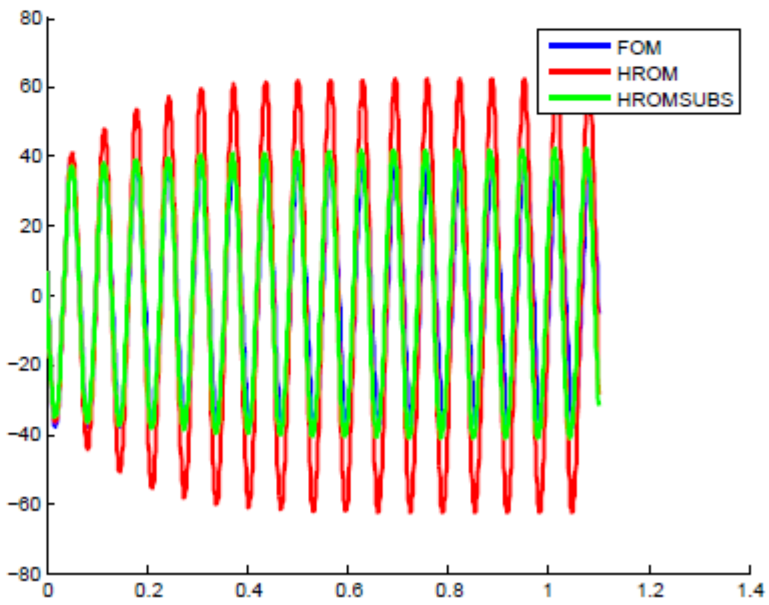
# Improving the performance of the ROM

Real subscales versus modelled subscales for a 5 degrees of freedom reduced-order model.



# Correcting errors of hyper-reduction

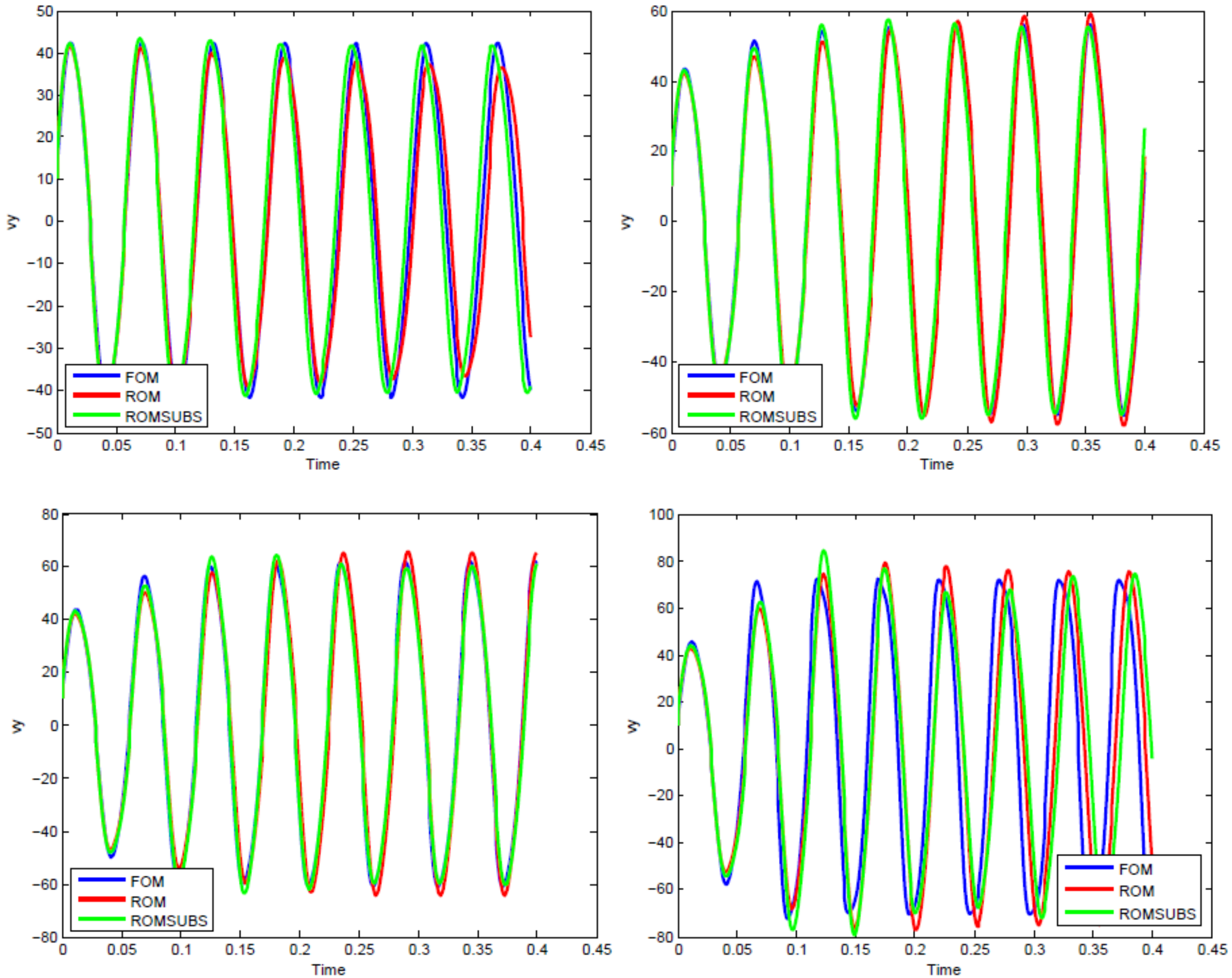
Time history for FOM, Hyper-Reduced ROM (2 degrees of freedom), Hyper-Reduced ROM with subscales (2 degrees of freedom)




FOM amplitude: 38 HROM amplitude: 63 ROM with subs amplitude: 42

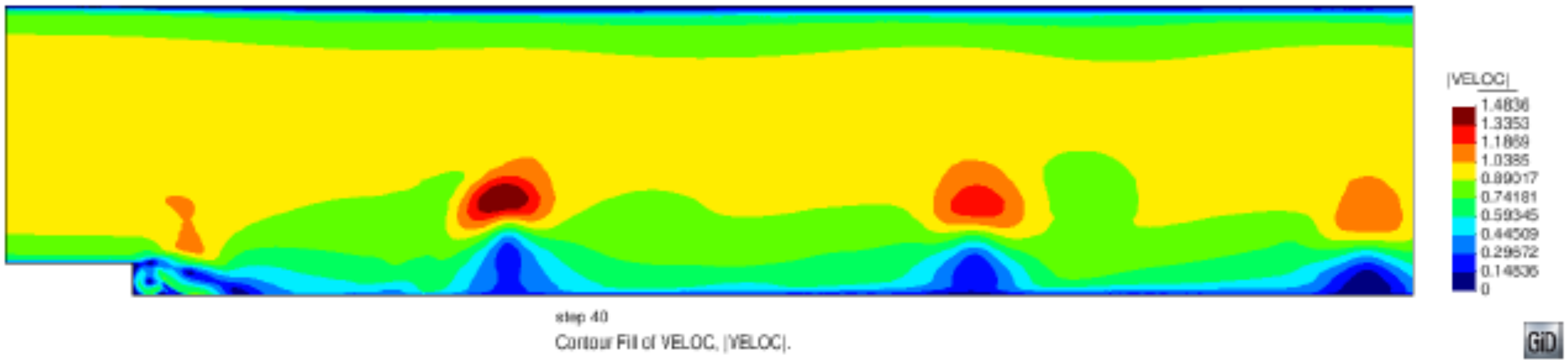
# Adapting to different physical parameters

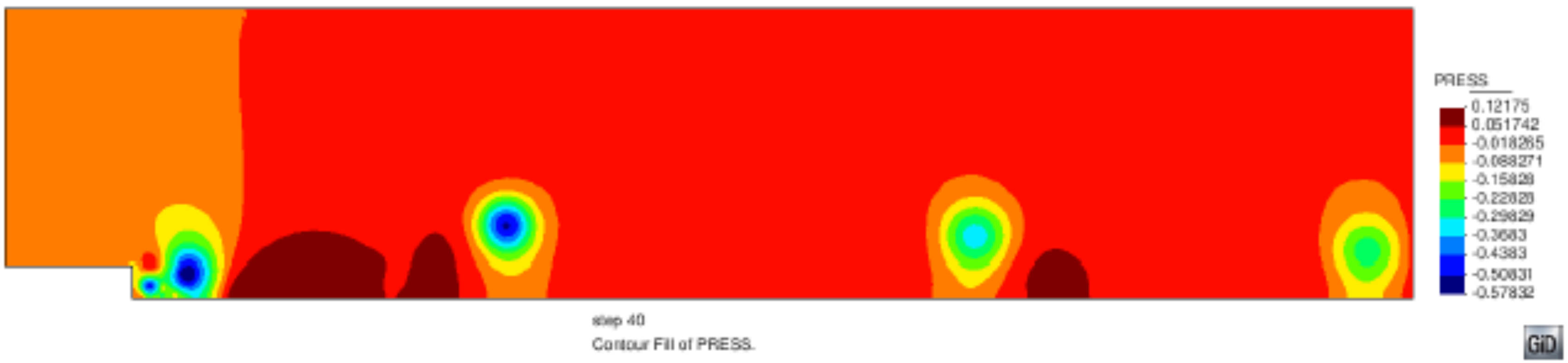
Reynolds from 100 to 1000 (trained at Re=100 and Re=200)



# Using the subscales to solve complex flow problems

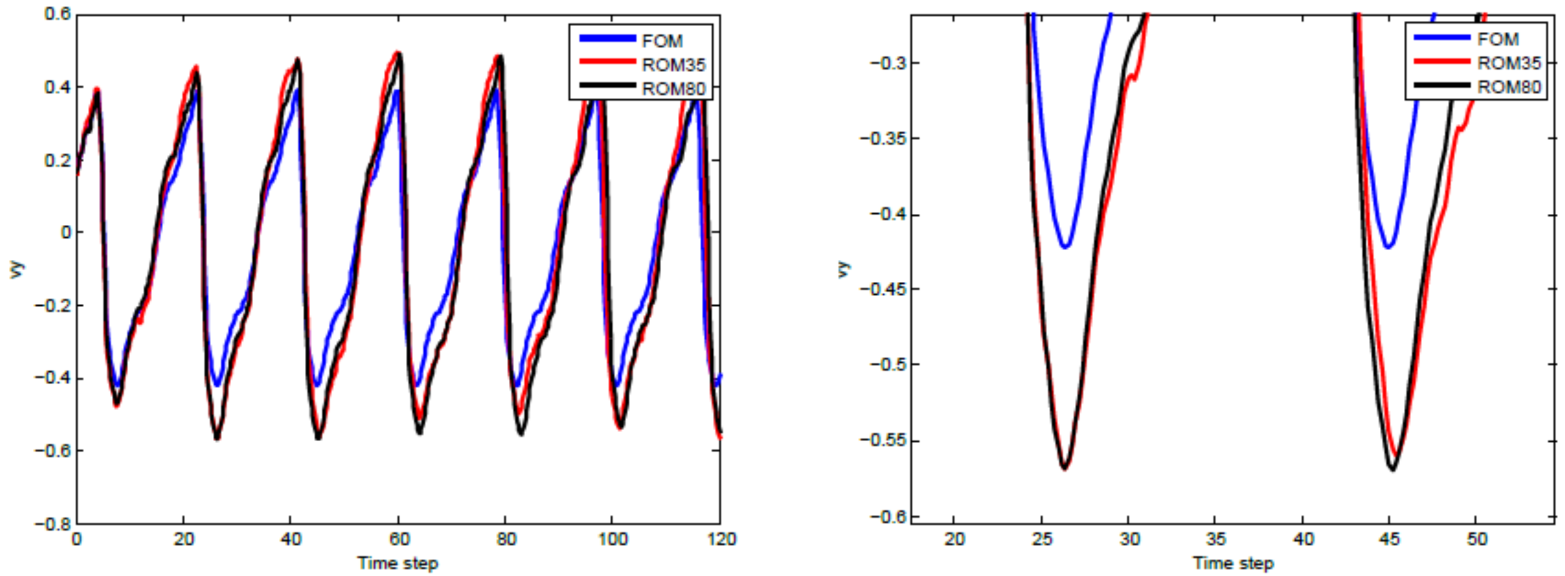
Backward facing step, Reynolds = 37000:



# Using the subscales to solve complex flow problems

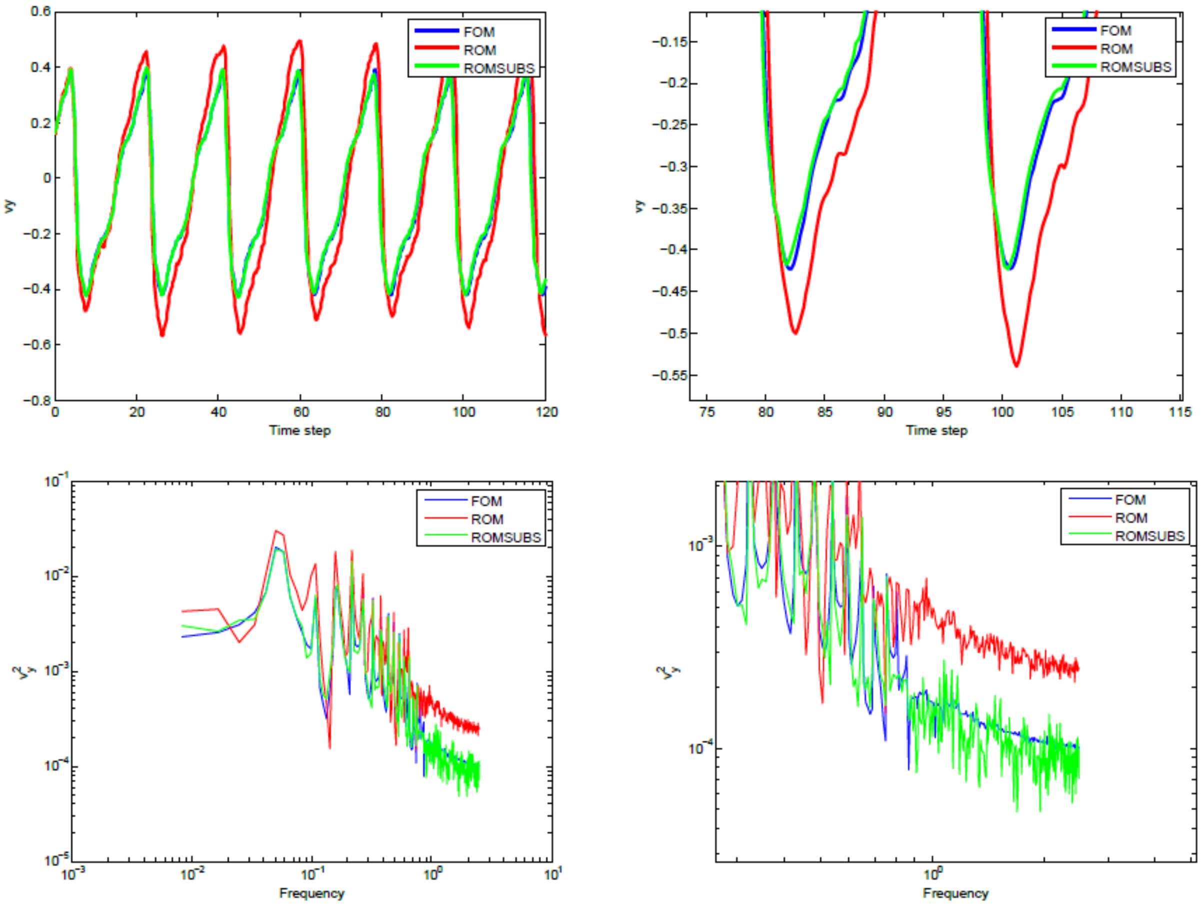
Comparison of results for FOM, ROM with 35 degrees of freedom and ROM with 80 degrees of freedom.




Little improvement is obtained by increasing from 35 to 80 dofs, many more degrees of freedom would be required.

# Using the subscales to solve complex flow problems

Comparison of results for FOM, ROM with 35 degrees of freedom and ROM with 35 degrees of freedom plus subscales.



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# Overview

- A model for the subscales in POD reduced-order models has been presented
- The basic idea is to split the full-order solution into the part which can be captured by the reduced-order model and the subscales.
- The proposed model is defined as a linear function of the solution of the reduced-order model.
- The coefficients for the linear model are obtained by comparing the reduced and the full-order solution at some trial configurations.
- The coefficients for the linear model can be computed independently, and some of them are dropped for accuracy and performance reasons.
- Numerical tests show that:
  - The subscales enhance the performance of the ROM.
  - When using hyper-reduction, they allow to correct the errors introduced by hyper-reduction.
  - The reduced-order model with the subscales is capable of adapting to different physical configurations.
  - The subscales can be used to solve complex flow problems using POD reduced-order models.
- Remark: We still need the reduced-order basis to be able to accurately enough represent the full-order solution.

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# Thank you!

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