Improvement of Reduced Order Modeling based on Proper Orthogonal Decomposition

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Summary

Context and flow configuration

I - A pressure extended Reduced Order Model based on POD

II - Stabilization of Reduced Order Models

- Residuals based stabilization method
- Classical SUPG and VMS methods

III - Improvement of the functional subspace

- ► An hybrid DNS/POD ROM method (Database modification)
- Krylov like method

Conclusions



Context and flow configuration

- > Context
 - Need of Reduced Order Model for Flow Control Purpose
 - \hookrightarrow To reduce the CPU time
 - \hookrightarrow To reduce the memory storage during adjoint-based minimization process
 - Optimization + POD ROM methods
 - ← Generalized basis, no POD basis actualization : fast but no "convergence" proof
 - \hookrightarrow Trust Region POD (TRPOD), POD basis actualization : proof of convergence !
 - Drawbacks
 - → Need to stabilize POD ROM (lack of dissipation, roundoff errors, pressure term)
 - \hookrightarrow Basis actualization : DNS \rightarrow high numerical costs !
 - Solutions
 - ← Efficient ROM & stabilization
 - \hookrightarrow Low costs functional subspace adaptation during optimization process



Context and flow configuration

Flow Configuration

- 2-D Confined flow past a square cylinder in laminar regime
- Viscous fluid, incompressible and newtonian
- No control



Numerical methods

Gear method in time

- Penalization method for the square cylinder
- Multigrids V-cycles method in space

C.-H. Bruneau solver



Ο



► Momentum conservation

Detailled model (exact)

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} = -\boldsymbol{\nabla}p + \frac{1}{Re}\Delta\boldsymbol{u}$$

Temporal discretization

$$\frac{\boldsymbol{u}^{n+1}}{\Delta t} + \boldsymbol{\nabla} p^{n+1} - \frac{1}{Re} \Delta \boldsymbol{u}^{n+1} = \frac{\boldsymbol{u}^n}{\Delta t} - (\boldsymbol{u}^n \cdot \boldsymbol{\nabla}) \boldsymbol{u}^n$$

Projection onto the pressure extended POD basis (correlations onto $U = (u, p)^T$)

$$\widetilde{\boldsymbol{u}}(\boldsymbol{x}, t) = \sum_{i=1}^{N} a_i(t) \boldsymbol{\phi}_i(\boldsymbol{x}) \text{ and } \widetilde{p}(\boldsymbol{x}, t) = \sum_{i=1}^{N} a_i(t) \psi_i(\boldsymbol{x})$$

$$\sum_{j=1}^{N} a_j^{(n+1)} \left(\frac{\phi_j}{\Delta t} + \nabla \psi_j - \frac{1}{Re} \Delta \phi_j \right) = \sum_{i=j}^{N} a_j^{(n)} \frac{\phi_j}{\Delta t} + \left(\sum_{j=1}^{N} a_j^{(n)} \phi_j^{(u)} \cdot \nabla \right) \sum_{k=1}^{N} a_k^{(n)} \phi_k^{(u)}$$



After some simplifications

$$\sum_{j=1}^{N} a_j^{(n+1)} \left(\frac{\boldsymbol{\phi}_i}{\Delta t} + \boldsymbol{\nabla}\psi_i - \frac{1}{Re} \Delta \boldsymbol{\phi}_i \right) = \sum_{j=1}^{N} a_j^{(n)} \frac{\boldsymbol{\phi}_j}{\Delta t} + \sum_{j=1}^{N} \sum_{k=1}^{N} a_j^{(n)} \left(\boldsymbol{\phi}_j^{(\boldsymbol{u})} \cdot \boldsymbol{\nabla} \right) \boldsymbol{\phi}_k^{(\boldsymbol{u})} a_k^{(n)}$$

$$\sum_{j=1}^{N} a_j^{(n+1)} \boldsymbol{\chi}_j = \sum_{j=1}^{N} a_j^{(n)} \boldsymbol{\xi}_j + \sum_{j=1}^{N} \sum_{k=1}^{N} a_j^{(n)} \boldsymbol{\zeta}_{jk} a_k^{(n)}$$

Least squares

$$\sum_{j=1}^{N} \boldsymbol{\chi}_{i}^{T} \boldsymbol{\chi}_{j} a_{j}^{(n+1)} = \sum_{j=1}^{N} \boldsymbol{\chi}_{i}^{T} \boldsymbol{\xi}_{j} a_{j}^{(n)} + \sum_{j=1}^{N} \sum_{k=1}^{N} a_{j}^{(n)} \boldsymbol{\chi}_{i}^{T} \boldsymbol{\zeta}_{jk} a_{k}^{(n)}$$
$$\sum_{j=1}^{N} L_{ij}^{qdm} a_{j}^{(n+1)} = \sum_{j=1}^{N} B_{ij} a_{j}^{(n)} + \sum_{j=1}^{N} \sum_{k=1}^{N} C_{ijk} a_{j}^{(n)} a_{k}^{(n)}$$

 \hookrightarrow The ROM does not satisfied *a priori* the mass conservation (for non divergence free modes, as NSE-Residual modes)





► Mass conservation

Detailled model

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

Projection onto the POD basis

$$\sum_{j=1}^{N} a_j^{(n+1)} \nabla \cdot \phi_j = \mathbf{0}$$
$$\sum_{j=1}^{N} (\nabla \cdot \phi_j)^T \nabla \cdot \phi_j a_j^{(n+1)} = \mathbf{0}$$
$$\sum_{j=1}^{N} L_{ij}^{div} a_j^{(n+1)} = \mathbf{0}$$

Modified ROM

$$\sum_{j=1}^{N} (\alpha L_{ij}^{qdm} + \beta L_{ij}^{div}) a_j^{(n+1)} = \sum_{j=1}^{N} \alpha B_{ij} a_j^{(n)} + \sum_{j=1}^{N} \sum_{k=1}^{N} \alpha C_{ijk} a_j^{(n)} a_k^{(n)}$$

 \hookrightarrow The ROM has moreover to satisfy the flow rate conservation..





► Flow rate conservation

For the 2-D confined flow

$$\int_{\mathcal{S}} u \, d\mathcal{S} = Cste$$
$$\sum_{i=1}^{N} a_j(t) \int_{\mathcal{S}} \phi_j^u \, d\mathcal{S} = Cste$$
$$\sum_{j=1}^{N} \frac{da_j}{dt} \int_{\mathcal{S}} \phi_j^u \, d\mathcal{S} = 0$$
$$\sum_{j=1}^{N} L_{ij}^{deb} a_j^{(n+1)} = \sum_{j=1}^{N} L_{ij}^{deb} a_j^{(n)}$$

Finally, the ROM writes

$$\sum_{j=1}^{N} (\alpha L_{ij}^{qdm} + \beta L_{ij}^{div} + \gamma L_{ij}^{deb}) a_j^{(n+1)} = \sum_{j=1}^{N} (\alpha B_{ij} + \gamma L_{ij}^{deb}) a_j^{(n)} + \sum_{j=1}^{N} \sum_{k=1}^{N} \alpha C_{ijk} a_j^{(n)} a_k^{(n)}$$





 $Re = 200, 11 \text{ modes} \Rightarrow$ convergence towards the exact limit cycles (= DNS)





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▶ Drawbaks same as usual, *i.e.* lack of dissipation...

 $Re = 200, 5 \text{ modes} \Rightarrow$ convergence towards an erroneous limit cycles (\neq DNS)



Fig. : Temporal evolution of the POD ROM coefficients over 25 vortex shedding periods **Fig.** : Limit cycles of the POD ROM coefficients over 25 vortex shedding periods

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► Drawbaks same as usual, *i.e.* lack of dissipation...

 $Re = 200, 3 \text{ modes} \Rightarrow \text{exponential divergence}$



Fig. : Temporal evolution of the POD ROM coefficients over 25 vortex shedding periods

Fig. : Limit cycles of the POD ROM coefficients over 25 vortex shedding periods

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Overview of stabilization methods (non-exhaustive)

- Eddy viscosity
 - \hookrightarrow Heisenberg viscosity
 - \hookrightarrow Spectral vanishing viscosity
 - \hookrightarrow Optimal viscosity
- Penalty method
- Calibration of POD ROM coefficients
- "New" stabilization methods in POD ROM context
- Residuals based stabilization method
 - Streamline Upwind Petrov-Galerkin (SUPG) and Variational Multi-scale (VMS) methods





Residuals based stabilization method

- \Rightarrow Idea add dominant POD-NSE residual modes to the existing basis
- \hookrightarrow The POD-NSE residuals are $\mathcal{L}(\widetilde{\boldsymbol{u}}(\boldsymbol{x}, t), \widetilde{p}(\boldsymbol{x}, t)) = \boldsymbol{R}(\boldsymbol{x}, t)$, where $\widetilde{\boldsymbol{u}}$ and \widetilde{p} obtained using POD and \mathcal{L} is the NSE operator

Model $A^{[N]}$, **unstable POD ROM** built with N basis functions $\Phi_i(x)$.

Algorithm

1. Integrate the ROM to obtain $a_i(t)$ and extract N_s snapshots $a_i(t_k)$, $k = 1, ..., N_s$.

2. Compute
$$\widetilde{\boldsymbol{u}}(\boldsymbol{x}, t_k) = \sum_{i=1}^N a_i(t_k) \boldsymbol{\phi}_i(\boldsymbol{x}), \ \widetilde{p}(\boldsymbol{x}, t_k) = \sum_{i=1}^N a_i(t_k) \psi_i(\boldsymbol{x}), \ \text{and} \ \boldsymbol{R}(\boldsymbol{x}, t_k).$$

- 3. Compute the POD modes $\Psi(x)$ of the NSE residuals.
- 4. Add the *K* firsts residual modes $\Psi(x)$ to the existing POD basis $\Phi_i(x)$ and built a new ROM (here the mass and flow rate constraints are important).

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Model $B^{[N;K]}$, PODRES ROM built with N POD basis functions $\Phi_i(x)$ + K RES basis functions $\Psi_i(x)$



SUPG and VMS methods

 \Rightarrow ldea approximate the fine scales using the NSE residuals $\mathbf{R} = (\mathbf{R}_M, R_C)^T$

$$\boldsymbol{u}'(\boldsymbol{x},\,t) = au_M \, \boldsymbol{R}_M(\boldsymbol{x},\,t) \quad \text{and} \quad p'(\boldsymbol{x},\,t) = au_C \, R_C(\boldsymbol{x},\,t)$$

 \hookrightarrow Class of penalty methods, *i.e.*

$$\sum_{j=1}^{N} L_{ij} \frac{da_j}{dt} = \sum_{j=1}^{N} B_{ij} a_j + \sum_{j=1}^{N} \sum_{k=1}^{N} C_{ijk} a_j a_k + F_i(t)$$

Model $C^{[N]}$, SUPG method

$$F_i^{SUPG}(t) = (\widetilde{\boldsymbol{u}} \cdot \nabla \boldsymbol{\Phi}_i + \nabla \Psi_i, \tau_M \boldsymbol{R}_M(\boldsymbol{x}, t))_{\Omega} + (\nabla \cdot \boldsymbol{\Phi}_i, \tau_C R_C(\boldsymbol{x}, t))_{\Omega}$$

Model $D^{[N]}$, VMS method

$$F_i^{VMS}(t) = F_i^{SUPG}(t) + (\widetilde{\boldsymbol{u}} \cdot (\nabla \boldsymbol{\Phi}_i)^T, \tau_M \boldsymbol{R}_M(\boldsymbol{x}, t))_{\Omega} - (\nabla \boldsymbol{\Phi}_i, \tau_M \boldsymbol{R}_M(\boldsymbol{x}, t) \otimes \tau_M \boldsymbol{R}_M(\boldsymbol{x}, t))_{\Omega}$$

 \hookrightarrow Parameters au_M and au_C are determined using adjoint based minimization method



ightarrow Re = 200 and N = 5 POD basis function ightarrow erroneous limit cylcles





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ightarrow Re = 200 and N = 3 POD basis function ightarrow divergence



Fig. : temporal evolution of the L_2 norm of the POD-NSE residuals

Fig. : Limit cycle of the POD ROM coefficients over 20 vortex shedding periods



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POD-NSE residuals

Fig. : Limit cycle of the POD ROM coefficients over 20 vortex shedding periods



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Functional subspace drawbacks, $\Phi_n(x)$: lack of representativity of 3D flows outside the database



Figures results from Buffoni etal. Journal of Fluid Mech. 569 (2006)

- Problems for 3D flow control
- Erroneous turbulence properties (spectrum, etc)





▷ Method 1 : hybrid ROM-DNS method to adapt the functional subspace $\Phi_n(\mathbf{x})$ Goal : determine $\Phi_n(\mathbf{x})$ at Re_2 starting from $\Phi_n(\mathbf{x})$ at Re_1 for low numerical costs.

• **Database modification :** statistics evolution $\Rightarrow \varphi : \Phi^{(k)} \mapsto \Phi^{(k+1)}$



1. Database modification $[\boldsymbol{U}(\boldsymbol{x}, t_1) \ \boldsymbol{U}(\boldsymbol{x}, t_2) \ \dots \ \boldsymbol{U}(\boldsymbol{x}, t_{N_r})]$

$$\widetilde{\boldsymbol{U}}^{[1,\cdots,N_r]}(\boldsymbol{x},t_k) = \sum_{n=1}^{N_r} a_n(t_k)\boldsymbol{\phi}_n(\boldsymbol{x}),$$

One snapshot modification using few DNS iterations

$$\boldsymbol{U}(\boldsymbol{x},t_s) = \widetilde{\boldsymbol{U}}^{[1,\cdots,N_r]}(\boldsymbol{x},t_s) + \boldsymbol{U}_s^{\perp}(\boldsymbol{x},t_s).$$

In a general way

$$\widetilde{\boldsymbol{U}}(\boldsymbol{x},t_k) = \widetilde{\boldsymbol{U}}^{[1,\cdots,N_r]}(\boldsymbol{x},t_k) + \delta_{ks} \boldsymbol{U}^{\perp}(\boldsymbol{x},t_s),$$



2 Modification temporal correlations tensor

$$C(t_k, t_l) = (\boldsymbol{U}(\boldsymbol{x}, t_k), \boldsymbol{U}(\boldsymbol{x}, t_l))_{\Omega}$$

$$= \left(\sum_{i=1}^{N_r} a_i(t_k)\boldsymbol{\phi}_i(\boldsymbol{x}) + \boldsymbol{U}^{\perp}(\boldsymbol{x}, t_k), \sum_{j=1}^{N_r} a_j(t_l)\boldsymbol{\phi}_j(\boldsymbol{x}) + \boldsymbol{U}^{\perp}(\boldsymbol{x}, t_l)\right)_{\Omega}$$

$$=\sum_{i=1}^{N_r}\sum_{j=1}^{N_r}a_i(t_k)a_j(t_l)\underbrace{(\boldsymbol{\phi}_i(\boldsymbol{x}),\boldsymbol{\phi}_j(\boldsymbol{x}))_{\Omega}}_{=\delta_{ij}} + \left(\boldsymbol{U}^{\perp}(\boldsymbol{x},t_k),\boldsymbol{U}^{\perp}(\boldsymbol{x},t_l)\right)_{\Omega}$$

$$+\sum_{i=1}^{N_r}a_i(t_k)\underbrace{\left(\boldsymbol{\phi}_i(\boldsymbol{x}),\boldsymbol{U}^{\perp}(\boldsymbol{x},t_l)\right)_{\Omega}}_{=0}+\sum_{j=1}^{N_r}a_{lj}\underbrace{\left(\boldsymbol{U}^{\perp T}(\boldsymbol{x},t_k),\boldsymbol{\phi}_j(\boldsymbol{x})\right)_{\Omega}}_{=0}.$$

Final approximation

$$C(t_k, t_l) = \sum_{i=1}^{N_r} a_i(t_k) a_i(t_l) + \delta_{ks} \delta_{ls} \int_{\Omega} \sum_{i=1}^{n_c} U^{\perp i}(\boldsymbol{x}, t_s) U^{\perp i}(\boldsymbol{x}, t_s) d\boldsymbol{x}.$$





Fig. : Comparison of the temporal correlation tensor eigenvalues evaluated from the exact field, U, and from the N_r -modes approximated one, $\widetilde{U}^{[1,\dots,N_r]}$.

 \hookrightarrow Very good approximation, and very low costs method!





3 Functional subspace adaptation

$$\boldsymbol{\phi}_{k}^{(n+1)}(\boldsymbol{x}) = \frac{1}{\lambda_{k}^{(n+1)}} \sum_{j=1}^{N} \widetilde{\boldsymbol{U}}^{(n)}(\boldsymbol{x}, t_{j}) a_{k}^{(n+1)}(t_{j})$$

$$\boldsymbol{\phi}_{k}^{(n+1)}(\boldsymbol{x}) = \frac{1}{\lambda_{k}^{(n+1)}} \sum_{i=1}^{N_{r}} \sum_{j=1}^{N} a_{k}^{(n+1)}(t_{j}) a_{i}^{(n)}(t_{j}) \, \boldsymbol{\phi}_{i}^{(n)}(\boldsymbol{x}) + \frac{1}{\lambda_{k}} \boldsymbol{U}^{\perp(n)}(\boldsymbol{x}, t_{s}) a_{k}^{(n+1)}(t_{s}).$$

$$\boldsymbol{\phi}_{k}^{(n+1)}(\boldsymbol{x}) = \sum_{i=1}^{N_{r}} K_{ki}^{(n+1)} \boldsymbol{\phi}_{i}^{(n)}(\boldsymbol{x}) + \boldsymbol{S}_{k}^{(n+1)}(\boldsymbol{x}).$$

Taken $S^{(n+1)}$ with elements $S_{ij}^{(n+1)} = S_i^{j(n+1)}$, the actualized basis is obtained using the linear application $\varphi : \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}^n \times \mathbb{R}^n$ defined as

$$\varphi: \phi^{(n)} \mapsto \phi^{(n+1)} = \phi^{(n)} K^{(n+1)} + S^{(n+1)}$$

Incrementation n = n + 1.





Example : we have a POD basis for $Re_1 = 100$, and we want a POD basis for $Re_2 = 200$.

- The POD ROM is evaluated with the current improved POD basis $\Phi_i^{(k)}$
- The DNS is performed for Re_2 .



Fig. : Modification of the POD basis functions under the application of the linear transfomation φ . Streamline representation of the velocity fields. Bifurcation from Re = 100 to Re = 200.

 \hookrightarrow Functional subspace modification



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▶ Results for a dynamical evolution from $Re_1 = 100$ to $Re_2 = 200$

 $Re_1 = 100$

 $Re_2 = 200$



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Observations

Results are very good if a sufficient amount of DNS is performed

- \hookrightarrow Good for a percentage $\frac{DNS}{DNS+PODROM}$ greater than 70%
- ► Possible explanation





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Observations

Results are very good if a sufficient amount of DNS is performed

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- **b** Method 2 : Krylov-like method to improve the functional subspace $\Phi_n(\boldsymbol{x})$
 - Use of the POD-NSE residuals : $\mathcal{L}(\widetilde{u}(x, t), \widetilde{p}(x, t)) = \mathbf{R}(x, t)$, \widetilde{u} and \widetilde{p} are POD fields, \mathcal{L} is the NSE operator

Algorithm

Start with the POD basis to be improved, Φ_i with i = 1, ..., N. Let $N_0 = N$.

1. Built and solve the corresponding ROM to obtain $a_i(t)$ and extract N_s snapshots $a_i(t_k)$ with i = 1, ..., N and $k = 1, ..., N_s$.

2. Compute
$$\widetilde{\boldsymbol{u}}(\boldsymbol{x}, t_k) = \sum_{i=1}^N a_i(t_k) \boldsymbol{\phi}_i(\boldsymbol{x})$$
, $\widetilde{p}(\boldsymbol{x}, t_k) = \sum_{i=1}^N a_i(t_k) \psi_i(\boldsymbol{x})$, and $\boldsymbol{R}(\boldsymbol{x}, t_k)$.

- 3. Compute the POD modes $\Psi({\boldsymbol{x}})$ of the NSE residuals.
- 4. Add the K firsts residual modes $\Psi(x)$ to the existing POD basis $\Phi_i(x)$
 - $\mathbf{\Psi} + \mathbf{\Phi}
 ightarrow \mathbf{\Phi} ullet$
 - $\bullet \ N \leftarrow N + K$
 - If N is below than a threshold, return to 1. Else, go to 5.
- 5. Perform a new POD compression with $N = N_0$.
 - If convergence is satisfied, stop. Else, return to 1.







First test case : 1D burgers equation $\underline{Re_1 = 50} \rightarrow \underline{Re_2 = 300} (\Phi^{Re_1} \cdot \Phi^{Re_2} \approx 0.5)$





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First test case : 1D burgers equation $\underline{Re_1} = 50 \rightarrow \underline{Re_2} = 300 \ (\Phi^{Re_1} \cdot \Phi^{Re_2} \approx 0.5)$





► Second test case : 2D NSE equations $\underline{Re_1 = 100} \rightarrow \underline{Re_2 = 200}$ ($\Phi^{Re_1} \cdot \Phi^{Re_2} \approx 0.5$)





Observations

- the decomposition $U'(x, t) = \tau R(x, t)$ is used to stabilize the ROM
 - $\, \hookrightarrow \ \ \, \text{Very good results for NSE}$
- the decomposition $U'(x, t) = \tau R(x, t)$ is used to improve POD basis
 - \hookrightarrow Very good results for Burgers, quite bad results for NSE

► Possible explanation

- the decomposition $m{U}'(m{x},\,t)= aum{R}(m{x},\,t)$ is only valid for :
 - \hookrightarrow small values of U'(x, t) (for instance, non resolved POD modes).
 - \hookrightarrow Can we find a good approximation τ of the elementary Green's function? Not sure...

► Future works

Look for an other decomposition for the missing scales $m{U}'(m{x},\,t)$:

$$\hookrightarrow U'(\boldsymbol{x}, t) = M(t)\boldsymbol{R}(\boldsymbol{x}, t)$$
, where $M \in \mathbb{R}^{3 \times 3}$

→ …??



Conclusions

A pressure extended Reduced Order Model

- The pressure is naturally included in the ROM \Rightarrow no modelisation of pressure term...
- ... but need of modelisation interaction with non resolved modes (dissipation)

Stabilization of Reduced Order Models based on POD

- $\circ \quad \text{Add some residual modes} \Rightarrow \text{Good results}$
- SUPG and VMS methods \Rightarrow Very good results

> Try to improve the functional subspace

- Database modification : an hybrid DNS/ROM method
 - \hookrightarrow Fast evaluation of temporal correlations tensor
 - \hookrightarrow Linear actualization of the POD basis
 - \hookrightarrow DNS must correct ROM \Rightarrow good results for amount of DNS greater than 70%
- Improvement using POD-NSE residuals (Krylov like method)
 - \hookrightarrow Very good for 1D burgers equation but quite poor results for 2D NSE equations
 - \hookrightarrow Problem with the continuity equation?
 - \hookrightarrow Missing scales \neq "fine scales" \Rightarrow approximation $U'(x, t) = \tau R(x, t)$ not good !

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