Interpolation of POD-ROMs for turbo-machinery by grassmannian kriging

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Context : French Research Agency project HECO

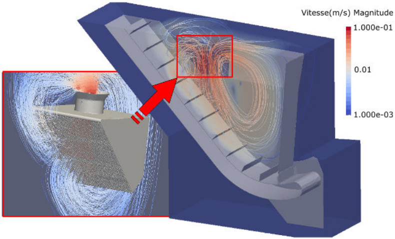
From HEating to COoling

The project : FE simulation of full scale industrial furnace/quenching tank for the prediction of thermal history of formed metal parts.

One problem : Simulation of the axial fans/agitators yields very fine mesh $\Rightarrow$ costly operation

But we are not interested in the high fidelity description of the flow around the rotating solids

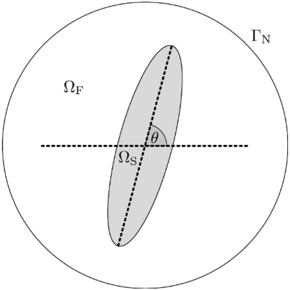
Solution replace them by reduced order models



Objective and approach

Objective

Build **adaptive POD-ROM** for a rigid bodies in forced rotation inside a fluid domain.



Difficulties with POD

1. moving boundaries : not compatible with spatial POD basis.
2. robustness w.r.t change of parameters.

Approach

1. Monolithic description of FSI and exploit the geometry [1].
2. Interpolation of POD-bases by novel grassmannian kriging [2].

1. Falaize, Liberge et Hamdouni, "POD-based reduced order model for flows induced by rigid solids in forced rotation", 2019.
2. Mosquera, "Interpolation sur les variétés grassmanniennes et applications la réduction de modles en mécanique", 2018.

Domains description

- Computational domain $\Omega = \Omega_{\mathrm{S}}(t) \cup \Omega_{\mathrm{F}}(t)$.
- Characteristic function $\chi_{\mathrm{S}}(\boldsymbol{x}, t) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \Omega_{\mathrm{S}}(t), \\ 0 & \text{otherwise.} \end{cases}$

Rotation velocity

$$\boldsymbol{u}_{\boldsymbol{\omega}}(\boldsymbol{x}, t) = \boldsymbol{\omega} \times (\boldsymbol{x} - \boldsymbol{x}_{\omega}), \quad \forall \boldsymbol{x} \in \Omega \text{ and } \forall t \in \mathrm{T}$$

Rotation constraint

$$\boldsymbol{u}(\boldsymbol{x}, t) - \boldsymbol{u}_{\boldsymbol{\omega}}(\boldsymbol{x}, t) = \mathbf{0}, \quad \forall \boldsymbol{x} \in \Omega_{\mathrm{S}}(t) \text{ and } \forall t \in \mathrm{T}, \tag{1}$$

Consequence : no deformation of the solid domain

$$\mathrm{D}(\boldsymbol{u}_{\mathrm{S}}) = \nabla \cdot \boldsymbol{u}_{\mathrm{S}} = 0, \quad \forall \boldsymbol{x} \in \Omega_{\mathrm{S}}(t), \ \forall t \in \mathrm{T}. \tag{2}$$

Multiphase MOR : Governing equations

Navier-Stokes + solid rotation constraint

$$\left\{ \begin{array}{rcl} \rho \left(\dfrac{\partial \boldsymbol{u}}{\partial t} + \nabla \boldsymbol{u} \cdot \boldsymbol{u} \right) & = & \nabla \cdot \boldsymbol{\sigma} + \boldsymbol{f} - \boldsymbol{\lambda}, \\ \nabla \cdot \boldsymbol{u} & = & 0, \\ \chi_{\mathrm{S}} (\boldsymbol{u} - \boldsymbol{u}_{\boldsymbol{\omega}}) & = & 0, \end{array} \right.$$

$\boldsymbol{\lambda}$ is the Lagrange multiplier associated with the rotation constraint.

Boundary conditions

$$\left\{ \begin{array}{llll} \boldsymbol{u}_{\mathrm{F}} = \boldsymbol{u}_{\mathrm{D}} & \forall \boldsymbol{x} \in \Gamma_{\mathrm{D}}, & \forall t \in \mathrm{T}, & \text{constant Dirichlet}, \\ \boldsymbol{\sigma}_{\mathrm{F}} \cdot \boldsymbol{n} = 0 & \forall \boldsymbol{x} \in \Gamma_{\mathrm{N}} = \Gamma \setminus \Gamma_{\mathrm{D}}, & \forall t \in \mathrm{T}, & \text{Outflow}. \end{array} \right.$$

Iterative relaxation of the solid rotation constraint [3]

At each time-step

Initial values $\boldsymbol{u}^0$, p^0 (*e.g.* from the previous time-step).
Initialize $\ell \leftarrow 0$, $\boldsymbol{\lambda}^\ell \leftarrow \mathbf{0}$

While not converge, do
Update $\ell \leftarrow \ell + 1$

Solve for $\boldsymbol{u}^\ell$, p^ℓ :

$$\rho \left(\delta_t \boldsymbol{u}^\ell + \nabla \boldsymbol{u}^\ell \cdot \boldsymbol{u}^\ell \middle| \boldsymbol{v}\right) - \left(\boldsymbol{f} - \chi_{\mathrm{S}} \boldsymbol{\lambda}^{\ell-1} \middle| \boldsymbol{v}\right) - \left(p^\ell \middle| \nabla \cdot \boldsymbol{v}\right) + 2\,\eta \left(\mathrm{D}\left(\boldsymbol{u}^\ell\right) \middle| \mathrm{D}\left(\boldsymbol{v}\right)\right) = 0,$$
$$\left(\nabla \cdot \boldsymbol{u}^\ell \middle| q\right) = 0$$

Uzawa update $\boldsymbol{\lambda}^\ell$:

$$\boldsymbol{\lambda}^\ell \leftarrow \boldsymbol{\lambda}^{\ell-1} + r\,\chi_{\mathrm{S}} \left(\boldsymbol{u}^\ell - \boldsymbol{u}_{\boldsymbol{\omega}}\right)$$

In the sequel, $\boldsymbol{v}$ will be chosen as the POD modes.

3. Glowinski et Le Tallec, Augmented Lagrangian and operator-splitting methods in nonlinear mechanics, 1989.

Standard ROM : POD of the fluctuating velocity

Ersatz

$$\widehat{\boldsymbol{u}}_h(\boldsymbol{x}, t_n) = \overline{\boldsymbol{u}}_h(\boldsymbol{x}) + \sum_{i=1}^{n_{\boldsymbol{u}}} \phi_i^{\boldsymbol{u}}(\boldsymbol{x})\, a_i(t_n)$$

with

- $\overline{\boldsymbol{u}}_h(\boldsymbol{x})$ the time averaged velocity,
- $\boldsymbol{\Phi}^{\boldsymbol{u}} = \big(\phi_i^{\boldsymbol{u}}(\boldsymbol{x})\big)_{1 \le i \le n_{\boldsymbol{u}}}$ the truncated POD basis,
- $\boldsymbol{a} = \big(a_i(t)\big)_{1 \le i \le n_{\boldsymbol{u}}}$ the temporal coefficients.

Remarks

- The velocity POD modes are divergence free $\nabla \cdot \phi_i^{\boldsymbol{u}} = 0$, $1 \le i \le n_{\boldsymbol{u}}$ and the approximation $\widehat{\boldsymbol{u}}_h$ automatically satisfies the continuity equation $\nabla \cdot \widehat{\boldsymbol{u}}_h = 0$.
- Dirichlet boundary conditions are all included in the mean field $\overline{\boldsymbol{u}}(\boldsymbol{x}) \Rightarrow$ POD modes vanish.

ROM1 : Galerkin projection of the momentum equations

Momentum equations

$$\mathbf{A} \cdot \frac{\mathrm{d}\boldsymbol{a}}{\mathrm{d}t} + \mathbf{B} \cdot \boldsymbol{a} + \mathbf{C} : \boldsymbol{a} \otimes \boldsymbol{a} + \mathbf{E}^{\ell} + \mathbf{F} = \mathbf{0}. \tag{3}$$

Uzawa update

$$\boldsymbol{\lambda}^{\ell+1} = \boldsymbol{\lambda}^{\ell} + r\,\chi_{\mathrm{S}} \left(\overline{\boldsymbol{u}} + \sum_{i=1}^{n_{\boldsymbol{u}}} \boldsymbol{\phi}_i^{\boldsymbol{u}}\, a_i - \boldsymbol{u}_{\boldsymbol{\omega}} \right), \tag{4}$$

Coefficients

$$\left\{ \begin{array}{lcl} A_{ij} & = & \rho \left(\boldsymbol{\phi}_j^{\boldsymbol{u}} \middle| \boldsymbol{\phi}_i^{\boldsymbol{u}} \right) \quad (= \rho\, \delta_{ij}), \\ B_{ij} & = & \rho \left(\nabla \boldsymbol{\phi}_j^{\boldsymbol{u}} \cdot \overline{\boldsymbol{u}} + \nabla \overline{\boldsymbol{u}} \cdot \boldsymbol{\phi}_j^{\boldsymbol{u}} \middle| \boldsymbol{\phi}_i^{\boldsymbol{u}} \right) + 2\eta \left(\mathrm{D}\left(\boldsymbol{\phi}_j^{\boldsymbol{u}}\right) \middle| \mathrm{D}\left(\boldsymbol{\phi}_i^{\boldsymbol{u}}\right) \right), \\ C_{ijk} & = & \rho \left(\nabla \boldsymbol{\phi}_j^{\boldsymbol{u}} \cdot \boldsymbol{\phi}_k^{\boldsymbol{u}} \middle| \boldsymbol{\phi}_i^{\boldsymbol{u}} \right), \\ E_i^{\ell} & = & \left(\chi_{\mathrm{S}}\, \boldsymbol{\lambda}^{\ell} \middle| \boldsymbol{\phi}_i^{\boldsymbol{u}} \right), \\ F_i & = & \rho \left(\nabla \overline{\boldsymbol{u}} \cdot \overline{\boldsymbol{u}} \middle| \boldsymbol{\phi}_i^{\boldsymbol{u}} \right) + 2\eta \left(\mathrm{D}\left(\boldsymbol{\phi}_j^{\boldsymbol{u}}\right) \middle| \mathrm{D}\left(\boldsymbol{\phi}_i^{\boldsymbol{u}}\right) \right) - \left(\boldsymbol{f} \middle| \boldsymbol{\phi}_i^{\boldsymbol{u}} \right). \end{array} \right. \tag{5}$$

Still depends on the high dimension due to projections !

Proposed ROM : POD of the characteristic function

Ersatz

$$\widehat{\chi_\mathrm{S}}(\boldsymbol{x}, t) = \overline{\chi_\mathrm{S}} + \sum_{i=1}^{n_\chi} \phi_i^\chi(\boldsymbol{x})\, c_i\,(\theta).$$

with

- $\overline{\chi_\mathrm{S}}(\boldsymbol{x})$ the <u>angle</u> averaged characteristic function,
- $\Phi^\chi = \left(\phi_i^\chi(\boldsymbol{x})\right)_{1 \leq i \leq n_\chi}$ the truncated POD basis,
- $\boldsymbol{c} = \left(c_i(\theta)\right)_{1 \leq i \leq n_\chi}$ the <u>angular</u> coefficients.

Remarks

- Forced rotation of the solid domain $\Rightarrow$ the $\theta : t \mapsto \theta(t)$ is known explicitly.
- The $\left(c_i(\theta)\right)_{1 \leq i \leq n_\chi}$ can be learned *a priori* (we use periodic splines).

ROM2 : Galerkin projection of the Uzawa iteration

Now, due to the iterative procedure for updating the Lagrange multiplier $\boldsymbol{\lambda}$, the reduced Lagrange multiplier $\widehat{\boldsymbol{\lambda}}^{\ell} = (\widehat{\lambda}_i^{\ell})_{1 \leq i \leq n_{\boldsymbol{u}}}$ can be used in place of $\mathbf{E}^{\ell}$ in the reduced momentum equation (3) :

Momentum equations

$$\mathbf{A} \cdot \frac{\mathrm{d}\boldsymbol{a}}{\mathrm{d}t} + \mathbf{B} \cdot \boldsymbol{a} + \mathbf{C} : \boldsymbol{a} \otimes \boldsymbol{a} + \widehat{\boldsymbol{\lambda}}^{\ell} + \mathbf{F} = \mathbf{0}.$$

Uzawa update

$$\widehat{\boldsymbol{\lambda}}^{\ell+1} = \widehat{\boldsymbol{\lambda}}^{\ell} + r \left(\mathbf{G} \cdot \boldsymbol{a} + \mathbf{H} \cdot \boldsymbol{c} + \mathbf{L} : \boldsymbol{c} \otimes \boldsymbol{a} + \mathbf{M} \right),$$

Coefficients

$$\left\{ \begin{array}{lcl} \widehat{\lambda}_i^{\ell} & = & \left(\chi_{\mathrm{S}}\, \boldsymbol{\lambda}^{\ell} \middle| \, \phi_i^{\boldsymbol{u}} \right), \\ G_{ij} & = & \left(\overline{\chi_{\mathrm{S}}}\, \phi_j^{\boldsymbol{u}} \middle| \, \phi_i^{\boldsymbol{u}} \right), \\ H_{ik} & = & \left(\phi_k^{\chi} \left(\overline{\boldsymbol{u}} - \boldsymbol{u}_{\omega} \right) \middle| \, \phi_i^{\boldsymbol{u}} \right), \\ L_{ijk} & = & \left(\phi_k^{\chi}\, \phi_j^{\boldsymbol{u}} \middle| \, \phi_i^{\boldsymbol{u}} \right), \\ M_i & = & \left(\overline{\chi_{\mathrm{S}}} \left(\overline{\boldsymbol{u}} - \boldsymbol{u}_{\omega} \right) \middle| \, \phi_i^{\boldsymbol{u}} \right). \end{array} \right.$$

Does not depend on the high dimension !

Interpolation of the reduced order models

Question

Provided a set of POD bases $\left(\Phi(\lambda_i)\right)_{1 \le i \le N}$ with ${}^t\Phi(\lambda_i)\,\Phi(\lambda_i) = \mathrm{I}_m$, how to derive the POD basis for a new parameter λ <u>without computing the full order solution</u> ?

One solution

Interpolate the set $\left(\Phi(\lambda_i)\right)_{1 \le i \le N}$ w.r.t the $\left(\lambda_i\right)_{1 \le i \le N}$

ROM1 : Interpolate POD basis for the velocity $\boldsymbol{\Phi}^{\boldsymbol{u}}$ only,

ROM2 : Interpolate POD bases for the velocity $\boldsymbol{\Phi}^{\boldsymbol{u}}$ and the characteristic function Φ^{χ} if the geometry changed

In this work, we focus on the interpolation over a set of Reynolds number (related with the solid rotation velocity), but the proposed method remains valid for multi-parameters setting.

What are the proper objects to interpolate ?

POD-Galerkin ROM is independent of the choice of the POD basis

For every orthogonal matrix $A \in O(m) = \{B \in \mathbb{R}^{m \times m} : \ ^T BB = I_m\}$, we have

$$\begin{aligned} u_{\phi A} &= \Phi A\,^T(\phi A)\,u \\ &= \Phi(A\,^T A)\,^T \phi u \\ &= \Phi\,^T \Phi\,u \\ &= u_\Phi \end{aligned}$$

$\Rightarrow$ Interpolate the vectorial subspaces [4] $(\overline{\phi}_i)_{i=1}^N$ engendered by the POD bases $(\phi_i)_{i=1}^N$

- Interpolate in the set of all ***m*-dimensional vectorial subspaces of the *n*-dimensional euclidian space**.
- This is the the **Grassmann manifold** $G_m(\mathbb{R}^n)$, a differential manifold of dimension $m \times (n - m)$.

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4. Amsallem et Farhat, "Interpolation method for adapting reduced-order models and application to aeroelasticity", 2008.

Grassmannian Kriging

Principle

1. Each point $\overline{\phi}_i$ is considered as the **realization of a random process** $Z = \mu + \delta$ with mean μ and δ a stationary random process with values in $T_{\overline{\phi}_r} G_m(\mathbb{R}^n)$:
$$Z_i = \exp^{-1}_{\overline{\phi}_r}(\overline{\phi}_i).$$
2. Construct an **experimental semivariogram** from the data $(\overline{\phi}_i)_{i=1}^N$ and using the geodesic distance over $G_m(\mathbb{R}^n)$ (information on the spatial autocorrelation).
3. Depending on the spatial autocorrelation, we can **choose an analytic semivariogram**.
4. The weights $\left(\alpha_i(\lambda)\right)_{i=1}^N$ for the combination over a reference tangent space so that the variance is minimized are fully determined by the analytic semivariogram.
$$Z^\star = \sum_{i=1}^N \alpha_i(\lambda^\star)\, Z_i.$$
5. Finally, combine the data in the tangent space at a reference point and get back on the Grassmann manifold
$$\overline{\phi}^\star = \exp_{\overline{\Phi_r}}(Z^\star).$$

Compute the experimental semi-variogram (step 2)

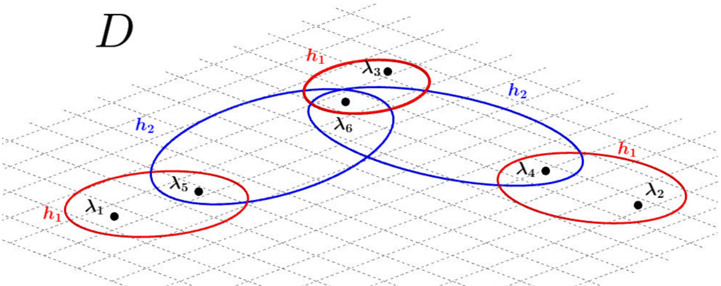
The semi-variogram associated with δ is **not known in practice**.
An **experimental semi-variogram** is built from the data $\left(\overline{\Phi_i}\right)_{1\leq i\leq n_p}$ as follows.

First, consider the following distances in the space of parameters

$$m(\Lambda) = \min\{\|\lambda_i - \lambda_j\| : 1 \leq i < j \leq N\}, \tag{6}$$

$$M(\Lambda) = \max\{\|\lambda_i - \lambda_j\| : 1 \leq i < j \leq N\}, \tag{7}$$

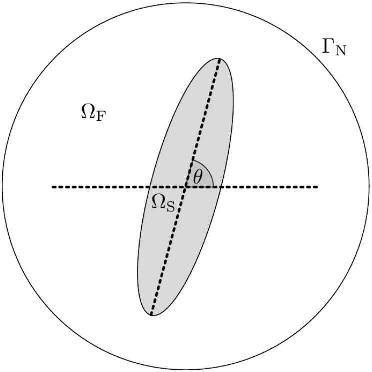
and $K \in \mathbb{N}$ such that $K \cdot m(\Lambda) < M(\Lambda)$.
Then ,define $h = (h_0, \cdots, h_{K+1}) \in \mathbb{R}^{K+2}$ where $h_k = k \cdot m(\Lambda)$ for all $k \in \{1, \cdots, K\}$, $h_0 = 0$ and $h_{K+1} = M(\Lambda)$.

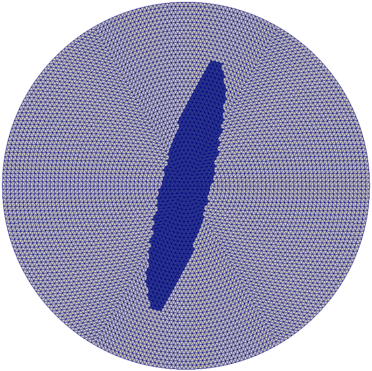


Algorithm to compute the experimental semi-variogram in step 2 (range and ceil)

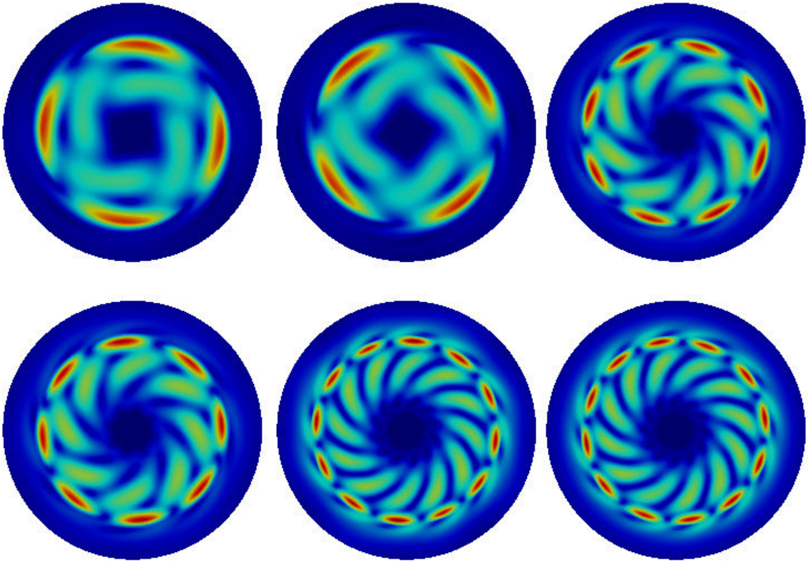
compute $m(\Lambda) = \min\{\|\lambda_i - \lambda_j\| : 1 \leq i < j \leq N\}$
compute $M(\Lambda) = \max\{\|\lambda_i - \lambda_j\| : 1 \leq i < j \leq N\}$
$h_0 = 0$
for $k = 1$ to $K + 1$ **do**
    $h_k = k \cdot m(\Lambda)$ if $k < K + 1$, else $h_k = M(\Lambda)$
    $D_k = \emptyset$ // **geodesic distances**
    for $i = 1$ to N **do**
        for $j = i + 1$ to N **do**
            if $h_{k-1} < \|\lambda_i - \lambda_j\| \leq h_k$ **then**
                Add $\widehat{d}^2\left(\widehat{log}(\Phi_i), \widehat{log}(\Phi_j)\right)$ **to the set** D_k // **geodesic** $d(\bullet)$
            end
        end
    end
    if $\mathrm{Card}(D_k) \neq 0$ **then**
        $\widetilde{v}_k = \frac{1}{\mathrm{Card}(D_k)} \mathrm{Sum}(D_k)$
    end
end
$a = h_{K+1}$ // Range
$c = \widetilde{v}_{K+1}$ // Ceil

Non-conforming mesh

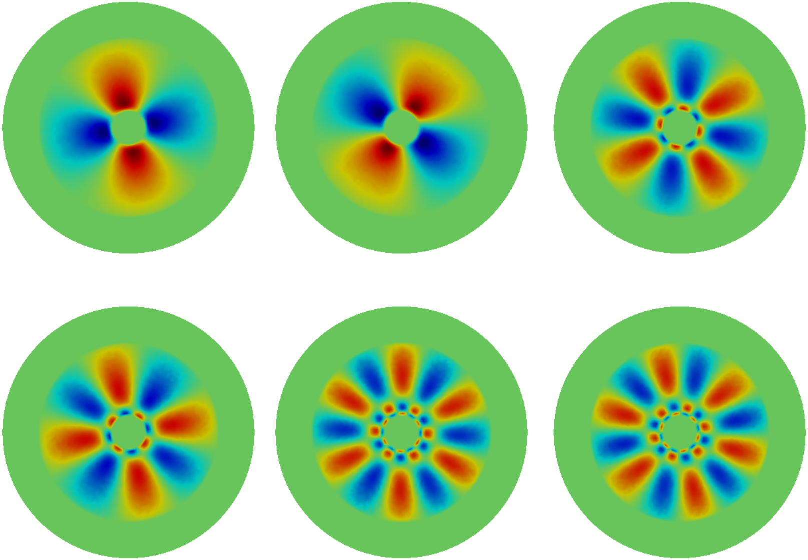




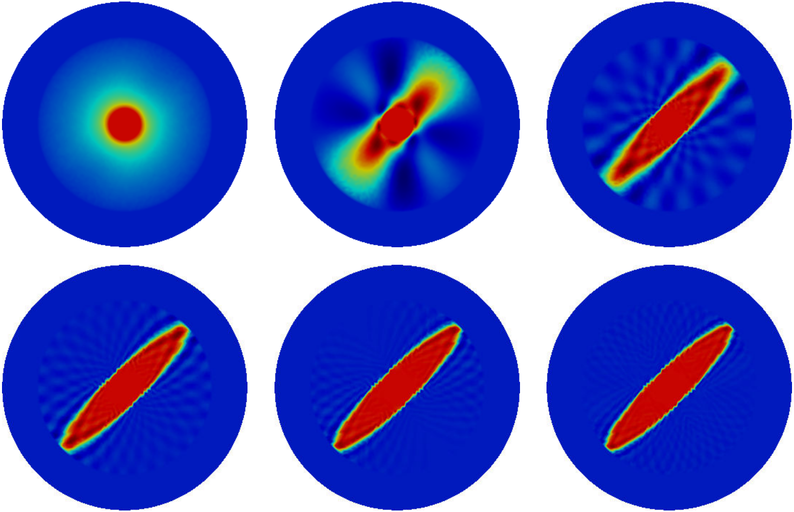
POD basis for the velocity



POD basis for the characteristic function

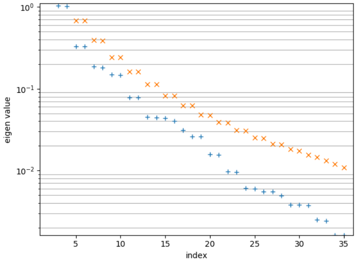


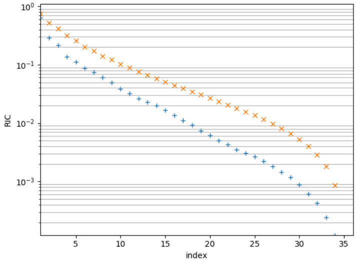
Reconstruction of the characteristic function



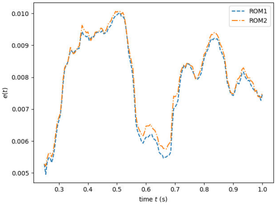
Overview

We choose $n_{\boldsymbol{u}} = 30$ and $n_{\chi} = 35$





Error $E(t) = \dfrac{\|\boldsymbol{u}(t) - \widehat{\boldsymbol{u}}(t)\|_2}{\|\boldsymbol{u}(t)\|_2}$



Time-saving

HDM $\simeq$7h,

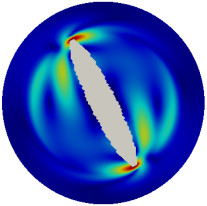
ROM1 $\simeq$20min,

ROM2 $\simeq$1min.

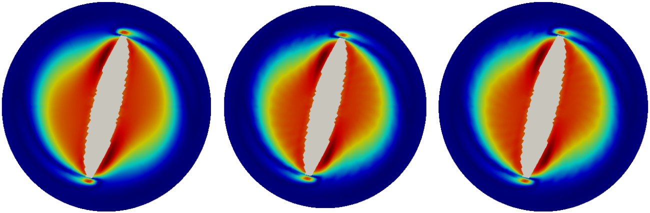
Numerical Results : Direct POD-ROMs

Fluctuating velocity

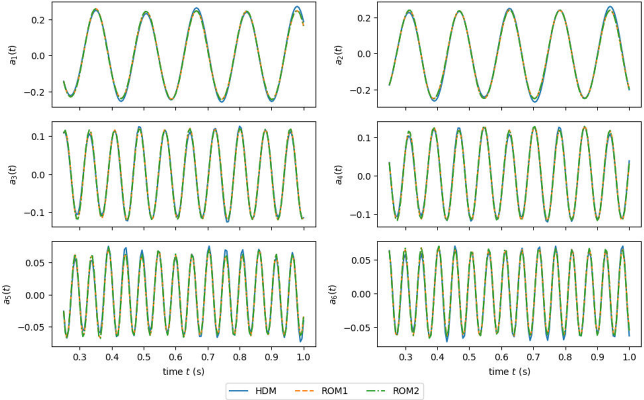
left : HDM center : ROM1 right : ROM2



Vorticity



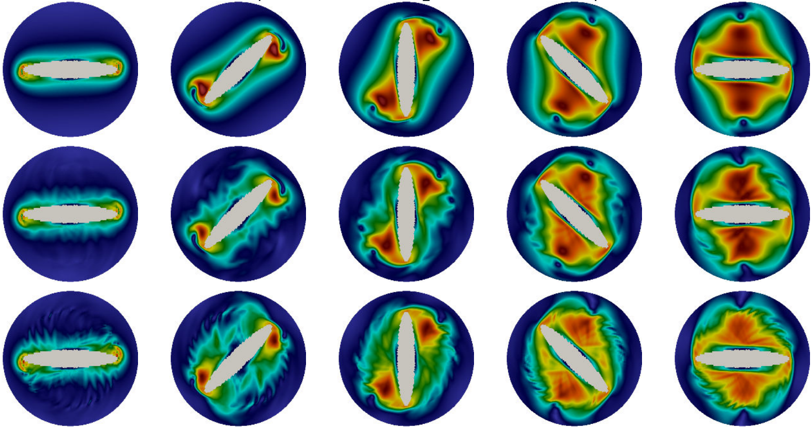
Temporal coefficients for the velocity



Numerical Results : Interpolated POD-ROMs on transient period

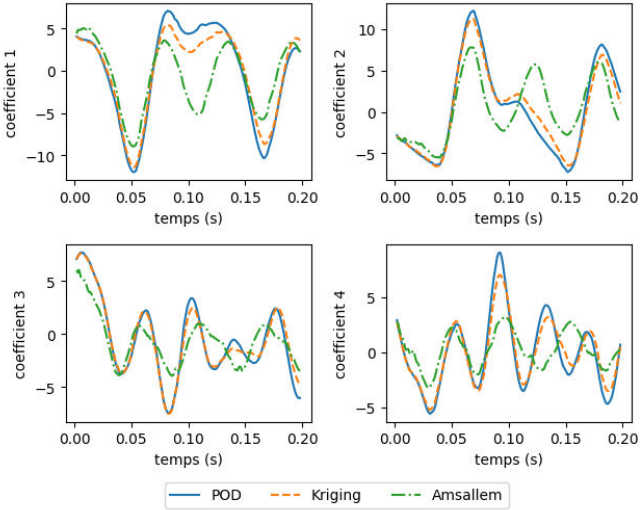
Parameter is the Reynolds number. Sampling : $\mathrm{Re} \in (1000, 1150, 1350, 1500)$.
Interpolate at $\mathrm{Re} = 1250$.

$\theta = 0$ | $\theta = \frac{\pi}{4}$ | $\theta = \frac{\pi}{2}$ | $\theta = \frac{3\pi}{4}$ | $\theta = \pi$



Numerical Results : Interpolated POD-ROMs on transient period

Temporal coefficients for the velocity



Conclusions

Contributions

- Efficient procedure to build POD-ROM for flows induced by rigid rotating bodies.
- Introduction of the grassmannian krging interpolator.

Perspectives

- Use of rotating frame for rotor subdomain $\Rightarrow$ Tearing-and-Coupling approach.
- Space/time Interpolations to avoid the resolution of the ROM.
- Extension of the proposed methods to tensor manifolds $\rightarrow$ PGD.
- Precise *a priori* estimation of interpolation errors.

Thank you for your attention.