Calibration of POD-based Reduced Order Models

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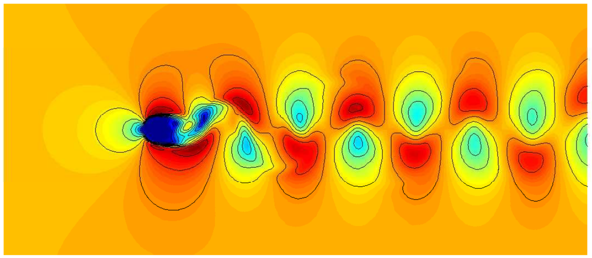
Snapshot Proper Orthogonal Decomposition

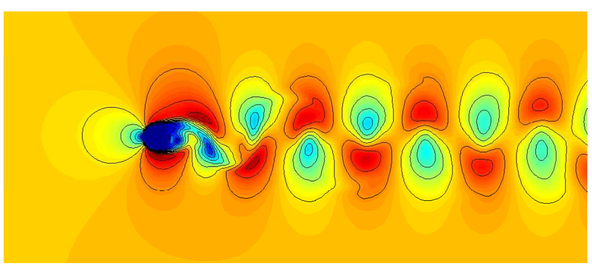
Input data set

$\mathbf{u}(\mathbf{x}, t_1)$



⋮

$\mathbf{u}(\mathbf{x}, t_{N_t})$



Time

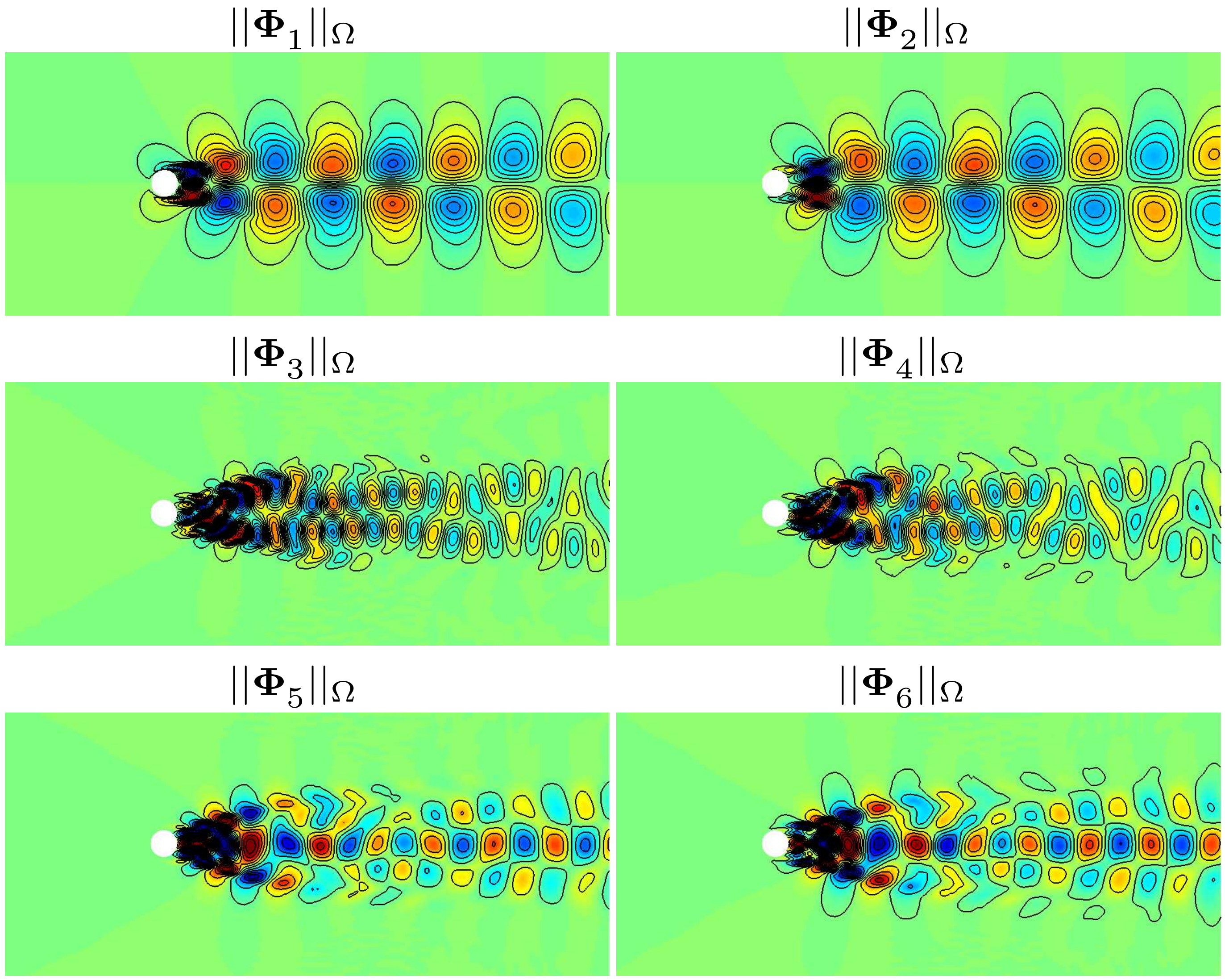
Cylinder wake flow - DNS

DNS code ICARE - *IMFT*

$Re = 200$

$N_t = 100$ snapshots corresponding to 1 period of vortex shedding ($T_o \simeq 6$)

$\mathbf{x} \in \Omega$



6 POD modes represent 99.9% of the flow energy.

POD Reduced Order Model

- POD Reduced Order Model (component i)

$$(\mathcal{P}_C)\begin{cases}\dot{a}_i^{ROM}(t) = C_i^{GP} + \sum_{j=1}^{N_{gal}} L_{ij}^{GP}\, a_j^{ROM}(t) + \sum_{j=1}^{N_{gal}}\sum_{k=1}^{N_{gal}} Q_{ijk}^{GP}\, a_j^{ROM}(t) a_k^{ROM}(t)\\ a_i^{ROM}(0) = a_i^{POD}(0)\end{cases}$$

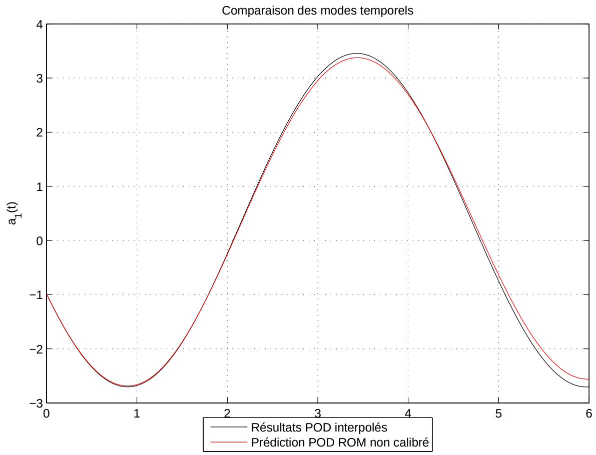
where

$$a_i^{POD}(t) = (\mathbf{u}(t) - \mathbf{u_m}(t), \mathbf{\Phi}_i)_\Omega$$

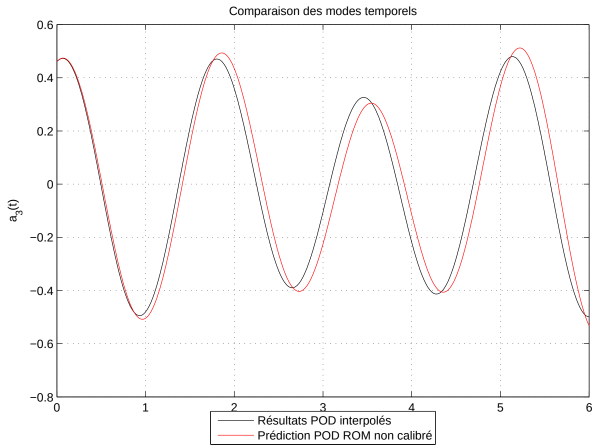
are the POD temporal modes.

- Integration in time (4th order Runge-Kutta)

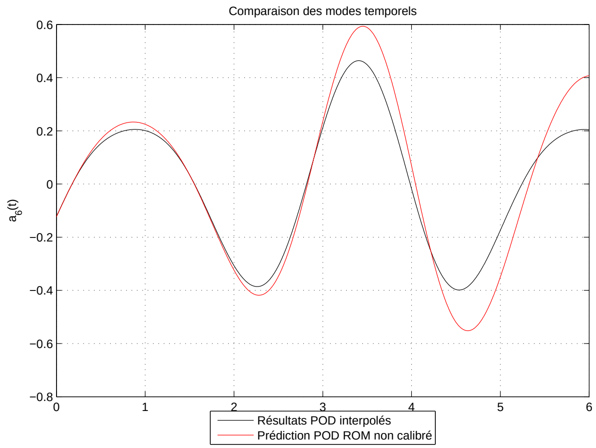
POD ROM with no calibration



$a_1(t)$



$a_3(t)$



$a_6(t)$

➡ **The accuracy of the POD ROM is not perfect.**

Temporal amplification and phase shifts.

Some explanations of the reconstruction errors

- Structural instability of the Galerkin projection (Iollo 2000, Rempfer 2000, Noack *et al.* 2003)
- Galerkin truncation: dissipative scales neglected
- Pressure contribution or boundary terms not (correctly) evaluated
- Incompressibility hypothesis not verified (experimental data).

⇨ **We need to calibrate the POD Reduced Order Models**

POD Reduced Order Model (component i)

$$\dot{a}_i^{ROM}(t) = C_i + \sum_{j=1}^{N_{gal}} L_{ij}\, a_j^{ROM}(t) + \sum_{j=1}^{N_{gal}} \sum_{k=1}^{N_{gal}} Q_{ijk}\, a_j^{ROM}(t) a_k^{ROM}(t)$$

$$= f_i(\underbrace{C_i, L_{i,:}, Q_{i,:,:}}_{\mathbf{y_i}}, \mathbf{a}^{ROM}(t)) = f_i(\mathbf{y_i}, \mathbf{a}^{ROM}(t))$$

where $\mathbf{y_i} = \begin{pmatrix} C_i \\ L_{i1} \\ \vdots \\ L_{iN_{gal}} \\ Q_{i11} \\ \vdots \\ Q_{iN_{gal}N_{gal}} \end{pmatrix} \in \mathbb{R}^{N_{c_i}}$ with $N_{c_i} = 1 + N_{gal} + \frac{N_{gal}(N_{gal}+1)}{2}$.

POD ROM calibration

- POD Reduced Order Model (vectorial notation)

$$\boxed{\dot{\mathbf{a}}^{ROM}(t) = \mathbf{f}(\mathbf{y}, \mathbf{a}^{ROM}(t))}$$

where

$$\mathbf{f} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{N_{gal}} \end{pmatrix} \in \mathbb{R}^{N_{gal}} \quad \text{and} \quad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{N_{gal}} \end{pmatrix} \in \mathbb{R}^{N_c}$$

with $N_c = N_{gal} N_{c_i} = N_{gal} \left(1 + N_{gal} + \frac{N_{gal}(N_{gal}+1)}{2}\right)$.

- When $\{C, L, Q\} = \{C^{GP}, L^{GP}, Q^{GP}\}$ then we note $\mathbf{f} = \mathbf{f}^{GP}$.

- State calibration method or "Floquet calibration" (Noack)

$$\mathbf{e}^{(1)}(\mathbf{f},t) = \mathbf{a}^{POD}(t) - \mathbf{a}^{ROM}(t) \in \mathbb{R}^{N_{gal}}$$

- Norm

$$\forall \mathbf{z} \in \mathbb{R}^{N_{gal}} \text{ we define } \|\mathbf{z}\|_\Lambda^2 = \mathbf{z}^T \Lambda \mathbf{z} \quad \text{with } \Lambda \in \mathbb{R}^{N_{gal} \times N_{gal}}$$

- Time average operator $\langle g(t) \rangle_{T_o} = \int_0^{T_o} g(t)\, dt = 1/N_t \sum_{k=1}^{N_t} g(t_k)$
- Natural minimization problem

Minimize $\langle \|\mathbf{e}^{(1)}(\mathbf{f},t)\|_\Lambda^2 \rangle_{T_o}$ with $\mathbf{a}^{ROM}$ solution of the Cauchy problem

$$(\mathcal{P}_C) \begin{cases} \dot{\mathbf{a}}^{ROM}(t) = \mathbf{f}(\mathbf{y}, \mathbf{a}^{ROM}(t)), \\ \mathbf{a}^{ROM}(0) = \mathbf{a}^{POD}(0). \end{cases}$$

This is a non linear constrained optimization problem !!

Constrained optimization problem

- $$\langle \|\mathbf{e}^{(1)}(\mathbf{f}, t)\|^2_{I_{N_{gal}}} \rangle_{T_o} = \frac{1}{N_t} \sum_{k=1}^{N_t} \sum_{i=1}^{N_{gal}} \left(a_i^{POD}(t_k) - a_i^{ROM}(t_k) \right)^2$$

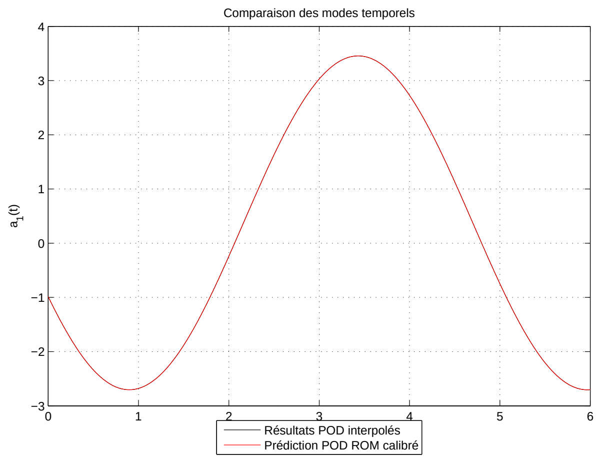
- Ex: Let C_i and L_{ij} be the calibration coefficients. We determine:
  1. adjoint equations

$$\frac{d\xi_i}{dt} = -\sum_{j=1}^{N_{gal}} L_{ji}\, \xi_j(t) - \sum_{j,k=1}^{N_{gal}} \xi_j(t) \left(Q_{jik} + Q_{jki} \right) a_k^{ROM}(t)$$
$$- 2 \left(a_i^{ROM}(t) - a_i^{POD}(t) \right) \quad \text{avec} \quad \xi_i(T_o) = 0$$

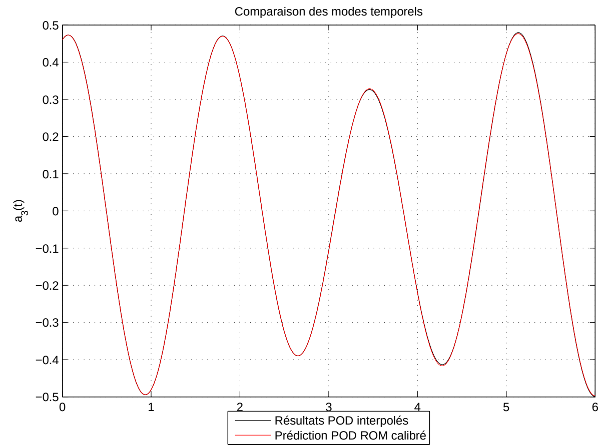
  2. optimality conditions

$$\int_0^{T_o} \xi_i(t)\, dt = 0 \quad \text{et} \quad \int_0^{T_o} \xi_i(t) a_j^{ROM}(t)\, dt = 0$$

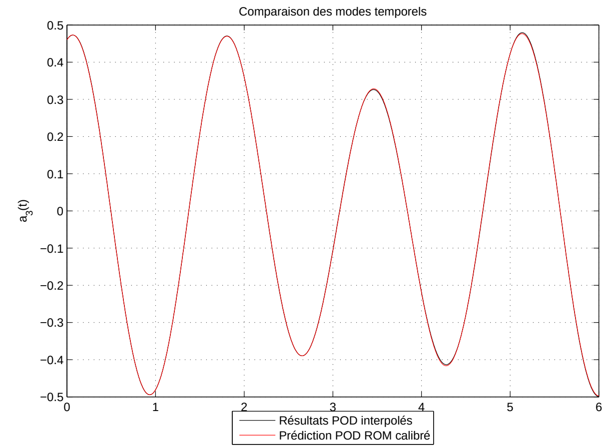
- Problem solved:
  - iteratively in Bergmann (2004) and Galletti et al. (2004)
  - in one shot (pseudo spectral method) in Galletti et al. (2007)



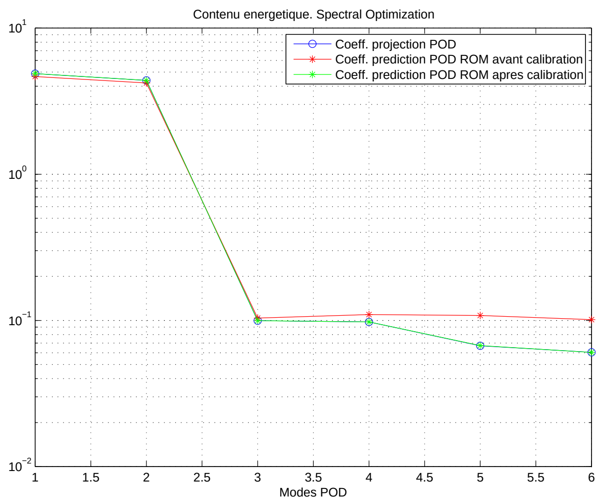
$a_1(t)$



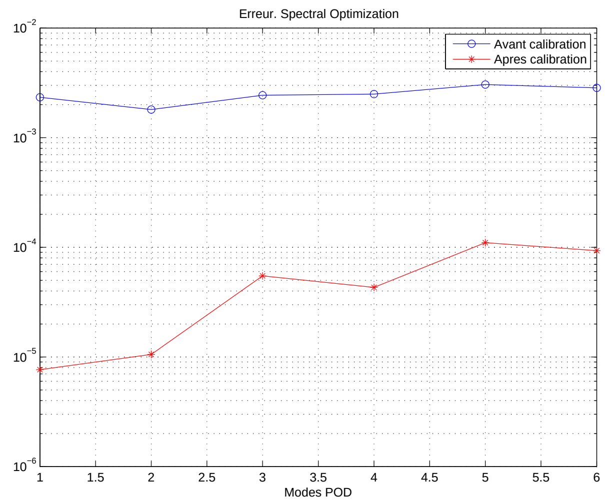
$a_3(t)$



$a_6(t)$



Energetic content



L^2 error

Two another definitions for e

- After integration in time of the state equations, we obtain:

$$\int_0^t \dot{\mathbf{a}}^{ROM}(\tau)\,d\tau = \mathbf{a}^{ROM}(t) - \mathbf{a}^{POD}(0) = \int_0^t \mathbf{f}(\mathbf{a}^{ROM}(\tau))\,d\tau$$

$$\Longrightarrow \mathbf{e}^{(1)}(\mathbf{f},t) = \mathbf{a}^{POD}(t) - \mathbf{a}^{POD}(0) - \int_0^t \mathbf{f}(\mathbf{a}^{ROM}(\tau))\,d\tau$$

- State calibration method with $\mathbf{a}^{ROM} \longrightarrow \mathbf{a}^{POD}$

$$\mathbf{e}^{(2)}(\mathbf{f},t) = \underbrace{\mathbf{a}^{POD}(t) - \mathbf{a}^{POD}(0)}_{\mathbf{e}^{(2)}(0,t)} - \int_0^t \mathbf{f}(\mathbf{a}^{POD}(\tau))\,d\tau$$

- Flow calibration method or "Poincaré calibration" (Noack)

$$\frac{d}{dt}\left(\mathbf{e}^{(1)}(f,t)\right) = \dot{\mathbf{a}}^{POD}(t) - \mathbf{f}(\mathbf{a}^{ROM}(t)) \text{ and } \mathbf{a}^{ROM} \longrightarrow \mathbf{a}^{POD}$$

$$\Longrightarrow \mathbf{e}^{(3)}(\mathbf{f},t) = \underbrace{\dot{\mathbf{a}}^{POD}(t)}_{\mathbf{e}^{(3)}(0,t)} - \mathbf{f}(\mathbf{a}^{POD}(t))$$

Some comments on $\mathrm{e}^{(3)}$

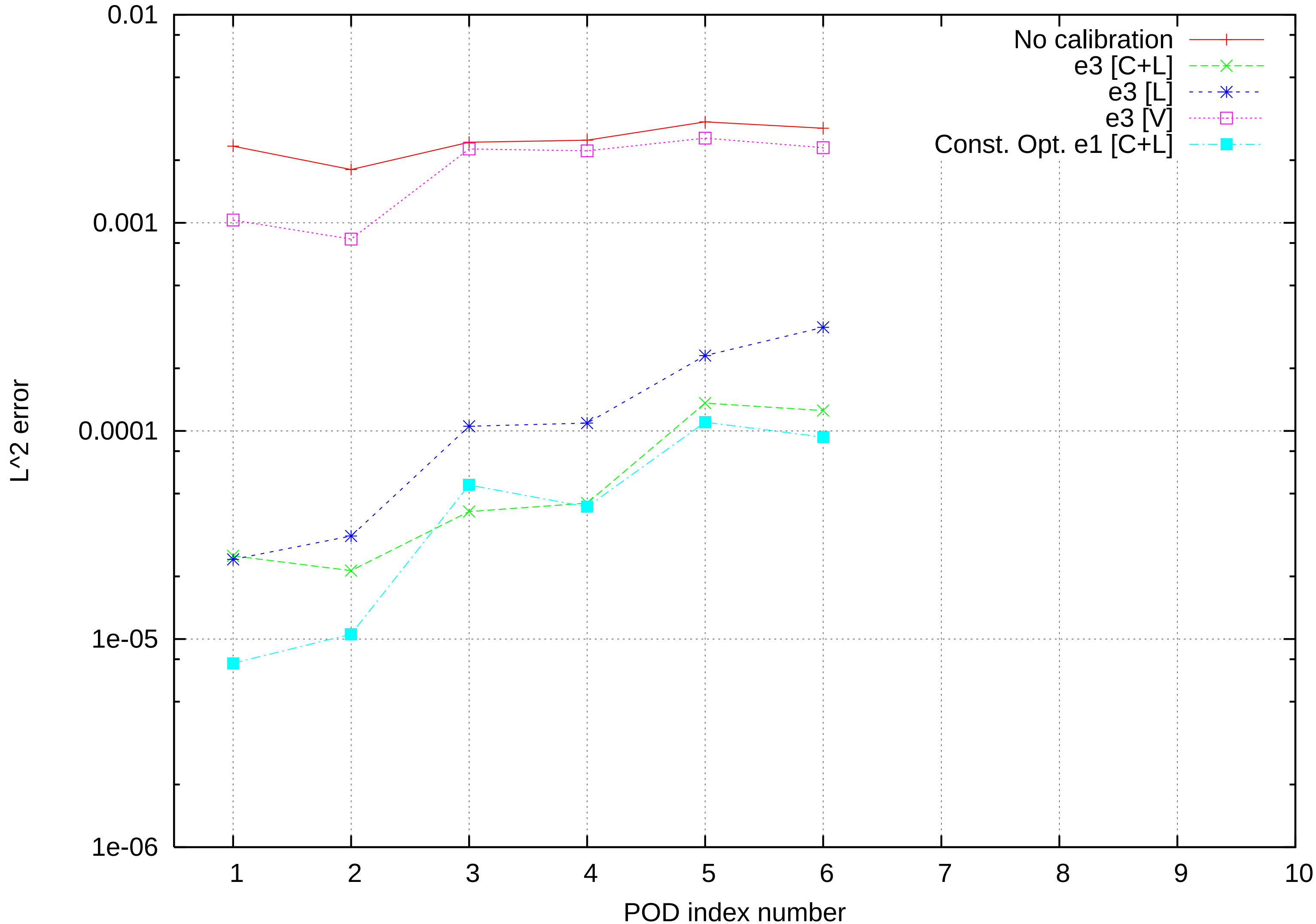
- $$\langle \|\mathbf{e}^{(3)}(\mathbf{f},t)\|^2_{I_{N_{gal}}}\rangle_{T_o} = \frac{1}{N_t}\sum_{k=1}^{N_t}\sum_{i=1}^{N_{gal}}\left(\dot{a}_i^{POD}(t_k) - f_i(a_i^{POD}(t_k))\right)^2$$
- Problem solved:
  - in Galletti et al. (2004) for C and L
  - in Favier (2007) for
    1. C
    2. C and L
    3. eddy viscosities ν_i (see Bergmann 2004)
  - in Bourguet et al. (2007) for C and L
- Buffoni et al. (2008) suggested to minimize the model prediction error in the H^1 norm

$$\int_0^{T_o} \dot{a}_i^P\, dt = C_i T_o + L_{ij}\int_0^{T_o} a_j^P\, dt + Q_{ijk}\int_0^{T_o} a_j^P a_k^P\, dt$$

$$\int_0^{T_o} \dot{a}_i^P a_l^P\, dt = C_i\int_0^{T_o} a_l^P\, dt + L_{ij}\int_0^{T_o} a_j^P a_l^P\, dt + Q_{ijk}\int_0^{T_o} a_j^P a_k^P a_l^P\, dt$$

It can be shown that this method is equivalent to the minimization of $\mathbf{e}^{(3)}$.

L^2 error for different calibration methods



For the first two modes, minimizing $\mathrm{e}^{(1)}$ is better than $\mathrm{e}^{(3)}$.

Error increases with the POD modes.

Minimization problems for $\mathrm{e}^{(2)}$ and $\mathrm{e}^{(3)}$

- $\mathbf{e}^{(2)}$ and $\mathbf{e}^{(3)}$ are affine function of $\mathbf{f}$ i.e. of $\mathbf{y} \in \mathbb{R}^{N_c}$. We introduce the application:

$$\mathbf{e}^{(i)}(\cdot, t) : \mathbb{R}^{N_c} \longrightarrow \mathbb{R}^{N_{gal}}$$

$$\mathbf{y} \mapsto E^{(i)}(t)\mathbf{y} + \mathbf{e}^{(i)}(0,t) \qquad \text{with} \quad E^{(i)}(t) \in \mathbb{R}^{N_{gal} \times N_c}.$$

$$E^{(2)}(t)\mathbf{y} = -\int_0^t \mathbf{f}(\mathbf{a}^{POD}(\tau))\, d\tau \quad \text{and} \quad E^{(3)}(t)\mathbf{y} = -\mathbf{f}(\mathbf{a}^{POD}(t))$$

- Minimizing $\mathcal{J}^{(i)}(\mathbf{f}) = \langle \|\mathbf{e}^{(i)}(\mathbf{f}, t)\|_\Lambda^2 \rangle_{T_o}$ for $i = 2$ or 3 is equivalent to solve the linear system:

$$\boxed{A^{(i)}\mathbf{y} = \mathbf{b}^{(i)}}$$

with

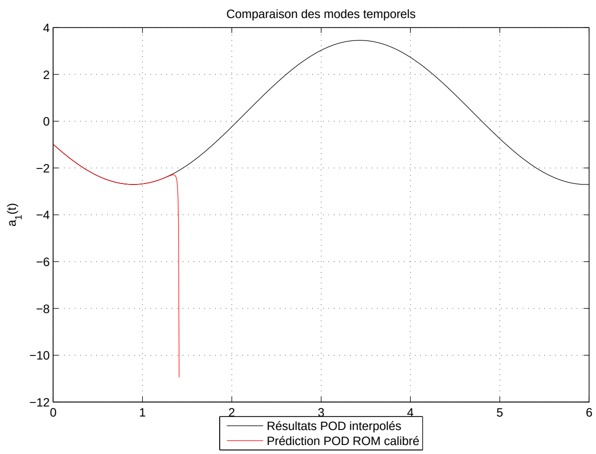
$$A^{(i)} = \langle E^{(i)T}(t)\Lambda E^{(i)}(t)\rangle_{T_o} \in \mathbb{R}^{N_c \times N_c}$$

and

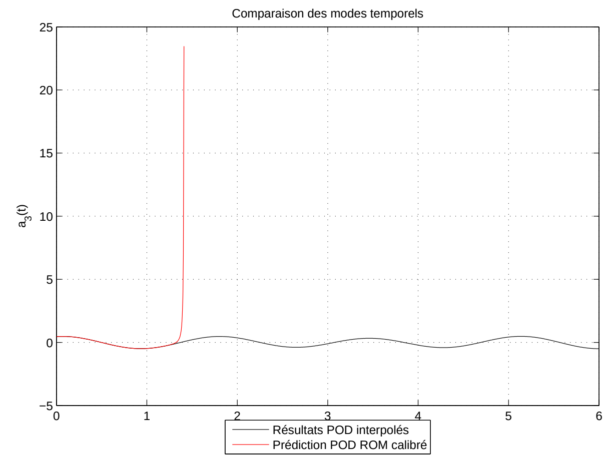
$$\mathbf{b}^{(i)} = -\langle E^{(i)T}(t)\Lambda \mathbf{e}^{(i)}(0,t)\rangle_{T_o} \in \mathbb{R}^{N_c}$$

POD ROM with calibration of C, L and Q

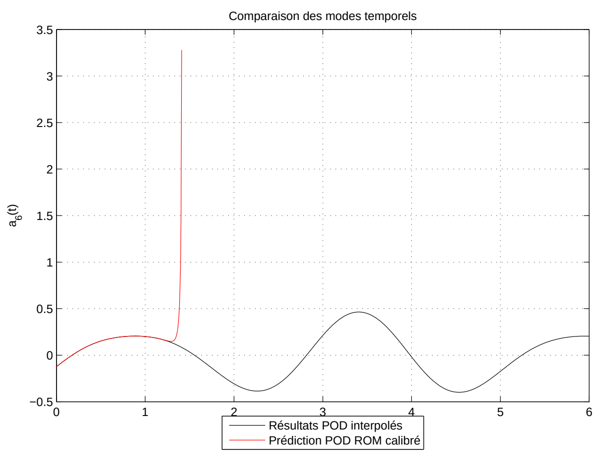
Error $\mathbf{e}^{(3)}$



$a_1(t)$



$a_3(t)$



$a_6(t)$

➩ **Divergence in the time integration.**

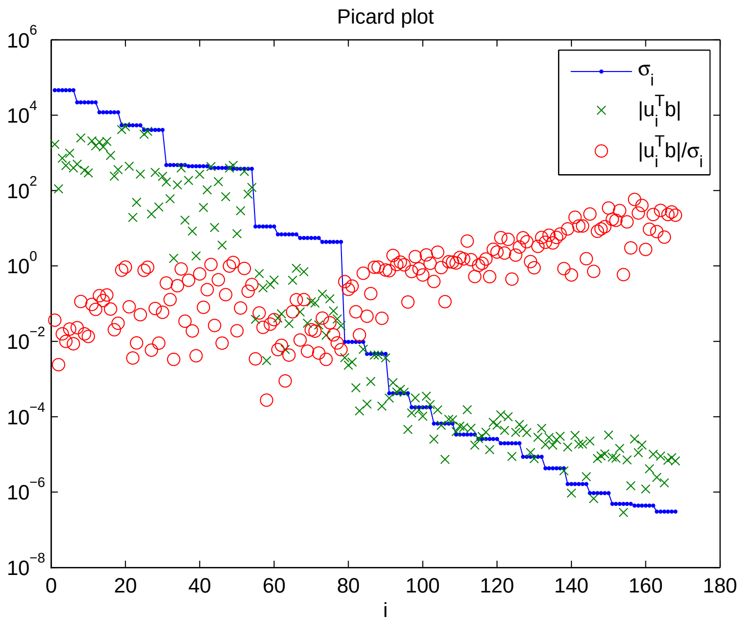
$A^{(3)}$ *is ill conditionned.*

Discrete Picard condition and filter factor

- Using the SVD decomposition of $A^{(i)}$ ($A^{(i)} = U\Sigma V^T = \sum_{j=1}^{n} \mathbf{u_j}\sigma_j \mathbf{v_j}^T$), we show that:

$$\mathbf{y} = \sum_{j=1}^{n} \frac{1}{\sigma_j} \mathbf{u_j}^T \mathbf{b} \mathbf{v_j} = \sum_{j=1}^{n} h_j \frac{1}{\sigma_j} \mathbf{u_j}^T \mathbf{b} \mathbf{v_j} \quad \text{with} \quad h_j = 1$$

- Picard plot



➡ **For $j \simeq 80$, σ_j decay faster than the Fourier coefficients $\mathbf{u_j}^T\mathbf{b}$.**

How can we regularize the solution?

- Following Couplet (2005), we introduce a new functional:

$$\mathcal{J}_{\alpha}{}^{(i)}(\mathbf{f}) = (1-\alpha)\mathcal{E}^{(i)}(\mathbf{f}) + \alpha\mathcal{D}^{(i)}(\mathbf{f})$$

with

$$\mathcal{E}^{(i)}(\mathbf{f}) = \frac{\langle \|\mathbf{e}^{(i)}(\mathbf{f},t)\|_{\Lambda}^2\rangle_{T_o}}{\langle \|\mathbf{e}^{(i)}(\mathbf{f}^{GP},t)\|_{\Lambda}^2\rangle_{T_o}} = \frac{\mathcal{J}^{(i)}(\mathbf{f})}{\mathcal{J}^{(i)}(\mathbf{f}^{GP})}$$

and

$$\mathcal{D}^{(i)}(\mathbf{f}) = \frac{\|\mathbf{f}-\mathbf{f}^{GP}\|_{\Pi}^2}{\|\mathbf{f}^{GP}\|_{\Pi}^2}$$

- Norm

$\forall \mathbf{f}(\mathbf{y}) \in \mathbb{R}^{N_{gal}}$ we define $\|\mathbf{f}\|_{\Pi}^2 = \mathbf{y}^T\Pi\mathbf{y}$ with $\Pi \in \mathbb{R}^{N_c \times N_c}$ and $\mathbf{y} \in \mathbb{R}^{N_c}$

- $\alpha \in [0;1]$ is a new constant to be tuned.

- Minimizing ${\mathcal{J}_\alpha}^{(i)}(\mathbf{f})$ for $i = 2$ or 3 is equivalent to solve the linear system:

$$\boxed{A_\alpha^{(i)} \mathbf{y}_\alpha^{(i)} = \mathbf{b}_\alpha^{(i)}}$$

with

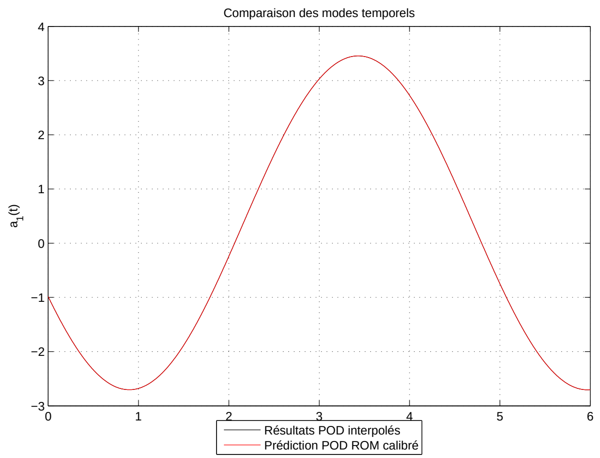
$$A_\alpha^{(i)} = \frac{1-\alpha}{\langle \|\mathbf{e}^{(i)}(\mathbf{f}^{GP}, t)\|_\Lambda^2 \rangle_{T_o}} A^{(i)} + \frac{\alpha}{\|\mathbf{f}^{GP}\|_\Pi^2} \Pi$$

and

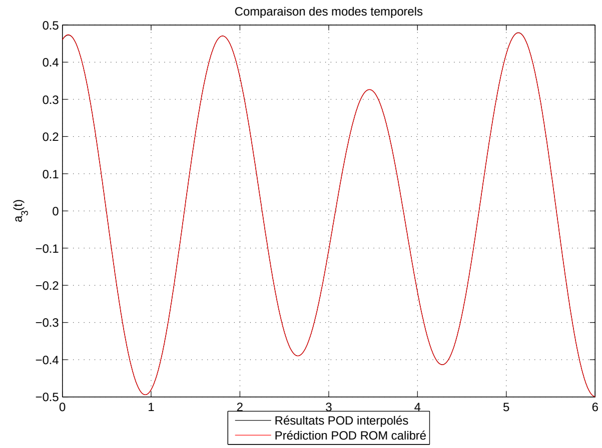
$$\mathbf{b}_\alpha^{(i)} = \frac{1-\alpha}{\langle \|\mathbf{e}^{(i)}(\mathbf{f}^{GP}, t)\|_\Lambda^2 \rangle_{T_o}} \mathbf{b}^{(i)} + \frac{\alpha}{\|\mathbf{f}^{GP}\|_\Pi^2} \Pi \mathbf{y}^{GP}$$

- Open questions:
  1. How can we choose α optimally?
  2. How can we use this approach for experimental data (no Galerkin Projection coefficients available)?

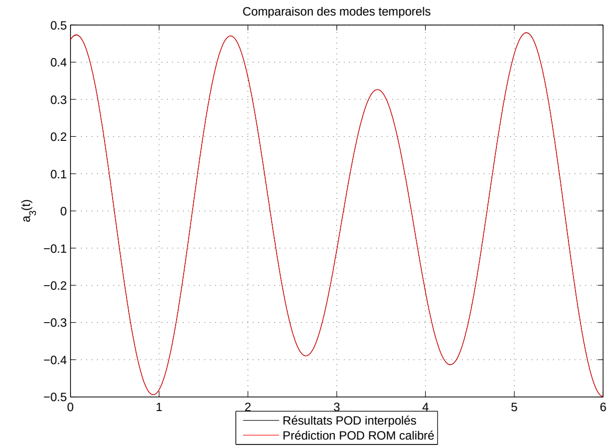
POD ROM with calibration of C, L and Q — $\alpha = 0.001$ (error $\mathbf{e}^{(3)}$)



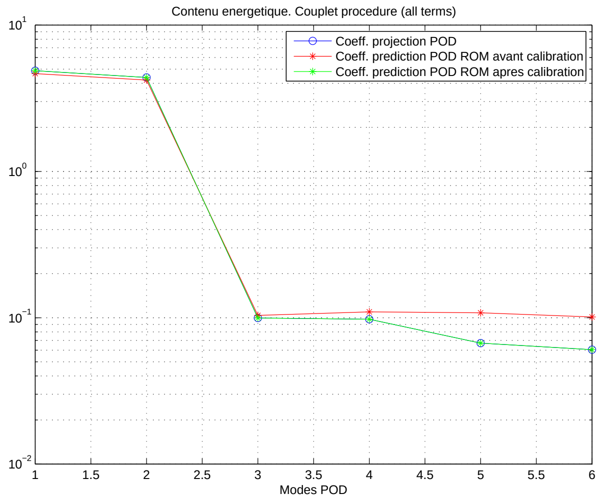
$a_1(t)$



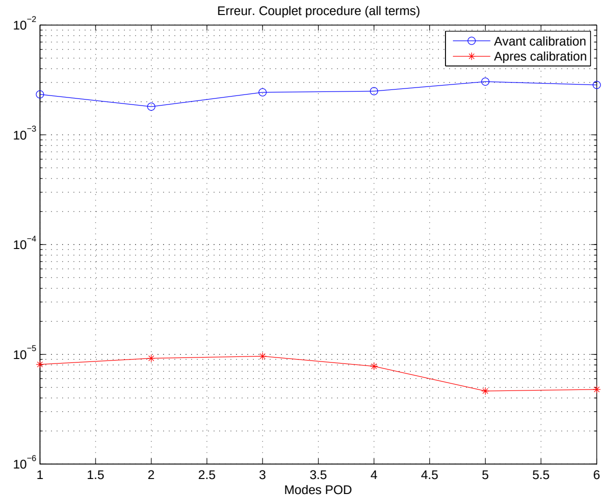
$a_3(t)$



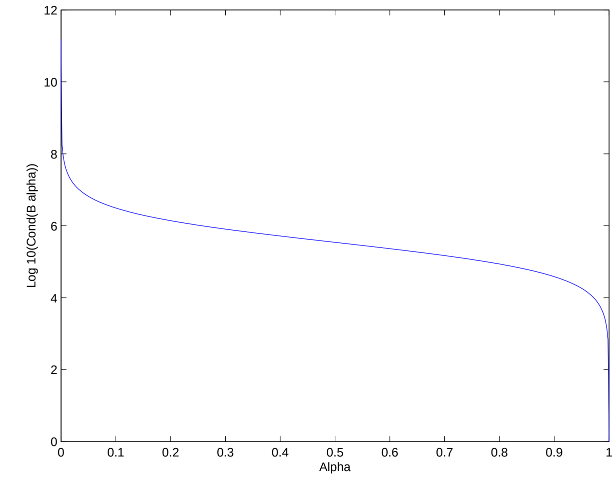
$a_6(t)$



Energetic content

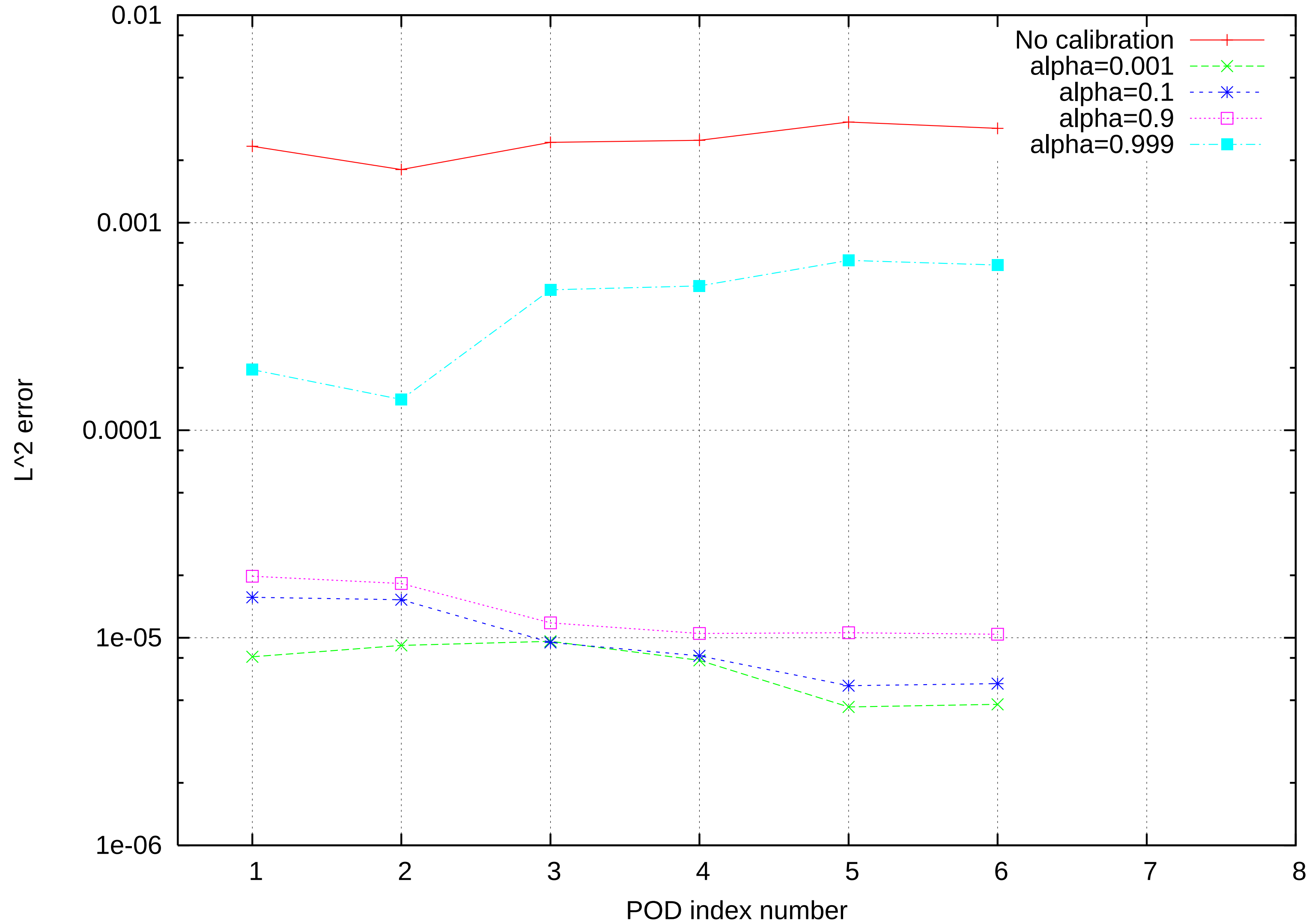


L^2 error



Log_{10} of the condition number

POD ROM with calibration of C, L and Q Influence of α (error $\mathbf{e}^{(3)}$)



Error increases with value of α.

The choice of α is difficult: compromise !!

Regularized solution

- For $A\mathbf{x} = \mathbf{b}$, the regularized solution is:

$$\mathbf{x}_\rho = \text{arg min}_{\mathbf{x}}\{\|A\mathbf{x} - \mathbf{b}\|^2 + \rho\|\mathbf{x}\|^2\}$$ where ρ is a regularization parameter.

➡ Regularization can be understood as a balance between two requirements:

1. $\mathbf{x}$ should give a small residual $A\mathbf{x} - \mathbf{b}$
2. $\mathbf{x}$ should be small in L^2 norm.

- This problem is equivalent to solve:

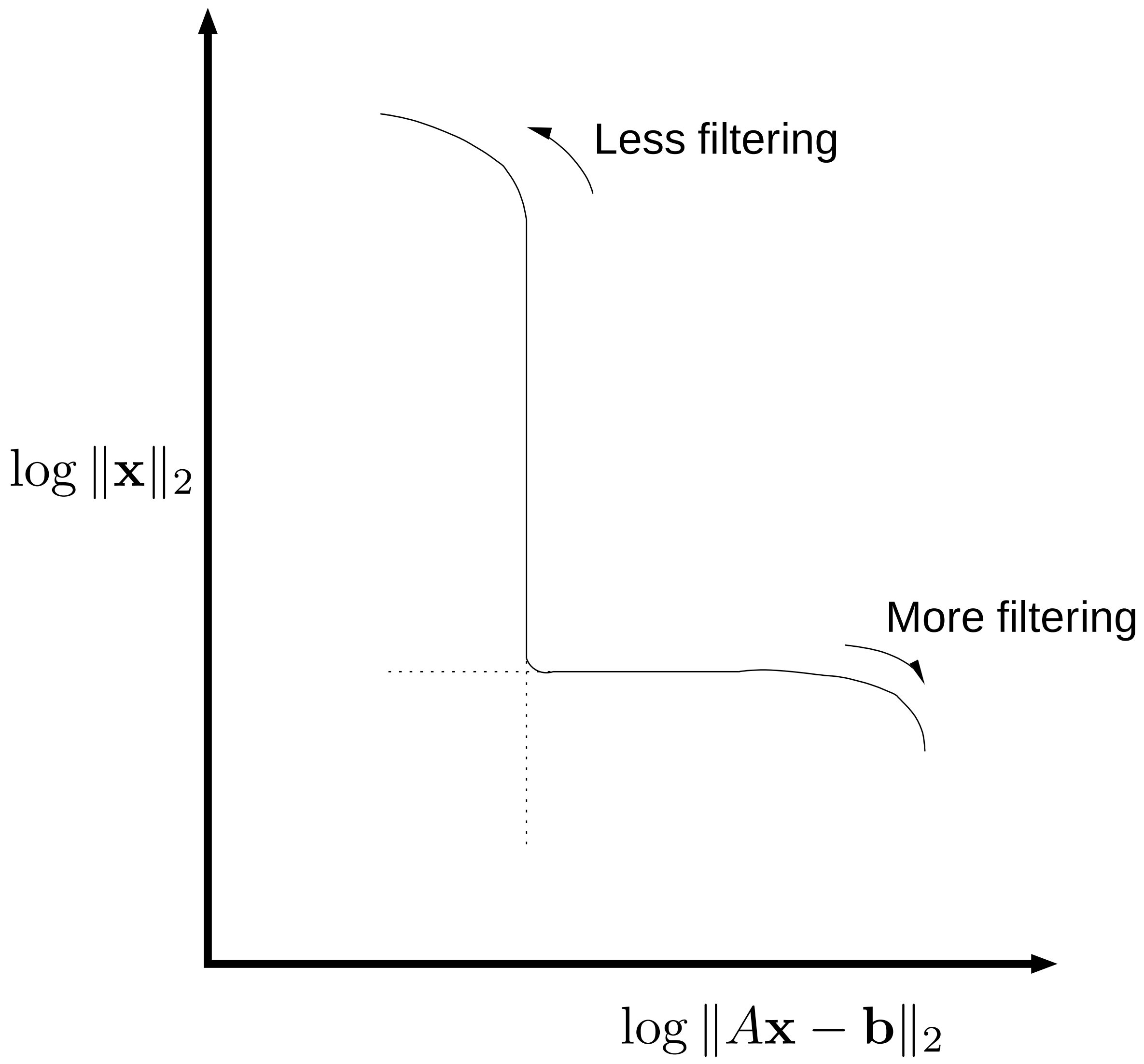
$$\left(A^T A + \rho I\right)\mathbf{x}_\rho = A^T\mathbf{b}$$

- Using the SVD decomposition of A, it can be shown that:

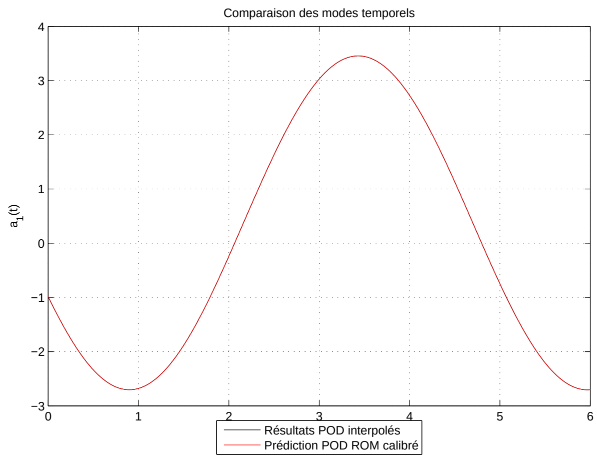
$$\mathbf{x}_\rho = \sum_{j=1}^{n} \frac{\sigma_j}{\sigma_j^2 + \rho}\mathbf{u_j}^T\mathbf{b}\mathbf{v_j} = \sum_{j=1}^{n} h_j \frac{1}{\sigma_j}\mathbf{u_j}^T\mathbf{b}\mathbf{v_j} \quad \text{with } h_j = \frac{\sigma_j^2}{\sigma_j^2 + \rho}$$

- ρ is based on the L-curve (Hansen, regularization tools).

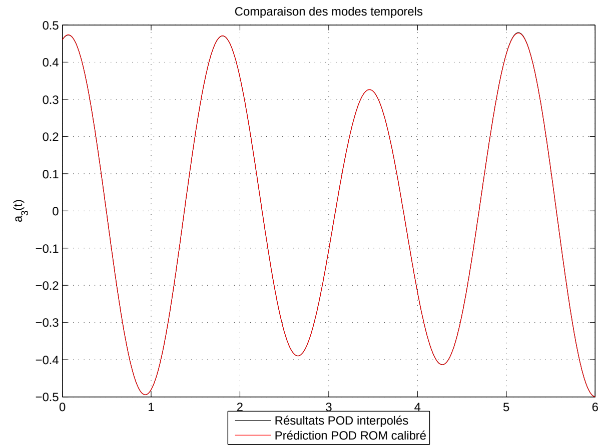
Principle of the L-curve



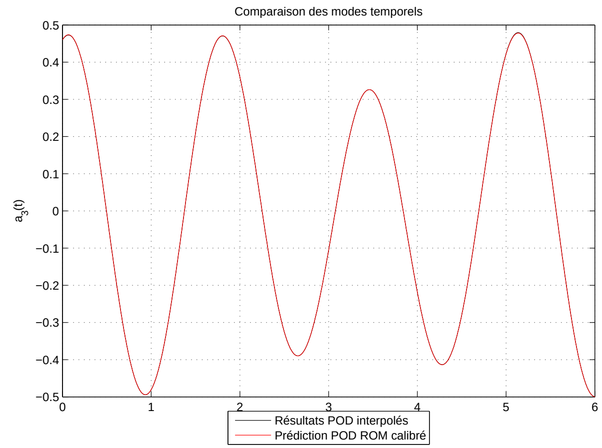
POD ROM with calibration of C, L and Q — Tikhonov regularization ($\mathbf{e}^{(3)}$)



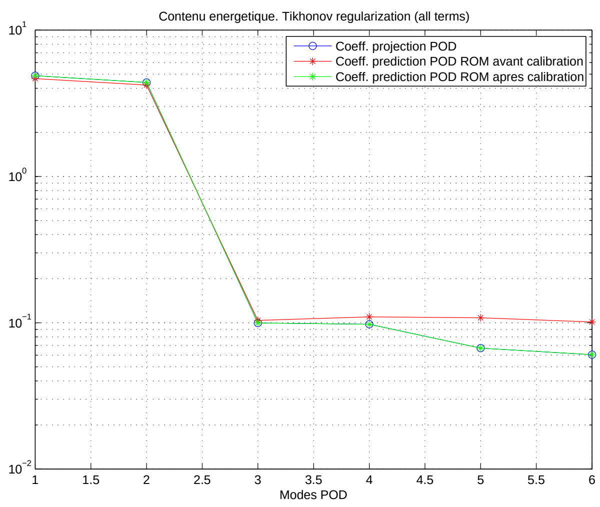
$a_1(t)$



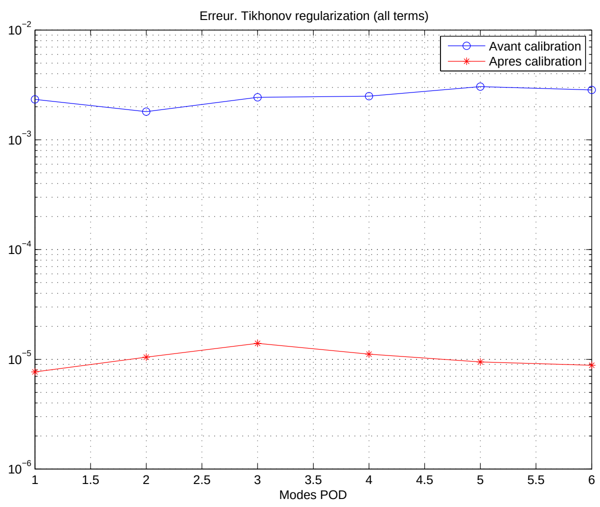
$a_3(t)$



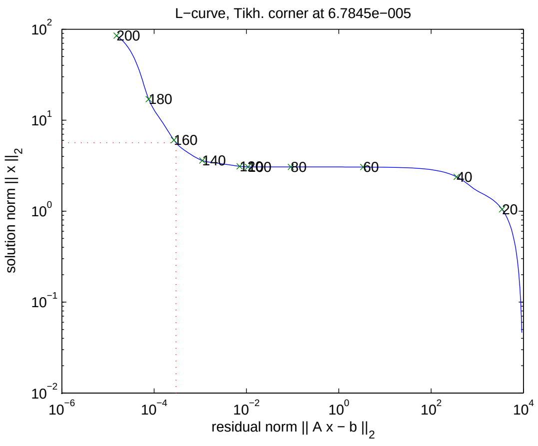
$a_6(t)$



Energetic content



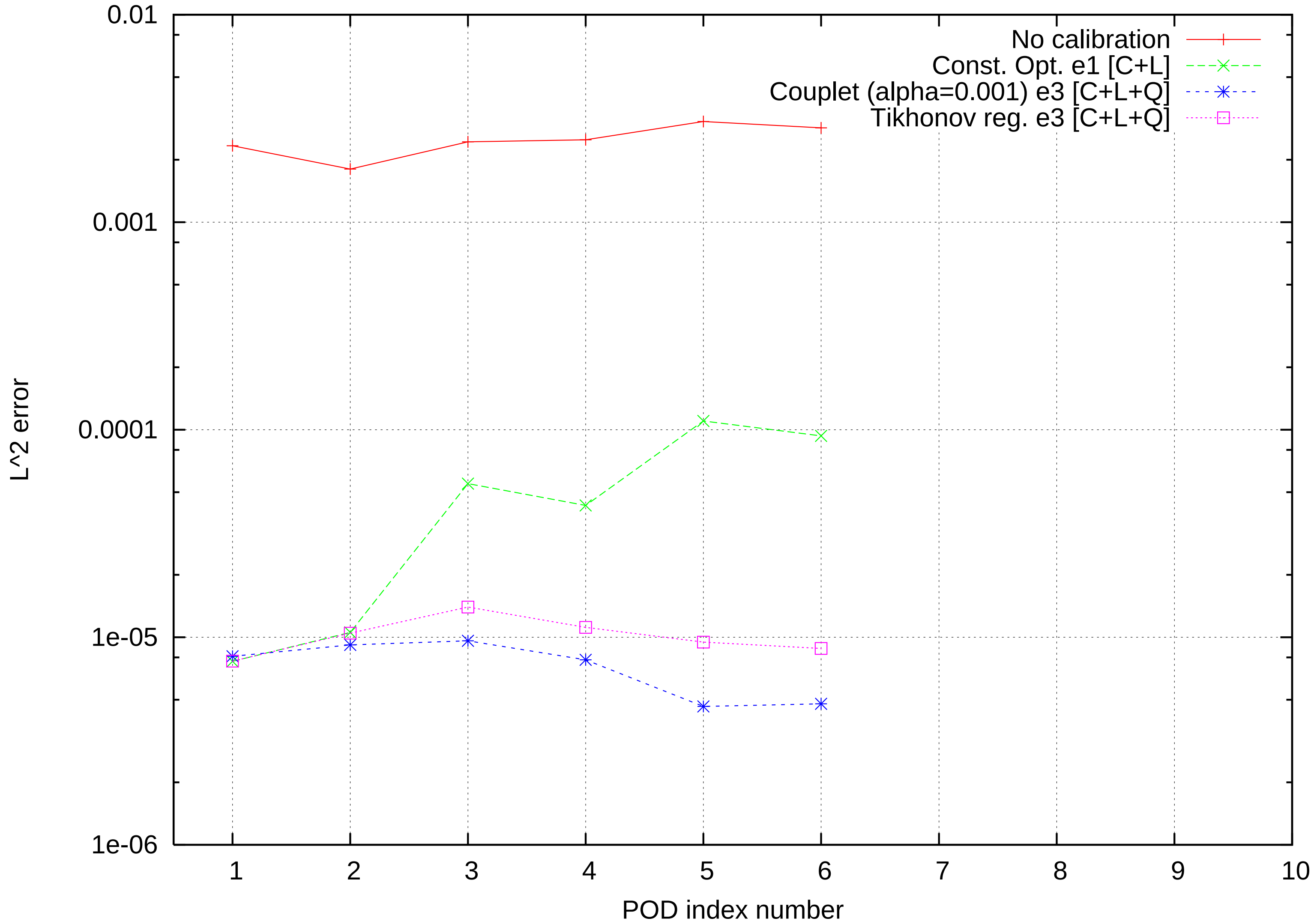
L^2 error



L-curve

Regularized solution

L^2 error for different calibration methods



For the first three modes, errors are similar.

For $\mathbf{e}^{(1)}$, error increases with the POD modes.

Conclusions and perspectives

- Conclusions (simple dynamics)
  - Minimizing $\mathbf{e}^{(1)}$ (constrained optimization) or minimizing $\mathbf{e}^{(3)}$ with regularization strategies is equivalent for the first POD modes.
  - For the higher POD modes, it seems better to minimize $\mathbf{e}^{(3)}$ with a regularization strategy.
- Perspectives
  - Extend this work to more complex dynamics
    - 3D plane mixing layer or cavity flow (Comte P.)
    - experimental PIV data of a turbulent boundary layer (European project Wallturb)

Questions ???