POD-based Reduced Order Models for Parameterized PDEs

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Outline

1. Setting of the problem – Numerical examples
2. Numerical analysis of POD-Galerkin and POD-Propagator for the Laplace problem
3. Nonlinear case
4. Partition-of-unity ROM
5. Looking forward : challenges

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Context

Operating requirements

θ

Design parameters

Environmental parameters

Uncertain variables

Computer-Assisted Engineering

Response surfaces

Performance

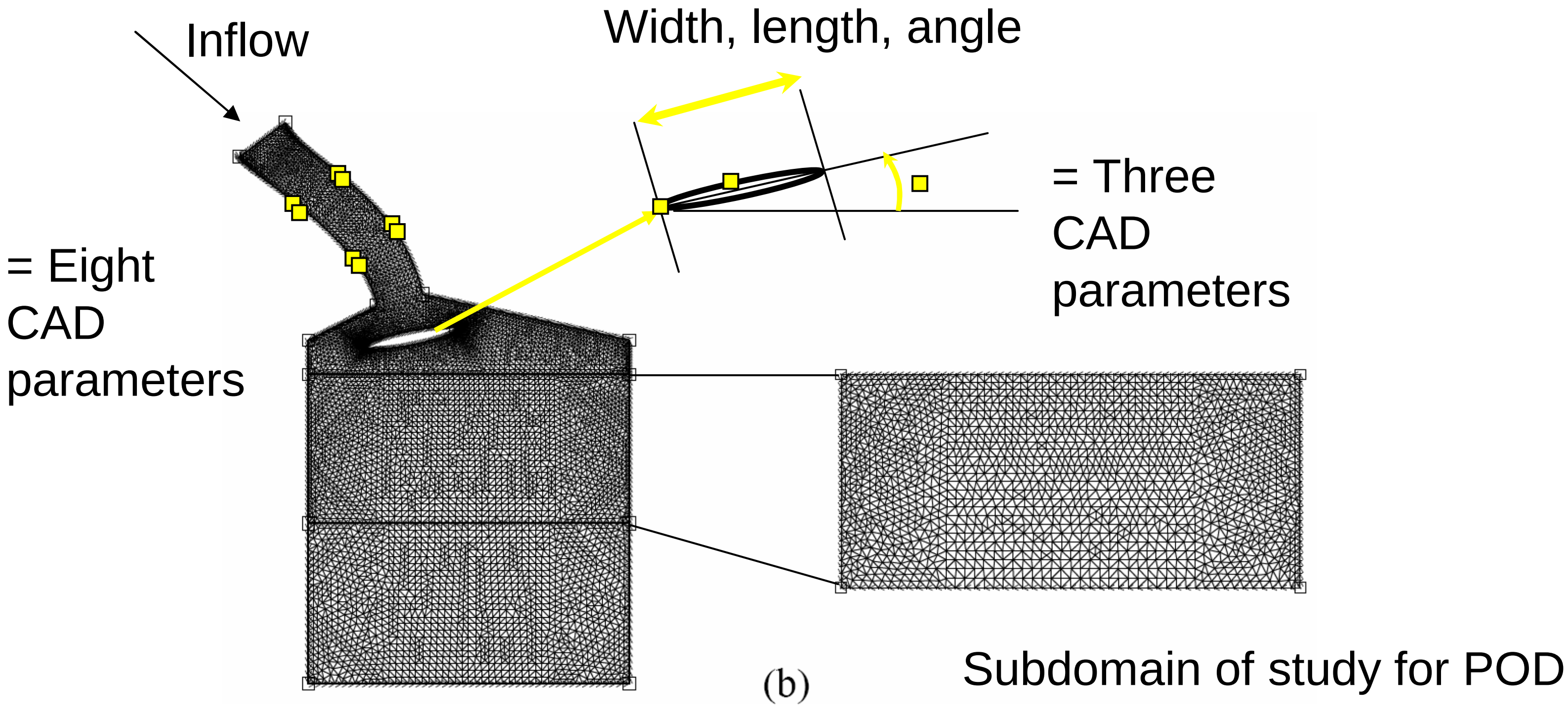
Cost

Flow fields

Parameter sensitivity analysis
Parameter optimization

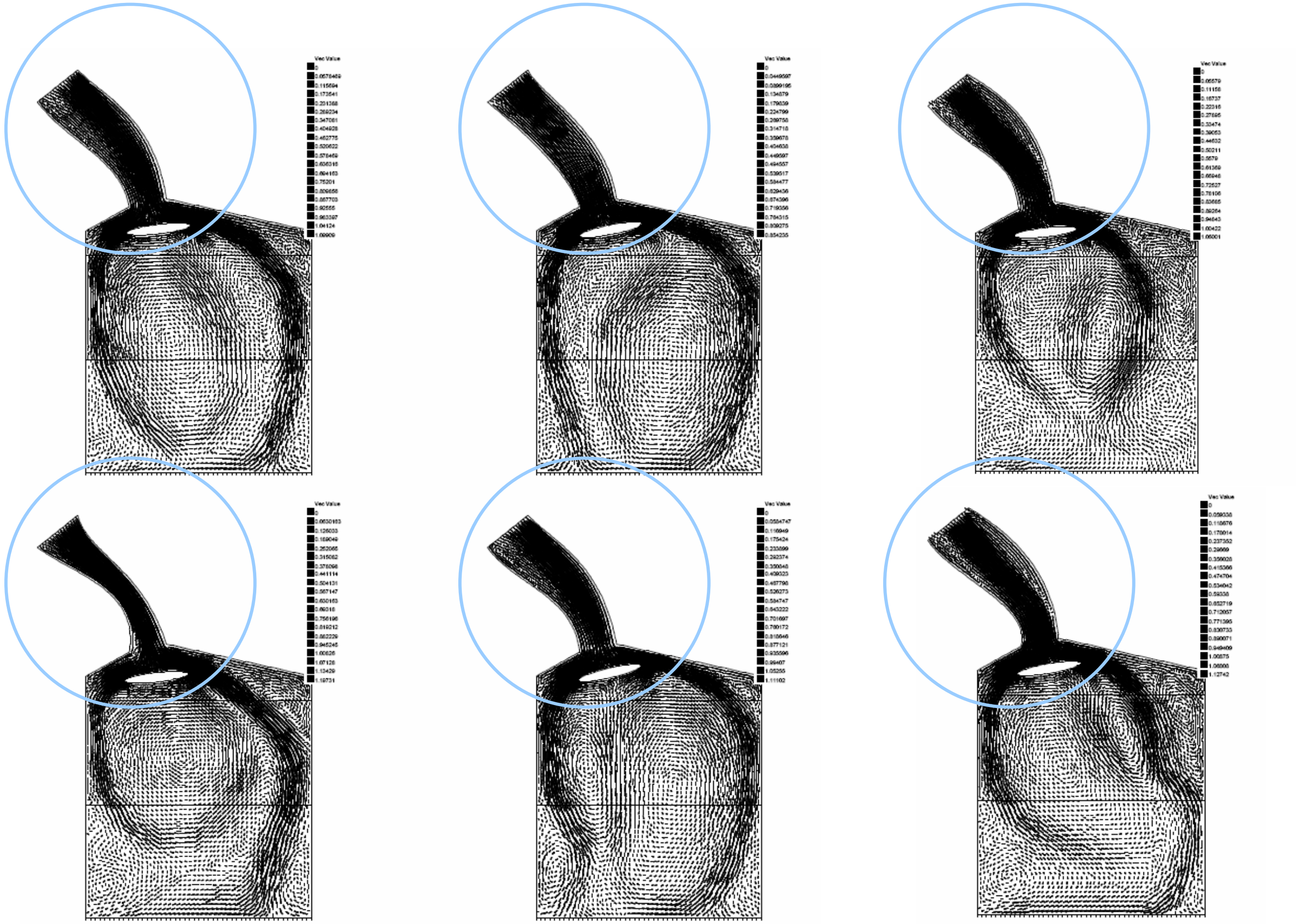
Case study – stationary Navier-Stokes solutions depending on 11 CAD parameters

[Audouze, De Vuyst 2008]



➔ Total 11 CAD parameters
Each Parameter may vary in a small given interval

Design of experiment (DoE) – Examples of FE solutions



Many kinds of solutions

Parameterized discrete FE solutions

$$u^h = u^h(\mathbf{x}, \boldsymbol{\theta})$$

space

vector parameter

Parameter space :

$$\boldsymbol{\theta} \in [0,1]^p$$

Q : is it possible to get a cheap estimator of

$$\boldsymbol{\theta} \mapsto u^h(.,\boldsymbol{\theta}) \ ?$$

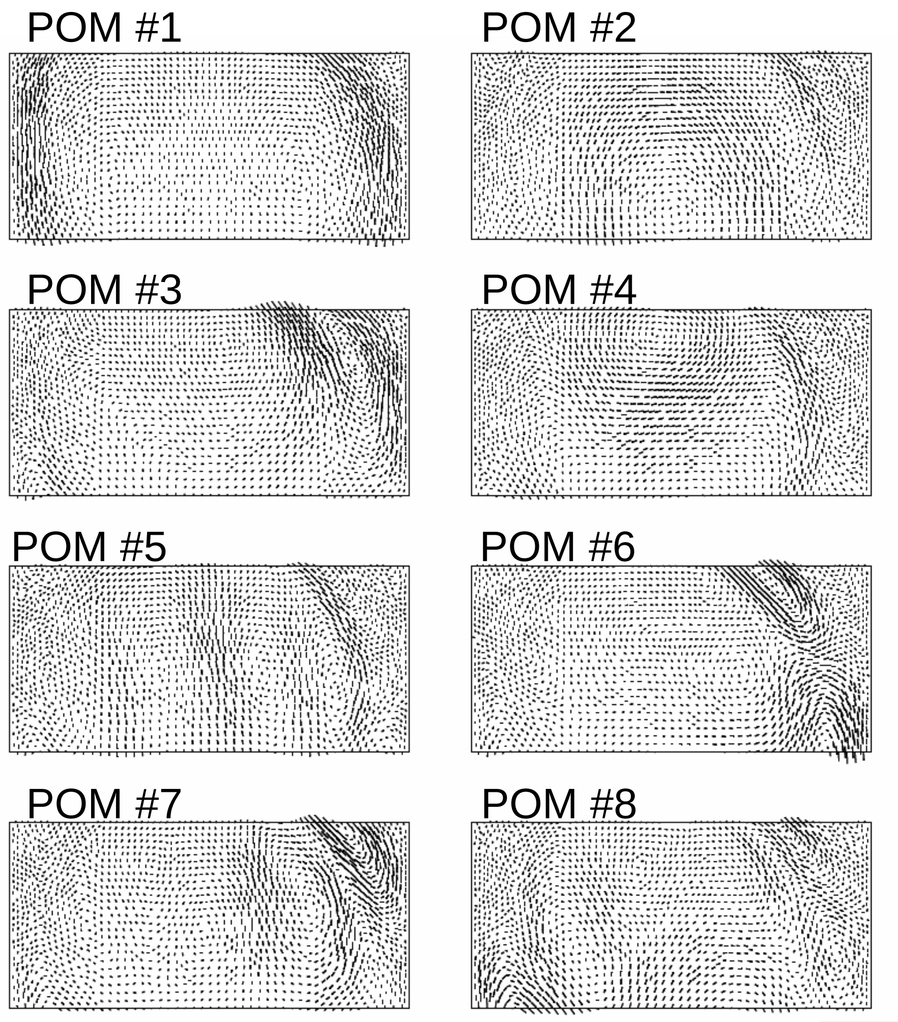
Proper Orthogonal Decomposition analysis

Velocity POD modes

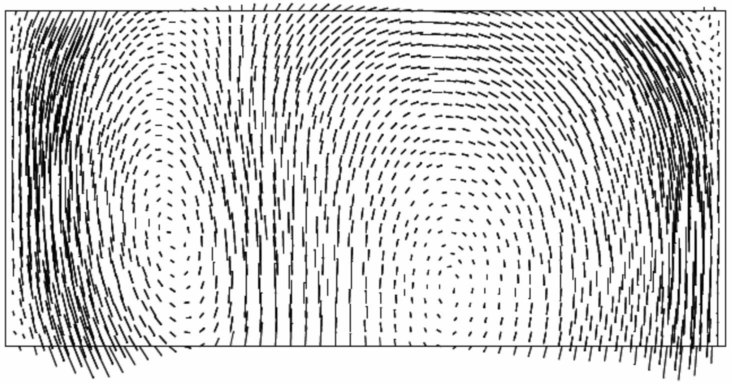
λ^1	23708.3	λ^5	328.89
λ^2	3667.95	λ^6	155.382
λ^3	735.854	λ^7	145.539
λ^4	505.24	λ^8	85.2643

First eigenvalues of the correlation matrix

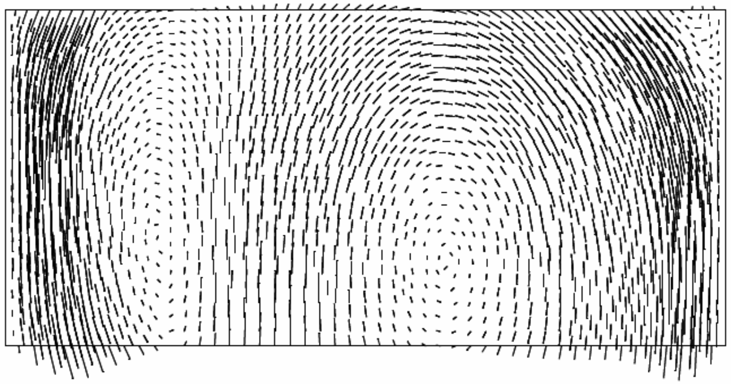
Rather good decreasing



Comparing a particular solution and its POD projection



$$u^{\theta,h}(\mathbf{x})$$



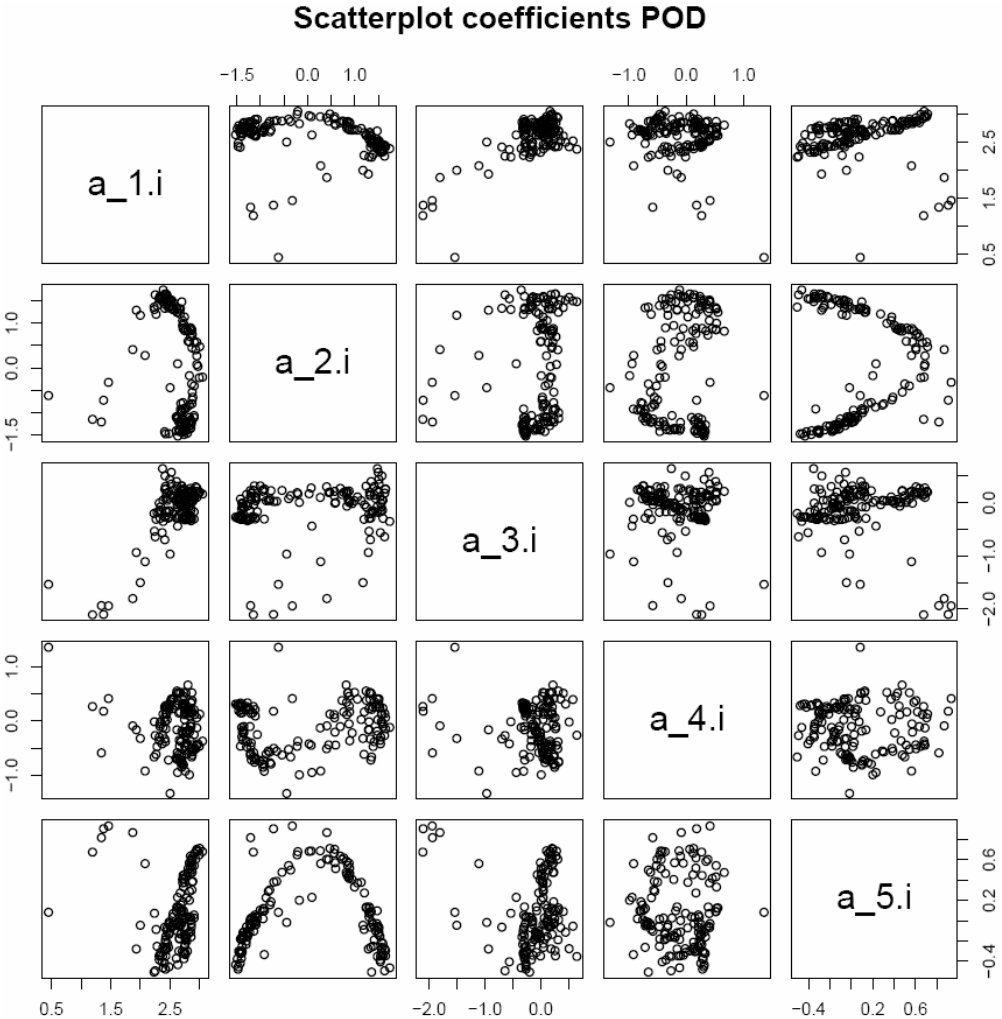
$$\Pi^K u^{\theta,h} = \sum_{k=1}^{K} a_k(\boldsymbol{\theta})\, \Psi^{k,h}(\mathbf{x}).$$

Using only K=5

(5 POD modes) !

Plotting all the POD coefficients (DoE made of N=150 simulations) - Scatterplot

$$a_k^i = a_k(\boldsymbol{\theta}^i),\ \ i = 1, \dots, N$$



Mysterious correlations ….

Design
and
Numerical Analysis
of some Reduced Order Models

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Basics on POD approximation

Proposition. Let $\varepsilon > 0$ be a small error criterion. If $K = K(\varepsilon)$ is chosen such that

Proper truncation rank

(H)
$$\frac{\displaystyle\sum_{k=K+1}^{N} \lambda^k}{\displaystyle\sum_{k=1}^{N} \lambda^k} \leq \varepsilon.$$

then

$$\sum_{i=1}^{N} ||u^i - \Pi^K u^i||^2 \leq \varepsilon^2 \sum_{i=1}^{N} ||u^i||^2.$$

(standard PCA analysis)

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1. POD-Galerkin approach on Laplace problem

Snapshots:

$$\mathscr{S}^N = \{u^{1,h}, \ldots, u^{N,h} \in V^h\}.$$

$$\boxed{u^{i,h} = u^{\theta^i,h}}$$

POD

$$W^h = \textit{span}\left(\Psi^{1,h}, \ldots, \Psi^{K,h}\right) \subset V^h$$

Variational formulation of Laplace problem:

$$\left(u^{\theta,h}, v^h\right)_{H_0^1} = (f^\theta, v^h) \; \forall v^h \in V^h.$$

➔ POD-Galerkin

$$\left(\tilde{u}^{\theta,h}, w^h\right)_{H_0^1} = (f^\theta, w^h) \; \forall w^h \in W^h.$$

ROM !

Closed form ROM solution and error estimate

If the H_0^1-inner product is used for the correlation matrix, then POD modes are orthogonal in H_0^1 and

$$\text{ROM} \qquad \tilde{u}^{\theta,h}(\mathbf{x}) = \sum_{k=1}^{K} \underbrace{(f^\theta, \Psi^{k,h})}_{= a_k(\boldsymbol{\theta})} \Psi^{k,h}(\mathbf{x})$$

Standard Galerkin error estimate :

$$||u^{\theta,h} - \tilde{u}^{\theta,h}||_{H_0^1} \leq ||u^{\theta,h} - w^h||_{H_0^1} \quad \forall w^h \in W^h.$$

Then under (H)-hypothesis, we get

$$\sum_{i=1}^{N} ||u^{i,h} - \tilde{u}^{i,h}||_{H_0^1}^2 \leq \varepsilon^2 \sum_{i=1}^{N} ||u^{i,h}||_{H_0^1}^2 \leq \varepsilon^2 \, C(\Omega^h) \sum_{i=1}^{N} ||f^i||_{L^2}^2.$$

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2. POD-propagator approach

- Now perform PCA on RHS rather than solutions

$$\mathscr{S}^N = \{f^1, \dots, f^N \in L^2(\Omega^h)\}.$$

POD basis : $\Psi^{1,h}, \dots, \Psi^{K,h} \in L^2(\Omega^h)$

- Then build a dual basis such that

$$(\varphi^{k,h}, v^h)_{H_0^1} = (\Psi^{k,h}, v^h)_{L^2} \; \forall v^h \in V^h.$$

Laplace problem with $\Psi^{k,h}$
as RHS == mode propagator

POD-propagator approach

Then the solution of the Laplace problem

$$(u^{\theta,h}, v^h)_{H_0^1} = (\underline{\Pi^K f^\theta}, v^h)\ \forall v^h \in V^h.$$

is in closed form

$$\tilde{u}^{\theta,h} = \sum_{k=1}^{K} (f^\theta, \underline{\Psi^{k,h}})\, \underline{\varphi^{k,h}}.$$

Same error estimate as POD-Galerkin

Comparison

	POD-Galerkin	POD-propagator
Closed form ROM	yes	yes
NB of required Laplace solutions	*N*	*K*
Intrusive approach	yes	no

Important aspect in Engineering

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3. Weighted residual approach

Remember the Laplace problem :

$$(\nabla u^{\theta,h}, \nabla v^h) - (f^\theta, v^h) = 0 \ \forall v^h \in V^h.$$

Let $\{w^{i,h}\}_{i=1,\ldots,d}$ be the FE “hat function”basis.

The residual is defined as :

$$R_i(\tilde{u}^{\theta,h}, f^\theta) = (\nabla \tilde{u}^{\theta,h}, \nabla w^{i,h}) - (f^\theta, w^{i,h}).$$

Guess

Residual

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Idea

$$\tilde{u}^{\theta,h}(\boldsymbol{a}) = \sum_{k=1}^{K} a_k \, \Psi^{k,h}$$

Find $\boldsymbol{a} = \boldsymbol{a}(\boldsymbol{\theta})$ solution of the minimization problem

$$\min_{\boldsymbol{a}\in\mathbb{R}^K} \frac{1}{2}\left|\left|\mathbf{R}(\tilde{u}^{\theta,h}(\boldsymbol{a}), f^{\theta})\right|\right|^2_{\mathbb{R}^d}.$$

Numerical complexity far less than a whole Laplace problem FE solution

Non intrusive approach (is the FE code is able to return a residual from a guess)

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Non linear problems

- POD-Galerkin OK
- POD-Propagator KO (only for linear operators)
- Weighted residual approach OK

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4. Data driven approach (non intrusive) Parameter space interpolation

$$\left(\mathcal{N}(u^{\theta,h}), v^h\right)_V = (f^\theta, v^h)_{L^2(\Omega^h)} \; \forall v^h \in V^h$$

Looking for a ROM in the form

$$\hat{u}^{\theta,h} = \sum_{k=1}^{K} \hat{a}_k(\boldsymbol{\theta})\, \Psi^{k,h}$$

Ideally, $\hat{a}_k(\boldsymbol{\theta})$ should be

$$a_k(\boldsymbol{\theta}) = (u^{\theta,h}, \Psi^{k,h}).$$

Not known

By a design of computer experiment DoCE

1. Generate a cloud of parameter N points $\boldsymbol{\theta}^i$ In $[0,1]^p$ (Latin Hypercube Sampling, Sobol, etc.) ;
2. Compute N FE solutions $u^{i,h} = u^{\theta^i,h}$;
3. Compute $a_k^i = a_k(\boldsymbol{\theta}^i) = \left(u^{i,h}, \Psi^{k,h}\right)$;
4. Then interpolate/approximate the a_k in the parameter space.

➔Requires high-dimensional interpolators/approximators.

Many candidates :

Low-order polynomials
Radial basis functions (RBF) [Wendland 2006]
Kriging approaches
Moving least squares (diffuse approximation)
SPH-like approximation, etc…

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Case of RBF approximators

RBF centers

$$\hat{a}_k(\boldsymbol{\theta}) = \sum_{j=1}^{J} \alpha_k^j \Phi\left(\frac{\left\|\boldsymbol{\theta} - \boldsymbol{\theta}'^j_k\right\|}{\sigma_k^j}\right) + P_k(\boldsymbol{\theta})$$

Weights Kernel Scaling factors Polynomial lifting

Parameters identification :

$$\min_{(\boldsymbol{\alpha}_k, \boldsymbol{\theta}'^1_k, \dots, \boldsymbol{\theta}'^J_k, \boldsymbol{\sigma}_k)} \frac{1}{2} \sum_{i=1}^{N} \left(\hat{a}_k(\boldsymbol{\theta}^i; \boldsymbol{\alpha}_k, \boldsymbol{\theta}'^1_k, \dots, \boldsymbol{\theta}'^J_k, \boldsymbol{\sigma}_k) - a_k^i\right)^2$$

$$+ \mu \left(\|\boldsymbol{\alpha}_k\|^2 + \left\|\boldsymbol{\theta}'^1_k\right\|^2 + \dots + \left\|\boldsymbol{\theta}'^J_k\right\|^2 + \|\boldsymbol{\sigma}_k\|^2\right)$$ Tykhonov-like

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Numerical experiment

Keller-Segel PDE system
(modeling skin patterns for living beings)

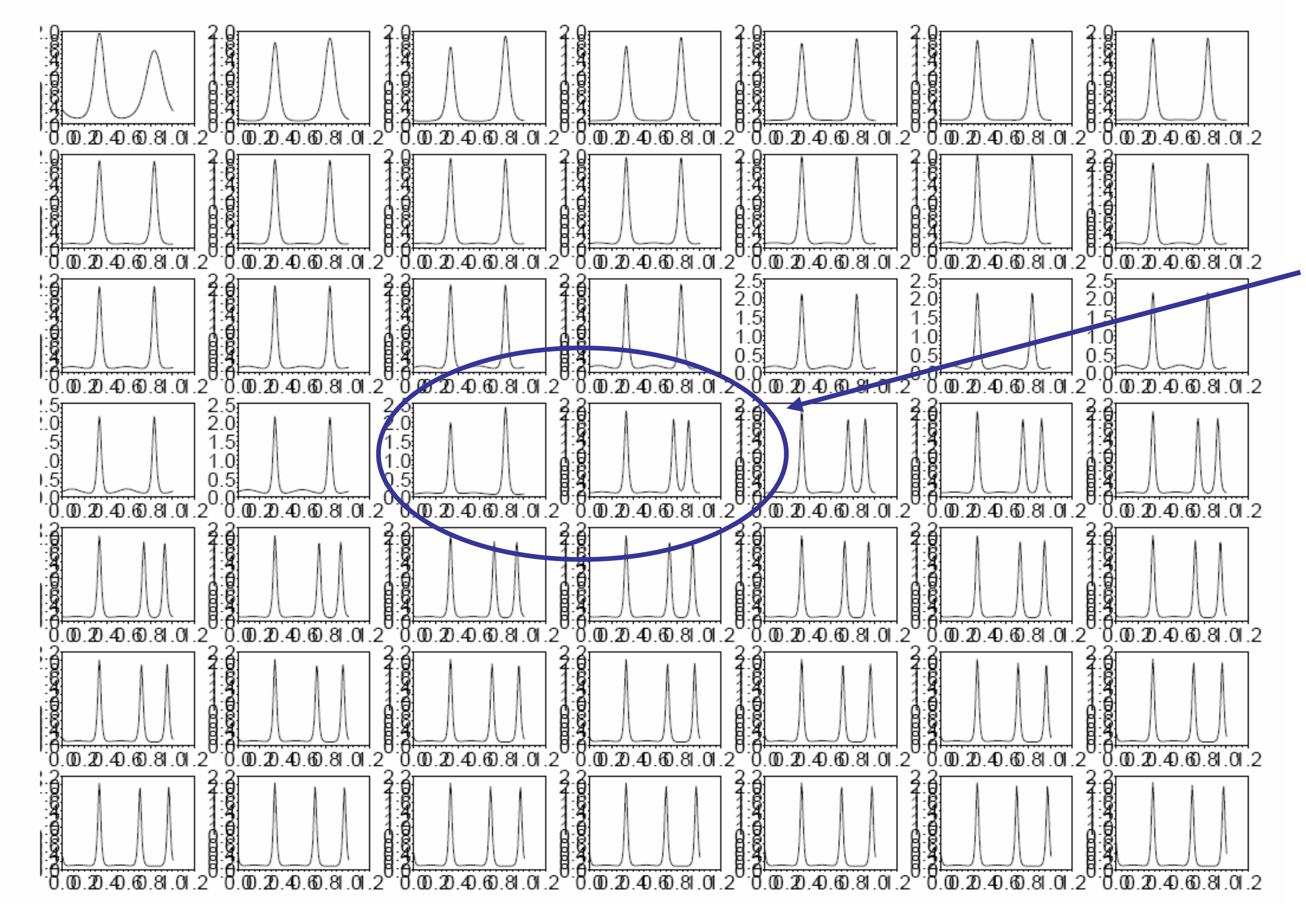
Nonlinear terms

$$\partial_t u - \Delta u + \alpha \nabla \cdot (u \nabla c) = \beta u(1-u),$$

$$\partial_t c - \delta \Delta c = \gamma \left(\frac{u}{1+u} - c \right).$$

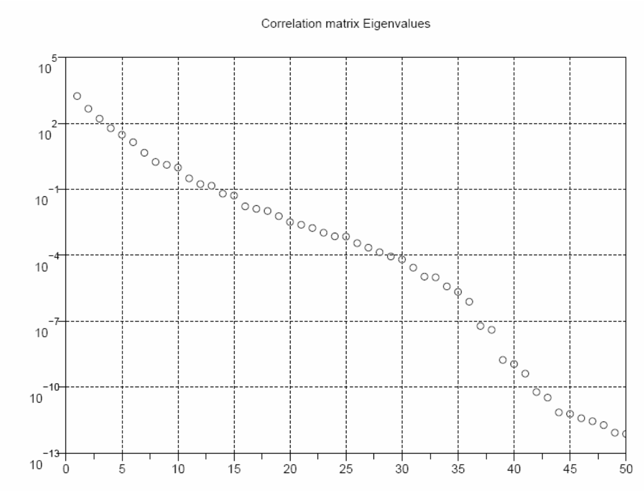
The system is known to have a rich variety of solutions
with respect to the different model coefficients.

Exemple of 1D steady-state solutions with periodical BC

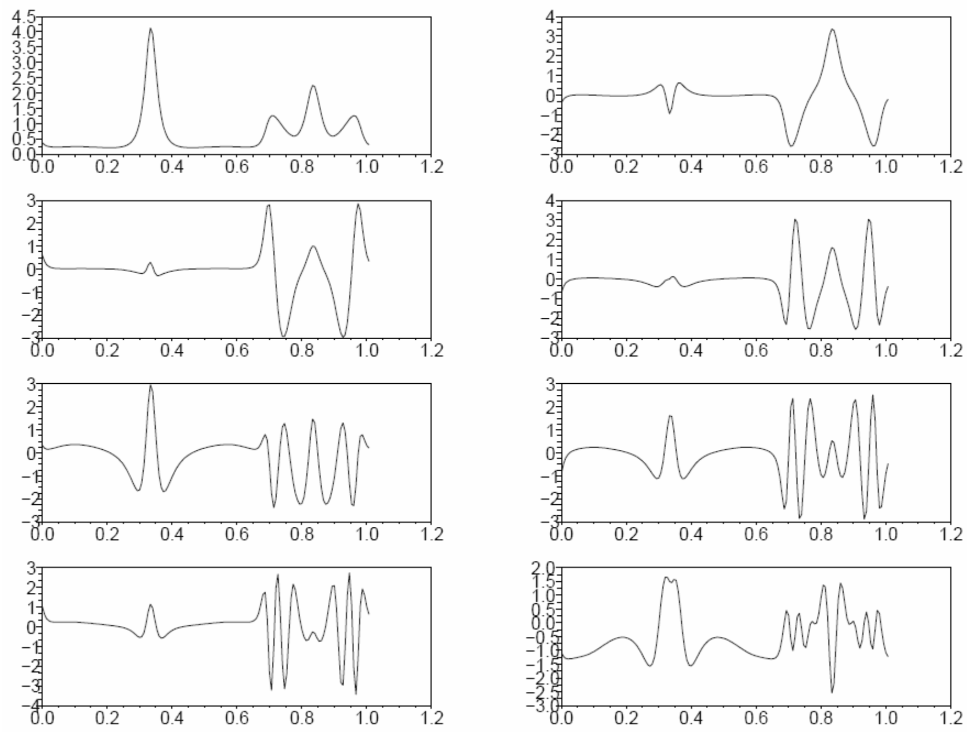


Here, only γ is varying in an interval.

Proper orthogonal decomposition

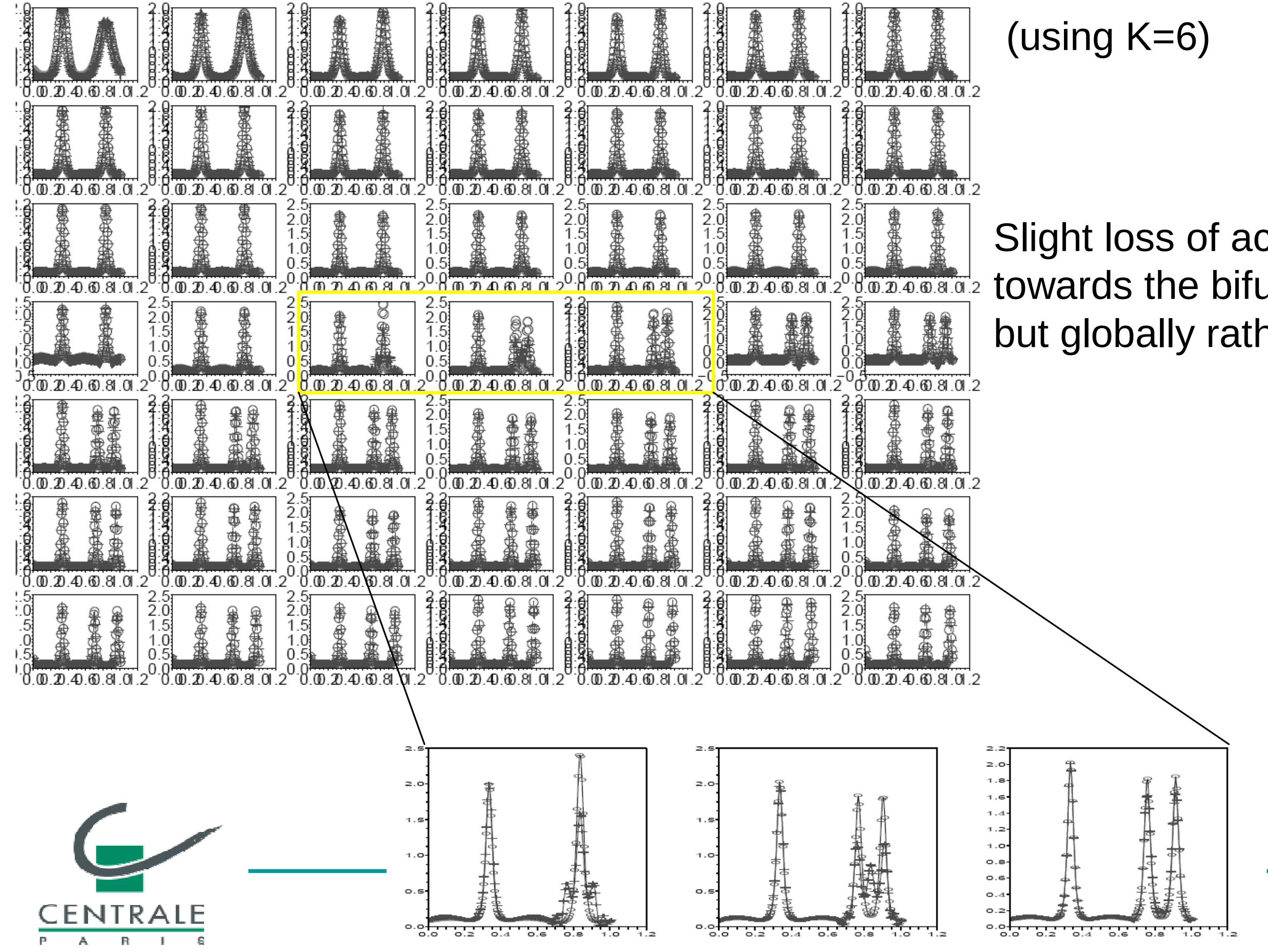


Spectrum of the
corrlation matrix



The eight first
POD eigenmodes

POD-RBF ROM solutions compared to FE ones



(using K=6)

Slight loss of accuracy towards the bifurcation but globally rather good ROM

ZOOM

5. Partition-of-unity local-POD basis ROM

- POD approximation is sometimes reproached to use a basis only dedicated to a particular regime (that means for a small parameter-space region)

Idea ➔ Use different locally-optimal POD basis dedicated to a particular parameter region, then reconstruct the global approximation in a smooth fashion.

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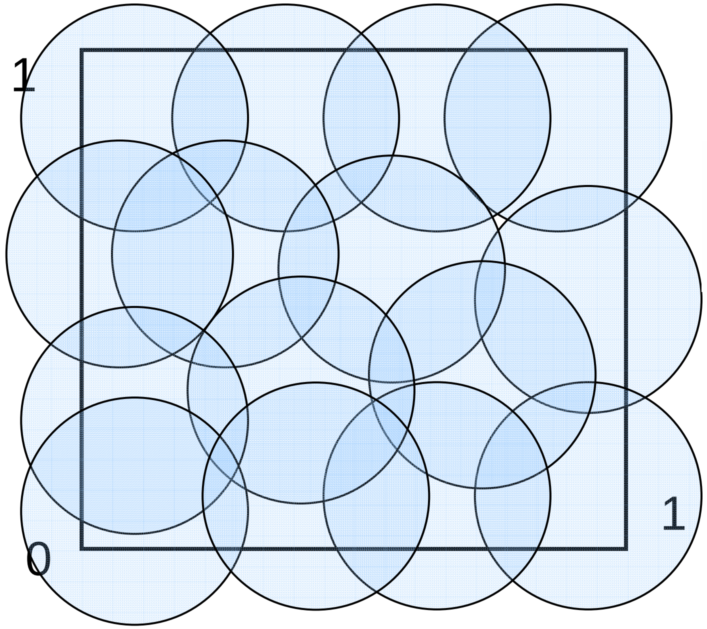
Partition-of-unity local-POD basis ROM

Parameter domain $[0,1]^p$



$$\omega^m(\boldsymbol{\theta})$$

$$\Psi^{k,h}_{m}$$

Practical construction of
a partition-of-unity:

$$\hat{\omega}^m(\boldsymbol{\theta}) = \Phi\left(\frac{||\boldsymbol{\theta} - \boldsymbol{\theta}^{c,m}||}{\sigma^m}\right).$$

Smooth positive compactly supported kernel

Then $\omega^m(\boldsymbol{\theta}) = \dfrac{\hat{\omega}^m(\boldsymbol{\theta})}{\sum_{\ell=1}^{M} \hat{\omega}^\ell(\boldsymbol{\theta})}$ has the expected properties :

$$\omega^m \geq 0, \sum_m \omega^m \equiv 1.$$

Algorithm

1. First, build a local POD basis attached to the partition function nb *m* :

$$\min_{\substack{(\Psi_m^{1,h},\ldots,\Psi_m^{K_m,h}) \\ (\Psi_m^{k,h},\Psi_m^{\ell,h})=\delta_{k\ell},\ 1\le k\le \ell\le K_m}} \frac{1}{2}\sum_{i=1}^{N} \omega_m(\boldsymbol{\theta}^i) \left\| u^{i,h} - \sum_{k=1}^{K_m} (u^{i,h}, \Psi_m^{k,h})\, \Psi_m^{k,h} \right\|^2$$

Weighted least squares

Local ROM :

$$\tilde{u}^{\theta,h} = \sum_{k=1}^{K_m} (u^h(\boldsymbol{\theta}), \Psi_m^{k,h})\, \Psi_m^{k,h}.$$

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Global reconstruction

- Then from the property:

$$\sum_{m=1}^{M} \omega_m(\boldsymbol{\theta}) = 1$$

one can propose the following reconstruction:

$$\tilde{u}^{\theta,h} = \sum_{m=1}^{M} \omega_m(\boldsymbol{\theta}) \sum_{k=1}^{K_m} (u^h(\boldsymbol{\theta}), \Psi_m^{k,h})\, \Psi_m^{k,h}.$$

in the form

Possible to use again RBF approximators !

$$\hat{u}^{\theta,h} = \sum_{m=1}^{M} \sum_{k=1}^{K_m} \hat{a}_m^k(\boldsymbol{\theta})\, \Psi_m^{k,h}$$

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Looking forward : challenges

- Multilevel ROM modeling for optimization process
- A posteriori estimators and DoCE enrichment at worst error locations for better approximation
- ROM for nonsmooth solutions (discontinuous solutions of hyperbolic equations for example)
- Extension/use in the uncertainty propagation community

References :

F. De Vuyst, C. Audouze, Réduction de modèles Eléments Finis par POD pour les problèmes paramétrés aux EDP, chapter in "Optimisation de Systèmes Mécaniques", collection "Mécanique et ingénierie des Matériaux", Hermès Sciences (2008).

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C. Audouze, F. De Vuyst, P.B. Nair, «Reduced-order modeling of parameterized PDEs using time-space-parameter principal component analysis : Part I », International Journal of Numerical Methods in Engineering, in press, 2008.

Thank you for your attention

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