Model Order Reduction techniques for CFD: nonlinear approximations and constrained formulation

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inventeurs du monde numérique

Institut de Mathématiques de Bordeaux

Acknowledgements

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Michel Bergmann, Sebastien Riffaud (Inria MEMPHIS)

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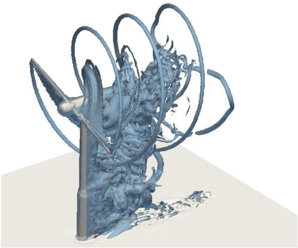
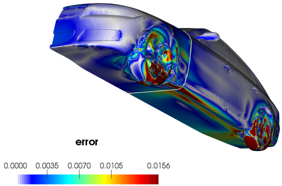
Objective

Parameterized Model Order Reduction (pMOR) for PDEs

The goal of pMOR is to reduce the **marginal** cost associated with the solution to parameterized problems.

pMOR is motivated by *real-time* and *many-query* problems
design and optimization, UQ, control[1]...





[1] Pictures show results of simulations performed by the MEMPHIS team: courtesy of Angelo Iollo.

The Reduced Basis method: general recipe

Pb: find $u_\mu \in \mathcal{X} : A_\mu(u_\mu, v) = F(v) \qquad \forall\, v \in \mathcal{Y}\ \mu \in \mathcal{P}$

Approx: $\hat{u}_\mu = \sum_{n=1}^{N} \alpha_\mu^n \zeta_n, \qquad \alpha^n : \mathcal{P} \to \mathbb{R},\ \zeta_n \in \mathcal{X}$

$N \ll N_{\mathrm{hf}} =$ dofs of the Full Order Model $\Big(\underbrace{\mathrm{FOM}}_{=\mathrm{FE},\dots}\Big)$

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Offline stage: (performed once)

compute $u_{\mu^1}, \dots, u_{\mu^{n_{\mathrm{train}}}}$ using a FE (or FV...) solver;

construct $\{\zeta_n\}_{n=1}^N$ and define $\mathcal{Z}_N = \mathrm{span}\{\zeta_n\}_{n=1}^N$.

Online stage: (performed for any new $\bar{\mu} \in \mathcal{P}$)

solve $\hat{u}_{\bar{\mu}} \in \mathcal{Z}_N :\ A_{\bar{\mu}}(\hat{u}_{\bar{\mu}}, v) = F(v), \quad \forall\, v \in \mathcal{Z}_N$;

estimate $\|\hat{u}_{\bar{\mu}} - u_{\bar{\mu}}\|_{\mathcal{X}}$.

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$N \ll N_{\mathrm{hf}} =$ dofs of the Full Order Model $\Big(\underbrace{\mathrm{FOM}}_{=\mathrm{FE},\dots}\Big)$

Successful applications of Reduced Basis methods

Past and current research on pMOR focuses on

1. data compression $\mathcal{Z}_N$
2. reduced formulation $\mathcal{Z}_N \Rightarrow \boldsymbol{\alpha}_{\bar{\mu}}$
3. *a posteriori* error estimation $\|\hat{u}_{\bar{\mu}} - u_{\bar{\mu}}\|_{\mathcal{X}}$

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PR-scRBE: Patera, Huynh, Knezevic, `Akselos S.A.`

Port-**R**educed **s**tatic **c**ondensation **RB E**lement method

component-based structures, solid mechanics.

LRB-Ms: Ohlberger, Schindler, ...

Localized **RB M**ulti**s**cale method

multiscale problems, porous media.

Akselos is a software company that provides a commercial implementation of PR-scRBE.

Data compression

Challenges: turbulence (wide spectrum of scales), approximation of shocks, boundary/internal layers...

Reduced formulation

Challenges: fragility of Galerkin models, nonlinearities.

Error estimation

Challenge: need for estimates of averaged QOIs.

Data compression

Challenges: turbulence (wide spectrum of scales), approximation of shocks, boundary/internal layers...

nonlinear approximation procedures.

Reduced formulation

Challenges: fragility of Galerkin models, nonlinearities.

stabilized formulations;
hyper-reduction.

Error estimation

Challenge: need for estimates of averaged QOIs.

time-averaged error indicators.

Outline of the talk

Goal: present two contributions for fluid problems.

1. A Lagrangian nonlinear approximation procedure for stationary problems.
2. A constrained Galerkin formulation for turbulent flows.

Iollo, Taddei, *A nonlinear approximation procedure for parameterized Model Order Reduction; in preparation*.

Fick, Maday, Patera, Taddei, *A stabilized POD model for turbulent flows over a range of Reynolds numbers: optimal parameter sampling and constrained projection;* JCP, 2018.

Nonlinear approximation

- pMOR for hyperbolic problems
- Registration algorithm
- Application to a linear transport problem

Nonlinear approximation

- pMOR for hyperbolic problems
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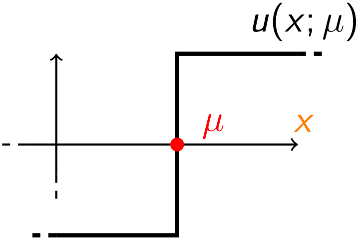
- Application to a linear transport problem

Develop a pMOR procedure for

hyperbolic stationary equations

in the presence of parameter-dependent shocks.

Example



$$u(x, \mu) = \mathrm{sign}\,(x - \mu),$$
$$x \in \Omega := (0, 1)$$
$$\mu \in \mathcal{P} = \left[\tfrac{1}{3}, \tfrac{2}{3}\right]$$

Failure of linear approximation strategies

Linear Reduced Order Models (ROMs) rely on N-term linear expansions to approximate u:

$$u_\mu(x) \approx \widehat{u}_\mu(x) = Z_N(x)\boldsymbol{\alpha}_\mu, \qquad Z_N = [\zeta_1, \ldots, \zeta_N]$$

If $u_\mu(x) = \mathrm{sign}(x - \mu)$,

$$\sup_{\mu \in \mathcal{P}} \inf_{(Z_N, \boldsymbol{\alpha})} \|u_\mu - Z_N(\cdot)\boldsymbol{\alpha}\|_{L^2(\Omega)} = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

for Lagrangian spaces (i.e., $Z_N = \left[u_{\mu^1}, \ldots, u_{\mu^N}\right]$).

Linear ROMs are ill-suited for travelling fronts.

Taddei, Perotto, Quarteroni, 2015.

Recipe: given $\mu \in \mathcal{P}$,

1. define the reduced operator $Z_{N,\mu} : \mathbb{R}^N \to L^2(\Omega)$;
2. determine the approximation $\widehat{u}_\mu = Z_{N,\mu}(\boldsymbol{\alpha}_\mu)$ using a projection method.

Selected references:

Manifold learning

Amsallem, Farhat, 2008; Lee, Carlberg, 2018[2].

"Transported/transformed snapshot" methods

Nair, Balajewicz, 2017; Welper, 2017.

hp-in-parameter adaptive refinement

Eftang et al., 2010; Carlberg, 2015; Peherstorfer, 2018.

[2]Here, the authors consider $\widehat{u}_\mu = g(x; \boldsymbol{\alpha}_\mu)$

Lagrangian approaches to nonlinear approximation

Recipe: given $\mu \in \mathcal{P}$,

1. define a bijective mapping $\Phi_\mu : \Omega \to \Omega$;
2. determine the approximation $\widehat{\tilde{u}}_\mu = \widetilde{Z}_N \boldsymbol{\alpha}_\mu$ of $\widetilde{u}_\mu := u_\mu \circ \Phi_\mu$ using a projection method.

Selected references:

Iollo, Lombardi, 2014; Ohlberger, Rave, 2015; Cagniart et al., 2017; Mojgani, Balajewicz, 2017.

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Example $u_\mu(x) = \mathrm{sign}\,(x - \mu)\,,\ x \in \Omega = (0,1)$.

If we choose $\Phi_\mu(X) = \begin{cases} 2\mu X & X < \frac{1}{2} \\ \mu + (1-\mu)(2X-1) & X \geq \frac{1}{2} \end{cases}$,

the mapped field is μ-independent.

$$\widetilde{u}_\mu(X) = \mathrm{sign}(2X - 1).$$

Lagrangian approaches: offline/online decomposition[3]

Offline stage: (performed once)

1. compute $u_{\mu^1}, \dots, u_{\mu^{n_{\text{train}}}}$ using a FE/FV solver;
2. define the mapping Φ_μ for all $\mu \in \mathcal{P}$;
3. define the ROM for $\tilde{u} = u \circ \Phi$.

ROM: $\mu \mapsto \widehat{\tilde{u}}_\mu = \widetilde{Z}_N \boldsymbol{\alpha}_\mu$

Online stage: (performed for any new $\bar{\mu} \in \mathcal{P}$)

1. query the ROM to compute $\widehat{\tilde{u}}_{\bar{\mu}}$;
2. (if needed) compute $\widehat{u}_{\bar{\mu}} = \widehat{\tilde{u}}_{\bar{\mu}} \circ \Phi_{\bar{\mu}}^{-1}$.
3. estimate the error $\|\widehat{u}_{\bar{\mu}} - u_{\bar{\mu}}\|_{\mathcal{X}}$.

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Refined goal: develop a *general* registration algorithm for the construction of Φ_μ for Lagrangian approaches.

Agenda:

1. Registration algorithm.
2. Application to a linear advection-reaction problem.

General = independent of the underlying PDE model.

Nonlinear approximation

- pMOR for hyperbolic problems
- Registration algorithm
- Application to a linear transport problem

Well-posedness

Projection is performed in the mapped configuration. Therefore, for all $\mu \in \mathcal{P}$, the map Φ_μ should satisfy

$$\Phi_\mu(\Omega) = \Omega, \; \mathfrak{J}_\mu(X) = \left|\nabla \Phi_\mu(X)\right| > 0, \;\; X \in \Omega.$$

Efficiency

The map Φ_μ should be designed such that the manifold

$$\widetilde{\mathcal{M}} = \{\widetilde{u}_\mu = u_\mu \circ \Phi_\mu : \; \mu \in \mathcal{P}\}$$

is "more favorable" than[4] $\mathcal{M} = \{u_\mu : \; \mu \in \mathcal{P}\}$ for linear approximation methods.

[4] This notion should be formalized by means of the introduction of a Kolmogorov N-width.

Overall strategy

Inputs: snapshots $\{u^k = u_{\mu^k}\}_{k=1}^{n_{\mathrm{train}}}$, reference[5] $\bar{u}$.

Output: mapping $\Phi_\mu : \Omega \to \Omega$ for all $\mu \in \mathcal{P}$.

1. Determine a family of mappings $\{\Psi(\cdot; \mathbf{a})\}_{\mathbf{a} \in \mathbb{R}^M}$ for the domain Ω;
2. choose $\Psi(\cdot; \mathbf{a}^k)$ using u^k and $\bar{u}$;

   $\to \{\mu^k, \mathbf{a}^k\}_{k=1}^{n_{\mathrm{train}}}$
3. learn $\mathbf{a} : \mathcal{P} \to \mathbb{R}^M$ based on $\{\mu^k, \mathbf{a}^k\}_{k=1}^{n_{\mathrm{train}}}$;

   regression problem
4. set $\Phi_\mu = \Psi(\cdot; \mathbf{a}(\mu))$.

[5] Here, $\bar{u}$ is set equal to $u_{\bar{\mu}}$, where $\bar{\mu} = \frac{1}{n_{\mathrm{train}}} \sum_k \mu^k$.

Family of mappings $\{\Psi(\cdot;\mathbf{a})\}_{\mathbf{a}}$: a theoretical result[6]

Let Ω be diffeomorphic to $\widehat{\Omega} = \{x \in \mathbb{R}^d : f(x) < 0\}$ where f is convex.

Let $\Phi : \Omega' \to \mathbb{R}^d$, $\Omega \subset\subset \Omega'$, satisfy

(i) $\Phi \in C^1(\Omega'; \mathbb{R}^d)$;

(ii) $\inf_{X\in\Omega} \mathfrak{J}(X) = |\nabla\Phi(X)| > 0$;

(iii) $\operatorname{dist}(\Phi(X), \partial\Omega) = 0$ for all $X \in \partial\Omega$.

i.e. $\Phi(\partial\Omega) \subset \partial\Omega$

Then, Φ is a bijection from Ω into itself.

Examples: $\widehat{\Omega} = (0,1)^d$, $\widehat{\Omega} = \mathcal{B}_1(0), \ldots$

[6] We thank Pierre Mounoud (University of Bordeaux) for fruitful discussions.

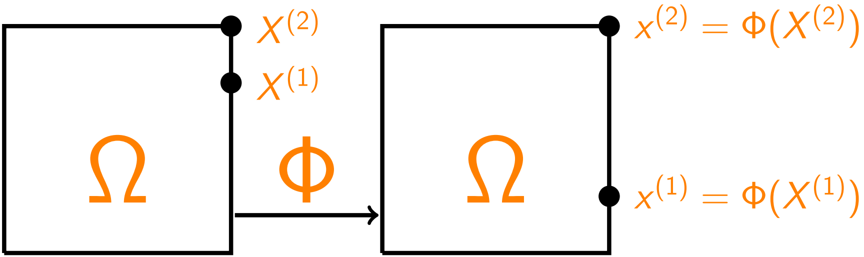
Family of mappings $\{\Psi(\cdot;\mathbf{a})\}_{\mathbf{a}}$: implications for $\Omega = (0,1)^2$

Consider $\Psi(X;\mathbf{a}) = X + \sum_{m=1}^{M} a_m \varphi_m(X)$, with

$$\varphi_m(X)\cdot\mathbf{e}_1 = 0 \ \text{ on } \{X_1 = 0, 1\},\ m = 1,\dots,M;$$

$$\varphi_m(X)\cdot\mathbf{e}_2 = 0 \ \text{ on } \{X_2 = 0, 1\},\ m = 1,\dots,M.$$

(ii) holds for $\mathbf{a} = \bar{\mathbf{a}} \Rightarrow \Psi(\cdot;\bar{\mathbf{a}})$ is bijective + $\Psi(\Omega;\bar{\mathbf{a}}) = \Omega$.



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In our implementation, we resort to a tensorized polynomial expansion.

$$\varphi_1(X) = \ell_0(X_1)\ell_0(X_2)X_1(1-X_1)\begin{bmatrix} 1 \\ 0 \end{bmatrix}, \ldots$$

$$\varphi_M(X) = \ell_p(X_1)\ell_p(X_2)X_2(1-X_2)\begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

ℓ_i = Legendre polynomial of degree i

Registration algorithm for $(u^k, \bar{u}) \to \mathbf{a}^k$

Find $\mathbf{a}^k$ to minimize

$$\min_{\mathbf{a}} \int_\Omega \| u^k(\Psi(X;\mathbf{a})) - \bar{u}(X) \|_2^2 dX \; + \xi \left| \Psi(\cdot;\mathbf{a}) \right|_{H^2(\Omega)}^2$$

$$\text{s.t.} \int_\Omega \exp\left(\frac{\epsilon - \mathfrak{J}_{\mathbf{a}}(X)}{C_{\exp}} \right) + \exp\left(\frac{\mathfrak{J}_{\mathbf{a}}(X) - 1/\epsilon}{C_{\exp}} \right) dX \; \leq \; \delta$$

Non-convex nonlinear optimization problem.

Solver: Matlab 2018b `fmincon` (interior-point).

Initial condition: $\mathbf{a}^1 = \mathbf{0}$, $\mathbf{a}^k = \mathbf{a}^{k-1}$.

We reorder $\mu^1, \ldots, \mu^{n_{\text{train}}}$ so that
$\mu^{k+1} = \arg\min_{\mu \in \{\mu^{k'}\}_{k'=k+1}^{n_{\text{train}}}} \|\mu^k - \mu\|_2$.

Registration algorithm for $(u^k, \bar{u}) \to \mathbf{a}^k$: interpretation

$\int_\Omega \| u^k(\Psi(X; \mathbf{a})) - \bar{u}(X) \|_2^2 dX$ measures the "distance" between u^k and $\bar{u}$ in the mapped configuration;

$\xi \left| \Psi(\cdot; \mathbf{a}) \right|^2_{H^2(\Omega)}$ is a regularization term to bound gradient and Hessian of $\Psi(\cdot; \mathbf{a})$;

the constraint

$$\int_\Omega \exp\left(\frac{\epsilon - \mathfrak{J}_{\mathbf{a}}(X)}{C_{\exp}} \right) + \exp\left(\frac{\mathfrak{J}_{\mathbf{a}}(X) - 1/\epsilon}{C_{\exp}} \right) dX \leq \delta$$

imposes weakly that $\mathfrak{J}_{\mathbf{a}}(X) \in [\epsilon, 1/\epsilon]$ for all $X \in \Omega$.

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imposes weakly that $\mathfrak{J}_{\mathbf{a}}(X) \in [\epsilon, 1/\epsilon]$ for all $X \in \Omega$.

The statement depends on $\xi, \epsilon, C_{\exp}, \delta$:

Here, we set $\xi = 10^{-3}, \epsilon = 0.1, C_{\exp} = 0.005, \delta = 1$.

Generalization: $\{\mu^k, \mathbf{a}^k\}_k \Rightarrow \mathbf{a} : \mathcal{P} \to \mathbb{R}^M$

We proceed as follows.

1. POD reduction: $\mathbf{a} \approx \mathbf{U}_\Phi \mathbf{a}_\mathrm{r}$, $\mathbf{U}_\Phi^T \mathbf{U}_\Phi = \mathbb{1}$, $\mathbf{a}_\mathrm{r} \in \mathbb{R}^{M_\mathrm{r}}$, $M_\mathrm{r} < M$.
2. RBF approximation: $\{\mu^k, \mathbf{a}_\mathrm{r}^k\}_k \Rightarrow \mathbf{a}_\mathrm{r} : \mathcal{P} \to \mathbb{R}^{M_\mathrm{r}}$.

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POD reduction: POD leads to a significant reduction in terms of online costs and reduces the dependence on the preliminary choice of M.

Drawback of RBF regression: there is no guarantee that

$$\min_{X \in \Omega, \mu \in \mathcal{P}} \mathfrak{J}_\mu(X) > 0$$

Potential fixes (work in progress): multi-fidelity approaches, constrained regression.

Nonlinear approximation

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Steady advection-reaction problem

Consider the problem

$$\begin{cases} \sigma_\mu\, u_\mu + \nabla \cdot (\mathbf{c}_\mu\, u_\mu) \;=\; f_\mu & \text{in } \Omega \\ u_\mu \;=\; u_{\mathrm{D},\mu} & \text{on } \Gamma_{\mathrm{in},\mu} \end{cases}$$

where $\Gamma_{\mathrm{in},\mu} = \{x \in \partial\Omega : \, \mathbf{c}_\mu \cdot \mathbf{n} < 0\}$, and

$$\mathbf{c}_\mu = [\cos(\mu_1), \sin(\mu_1)], \quad \sigma_\mu = 1 + \mu_2\, e^{x_1 + x_2},$$

$$f_\mu = 1 + x_1 x_2, \quad u_{\mathrm{D},\mu} = 4 \arctan\left(\mu_3\left(x_2 - 1/2\right)\right) x_2(1 - x_2)$$

$\mu_1 \in \left[-\frac{\pi}{10}, \frac{\pi}{10}\right]$, $\mu_2 \in [0.3,\, 0.7]$, $\mu_3 \in [60,\, 100]$.

The problem is discretized using a Q2 DG discretization with Local Lax-Friedrichs flux.

65790 dofs.

Mapped configuration; reduced formulation

Offline computations are based on $n_{\mathrm{train}} = 250$ snapshots.

Reduced operator $\widetilde{Z}_N$ built using POD.

Reduced formulation: Galerkin.

Hyper-reduction based on POD with EIM point selection.
[Barrault et al., 2004], [Grepl et al., 2007]

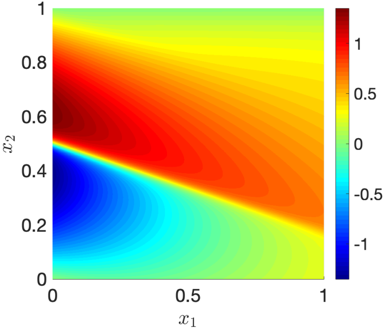
Mapping based on Q7 tensorized polynomials ($M = 72$).

Remark: $\tilde{u}_\mu$ satisfies an AR problem with

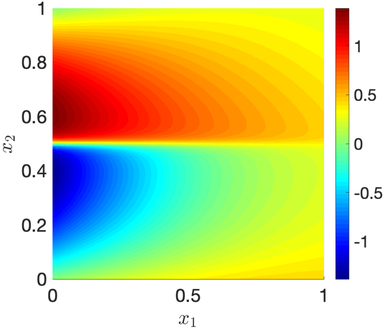
$$\tilde{\sigma}_\mu = \mathfrak{J}_\mu \, \sigma_\mu, \quad \widetilde{\mathbf{c}}_\mu = \mathfrak{J}_\mu \, \nabla \Phi_\mu^{-1} \, \mathbf{c}_\mu, \quad \tilde{f}_\mu = \mathfrak{J}_\mu \, f_\mu, \quad \tilde{u}_{\mathrm{D},\mu} = u_{\mathrm{D},\mu}.$$

The mapping Φ_μ reduces the sensitivity of the solution to changes in μ_1.

$$\mathbf{c}_\mu = [\cos(\mu_1), \sin(\mu_1)];$$
$$\bar{\mu} = [0, 0.5, 80].$$



(a) $u(\mu)$



(b) $\bar{u}$

Visualization of the solution field: $\mu = [-\pi/10, 0.3, 60]$

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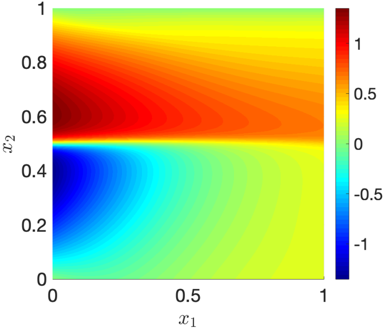
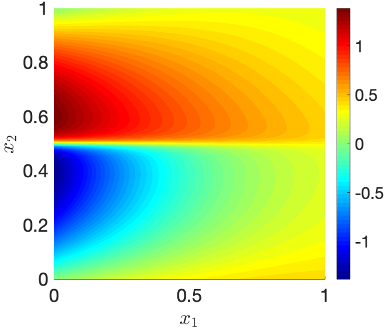


(a) $\tilde{u}(\mu)$

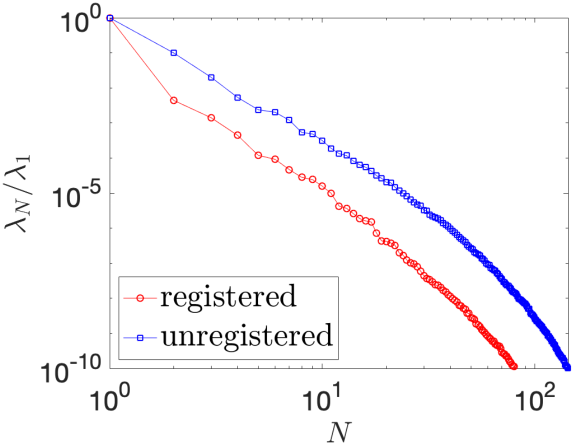


(b) $\bar{u}$

Behavior of the POD eigenvalues

Decay rate is nearly the same for both registered and unregistered configurations, **but**

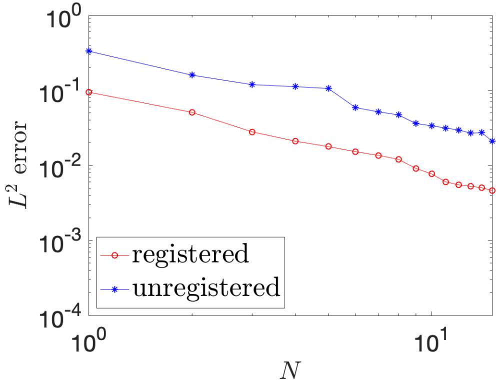
we have $(\lambda_n^{\mathrm{reg}}/\lambda_1^{\mathrm{reg}})/(\lambda_n^{\mathrm{unreg}}/\lambda_1^{\mathrm{unreg}}) = \mathcal{O}(10^2)$.



Performance of the Reduced Basis ROM

Relative error is computed based on $n_{\mathrm{test}} = 20$ parameters, in the physical configuration.

The nonlinear ROM is approximately 4 times more accurate than the linear ROM.



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Develop a pMOR procedure for

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in the turbulent regime.

We wish to *efficiently* and *accurately* estimate QOIs associated with the velocity field

$$u(\mu) = u(x, t; \mu), \qquad x \in \Omega \subset \mathbb{R}^d, \quad t \in (0, \infty), \quad \mu \in \mathcal{P} \subset \mathbb{R}^P$$

in the limit of many queries.

Efficiency: measured wrt the FOM in terms of

memory requirements;

computational time.

Accuracy: measured wrt the FOM in terms of

the long-time averaged flow $\langle u \rangle = \lim_{T\to\infty} \frac{1}{T} \int_0^T u(t)\, dt,$

the TKE[7] $\mathrm{TKE}(t) = \frac{1}{2} \int_\Omega \|u(x,t) - \langle u \rangle(x)\|_2^2 \, dx.$

For chaotic flows, prediction of the *instantaneous* velocity is out of reach.

[7] More precisely, we shall estimate the *moments* of the TKE.

A simplified task: solution reproduction problem ($\mathcal{P} = \{\bar{\mu}\}$)

We seek an estimate of $u(\bar{\mu})$ s.t.

$$\hat{u}(x,t) = \sum_{n=1}^{N} \alpha_n(t)\zeta_n(x)$$

Offline stage:

given $\{u(\cdot, t^k, \bar{\mu})\}_{k=1}^{K}$,

generate the reduced space $\mathcal{Z}_N = \mathrm{span}\{\zeta_n\}_{n=1}^{N}$, and

formulate the Reduced Order Model

Online stage:

query the ROM for **the same** $\mu = \bar{\mu}$ to estimate $\{\alpha_n(t)\}_{n=1}^{N}$ for $t > 0$.

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Limited practical interest, but key intermediate step toward the development of the ROM formulation.

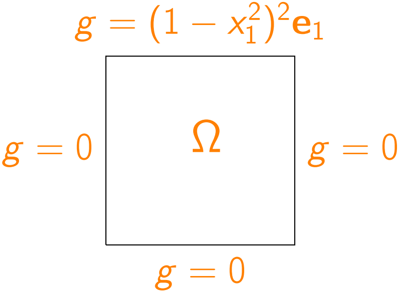
Constrained formulation

- pMOR for turbulent flows
- Lid-driven cavity problem
- A first attempt: POD-Galerkin
- Our proposal: POD-constrained Galerkin

A lid-driven cavity problem[8]

Consider the problem:

$$\begin{cases} \partial_t u + (u \cdot \nabla) u - \frac{1}{\mathrm{Re}} \Delta u + \nabla p = 0 & \Omega \times \mathbb{R}_+ \\ \nabla \cdot u = 0 & \Omega \times \mathbb{R}_+ \\ u|_{\partial\Omega} = g, \qquad u(0) = 0 & \end{cases}$$



$\Omega = (-1, 1)^2$

$\mathrm{Re} = 15000$
(turbulent regime)

[8]Model problem considered in Balajewicz, Dowell, Nonlinear Dyn (2012).

Weak formulation for the lifted equations ($\mathring{u} := u - R_g$)

Given R_g s.t. $R_g|_{\partial\Omega} = g$, $\nabla \cdot R_g \equiv 0$, find $(\mathring{u}, p)$ s.t.

$$\begin{cases} \langle \partial_t \mathring{u}(t), v \rangle_\star + \dfrac{1}{\mathrm{Re}} \displaystyle\int_\Omega \nabla(\mathring{u}(t) + R_g) : \nabla v \, dx \\ \qquad + c(\mathring{u}(t) + R_g, \mathring{u}(t) + R_g, v) + b(v, p(t)) = 0 \\ b(\mathring{u}(t), q) = 0 \qquad \forall\, v \in V, \quad q \in Q, \quad \text{a.e. } t > 0. \end{cases}$$

where $V = [H_0^1(\Omega)]^2$, $Q = \{q \in L^2(\Omega) : \int_\Omega q = 0\}$, and

$$c(w, v, z) = \int_\Omega (w \cdot \nabla) v \cdot z \, dx, \; b(v, q) = -\int_\Omega (\nabla \cdot v) q \, dx.$$

Choice for the lift: $R_g =$ Stokes solution

The choice $R_g = \langle u \rangle$ is not suitable for the parametric case.

High-fidelity model: SEM in Nek5000

We rely on the **spectral element** solver Nek5000 to generate the DNS data.

We refer to nek5000.mcs.anl.gov for details concerning the software.

Simulations were performed by Dr. Lambert Fick (Texas A&M) at Argonne National Lab.

Deville, Fischer, Mund, Cambridge University Press (2002).

Constrained formulation

- pMOR for turbulent flows
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- A first attempt: POD-Galerkin
- Our proposal: POD-constrained Galerkin

Galerkin ROM (semi-implicit time integration)

Given $\mathcal{Z}_N := \mathrm{span}\{\zeta_n\}_{n=1}^N \subset V_{\mathrm{div}} = \{v \in V : \nabla \cdot v = 0\}$, and $\{t^j = j\Delta t\}_{j=0}^J$, find $\{\hat{u}^j\}_j \subset \mathcal{Z}_N$ such that

$$\left(\frac{\hat{u}^{j+1} - \hat{u}^j}{\Delta t}, v\right)_{L^2(\Omega)} + \frac{1}{\mathrm{Re}} \int_\Omega \nabla(\hat{u}^{j+1} + R_g) : \nabla v \, dx$$
$$+ c(\hat{u}^j + R_g, \hat{u}^{j+1} + R_g, v) = 0 \;\; \forall v \in \mathcal{Z}_N, \;\; j = 0, 1, \ldots$$

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$$+ c(\hat{u}^j + R_g, \hat{u}^{j+1} + R_g, v) = 0 \;\; \forall v \in \mathcal{Z}_N, \;\; j = 0, 1, \ldots$$

The space $\mathcal{Z}_N$ is built through the DNS data $\{\mathring{u}^k = u(t^k) - R_g\}_{k=1}^K \subset V_{\mathrm{div}}$ using POD.

We consider the following choice of the inner product $(\cdot, \cdot)$:

$$(w, v) = \int_\Omega \nabla w : \nabla v \, dx \quad H^1 - \mathrm{POD}$$

Iollo, Lanteri, Désidéri, Theor Comp Fluid Dyn (2000).

Galerkin ROM: algebraic formulation (semi-implicit in time)

The coefficients $\boldsymbol{\alpha}^j = [\alpha_1^j, \ldots, \alpha_N^j]$ ($\leftrightarrow \{\hat{u}^j\}_j$) solve

$$\mathbb{A}(\boldsymbol{\alpha}^j)\,\boldsymbol{\alpha}^{j+1} = \mathsf{F}(\boldsymbol{\alpha}^j) \quad j = 0, 1, \ldots, \quad (\hat{u}^{\cdot} = \sum_n \alpha_n^{\cdot} \zeta_n)$$

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where $\mathbb{A} : \mathbb{R}^N \to \mathbb{R}^{N,N}$, and $\mathbf{F} : \mathbb{R}^N \to \mathbb{R}^N$ are

$$\mathbb{A}_{m,n}(\mathbf{w}) = \frac{1}{\Delta t}\int_\Omega \zeta_n \cdot \zeta_m \, dx + \frac{1}{\mathrm{Re}}\int_\Omega \nabla\zeta_n : \nabla\zeta_m \, dx$$
$$+ c(R_g, \zeta_n, \zeta_m) + \sum_{i=1}^N w_i \, c(\zeta_i, \zeta_n, \zeta_m)$$

$$\mathbf{F}_m(\mathbf{w}) = \sum_{n=1}^N w_n \left(\frac{1}{\Delta t}\int_\Omega \zeta_n \cdot \zeta_m \, dx - c(\zeta_n, R_g, \zeta_m) \right)$$
$$- \frac{1}{\mathrm{Re}}\int_\Omega \nabla R_g : \nabla\zeta_m \, dx$$

Computational summary (POD-Galerkin)

Offline stage:

Compute DNS data $\{u^k = u(\cdot, t^k)\}_{k=1}^K$, $t^k = T_0 + k$

$T_0 = 500$, $K = 500$

Use POD to build the space $\mathcal{Z}_N = \mathrm{span}\{\zeta_n\}_{n=1}^N$

Define $\mathbb{A} : \mathbb{R}^N \to \mathbb{R}^{N,N}$, and $\mathbf{F} : \mathbb{R}^N \to \mathbb{R}^N$

Online stage:

Solve the discrete dynamical system:

$$\mathbb{A}(\boldsymbol{\alpha}^j)\boldsymbol{\alpha}^{j+1} = \mathbf{F}(\boldsymbol{\alpha}^j), \qquad j = 0, \ldots, J-1$$

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Online stage:

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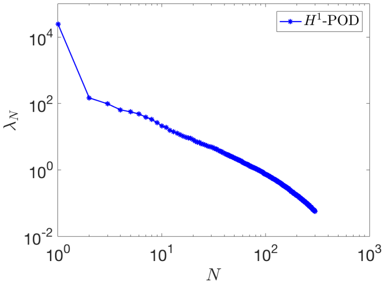
$$\mathbb{A}(\boldsymbol{\alpha}^j)\boldsymbol{\alpha}^{j+1} = \mathbf{F}(\boldsymbol{\alpha}^j), \qquad j = 0, \ldots, J-1$$

Online memory requirements: $\mathcal{O}(N^3)$.

Online cost: $\mathcal{O}(N^3 J)$.

POD eigenvalues ($\mathrm{Re} = 15000$)

POD eigenvalues $\{\lambda_N\}_N$ decay slowly with N.

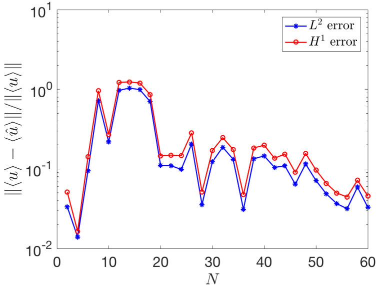


$u^k := u(\cdot, t^k)$
$t^k := 500 + k,$
$k = 1, \dots, K = 500$

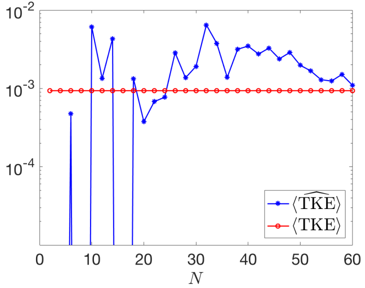
$\zeta_1 \approx C(\langle u \rangle - R_g)$ $\Rightarrow$ no contribution to fluctuating field

$$\frac{\sum_{k'=2}^{N} \lambda_{k'}}{\sum_{k=2}^{K} \lambda_k} = \begin{cases} 16.5\% & N = 2 \\ 73.1\% & N = 20 \\ 79.7\% & N = 30 \\ 87.0\% & N = 50 \end{cases}$$

Numerical results ($\mathrm{Re} = 15000$): performance (I)



Rel. error in $\langle u\rangle$



Mean TKE

We observe several **spurious** effects for moderate N:

false stable steady flows,

overly unstable flows...

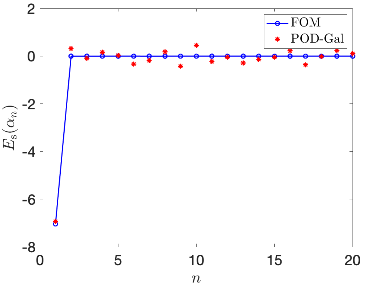
For $N \gtrsim 50$, accuracy improves.

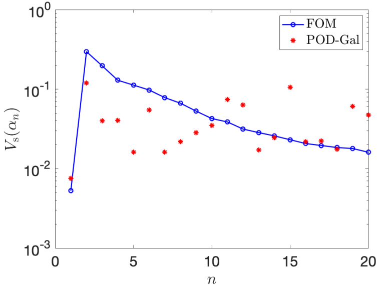
Numerical results ($\mathrm{Re} = 15000$): performance (II)

Moments of $\{\alpha_n\}_n$ ($\mathring{u}(\cdot, t) = \sum_{n=1}^{\infty} \alpha_n(t)\zeta_n$): **N = 20**

$$E_\mathrm{s}(\alpha_n, \{t^k\}) = \frac{1}{K}\sum_{k=1}^{K} \alpha_n(t^k),$$

$$V_\mathrm{s}(\alpha_n, \{t^k\}) = \frac{1}{K-1}\sum_{k=1}^{K} \left(\alpha_n(t^k) - E_\mathrm{s}(\alpha_n, \{t^k\})\right)^2$$



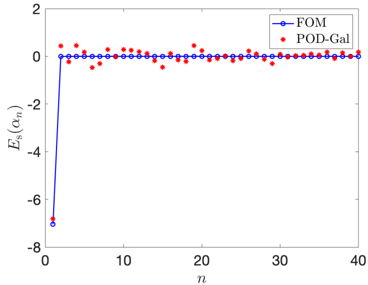


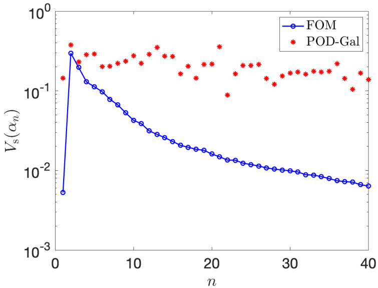
Numerical results ($\mathrm{Re} = 15000$): performance (II)

Moments of $\{\alpha_n\}_n$ $\left(\mathring{u}(\cdot, t) = \sum_{n=1}^{\infty} \alpha_n(t)\zeta_n\right)$: **N = 40**

$$E_{\mathrm{s}}(\alpha_n, \{t^k\}) = \frac{1}{K}\sum_{k=1}^{K} \alpha_n(t^k),$$

$$V_{\mathrm{s}}(\alpha_n, \{t^k\}) = \frac{1}{K-1}\sum_{k=1}^{K} \left(\alpha_n(t^k) - E_{\mathrm{s}}(\alpha_n, \{t^k\})\right)^2$$





Numerical results ($\mathrm{Re} = 15000$): performance (II)

Moments of $\{\alpha_n\}_n$ $(\mathring{u}(\cdot,t) = \sum_{n=1}^{\infty} \alpha_n(t)\zeta_n)$: **N = 60**

$$E_{\mathrm{s}}(\alpha_n, \{t^k\}) = \frac{1}{K}\sum_{k=1}^{K} \alpha_n(t^k),$$

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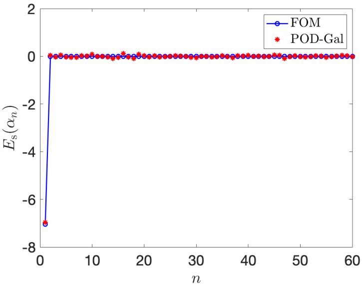

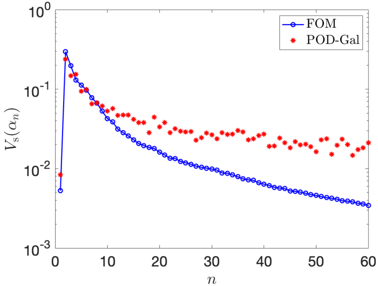

Comments

POD-Galerkin approach does not provide an adequate approximation of the long-time system dynamics, particularly for moderate N.

We observe several spurious effects

false stable steady flows,

overly unstable flows...

This behavior is similar to the one observed for highly-truncated spectral approximations to turbulent flows.

Curry, Herring, Loncaric, Orszag, J Fluid Mech (1984).

Constrained formulation

- pMOR for turbulent flows
- Lid-driven cavity problem
- A first attempt: POD-Galerkin
- Our proposal: POD-constrained Galerkin

We propose the following ROM (`cGalerkin`):

$$\boldsymbol{\alpha}^{j+1} := \arg\min_{\mathbf{w}\in\mathbb{R}^N} \|\mathbb{A}(\boldsymbol{\alpha}^j)\mathbf{w} - \mathbf{F}(\boldsymbol{\alpha}^j)\|_2^2,$$

$$\text{subject to } a_n \leq w_n \leq b_n, \; n = 1, \ldots, N.$$

$\mathbb{A}$ and $\mathbf{F}$ are the matrix-valued and vector-valued functions introduced for the Galerkin ROM.

cGalerkin formulation (semi-implicit in time)

We propose the following ROM (cGalerkin):

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$\mathbb{A}$ and $\mathbf{F}$ are the matrix-valued and vector-valued functions introduced for the Galerkin ROM.

If $\boldsymbol{\alpha}_{\mathrm{Gal}}^{j+1} := \mathbb{A}(\boldsymbol{\alpha}^j)^{-1}\,\mathbf{F}(\boldsymbol{\alpha}^j)$ satisfies the constraints, cGalerkin = Galerkin.

For semi-implicit and explicit time discretizations, cGalerkin corresponds to a **convex quadratic programming** problem, which can be solved using an interior point method.

Estimates of $\{a_n\}_n$ and $\{b_n\}_n$

a_n and b_n are lower and upper bounds for[9]

$$\alpha_n(t) := (\mathring{u}(t) = u(t) - R_g, \zeta_n).$$

Given the snapshots $\{u^k\}_{k=1}^K$, we set $\{a_n\}_n$ and $\{b_n\}_n$ as

$$a_n = m_n^{\mathrm{u}} - \epsilon(M_n^{\mathrm{u}} - m_n^{\mathrm{u}}), \qquad b_n = M_n^{\mathrm{u}} + \epsilon(M_n^{\mathrm{u}} - m_n^{\mathrm{u}});$$

where $\epsilon = 0.01$[10], and

$$m_n^{\mathrm{u}} := \min_{k=1,\ldots,K} (\mathring{u}^k, \zeta_n)_V, \qquad M_n^{\mathrm{u}} := \max_{k=1,\ldots,K} (\mathring{u}^k, \zeta_n)_V.$$

[9] **NOTE 1:** $(\zeta_m, \zeta_n) = \delta_{m,n}$

[10] **NOTE 2:** $\{t^k\}_k$ sampling times, $\{t^j\}_j$ time grid, $K \ll J$.

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The hyper-parameters $\{a_n\}_n$ and $\{b_n\}_n$ of `cGalerkin`

admit a simple interpretation, and

can be easily tuned based on **sparse DNS data**.

[9] **NOTE 1:** $(\zeta_m, \zeta_n) = \delta_{m,n}$

[10] **NOTE 2:** $\{t^k\}_k$ sampling times, $\{t^j\}_j$ time grid, $K \ll J$.

Computational summary (constrained POD-Galerkin)

Offline stage:

Compute DNS data $\{u^k = u(\cdot, t^k)\}_{k=1}^K$

Use POD to build the space $\mathcal{Z}_N = \mathrm{span}\{\zeta_n\}_{n=1}^N$

Define $\mathbb{A} : \mathbb{R}^N \to \mathbb{R}^{N,N}$, and $\mathbf{F} : \mathbb{R}^N \to \mathbb{R}^N$

Define $\{a_n\}_n$ and $\{b_n\}_n$ based on the DNS data $\{\mathring{u}^k\}_k$

Online stage:

Solve the discrete dynamical system:

$$\boldsymbol{\alpha}^{j+1} = \arg\min_{\mathbf{w}\in\mathbb{R}^N} \|\mathbb{A}(\boldsymbol{\alpha}^j)\mathbf{w} - \mathbf{F}(\boldsymbol{\alpha}^j)\|_2^2, \ \ \text{s.t. } a_n \le w_n \le b_n$$

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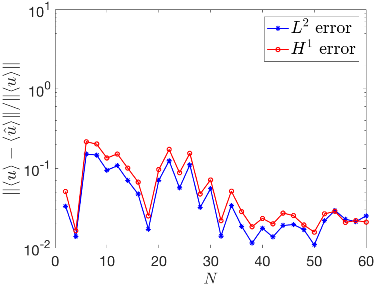
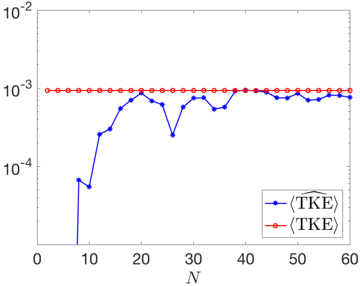
Online memory requirements: $\mathcal{O}(N^3)$.

Online cost: $\mathcal{O}(N^3 \underbrace{J_{\text{pure}}}_{\text{Gal. solves}} + \underbrace{\kappa N^3}_{\text{cost QP}} (J - J_{\text{pure}}))$.

Numerical results ($\mathrm{Re} = 15000$): performance (I)



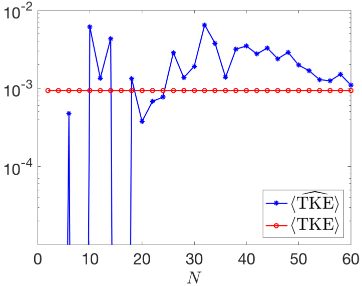
Rel. error in $\langle u \rangle$



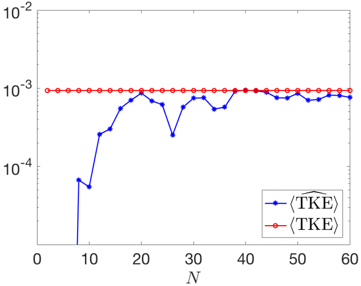
Mean TKE

The constrained Galerkin formulation consistently underestimates the TKE.

Numerical results ($\mathrm{Re} = 15000$): performance (II)



Galerkin



constrained Galerkin

For some values of N, $\langle \mathrm{TKE}_{\mathrm{cGal}} \rangle > \langle \mathrm{TKE}_{\mathrm{Gal}} \rangle$. For some other values $\langle \mathrm{TKE}_{\mathrm{cGal}} \rangle < \langle \mathrm{TKE}_{\mathrm{Gal}} \rangle$.

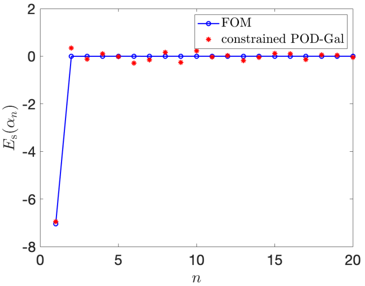
$\Rightarrow$ `cGalerkin` does **not** add artificial viscosity to `Galerkin`.

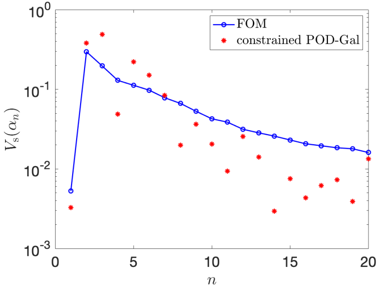
Numerical results ($\mathrm{Re} = 15000$): performance (III)

Moments of $\{\alpha_n\}_n$ ($\mathring{u}(\cdot, t) = \sum_{n=1}^{\infty} \alpha_n(t)\zeta_n$): **N = 20**

$$E_{\mathrm{s}}(\alpha_n, \{t^k\}) = \frac{1}{K}\sum_{k=1}^{K} \alpha_n(t^k),$$

$$V_{\mathrm{s}}(\alpha_n, \{t^k\}) = \frac{1}{K-1}\sum_{k=1}^{K} \left(\alpha_n(t^k) - E_{\mathrm{s}}(\alpha_n, \{t^k\})\right)^2$$





Numerical results ($\mathrm{Re} = 15000$): performance (III)

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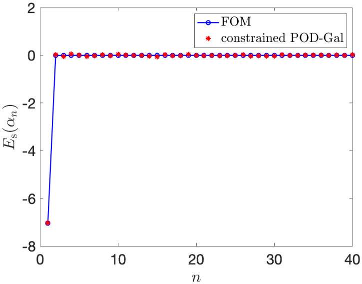

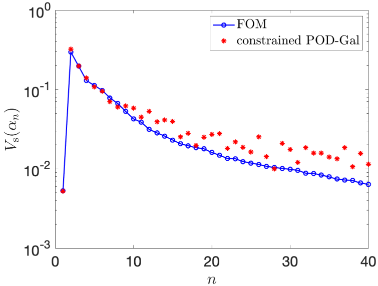

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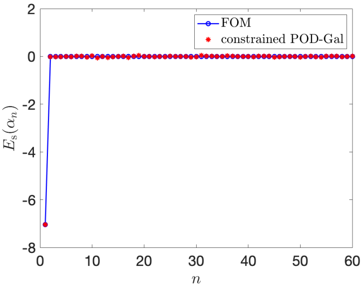
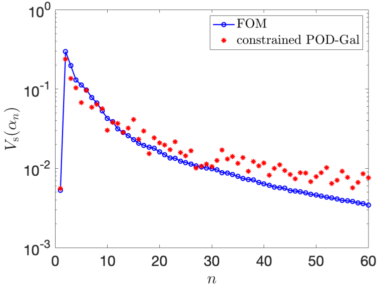
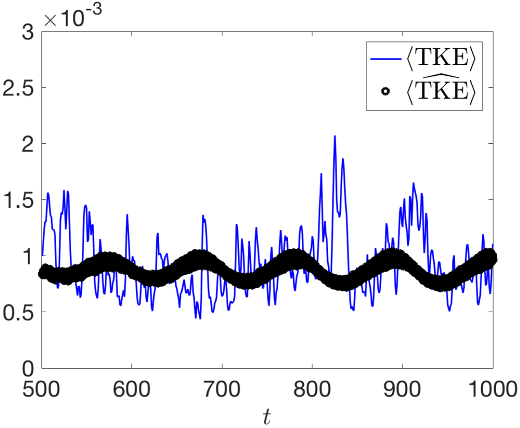
$$E_\mathrm{s}(\alpha_n, \{t^k\}) = \frac{1}{K}\sum_{k=1}^{K} \alpha_n(t^k),$$

$$V_\mathrm{s}(\alpha_n, \{t^k\}) = \frac{1}{K-1}\sum_{k=1}^{K} \left(\alpha_n(t^k) - E_\mathrm{s}(\alpha_n, \{t^k\})\right)^2$$





Behavior of the turbulent kinetic energy ($N = 20$)



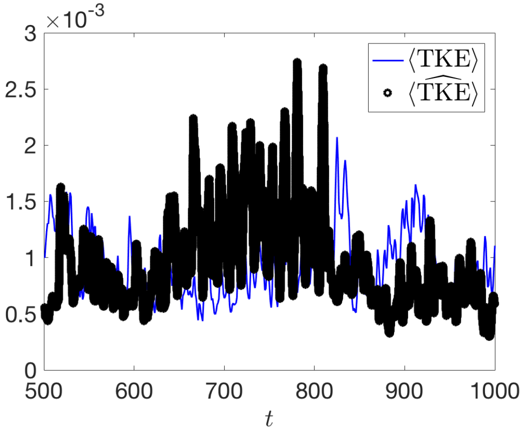
$\langle \text{TKE} \rangle = 9.4 \cdot 10^{-4}$,

$\langle \widehat{\text{TKE}} \rangle = 8.6 \cdot 10^{-4}$;

$\mathbb{V}(\text{TKE}) = 8.5 \cdot 10^{-8}$;

$\mathbb{V}(\widehat{\text{TKE}}) = 5.5 \cdot 10^{-9}$.

Behavior of the turbulent kinetic energy ($N = 40$)



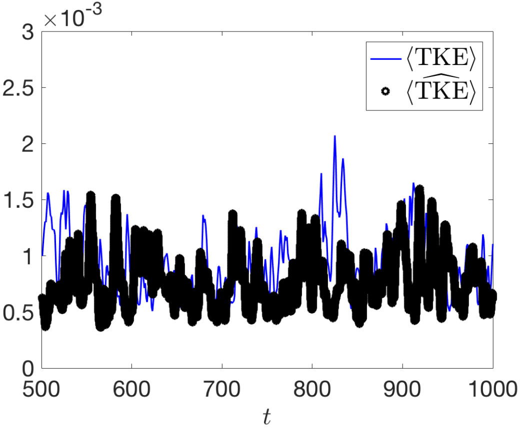
$\langle \text{TKE} \rangle = 9.4 \cdot 10^{-4}$,

$\langle \widehat{\text{TKE}} \rangle = 9.4 \cdot 10^{-4}$;

$\mathbb{V}(\text{TKE}) = 8.5 \cdot 10^{-8}$;

$\mathbb{V}(\widehat{\text{TKE}}) = 1.7 \cdot 10^{-7}$.

Behavior of the turbulent kinetic energy ($N = 60$)



$\langle \text{TKE} \rangle = 9.4 \cdot 10^{-4}$,

$\langle \widehat{\text{TKE}} \rangle = 7.65 \cdot 10^{-4}$;

$\mathbb{V}(\text{TKE}) = 8.5 \cdot 10^{-8}$;

$\mathbb{V}(\widehat{\text{TKE}}) = 5.8 \cdot 10^{-8}$.

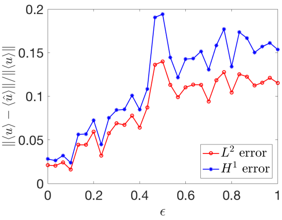
Prediction of instantaneous TKE is out of reach.

Our results suggest that estimation of TKE moments is achievable.

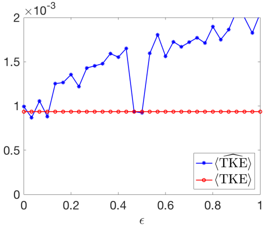
Sensitivity analysis wrt ϵ ($\mathrm{Re} = 15000$, $N = 40$)

ϵ enters in the definition of the bounds a_n and b_n:

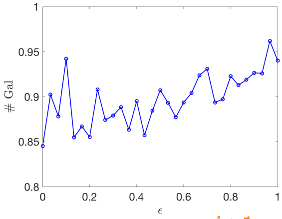
$$a_n = m_n^{\mathrm{u}} - \epsilon(M_n^{\mathrm{u}} - m_n^{\mathrm{u}}), \qquad b_n = M_n^{\mathrm{u}} + \epsilon(M_n^{\mathrm{u}} - m_n^{\mathrm{u}});$$



Rel. error in $\langle u\rangle$



Mean TKE

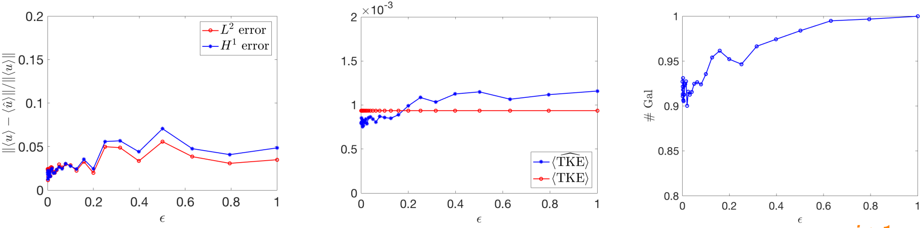


% $\alpha^{j+1} = \alpha^{j+1}_{\mathrm{Gal}}$

Sensitivity analysis wrt ϵ ($\mathrm{Re} = 15000$, $N = 60$)

ϵ enters in the definition of the bounds a_n and b_n:

$$a_n = m_n^{\mathrm{u}} - \epsilon(M_n^{\mathrm{u}} - m_n^{\mathrm{u}}), \qquad b_n = M_n^{\mathrm{u}} + \epsilon(M_n^{\mathrm{u}} - m_n^{\mathrm{u}});$$



Rel. error in $\langle u\rangle$ Mean TKE % $\alpha^{j+1} = \alpha_{\mathrm{Gal}}^{j+1}$

Interpretation: as N increases, the Galerkin model becomes more and more accurate, and box constraints become less and less important.

Conclusions and perspectives

Fluid problems present unique challenges for MOR.

Data compression

boundary layers, shocks;

wide spectrum of scales (turbulence).

Reduced formulation

fragility of Galerkin ROMs;

presence of nonlinearities.

Error estimation

Summary

Fluid problems present unique challenges for MOR.

Data compression

boundary layers, shocks;

$\rightarrow$ Lagrangian nonlinear approximation procedure.

wide spectrum of scales (turbulence).

Reduced formulation

fragility of Galerkin ROMs;

$\rightarrow$ constrained Galerkin formulation.

presence of nonlinearities.

Error estimation

$\rightarrow$ time-avg error indicators (Fick et al., 2018).

Ongoing work

Nonlinear approximation (with A Iollo)

definition of the reference field $\leftrightarrow$ clustering

reduction of offline costs for map generation $\leftrightarrow$ hierarchy of models

Constrained Galerkin (with P Fischer[11], AT Patera)

identification of new sets of constraints;

extension to more challenging problems.

[11] Two PhD theses were funded on this subject at University of Illinois (PI: Paul Fischer).

Thank you for your attention!

Reference: (constrained Galerkin)
Fick, Maday, Patera, Taddei. *A stabilized POD model for turbulent flows over a range of Reynolds numbers: Optimal parameter sampling and constrained projection*, 2018; JCP.