POD on the fly: an adaptive combination of CFD and POD to simulate complex dynamics

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**Motivation**

- Flow simulations are required for various **tasks** (design, control, stability analysis, ...) in many **fields** (engineering, physics, biology, ...)
- **Huge computational resources** are often involved ($Re \gg 1$)

- **Reducing the computational resources** required by standard numerical solvers is crucial in industrial applications. Huge acceleration factors (say, 100-1000 or more) are required

- **Numerical complexity** (number of grid points or cells) is often *much larger* than **physical complexity** (spatio-temporal features)

- **POD** (combined with additional ingredients) is a very powerful **tool** to identify the physical complexity

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1 Lucia et al., *Prog. Aerosp. Sci.* 40 (2004), 51–117
POD is extensively used to construct reduced order models (ROMs) after seminal ideas by Sirovich\(^2\) (method of snapshots)

**Two classes of POD-based ROMs** (among many others):

**Pre-processed ROMs**, in three steps: (i) CFD-calculate a representative set of snapshots (expensive pre-process), (ii) identify the most energetic POD modes, and (iii) project (e.g., Galerkin) the governing equations onto the POD modes (inexpensive online operation) \( q = \sum A_j(t)Q_j(x) \).

**POD on the fly** (this talk) combines POD and CFD

1 SOME IDEAS
- The magic of POD
- Switching between CFD and POD
- Updating the set of POD modes
- Additional ingredients
- Summary of the method

2 SOME PLOTS
- Ginzburg-Landau and laminar flows
- Aeroelasticity
- Subsurface oil-reservoir simulations
Outline

1 Some ideas
- The magic of POD
- Switching between CFD and POD
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2 Some plots
- Ginzburg-Landau and laminar flows
- Aeroelasticity
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The magic of POD (facts)

Complex 1D Ginzburg-Landau equation (GLE): transient dynamics converging to a periodic solution at $\mu = 20$ provides 17 useful POD modes.

Then$^3$:

- A preprocessed ROM based on the 7 most energetic POD modes approximates the bifurcation diagram in $0 \leq \mu \leq 300$.
- Using 14 modes approximates the diagram in $0 \leq \mu \leq 2000$

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The magic of POD (opportunities)

- Continuity of the approximating low-dimensional manifold: For a given accuracy, as a parameter (or time) is varied, new POD modes (new dimensions of the manifold) come into play with a very small amplitude.

- **Spatial complexity** (provided by CFD) varies smoothly. **Temporal complexity** (calculated by the ROM), instead, may show very steep jumps.

Additional observations:

- POD modes calculated for a set of parameter values are useful for other parameter values as well.
- Unconverged/transient snapshots are useful.
- POD modes calculated for related equations (e.g., quintic GLE) are useful for other parameter values as well.
Need to update POD modes detected

The need to update the POD modes detected when either:

- **Truncation error** not small enough

\[ E_n^{n_1} = \| q_{n_1}^{n_1} - q_n^{GS} \| \equiv \sqrt{\sum_{j=n+1}^{n_1} |A_j|^2} < \varepsilon \]

- The Galerkin system (GS) is being destabilized by the neglected modes (mode truncation instability). Can be monitored:
  - Comparing with a second instrumental GS retaining more modes\(^a\)
  - Using a normalized residual \(^b\) of the GS

\[ E_{res}^{n_1} < \varepsilon/k \]

Residuals already used in ROMs for different purposes \(^c\)


**Upd ating strategy**

When updating is needed, new snapshots are calculated using CFD. These are used to update (rotate/enlarge/contract) the POD manifold. New POD modes can be calculated.

**Observations**

- **Weighted** old and new POD modes are mixed using POD (mixing snapshots is no good).
- The weights must ensure that:
  - Contamination of the POD manifold is avoided.
  - Modes that showed very small amplitude in the last GS are eliminated.
• Projection of the governing equations onto the POD modes based on a few number of mesh-points. Sophisticated sampling\(^a\) not necessary
• Mode libraries\(^b\) can be used to shorten the first CFD run


POD ON THE FLY (SUMMARY)

- POD basis construction (improved by mode libraries)
- residual control (instabilities)
- amplitudes control (accuracy)

POD basis update (old + new modes)

- CFD
- POD
- CFD
- POD
- CFD
- POD

- full integration (snapshots)
- reduced integration
- full integration (snapshots)
- reduced integration
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1D CGLE: moderate complexity

- Required accuracy $\varepsilon = 10^{-2}$
- Errors set to zero where snapshots are computed
- Comparison restricted to a suitable timescale (needed for unstable dynamics)

$E_n^1$ is a good estimate of the actual relative RMS error $E_{L_2}$ (vs. NS)

Speedup $\approx 7.06$
1D CGLE: HIGH COMPLEXITY

Speedup = 3.63

Speedup = 3.7
For the CGLE

- For the 2D CGLE, the speedups are similar to their maximum values.
- **Mode libraries**, either generic (i.e., Fourier expansions) or resulting from former applications of the methods, allow to shorten the first CFD interval, obtaining speedups as large as 30 for the 1D CGLE and 350 for the 2D CGLE.

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- The method works also well for laminar flows, such as the **unsteady lid-driven cavity** at moderate Re\(^a\) and thermal convection problems\(^b\).
- Turbulent flows would require additional ingredients.

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2 DOF AEROELASTIC FLOW IN 2D (ONGOING)
Constructing ROMs for these flows involves additional difficulties:

⭐ Purely convective equations + Darcy law. Very rough discretizations.
⭐ High contrast (between neighboring cells) in physico-chemical properties, which are not-well-determined.
⭐ Steep fronts near the water/oil interfaces are quite demanding for POD.
Subsurface flow simulations (II)

Oil rates at a representative production well over 30 years obtained by the full model (green) and the ROM (blue):
Subsurface flow simulations (III)

Water saturation distribution after 30 years using the full model (left) and the ROM (right):