An approach to perform shape optimisation by means of hybrid ROM-CFD simulations

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Introduction

Shape optimisation in fluid dynamics

- Need to perform several function evaluations
- Very expensive CFD simulations when dealing with 3D turbulent flows
- Need of simple and general tools (non-intrusive)

Reduced Order Modelling can provide low cost surrogates for predictive simulations.

Examples of industrial problems studied by means of hybrid CFD-POD simulations at Optimad Engineering
Proper Orthogonal Decomposition

Snapshots from CFD simulation:

\[ U_{POD}(x, t) = \sum_{i=1}^{N} a_i(t) \Phi_i(x) \]

\( t \) represents time in an unsteady problem or a generic design parameter in a steady problem

\[
\Phi_i = \sum_{j=1}^{N_s} b_{i}^{j} U_{s}^{j}
\]

(Sirovich approach)

\[
F = \sum_{k=1}^{N_s} (U_{s}^{k} \cdot \phi)^2 - \lambda (\Phi \cdot \Phi - 1) = \frac{\partial F}{\partial b_j} = 0 \quad \text{Constrained maximisation problem}
\]

\[
[A] b = \lambda b \quad \text{Eigenvalue problem}
\]

\[
A_{mn} = U_{s}^{m} \cdot U_{s}^{n} \quad \text{Correlation matrix}
\]
**POD Galerkin**

- Gives a set of ODEs for the evolution of the modes coefficients
- Strong reduction in the computational cost
- Stability and robustness issues: difficult to perform predictive simulations

**Hybrid CFD-POD**

- Moderate reduction of the computational cost
- Robustness thanks to CFD feedback
- Stability linked to the effects of the numerical scheme
  - Two considered approaches for incompressible NS equations:
    - Domain decomposition
    - Poisson problem solved by POD
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Recent developments in numerical methods for model reduction

7–10 November 2016, Paris

Domain decomposition

• POD can identify the main structures in a flow field by extracting the information from a database of snapshots

• Need for a robust POD model: ability to predict flows with parameter’s values not present in the database

Possible approach: domain decomposition

• The POD model is used to define the boundary conditions for a reduced CFD domain

• The non-linearities which are difficult to describe by POD and the phenomena not included in the database are directly taken into account by the CFD

Hybrid CFD-POD: domain decomposition

**Coupling in the overlapping zone**

\[ U_{ROM}(x, t) = U_{avg}(x) + \sum_{i=1}^{N} a_i(t)\Phi_i(x) \]

with \( a_i \) obtained at each time step by

\[ \min \left( \| U_{CFD} - U_{ROM} \|_{\Omega_o} \right) \]

- \( U_{avg} \) fixes the far field value
- The modes are zero in the far field
- The far field values which characterise the working condition (e.g. Reynolds number) are automatically satisfied
- Two completely independent models, one for velocity and one for pressure
An example: flow around a cylinder
Recursive hybrid simulations: numerical zoom

Level 0
Mesh 300x200
DX=DY=0.16

CPU time for 1 period = 190 s
Recursive hybrid simulations: numerical zoom

Level 1

Mesh
300x200

DX=DY=0.08

CPU time for 1 period = 290 s
Recursive hybrid simulations: numerical zoom

Level 2

Mesh
300x200

DX=DY=0.04

CPU time for 1 period = 720 s
Recursive hybrid simulations: numerical zoom

Level 3

Mesh 300x200

DX=DY=0.02

CPU time for 1 period = 2100 s
Recursive hybrid simulations: numerical zoom

Reference

Mesh
2400x1600

DX=DY=0.02

CPU time for 1 period = 80000 s
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Hybrid CFD-POD: domain decomposition

Numerical zoom: reference CFD vs Hybrid CFD-POD (level 1)

Cd_avg=1.37
Cd_avg=1.22

St=0.165
St=0.168
Numerical zoom: reference CFD vs Hybrid CFD-POD (level 2)

Cd_avg=1.24
Cd_avg=1.22

St=0.167
St=0.168
Recent developments in numerical methods for model reduction
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Hybrid CFD-POD: domain decomposition

Numerical zoom: reference CFD vs Hybrid CFD-POD (level 3)

Cd_avg=1.22
St=0.168
When does domain decomposition pay?

Simple external flow around an isolated body

Most of the degrees of freedom of the discretisation should be concentrated close to the body (by means of adaptive meshes) so the reduction of the computational cost between the full CFD and the hybrid simulation could be small.

Multi-body configurations or local analyses

The hybrid simulation is significantly cheaper than the full CFD simulation, even when adaptive meshes are employed.
Robust POD basis

• The coupled POD-CFD simulation requires a preliminary database of full CFD (expensive) simulations to build the POD model

• The POD is useful for shape optimisation only if it is robust: it must be able to predict a configuration not in the database

• Is the hybrid approach suitable for prediction?
Vortex-airfoil interaction: robustness test

Model problem: NACA0012 (Re=1000, α=5°) and vortex
Uniform cartesian meshes, same mesh size in full CFD and hybrid simulations. Measured speedup from full CFD to hybrid: 65
Hybrid CFD-POD: domain decomposition

Space of the parameters: intensity and size of the vortex

Uniform sampling of the space of parameters:
9 full CFD simulations are performed to build the POD basis
Evolution of the lift coefficient (Cl) for the configurations in the database
Hybrid CFD-POD: domain decomposition

Space of the parameters: configurations used for building the POD database (blue) and test configurations for hybrid prediction (red)
Prediction with hybrid CFD-POD for the configurations out in the database: comparison with full CFD
Residual minimisation: POD for Poisson problem

• Classical incompressible NS solvers require the solution of a Poisson problem on pressure to get a diverge free velocity field

• The solution of the Poisson problem represents a significant contribution to the CPU time

• Dimension of the Poisson matrix: $N_{DOF} \times N_{DOF}$

• A POD basis $(\Psi_i)$ can be used to describe the pressure field:

$$P = P_{avg} + \sum_{i=1}^{N_{POD}} b_i \Psi_i$$
Poisson problem approximated by POD

Find the “best” solution of the Poisson prob. in the space of the POD basis

\[ \Delta \hat{\phi} = \rho \nabla \cdot u^* \]

Introduction of the POD expansion in the “correction” variable \( \hat{\phi} \):

\[ \hat{\phi} = (P^{n+1} - P^n) \Delta t = \left( P_{avg} + \sum_{i=1}^{N_{POD}} a_i \Phi_i - P^n \right) \Delta t \]

\[ R = \Delta \hat{\phi} - \rho \nabla \cdot u^* \]

\[ f = \sum_{i=1}^{N_{points}} R^2 \]

Norm-2 of the residuals

\[ \frac{\partial f}{\partial b_i} = 0 \quad 1 \leq i \leq N_{POD} \rightarrow \text{Linear system of dimension } N_{POD} \]
Cylinder at Re=100 with snapshots at Re=100

Full CFD vs Hybrid CFD-POD (5 modes)
Cylinder at $Re=100$ with snapshots at $Re=100$

Full CFD vs Hybrid CFD-POD (10 modes)
Cylinder at Re=100 with snapshots at Re=100
Full CFD vs Hybrid CFD-POD (20 modes)
Cylinder at Re=125 with snapshots at Re=100, 150, 200

Full CFD vs Hybrid CFD-POD (40 modes)
Dynamic POD update

• The POD basis could not contain enough information to solve properly the Poisson problem
  • \( \nabla \cdot \mathbf{u}^n \) will increase in time

• When the divergence is larger than a threshold, call a Krylov solver:
  • Krylov solver initialised with POD solution
  • Divergence of velocity is set to zero
  • The new pressure field is used to enrich the basis: it is orthonormalised w.r.t. the existing modes and then it is added to the basis
Cylinder at $\text{Re}=125$ with snapshots at $\text{Re}=100, 150, 200$

Full CFD vs Hybrid CFD-POD (40 modes) + automatic POD update

- At each call of the Krylov solver there is a jump in the forces
- 45 new modes are added to the database
- The new modes are mainly taken from the first period
- 45 calls to Krylov solver in 750 time steps of the first period
Car shape optimisation example

- **Objective function**: overall drag coefficient
- **Design parameters** which control the shape of the car by means of free form deformation

Function evaluations are done by three different tools:
- High fidelity tool: OpenFoam with Spalart-Allmaras RANS
- Hybrid CFD-POD simulations based on domain decomposition
- Low fidelity tool: Kriging interpolation
Geometry parametrisation

Free form deformation

Given a 3D object embedded into a grid of \((K+1)\times(L+1)\times(M+1)\) control nodes, the deformation of its generic point \(x_0\) is defined as a tensorial Bézier parametrisation:

\[
x(t_1, t_2, t_3) = x_0 + \sum_{k=0}^{K} \sum_{l=0}^{L} \sum_{m=0}^{M} B^K_k(t_1) B^L_l(t_2) B^M_m(t_3) p_{klm}
\]

where \(B^J_J(t) = \binom{J}{j} t^j (1 - t)^{J-j}\) are Bernstein polynomials and \(p_{klm}\) is a generic control point.

- Efficient to compute (embarrassingly parallel)
- Well controlled deformation over the entire grid/sub-grid
- Suitable for big/small deformations

\(\text{time(mesh morphing)} \ll \text{time(mesh generation)}\)
Efficient Global Optimisation (EGO)

EGO is a global optimization technique based on response surface surrogates. The implementation of this algorithm provided by the DAKOTA package is used.

The general algorithm behind the method is the following:

1. **Build an initial Gaussian Process (GP) model** of the objective function, based on a sample of high fidelity simulations (i.e. CFD simulations + hybrid ROM-CFD simulations)

2. **Find the point maximizing the Expected Improvement Function (EIF)**
   The EIF is a function of the expected values and variances predicted by the GP model (exploitation + exploration), and it is defined as the expectation that any point in the search space will provide an improvement on the best solution. → *if the maximum EIF is sufficiently small, stop*

3. **Evaluate the objective function at the new point** (i.e. hybrid ROM-CFD simulation)

5. **Update the GP model using this new point**

7. **Go to 2**
Hybrid CFD-POD based on domain decomposition

Low cost function evaluations called by the optimisation algorithm

Domain decomposition:
- Grey domain: ROM
- Red domain: hybrid ROM-CFD simulation

Original CFD domain: 93388 cells
Hybrid ROM-CFD domain: 12542 cells
Optimisation results

Initial configuration
Point (x=0, z=0)
Cd = 0.0152989

Best configuration after optimisation
Point (x=-0.102, z=-0.299)
Cd = 0.0147753
“true” Cd = 0.0147027

Expected improvement (drag reduction)
(based on hybrid ROM-CFD) → 3.42%
Real improvement (drag reduction)
(based on CFD) → 3.89%

Error on output → 0.49%
Cost of a CFD simulation: 1600 s
Cost of a hybrid ROM-CFD simulation: 220 s
Cost of surrogate model: negligible

(1) EGO with hybrid ROM-CFD
   5 CFD simulations (POD basis computation)
   30 hybrid ROM-CFD simulations
   Total optimization cost: 14600 s

(2) EGO with CFD
   35 CFD simulations
   Total optimization cost: 56000 s

→ save 74%
Conclusions

• Hybrid CFD-POD simulations can be efficiently used as low cost prediction tools for industrial flows

• The hybrid approach based on domain decomposition can be easily implemented: it only requires a projection of the CFD solution on the POD basis

• The projection used in the domain decomposition approach is equivalent to minimise the distance between the CFD solution and the POD reconstruction: it is possible to enforce a constraint in the minimisation process

• The solution of the Poisson problem for incompressible NS solvers can be accelerated by POD but further work is required to improve the robustness of the method
Thank you for your attention

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