Modal representation for reduced order models

Angelo Iollo

Université Bordeaux I
Thierry Colin
Damiano Lombardi
Olivier Saut

Jean Paloussière

Michel Bergmann
Marcelo Buffoni
Edoardo Lombardi
Jessie Weller
Discrete instantaneous velocity expanded in terms of empirical eigenmodes:

\[ u(x, t) = \overline{u}(x) + \sum_{n=1}^{N_r} a_n(t) \phi_n(x) \]

where \( \overline{u}(x) \) is a reference velocity field.

Eigenmodes \( \phi_n(x) \) are found by proper orthogonal decomposition (POD) using the "snapshots method" of Sirovich (1987).

Limited number of POD modes, \( N_r \), is used in the representation of velocity fields (snapshots) → they are the modes giving the main contribution to the flow energy.

Galerkin projection of the Navier-Stokes equations over the retained POD modes leading to the low-order model:

\[ \dot{a}_r(t) = A_r + C_{k_r}a_k(t) - B_{k_s r}a_k(t)a_s(t) \]
\[ a_r(0) = (u(x, 0) - \overline{u}(x), \phi_r) \]

Coefficient \( B_{k_s r} \) derives directly from the Galerkin projection of the non-linear terms in the Navier-Stokes equations
Tumor growth modeling

- PDE models: **they are all parametric models**

- Parameters take into account microscopic and mesoscopic scales phenomena **that we do not model directly**

- As consequence, parameters do not have a biological meaning and can not be measured; they **need to be identified**.
**Identification:**

\[ \partial_t Y(x; t) = f(Y, P, \pi) \]

The model describes the evolution: non-observables and parameters to be determined!

\[ \text{Im}_i = \text{Im}(x; t_i) \]

The data: in general, medical images

\[ E_i = \text{Im}_i - Y(x; t_i) \]

We want to minimize the error between the simulated history and measurements
The model

\[ Y = P + Q \]

\[ \gamma = \frac{1}{1 + \tanh(R(C - C_{hyp}))} \]

- Porosity
- Diffusivity
- Hypoxia function
- Mechanical closure
- Nutrient equation
- "Mitosis equation"
- "Saturation model"
- Dead cells density
- Proliferating cells density

\[ \frac{\partial P}{\partial t} + \nabla \cdot (vP) = (2\gamma - 1)P \]

\[ -\nabla \cdot (k\nabla) = -\gamma P \]

\[ \alpha P + \nabla \cdot (vQ) = (1 - \gamma)P \]

\[ k = k_0 + (k_2 - k_1)(P + Q) \]

\[ D = D_{\text{max}} - K(P + Q) \]
Inverse problems:

1) **Reduced approach**: compute a database of solutions, extract “important” structures and minimize residuals

Compute a database, varying both $P$, $\pi$

Extract coherent structures by means of POD

Inject informations in the model:
1) Equations are satisfied
2) The model fits at best the data

Offline stage: you do it once

$$\partial_t Y = f(Y, P, \pi); \quad (\pi_j, P_r) = \arg\min_{\tilde{P}, \tilde{\pi}} \left\{ \sum_i \| f(Im_i, \tilde{P}, \tilde{\pi}) - \partial_t Y \|^2 \right\}$$
Inverse problems:

- The POD expansions are substituted into the equations written for the observable $Y$

\[
\dot{Y} + a_i^v \nabla \cdot (Y \phi_i^v) = a_i^{\gamma P} \phi_j^{(\gamma P)}
\]

\[
a_i^v \nabla \cdot (\phi_i^v) = a_i^{\gamma P} \phi_j^{\gamma P}
\]

\[
k(Y) a_i^v \nabla \wedge \phi_i^v = \nabla k(Y) \wedge a_i^v \phi_i^v
\]

\[
ad_i^C \phi_i^C - a_i^C \nabla \cdot (K(Y) \nabla \phi_i^C) = -\alpha a_i^P a_i^C \phi_i^C \phi_i^{\gamma P} - \lambda a_i^C \phi_i^C
\]

\[
2a_i^{\gamma P} \phi_i^{\gamma P} = 1 + \tanh(R(a_i^C \phi_i^C - C_{hyp}))
\]

- Unknowns:
  - $k_2/k_1, D_{max}, K, \alpha, \lambda, C_{hyp}$
  - $a_i^P, a_i^C, a_i^v, a_i^{\gamma P}$

- Parameters
- Expansion Coefficients: functions of time only
Inverse problems:

- In the equation for the observable the time derivative $dY/dt$ is unknown.

- To solve the problem the time derivative is approximated by interpolation.

- Several type of interpolation have been tested:
  - Linear: $Y = tA + (1 - t)B$
  - Exponential: $\dot{Y} \approx A exp\{\zeta t\} + B exp\{-\zeta t\} = f(\zeta)$
  - Logistic: $Y \approx AG(\omega, \sigma) + BG(-\omega, -\sigma)$
    $G(\omega, \sigma) = \frac{\omega e^{\omega t}}{\omega - \sigma e^{\omega t}}$
Inverse problems:

- Solution of the non-linear system written at the time $t$, when $Y$ is observed: minimization of the residual

$$
\left( a_i^{(i)}(t_0), \pi_j \right) = \arg\min \{ F \} = \arg\min \left\{ \sum_l R_l^2 \right\}
$$

- Residual is minimized using a Newton solver (Levenberg-Marquardt).

- Condition on the variable $P$ are imposed via a penalisation technique.

- Reaction-Diffusion equation for the oxygen is critical since the variable is not observed, but entirely regularized.
2) **Sensitivity**: minimization of the error with respect to parameters and non-observed quantities.

\[
E_T^2 = \sum_i E_i^2 = \sum_i \int_\Omega (I m_i - Y(x; t_i))^2 \, dx
\]

\[
\frac{\partial E_T^2}{\partial \pi_j} = 2 \sum_i \int_\Omega E_i \frac{\partial Y}{\partial \pi_j} \, dx
\]

**Sensitivity**: quantifies changes in the solution for a small perturbation of the j-th parameter.
Slow growth nodule

Metastatic nodules in lungs: slow dynamics

- Given two, or three images, can we recover the following scans?
Computational set up:
- Finite Volume schemes on cartesian mesh;
  - WENO 5 scheme for transport;
  - RK2 scheme for time discretization;
- Level set methods;
- Resolution: 200 x 200, domain [0,8]x[0,8]
- Time: 2 min on one CPU

Control set:
- Parameters + Initial Condition for P
- P is supposed to be an external layer: $P_0 = A \exp(-\delta \varphi^2)$
Slow growth nodule

Tumor density distribution.  
Active part of the tumor  
Isocontours of nutrients
Slow growth nodule

Fig. 12. POD modes for the oxygen field, Case I: a) First mode, b) Third mode c) Fith mode.

Initially the proportion of proliferating cells is fixed to \( P_{\text{on the tumor}} = 1 \) on the tumor support, that is, at the beginning the tumor is totally proliferating. This value is of course not always realistic, but the results of the identification proved to be weakly
Slow growth nodule

Volume curve:

Distribution of radio-resistant cells:
Reduced model:

POD expansion:
• $N_p = 15$, $N_c = 5$, $N_v = 10$; $N_{gp} = 15$

Volume curve:

Comparison between sensitivity (blue) and ROM (black); at the beginning they have the same behavior
Slow growth nodule

Scan:  Simulation:  

Error is essentially a shape error:
Two nodules case
How far we can represent a PDE solution by POD?

1 - Problème base POD, $\Phi_n(x)$ : mauvaise représentation écoulements 3D turbulents

- Problèmes contrôle écoulements 3D turbulents
- Propriétés de turbulence érronées (spectre, etc)
Coherence by optimal mass transport

How to displace a certain amount of mass in such a way that a cost functional is minimized?

\[ X(\xi) = \arg \min \{ C(X(\xi)) \} \]

1. **Mathematical formulation**

- \( \rho_0(\xi) \quad \rho_1(x) \) are two density distributions such that:
  - \( \int_{\Omega_0} \rho_0(\xi) \, d\xi = \int_{\Omega_1} \rho_1(x) \, dx = 1 \) mass is conserved
  - \( \text{det} \left( \nabla \xi X \right) \rho_1(X(\xi)) = \rho_0(\xi) \) if and only if \( X \) is one-to-one

- Infinitely many \( X \) exists. Among them we look for the optimal one:
  - \( \int_{\Omega_0} \rho_0(\xi) \| X^*(\xi) - \xi \|^2 \, d\xi \leq \int_{\Omega_0} \rho_0(\xi) \| X(\xi) - \xi \|^2 \, d\xi \)
Mathematical formulation

- **Theorem:** the solution of this problem exists unique, and has this form:
  \[ X^*(\xi) = \nabla_\xi \Psi(\xi) \]
  where the potential is a convex function (a.e.)

- This problem can be formulated as the minimum of an action:
  \[ J = \frac{1}{2} \int_0^T \int_{\mathbb{R}^d} \rho(x, \tau) \|U(x, \tau)\|^2 \, dx d\tau \]

- Enforcing mass conservation \( \partial_\tau \rho + \nabla_x \cdot (\rho U) = 0 \) by means of a lagrangian multiplier lead to:
  \[ \partial_\tau \psi + U \cdot \nabla \psi = \frac{\|U\|^2}{2} \quad U = \nabla \psi \]
Introducing a space-time Lagrange multiplier subject to equations (11), (19), (20).

Optimal mass transfer problem is equivalent to the minimization of the constrained minimum of the density function
under mass conservation constraint, by a sequential quadrature step iterations are needed, the error in mass conservation level. Therefore if the initial map is far from the minimum an approach. This method, however, leads to an optimization problem of the size on may be large.

In [20] it is shown that the optimal mass transfer problem is equivalent to the minimization with respect to the velocity distribution of the size of the resolution in one space and a time-dependent solution of the size of the resolution in one space for the potential

\[ \partial_t \rho + \nabla_x \cdot (\rho U) = 0 \] mass conservation

\[ \partial_\tau \psi + \frac{\nabla \psi}{2} = 0 \] H-J equation for the potential

\[ U = \nabla \psi \] flow is irrotational

**Key Properties**

- \[ \rho(x, 0) = \rho_0(x) \] Time conditions concern the density only.
- \[ \rho(x, T) = \rho_1(x) \]
- \[ + \text{B.C. for the potential} \]

- This is a pressureless (infinitely compressible) Euler flow
- Since \[ \partial_\tau U + (U \cdot \nabla)U = 0 \] information is propagated along rays
- Difficult to integrate: two time conditions for the density and no initial neither final condition for the potential
A Lagrangian scheme:

**Information moves along straight lines:** Transport PDE has a simple lagrangian solution.

A set of particles is defined such that:

\[ \int_{\Omega_r} \sigma(\xi) \, d\xi = 1 \]

**Lagrangian mass formulation:** mass conservation is strongly imposed:

\[ \frac{d}{d\tau} \int_{\Omega(\tau)} \rho \, dx = 0 \quad \rho(x, \tau) \approx \sum_{j=1}^{N_p} c_j(t) \sigma(x - X_j(\tau)) \]

\[ \frac{d}{d\tau} \int_{\Omega(\tau)} \rho \, dx = \sum_{j=1}^{N_p} \partial_{\tau} c_j(\tau) \quad \partial_{\tau} c_j(\tau) = 0 \]

**The solution of the H-J equation, once the initial condition is set, reduces to:**

\[ X_j(\tau) = \xi_j + V(\xi_j) \tau \]
A Lagrangian scheme:

- Initial and final conditions have to be imposed: the problem reduces to an algebraic optimization problem.

Initial condition:

\[ c_j = \arg \left\{ \min_{d_j} \sum_{k=1}^{N_g} \left[ \rho(x_k, 0) - \sum_{j=1}^{N_p} d_j \sigma(x_k - X_j(0)) \right]^2 \right\} \]

Final Condition:

\[ \psi_l = \arg \left\{ \min_{\psi_l} \mathcal{E}(\psi_l) \right\} = \arg \left\{ \min_{\psi_l} \sum_{k=1}^{N_g} \left[ \rho(x_k, T) - \sum_{j=1}^{N_p} c_j \sigma(x_k - \xi_j - \sum_{l=1}^{N_d} D_{jl} \psi_l T) \right]^2 \right\} \]

- A regularization is added in order to speed up convergence:

\[ \mathcal{E}_p(\psi_l) = \mathcal{E}(\psi_l) + \beta \sum_j c_j \frac{\left\| \sum_{l=1}^{N_d} D_{jl} \psi_l \right\|^2}{2} \]
3D Tests:

- **3D example:** mapping a uniform cube into the MRI of a human head
The objective is to approximate the metric space defined by Wasserstein distance by an euclidean space.

A set of snapshots:
\[
\int_{\Omega \subset \mathbb{R}^d} \rho_i \, dx = 1, \quad \forall i = 0, \ldots, N_s
\]

Wasserstein distance:
\[
W^2(\rho_i, \rho_j) = \inf_{\tilde{X}} \left\{ \int_{\Omega} \rho_i(\xi)|\tilde{X}(\xi) - \xi|^2 \, d\xi \right\},
\]
\[
\rho_i(\xi) = \rho_j(\tilde{X}(\xi)) \det(\nabla_\xi \tilde{X}).
\]

Distance Matrix:
\[
D_{ij} = W^2(\rho_i, \rho_j)
\]

An euclidean space is sought, such that the distances between its elements recover at best the matrix distance.

Embedding Matrix:
\[
B = -\frac{1}{2}JDJ \quad \text{where:} \quad J = I - \frac{1}{N_s}11^T
\]

B is PSD <=> D is a distance matrix. Then B=X X'.

X is the matrix whose rows are the coordinates of the euclidean space elements.
The dynamics is governed by an Hamiltonian system: three different trajectories are represented, varying the offset

- a) meeting;
- b) mating;
- c) weak interaction.
Ideal Vortex Scattering

- Spectra of the embedding matrix in the three cases:
  - a) Two eigenvalues are significant;
  - b) Two eigenvalues are significant;
  - c) Only one eigenvalue is significant.
Eigenvectors in the three cases:

- a) Phase plot for meeting;
- b) Phase plot for mating;
- c) First eigenvector for the weak interaction.
Vortex Shedding

- The same analysis is performed in the case of a vortex shedding, for an incompressible flow around a confined circular cylinder.

- Kinetic Energy is studied, which is almost satisfying normalization condition; 10 snapshots are taken on half a period of vortex shedding.

- Spectrum of the embedding matrix and phase portrait of the first two eigenvectors.
Vortex Shedding

The following test was performed:

- a) Three snapshots are taken: at t=0, t=T/4, t=T/2, where T is the period
- b) The distribution that corresponds to the center of the circle is computed
- c) The flow is recovered mapping the center distribution in the snapshots:

\[ \Phi(t) = \cos(2\pi t)\phi_1 + \sin(2\pi t)\phi_2 \]

Center Distribution: it is not a physical configuration!
Vortex Shedding

- Contours of first and second mappings:

- Representation of the kinetic energy of the flow:

  - Best (t=0)
  - Worst (t=T/8)
Euclidean embedding

- Korteweg-de Vries equation with diffusion

\[ \partial_t u + \mu \partial_x^3 u + 2u \partial_x u - \nu \partial_x^2 u = 0 \]

- Standard POD modal approximation

- Transport approximation + POD modal approximation of the residual
Euclidean embedding
Euclidean embedding

\[ n \]

\[ \frac{e}{e(1)} \]
Euclidean embedding

3 modes
Euclidean embedding

5 modes

Solution
POD
WME
Euclidean embedding

9 modes