Modal representation for reduced order models

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- Discrete instantaneous velocity expanded in terms of empirical eingenmodes:

$$\boldsymbol{u}(\boldsymbol{x},t) = \overline{\boldsymbol{u}}(\boldsymbol{x}) + \sum_{n=1}^{N_r} a_n(t)\boldsymbol{\phi}_n(\boldsymbol{x})$$

  where $\overline{\boldsymbol{u}}(\boldsymbol{x})$ 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) $\longrightarrow$ 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:

$$\dot{a}_r(t) = A_r + C_{kr}a_k(t) - B_{ksr}a_k(t)a_s(t)$$
$$a_r(0) = (\boldsymbol{u}(\boldsymbol{x},0) - \overline{\boldsymbol{u}}(\boldsymbol{x}), \boldsymbol{\phi}_r)$$

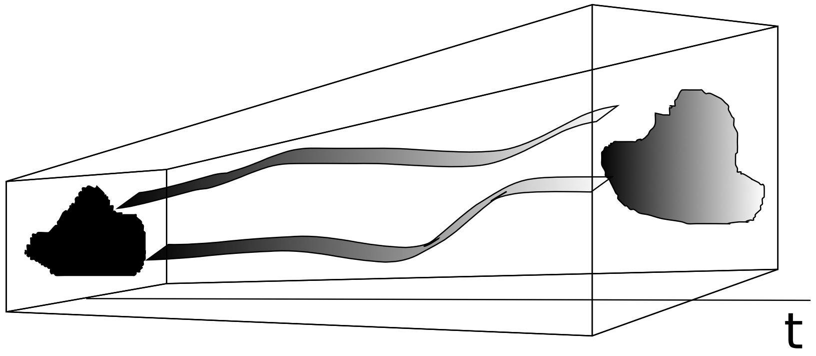
- Coefficient B_{ksr} derives directly from the Galerkin projection of the non-linear terms in the Navier-Stokes equations

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.

Inverse problems

- <u>Identification</u>:



$$\partial_t Y(x;t) = f(Y, P, \pi)$$ → The <u>model</u> describes the evolution: non-observables and parameters to be determined!

$$Im_i = Im(x; t_i)$$ → <u>The data</u>: in general, medical images

$$E_i = Im_i - Y(x; t_i)$$ → <u>We want to minimize the error beween the simulated history and measurements</u>

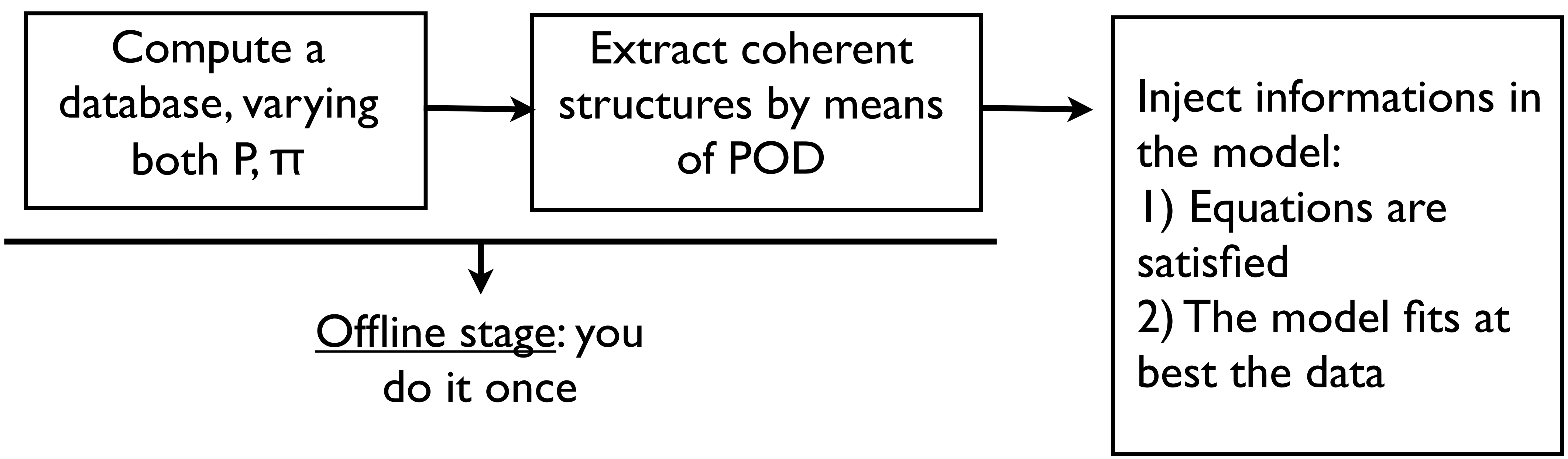
The model

$\dfrac{\partial P}{\partial t} + \nabla \cdot (\mathbf{v}P) = (2\gamma - 1)P$	$\longleftarrow$	Proliferating cells density
$\dfrac{\partial Q}{\partial t} + \nabla \cdot (\mathbf{v}Q) = (1 - \gamma)P$	$\longleftarrow$	Dead cells density
$\nabla \cdot (k\nabla\Pi) = -\gamma P$	$\longleftarrow$	Saturation, “mitosis equation”
$\mathbf{v} = -k\nabla\Pi$	$\longleftarrow$	Mechanical closure
$-\nabla \cdot (D\nabla C) = -\alpha PC - \lambda C$	$\longleftarrow$	Nutrient equation
$k = k_1 + (k_2 - k_1)(P + Q),$	$\longleftarrow$	Porosity
$D = D_{max} - K(P + Q)$	$\longleftarrow$	Diffusivity
$\gamma = \dfrac{1 + \tanh(R(C - C_{hyp}))}{2}$	$\longleftarrow$	Hypoxia function

Y= P+Q

Inverse problems:

1) <u>Reduced approach</u>: compute a database of solutions, extract "important" structures and minimize residuals



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

Inverse problems:

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

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

$$a_i^v \nabla \cdot (\phi_i^v) = a_j^{\gamma P} \phi_j^{\gamma P}$$

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

$$\dot{a}_i^C \phi_i^C - a_i^C \nabla \cdot (K(Y) \nabla \phi_i^C) = -\alpha a_i^p a_i^C \phi_i^C \phi_i^P - \lambda a_i^C \phi_i^C$$

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

- Unknowns:
  - $k_2/k_1, D_{max}, K, \alpha, \lambda, C_{hyp}$ ⟶ Parameters
  - $a_i^P, a_i^C, a_i^v, a_i^{\gamma P}$ ⟶ 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: $$\dot{Y} \approx Aexp\{\zeta t\} + Bexp\{-\zeta t\} = f(\zeta)$$
  - 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

$$\left(a_i^{(\cdot)}(t_0), \pi_j\right) = argmin\left\{F\right\} = argmin\left\{\sum_l R_l^2\right\}$$

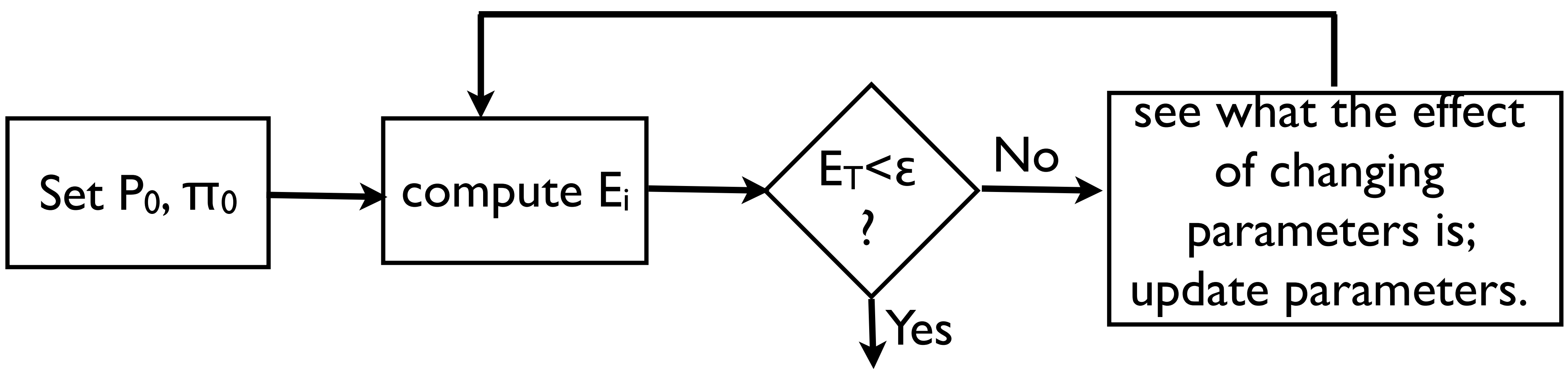
- Residual is minimized using a Newton solver (Levemberg-Marquardt).

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

- Reaction-Diffusion equation for the oxygen is critical since the variable is not observed, but entirely regularized.

Inverse problems:

2) Sensitivity: minimization of the error with respect to parameters and non-observed quantities.



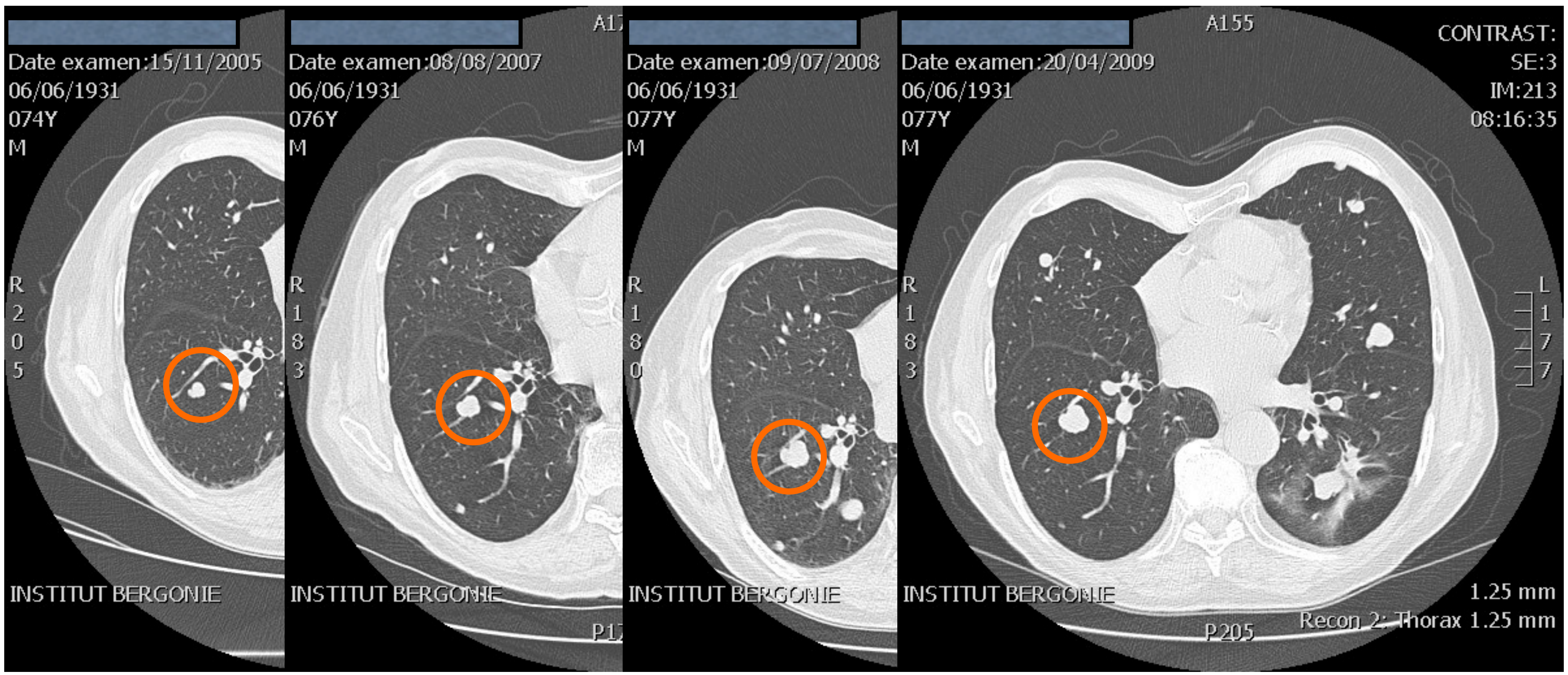
$$E_T^2 = \sum_i E_i^2 = \sum_i \int_\Omega (Im_i - Y(x;t_i))^2 \; dx$$

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

Sensitivity: quantifies changes in the solution for a small perturbation of the j-th parameter

Slow growth nodule

Metastatic nodules in lungs: slow dynamics



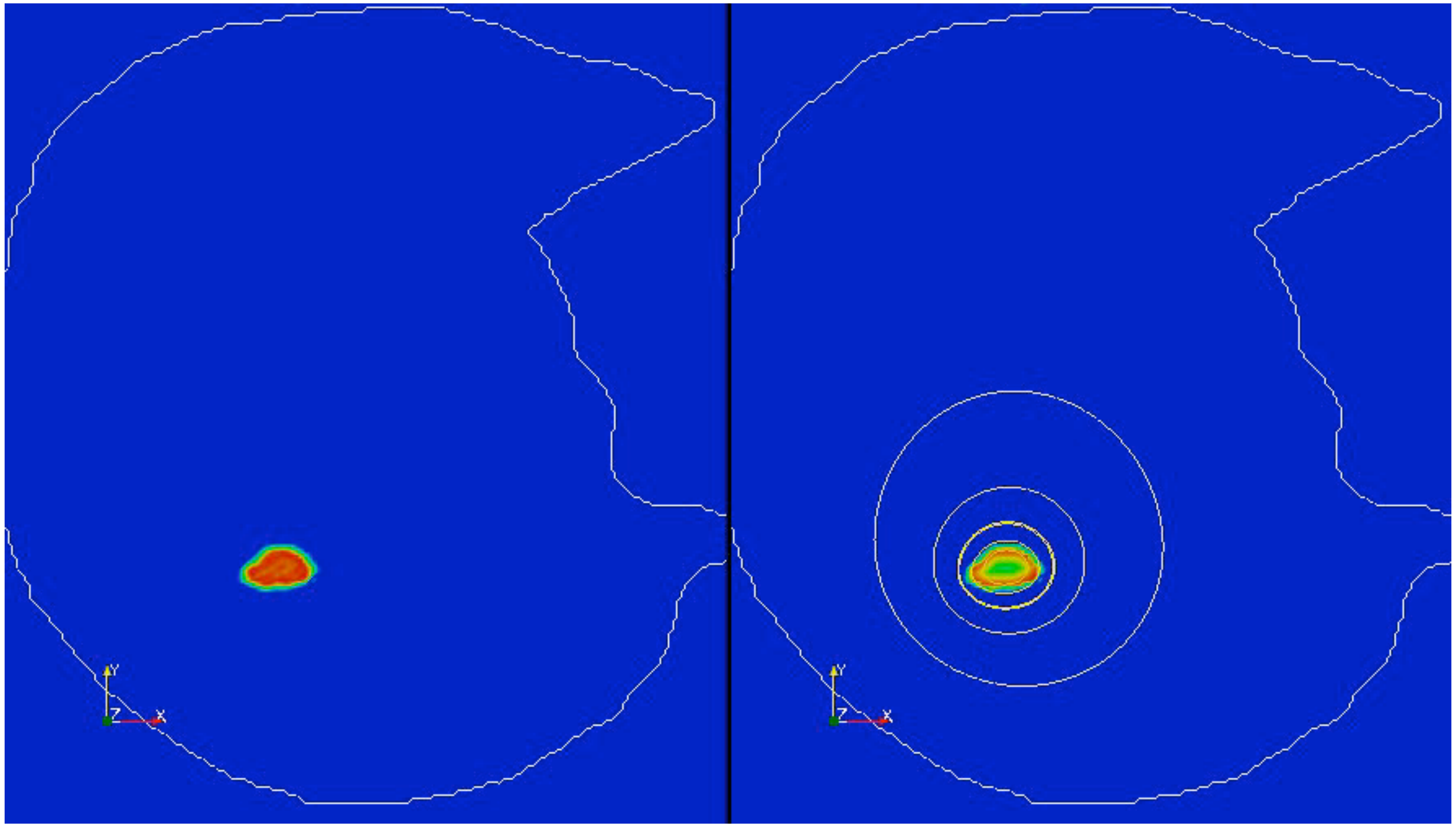
- Given two, or three images, can we recover the following scans?

Slow growth nodule

- 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

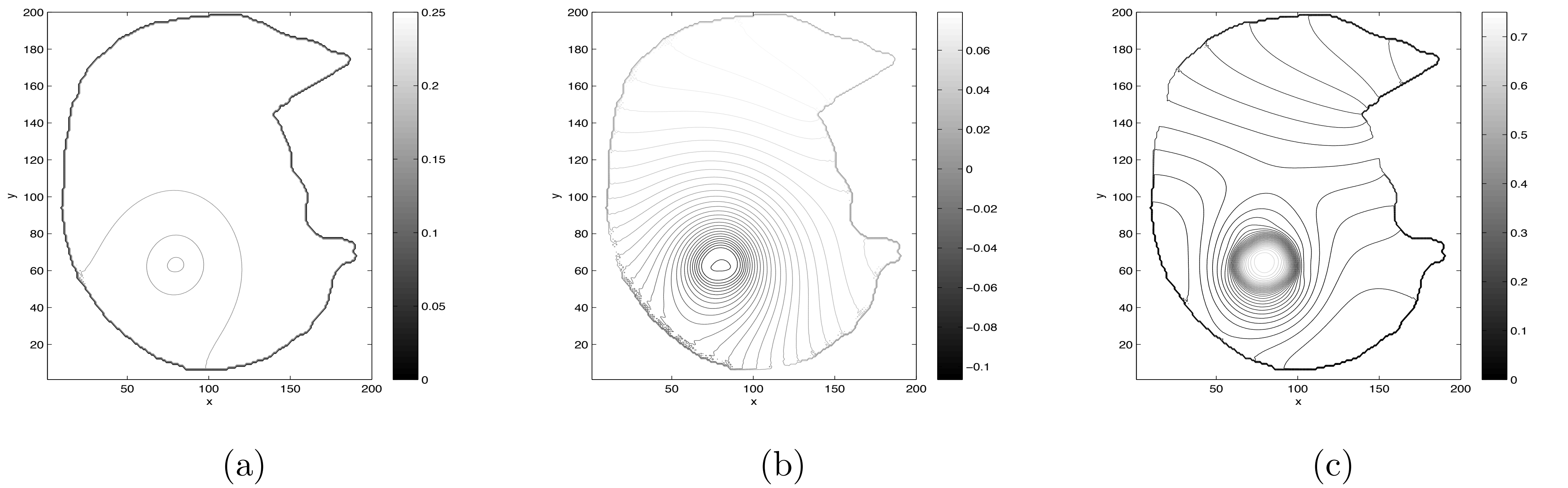
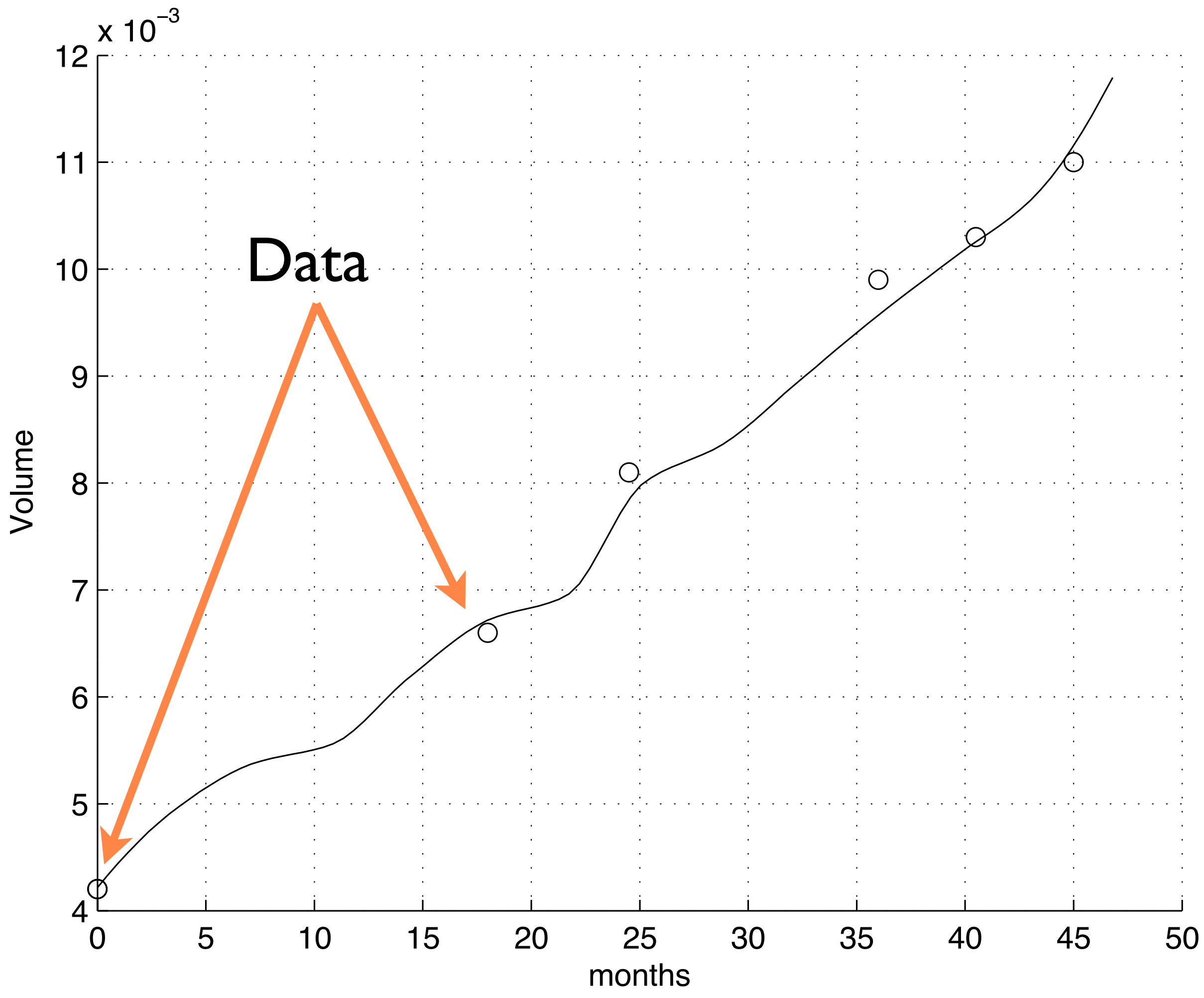


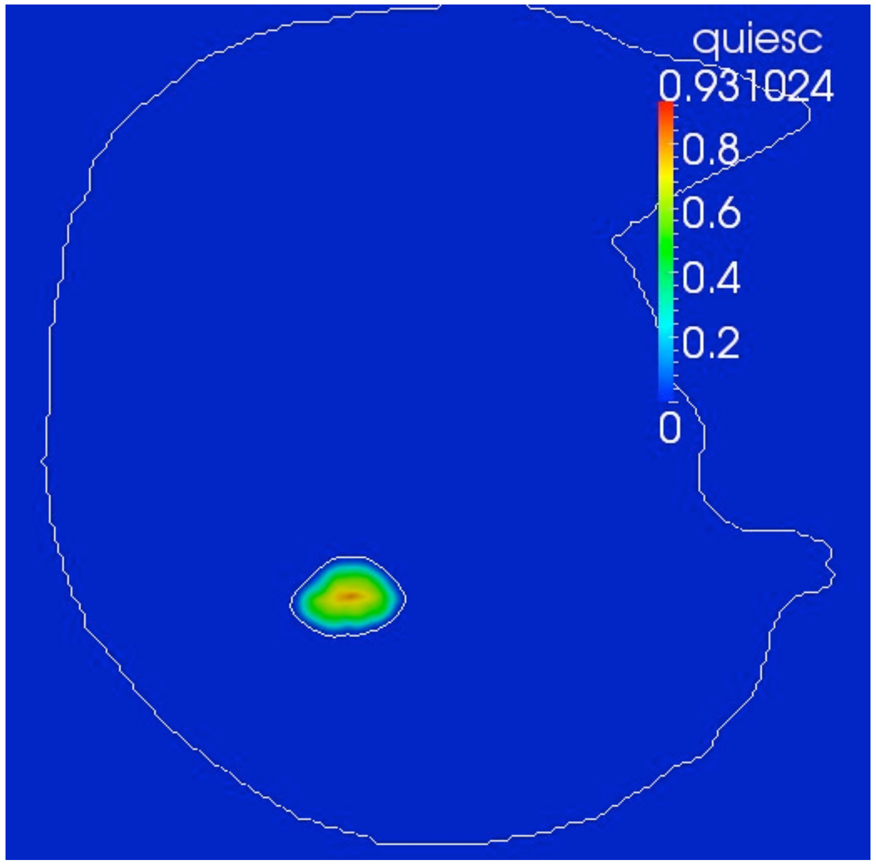
Fig. 12. POD modes for the oxygen field, Case I: a) First mode, b) Third mode c) Fith mode.

Slow growth nodule

Volume curve:



Distribution of radio-resistant cells:



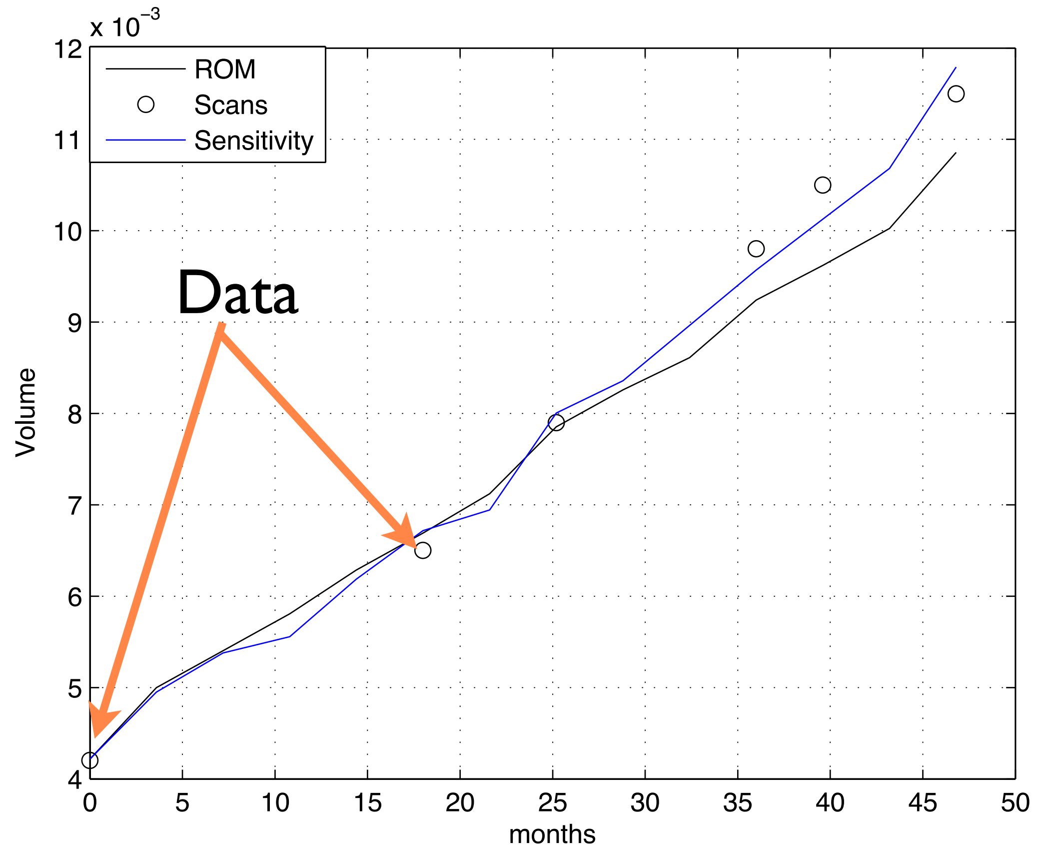
Slow growth nodule

- Reduced model:

POD expansion:

- Np = 15, Nc = 5, Nv = 10; Ngp = 15

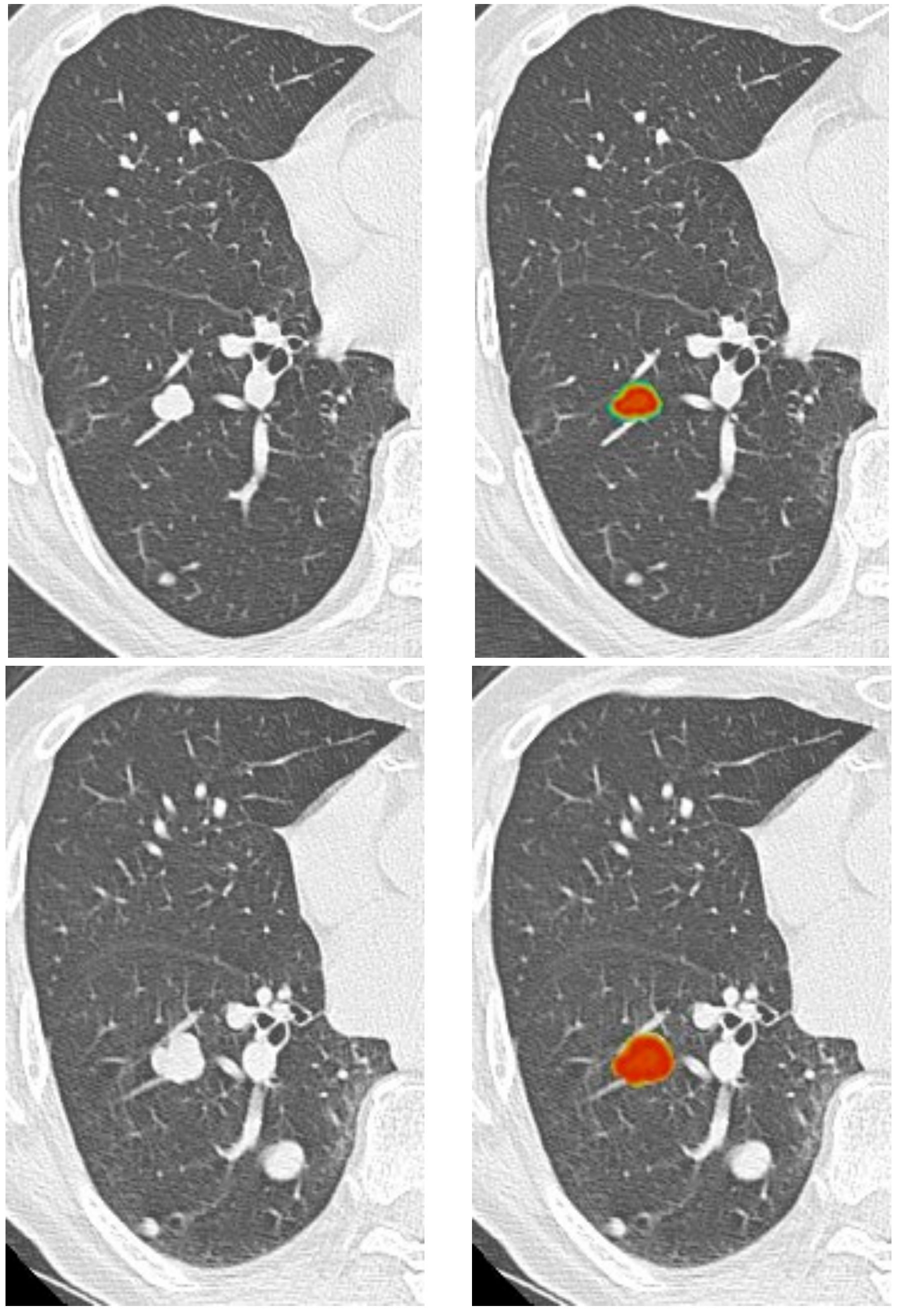
Volume curve:



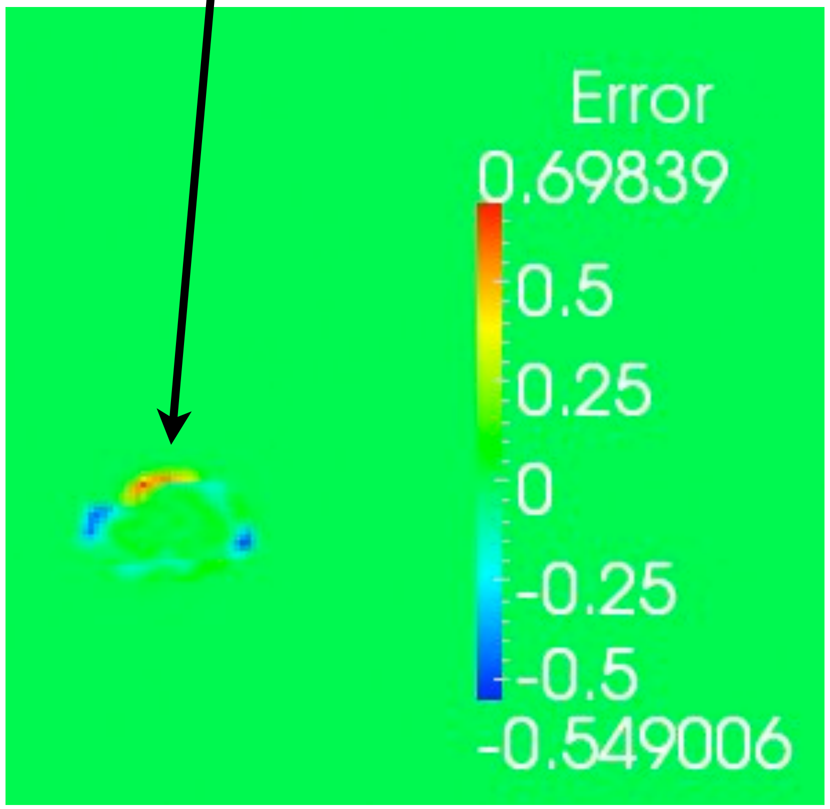
Comparison between sensitivity (blue) and ROM (black); at the beginning they have the same behavior

Slow growth nodule

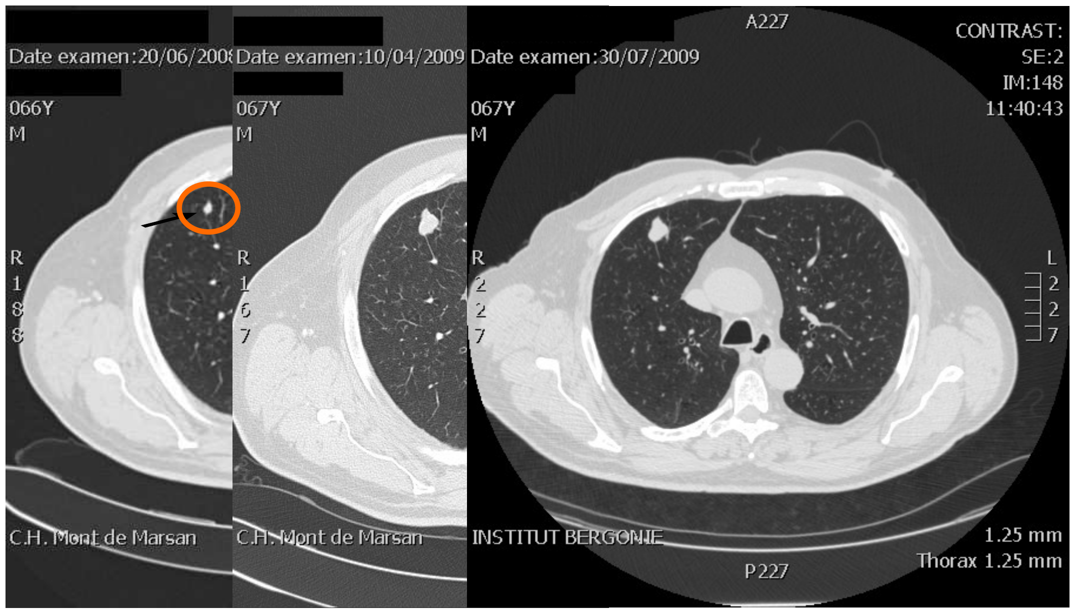
Scan: Simulation:

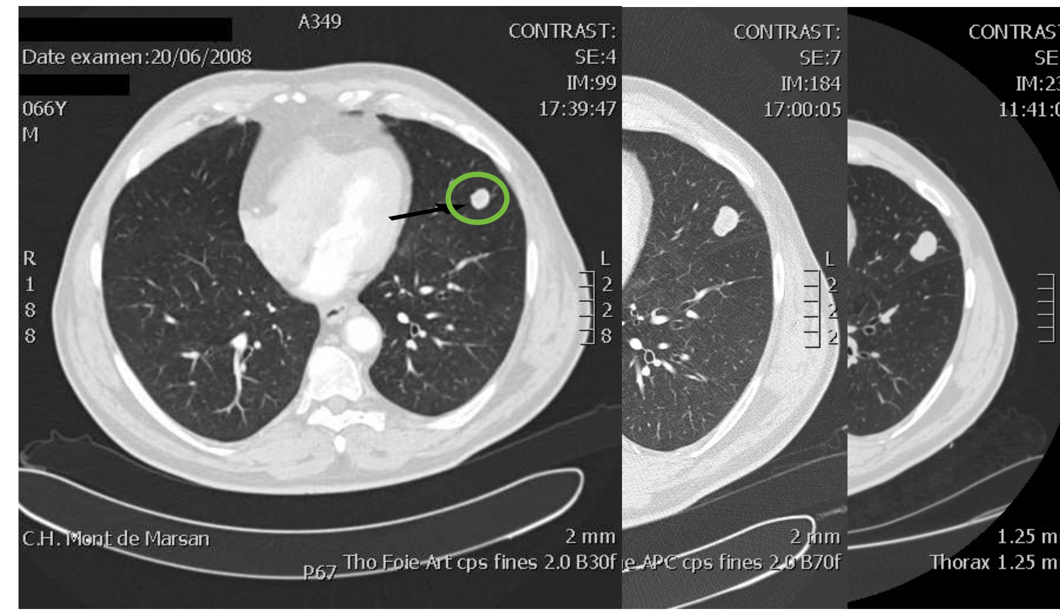


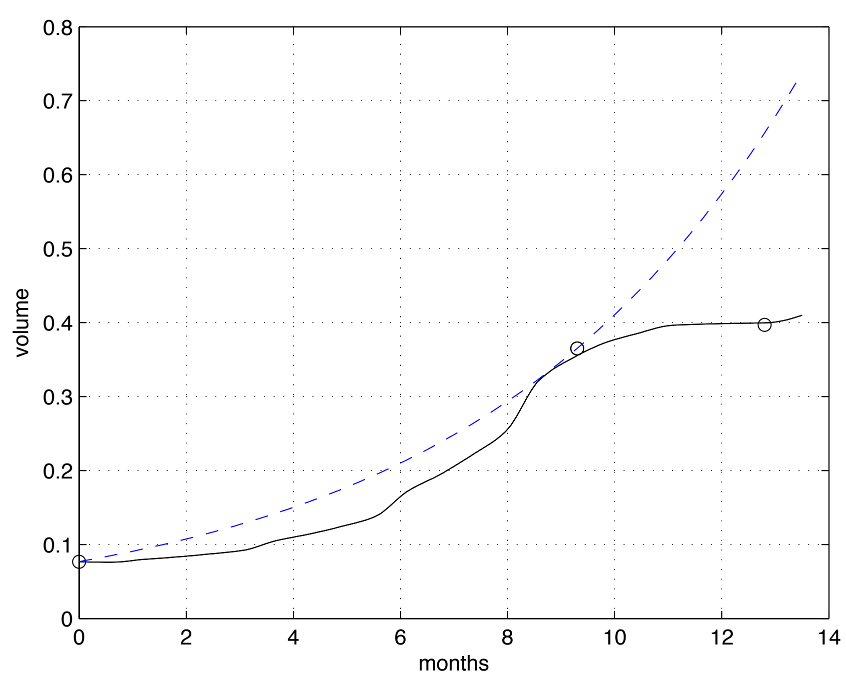
Error is essentially a shape error:

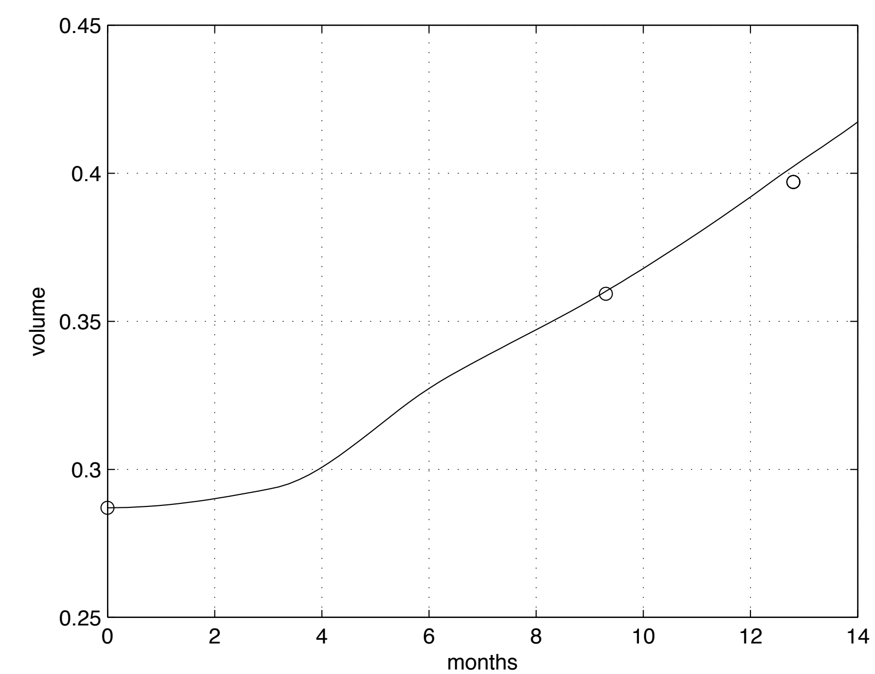


Two nodules case



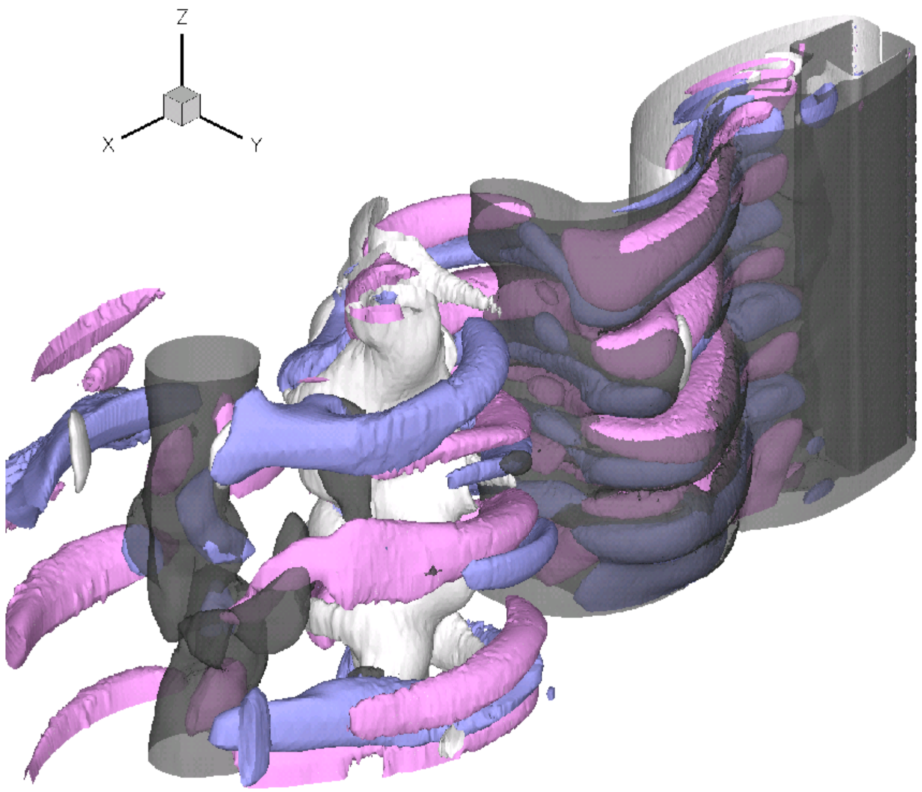


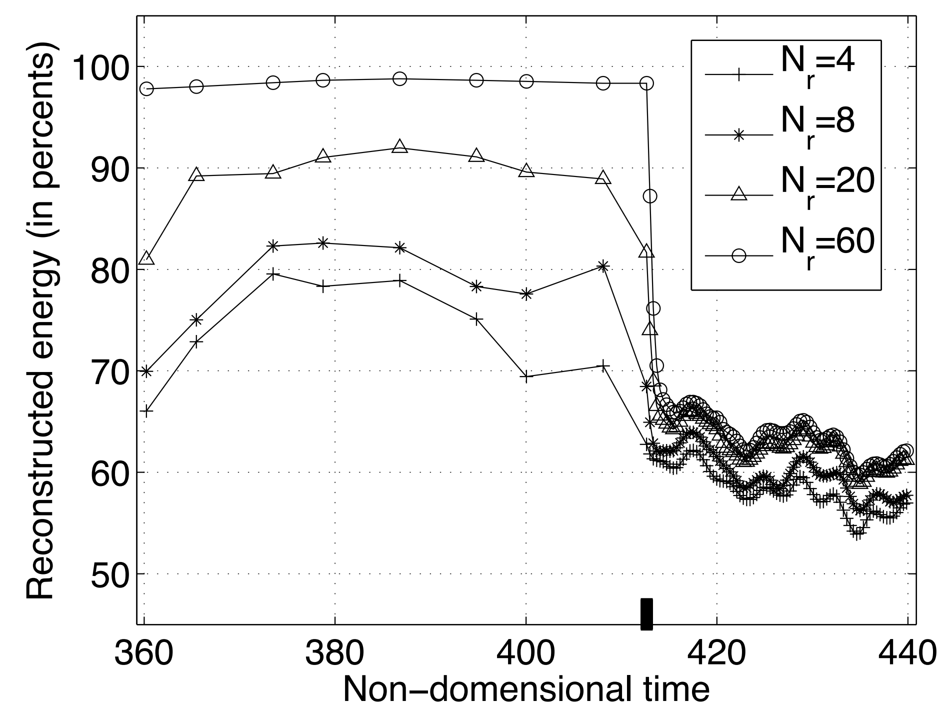




How far we can represent a PDE solution by POD ?

1 - Problème base POD, $\Phi_{\mathbf{n}}(\mathbf{x})$: mauvaise représentation écoulements 3D turbulents *hors base de données*

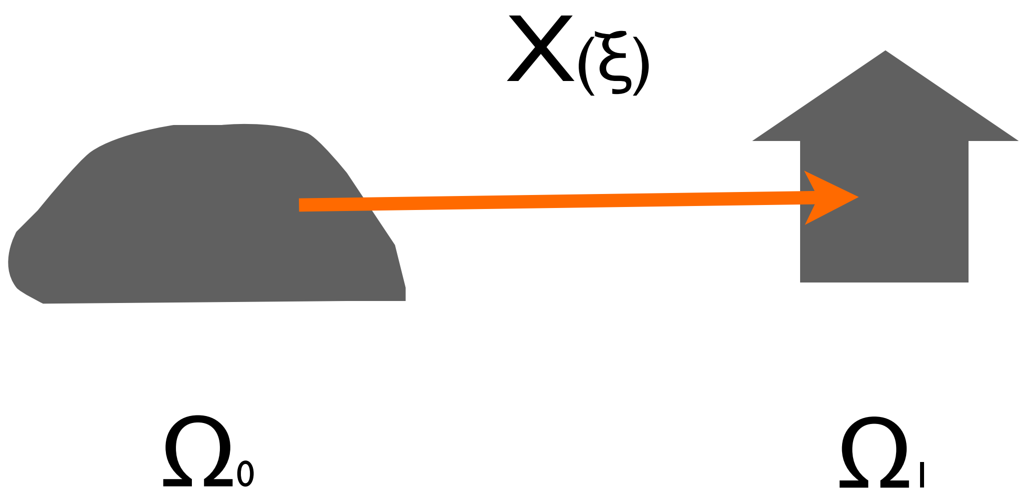




- Problèmes contrôle écoulements 3D turbulents
- Propriétés de turbulence érronées (spectre, *etc*)

Coherence by optimal mass transport

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



$$x_{(\xi)} = \arg\min\{C(X_{(\xi)})\}$$

* Histoire de l'Academie de Science de Paris: "Mémoire sur la théorie des déblais remblais"

Mathematical formulation

- $\rho_0(\xi)$ $\rho_1(x)$ 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
  - $det\,(\nabla_\xi X)\,\rho_1(X(\xi)) = \rho_0(\xi)$ 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:

  $$J = \frac{1}{2} \int_0^T \int_{R^d} \rho(x, \tau) \| U(x, \tau) \|^2 \ dx d\tau$$

- Enforcing mass conservation $\partial_t \rho + \nabla_x \cdot (\rho U) = 0$ by means of a lagrangian multiplier lead to:

  $$\partial_\tau \psi + U \cdot \nabla \psi = \frac{\|U\|^2}{2} \qquad U = \nabla \psi$$

Key Properties

- $\partial_t \rho + \nabla_x \cdot (\rho U) = 0$ mass conservation
- $\partial_\tau \psi + \frac{|\nabla \psi|^2}{2} = 0$ H-J equation for the potential
- $U = \nabla \psi$ flow is irrotational

time conditions:

- $\rho(x,0) = \rho_0(x)$
- $\rho(x,T) = \rho_1(x)$

Time conditions concerns the density only.

+ B.C. for the potential

- This is a presureless (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:
    - $$\frac{d}{d\tau}\int_{\Omega(\tau)} \rho\; dx\; = 0 \qquad \rho(x,\tau) \approx \sum_{j=1}^{N_p} c_j(t)\sigma(x - X_j(\tau))$$
    $$\frac{d}{d\tau}\int_{\Omega(\tau)} \rho\; dx = \sum_{j=1}^{N_p} \partial_\tau c_j(\tau) \qquad \partial_\tau c_j(\tau) = 0$$
  - 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:

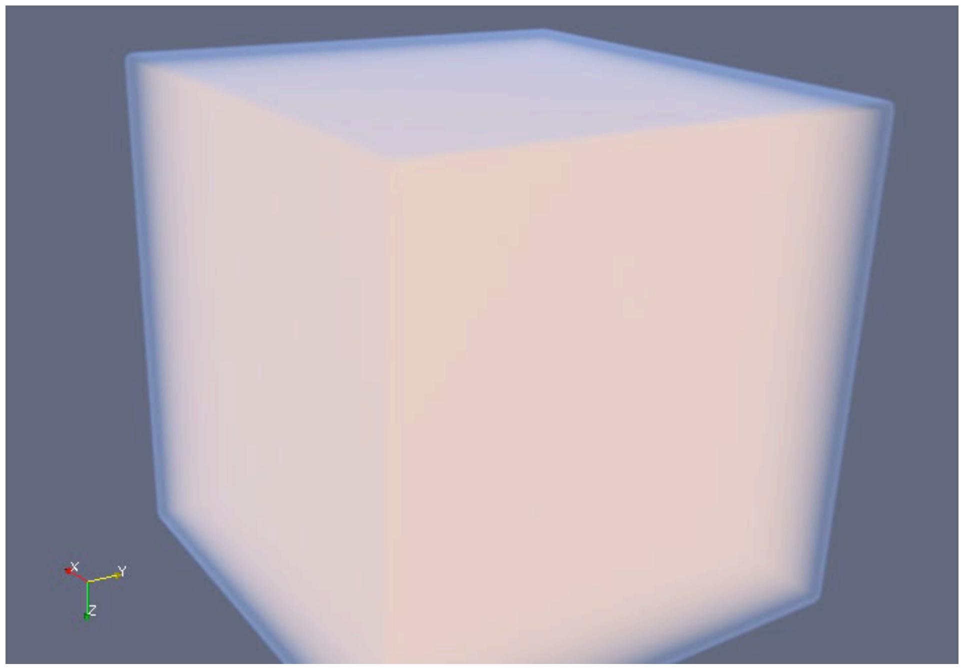
$$\psi_l = \arg\left\{\min_{\Psi_l} \mathcal{E}(\Psi_l)\right\} = \arg\left\{\min_{\Psi_l} \sum_{k=1}^{N_g}\left[\rho(x_k,T) - \sum_{j=1}^{N_p} c_j\ \sigma(x_k - \xi_j - \sum_{l=1}^{N_d} D_{jl}\Psi_l\ T)\right]^2\right\}$$

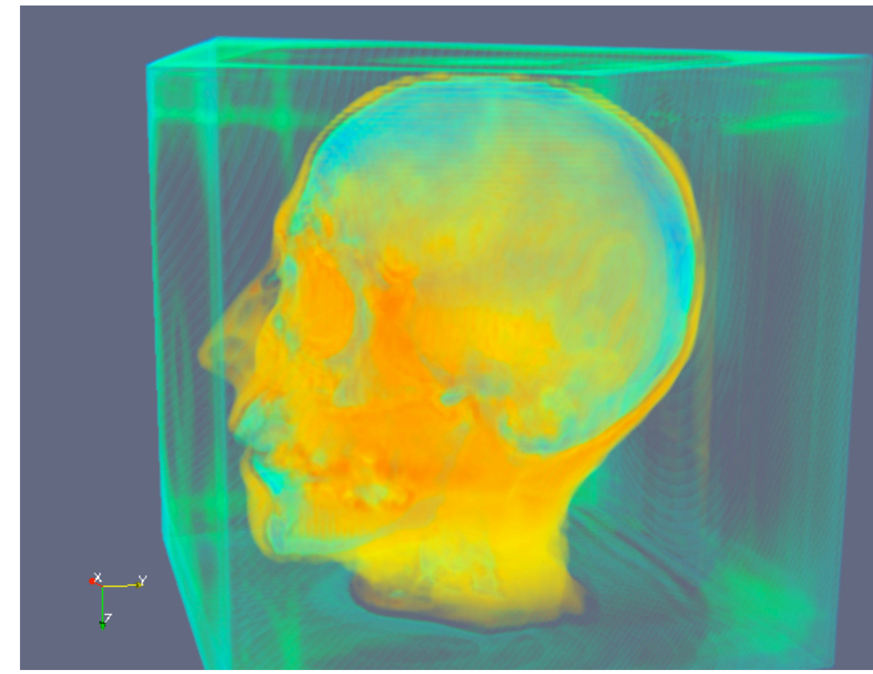
- A regularization is added in order to speed up convergence:

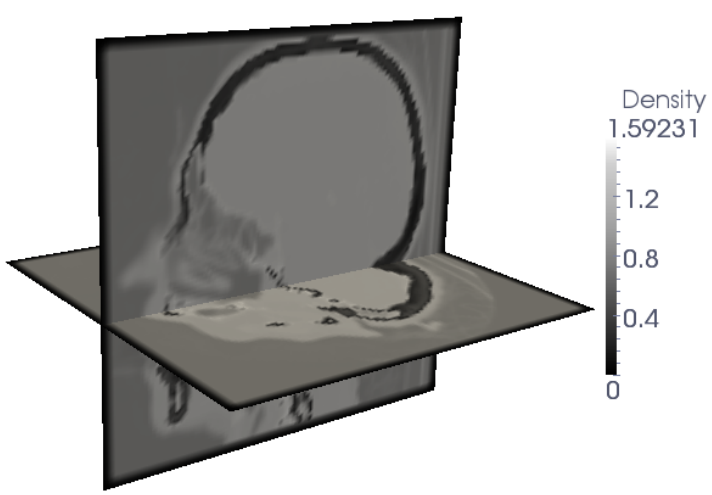
$$\mathcal{E}_p(\Psi_l) = \mathcal{E}(\Psi_l) + \beta\ \sum_{j}^{N_p} c_j \frac{\| \sum_{l=1}^{N_d} D_{jl}\Psi_l\|^2}{2}$$

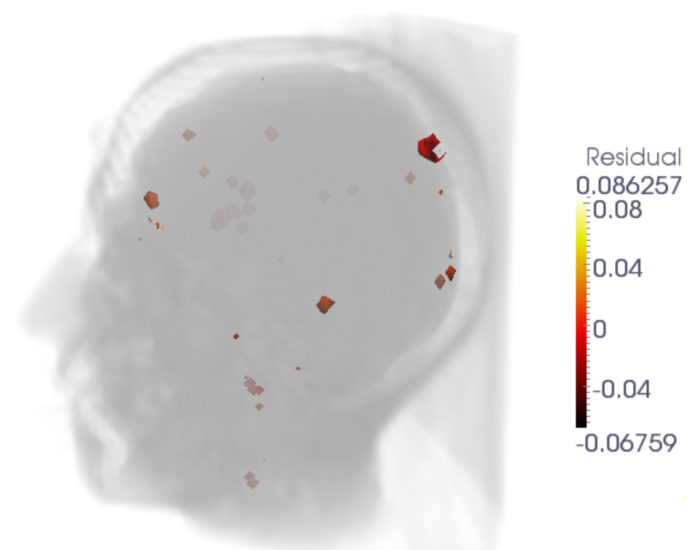
3D Tests:

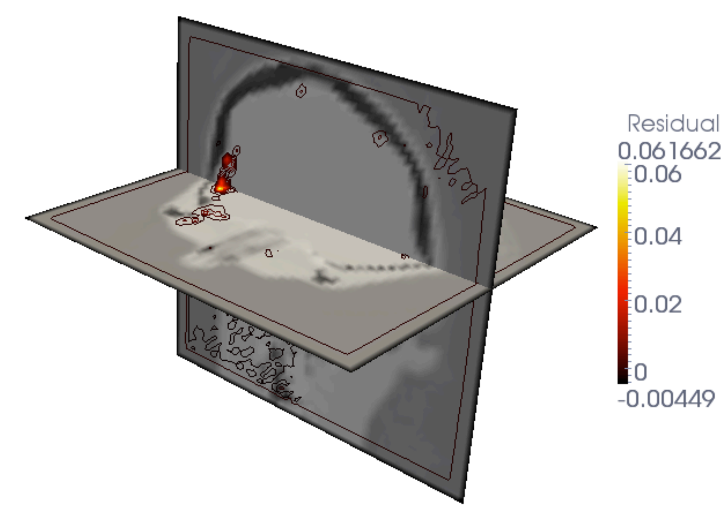
- 3D example: mapping a uniform cube into the MRI of a human head











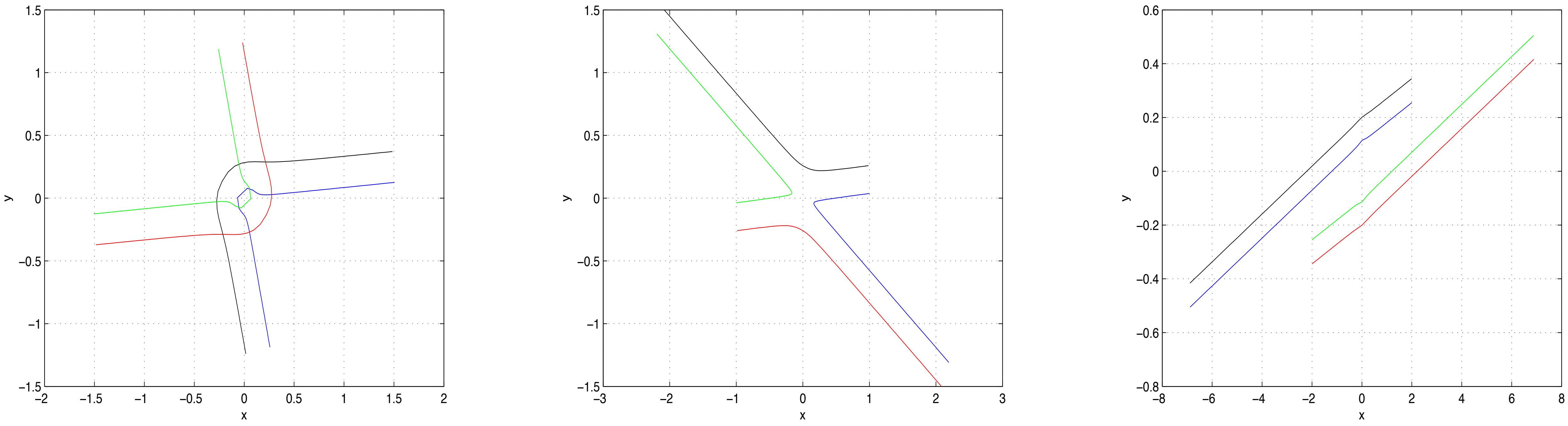
Euclidean embedding

- The objective is to approximate the metric space defined by Wasserstein distance by an euclidean space
  - A set of snapshots: $\int_{\Omega \subset R^d} \rho_i \, dx = 1, \quad \forall i = 0, ..., N_s$
  - Wasserstein distance: $\mathcal{W}^2(\rho_i, \rho_j) = \inf_{\tilde{X}} \left\{ \int_\Omega \rho_i(\xi) |\tilde{X}(\xi) - \xi|^2 \, d\xi \right\},$
    $\rho_i(\xi) = \rho_j(\tilde{X}(\xi)) \det(\nabla_\xi \tilde{X}).$
  - Distance Matrix: $\mathcal{D}_{ij} = \mathcal{W}^2(\rho_i, \rho_j)$

- An euclidean space is sought, such that the distances between its elements recover at best the matrix distance
  - Embedding Matrix: $B = -\frac{1}{2} J \mathcal{D} J$ where: $J = I - \frac{1}{N_s} \mathbb{1}\mathbb{1}^T$
  - 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

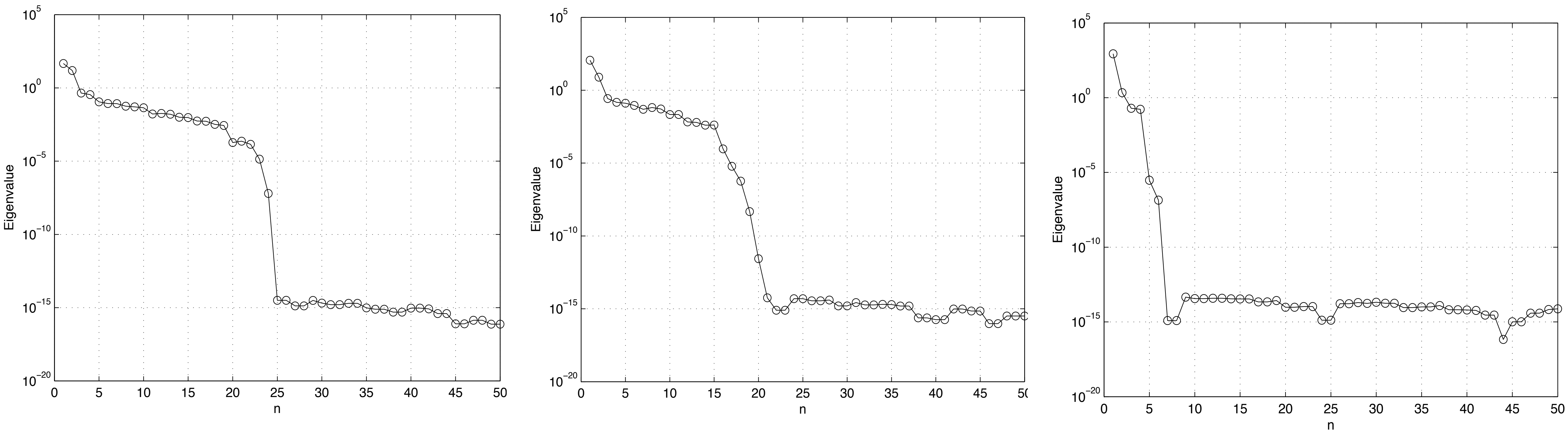
Ideal Vortex Scattering



(a) (b) (c)

- The dynamics is governed by an Hamiltonian system: three different trajectories are represented, varying the offset
  - a) meeting;
  - b) mating;
  - c) weak interaction.

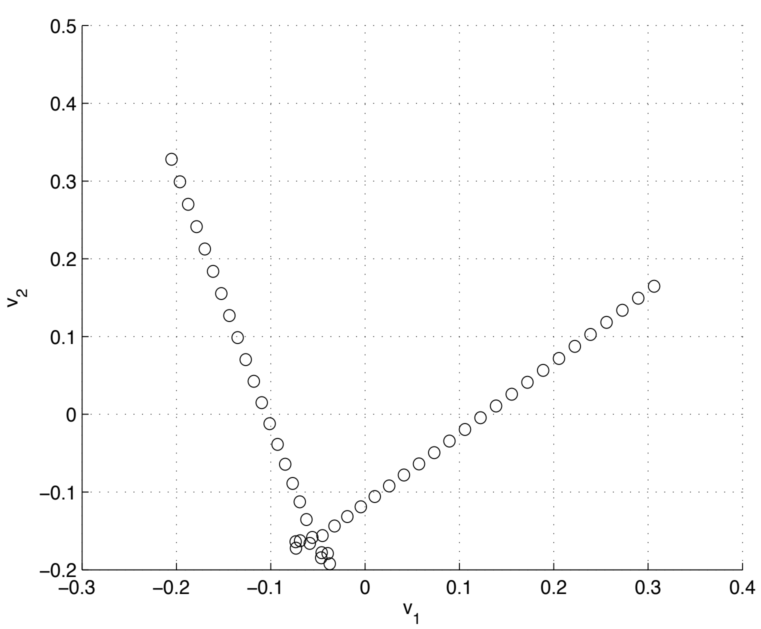
Ideal Vortex Scattering

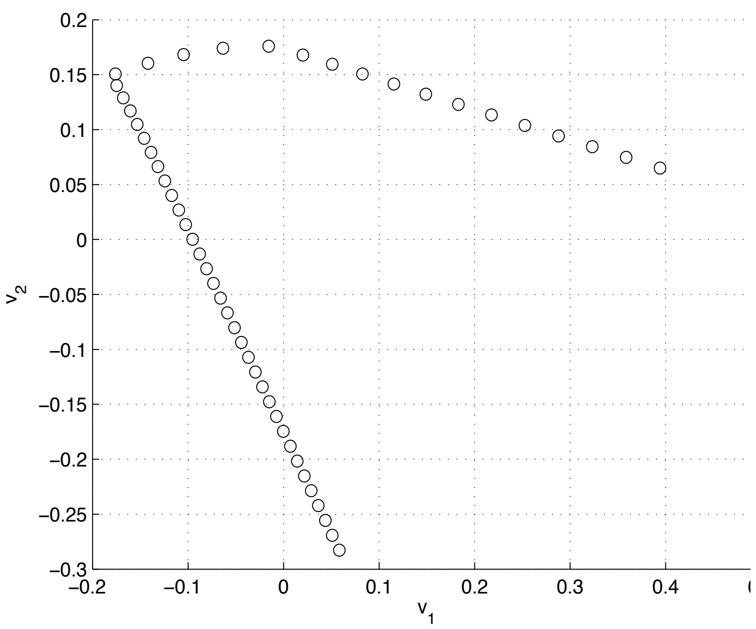


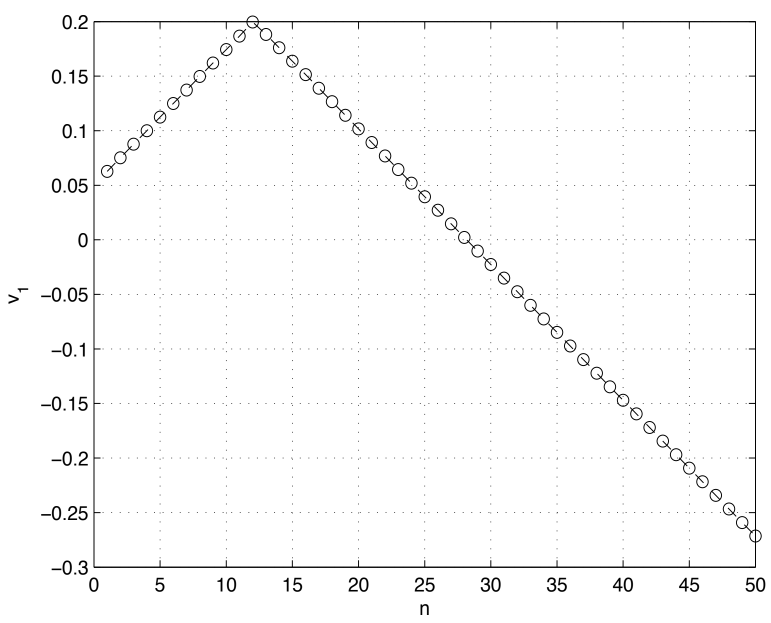
- Spectra of the embedding matrix in the three cases:
  - a) Two eigenvalues are significant;
  - b) Two eigenvalues are significant;
  - c) Only one eigenvalue is significant.

Ideal Vortex Scattering

- Eigenvectors in the three cases:





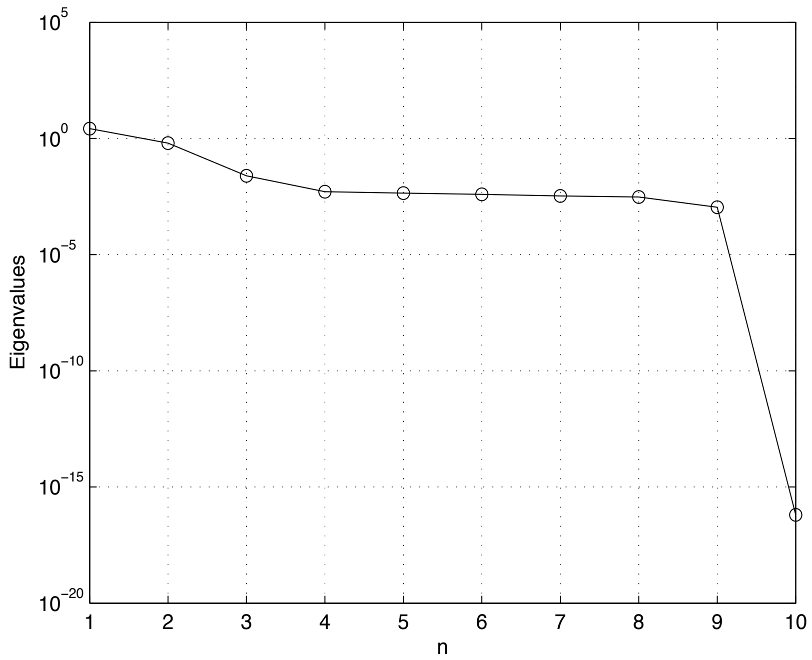


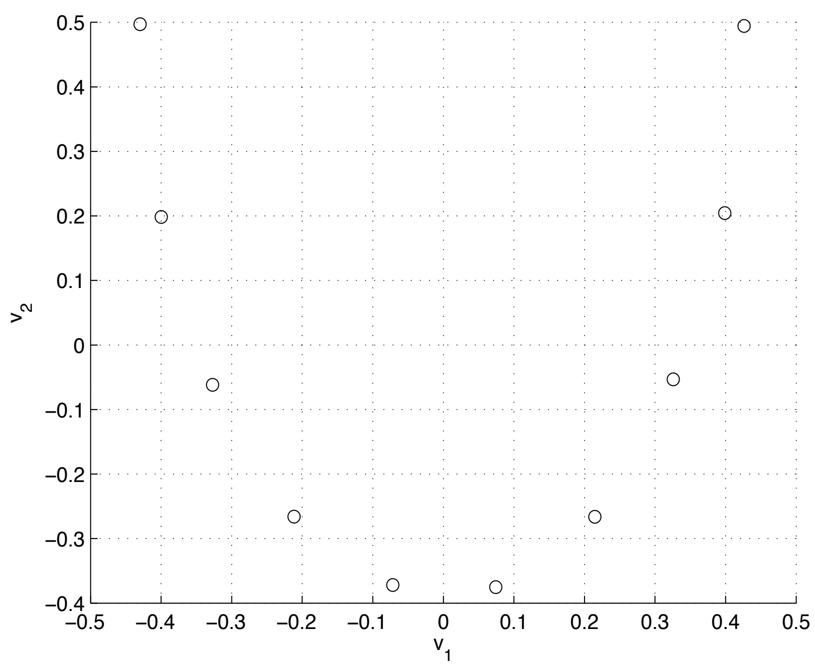
- a) Phase plot for meeting;
- b) Phase plot for mating;
- c) First eigenvector for the weak interaction.

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



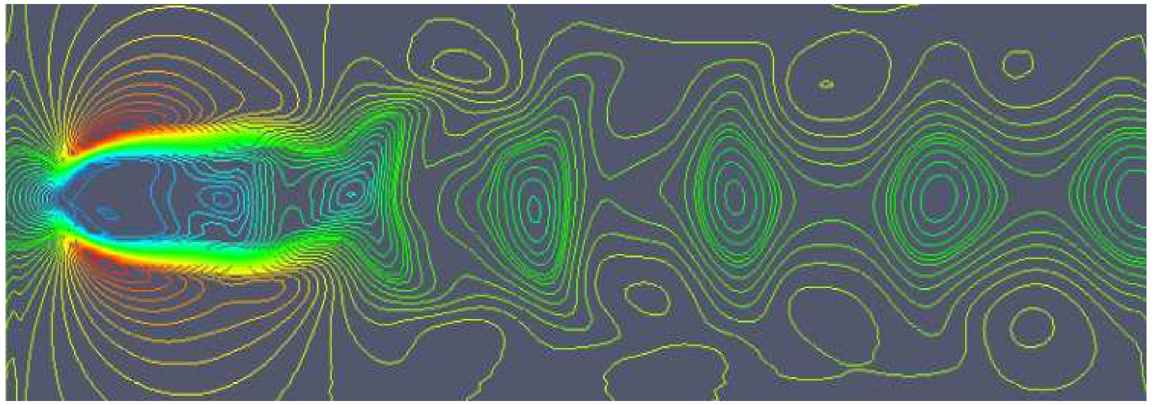


- Spectrum of the embedding matrix and phase portait of the first two eigenvectors

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 snapsnots:

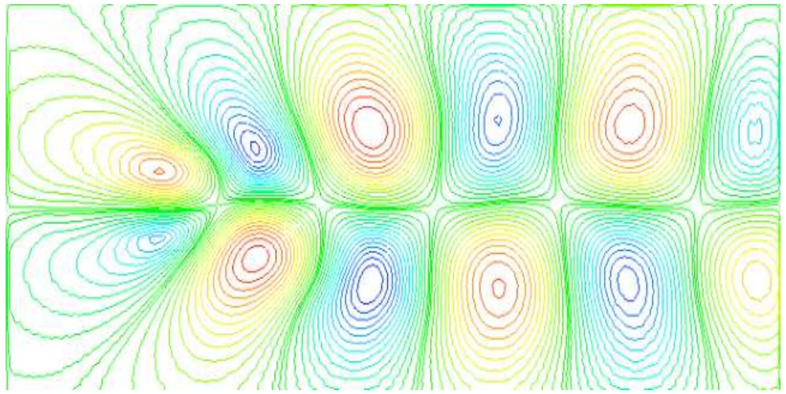
$$\Phi(t) = cos(2\pi t)\phi_1 + sin(2\pi t)\phi_2$$

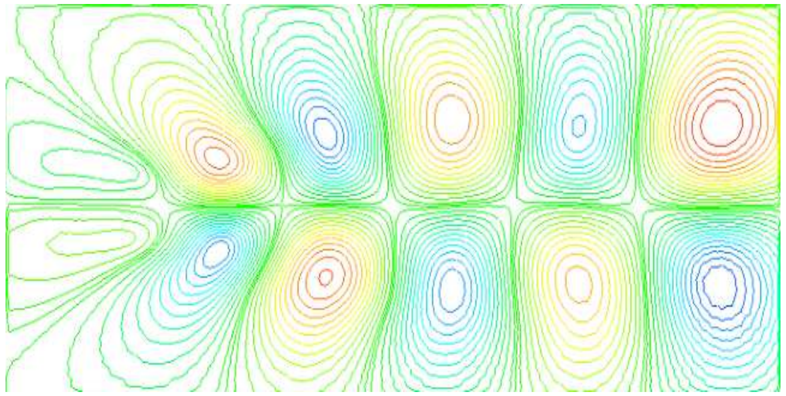


- Center Distribution: it is not a physical configuration!

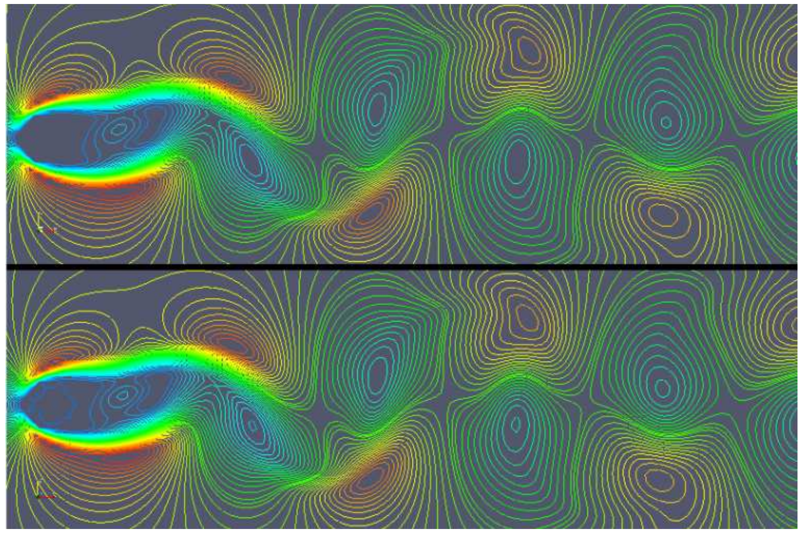
Vortex Shedding

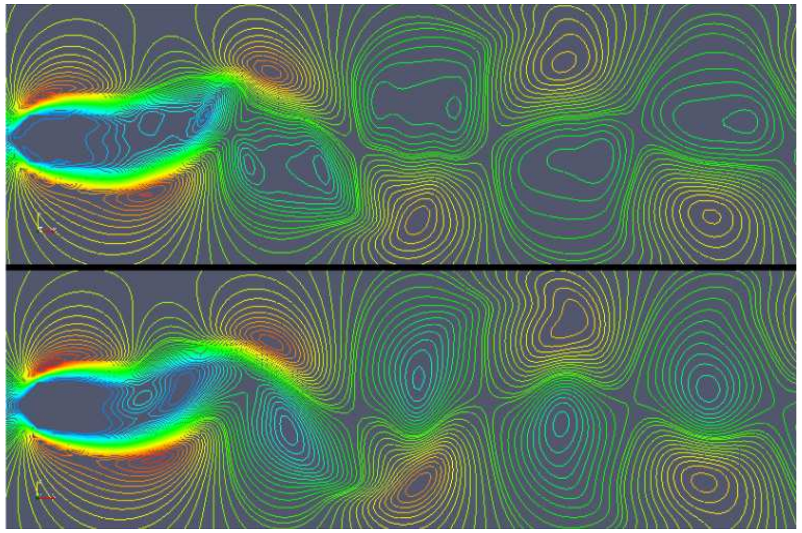
- Contours of first and second mappings:





- Representation of the kinetic energy of the flow:





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

Euclidean embedding

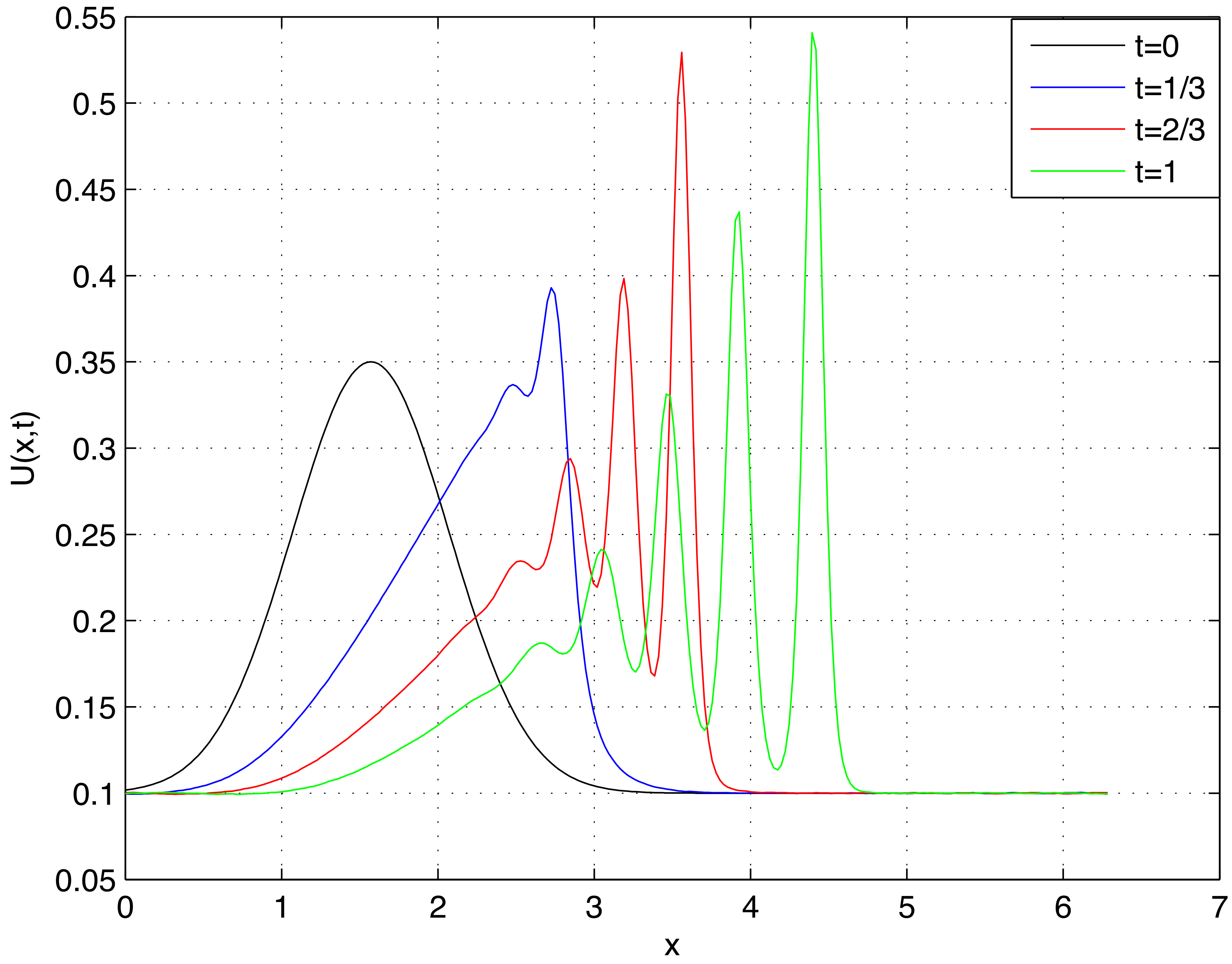
- Korteweg-de Vries equation with diffusion

  - $$\partial_t u + \mu \, \partial_x^3 u + 2 \, u \, \partial_x u - \nu \, \partial_x^2 u = 0$$

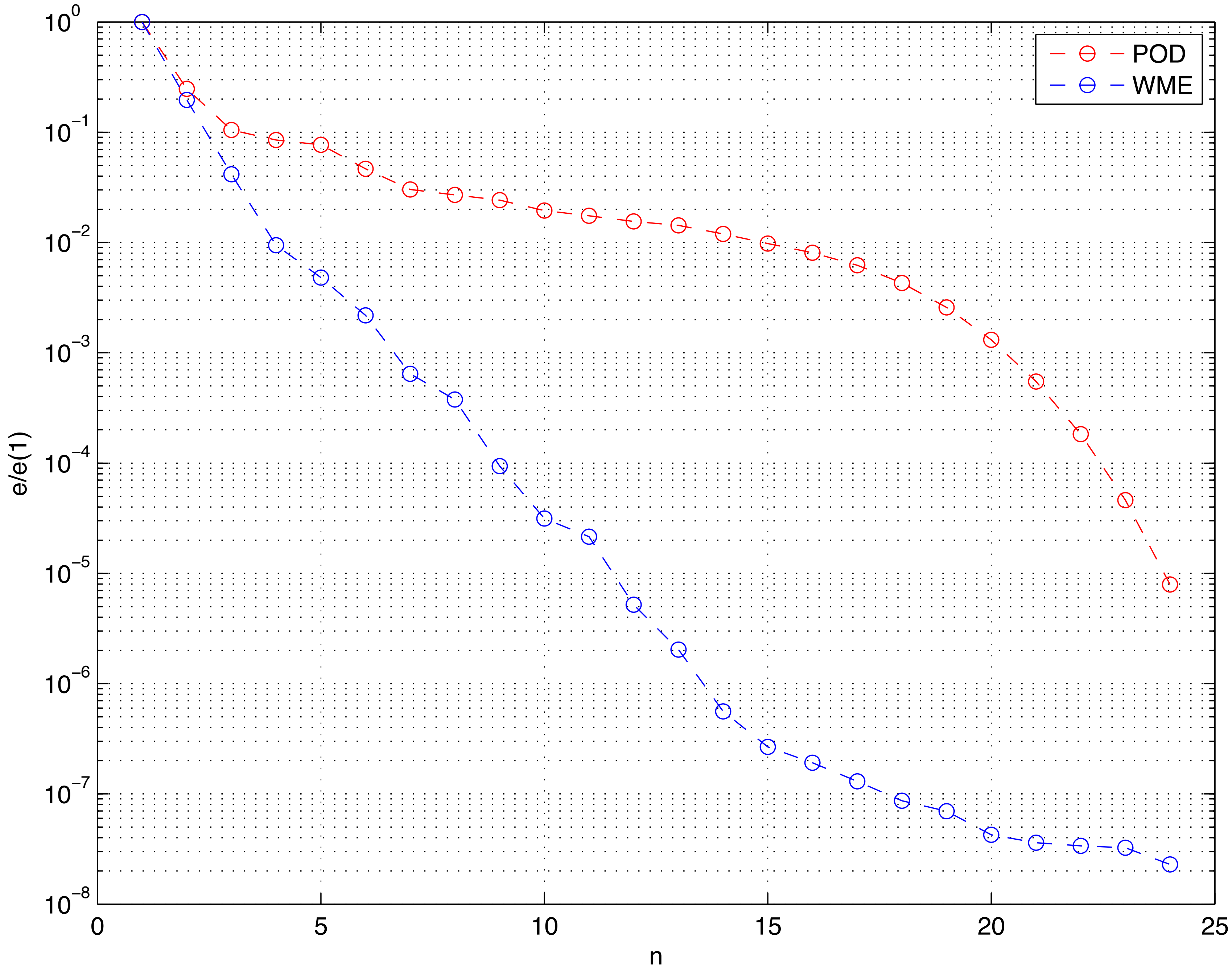
  - Standard POD modal approximation

  - Transport approximation + POD modal approximation of the residual

Euclidean embedding

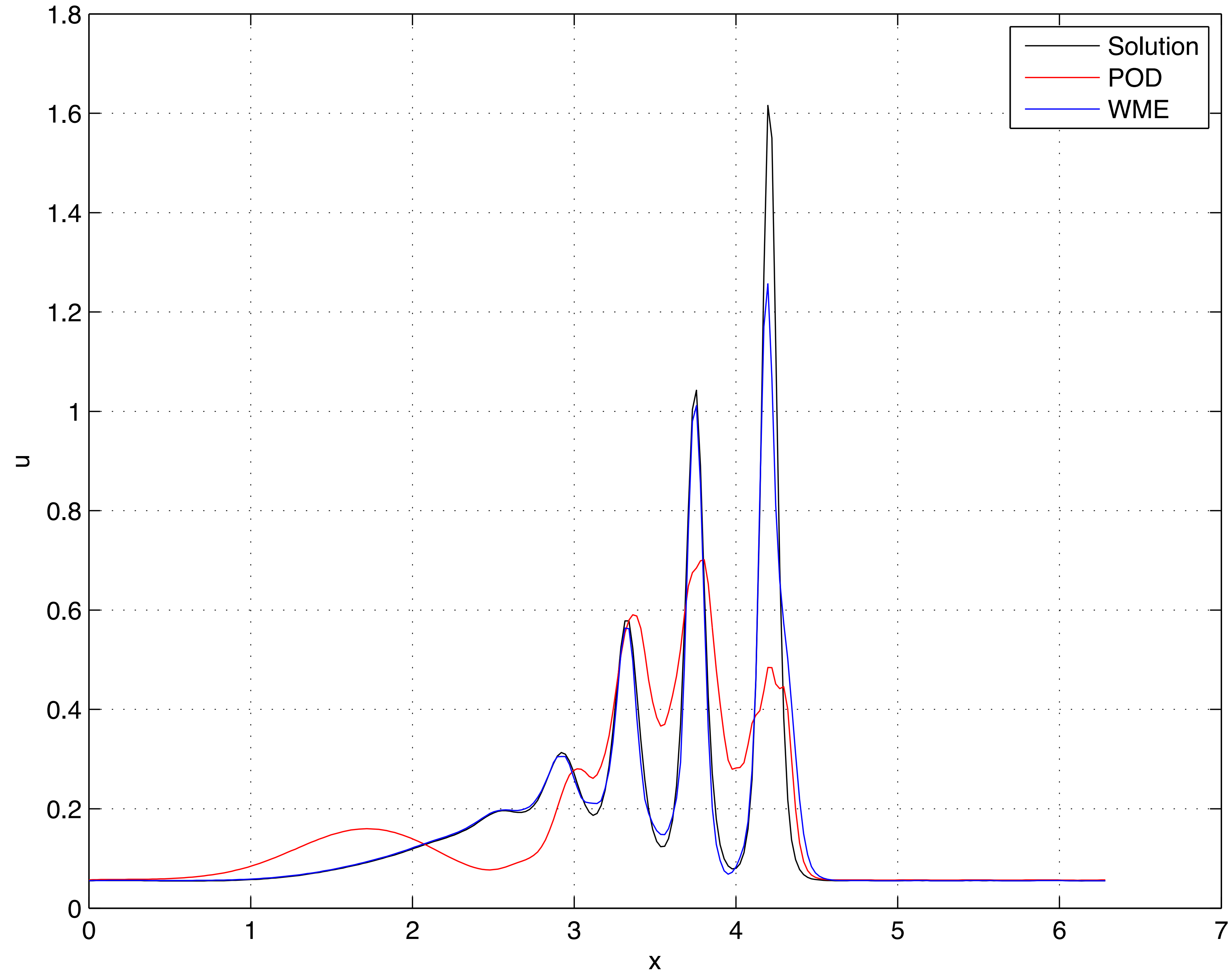


Euclidean embedding



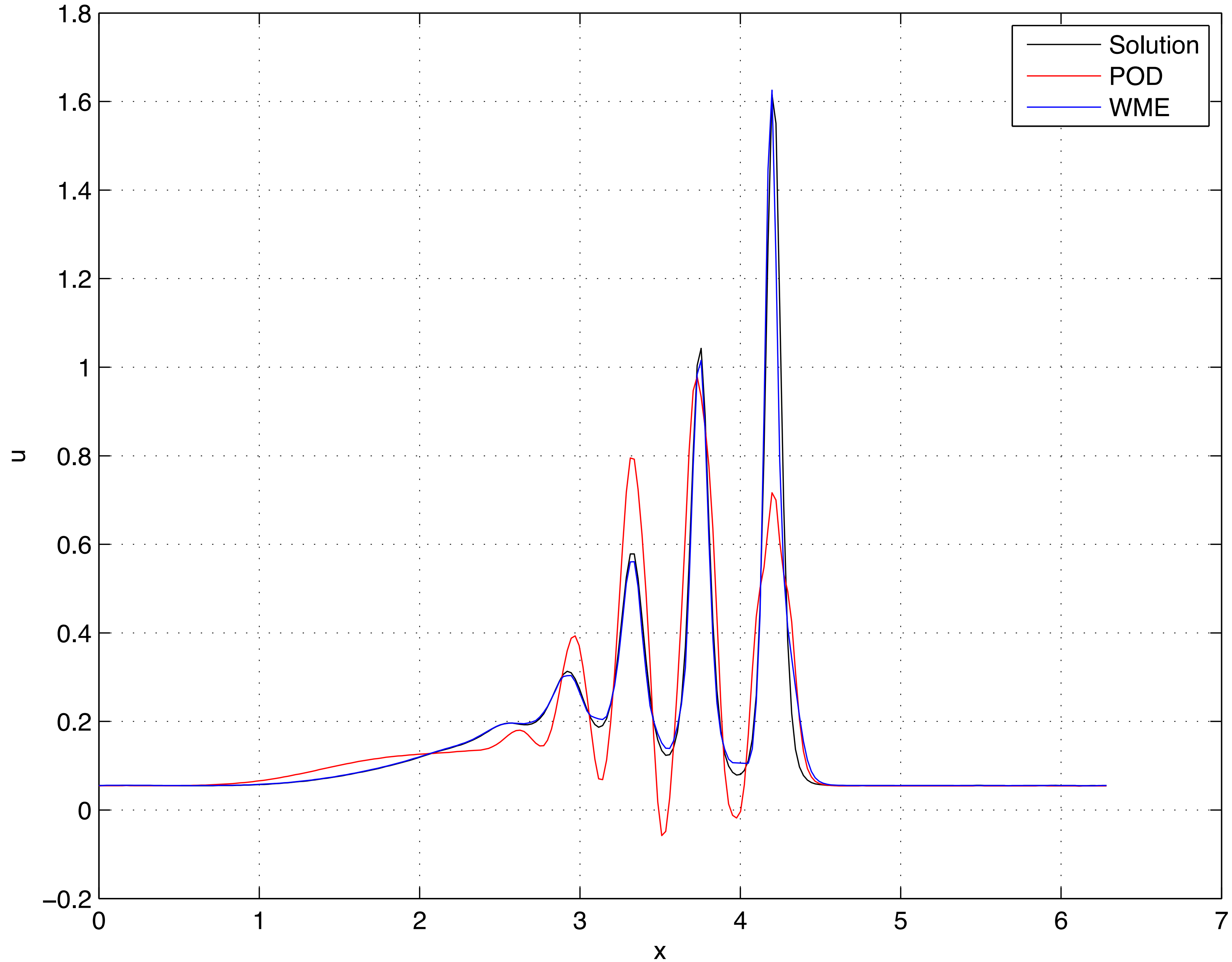
Euclidean embedding

3 modes



Euclidean embedding

5 modes



Euclidean embedding

9 modes