Optimization and uncertainty quantification of 1D arterial models

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1 Introduction

2 The hemodynamic model : blood flow computation in the arterial tree

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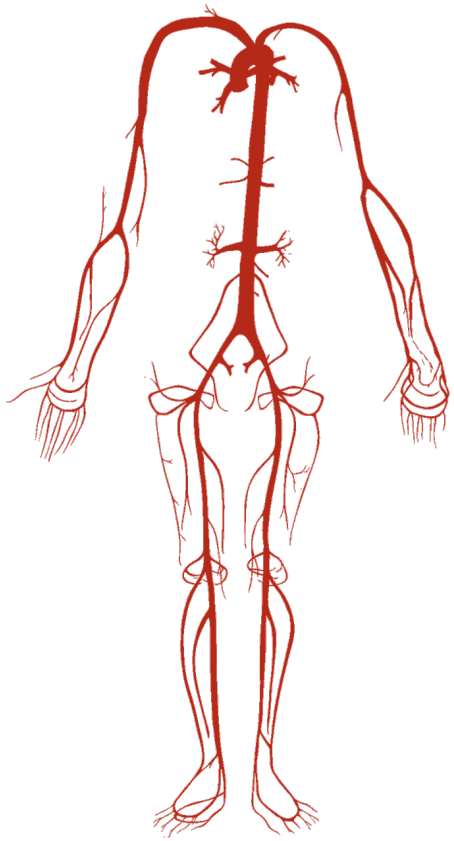
Introduction

- The numerical simulation of blood flow in the human arterial tree is a very complex problem, as it involves, in the more general approach, 3D fluid/structure simulations.

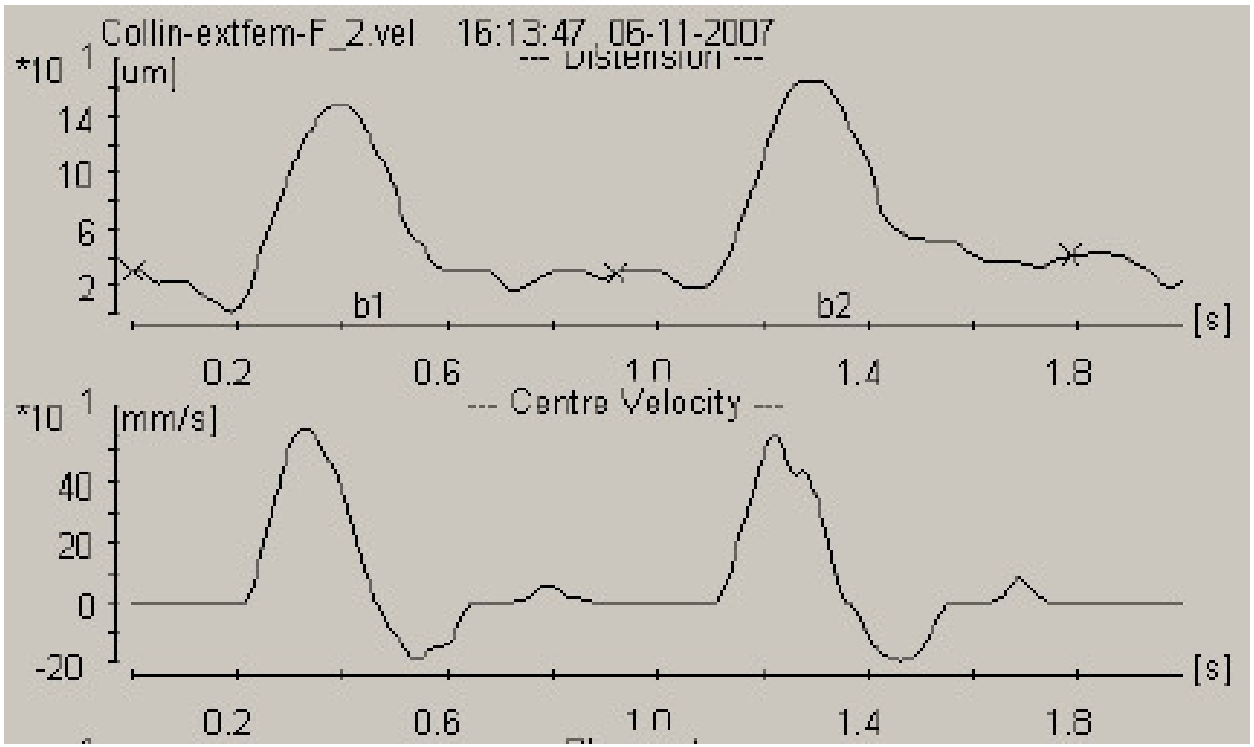


Introduction

- In order to reduce the computational cost, a simplified fluid/structure model for the blood flow in the arterial tree will be presented (direct problem).
- A major concern that remains, is to determine the parameters of the numerical model for a given patient (inverse problem).
- The parameters are patient-specific and will be obtained with the help of a non invasive, non costly experimental device.
- A robustness study, also called uncertainty quantification, around the chosen parameters need also to be done.

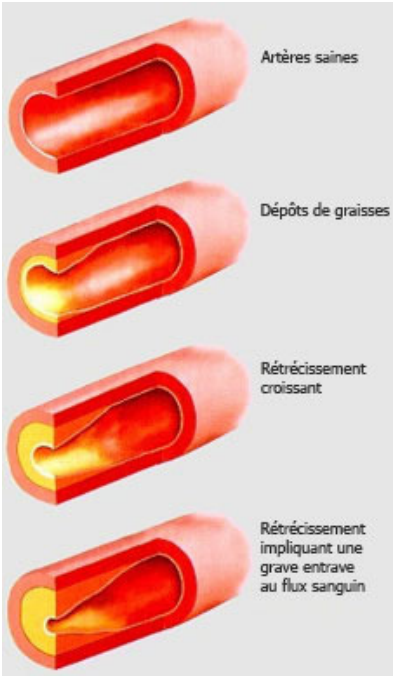
Introduction

- The non invasive measurements that will be used here, are based on Doppler techniques and are made with a device called echotracking.
- The echotracking measurements that will be used are the time profiles of diameter and velocity at various positions of the arterial tree :



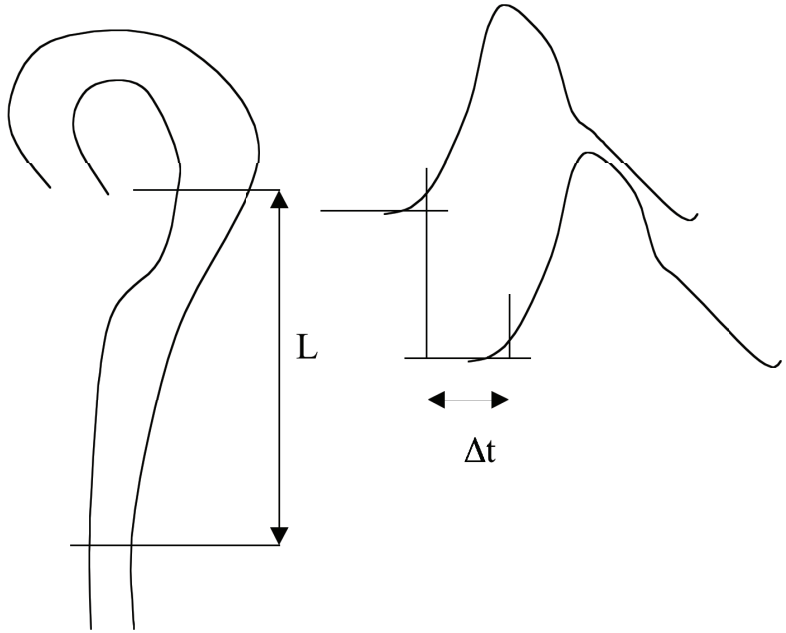
Introduction

- Once validated, such numerical reconstruction will help practionners for an early diagnosis of cardiovascular diseases, like atherosclerosis.



Introduction

- Among parameters, the arterial stifness is a well-known index for predicting cardiovascular risks.
- It is currently estimated with echotracking measurements after computing the pulse wave velocity, also called PWV :



by using the Moens-Korteweg equation : $PWV = \sqrt{\frac{Eh}{2r\rho}}$

- A full numerical reconstruction will give a more accurate and a local estimation of PWV.

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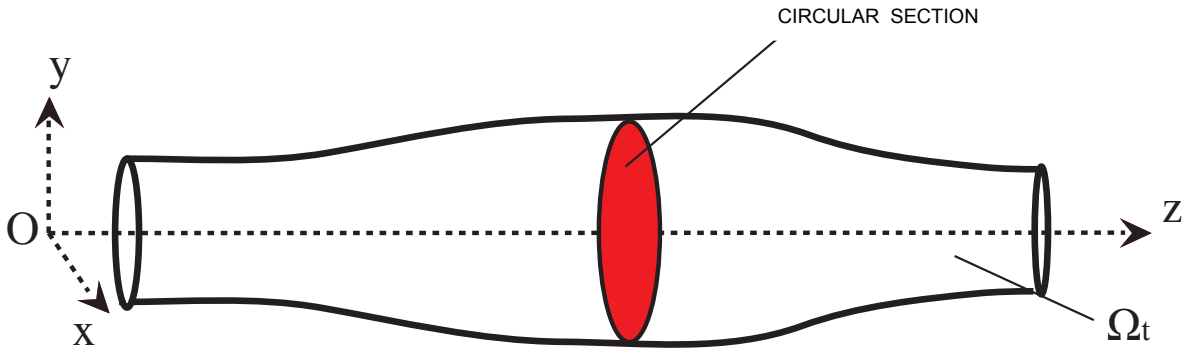
The 1D model



- For a given artery, the domain Ω_t is assumed to be cylindrical along the Oz axis and of constant length L.
- A simplified fluid/structure interaction model is derived on this geometry.
- References : *Formaggia, Nobile, Quarteroni* (2001),*Sherwin et al.* (2003), *Gerbeau et al.* (2005), *Stergiopoulos et al.* (2009).

The 1D model : the equations

- For a given artery, the two unknowns $A(t,z)$ (cross section) and $Q(t,z)$ (mean flux) satisfy the following set of equations :

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial z} = 0$$
$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial z}\left(\frac{Q^2}{A}\right) + \frac{A}{\rho}\frac{\partial P}{\partial z} + K_r \frac{Q}{A} = 0$$

- An elastic linear law closes the system :

$$P - P_{ext} = \beta(z)\left(\sqrt{A(z,t)} - \sqrt{A_0(z)}\right)$$

The 1D model : conservative form

- The 1D model can be rewritten in a conservative form :

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial z} = B(U)$$

where $U = (A, Q)^t$ and $F(U) = \begin{pmatrix} Q \\ \frac{Q^2}{A} + \frac{\beta}{3\rho} A^{\frac{3}{2}} \end{pmatrix}$.

- It can be observed that this system is hyperbolic, as the Jacobian $H = \frac{\partial F}{\partial U}$ has always two real and distinct eigenvalues for all the allowable values of U : $\lambda_i = \frac{Q}{A} \pm c$ where

$$c = \sqrt{\frac{A}{\rho} \frac{\partial p}{\partial A}}$$

The 1D model : the discretization scheme

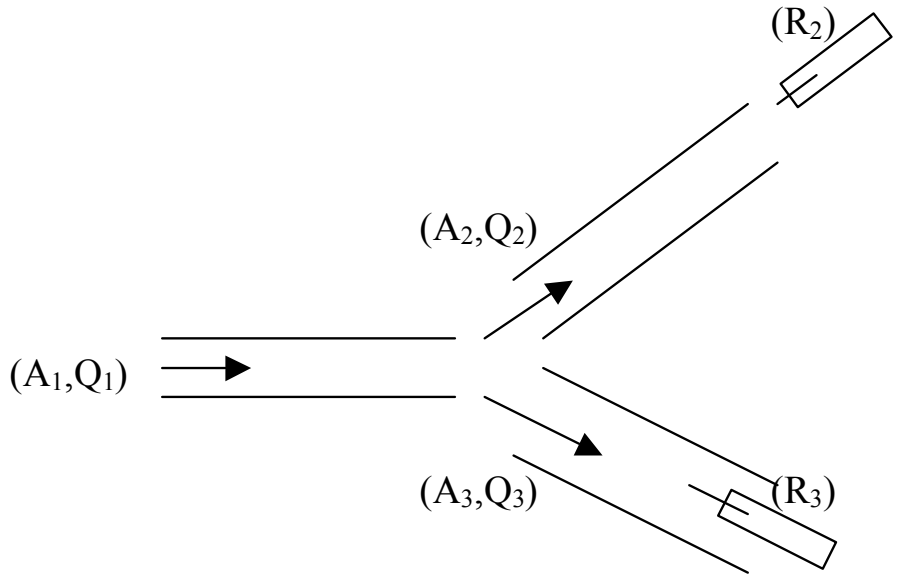
- The equations are discretized in time in their conservative form by using a second order Taylor Galerkin scheme :

$$U^{n+1} = U^n - \Delta t \frac{\partial}{\partial z}(F^n + \frac{\Delta t}{2}\frac{\partial F}{\partial U}^n B^n) - \frac{\Delta t^2}{2}(\frac{\partial B}{\partial U}^n \frac{\partial F^n}{\partial z} - \frac{\partial}{\partial z}(\frac{\partial F}{\partial U}^n \frac{\partial F^n}{\partial z})) + \Delta t(B^n + \frac{\Delta t}{2}\frac{\partial B}{\partial U}^n B^n)$$

- The spatial discretization is then done by using linear finite elements on a subdivision of $[0, L]$.
- As $\lambda_1 > 0$ and $\lambda_2 < 0$, the system is completed by two appropriate boundary conditions, one at each end for the characteristic variables W_1 and W_2.
- After some algebraic manipulations, it can be seen that a pressure profile can be imposed at the entrance.

The 1D model : network and boundary conditions

- At a bifurcation in a network of arteries, three additional conditions are imposed (conservation of mass and two pressure conditions).



- Resistance conditions are put at the exit to simulate the effect of the downtream resistance network.

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The inverse model : the parameters

- The main parameters that need to be fixed are the rigidity coefficients $z \to \beta_i(z)$ of each artery. They can be a function of z in the case of an artery with a plaque.
- The reference cross sections $z \to A_{0,i}(z)$ of each artery are also unknown.
- The parameter K_r is linked to the blood viscosity and is supposed to be known here.
- Among the numerical parameters, the equivalent resistances at each exit of the arterial tree are the most sensitive for the simulation results.

The inverse problem : the cost function

- In view of constructing an optimal network with respect to experimental values from echotracking, the cost function to minimize has the following form :

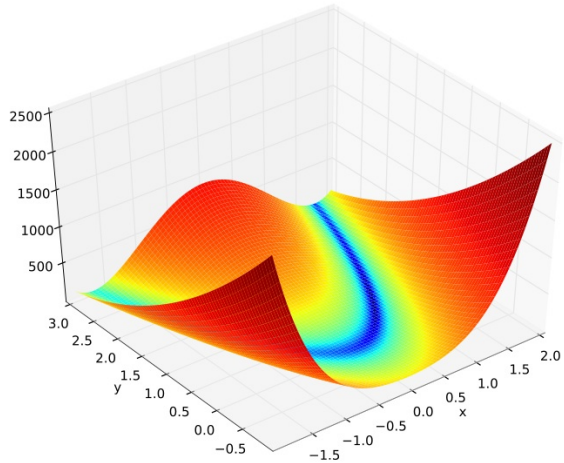
$$J(\beta_i, A_{0,i}, R_i) = \sum_{pts \in \{P_1,\dots,P_N\}} \sum_{j=1}^{M} (errA(t_j, pts) + errQ(t_j, pts))$$

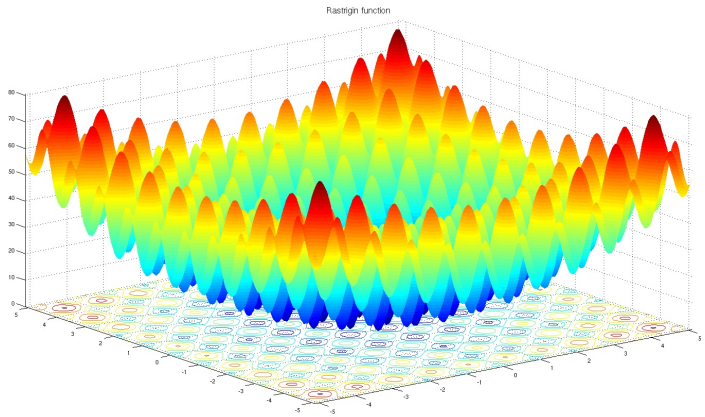
with

$$\begin{cases} errA(t_j, pts) = |A(t_j, pts) - A_{exp}(t_j, pts)|^2 \\ errQ(t_j, pts) = |Q(t_j, pts) - Q_{exp}(t_j, pts)|^2 \end{cases}$$

The optimization problem

- The inverse problem can be viewed as a global minimization problem of a cost function $J : \mathcal{O} \subset \mathbb{R}^n \to \mathbb{R}$.





- In this case, the cost function J is obtained through the resolution of a coupled system of PDEs.

Existing methods

- The most classical method is based on the computation of the gradient of J and the evaluation of the following sequence :

$$x_{k+1} = x_k - \alpha_k \nabla J(x_k)$$

  to approximate a local minima of J.
- The use of second order informations on the cost function J (if it is C^2) allows a faster convergence rate (Newton method) :

$$x_{k+1} = x_k - \alpha_n \nabla^2(x_k)^{-1} \cdot \nabla J(x_k)$$

Existing methods

- As the gradient evaluation of J is very difficult here, the use of derivative free optimization (DFO) methods is almost mandatory.
- A first class of DFO method is based on the evolution of a set of $n+1$ points in $\mathbb{R}^n$ (Nelder Mead).
- Another popular set of DFO methods is the family of evolutionary algorithms based on the evolution of a population of solutions.

Genetic algorithm (GA)

- Choice of a random initial population $P_1 = \{X_i^1 \in \mathcal{O}, 1 \leq i \leq N_p\}$
- for n_g from 1 to $Ngen$
- Evaluation of $\{J(X_i^{n_g}), 1 \leq i \leq N_p\}$.
- for k from 1 to $\frac{N_p}{2}$
  - Selection of $(X_\alpha^{n_g}, X_\beta^{n_g})$ with respect to their fitness.
  - Crossover : with probability p_c, replace $(X_\alpha^{n_g}, X_\beta^{n_g})$ par $(Y_\alpha^{n_g}, Y_\beta^{n_g})$.
  - Mutation : with probability p_m, replace $Y_i^{n_g}$ by $Z_i^{n_g}$
  - end for
- Generation of the new population P_{n_g}.
- end for

Evolution strategy (ES)

- Choice of a random initial population of μ 'parents' : $P_1 = \{X_i^1 \in \mathcal{O}, \quad 1 \leq i \leq \mu\}$
- for n_g from 1 to *Ngen*
- Creation of a population of $\lambda \geq \mu$ 'childrens' O_{n_g} by :
  - Crossover of ω 'parents' $Y_i^{n_g} = \frac{1}{\omega}(\sum_{j=1}^{\omega} X_j^{n_g})$
  - Mutation : replace $Y_i^{n_g}$ by $Z_i^{n_g}$
  - Evaluation of $\{J(Z_i^{n_g}), 1 \leq i \leq \lambda\}$
- Selection of the best μ parents in the population $P_{n_g} \cup O_{n_g}$.
- end for

Particle Swarm Optimization (PSO)

- Choice of a random initial population $P_1 = \{(X_i^1, v_i^1, p_i^1), 1 \leq i \leq N_p\}$ of 'particles' with the current position $X_i \in \mathcal{O}$, velocity v_i and the current best visited position p_i.
- for n_g from 1 to $Ngen$
- Evaluation of $\{J(X_i^{n_g}), 1 \leq i \leq N_p\}$.
- Computation of the best position so far, globally and individually $(p_g^{n_g})$
  - Computation of the new velocities of each particle :

$$v_i^{n_g+1} = \omega v_i^{n_g} + c_1\rho_1(p_i^{n_g} - x_i^{n_g}) + c_2\rho_2(p_g^{n_g} - x_i^{n_g})$$

  - Computation of the new position of each particle :

$$X_i^{n_g+1} = X_i^{n_g} + v_i^{n_g+1}$$

- end for

Uncertainty quantification

- Once the optimal parameters of the model have been found, the robustness of these parameters must be studied.
- A non intrusive method called uncertainty quantification by polynomial chaos can been chosen.
- It consists in choosing an uncertainty probability distribution function for n parameters (density f_j on $[-1,1]$) and to decompose a well chosen quantity at the exit, $A(t,x)$, in an orthonormal polynomial basis of the form :

$$A(x,t,\omega) = \sum_{j=0}^{M-1} a_j(x,t)\psi_j(\xi_1(\omega),\xi_2(\omega),...,\xi_n(\omega))$$

Uncertainty quantification

- The deterministic coefficients are obtained by a non intrusive method in the following way :

$$a_j(x,t) = \frac{< A(x,t,.), \psi_j(\xi(.)) >}{< \psi_j^2(\xi(.)) >}$$

  for $1 \leq j \leq M = \frac{(n+p)!}{n!p!}$.
- A Gauss quadrature can be used for the computation of the multi-dimensional integral.
- In case of a large n, a sparse grid interpolation technique is required to reduce the computational cost.

Sparse grids : hierarchical construction in dimension 1

- The objective is to interpolate the function :

$$f : [0,1] \to \mathbb{R}.$$

- For $i \in \mathbb{N}$, denote X^i the set of Chebychev points on $[0,1]$ of level i. More precisely, $x_j^i \in X^i$ is such that :

$$x_j^i = \begin{cases} \frac{1}{2} & \text{for } j = 1 \text{ and } i = 1 \\ \frac{1}{2}(-\cos(\pi \frac{j-1}{n_i - 1}) + 1) & \text{for } j = 1, \ldots, n_i = 2^{i-1} + 1 \text{ and } i > 1. \end{cases}$$

Sparse grids : hierarchical construction in dimension 1

- Denote $a_j^i$the set of Lagrange polynomials associated to $x_j^i \in X^i$:

$$a_j^i(x) = \begin{cases} 1 & \text{pour } j = 1 \text{ et } i = 1 \\ \prod_{k=1, k\neq j}^{n_i} \frac{x - x_k^i}{x_j^i - x_k^i} & \text{pour } j = 1, \ldots, n_i \text{ et } n_i > 1. \end{cases} .$$

- The interpolation model of level i of f, denoted $m_i(f)$, writes as :

$$m_i(f) = \sum_{x_j^i \in X^i} f(x_j^i) a_j^i. \tag{1}$$

Sparse grids : hierarchical construction in dimension 1

- Denote Δ^i the difference between levels i and $i-1$:

$$\Delta^i = m_i(f) - m_{i-1}(f) = \sum_{x_j^i \in X^i} (f(x_j^i) - m_{i-1}(f)(x_j^i)) \ . \ a_j^i.$$

- With $X_\Delta^i = X^i \backslash X^{i-1}$, we get

$$\Delta^i = \sum_{x_j^i \in X_\Delta^i} \underbrace{(f(x_j^i) - m_{i-1}(f)(x_j^i))}_{w_j^i} \ . \ a_j^i, \tag{2}$$

- The hierarchical construction of $m_i(f)$ is thus :

$$\begin{aligned} m_i(f) &= m_{i-1}(f) + \Delta^i \\ &= \sum_{k=1}^i \Delta^k. \end{aligned}$$

Sparse grids : hierarchical construction in dimension n

- In order to interpolate $f : [0,1]^n \to \mathbb{R}$, a tensor product gives :

$$m_{(i_1,i_2,\dots i_n)}(f) = \sum_{x_{j_1}^{i_1} \in X^{i_1}} \dots \sum_{x_{j_n}^{i_n} \in X^{i_n}} f(x_{j_1}^{i_1}, \dots, x_{j_n}^{i_n})(a_{j_1}^{i_1} \otimes \dots \otimes a_{j_n}^{i_n}).$$

- As before, the hierachical expression in dimension n on a full grid is thus :

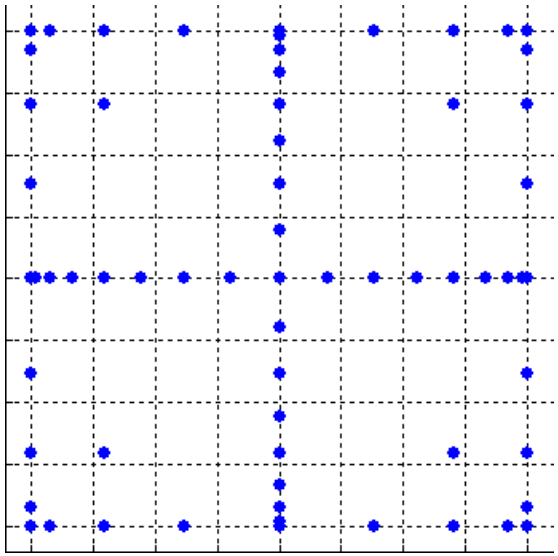
$$m_{(i_1,i_2,\dots i_n)}(f) = \sum_{k_1=1}^{i_1} \dots \sum_{k_l=1}^{i_l} \dots \sum_{k_n=1}^{i_n} \underbrace{(\Delta^{k_1} \otimes \dots \otimes \Delta^{k_l} \otimes \dots \otimes \Delta^{k_n})}_{\Delta^{\mathbf{k}}},$$

Sparse grids interpolation : the general expression

- The sparse grid interpolation, first proposed by Smolyak , consists in neglecting the basis functions with smallest support range :

$$SG_N(f) = \sum_{|\mathbf{k}|_1 \leq n+N-1} (\Delta^{k_1} \otimes \ldots \otimes \Delta^{k_n}).$$

- For instance, in dimension 2 and at level $N = 4$, it gives the following set of points :



Sparse grids interpolation : the error estimation

- Sparse grids interpolation allows to decrease the number of interpolation points needed by a large factor, while keeping a good interpolation error :

Level N	Interpolation points number	L^2 norm error
Full Grid	$\mathcal{O}(N^n)$	$\mathcal{O}(N^{-2})$
Sparse Grid	$\mathcal{O}(N(\log N)^{n-1})$	$\mathcal{O}(N^{-2}(\log N)^{n-1})$

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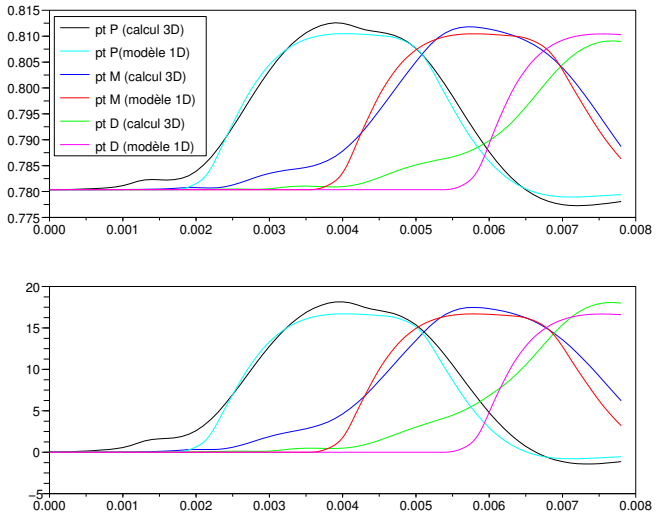
Comparison 3D model vs 1D model

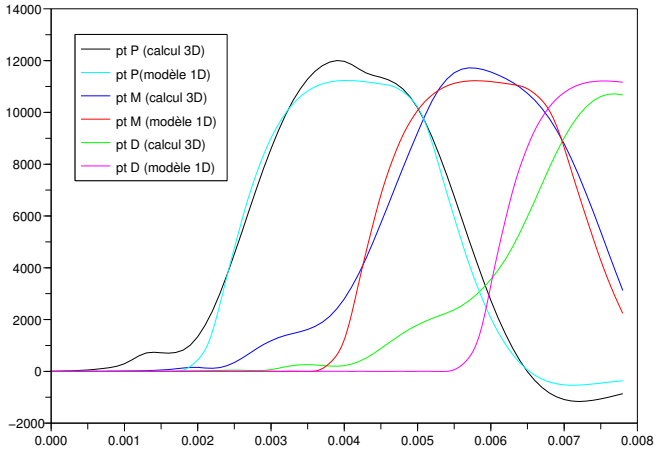
- The objective of this first inverse problem is to fit the 1D model with the results of an existing 3D computation (done with the LifeV software).

- A classical Evolution Strategy is used here to find the optimal value of β. The cost function is based on the profile of A and Q at three positions.

Comparison 3D model vs 1D model

- The results show in particular that the 1D model can fit relatively well with the complex 3D model at a very lower computational cost.





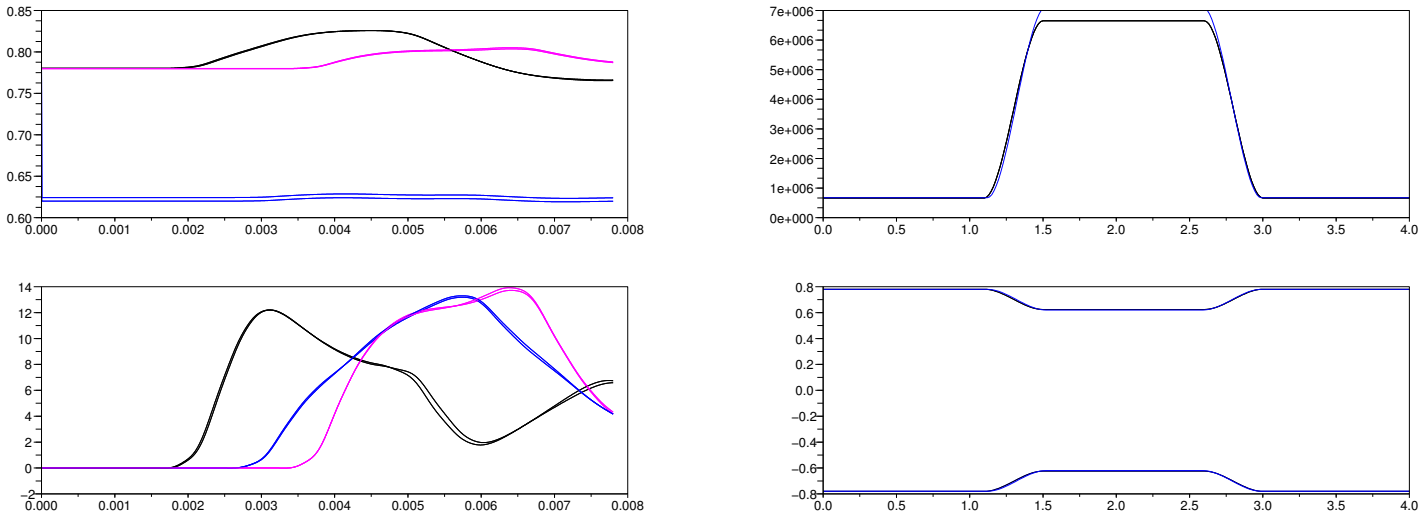
- Note also that the optimal value of β which allows the 1D model to fit to the corresponding 3D model is far below the value issued from a formal derivation.

A toy problem : recovering the parameters of a diseased artery

- The objective of this second inverse problem is to reconstruct the functions $z \mapsto \beta(z)$ and $z \mapsto A_0(z)$ in the case where it takes two distinct values.
- In this case, the six unknowns are respectively a_1, a_2, β_1, β_2, S_1 and S_2.
- As a first validation test case, the target results are issued from synthetic data computed with the 1D model.
- The objective is to show that with a reduced number of spatial information, the model can recover the artery geometry and properties.

A toy problem : recovering the parameters of a diseased artery

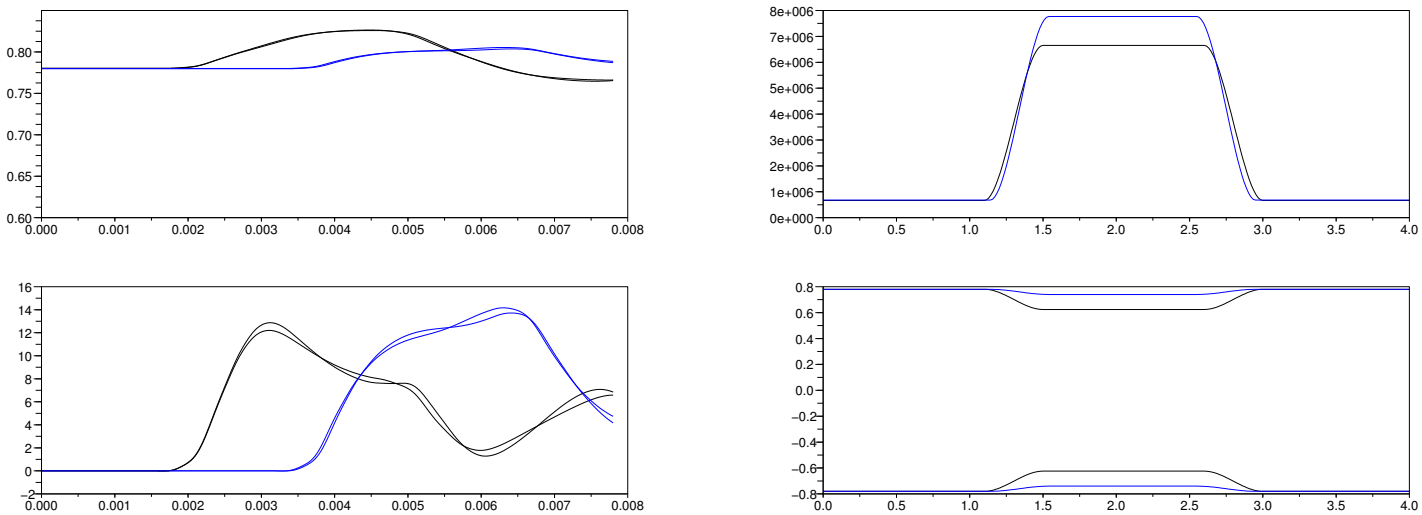
- When the profiles of A and Q are known at three different positions, the optimization process is able to reconstruct a very precise shape of $z \mapsto \beta(z)$ and $z \mapsto A_0(z)$:



- The values of A and Q are also perfectly recovered at the three sections.

A toy problem : recovering the parameters of a diseased artery

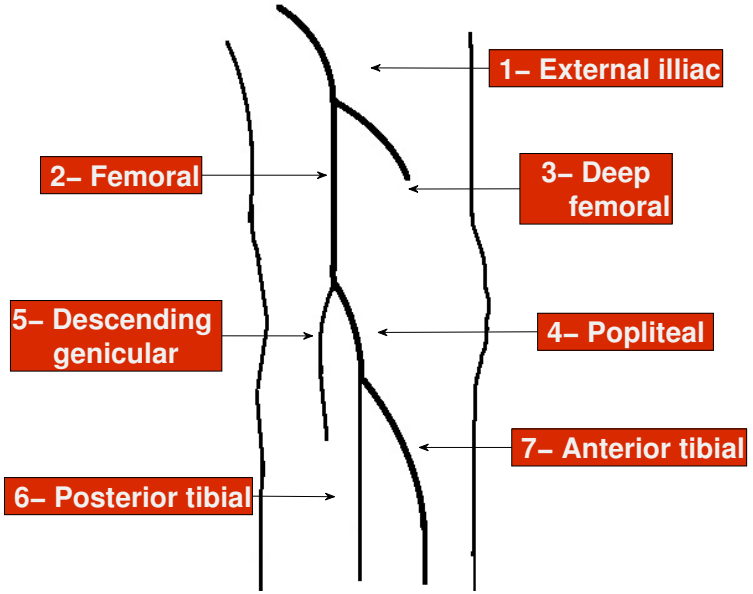
- When the profiles of A and Q are only known at two different positions (outside the plaque area), the optimization process is still able to reconstruct a rather precise shape of $z \mapsto \beta(z)$ and $z \mapsto A_0(z)$:



- The values of A and Q are still perfectly recovered at the two sections.

Numerical reconstruction of an arterial network from echotraking (patient P1)

- The arterial network studied here, is made of 7 arteries of the lower limb.



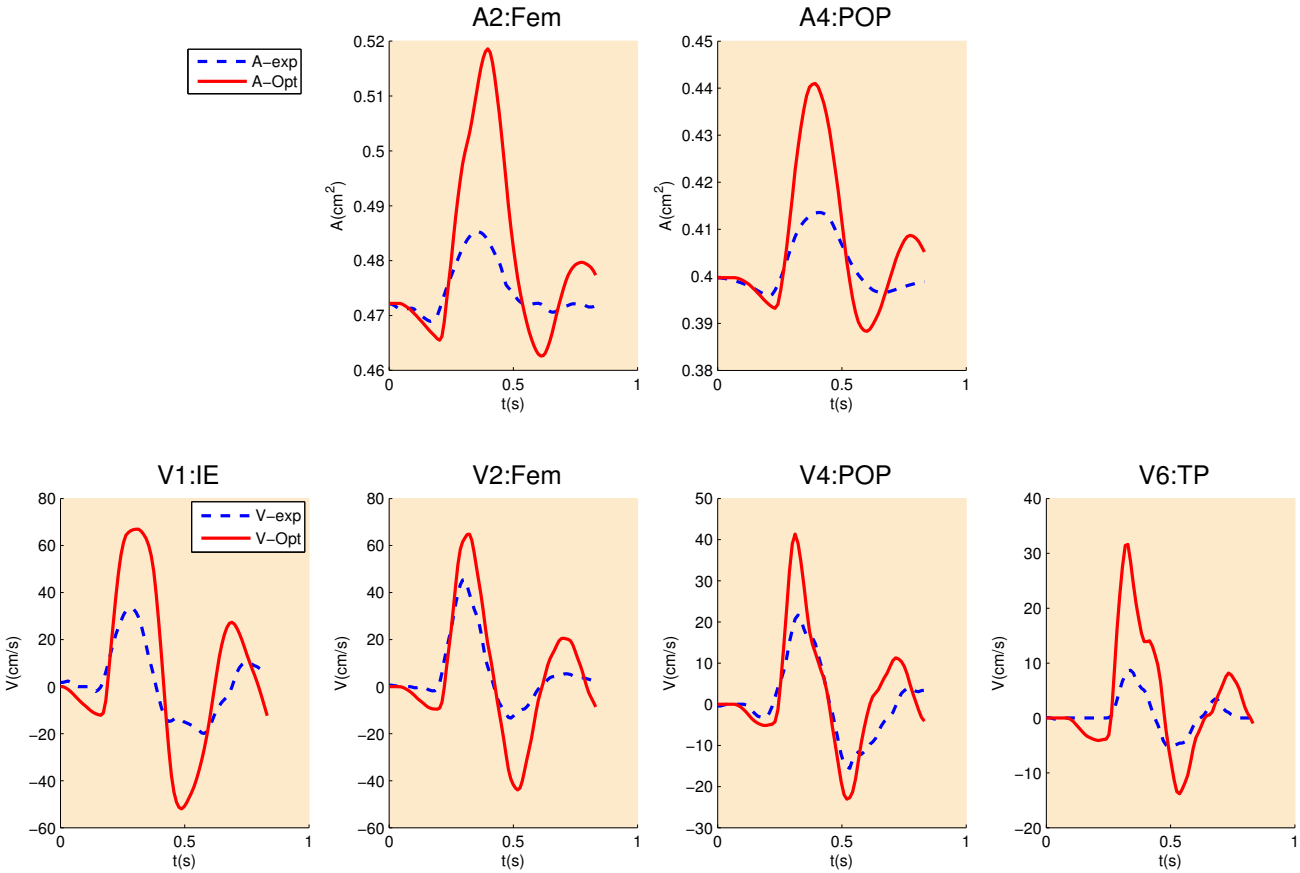
- The echotracking measurements consist in 4 velocity profiles (arteries 1,2 4 and 6) and 3 cross section profiles (arteries 1, 2 and 4).
- The cross section measurement at artery 1 is taken as the entrance condition.

The nominal parameters for patient P1

Artery denomination	L (cm)	A_0 (cm^2)	c_0 (m/s)	R
1 : external iliac	14.4	**0.53**	7.20	-
2 : femoral	44.3	**0.47**	9.15	-
3 : deep femoral	15	0.30	8.32	0.65
4 : popliteal	5	**0.40**	9.50	-
5 : genicular	10	0.30	9.95	0.65
6 : posterior tibial	32.1	0.20	11.12	0.65
7 : anterior tibial	34.3	0.20	14.03	0.65

TABLE: Nominal set of parameters for Patient P1, partially chosen from the literature. Bold figures refer to measured clinical values

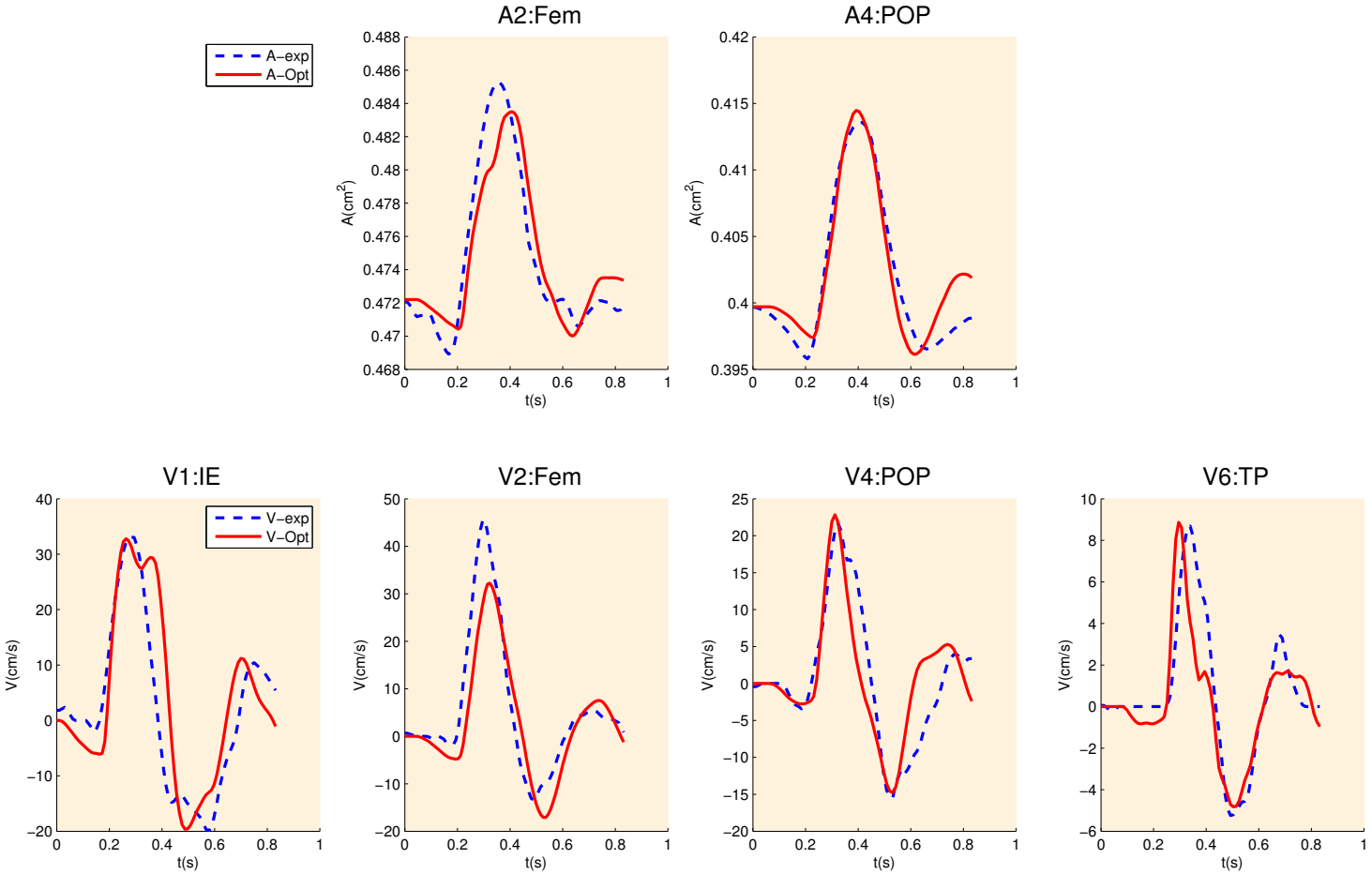
First results for patient P1, nominal parameters



Parameter identification for patient P1

- The physical parameters to determine are :
  - the 7 arterial stiffness β_i, $i \in \{1, ..., 7\}$. for each artery,
  - the 4 cross sections at rest $A_{0,i}$ of arteries $i \in \{3, 5, 6\}$.
- Another set of unknowns parameters, of numerical type, are :
  - the 4 output resistances R_i for $i \in \{3, 5, 6, 7\}$.
- The function to minimize is obtained by using 4 experimental velocity measurements (arteries 1, 2, 4 and 6) and 2 cross section measurements (arteries 2 and 4).
- A CMA-ES method is used to minimize the associated cost function in $\mathbb{R}^{15}$.

Parameter identification, the 'patient P1 model'



the 'patient P1' optimal parameters

	Patient P1			Patient P2		
Artery	$\overline{\mathbf{A_0}}$ (cm^2)	$\overline{\mathbf{c_0}}$ (m/s)	$\overline{\mathbf{R}}$	$\overline{\mathbf{A_0}}$ (cm^2)	$\overline{\mathbf{c_0}}$ (m/s)	$\overline{\mathbf{R}}$
1 : EI	**0.53**	4.99	-	**0.53**	6.57	-
2 : Fem	**0.47**	11.96	-	**0.38**	11.80	-
3 : DF	0.27	7.39	0.48	0.32	7.58	0.7
4 : Po	**0.40**	10.51	-	**0.34**	8.85	-
5 : Ge	0.32	9.93	0.42	0.22	13.47	0.33
6 : PT	0.23	11.61	0.95	0.24	11.67	0.68
7 : AT	0.22	9.91	0.73	0.13	14.12	0.97

TABLE: The mean optimal parameters for Patients P1 and P2 after 10 CMA-ES runs.

Robustness study of the 'patient P1 model'

- The effect of the number of experimental measurements available is first investigated.
- The influence of uncertainty among the previously obtained parameters have also to be studied before a complete validation of the model.
- The effect of such uncertainty at the entrance of the model(observables), have been tested on various outputs : local pulse pressure, reflection index, etc...

Robustness study of the 'patient P1 model'

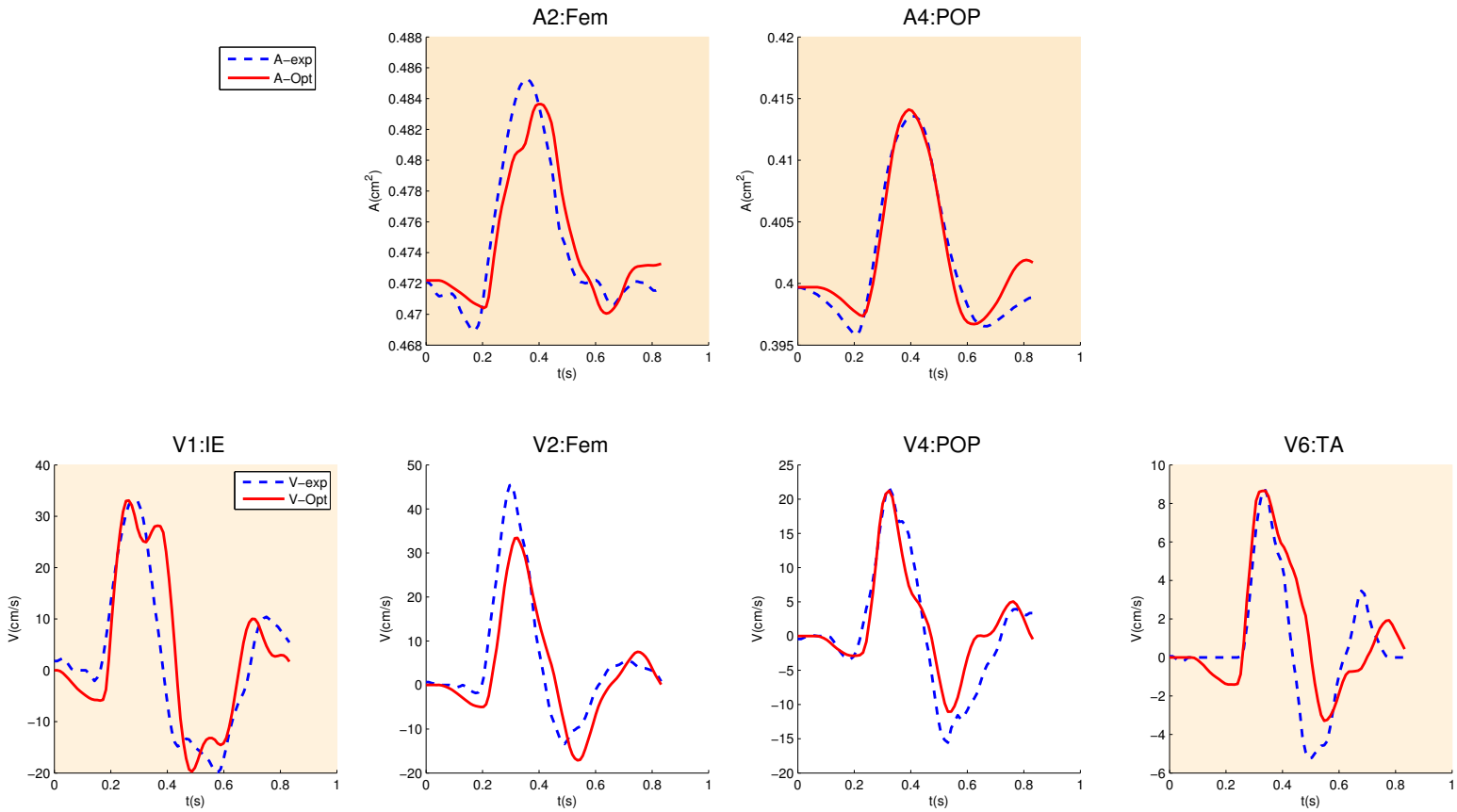


FIGURE: Numerical luminal cross-section and velocity profiles compared to clinical data (dashed curves) for Patient P1 with optimal parameters obtained with the error function

Robustness study of the 'patient P1 model'

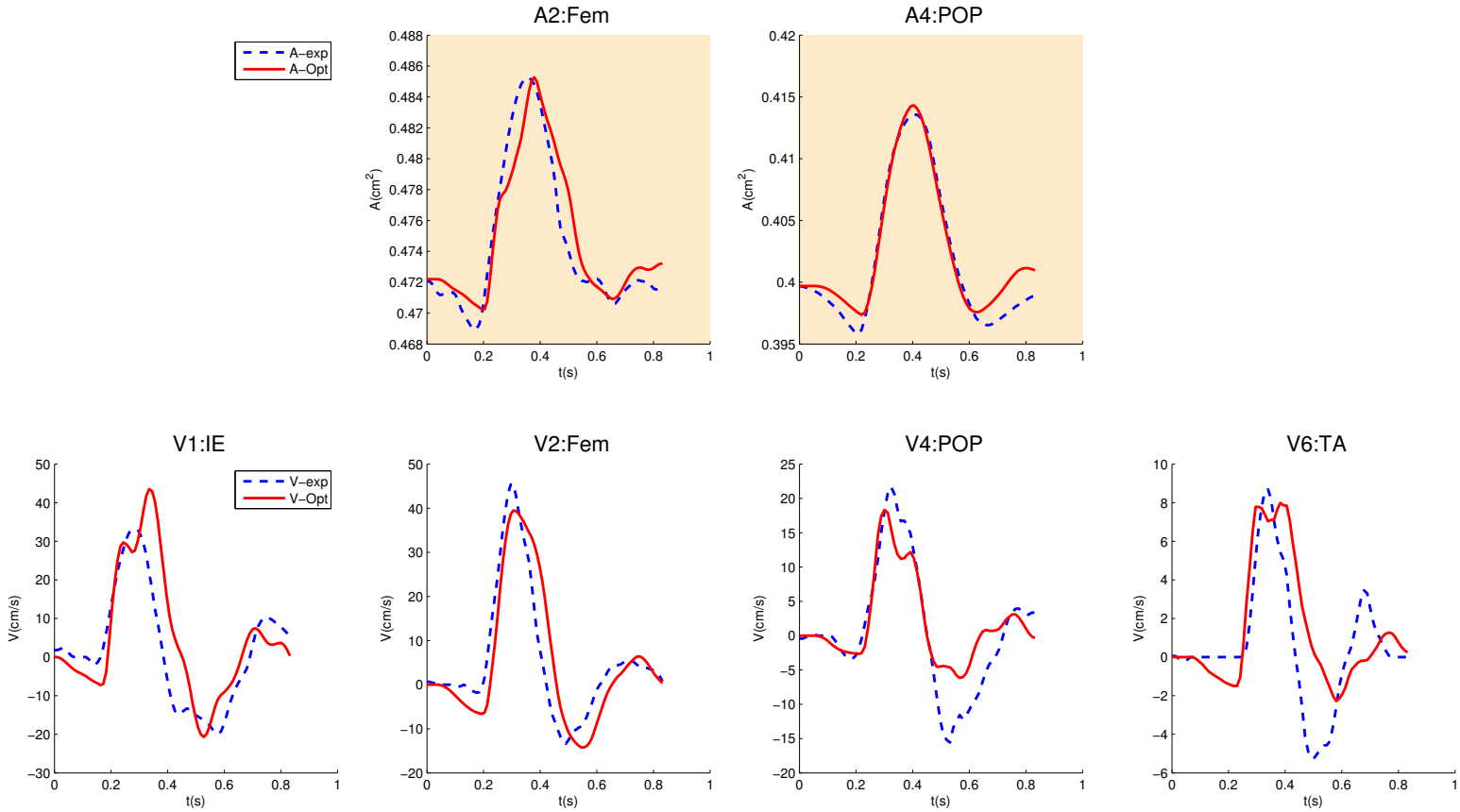


FIGURE: Numerical section and velocity profiles compared to clinical data (dashed curves) for Patient P1 with optimal parameters obtained with the error function defined

Robustness study of the 'patient P1 model'

- Three uncertainty analysis for patient P1 have been carried out :
  - 2 studies on local parametric uncertainty, namely the section $A_{0,k}$ and pulse wave velocity at rest $c_{0,k}$ for artery 3 and 6 respectively.
  - 1 study on the effect of external parametric uncertainty, namely peripheral resistances $(R_m)_{m\in\{3,5,6,7\}}$ at the exit.
- The random parameters for this three cases are thus respectively $(A_{0,3}, c_{0,3})$, $(A_{0,6}, c_{0,6})$ and (R_3, R_5, R_6, R_7).
- The type of uncertainty that has been chosen is of uniform type with a $\pm 25\%$ variation around the deterministic value.
- A polynomial chaos approximation of order 3 is chosen. A Gauss (respectively sparse grid) quadrature have been used for case 1 and 2 (respectively 3).

Robustness study of the 'patient P1 model'

Artery denomination	$A_{0,3}, c_{0,3}$ (N=2)	$A_{0,6}, c_{0,6}$ (N=2)	$R_{\{3,5,6,7\}}$ (N=4)
1 : external iliac	1.37	0.17	1.91
2 : femoral	2.90	5.56	10.44
3 : deep femoral	2.86	1.58	4.71
4 : popliteal	2.58	5.74	14.38
5 : genicular	1.95	6.02	14.46
6 : posterior tibial	**4.37**	**7.76**	**16.26**
7 : anterior tibial	3.96	3.64	15.73

TABLE: The pulse pressure (PP) coefficient of variation (in percentage) for each artery and for the three UQ studies.

Robustness study of the 'patient P1 model'

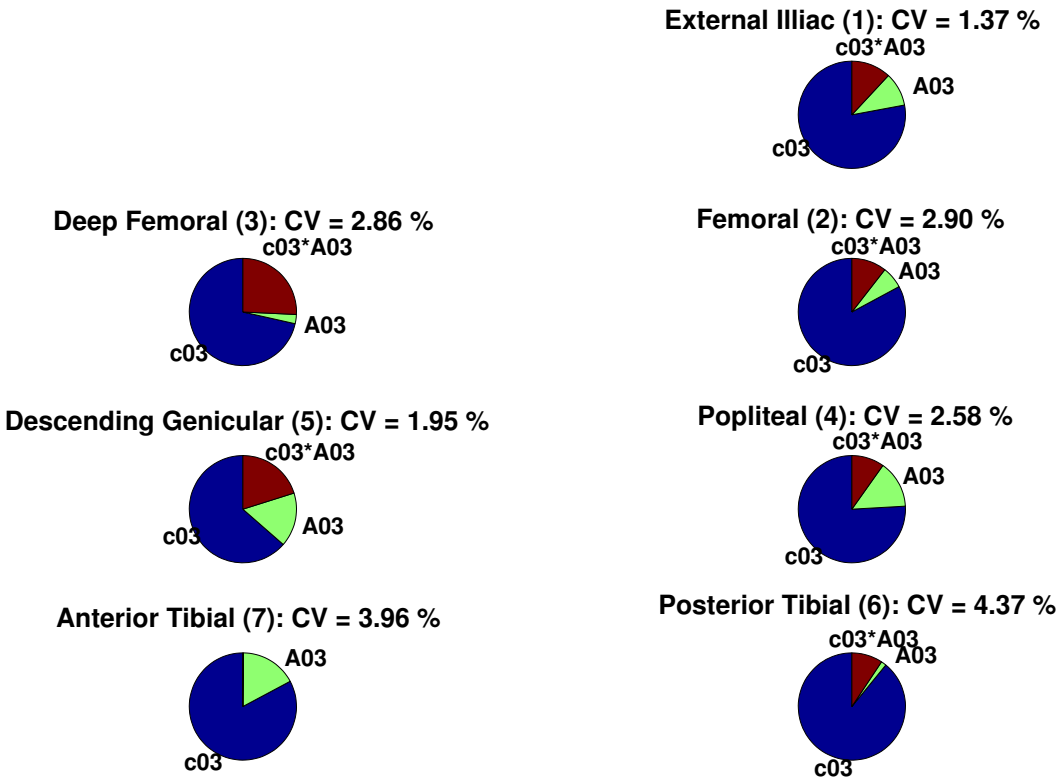


FIGURE: Patient P1 : First and second order Sobol coefficients contribution to PP uncertainty for the first UQ computation.

Robustness study of the 'patient P1 model'

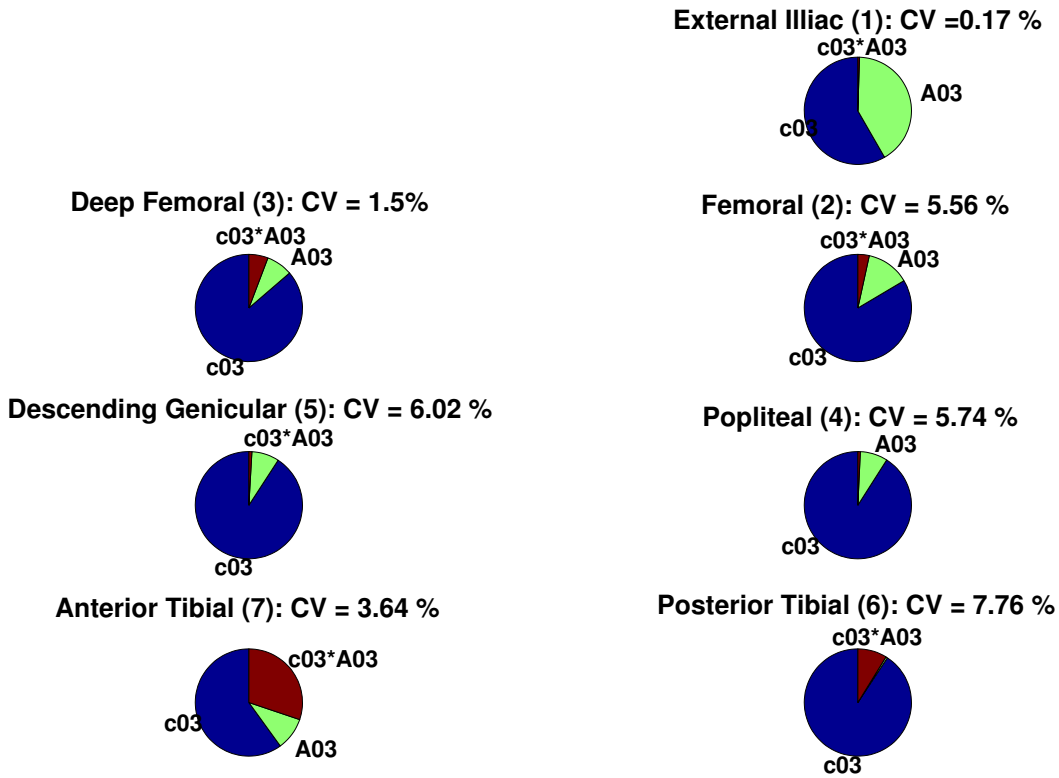


FIGURE: Patient P1 : First- and second-order Sobol coefficients contribution to PP uncertainty for the second UQ computation.

Robustness study of the 'patient P1 model'

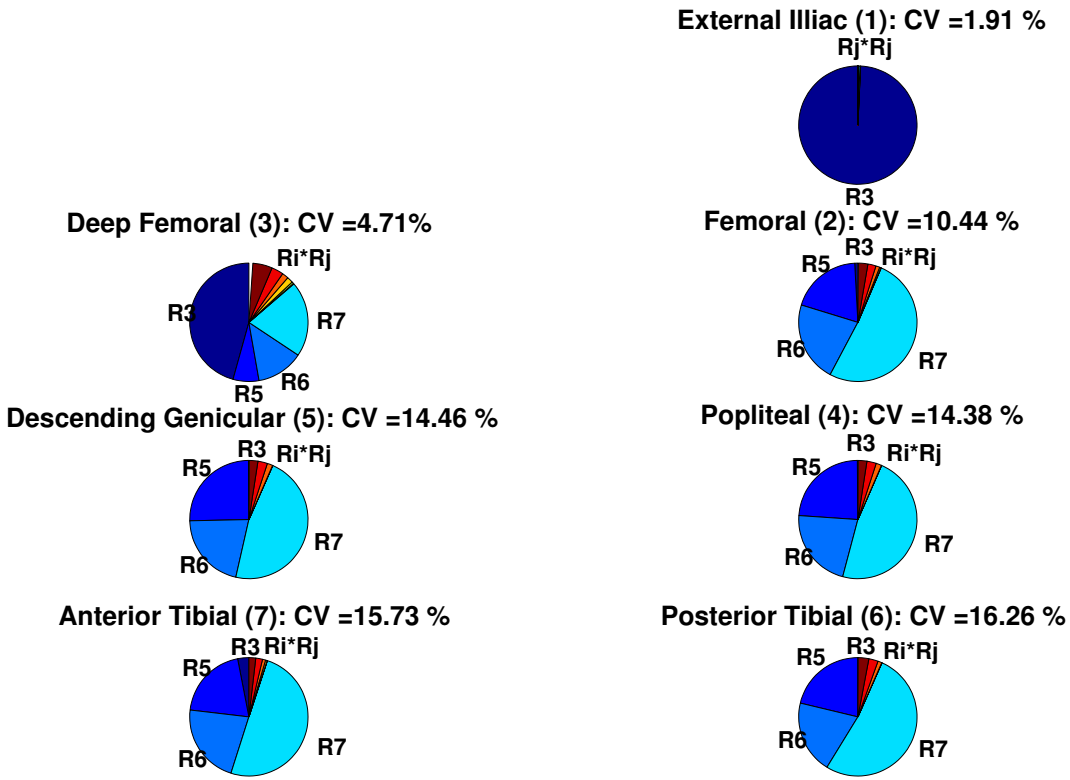


FIGURE: Patient P1 : First- and second-order Sobol coefficients contribution to PP uncertainty for the third UQ computation.

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