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Computational Issues for Optimal Shape Design in Hemodynamics

Olivier Pironneau *

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Abstract

A Fluid-Structure Interaction model is studied for aortic flow, based on Koiter's shell model for the structure, Navier-Stokes equation for the fluid and transpiration for the coupling. It accounts for wall deformation while yet working on a fixed geometry. The model is established first. Then a numerical approximation is proposed and some tests are given. The model is also used for optimal design of a stent and possible recovery of the arterial wall elastic coefficients by inverse methods.

Introduction

Hemodynamics, a special branch of computational fluid dynamics, poses many problems of modeling, data acquisition, computation and visualization. However even as of now it is a valuable tools to understand aneurisms, to design stents and heart valves, etc (see for example [10, 4, 11]).

In this paper we shall focus on a rtic flow, its modelisation, numerical simulation and inverse techniques.

Blood in large vessels like the aorta is newtonian and flows in a laminar regime with Reynolds number of a few thousands. The Navier-Stokes equation for incompressible fluid is a good model for it.

A blood vessel on the other hand is a complex structure for which linear elasticity is only a first crude approximation and for which the Lamé coefficients do not have a universal value and can vary with individuals.

Nevertheless, like many authors ([1, 8] for instance) we shall use Koiter's linear shell theory.

1 Koiter's Shell Model for Arteries

The following hierarchy of approximations for the displacement \vec{d} of the aortic wall will be made:

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- Small displacement linear elasticity instead of large displacement (needed for the heart).
- No contact inequalities with the surrounding organs.
- Shell model for the mean surface,
- With reference to the mean surface, normal displacement of the walls only.

Let Σ be the shell surface representing the mean position of the blood vessel. Let $\vec{n}(x)$ be the normal at $x \in \Sigma$. Let $\vec{d}(x,t)$ be the displacement of the wall at x at time t. Normal displacement implies $\vec{d} = \eta \vec{n}$.

In [8] it is shown that under such conditions, Koiter's model reduces to the following equation of η on Σ

$$\rho_s h \partial_{tt} \eta - \nabla \cdot (\mathbf{T} \nabla \eta) - \nabla \cdot (\mathbf{C} \nabla \partial_t \eta) + a \partial_t \eta + b \eta = f^s, \tag{1}$$

where ρ_s is the density and *h* the thickness of the vessel, **T** is the pre-stress tensor, **C** is a damping term, *a*, *b* are viscoelastic terms and f^s the external normal force, i.e. the normal component of the normal stress tensor $-\sigma_{nn}^s$. As with all second order wave type equations two conditions must be given at t = 0, for instance

$$\eta_{|t=0} = \eta_0, \qquad \partial_t \eta_{|t=0} = \eta'_0$$

Remark 1 When $[h, T, C, a] \ll b$, (1) leads to the so-called surface pressure model

$$-\sigma^{\mathbf{s}}{}_{nn} = b\eta, \quad with \ b = \frac{Eh\pi}{A(1-\xi^2)} \tag{2}$$

where A is the artery's cross section, E the Young modulus, ξ the Poisson coefficient.

Some typical values are (in the metric system MKSA) for a heart beat of one pulsation per second:

$$E = 3MPa, \ \xi = 0.3, \ A = \pi R^2, \ R = 0.013, \ h = 0.001, \ \rho^f = 9.81 \ 10^6$$

leading to $b=3.310^7ms^{-2}$ and giving displacements in the range of 0.1 $10^{-3}{\rm m}$ and flow rates around 2 $10^{-5}{\rm m}^3{\rm s}^{-1}$

2 Fluid Equations

The Navier-Stokes equations in a moving domain $\Omega(t)$ define the velocity \vec{u} and the pressure p:

$$\rho^{f}\left(\frac{\partial \vec{u}}{\partial t} + u \cdot \nabla u\right) + \nabla p - \mu \nabla \cdot \left(\nabla \vec{u} + \nabla \vec{u}^{T}\right) = 0, \quad \nabla \cdot \vec{u} = 0, \tag{3}$$

where ρ^f is the density of the fluid and μ its viscosity.

Continuity on Σ of fluid and solid velocities implies

$$\vec{u} = rac{\partial d}{\partial t} := \vec{n} rac{\partial \eta}{\partial t}, \text{ on } \Sigma$$

Continuity of normal stresses implies

$$\sigma^f_{nn} := \vec{n} \cdot (\mu (\nabla u + \nabla u^T) - p) \vec{n} = -\sigma^s_{nn} := b\eta$$

Notice that as a consequence of the hypothesis of normal displacements only of the structure, there is no provision to write the continuity of the tangential stresses.

For a ortic flow there also an inflow and an outflow boundary Γ_i and Γ_o on which we will prescribe pressure and no tangential velocity. If $S = \Gamma_i \cup \Gamma_o$, then the boundary Γ is

$$\Gamma := \partial \Omega(t) = \Sigma \cup S = \Sigma \cup \Gamma_i \cup \Gamma_o$$

In [9] and many other authors, the matching conditions on Σ are written on the boundary of a fixed reference domain $\partial \Omega_0$ because Koiter's shell model works with a fixed mean surface Σ .

With the notations of [7], assume that the domain of the fluid is $\Omega_t = \mathcal{A}_t(\Omega_0)$ with $\mathcal{A}_t : x_0 \to x_t := \mathcal{A}_t(x_0)$. Let

$$u_{\tau}(x,t) = u(\mathcal{A}_t(\mathcal{A}_{\tau}^{-1}(x)), t), \ \forall x \in \Omega_{\tau}$$

$$\tag{4}$$

Then in Ω_t at $t = \tau$, the Navier-Stokes equations are in ALE format

$$\rho^{f} \frac{\partial \vec{u}_{\tau}}{\partial t} + (\vec{u}_{\tau} - \vec{c}_{\tau}) \cdot \nabla \vec{u}_{\tau} + \nabla p - -\mu \nabla \cdot (\nabla \vec{u}_{\tau} + \nabla \vec{u}_{\tau}^{T}) = 0,$$

$$\nabla \cdot \vec{u}_{\tau} = 0, \quad \text{with} \quad c_{\tau}(x) = -\frac{\partial \mathcal{A}_{t}(\mathcal{A}_{\tau}^{-1}(x))}{\partial t}|_{t=\tau}$$
(5)

3 Transpiration Conditions for the Fluid

3.1 Conservation of Energy

We begin with an important remark on the conservation of energy. The variational formulation of (3)- divided by ρ^s - is, $\forall \hat{u}, \hat{p}$

$$\int_{\Omega(t)} [\hat{u} \cdot (\partial_t u + u \cdot \nabla u) + \nabla p \cdot \hat{u} - \hat{p} \nabla \cdot u + \frac{\nu}{2} (\nabla u + \nabla u^T) : (\nabla \hat{u} + \nabla \hat{u}^T)] = \int_{\Omega(t)} f^s \cdot \hat{u}$$
(6)

An energy balance is obtained by taking $\hat{u} = u$ and $\hat{p} = -p$,

$$\partial_t \int_{\Omega(t)} \frac{u^2}{2} + \frac{\nu}{2} \int_{\Omega} |\nabla u + \nabla u^T|^2 = \int_{\Omega} f^s \cdot \hat{u} - \int_{\partial \Omega} p u \cdot n \tag{7}$$

because

$$\partial_t \int_{\Omega(t)} u \cdot w = \int_{\Omega(t)} \partial_t (u \cdot w) + \int_{\partial \Omega} v \ u \cdot w$$
$$\int_{\Omega} ((u\nabla u) \cdot u) = \int_{\partial \Omega} u \cdot n \frac{u^2}{2} = \int_{\partial \Omega} \frac{v}{2} u \cdot u$$
(8)

when $v = u \cdot n$, the normal speed of $\partial \Omega$.

With transpiration conditions we intend to work on a fixed domain with zero tangential velocity but non zero normal velocity $u \cdot n = w$. In that case, in order to preserve energy, (6) needs to be modify into

$$\int_{\Omega} [\hat{u} \cdot (\partial_t u + u \cdot \nabla u) + \nabla p \cdot \hat{u} - \hat{p} \nabla \cdot u + \frac{\nu}{2} (\nabla u + \nabla u^T) : (\nabla \hat{u} + \nabla \hat{u}^T)] - \int_{\partial \Omega} \frac{w}{2} u \cdot \hat{u} = \int_{\Omega} f^s \cdot \hat{u}$$
(9)

or equivalently into

$$\int_{\Omega} [\hat{u} \cdot (\partial_t u - u \times \nabla \times u) + \nabla p \cdot \hat{u} - \hat{p} \nabla \cdot u + \frac{\nu}{2} (\nabla u + \nabla u^T) : (\nabla \hat{u} + \nabla \hat{u}^T)] = \int_{\Omega} f^s \cdot \hat{u}$$
(10)

Finally we recall an identity (see [3] for instance) which shows that we can use several forms for the viscous terms:

$$\int_{\Omega} [\nabla \times u \cdot \nabla \times v + \nabla \cdot u \nabla \cdot v] = \int_{\Omega} \nabla u : \nabla v$$
$$= \int_{\Omega} [\frac{1}{2} (\nabla u + \nabla u^{T}) : (\nabla v + \nabla v^{T}) - \nabla \cdot u \nabla \cdot v]$$
(11)

Hence a variational formulation adapted to the problem is to find u with $u\times n=0$ and, for all \hat{p} and all \hat{u} with $\hat{u}\times n=0$

$$\int_{\Omega} [\hat{u} \cdot (\partial_t u - u \times \nabla \times u) - p \nabla \cdot \hat{u} - \hat{p} \nabla \cdot u + \nu \nabla \times u \cdot \nabla \times v] + \int_{\partial \Omega} p u \cdot n = \int_{\Omega} f^s \cdot \hat{u}$$
(12)

3.2 Transpiration

As the wall vessel is $\{x + \eta \vec{n} : x \in \Sigma\}$ and as, by Taylor,

$$\vec{u}(x+\eta\vec{n}) = \vec{u}(x) + \eta\nabla\vec{u}\cdot\vec{n}(x) + o(\eta)$$

matching the velocities of fluid and structure may be written as

$$u + \eta \frac{\partial u}{\partial n} = \vec{n} \frac{\partial \eta}{\partial t} + o(\eta) \text{ on } \Sigma, \quad u \times n = 0$$
 (13)

On a torus of small radius r and large radius R, at a point of coordinates $(R+r\cos\theta)\cos\varphi, (R+r\cos\theta)\cos\varphi, r\sin\theta)$, a straightforward calculation shows that

$$u \times n = 0, \ \nabla \cdot u = 0 \Rightarrow n \cdot \frac{\partial u}{\partial n} = (1 + \frac{r}{R} \cos^2 \theta) \frac{u \cdot n}{r}$$

So (13) becomes

$$u \cdot n = \partial_t \eta \left(1 + \frac{\eta}{r} \left(1 + \frac{r}{R} \cos^2 \theta \right) \right)^{-1}, \quad u \times n = 0 \tag{14}$$

Similarly the normal component of the normal fluid stress tensor is

$$\sigma_{nn}^f = p + 2(1 + \frac{r}{R}\cos^2\theta)\frac{\mu}{r}u \cdot n$$

Therefore for a quasi toroidal geometry, for large R, (1) is

$$\rho_s h \partial_{tt} \eta - \nabla \cdot (\mathbf{T} \nabla \eta) - \nabla \cdot (\mathbf{C} \nabla \partial_t \eta) + a \partial_t \eta + b \eta$$

= $p + 2(1 + \frac{r}{R} \cos^2 \theta) \frac{\mu}{r} \partial_t \eta \left(1 + \frac{\eta}{r} (1 + \frac{r}{R} \cos^2 \theta)\right)^{-1}$ (15)

So, in fine, the domain Ω no longer varies with time but on part of its boundary

$$u \cdot n = \partial_t \eta \left(1 + \frac{\eta}{r} (1 + \frac{r}{R} \cos^2 \theta) \right)^{-1}, \quad u \times n = 0,$$

$$\rho_s h \partial_{tt} \eta - \nabla \cdot (\mathbf{T} \nabla \eta) - \nabla \cdot (\mathbf{C} \nabla \partial_t \eta) + a \partial_t \eta + b \eta = p$$
(16)

where a is a non linear function of η .

Remark 2 Notice that $\eta \ll r$, i.e. large vessels, allows us to eliminate η and write everything in terms of $\partial_t p$ and $u_n := u \cdot n$. It suffices to differentiates the last equation with respect to t and use the first one and integrate in time:

$$p = p_0 + \mathcal{L}(u \cdot n) := \int_0^t \left(\rho_s h \partial_{tt} u_n - \nabla \cdot (T \nabla u_n) - \nabla \cdot (C \nabla \partial_t u_n) + a \partial_t u_n + b u_n \right)$$
(17)

4 Variational Formulation and Approximation

Coming back to (4) and using (17):

Continuous Problem Find u with $u \times n = 0$ and, for all \hat{p} and all \hat{u} with $\hat{u} \times n = 0$

$$\int_{\Omega} [\hat{u} \cdot (\partial_t u - u \times \nabla \times u) - p\nabla \cdot \hat{u} - \hat{p}\nabla \cdot u + \nu\nabla \times u \cdot \nabla \times v] \\ + \int_{\Sigma} \Big(p_0 + \mathcal{L}(u \cdot n) \Big) u \cdot n = - \int_S p_{\Gamma} \hat{u} \cdot n$$

4.1 Approximation in Time

From now on, for clarity, we consider only the case of the surface pressure model, i.e. h = T = C = a = 0, $\mathcal{L}(u \cdot n) = bu \cdot n$. However everything below extends to the full model.

So define

$$U(t) = \int_0^t u(s) ds$$
 and use the integration rule $U^{m+1} = U^m + u^{m+1} dt$.

Then

Time discrete Problem $p(t) = p_0 + bU(t)$ and we seek $u^{m+1} \in V, \hat{p}^{m+1} \in Q$, satisfying for all $\hat{u} \in V, \hat{p} \in Q$,

$$\int_{\Omega} \left[\hat{u} \cdot \left(\frac{u^{m+1} - u^m}{\delta t} - u^{m+\frac{1}{2}} \times \nabla \times u^m \right) - p^{m+1} \nabla \cdot \hat{u} - \hat{p} \nabla \cdot u^{m+\frac{1}{2}} + \nu \nabla \times u^{m+\frac{1}{2}} \cdot \nabla \times \hat{u} \right] + \int_{\Sigma} \left[b \hat{u} \cdot \vec{n} (u^{m+\frac{1}{2}} \delta t + U^m) \cdot \vec{n} \right] = - \int_{S} p_{\Gamma} \hat{u} \cdot n$$
(18)

where $u^{m+\frac{1}{2}} = \frac{1}{2}(u^{m+1} + u^m).$

4.2 Convergence

A convergence analysis was done in [2]; we recall the results. We denote u_{δ} the linear in time interpolate of $\{u^m\}_1^M$ on $(0,T) = \bigcup_1^M [(m-1)\delta t, m\delta t]$. For clarity let's assume that $S = \emptyset$.

Lemma 1 If Ω is $\mathcal{C}^{1,1}$ or polyhedral and $u_0 \in L^2(\Omega)^3$, $p_0 \in H^{1/2}(\Sigma)$, then the weak solution of the continuous problem verifies $u \in L^2(\mathbf{H}^2)$, $\partial_t u \in L^2(\mathbf{L}^2)$, $p \in L^2(H^1)$, and $u \times n = 0$ in $L^2(L^4(\Sigma))$, $\partial_t p = bu \cdot n$ in $L^2(H^{1/2}(\Sigma))$, $p(0) = p_0$

Theorem 1 The solution of the time discretized variational problem satisfies

$$\begin{aligned} \|u_{\delta}\|_{L^{\infty}(\mathbf{L}^{2})} + \sqrt{\nu} \,\|u_{\delta}\|_{L^{2}(\mathbf{H}^{1})} + b \,\|\delta t \,\sum_{k=1}^{n+1} u^{k} \cdot n\|_{L^{\infty}(\mathbf{L}^{2}(\Sigma))} \\ &\leq C \,\left(\|u_{0}\|_{0,2,\Omega} + \frac{1}{\sqrt{\nu}}\|p_{0}\|_{L^{2}(\Sigma)}\right) \end{aligned}$$

Theorem 2 If Ω is simply connected, there is a subsequence $(u_{\delta'}, p_{\delta'})$ which converges to the continuous problem in $L^2(\mathbf{W}) \times H^{-1}(L^2)$ where

$$\mathbf{W} = \{ w \in L^2(\Omega) \, | \, \nabla \times w \in L^2(\Omega), \, \nabla \cdot w \in L^2(\Omega), \, n \times \mathbf{w}_{|_{\Sigma}} = \mathbf{0} \, \}.$$



Figure 1: An implementation using freefem++ for problem (18)

4.3Spatial Discretization with Finite Elements

The easiest is to use penalization to enforce $u \times n = 0$ by adding to the boundary integral $\frac{1}{\epsilon} \int_{\Sigma} u^{m+1} \times n \cdot \hat{u} \times n$. Then we may use conforming triangular or tetrahedral elements P^2 or P^1 +bubble for the velocities and P^1 for the pressure.

A freefem++ implementation (see [6]) is shown on Figure 1

Optimization and Inverse Problems $\mathbf{5}$

5.1**Optimal Stents with the Surface Pressure Model**

A stent is a device to reinforce part of a cardiac vessel and/or to change the topology of the flow by its rigidity. This results in a change of the coefficient b. So with a first order scheme in time we can consider

$$\min_{b(x)} J = \int_{\Sigma \times (0,T)} F(p) dx dt : \text{Subject to}
\int_{\Omega} [\hat{u} \cdot (\frac{u^{m+1} - u^m}{\delta t} - u^{m+1} \times \nabla \times u^m) - p^{m+1} \nabla \cdot \hat{u} - \hat{p} \nabla \cdot u^{m+1}]
+ \int_{\Omega} \nu \nabla \times u^{m+1} \cdot \nabla \times \hat{u} + \int_{\Sigma} (u^{m+1} b \delta t + p^m n) \cdot \hat{u} = -\int_{S} p_{\Gamma} \hat{u} \cdot n
\forall \hat{u} \in V_h, \hat{p} \in Q_h \text{ with } \hat{u} \times n|_{\Gamma} = 0$$
(19)

For instance $F = |p|^4$ will minimize the time averages pressure peak on Σ .

5.1.1 First order discretization and adjoint

Consider the adjoint state

$$\begin{split} &\int_{\Omega} [\hat{v} \cdot \frac{v^m - v^{m+1}}{\delta t} - \hat{v} \times \nabla \times u^{m-1} \cdot v^m - u^{m+1} \times \nabla \times \hat{v} \cdot v^{m+1} \\ &+ \nu \nabla \times v^m \cdot \nabla \times \hat{v} + \nabla \hat{q} \cdot v^m - q^m \nabla \cdot \hat{v}] + \int_{\Sigma} \delta t b v^m \cdot \hat{v} \end{split}$$

$$= \int_{\Sigma} F'(p^m)\hat{q} \tag{20}$$

for all \hat{v}, \hat{q} such that $\hat{v} \times n = 0$ on $\partial \Omega$.

Letting $\hat{v} = \delta u^m$, $\hat{q} = \delta p^m$ and summing in *m*, from 1 to M gives

$$\sum_{1}^{M} \int_{\Sigma} F'(p^{m}) \delta p^{m} \delta t = \sum_{1}^{M} \delta t \int_{\Omega} \delta u^{m} \cdot \frac{v^{m-1} - v^{m}}{\delta t}$$
$$+ \sum_{1}^{M} \delta t \int_{\Omega} \left(-\delta u^{m} \times \nabla \times u^{m-1} \cdot v^{m-1} - u^{m+1} \times \nabla \times \delta u^{m} \cdot v^{m} \right)$$
$$+ \nu \nabla \times v^{m} \cdot \nabla \times \delta u^{m} \right)$$
$$+ \sum_{1}^{M} \delta t \int_{\Omega} \left(\nabla \delta p^{m} \cdot v^{m} - q^{m} \nabla \cdot \delta u^{m} \right) + \int_{\Sigma} \delta t b v^{m} \cdot \delta u^{m}$$
(21)

5.1.2 Optimality Conditions

As $\delta u^0 = 0$ and by choosing $v^M = 0$ it is also

$$\delta J = \sum_{0}^{M-1} \delta t \int_{\Omega} \left(v^m \frac{\delta u^{m+1} - \delta u^m}{\delta t} + v \nabla \times v^{m+1} \cdot \nabla \times \delta u^{m+1} \right)$$
$$- \sum_{0}^{M-1} \delta t \int_{\Omega} \left(\delta u^{m+1} \times \nabla \times u^m \cdot v^m + u^{m+1} \times \nabla \times \delta u^m \cdot v^m \right)$$
$$- \sum_{0}^{M-1} \delta t \left(\int_{\Omega} [\delta p^{m+1} \nabla \cdot v^{m+1} + q^{m+1} \nabla \cdot \delta u^{m+1}] + \int_{\Sigma} (\delta t b \delta u^{m+1} + \delta p^{m+1} n) \cdot v^{m+1} \right)$$
(22)

The same is found by linearizing (19) and taking $\hat{u} = v^m$, $\hat{q} = q^m$, except that there is an additional term due to δb . In fine

$$\delta J = \delta t^2 \int_{\Sigma} \delta b \left(\sum_{0}^{M-1} u^{m+1} \cdot v^m \right)$$
(23)

5.1.3 Preliminary Computer Experiments

Experiment 1 This is only a feasibility test with $F = p^4$; The geometry is a quarter of a torus with R=4 and r=1. It is discretized with 1395 vertices and 6120 elements. The number of unknown of the coupled system $[\vec{u}, p]$ is 23940 with the P^1 -bubble/ P^1 element and Crank-Nicolson implicit scheme. The viscosity is $\nu = 0.01$; we chose $\epsilon = \nu$. The final time is T = 1, the time step is dt = 0.1 and the pressure difference imposed at Γ_i (top) and Γ_o bottom is $6 \cos^2(\pi t)$.

The flow is stored on disk at every iteration ready to be reused backward in time for the adjoint equations.

Starting with b=200, after 3 iterations of steepest descent with fixed step size, the cost function is decreased from 1200 to 900. But as there is no constraint b is much reduced at the top near Γ_i . Consequently the vessel wall becomes fragile as shown by a simulated wall motion by $x \to x + \sum u^m \cdot ndt$ at every time step, as shown on Figure 2.



Figure 2: Top left: Optimization criteria versus iteration number. Top right: the coefficient b(x) after 3 iterations. Bottom Left: effect of the change of b on the dilatation of the vessel and some iso surfaces of constant pressure. Bottom right: a snap shot of the adjoint pressure and some iso surfaces.

Experiment 2 The same computations has been made but now b is constrained to be greater than $b_0/2$. A mesh double the size of the previous one has been used, with 191808 degrees of freedom. The initial value of b is $b_0 = 200$. Af-

ter 10 iterations, similar to Experiment 1 but with a projected gradient method for the optimization, the results of Figure 3 are found.



Figure 3: Left: Optimization criteria $\int_{\Sigma \times (0,T)} p^4$ versus iteration number. Right: the coefficient b(x) after 4 iterations. Right: effect of the change of b on the dilatation of the vessel.

5.2 Identification of b

Finally we run an identification test of b from the observation of the wall displacement, ideally, $u \cdot n$. However the formulation does not allow it becausze the extra integral in the adjoint variational formulation is in competition with a similar term from the surface pressure model, so we used p/b. For this first test the criteria is

$$J = \int_{\Sigma \times (0,T)} |p - p_d|^2 \mathrm{d}x \mathrm{d}t$$

where p_d is obtained from a reference computation (introduction of b in the criteria makes the problem harder) with

$$b = 200 + 100\cos x \cos y \cos z.$$

The results are shown on figure 4.

Because of the computing cost, we made only an initial study; the target is not reached, but 5 iterations go into the right direction. To do better one would have to used a varying step size gradient method and a better computer (this being done on a macbook pro, takes about 15 min).

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Figure 4: Left: Optimization criteria $\int_{\Sigma \times (0,T)} (p-p_d)^2$ versus iteration number. Right: the coefficient b(x) after 5 iterations. middle: The target b.

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