Méthode de quasi-Newton en interaction fluide-structure

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Motivations médicales

Athérosclérose :









Ce que pourrait permettre la simulation :

- mieux comprendre le phénomène
- prévoir les conséquences d'opérations chirurgicales
- améliorer les prothèses



1. Problem statement

Purpose : simulate the mechanical interaction between the wall and the blood in a portion of large vessels





1.1. General equations Fluid models :

Navier-Stokes 2D or 3D (u, p) in Arbitrary Lagrange Euler formulation (w)

Structure models :

• Structure 1D ($d = d_r e_r$) : cylindrical geometry, linear elasticity

$$\rho_w h \frac{\partial^2 d_r}{\partial t^2} - kGh \frac{\partial^2 d_r}{\partial z^2} + \frac{Eh}{1 - \nu^2} \frac{d_r}{R_0^2} - \gamma \frac{\partial^3 d_r}{\partial z^2 \partial t} = \boldsymbol{f}_{\Sigma}$$

• Structure 2D (d). Shell model in large displacements (MITC)

Coupling Fluid-Structure interface Σ_t (reference configuration $\hat{\Sigma}$) :

$$oldsymbol{u}|_{\Sigma_t}=rac{\partialoldsymbol{d}}{\partial t}|_{\hat{\Sigma}}$$

$$=\int_{\Sigma_t}(poldsymbol{n}-2\mu\epsilon(oldsymbol{u})\cdotoldsymbol{n})\cdotoldsymbol{arphi}\,d\sigma$$



1.2. Variational formulation

Let \hat{v} and φ test fonctions independent of t on $\hat{\Omega}$, with v = 0 on Σ_t .

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_{F}(t)} \rho_{F} \boldsymbol{u} \cdot \boldsymbol{v} \, dx + \int_{\Omega_{F}(t)} \rho_{F}(\boldsymbol{u} - \boldsymbol{w}) \cdot \boldsymbol{\nabla} \boldsymbol{u} \cdot \boldsymbol{v} \, dx \\ - \int_{\Omega_{F}(t)} \rho_{F} \boldsymbol{u} \cdot \boldsymbol{v} \, \operatorname{div} \, \boldsymbol{w} \, dx - \int_{\Omega_{F}(t)} p \, \operatorname{div} \, \boldsymbol{v} \, dx + \int_{\Omega_{F}(t)} 2\mu\epsilon(\boldsymbol{u}) \cdot \epsilon(\boldsymbol{v}) \, dx &= 0 \\ \int_{\Omega_{F}(t)} q \, \operatorname{div} \, \boldsymbol{u} &= 0 \\ \int_{\Omega_{F}(t)} \boldsymbol{\nabla} \boldsymbol{w} \cdot \boldsymbol{\nabla} \boldsymbol{v} &= 0 \\ \int_{\Omega_{F}(t)} \rho_{S} \frac{\partial^{2} \boldsymbol{d}}{\partial t^{2}} \cdot \boldsymbol{\varphi} \, d\hat{x} + a(\boldsymbol{d}, \boldsymbol{\varphi}) = \langle \boldsymbol{f}_{\Sigma_{t}}, \boldsymbol{\varphi} \rangle \end{aligned}$$



1.3. Time discretization. Fluid. (implicit Euler)

$$\frac{1}{\delta t} \int_{\Omega_{F}^{n+1}} \rho_{F} u^{n+1} \cdot v + \int_{\Omega_{F}^{n+1}} \rho_{F} (u^{n+1} - w^{n+1}) \cdot \nabla u^{n+1} \cdot v -$$

$$\int_{\Omega_{F}^{n+1}} \rho_{F} u^{n+1} \cdot v \operatorname{div} w^{n+1} - \int_{\Omega_{F}^{n+1}} p \operatorname{div} v + \int_{\Omega_{F}^{n+1}} 2\mu \epsilon (u^{n+1}) \cdot \epsilon (v) = \frac{1}{\delta t} \int_{\Omega_{F}^{n}} u^{n} \cdot v$$

$$\int_{\Omega_{F}^{n+1}} q \operatorname{div} u^{n+1} = 0$$

$$u^{n+1}|_{\Sigma^{n+1}} = \frac{d^{n+1} - d^{n}}{\delta t}$$

$$\int_{\Omega^{n+1}} \nabla w^{n+1} \cdot \nabla v = 0$$

$$w^{n+1}|_{\Sigma^{n+1}} = u^{n+1}|_{\Sigma^{n+1}}$$

$$f_{\Sigma^{n+1}} = \mathcal{F}(d^{n+1})$$



1.4. Time discretization. Structure. (mid-point)

$$\begin{split} \int_{\hat{\Omega}_{S}} \rho_{S} \frac{\boldsymbol{v}_{S}^{n+1} - \boldsymbol{v}_{S}^{n}}{\delta t} \cdot \boldsymbol{\varphi} \, d\hat{x} + \frac{1}{2} a(\boldsymbol{d}^{n}, \boldsymbol{\varphi}) + \frac{1}{2} a(\boldsymbol{d}^{n+1}, \boldsymbol{\varphi}) &= -\langle \boldsymbol{f}_{\Sigma^{n+1}}, \boldsymbol{\varphi} \rangle \\ & \frac{\boldsymbol{d}^{n+1} - \boldsymbol{d}^{n}}{\delta t} &= -\frac{\boldsymbol{v}_{S}^{n+1} + \boldsymbol{v}_{S}^{n}}{2} \end{split}$$

where $<m{f}_{\Sigma^{n+1}},m{arphi}>$ is the "residual" of the fluid problem

$$oldsymbol{d}^{n+1} = \mathcal{S}(oldsymbol{f}_{\Sigma^{n+1}})$$



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1.5. Fluid/structure coupling.

Two main approaches :

(i) Staggered schemes (Piperno, Fahrat, Larrouturou, ...)

At each time step : basically one resolution of \mathcal{F} and one resolution of \mathcal{S} .

 \longrightarrow this seems to be unsuitable for blood flows

(ii) Implicit schemes (Le Tallec & Mouro)

At each time step a nonlinear problem to be solved :

$$d^{n+1} = S \circ \mathcal{F}(d^{n+1})$$

Advantages : stability (energy balance)

Drawback : expensive !

2. Numerical algorithms

2.1. Fixed point algorithms

"Naive" fixed point algorithm

(i) $\boldsymbol{d}_0 = \boldsymbol{d}^n$

(ii) $\boldsymbol{d}_{k+1} = \mathcal{S} \circ \mathcal{F}(\boldsymbol{d}_k)$

 \rightarrow does not converge !





Relaxed fixed point algorithm with prediction

(i)
$$\boldsymbol{d}_0 = \boldsymbol{d}^n + \frac{3\delta t}{2} \boldsymbol{v}_S^n - \frac{\delta t}{2} \boldsymbol{v}_S^{n-1}$$

(ii) $\tilde{\boldsymbol{d}}_{k+1} = S \circ \mathcal{F}(\boldsymbol{d}_k)$
(iii) $\boldsymbol{d}_{k+1} = \omega_k \tilde{\boldsymbol{d}}_{k+1} + (1 - \omega_k) \boldsymbol{d}_k$



How to choose ω_k ?: (i) "by hand": $\omega_k = \omega$

- (ii) Domain decomposition (Le Tallec Mouro) : reformulate the fixed point algorithm as a preconditioned gradient method applied to an interface problem
- (iii) Aitken-like acceleration formula (*Mok Wall Ramm*) : heuristic generalization in *n* dimensions, of the formula that gives the exact solution for affine functions in 1D :

$$\omega_k = \frac{(\boldsymbol{d}_k - \boldsymbol{d}_{k-1}) \cdot (\boldsymbol{d}_k - \boldsymbol{\mathcal{S}} \circ \boldsymbol{\mathcal{F}}(\boldsymbol{d}_k) - \boldsymbol{d}_{k-1} + \boldsymbol{\mathcal{S}} \circ \boldsymbol{\mathcal{F}}(\boldsymbol{d}_{k-1}))}{|\boldsymbol{d}_k - \boldsymbol{\mathcal{S}} \circ \boldsymbol{\mathcal{F}}(\boldsymbol{d}_k) - \boldsymbol{d}_{k-1} + \boldsymbol{\mathcal{S}} \circ \boldsymbol{\mathcal{F}}(\boldsymbol{d}_{k-1})|^2}$$

Mok & co. concluded that (iii) gave slightly better results compared to (ii).



Domain decomposition method (formal)

$$\begin{bmatrix} A_{II}^{F} & A_{I\Sigma}^{F} & 0\\ A_{\Sigma I}^{F} & A_{\Sigma\Sigma}^{F} + A_{\Sigma\Sigma}^{S} & A_{\Sigma I}^{S}\\ 0 & A_{I\Sigma}^{S} & A_{II}^{S} \end{bmatrix} \begin{bmatrix} d_{I}^{F} \\ d_{\Sigma} \\ d_{I}^{S} \end{bmatrix} = \begin{bmatrix} b_{I}^{F} \\ b_{\Sigma} \\ b_{I}^{S} \end{bmatrix} \quad (d_{I}^{F} = \delta t \, u_{I}^{F})$$

(i) Fluid solver with Dirichlet boundary conditions : $A_{II}^F d_{I,k+1}^F = b_I^F - A_{I\Sigma}^F d_{\Sigma,k}$ (ii) Residual (force) computation : $F_{\Sigma,k+1} = A_{\Sigma I}^F d_{I,k+1}^F + A_{\Sigma\Sigma}^F d_{\Sigma,k}$ (iii) Structure solver with Neumann boundary conditions :

$$\begin{bmatrix} A_{\Sigma\Sigma}^S & A_{\Sigma I}^S \\ A_{I\Sigma}^S & A_{II}^S \end{bmatrix} \begin{bmatrix} \tilde{d}_{\Sigma,k+1} \\ d_{I,k+1}^S \end{bmatrix} = \begin{bmatrix} b_{\Sigma} - F_{\Sigma,k+1} \\ b_I^S \end{bmatrix}$$

(iv) $d_{\Sigma,k+1} = \omega_k \tilde{d}_{\Sigma,k+1} + (1 - \omega_k) d_{\Sigma,k}$



• Eliminate $d_{I,k+1}^F$ in (i) and (ii) ($S^F = A_{\Sigma\Sigma}^F - A_{\Sigma I}^F (A_{II}^F)^{-1} A_{I\Sigma}^F$)

$$F_{\Sigma,k+1} = S^F d_{\Sigma,k}^F + A_{\Sigma I}^F (A_{II}^F)^{-1} b_I^F$$

• Eliminate $d_{I,k+1}^S$ in (iii) ($S^S = A_{\Sigma\Sigma}^S - A_{\Sigma I}^S (A_{II})^{-1} A_{I\Sigma}^S$)

$$S^{S}\tilde{d}_{\Sigma,k+1} = b_{\Sigma} - A^{S}_{\Sigma I}(A^{S}_{II})^{-1}b^{S}_{I} - F_{\Sigma,k+1}$$

$$S^{S}\tilde{d}_{\Sigma,k+1} = -S^{F}d_{\Sigma,k} + b_{\Sigma} - A^{S}_{\Sigma I}(A^{S}_{II})^{-1}b^{S}_{I} - A^{F}_{\Sigma I}(A^{F}_{II})^{-1}b^{F}_{I}$$

$$\tilde{d}_{\Sigma,k+1} = (S^S)^{-1}(\tilde{b} - S^F d_{\Sigma,k})$$



• Relaxation :

$$d_{\Sigma,k+1} = \omega_k \tilde{d}_{\Sigma,k+1} + (1 - \omega_k) d_{\Sigma,k}$$

= $d_{\Sigma,k} + \omega_k (\tilde{d}_{\Sigma,k+1} - d_{\Sigma,k})$
= $d_{\Sigma,k} + \omega_k \left[(S^S)^{-1} (\tilde{b} - S^F d_{\Sigma,k}) + d_{\Sigma,k} \right]$
= $d_{\Sigma,k} + \omega_k (S^S)^{-1} \left[\tilde{b} - (S^F + S^S) d_{\Sigma,k} \right]$

• We recognize a gradient method for the solution of

$$(S^F + S^S)d_{\Sigma} = \tilde{b}$$

preconditionned by S^S .

 \longrightarrow this gives a way to design ω_k (e.g. steepest descent)



Benchmark test (Mok, Wall, Ramm in 2D)

Fluid : $\rho_F = 1$, $\mu = 0.01$ Structure : $\rho_S = 500$, E = 250, h = 0.002









Pressure wave in artery

 $\text{Fluid} \approx \text{blood}$









2.2. Quasi-Newton algorithms

$$\mathcal{R} = \mathcal{I} - \mathcal{S} \circ \mathcal{F}$$
$$\mathcal{R} d = 0$$

(i) $d_0 = d^n + \frac{3\delta t}{2} v_S^n - \frac{\delta t}{2} v_S^{n-1}$ (ii) $\tilde{\mathcal{R}}'(d_k) \delta d_k = -\mathcal{R}(d_k)$ (iii) $d_{k+1} = d_k + \lambda_k \delta d_k$

 $\tilde{\mathcal{R}}'$ is a suitable approximation of \mathcal{R}'

 λ_k is determined *via* a linesearch strategy.



First possibility : automatic differentiation

Second possibility : (Brown & Saad)

The linear system at step (ii) is solved approximatively with a few iterations of GMRES. The matrix/vector products $\mathcal{R}'(d_k)z$ are evaluated by computing :

$$\frac{\mathcal{R}(\boldsymbol{d}_k + hz) - \mathcal{R}(\boldsymbol{d}_k)}{h}$$

or (better)

$$\frac{\mathcal{R}(\boldsymbol{d}_k + hz) - \mathcal{R}(\boldsymbol{d}_k - hz)}{2h}$$

It works, but it's expensive and it's difficult to choose h.

Third possibility : evaluate the continuous Jacobian of the fluid structure problem (*Fernandez & Moubachir*). To be tested !

Fourth possibility :

use a reduced model.

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3. Reduced FSI models

- 3.1. Classical 1D model :
- cylinder
- axial symmetry
- no radial velocity



-
$$|\mathcal{S}|$$
 (area of \mathcal{S})

-
$$Q = \int_{\mathcal{S}} u_z \, d\sigma$$

(flux through
$$S$$
) ou \overline{u}

-
$$\overline{p} = \frac{1}{A(z)} \int_{\mathcal{S}} p \, d\sigma$$

(mean pressure moyenne)



mass conservation :

div
$$\mathbf{u} = 0 \implies \qquad \frac{\partial A}{\partial t} + \frac{\partial Q}{\partial z} = 0$$

momentum along z:

$$\frac{\partial u_z}{\partial t} + \operatorname{div}\left(u_z \mathbf{u}\right) + \frac{1}{\rho_F} \frac{\partial p}{\partial z} - \nu \Delta u_z = 0 \Longrightarrow \left| \frac{\partial Q}{\partial t} + \frac{\partial}{\partial z} \left(\alpha \frac{Q^2}{A} \right) + \frac{A}{\rho_F} \frac{\partial \overline{p}}{\partial z} + K_R \frac{Q}{A} = 0 \right|$$

wall law : relation between \overline{p} and A

e.g.:
$$\Phi(A) = p_0 + \frac{\sqrt{\pi}h_0E}{(1-\nu^2)A_0} \left(\sqrt{A} - \sqrt{A_0}\right) \Longrightarrow \qquad \overline{p} = \beta_0 + \beta\sqrt{A}$$

Main difficulties :

- geometry : cylinder
- mean value variables : 3D \rightarrow 1D \rightarrow 3D



3.2. A new reduced model

An important feature in fluid structure interaction problems in blood flow is the so-called "mass added effect".

This effect can be captured with a non-viscous linear fluid model :

$$\begin{cases} \rho_F \partial_t \boldsymbol{u} + \boldsymbol{\nabla} p &= 0 & \text{on } \bar{\Omega}_F \\ \text{div } \boldsymbol{u} &= 0 & \text{on } \bar{\Omega}_F \\ \boldsymbol{u} \cdot \boldsymbol{n} &= \partial_t \boldsymbol{d} \cdot \boldsymbol{n} & \text{on } \bar{\Sigma} \end{cases}$$

or,

$$\begin{cases} -\Delta p &= 0 & \text{on } \bar{\Omega}_F \\ \frac{\partial p}{\partial n} &= -\rho_F \frac{\partial \boldsymbol{u}}{\partial t} \cdot \boldsymbol{n} & \text{on } \bar{\Sigma} \end{cases}$$



3.3. The special case of the generalized wave equation

Notation :
$$\begin{cases} -\triangle p = 0 & \text{on } \Omega_F \\ \frac{\partial p}{\partial n} = g & \text{on } \Sigma & \longrightarrow \end{cases} \begin{array}{c} p|_{\Sigma} = \mathcal{M}_{\mathcal{A}} g \\ p = p^d & \text{on } \Gamma \end{array}$$

Generalized wave equation for the structure :

$$\rho_S \frac{\partial^2 d_r}{\partial t^2} - a \frac{\partial^2 d_r}{\partial z^2} + b d_r - c \frac{\partial^3 d_r}{\partial z^2 \partial t} = p_{\Sigma}$$

Simplified fluid model : $p_{\Sigma} = -\rho_F \mathcal{M}_A \frac{\partial u}{\partial t} \cdot \boldsymbol{n} = -\rho_F \mathcal{M}_A \frac{\partial^2 d_r}{\partial t^2}$

Simplified fluid-structure problem :

$$(\rho_S + \rho_F \mathcal{M}_{\mathcal{A}}) \frac{\partial^2 d_r}{\partial t^2} - a \frac{\partial^2 d_r}{\partial z^2} + b d_r - c \frac{\partial^3 d_r}{\partial z^2 \partial t} = 0$$



3.4. Three possible applications of the reduced model

With 1D model structure (wave equation) :

(i) A good candidate for studying fluid-structure algorithms(ii) A possible alternative for classical FSI 1D models

With general structure models :

(iii) A good candidate for approximating the jacobian in Quasi-Newton algorithms



(i) A good candidate for studying fluid-structure algorithms

- it is rather simple (linear)
- it shares two important features with the real model :
 - \longrightarrow lots of sub-structuring iterations are needed to converge
 - \longrightarrow analogous property of propagation







Why staggered algorithm does not work in blood flows? Implicit algorithm :

$$\boldsymbol{u}^{n+1} \cdot \boldsymbol{n} = \boldsymbol{v}_S^{n+1} \cdot \boldsymbol{n}$$
$$(\rho_S + \rho_F \mathcal{M}_A) \frac{\boldsymbol{v}_S^{n+1} - \boldsymbol{v}_S^n}{\delta t} - a \frac{\partial^2 d_r^{n+1/2}}{\partial z^2} + b d_r^{n+1/2} - c \frac{\partial^3 d_r^{n+1/2}}{\partial z^2 \partial t} = 0$$

Staggered algorithm :

$$\boldsymbol{u}^{n+1} \cdot \boldsymbol{n} = \boldsymbol{v}_{S}^{n} \cdot \boldsymbol{n}$$

$$\rho_{S} \frac{\boldsymbol{v}_{S}^{n+1} - \boldsymbol{v}_{S}^{n}}{\delta t} + \rho_{F} \mathcal{M}_{\mathcal{A}} \frac{\boldsymbol{v}_{S}^{n} - \boldsymbol{v}_{S}^{n-1}}{\delta t} - a \frac{\partial^{2} d_{r}^{n+1/2}}{\partial z^{2}} + b d_{r}^{n+1/2} - c \frac{\partial^{3} d_{r}^{n+1/2}}{\partial z^{2} \partial t} = 0$$



$$\begin{bmatrix} D_{n+1} \\ V_{n+1} \\ W_{n+1} \end{bmatrix} = P \begin{bmatrix} D_n \\ V_n \\ W_n \end{bmatrix}$$

Spectral property of the iteration matrix P:

- For $\rho_F/\rho_S > 0.001$ (roughly) : $|\lambda_k| >> 1$
- $|\lambda_k|$ increases when δt decreases



(ii) A possible alternative for classical FSI 1D models

$$\frac{\partial}{\partial t} \begin{bmatrix} A \\ Q \end{bmatrix} + \frac{\partial}{\partial z} \begin{bmatrix} Q \\ \frac{Q^2}{A} + \frac{\beta}{3} A^{3/2} \end{bmatrix} = \begin{bmatrix} 0 \\ -K \frac{Q}{A} \end{bmatrix}$$

versus

$$(\rho_S + \rho_F \mathcal{M}_{\mathcal{A}}) \frac{\partial^2 \boldsymbol{d}}{\partial t^2} - a \frac{\partial^2 \boldsymbol{d}}{\partial z^2} + b \boldsymbol{d} - c \frac{\partial^3 \boldsymbol{d}}{\partial z^2 \partial t} = 0$$

What has been lost?

- nonlinearity
- viscous effect

What has been gained?

- same variables as the complete model (3D-3D)
- realistic structure response

(iii) Approximate the tangent operator of the real problem

(i) Prediction : $\boldsymbol{d}_0 = \boldsymbol{d}^n + rac{3\delta t}{2} \boldsymbol{v}_S^n - rac{\delta t}{2} \boldsymbol{v}_S^{n-1}$

(ii) Resolution of $\tilde{\mathcal{R}}'(\boldsymbol{d}_k)\delta\boldsymbol{d}_k = -\mathcal{R}(\boldsymbol{d}_k)$

- evaluate $-\mathcal{R}(d_k)$ (with $\mathcal{R} = \mathcal{I} \mathcal{S} \circ \mathcal{F}$)
- Solve the linear system with GMRES (tolerance 10^{-3} , about 8 iterations). The matrix/vector products being evaluated by :

$$\tilde{\mathcal{R}}'(d_k)z = z - \mathcal{S}'(\mathcal{F}(d_k)) \cdot \tilde{\mathcal{F}}'(d_k)z$$

 \longrightarrow one resolution of a scalar Poisson problem

(instead of Navier-Stokes)

→ one resolution of the linearized structure (already computed and factorized during the structure solution)

(iii) $d_{k+1} = d_k + \lambda_k \delta d_k$

In practice the linesearch procedure is never activated ($\lambda_k = 1$) : the approximated jacobian is not so bad !











Mean number of fluid-structure evaluations :

	Aitken	Quasi-Newton	Speed up
2D	24.7	6.1	4.
3D	33.9	8.9	3.8

Computational time :

	Aitken	Quasi-Newton	Speed up
2D	43 min	16 min	2.7
3D	12 h 16	5 h 13	2.4

