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FREE BOUNDARY FLOWS



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FREE BOUNDARY FLOWS WITH STRONG INTERFACIAL EFFECTS



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MODELING ANALYSIS AND SIMULATIONS

Free Boundary Flows

Free boundary flows involve deformable interfaces



Free Boundary vs Fixed Domains



▷ Additional Unknowns. one has to solve not only for the fluid velocity and pressure, but simultaneously also for the location of the interface and its evolution in time:

$$\mathbf{u}(x,y;t), \ p(x,y;t), \ \eta(x;t)$$
 (1)

Fluid-structure interaction: solve elasticity equations

▷ Additional Nonlinearities. The interface deformation is coupled to the fluid flow both <u>kinematically</u> (continuity of the velocities) and <u>dynamically</u> (balance of stresses), and the coupling is nonlinear. Coating Flows

flow dominated by capillary effects

 $Ca = \mu V/\sigma < 1$

- Ca: Capillary number
 μ: fluid viscosity
 V: characteristic velocity
 - σ : surface tension

Arterial Blood Flow

fluid and structure of comparable densities

 $\varrho_s/\varrho_f \leq 1$

 ϱ_s : structure density ϱ_f : fluid density

When interfacial effects are strong the coupling at the deformable interface is higly non-linear \rightarrow numerical instabilities

STATE OF THE ART: Several commercial and non-commercial codes. Free boundary flows with strong interfacial effects are usually solved using strongly coupled schemes: robust and stable

but with high computational costs and convergence issues

MAIN GOAL: Design schemes which combine stability low computational costs modularity

STRATEGY: use <u>operator splitting</u> method for time-discretization. Numerical instabilities can be controlled by treating carefully the kinematic and the dynamic coupling conditions.

\triangleright Arterial Blood Flow

- Modeling: blood and vessel wall
- Full Problem vs Reduced Effective Models
- Numerical solutions of the Full Problem
 - \rightarrow Kinematically-coupled algorithm

 \triangleright Coating Flow

- Slot Coater
- Comparison with Monolothic Scheme by Pasquali (Rice U.)

Arterial Blood Flow - Motivation



- cardiovascular diseases \leftrightarrow changes in blood flow and wall deformation (e.g. atherosclerosis, aneurysms,...)
- \bullet long-term success of clinical treatments \leftrightarrow changes induced on blood flow and body reaction
- fluid-structure interaction are mathematically very challenging

Proper resolution of fluid-structure interaction is one of the core problems!

Arterial Blood Flow - Modeling







heterogeneous and anisotropic nonlinear and viscoelastic pre-stressed suspension cells and plasma complex rehology

Arterial Blood Flow - Modeling



Models for vessel wall (structure) and blood (fluid) which is:

- complicated enough to catch the interesting phenomena
 - simple enough to be solved in a reasonable way

 \rightarrow Reduced Effective Models helps!

- based multiscale analysis (e.g. $R/L = \varepsilon$). Huge literature Barnard et al. 1964, Noseda 1974, Quarteroni et al. 2000, Olufsen et al. 2000, Formaggia et al. 2002, Smith et al. 2002
- avaraged equations on cross section \rightarrow ad hoc closure
- homogenization theory (Canic and Mikelic 2002) \rightarrow no ad hoc closure



Wall viscoelasticity: mathematical or physiological?



Left: In Vivo. Armentano et al. 1995

Right: Reduced Effective Model. Canic, Tambaca, Guidoboni, Mikelic, Hartley, Rosenstrauch 2006 (large-to-medium arteries, linear elasticity, thin shell, Kelvin-Voigt viscoelasticity)



- Prestress: present but not very important (Mikelic, Guidoboni, Canic 2007)
- Wall Displacement: radial >> longitudinal \rightarrow consider only radial
- Wall Thickness: we will consider thin walls
- Blood: large arteries: small non-Newtonian effects \rightarrow Navier-Stokes
- Well-posedness: open field!!!

Now we will see a specific model as a benchmark to present and test our novel numerical approach

Benchmark Problem: Mathematical Model



Fluid: Navier-Stokes eqs

$$\begin{split} \varrho_f(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) &= -\nabla p + \mu \Delta \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega \times (0, T), \\ \mathbf{u} &= (u_1, u_2) \text{: fluid velocity; } p \text{: pressure, } \varrho_f \text{: fluid density, } \mu \text{: fluid viscosity.} \\ \\ \hline \frac{\text{Dynamic and Kinematic Interfacial Coupling:}}{\varrho_s h_s \partial_t^2 \eta + a\eta - b \partial_x^2 \eta - \gamma \partial_t \partial_x^2 \eta = p|_{y=\eta(x,t)} \quad \text{on } (0, L) \times (0, T) , \\ \partial_t \eta &= u_2|_{y=\eta(x,t)}, \quad u_1|_{y=\eta(x,t)} = 0 \end{split}$$

 η : transverse displacement; ϱ_s : structure density; h_s : structure thickness; a, b, γ : elastic constants. (Causin, Gerbeau, Nobile 2005)

Traditional Partitioned Schemes (Loosely Coupled)

Farhat et al. 1998, Zhao et al. 1998, Quarteroni et al. 2000

- 1. Given η and $\partial_t \eta$ at t^n
- 2. Use $\partial_t \eta$ at t^n as Dirichlet condition for the fluid \rightarrow compute \mathbf{u} , p fluid solver with given b.c.
- 3. Use it to force the structure \rightarrow compute η and $\partial_t \eta$ structure solver with given load
- 4. go to t^{n+1} and Step1



• Implicit: iterate between fluid and structure till the coupling conditions are satisfied to a certain tolerance. Quarteroni, Nobile, Formaggia



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- Semi-Implicit: strong coupling between fluid pressure and structure displacement, while the fluid velocity is decoupled. Gerbeau, Grandmont, Quaini, Quarteroni

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Our Goal: combine stability of strongly coupled schemes with low computational cost and modularity of loosely coupled schemes

Kinematically-coupled scheme: Main Ideas

Guidoboni, Glowinski, Cavallini, Canic, Lapin (AML)

 \rightarrow Time-discretization via operator splitting. Splitting at differential level: freedom to use different time steps and/or space approximations in different substeps

→ Cardinal role of kinematic condition. (Kinematically-coupled scheme)
(1) first-order formulation → operator-splitting theory
(2) link velocities of fluid & structure → Added-Mass Effect

\rightarrow Split hyperbolic & parabolic parts.

Traditional schemes follow <u>multi-physics</u>: fluid vs structure Our scheme follows <u>multi-math</u>: hyperbolic vs parabolic Deeply related to our analytical studies on well-posedness Kim, Canic, Guidoboni, Mikelic

Mathematical Model: New notation

Assume small displacement \rightarrow fix fluid domain

$$\begin{split} \varrho_f \partial_t \mathbf{u} &= \Phi(\mathbf{u}, p), \quad \nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega \times (0, T), \\ \varrho_s h_s \partial_t^2 \eta &= \Psi(\eta) + \Pi(\partial_t \eta) + \Upsilon(\mathbf{u}, p) \quad \text{on } (0, L) \times (0, T), \\ \partial_t \eta &= u_2|_{y=H} \quad \text{on } (0, L) \times (0, T), \end{split}$$

with:

$$\begin{split} \Phi(\mathbf{u}, p) &= -\varrho_f \mathbf{u} \cdot \nabla \mathbf{u} - \nabla p + \mu \Delta \mathbf{u} \\ \Psi(\eta) &= -a\eta + b\partial_x^2 \eta \to \text{elasticity} \\ \Pi(\partial_t \eta) &= \gamma \partial_x^2 \partial_t \eta \to \text{viscoelasticity} \\ \Upsilon(\mathbf{u}, p) &= p|_{y=H} \to \text{interfacial hydrodynamic load} \end{split}$$

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Use the kinematic condition $\partial_t \eta = u_2|_{y=H}$ to obtain a first-order formulation

$$\begin{split} \varrho_f \partial_t \mathbf{u} &= \Phi(\mathbf{u}, p), \quad \nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega \times (0, T), \\ \varrho_s h_s \partial_t^2 \eta &= \Psi(\eta) + \Pi(\partial_t \eta) + \Upsilon(\mathbf{u}, p) \quad \text{on } (0, L) \times (0, T), \\ \partial_t \eta &= u_2|_{y=H} \quad \text{on } (0, L) \times (0, T), \end{split}$$

becomes:

$$\begin{split} \varrho_f \partial_t \mathbf{u} &= \Phi(\mathbf{u}, p), \quad \nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega \times (0, T) ,\\ \varrho_s h_s \partial_t u_2|_{y=H} &= \Psi(\eta) + \Pi(u_2|_{y=H}) + \Upsilon(\mathbf{u}, p) \quad \text{on } (0, L) \times (0, T) \\ \partial_t \eta &= u_2|_{y=H} \quad \text{on } (0, L) \times (0, T) . \end{split}$$

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Now we can properly apply the operator splitting technique for the time discretization

Operator Splitting Method

Consider the initial value problem:

 $\partial_t \varphi + A(\varphi, t) = 0$ in $(0, T), \quad \varphi(0) = \varphi_0$ (2)

Assume $A = A_1 + A_2$.

Let $\varphi^n = \varphi(t^n)$ be given.

1. Solve first

 $\partial_t \varphi + A_1(\varphi, t) = 0 \quad \text{in} \quad (t^n, t^{n+1}), \quad \varphi(t^n) = \varphi^n \tag{3}$ and then set $\varphi(t^{n+1}) = \varphi^{n+1/2}.$

2. Then solve

$$\partial_t \varphi + A_2(\varphi, t) = 0 \quad \text{in} \quad (t^n, t^{n+1}), \quad \varphi(t^n) = \varphi^{n+1/2}$$
(4)
and then set $\varphi(t^{n+1}) = \varphi^{n+1}$.

(see e.g. Yanenko (1971), Marchuk(1975,1990), Glowinski (2003))

- the decomposition is not unique
- \bullet the communication between sub-steps is through the initial conditions \rightarrow modules of black boxes
- freedom of using different time steps and/or spatial approx. for the same variable in different substeps
- \bullet stability may be achieved with different choices for the decomposition of A
- splitting error may compromise accuracy
 - \rightarrow symmetrization

Step1:

$$\begin{split} \varrho_f \partial_t \mathbf{u} &= \Phi(\mathbf{u}, p), \quad \nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega \times (0, T) ,\\ \varrho_s h_s \partial_t u_2|_{y=H} &= \Psi(\eta) + \Pi(u_2|_{y=H}) + \Upsilon(\mathbf{u}, p) \quad \text{on } (0, L) \times (0, T) \\ \partial_t \eta &= u_2|_{y=H} \quad \text{on } (0, L) \times (0, T) . \end{split}$$

Step2:

$$\begin{split} \varrho_f \partial_t \mathbf{u} &= \Phi(\mathbf{u}, p), \quad \nabla \cdot \mathbf{u} = 0, \quad \text{in } \ \Omega \times (0, T) \ ,\\ \varrho_s h_s \partial_t u_2|_{y=H} &= \Psi(\eta) + \Pi(u_2|_{y=H}) + \Upsilon(\mathbf{u}, p) \quad \text{on } (0, L) \times (0, T) \\ \partial_t \eta &= u_2|_{y=H} \quad \text{on } (0, L) \times (0, T) \ . \end{split}$$



Kinematically-coupled scheme: Step1

Given
$$\mathbf{u}(t^n) = \mathbf{u}^n$$
, $\eta(t^n) = \eta^n$, and $\partial_t \eta(t^n) = g^n$, solve:

$$\varrho_f \partial_t \mathbf{u} = \Phi(\mathbf{u}, p), \quad \nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega \times (t^n, t^{n+1}),$$

 $\varrho_s h_s \partial_t u_2|_{y=H} = \Pi(u_2|_{y=H}) + \Upsilon(\mathbf{u}, p), \text{ on } (0, L) \times (t^n, t^{n+1}),$

and then set
$$\mathbf{u}(t^{n+1}) = \mathbf{u}^{n+1/2}$$
 and $p(t^{n+1}) = p^{n+1}$.

MAIN IDEA:

The hydrodynamic part of the structure equation $\Pi(u_2|_{y=H}) + \Upsilon(\mathbf{u}, p)$ (viscoelasticity and fluid stress on the interface) are treated together with the fluid equations \rightarrow more inertia on the interface avoiding Added-Mass effect Kinematically-coupled scheme: Step2

Given
$$\eta(t^n) = \eta^n$$
, and $\partial_t \eta(t^n) = u_2|_{y=H}^{n+1/2}$, solve:

 $\partial_t \eta = u_2|_{y=H}$ $\varrho_s h_s \partial_t u_2|_{y=H} = \Psi(\eta)$

on $(0, L) \times (t^n, t^{n+1})$, and then set $\eta(t^{n+1}) = \eta^{n+1}$ and $\partial_t \eta(t^{n+1}) = u_2|_{y=H}^{n+1}$.

MAIN IDEA:

The elastic part of the structure equation $\Psi(\eta)$ is non-dissipateive and it is treated in a separate step \rightarrow non-dissipative solver

Blood Flow - Numerical Test

Benchmark Test: Formaggia et al. 2001. SHOW MOVIE



viscosity	μ	0.035	poise
fluid density	$ ho_f$	1	g/cm^3
young modulus	E	$0.75 \ 10^6$	$dynes/cm^3$
poisson coefficient	σ	0.5	[1]
structure density	$ ho_s$	1.1	g/cm^2
structure thickness	h_s	0.1	cm
shear modulus	G	$\frac{E \ hs}{2(1+\sigma)}$	dynes/cm
structure viscoelasticity	γ	0.01	poise \cdot cm
inlet pressure	\bar{p}_{max}	$2 \ 10^4$	$dynes/cm^2$
inlet pressure duration	$ au_{max}$	5	ms

Results with the kinematically-coupled scheme



Results with implicit scheme by Formaggia et al. 2001



Different time steps: displacement



Different time steps: pressure



Different time steps and mesh size: displacement



Different time steps and mesh size: pressure



Blood Flow - Numerical Test

Benchmark Test: density ratio beyond critical limit

viscosity	μ	0.035	poise
fluid density	$ ho_f$	10	g/cm^3
young modulus	E	$0.75 \ 10^6$	$dynes/cm^3$
poisson coefficient	σ	0.5	[1]
membrane density	$ ho_s$	1.1	g/cm^2
membrane thickness	h_s	0.1	cm
shear modulus	G	$\frac{E \ hs}{2(1+\sigma)}$	dynes/cm
membrane viscoelasticity	γ	0.01	poise \cdot cm
inlet pressure	\bar{p}_{max}	$2 \ 10^4$	$dynes/cm^2$
inlet pressure duration	$ au_{max}$	5	ms

SHOW MOVIE

Comparison with implicit schemes - Flow rate



(Implict scheme results from Nobile PhD Thesis)



Milestone work: Silliman (1979)

Monolithic Algorithm: Pasquali and Scriven (2004).

Comparison splitting/monolithic:

G. Guidoboni, R. Glowinski, M. Pasquali. Submitted to JCAM.

Time evolution of the free surface profile



Time evolution of the height of the free surface at x = 8



- Thick structure: work in progress
- Accuracy: first-order. Symmetrization?
- 3-D
- Clinically relevant problems

COLLABORATORS

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GRANTS

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