Automatic differentiation of a fluid-structure interaction problem

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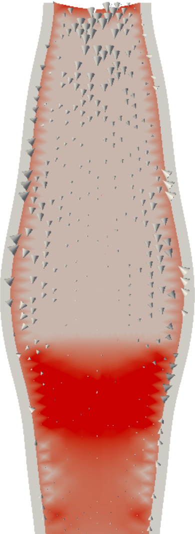
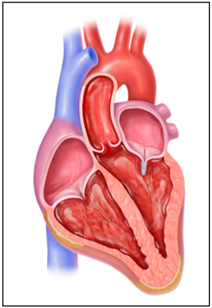
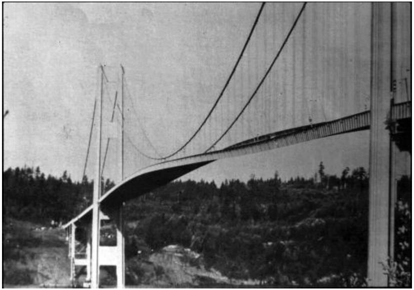
University of Oslo FEniCS Worksop 2013, Cambridge 2013–03–18



March 20, 2013

Examples of Fluid–structure interaction





Modelling Challenges

- model must integrate solid and fluid mechanics
- fluid geometry depends on structure deformation

Solving the FSI problem

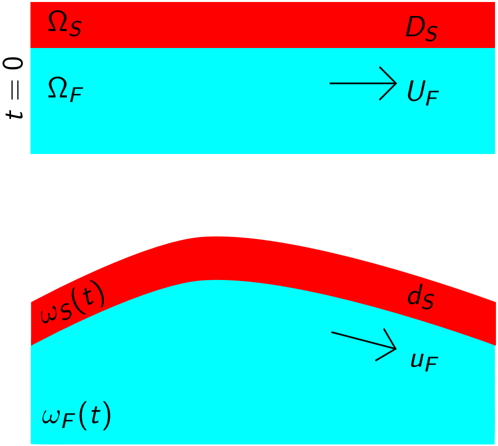
Issues:

- Continuum mechanics formulation
- Partitioned vs monolithic
- Fixed-pointed vs Newton
- Approximation of the Jacobian

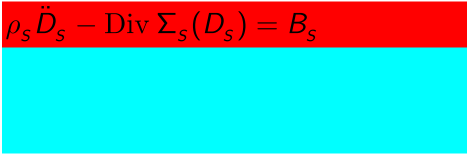
In this work we:

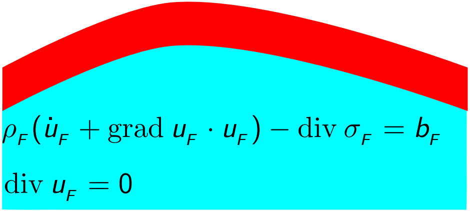
- derive a **Newton's** method with exact Jacobians for FSI problems using the **arbitrary Lagrangian Eulerian** formulation
- implement a **monolithic** solver in Python (using FEniCS)
- investigate various **optimizations** and **simplifications**

Setup of the FSI problem

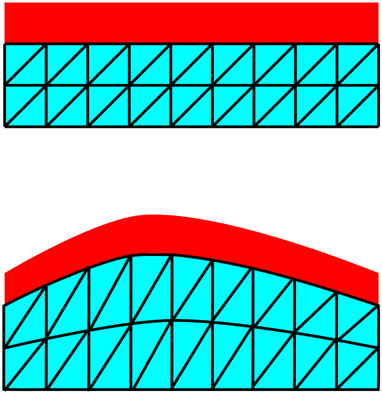


Mismatch in standard fluid and solid models





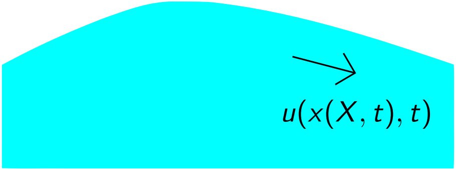
Mesh smoothing problem



Mesh equation

$$\dot{D}_M - \mathrm{Div}\ \Sigma_M(D_M) = 0$$

Arbitrary Lagrangian-Eulerian framework



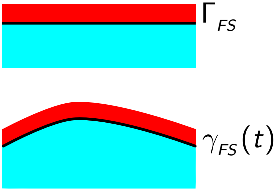
ALE time derivative:

$$\frac{d}{dt}(\rho u) = \rho \dot{u} + \rho \left(\mathrm{grad}\; u \cdot (u - \dot{D}_M)\right)$$

ALE fluid equation:

$$\begin{aligned} \rho_F(\dot{u}_F + \mathrm{grad}\; u_F \cdot (u_F - \dot{D}_M)) - \mathrm{div}\; \sigma_F(u_F, p_F) &= b_F && \text{in } \omega_F(t) \\ \mathrm{div}\; u_F &= 0 && \text{in } \omega_F(t) \end{aligned}$$

Interface conditions



- Stress continuity:

$$\sigma_S \cdot n = \sigma_F \cdot n \quad \text{on } \gamma_{FS}(t)$$

- Kinematic continuity:

$$u_F = u_S \quad \text{on } \gamma_{FS}(t)$$

- Domain continuity:

$$d_M = d_S \quad \text{on } \gamma_{FS}(t)$$

Linearization of the FSI problem

Two challenges:

- Derivative of fluid equation with respect to geometry?

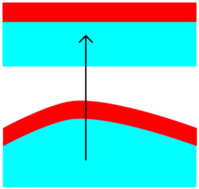
$$\begin{aligned} \frac{d}{dt}(\rho u) - \operatorname{div} \sigma_F(u_F, p_F) &= b_F && \text{in } \omega_F(t) \\ \operatorname{div} u_F &= 0 && \text{in } \omega_F(t) \end{aligned}$$

- Linearization of essential BCs

$$u_F = u_S \quad \text{on } \gamma_{FS}(t)$$

$$d_M = d_S \quad \text{on } \gamma_{FS}(t)$$

The reference domain approach



- Map the fluid problem to the reference domain
- Use standard techniques to differentiate
- Straightforward but tedious
- *Can be automated!*

Navier–Stokes pulled back to reference domain

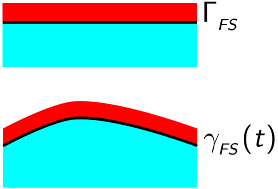
- Equation:

$$\rho_F J_M(\dot{U}_F + \mathrm{Grad}\, U_F \cdot F_M^{-1} \cdot (U_F - \dot{D}_M)) - \mathrm{Div}\;\Sigma_F = B_F$$
$$\mathrm{Div}\,(J_M\; F_M^{-1} \cdot U_F) = 0$$

- Pulled-back fluid stress:

$$\Sigma_F = J_M \left(\mu_F(\mathrm{Grad}\, U_F \cdot F_M^{-1} + F_M^{-\top} \cdot \mathrm{Grad}\, U_F^{\top}) - P_F I\right) \cdot F_M^{-\top}$$

Interface conditions: How to linearize?



Stress continuity:

$$\Sigma_S \cdot N = \Sigma_F \cdot N \quad \text{on } \Gamma_{FS}$$

Kinematic continuity:

$$U_F = U_S \quad \text{on } \Gamma_{FS}$$

Domain continuity:

$$D_M = D_S \quad \text{on } \Gamma_{FS}$$

Linearization of essential boundary conditions

Introduce Lagrange multipliers (τ_F, τ_M) and corresponding trial functions (χ_F, χ_M)

Kinematic continuity:

$$U_F - U_S \tau_{F\,\Gamma_{FS}} + \chi_F v_{F\,\Gamma_{FS}}$$

Domain continuity:

$$D_M - D_S \tau_{M\,\Gamma_{FS}} + \chi_M v_{M\,\Gamma_{FS}}$$

The linearized FSI operator (the Jacobian)

$$R'^{n}(v, \delta U; U^{n}, U^{n-1}) =$$

$$\left\langle v_{F},\ \rho_{F} J_{F}^{n}(\delta \dot{U}_{F}^{n} + \mathrm{Grad}\,\delta U_{F}^{n-\frac{1}{2}} \cdot F_{F}^{-1,n} \cdot (U_{F}^{n-\frac{1}{2}} - \dot{D}_{F}^{n}) + \mathrm{Grad}\,U_{F}^{n-\frac{1}{2}} \cdot F_{F}^{-1,n} \cdot \delta U_{F}^{n-\frac{1}{2}}\right\rangle_{F}$$

$$+ \left\langle \mathrm{Grad}\,v_{F},\ J_{F}^{n}\mu_{F}(\mathrm{Grad}\,\delta U_{F}^{n-\frac{1}{2}} \cdot F_{F}^{-1,n} + F_{F}^{-\top,n} \cdot \mathrm{Grad}\,\delta U_{F}^{\top,n}) \cdot F_{F}^{-\top,n}\right\rangle_{F}$$

$$- \left\langle \mathrm{Grad}\,v_{F},\ J_{F}^{n}\delta P_{F}^{n} \cdot F_{F}^{-\top,n}\right\rangle_{F} + \left\langle q_{F},\ \mathrm{Div}\,(J_{F}^{n}F_{F}^{-1,n} \cdot \delta U_{F}^{n-\frac{1}{2}})\right\rangle_{F}$$

$$- \langle v_{F},\ J_{F}^{n}\,\mathrm{tr}(\mathrm{Grad}\,\delta D_{F}^{n} \cdot F_{F}^{-1,n}) b_{F}\rangle_{F}$$

$$+ \left\langle v_{F},\ \rho_{F} J_{F}^{n}\mathrm{tr}(\mathrm{Grad}\,\delta D_{F}^{n} \cdot F_{F}^{-1})(\dot{U}_{F}^{n} + \mathrm{Grad}\,U_{F}^{n-\frac{1}{2}} \cdot F_{F}^{-1,n} \cdot (U_{F}^{n-\frac{1}{2}} - \dot{D}_{F}^{n}))\right\rangle_{F}$$

$$- \left\langle v_{F},\ \rho_{F} J_{F}^{n}\mathrm{Grad}\,U_{F}^{n-\frac{1}{2}} \cdot F_{F}^{-1,n}(\mathrm{Grad}\,\delta D_{F}^{n} \cdot F_{F}^{-1,n} \cdot (U_{F}^{n-\frac{1}{2}} - \dot{D}_{F}^{n}) + \delta \dot{D}_{F}^{n})\right\rangle_{F}$$

$$+ \left\langle \mathrm{Grad}\,v_{F},\ J_{F}^{n}\mathrm{tr}(\mathrm{Grad}\,\delta D_{F}^{n} \cdot F_{F}^{-1,n})\Sigma_{F} \cdot F_{F}^{-\top,n}\right\rangle_{F}$$

$$- \left\langle \mathrm{Grad}\,v_{F},\ J_{F}^{n}(\mu_{F}\mathrm{Grad}\,U_{F}^{n-\frac{1}{2}} \cdot F_{F}^{-1} \cdot \mathrm{Grad}\,\delta D_{F}^{n} \cdot F_{F}^{-1,n}) \cdot F_{F}^{-\top,n}\right\rangle_{F}$$

$$- \left\langle \mathrm{Grad}\,v_{F},\ J_{F}^{n}(\mu_{F}F_{F}^{-\top,n} \cdot \mathrm{Grad}\,\delta D_{F}^{\top,n} \cdot F_{F}^{-\top,n} \cdot \mathrm{Grad}\,U_{F}^{\top,n-\frac{1}{2}}) \cdot F_{F}^{-\top,n}\right\rangle_{F}$$

$$- \left\langle \mathrm{Grad}\,v_{F},\ J_{F}^{n}\Sigma_{F}(U_{F}^{n-\frac{1}{2}}, P_{F}^{n}, D_{F}^{n}) \cdot F_{F}^{-\top,n} \cdot \mathrm{Grad}\,\delta D_{F}^{\top,n} \cdot F_{F}^{-\top,n}\right\rangle_{F}$$

$$+ \left\langle q_{F},\ \mathrm{Div}\,(J_{F}^{n}(\mathrm{tr}(\mathrm{Grad}\,\delta D_{F}^{n} \cdot F_{F}^{-1,n})I - F_{F}^{-1,n} \cdot \mathrm{Grad}\,\delta D_{F}^{n}) \cdot F_{F}^{-1,n} \cdot U_{F}^{n-\frac{1}{2}})\right\rangle_{F}$$

$$+ \left\langle c_{S},\ \rho_{S}\delta \dot{U}_{S}^{n}\right\rangle_{S} + \left\langle v_{S},\ \delta \dot{D}_{S}^{n} - \delta U_{S}^{n-\frac{1}{2}}\right\rangle_{S}$$

$$+ \left\langle \mathrm{Grad}\,c_{S},\ \mathrm{Grad}\,\delta D_{S}^{n-\frac{1}{2}} \cdot (2\mu_{S}E_{S}^{n-\frac{1}{2}} + \lambda_{S}\mathrm{tr}(E_{S}^{n-\frac{1}{2}})I)\right\rangle_{S}$$

$$+ \left\langle \mathrm{Grad}\,c_{S},\ F_{S}^{n-\frac{1}{2}} \cdot (\mu_{S}(\mathrm{Grad}\,\delta D_{S}^{\top,n-\frac{1}{2}}(I + \mathrm{Grad}\,D_{S}^{n-\frac{1}{2}}) + (I + \mathrm{Grad}\,D_{S}^{\top,n-\frac{1}{2}}) \cdot \mathrm{Grad}\,\delta D_{S}^{n-\frac{1}{2}})\right\rangle_{S}$$

$$+ \Big\langle \mathrm{Grad}\,c_{S},\ F_{S}^{n-\frac{1}{2}} \cdot \lambda_{S}\mathrm{tr}(\tfrac{1}{2}(\mathrm{Grad}\,\delta D_{S}^{\top,n-\frac{1}{2}}(I + \mathrm{Grad}\,D_{S}^{n-\frac{1}{2}}) + (I + \mathrm{Grad}\,D_{S}^{\top,n-\frac{1}{2}}) \cdot \mathrm{Grad}\,\delta D_{S}^{n-\frac{1}{2}}))$$

$$+ \left\langle c_{F},\ \delta \dot{D}_{F}^{n}\right\rangle_{F} + \left\langle \mathrm{Grad}^{s} c_{F},\ 2\mu_{FD}\mathrm{Grad}^{s}\delta D_{F}^{n-\frac{1}{2}} + \lambda_{FD}\,\mathrm{tr}(\mathrm{Grad}\,\delta D_{F}^{n-\frac{1}{2}})I\right\rangle_{F}.$$

$$- \left\langle c_{S},\ J_{F}^{n-\frac{1}{2}}\mu_{F}(\mathrm{Grad}\,\delta U_{F}^{n-\frac{1}{2}} \cdot F_{F}^{-1} + F_{F}^{-\top,n-\frac{1}{2}} \cdot \mathrm{Grad}\,\delta U_{F}^{\top,n-\frac{1}{2}}) \cdot F_{F}^{-\top,n-\frac{1}{2}} \cdot N_{F}\right\rangle_{\Gamma_{FSI}}$$

$$+ \left\langle c_{S},\ J_{F}^{n-\frac{1}{2}}\delta P_{F}^{n} I \cdot F_{F}^{-\top,n-\frac{1}{2}} \cdot N_{F}\right\rangle_{\Gamma_{FSI}}$$

$$+ \left\langle c_{S},\ J_{F}^{n-\frac{1}{2}}(\mathrm{tr}(\mathrm{Grad}\,\delta D_{F}^{n-\frac{1}{2}} \cdot F_{F}^{-1,n-\frac{1}{2}})\mu_{F}F_{F}^{-\top,n-\frac{1}{2}} \cdot \mathrm{Grad}\,U_{F}^{\top,n-\frac{1}{2}}) \cdot F_{F}^{-\top,n-\frac{1}{2}} \cdot N_{F}\right\rangle_{\Gamma_{FSI}}$$

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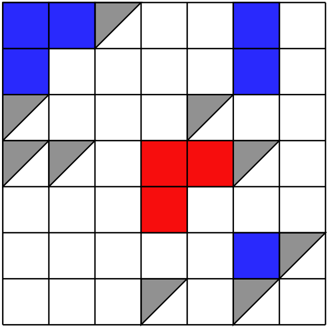
$$- \left\langle c_{S},\ J_{F}^{n-\frac{1}{2}}(\mu_{F}F_{F}^{-\top,n-\frac{1}{2}} \cdot \mathrm{Grad}\,\delta D_{F}^{\top,n-\frac{1}{2}} \cdot F_{F}^{-\top,n-\frac{1}{2}} \cdot \mathrm{Grad}\,U_{F}^{\top,n-\frac{1}{2}}) \cdot F_{F}^{-\top,n-\frac{1}{2}} \cdot N_{F}\right\rangle_{\Gamma_{FSI}}$$

$$- \left\langle c_{S},\ J_{F}^{n-\frac{1}{2}}(\mu_{F}F_{F}^{-\top,n-\frac{1}{2}} \cdot \mathrm{Grad}\,U_{F}^{\top,n-\frac{1}{2}}) \cdot F_{F}^{-\top,n-\frac{1}{2}} \cdot \mathrm{Grad}\,\delta D_{F}^{\top,n-\frac{1}{2}} \cdot F_{F}^{-\top,n-\frac{1}{2}} \cdot N_{F}\right\rangle_{\Gamma_{FSI}}$$

$$+ \langle v_{F},\ \delta L_{U}\rangle_{\Gamma_{FSI}} + \langle m_{U},\ \delta U_{F} - \delta U_{S}\rangle_{\Gamma_{FSI}} + \langle c_{F},\ \delta L_{D}\rangle_{\Gamma_{FSI}} + \langle m_{D},\ \delta D_{F} - \delta D_{S}\rangle_{\Gamma_{FSI}}.$$



FEniCS implementation

```
J = derivative(R, U)
```

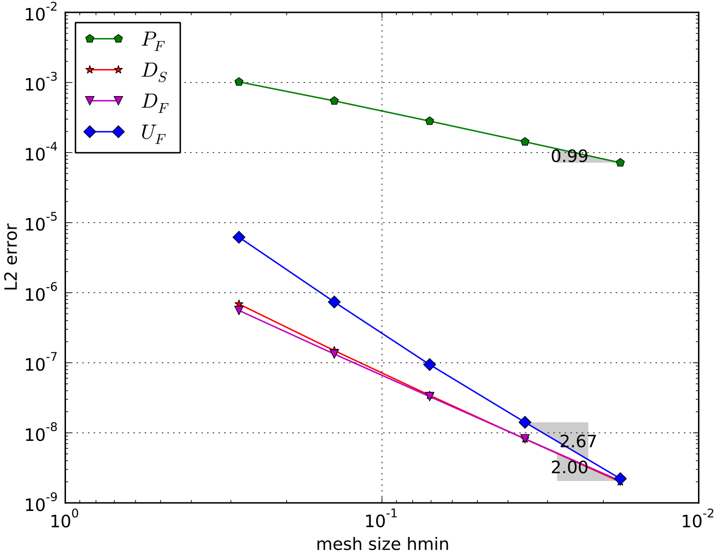
An analytic test problem

pdf/pdf/analyticproblem.pdf$_t ex$

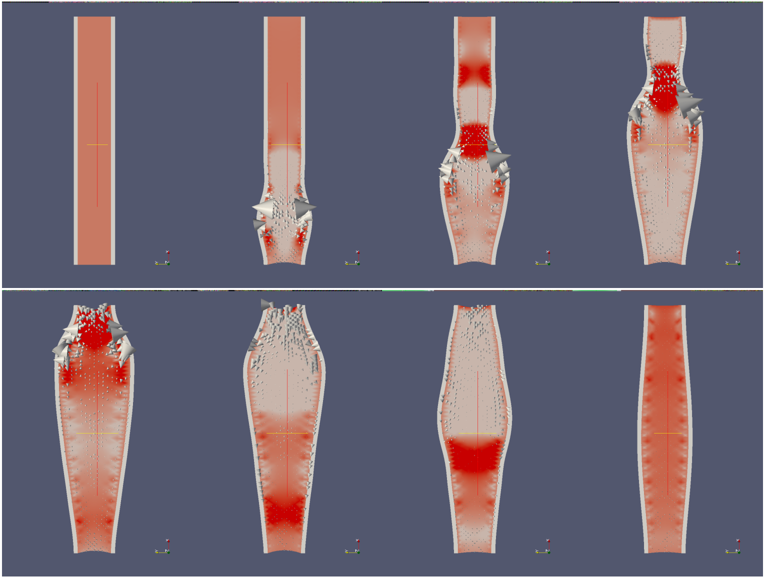
Primary variables:

$$
\begin{aligned}
U_{_F} &= y(1-y)\sin t \\
P_{_F} &= 2C\sin t(1-x-Cxy(1-y)(1-\cos t)) \\
D_{_S} &= Cy(1-y)(1-\cos t) \\
U_{_S} &= Cy(1-y)\sin t \\
D_{_M} &= Cxy(1-y)(1-\cos t)
\end{aligned}
$$

Convergence for analytic test problem



A two-dimensional blood vessel



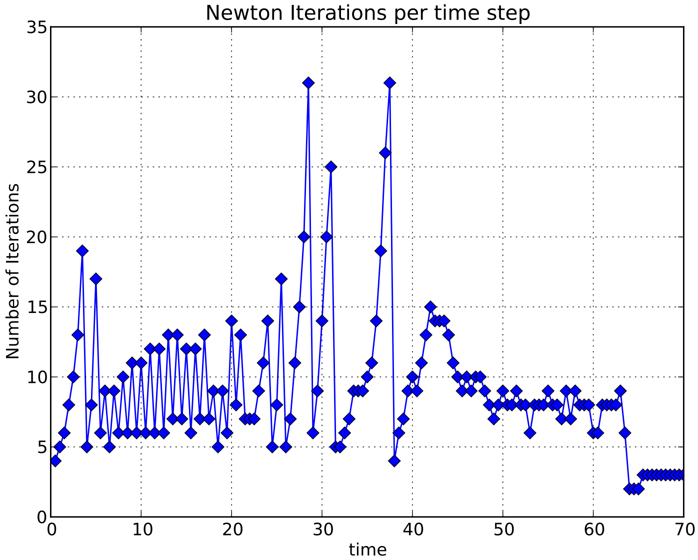
Break-down of run-time

Problem	Routine	Calls	Time (s)	
Analytic problem	Jacobian assembly	28	83.9s	**90%**
mesh size = 231	Linear solve	28	1.86s	2%
time steps = 10	Residual assembly	38	0.915s	1%
Blood vessel	Jacobian assembly	343	2980s	**81%**
mesh size = 1271	Linear solve	343	254s	18%
time steps = 140	Residual assembly	483	64.1s	1%

Effect of Jacobian reuse

Problem	Routine	Calls	
Analytic problem	Jacobian assembly	1 (-27)	-95 %
mesh size = 231	Linear solve	51 (+23)	-96%
time steps = 10	Residual assembly	61 (+23)	+54%
	Total Runtime:		**-93 %**
Blood vessel	Jacobian assembly	25 (-308)	-93 %
mesh size = 1271	Linear solve	1287 (+944)	-92 %
time steps = 140	Residual assembly	1427 (+944)	+192%
	Total		**-91 %**

Effect of Jacobian reuse

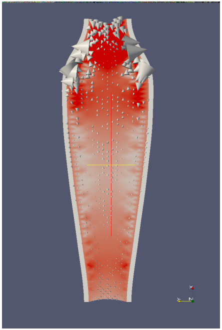


Optimization summary

Optimization	*Runtime*	*Memory*	*Robustness*
Jacobian Reuse			
Jacobian Simplification			
Jacobian Buffering			
Reduced Quadrature Order			

Summary: How to use the automatic derivative to solve FSI problems

- Map the fluid equation to the reference domain
- Impose essential BC's using Lagrange multipliers
- Let the automatic derivative compute the Jacobian



Challenges / work in progress:

- Long FFC compilation times
- Preconditioning