

# Decoupling Navier-Stokes / St. Venant-Kirchhoff Fluid-Structure Interaction by Optimization

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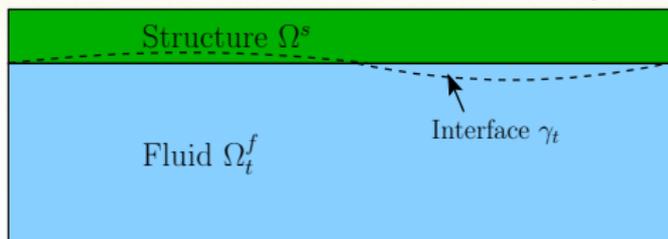
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# A Basic Fluid-Structure Interaction (FSI) Problem



- Fluid (**Navier–Stokes**) and structure (**linear elasticity**) in contact over an interface

$$\rho_f \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) - 2\nu_f \nabla \cdot D(\mathbf{u}) + \nabla p = \mathbf{f}_f \quad \text{in } \Omega_t^f$$

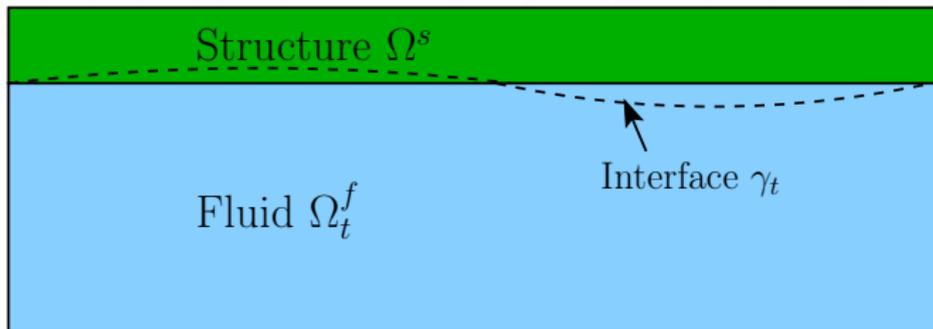
$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega_t^f$$

$$\rho_s \frac{\partial^2 \boldsymbol{\eta}}{\partial t^2} - \nabla \cdot \boldsymbol{\sigma}^s = \mathbf{f}_s \quad \text{in } \Omega^s$$

- Continuity of **velocity**:  $\mathbf{u} = \dot{\boldsymbol{\eta}} \quad \text{on } \gamma_t$
- Continuity of **traction force**:  $\boldsymbol{\sigma}^f \cdot \mathbf{n}_f = -\boldsymbol{\sigma}^s \cdot \mathbf{n}_s \quad \text{on } \gamma_t$

where  $D(\mathbf{v}) := (\nabla \mathbf{v} + \nabla \mathbf{v}^T)/2$  and  $(\boldsymbol{\sigma}^s)_{ij} := 2\mu D(\boldsymbol{\eta})_{ij} + \lambda D(\boldsymbol{\eta})_{kk} \delta_{ij}$

# Challenges of Solving FSI Problems



Solution of FSI problems is challenging because of:

- nonlinear mathematical models
- strong coupling between constituent model components
- moving domain, which require mesh update and/or reassembly
- shape of the fluid domain is part of the solution

# Description of the Optimization Problem

Fluid, Structure

$$\begin{aligned} \rho_f \left[ \left( \frac{\partial \mathbf{u}}{\partial t}, \mathbf{v} \right)_{\Omega^f} + (\mathbf{u} \cdot \nabla \mathbf{u}, \mathbf{v}) \right] + (\boldsymbol{\sigma}^f, \nabla \mathbf{v})_{\Omega^f} - (\rho, \nabla \cdot \mathbf{v})_{\Omega^f} \\ = (\mathbf{f}_f, \mathbf{v})_{\Omega^f} + (\boldsymbol{\sigma}^f \cdot \mathbf{n}_f, \mathbf{v})_{\gamma_t} \\ (\nabla \cdot \mathbf{u}, q)_{\Omega^f} = 0 \end{aligned}$$

$$\rho_s \left( \frac{\partial^2 \boldsymbol{\eta}}{\partial t^2}, \boldsymbol{\xi} \right)_{\Omega^s} + (\boldsymbol{\sigma}^s, \nabla \boldsymbol{\xi})_{\Omega^s} = (\mathbf{f}_s, \boldsymbol{\xi})_{\Omega^s} + (\boldsymbol{\sigma}^s \cdot \mathbf{n}_s, \boldsymbol{\xi})_{\gamma_t}$$

Use  $\boldsymbol{\sigma}^f \cdot \mathbf{n}_f = -\boldsymbol{\sigma}^s \cdot \mathbf{n}_s$  to replace  $(\boldsymbol{\sigma}^f \cdot \mathbf{n}_f, \mathbf{v})_{\gamma_t}$  with  $(\mathbf{g}, \mathbf{v})_{\gamma_t}$  and  $(\boldsymbol{\sigma}^s \cdot \mathbf{n}_s, \boldsymbol{\xi})_{\gamma_t}$  with  $-(\mathbf{g}, \boldsymbol{\xi})_{\gamma_t}$ , i.e., **unknown traction force as a control**.

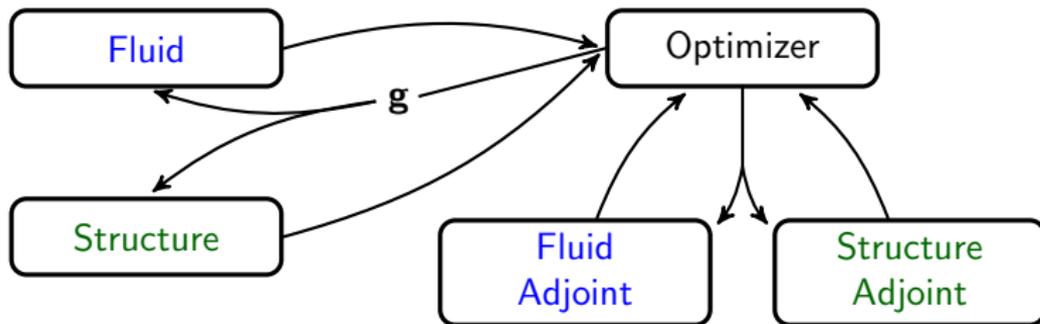
Find a  $\mathbf{g}^n$  that minimizes the functional

$$\mathcal{J}_n^\delta(\mathbf{u}^n, p^n, \boldsymbol{\eta}^n, \dot{\boldsymbol{\eta}}^n, \mathbf{g}^n) = \frac{1}{2} \int_{\gamma_n} |\mathbf{u}^n - \mathcal{V}(\dot{\boldsymbol{\eta}}^n)|^2 d\gamma_n + \frac{\delta}{2} \int_{\gamma_n} |\mathbf{g}^n|^2 d\gamma_n,$$

subject to the flow and structure constraint equations.

# An Optimization-Based FSI Approach

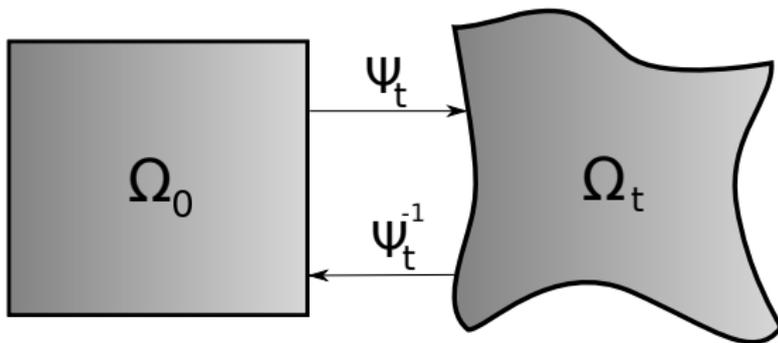
- Use optimization techniques to find an optimal  $\mathbf{g}$  that satisfies continuity of velocity to within some desired tolerance
  - Solve adjoint equations to use steepest descent method
  - **OR** solve linearized (and possibly adjoint) equations to use Gauss-Newton + BICGSTAB/CGLES/GMRES



# Arbitrary Lagrangian–Eulerian (ALE)

- Allows for formulation of the fluid on a moving domain
- Introduces a mesh that moves in time and space

$\Psi_t$  is the time-dependent bijective mapping which maps the reference domain  $\Omega_0$  to the physical domain  $\Omega_t$ :



$$\Psi_t : \Omega_0 \rightarrow \Omega_t, \quad \Psi_t(\hat{\mathbf{x}}) = \mathbf{x}(\hat{\mathbf{x}}, t),$$

where  $\hat{\mathbf{x}}$  and  $\mathbf{x}$  are the spatial coordinates in  $\Omega_0$  and  $\Omega_t$ , respectively.

# Variational Formulation of the Fluid Governing Equations

Using the Reynold's Transport theorem

$$\frac{d}{dt} \int_{\Omega_t} \phi \mathbf{v} \, d\Omega = \int_{\Omega_t} \left( \frac{\partial \phi}{\partial t} \Big|_{\hat{\mathbf{x}}} + \phi \nabla_{\mathbf{x}} \cdot \mathbf{z} \right) \mathbf{v} \, d\Omega,$$

with  $\phi = \mathbf{u}$ , the chain rule, and integration by parts, the variational formulation of the flow equations becomes:

$$\begin{aligned} \rho_f \frac{d}{dt} (\mathbf{u}, \mathbf{v})_{\Omega_t^f} + \rho_f ((\mathbf{u} - \mathbf{z}) \cdot \nabla \mathbf{u}, \mathbf{v})_{\Omega_t^f} - \rho_f (\mathbf{u}(\nabla \cdot \mathbf{z}), \mathbf{v})_{\Omega_t^f} + 2\nu_f (D(\mathbf{u}), D(\mathbf{v}))_{\Omega_t^f} \\ - (p, \nabla \cdot \mathbf{v})_{\Omega_t^f} - (2\nu_f D(\mathbf{u}) \cdot \mathbf{n}_f - p \mathbf{n}_f, \mathbf{v})_{\gamma_t} \\ = (\mathbf{f}_f, \mathbf{v})_{\Omega_t^f} \quad \forall \mathbf{v} \in \mathbf{H}_D^1(\Omega_t^f), \end{aligned}$$

$$(q, \nabla \cdot \mathbf{u})_{\Omega_t^f} = 0 \quad \forall q \in L^2(\Omega_t^f),$$

where  $\mathbf{z}$  is the mesh velocity,  $\mathbf{z} = \frac{d\Psi_t}{dt} \approx \frac{\Psi_n - \Psi_{n-1}}{\Delta t}$ .

# Time Discretization of the Flow Equations

Time discretization by implicit Euler yields

$$\begin{aligned}
 & \frac{\rho^f}{\Delta t} \left[ (\mathbf{u}^n, \mathbf{v})_{\Omega_n^f} - (\mathbf{u}^{n-1}, \mathcal{V}(\mathbf{v}))_{\Omega_{n-1}^f} \right] + \rho^f \left[ ((\mathbf{u}^n - \mathbf{z}^n) \cdot \nabla \mathbf{u}^n, \mathbf{v})_{\Omega_n^f} - (\mathbf{u}^n (\nabla \cdot \mathbf{z}^n), \mathbf{v})_{\Omega_n^f} \right] \\
 & + 2\nu_f (D(\mathbf{u}^n), D(\mathbf{v}))_{\Omega_n^f} - (\rho^n, \nabla \cdot \mathbf{v})_{\Omega_n^f} \\
 & - (2\nu_f D(\mathbf{u}^n) \cdot \mathbf{n}_f - \rho^n \mathbf{n}_f, \mathbf{v})_{\gamma_t} \\
 & = (\mathbf{f}_f^n, \mathbf{v})_{\Omega_n^f} \quad \forall \mathbf{v} \in \mathbf{H}_D^1(\Omega_n^f),
 \end{aligned}$$

$$(q, \nabla \cdot \mathbf{u}^n)_{\Omega_n^f} = 0 \quad \forall q \in L^2(\Omega_n^f).$$

- It is expected that the overall order of the time discretization (fluid and structure) will be only first order.
- Second order time scheme of the structure will be used for analysis because of extra accuracy needed.

# Second Order Time Discretization of the Structure

A second order time discretization of the structure problem is

$$\begin{aligned}
 & \frac{\rho_s}{\Delta t} (\dot{\eta}^n - \dot{\eta}^{n-1}, \xi)_{\Omega^s} \\
 & + 2 \mu \left( \frac{D(\eta^n) + D(\eta^{n-1})}{2}, D(\xi) \right)_{\Omega^s} + \lambda \left( \nabla \cdot \left( \frac{\eta^n + \eta^{n-1}}{2} \right), \nabla \cdot \xi \right)_{\Omega^s} \\
 & - \left( 2 \mu \left( \frac{D(\eta^n) + D(\eta^{n-1})}{2} \right) \cdot \mathbf{n}_s \right) + \lambda \left( \nabla \cdot \left( \frac{\eta^n + \eta^{n-1}}{2} \right) \right) \mathbf{n}_s, \xi \Big|_{\gamma_0} \\
 & = \left( \frac{\mathbf{f}_s^n + \mathbf{f}_s^{n-1}}{2}, \xi \right)_{\Omega^s} \quad \forall \xi \in \mathbf{H}_D^1(\Omega^s), \\
 & \left( \frac{\dot{\eta}^n + \dot{\eta}^{n-1}}{2}, \gamma \right)_{\Omega^s} - \left( \frac{\eta^n - \eta^{n-1}}{\Delta t}, \gamma \right)_{\Omega^s} = 0 \quad \forall \gamma \in \mathbf{L}^2(\Omega^s).
 \end{aligned}$$

# Optimization Constraints

- Set  $\mathbf{g}^n := (2\nu_f D(\mathbf{u}^n) \cdot \mathbf{n}_f - p\mathbf{n}_f - \frac{1}{2}((\mathbf{u}^n - \mathbf{z}^n) \cdot \mathbf{n}_f)\mathbf{u}^n) |_{\gamma_n}$  as our control
- $\frac{1}{2}((\mathbf{u}^n - \mathbf{z}) \cdot \mathbf{n}_f)\mathbf{u}^n$  will be approximately zero since at an optimal solution  $-\mathbf{g}^n$  can be used as the stress for the structure
- $-(\mathbf{g}^n \circ \Psi_n^{-1})J_n$  representing  $(2\mu D(\boldsymbol{\eta}^n) \cdot \mathbf{n}_s + \lambda(\nabla \cdot \boldsymbol{\eta}^n)\mathbf{n}_s) |_{t_0}$

Making this substitution and introducing  $c(\mathbf{u}, \mathbf{v}, \mathbf{w}) = \frac{1}{2}((\mathbf{u}\nabla\mathbf{v}, \mathbf{w})_{\Omega_n^f} - (\mathbf{u}\nabla\mathbf{w}, \mathbf{v})_{\Omega_n^f})$ , the flow constraints become

$$\begin{aligned}
 & \frac{\rho^f}{\Delta t} [(\mathbf{u}^n, \mathbf{v})_{\Omega_n^f} - (\mathbf{u}^{n-1}, \mathcal{V}(\mathbf{v}))_{\Omega_{n-1}^f}] + \rho^f [c(\mathbf{u}^n, \mathbf{u}^n, \mathbf{v})_{\Omega_n^f} + \frac{1}{2}((\mathbf{u}^n \cdot \mathbf{n}_f)\mathbf{u}^n, \mathbf{v})_{\Gamma_n^f}] \\
 & \quad - \frac{1}{2}((\nabla \cdot \mathbf{z}^n)\mathbf{u}^n, \mathbf{v})_{\Omega_n^f} - c(\mathbf{z}^n, \mathbf{u}^n, \mathbf{v})_{\Omega_n^f}] \\
 & \quad + 2\nu_f (D(\mathbf{u}^n), D(\mathbf{v}))_{\Omega_n^f} + (p^n, \nabla \cdot \mathbf{v})_{\Omega_n^f} \\
 & \quad = (\mathbf{f}_f^n, \mathbf{v})_{\Omega_n^f} + (\mathbf{g}^n, \mathbf{v})_{\gamma_n} \quad \forall \mathbf{v} \in \mathbf{H}_D^1(\Omega_n^f), \\
 & (q, \nabla \cdot \mathbf{u}^n)_{\Omega_n^f} = 0 \quad q \in L^2(\Omega_n^f).
 \end{aligned}$$

# Optimization Constraints

Also, the structure equations constraint can be rewritten as

$$\begin{aligned}
 & \frac{\rho_s}{\Delta t} (\dot{\eta}^n - \dot{\eta}^{n-1}, \xi)_{\Omega^s} \\
 & + 2 \mu \left( \frac{D(\eta^n) + D(\eta^{n-1})}{2}, D(\xi) \right)_{\Omega^s} + \lambda \left( \nabla \cdot \left( \frac{\eta^n + \eta^{n-1}}{2} \right), \nabla \cdot \xi \right)_{\Omega^s} \\
 & = \left( \frac{\mathbf{f}_s^n + \mathbf{f}_s^{n-1}}{2}, \xi \right)_{\Omega^s} - \left( \frac{\mathcal{V}(\mathbf{g}^n)J_n + \mathcal{V}(\mathbf{g}^{n-1})J_{n-1}}{2}, \xi \right)_{\gamma_0} \quad \forall \xi \in \mathbf{H}_D^1(\Omega^s), \\
 & \left( \frac{\dot{\eta}^n + \dot{\eta}^{n-1}}{2}, \gamma \right)_{\Omega^s} - \left( \frac{\eta^n - \eta^{n-1}}{\Delta t}, \gamma \right)_{\Omega^s} = 0 \quad \forall \gamma \in \mathbf{L}^2(\Omega^s).
 \end{aligned}$$

# A New Functional

Expected difficulties:

- Not possible to get a stability estimate for  $\dot{\boldsymbol{\eta}}^n$  in  $\mathbf{H}^1(\Omega^s)$
- An optimal  $\hat{\boldsymbol{\eta}}^n$  can be shown only in  $\mathbf{L}^2(\Omega^s)$
- The previous functionals are not well-defined (trace of optimal  $\dot{\boldsymbol{\eta}}^n$  is not well-defined)

We introduce a first order finite difference approximation of  $\dot{\boldsymbol{\eta}}^n$ , and define the new optimization problem as

$$\begin{aligned} \mathcal{J}_n^\delta(\mathbf{u}^n, p^n, \boldsymbol{\eta}^n, \dot{\boldsymbol{\eta}}^n, \bar{\boldsymbol{\eta}}^n, \mathbf{g}^n) &= \frac{1}{2} \int_{\gamma_n} \left| \mathbf{u}^n - \frac{\mathcal{V}(\boldsymbol{\eta}^n) - \mathcal{V}(\boldsymbol{\eta}^{n-1})}{\Delta t} \right|^2 d\gamma_n \\ &\quad + \frac{\delta}{2} \int_{\gamma_n} |\mathbf{g}^n|^2 d\gamma_n, \end{aligned}$$

subject to the flow and structure constraints.

# Penalized Functional as Norm of Nonlinear Function

Define the nonlinear operator  $N_n : \mathbf{L}^2(\gamma_n) \rightarrow \mathbf{L}^2(\gamma_n) \times \mathbf{L}^2(\gamma_n)$  by

$$N_n(\mathbf{g}^n) = \begin{pmatrix} (\mathbf{u}^n - \dot{\eta}^n \circ \Psi_n^{-1})|_{\gamma_n} \\ \sqrt{\epsilon} \mathbf{g}^n \end{pmatrix},$$

where  $\mathbf{u}^n$ ,  $\dot{\eta}^n$  are the fluid and structure velocities when  $\mathbf{g}^n$  is the stress function on the interface. Then, the functional can be written as

$$\mathcal{J}_n(\mathbf{g}^n) = \frac{1}{2} \|N_n(\mathbf{g}^n)\|_{\mathbf{L}^2(\gamma_n) \times \mathbf{L}^2(\gamma_n)}^2$$

and the nonlinear least squares problem we consider is to

*seek  $\mathbf{g}^n \in \mathbf{L}^2(\gamma_n)$  such that  $\mathcal{J}_n(\mathbf{g}^n)$  is minimized.*

# Linearization of Nonlinear Function

We can linearize  $N_n(\mathbf{g}^n)$  using the Fréchet derivative of  $N_n(\cdot)$  at  $\bar{\mathbf{g}}^n$ ,  $N'_n(\bar{\mathbf{g}}^n)$ , by

$$N_n(\mathbf{g}) = N_n(\bar{\mathbf{g}}^n) + N'_n(\bar{\mathbf{g}}^n)(\mathbf{g}^n - \bar{\mathbf{g}}^n) + O(\|\mathbf{g}^n - \bar{\mathbf{g}}^n\|_{\mathbf{L}^2(\gamma_n) \times \mathbf{L}^2(\gamma_n)}^2)$$

so that solutions of the nonlinear least squares problem can be obtained by repeatedly solving the linear least squares problem

$$\min_{\mathbf{h}^n \in \mathbf{L}^2(\gamma_n)} \frac{1}{2} \|N(\bar{\mathbf{g}}^n) + N'_n(\bar{\mathbf{g}}^n)\mathbf{h}^n\|_{\mathbf{L}^2(\gamma_n) \times \mathbf{L}^2(\gamma_n)}^2,$$

where  $\mathbf{h}^n = \mathbf{g}^n - \bar{\mathbf{g}}^n$ . Hence, starting with arbitrary  $\mathbf{g}_{(0)}^n$ , we can find a sequence  $\{\mathbf{g}_{(k)}^n\}$  obtained by  $\mathbf{g}_{(k)}^n = \mathbf{g}_{(k-1)}^n + \mathbf{h}_{(k)}^n$ , where  $\mathbf{h}_{(k)}^n$  is a solution of the linear least squares problem.

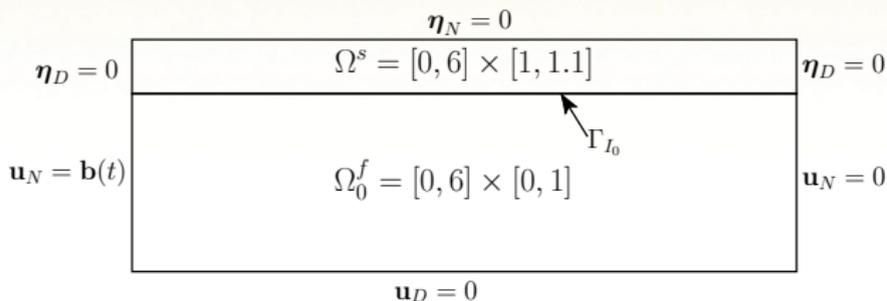
# Gauss-Newton Algorithm

## Algorithm (Gauss-Newton)

1. Choose  $\mathbf{g}_{(0)}^n$ .
2. For  $k = 1, 2, 3, \dots$ ,
  - a. *computable in parallel:*
    - i. find  $\mathbf{u}_{(k)}^n$  and  $p_{(k)}^n$  on  $\Omega_{n,(k-1)}^f$  using  $\mathbf{z}_{(k-1)}^n$  and  $\mathbf{g}_{(k-1)}^n$ ,
    - ii. find  $\boldsymbol{\eta}_{(k)}^n$  and  $\dot{\boldsymbol{\eta}}_{(k)}^n$  using  $\mathbf{g}_{(k-1)}^n$ ,
  - b. update  $\gamma_{n(k)}$ ,  $\mathbf{z}_{(k)}^n$ ,  $\Psi_n^{(k)}$ , and  $\Omega_{n,(k)}^f$  using  $\boldsymbol{\eta}_{(k)}^n$ ,
  - c. if  $\frac{1}{2} \int_{\gamma_{n(k-1)}} |\mathbf{u}^n - \dot{\boldsymbol{\eta}}^n \circ (\Psi_n^{(k-1)})^{-1}|^2 d\gamma < \epsilon_{tol}$ , break,
  - d. compute  $\mathbf{h}_{(k)}^n$  by CGLES, or in some other way solve the least squares problem with  $A = N'_n(\mathbf{g}_{(k-1)}^n)$ ,  $b = -N_n(\mathbf{g}_{(k-1)}^n)$ , and  $x = \mathbf{h}_{(k)}^n$ ,
  - e. set  $\mathbf{g}_{(k)}^n = \mathbf{g}_{(k-1)}^n + \mathbf{h}_{(k)}^n$ .



# Haemodynamic Experiment



$$\mathbf{b}(t) = \begin{cases} (-10^3(1 - \cos \frac{2\pi t}{0.025}), 0) \text{ dyne/cm}^2, & t \leq 0.025 \\ (0, 0), & 0.025 < t < T. \end{cases}$$

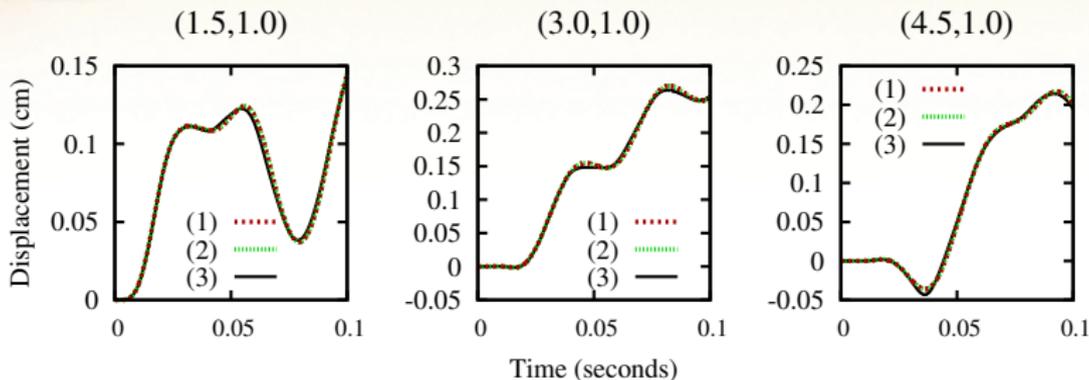
$$\rho_f = 1 \text{ g/cm}^3, \nu_f = 0.035 \text{ g/cm}\cdot\text{s}.$$

$\rho_s = 1.1 \text{ g/cm}^3, E = 3 \times 10^6 \text{ dyne/cm}^2, \nu = 0.3$ . The Lamé-Navier parameters  $\lambda$  and  $\mu$  are defined as follows:

$$\lambda = \frac{\nu E}{(1 - 2\nu)(1 + \nu)} \text{ dyne/cm}^2, \quad \mu = \frac{E}{2(1 + \nu)} \text{ dyne/cm}^2.$$

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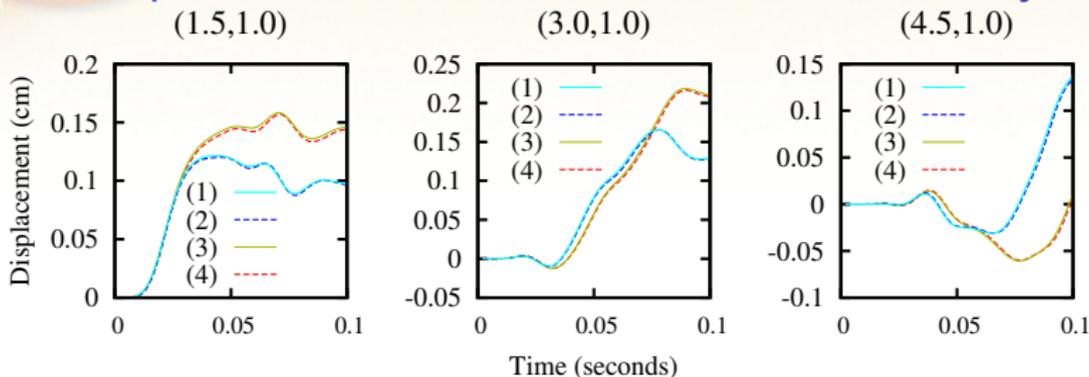
# Comparison with Aitken's Relaxation



**Figure:** Vertical displacement at three points on the interface using first (1) and second (2) order formulations with the optimal control algorithm beside vertical displacement using Aitken's relaxation (3)

Spatial discretization horizontally: 0.2 cm  
 Spatial discretization vertically: 0.1 cm  
 Temporal discretization:  $\Delta t=1e-4$  s,  $T=0.1$  s  
 Aitken's stopping tolerance:  $1e-7$   
 Optimization stopping tolerance:  $1e-4$

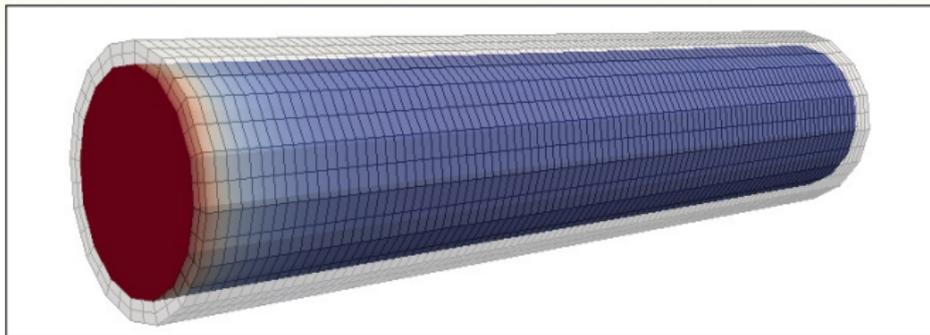
# Comparison of Linear vs. Nonlinear Elasticity



**Figure:** Vertical displacement at three points on the interface using (1) optimization and (2) Aitken's relaxation with the St. Venant–Kirchhoff constitutive equation and (3) optimization and (4) Aitken's relaxation with the linear elastic constitutive equation.

Spatial discretization horizontally: 0.2 cm  
 Spatial discretization vertically: 0.1 cm  
 Temporal discretization:  $\Delta t=1e-4$  s,  $T=0.1$  s  
 Aitken's stopping tolerance:  $1e-7$   
 Optimization stopping tolerance:  $1e-4$

# 3D Pulsatile Flow with Nonlinear Elastic



- Navier–Stokes fluid,  $\mu = 0.035$  poise,  $\rho_f = 1$  g/cm<sup>3</sup>, straight vessel of radius 0.5 cm and length 5 cm
  - St. Venant–Kirchhoff structure,  $\rho_s = 1.2$  g/cm<sup>3</sup>,  $E = 3.0e + 6$  dynes/cm<sup>2</sup>,  $\nu = 0.3$ , surrounding structure thickness of 0.1 cm
  - Overpressure on inlet boundary of  $1.3332e+4$  dynes/cm<sup>2</sup> for  $t \in [0, .005]$  s, inlet and outlet boundaries clamped
  - $\Delta t = 1e-4$  s
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# 3D Pulsatile Flow Computational Effort

Refinement	$h$	DOFs	Gauss-Newton Iterations	GMRES / Gauss-Newton	Fluid Solves (Total)	Fluid Solves (Stress Determined)	Work Factor
1	5/12	3975	3807	11.54	14302	2570	8.53
2	5/24	17983	4472	15.39	16608	2473	10.33
3	5/48	128790	5185	24.84	20006	2791	10.88

$$\text{Work Factor} = \frac{\text{Fluid Solves (Total)} + 2 \text{ Gauss-Newton Iterations}}{\text{Fluid Solves (Stress Determined)}}$$

- Even without preconditioning, the cost of optimization does not grow significantly with DOFs

## Significance of these Results

- Very few outer optimization iterations are performed per timestep (3-5 generally)
- The assembled matrix does not change between inner optimization iterations
  - We can **reuse the matrix factorization** over all linear optimization iterations!
- We can solve the coupled FSI problem in a **constant multiple** of the computational effort needed to solve the forward problems, had the correct boundary condition been known
- We use partitioned solvers, so the forward solves are cheap in comparison to a monolithic approach

# Completed Research

## Navier–Stokes / Linear Elasticity

- Recast FSI problem as a constrained minimization of the velocity mismatch
- Proved the existence of an optimal solution
- Proved the existence of Lagrange multipliers
- Applied Brezzi-Rappaz-Raviart (BRR) theory to prove convergence rates over a single time step
- Proved convergence of steepest descent algorithm
- Demonstrated theoretical rate of convergence via computation for fixed domain over a single time step

## Navier–Stokes / St. Venant–Kirchhoff

- Derived linearization of St. Venant–Kirchhoff constitutive equation
- Executed computational complexity experiments on 3D flow through a cylinder





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