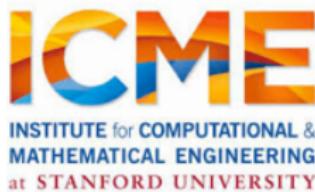


A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction

Ju Liu and Alison L. Marsden

Cardiovascular Biomechanics Computation Laboratory

Stanford University



Introduction: Two-field variational principle and its CFD analogue

G.A. Holzapfel, Nonlinear Solid Mechanics: a continuum approach for engineering, Chapter 8.

$$(S) \begin{cases} \int_{\Omega_x} \mathbf{w} \cdot \rho (\ddot{\mathbf{u}} - \mathbf{b}) + \nabla_x \mathbf{w} : \boldsymbol{\sigma}^{dev} - \nabla_x \cdot \mathbf{w} p dV = 0, \\ \int_{\Omega_x} \left(\frac{dH_{vol}}{dJ}(J) + \frac{p}{\kappa} \right) q dV = 0. \end{cases}$$

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$$\Updownarrow \quad \rho J = \rho_0$$

$$(F) \begin{cases} \int_{\Omega_x} \mathbf{w} \cdot \left(\frac{\partial(\rho \mathbf{v})}{\partial t} - \rho \mathbf{b} \right) - \nabla_x \mathbf{w} : (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla_x \mathbf{w} : \boldsymbol{\sigma}^{dev} - \nabla_x \cdot \mathbf{w} p = 0, \\ \int_{\Omega_x} (\rho R \theta - p) q dV = 0. \end{cases}$$

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G. Scovazzi, B. Carnes, and X. Zeng, IJNME v106:799-839, 2016.

$$(\times) \begin{cases} (\mathbf{w}, \dot{\mathbf{u}} - \mathbf{v}) = 0, \\ (\mathbf{w}, \rho_0 (\dot{\mathbf{v}} - \mathbf{b})) + (\nabla \cdot \mathbf{w}, p) + (\nabla \mathbf{w}, \boldsymbol{\sigma}^{dev}) = 0, \\ (\mathbf{q}, p - \kappa \nabla \cdot \mathbf{u}) + \text{Stabilization} = 0. \end{cases}$$

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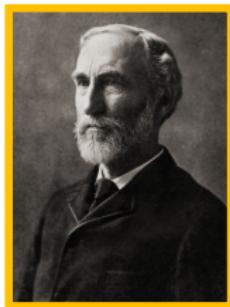
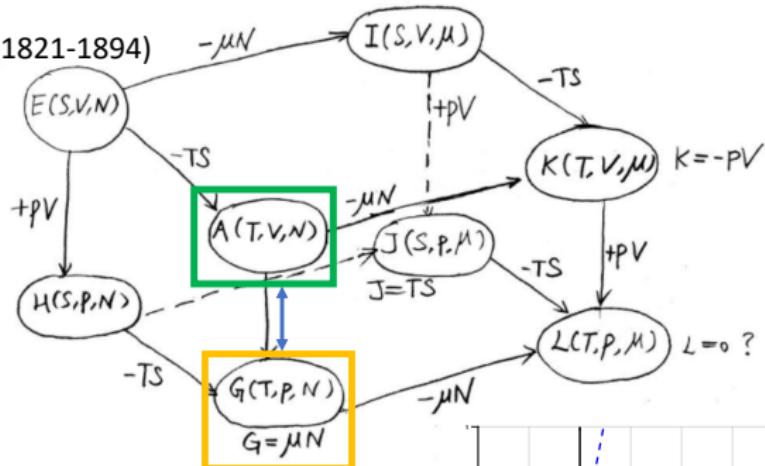
G. Hauke and T.J.R. Hughes. A comparative study of different sets of variables for solving compressible and incompressible flows. CMAME 1998.

J. Lowengrub and L. Truskinovsky. Quasi-incompressible Cahn-Hilliard fluids and topological transitions. Proceedings of the Royal Society A, 1998.

Constitutive modeling: Gibbs vs. Helmholtz

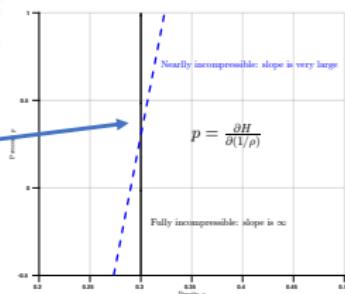


H. Helmholtz (1821-1894)



J.W. Gibbs (1839-1903)

How to take derivative
if the variable is fixed?



J. Lowengrub and L. Truskinovsky. Quasi-incompressible Cahn-Hilliard fluids and topological transitions. *Proceedings of the Royal Society A*, 1998.

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Continuum basis: Constitutive law based on the Gibbs free energy

Gibbs free energy per unit mass $G := \iota - \theta s + p/\rho$.

Coleman-Noll approach \Rightarrow

$$\text{dev}[\sigma] = \rho \tilde{\mathbf{F}} (\mathbb{P} : \tilde{\mathbf{S}}) \tilde{\mathbf{F}}^T + 2\bar{\mu} \text{dev}[d],$$

$$\frac{1}{3} \text{tr}[\sigma] = -p + \left(\frac{2}{3} \bar{\mu} + \bar{\lambda} \right) \nabla_{\mathbf{x}} \cdot \mathbf{v},$$

$$\mathbf{q} = -\kappa \nabla_{\mathbf{x}} \theta,$$

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Proposition (Additive split): $G(\tilde{\mathbf{C}}, p, \theta) = G_{iso}(\tilde{\mathbf{C}}, \theta) + G_{vol}(p, \theta)$.

Proof: $\frac{\partial G(\tilde{\mathbf{C}}, p, \theta)}{\partial p} = \rho^{-1}(p, \theta)$. Integrating the partial derivative gives the split of energy, where $G_{vol}(p, \theta) = \int \rho^{-1} dp$.

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Neo-Hookean material:

$$(?) \quad H = \frac{1}{2} \mu (\text{tr} \mathbf{C} - 3) - \mu \log(J) + H_{vol}(J),$$

$$(\checkmark) \quad H = \frac{1}{2} \mu (\text{tr} \tilde{\mathbf{C}} - 3) + H_{vol}(J).$$

Examples of closed system of equations within this framework

- Compressible Navier-Stokes equations
- Incompressible Navier-Stokes equations
- Compressible hyper-elastodynamics
- Incompressible hyper-elastodynamics
- Anisotropic incompressible visco-hyper-elasticity \iff Soft tissue solver

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$$\begin{cases} \mathbf{0} = \frac{d\mathbf{u}}{dt} - \mathbf{v}, \text{ or a mesh motion equation for ALE-CFD ,} \\ 0 = \beta_\theta \frac{dp}{dt} + \nabla_{\mathbf{x}} \cdot \mathbf{v} \\ \mathbf{0} = \rho \frac{d\mathbf{v}}{dt} - \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma}^{dev} + \nabla_{\mathbf{x}} p - \rho \mathbf{b}, \end{cases}$$

Elasticity:

$$\boldsymbol{\sigma}^{dev} = \boldsymbol{\sigma}^{ela} = J^{-1} \tilde{\mathbf{F}} (\mathbb{P} : \tilde{\mathbf{S}}) \tilde{\mathbf{F}}^T, \quad \tilde{\mathbf{S}} = 2 \frac{\partial \tilde{G}(\tilde{\mathbf{C}})}{\partial \tilde{\mathbf{C}}}.$$
$$\rho^{-1} = \rho(p)^{-1} = \frac{d\hat{G}(p)}{dp}, \quad \beta_\theta = \beta_\theta(p) = \frac{1}{\rho} \frac{\partial \rho}{\partial p} = - \frac{d^2 \hat{G}(p)}{dp^2} / \frac{d\hat{G}(p)}{dp}.$$

Fluids:

$$\boldsymbol{\sigma}^{dev} = \boldsymbol{\sigma}^{vis} = \bar{\mu} (\nabla_{\mathbf{x}} \mathbf{v} + \nabla_{\mathbf{x}} \mathbf{v}^T) + \bar{\lambda} \nabla_{\mathbf{x}} \cdot \mathbf{v} \mathbf{I}.$$

One (simplest) VMS formulation:

$$\mathbf{0} = \int_{\Omega_x^t} \psi \left(\frac{d\mathbf{u}}{dt} - \mathbf{v} \right) d\Omega_x,$$

$$0 = \int_{\Omega_x^t} q\beta_\theta \frac{dp}{dt} + q\nabla_x \cdot \mathbf{v} d\Omega_x + \int_{\Omega_x^{t'}} \nabla_x q \cdot \boldsymbol{\tau}_M \left(\rho \frac{d\mathbf{v}}{dt} - \nabla_x \cdot \overset{0}{\sigma^{dev}} + \nabla_x p - \rho \mathbf{b} \right) d\Omega_x,$$

$$\begin{aligned} \mathbf{0} = & \int_{\Omega_x^t} \mathbf{w}\rho \frac{d\mathbf{v}}{dt} + \nabla_x \mathbf{w} : \boldsymbol{\sigma}^{dev} - \nabla_x \cdot \mathbf{w}p - \rho \mathbf{b} d\Omega_x + \int_{\Gamma_x^{h,t}} \mathbf{w} \cdot \mathbf{h} d\Gamma_x \\ & + \int_{\Omega_x^{t'}} \nabla_x \cdot \mathbf{w} \boldsymbol{\tau}_C \left(\beta_\theta \frac{dp}{dt} + \nabla_x \cdot \mathbf{v} \right) d\Omega_x. \end{aligned}$$

$$\boldsymbol{\tau}_M = C_M \frac{\Delta x}{c\rho} \mathbf{I}_3, \quad \boldsymbol{\tau}_C = C_c c \Delta x \rho, \quad c \text{ is the elastic wave speed.}$$

T.J.R. Hughes and G.M. Hulbert. Space-time finite element methods for elastodynamics: formulation and error estimates. CMAME 1988.

G. Scovazzi, et al. Implicit finite incompressible elastodynamics with linear finite elements: A stabilized method in rate form. CMAME 2017.

J. Liu and A.L. Marsden. A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction. CMAME 2018.

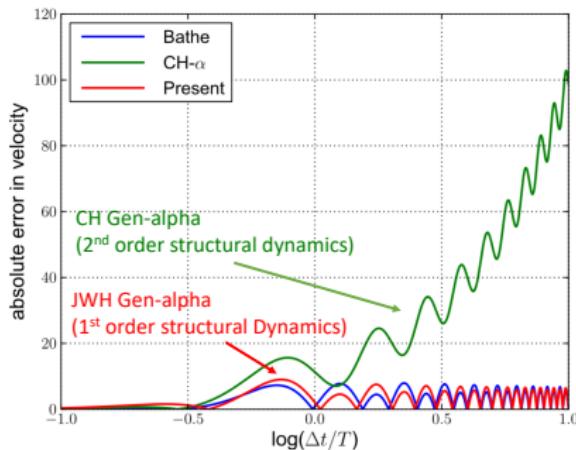
Dynamic response of the generalized- α method

$$R(\mathbf{d}_{n+\alpha_f}, \mathbf{v}_{n+\alpha_f}, \mathbf{a}_{n+\alpha_m}) = \mathbf{0}$$

Jansen-Whiting-Hulbert CMAME 2000

$$\text{First-order ODE: } \alpha_m = \frac{3-\rho_\infty}{2+2\rho_\infty}, \quad \alpha_f = \frac{1}{1+\rho_\infty}$$

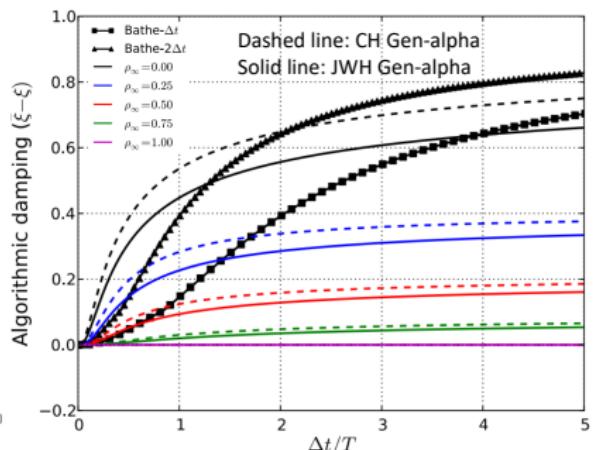
JWH- α does not suffer from 'overshoot'.



Chung-Hulbert J. Appl. Mech. 1993

$$\text{Second-order ODE: } \alpha_m = \frac{2-\rho_\infty}{1+\rho_\infty}, \quad \alpha_f = \frac{1}{1+\rho_\infty}$$

JWH- α is better in dissipation and dispersion



H.M. Hilber and T.J.R. Hughes. Collocation, dissipation, and 'overshoot' for time integration schemes in structural dynamics. *Earthquake Engineering and Structural Dynamics*, 1978.
 C. Kadapa, W.G. Dettmer, and D. Perić. On the advantage of using the first-order generalised-alpha scheme for structural dynamic problems. *Computers and Structures*, 2017

A segregated algorithm for the nonlinear solver

$$\begin{bmatrix} \alpha_m \mathbf{I} & \mathbf{0} & -\alpha_f \gamma \Delta t_n \mathbf{I} \\ \mathbf{K}_{(i), \dot{\mathbf{U}}}^p & \mathbf{K}_{(i), \dot{\mathbf{P}}}^p & \mathbf{K}_{(i), \dot{\mathbf{V}}}^p \\ \mathbf{K}_{(i), \dot{\mathbf{U}}}^m & \mathbf{K}_{(i), \dot{\mathbf{P}}}^m & \mathbf{K}_{(i), \dot{\mathbf{V}}}^m \end{bmatrix} \begin{bmatrix} \Delta \dot{\mathbf{U}}_{n+1,(i)} \\ \Delta \dot{\mathbf{P}}_{n+1,(i)} \\ \Delta \dot{\mathbf{V}}_{n+1,(i)} \end{bmatrix} = - \begin{bmatrix} \bar{\mathbf{R}}_{(i)}^k \\ \mathbf{R}_{(i)}^p \\ \mathbf{R}_{(i)}^m \end{bmatrix}$$

$$\Downarrow$$
$$\begin{bmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \frac{1}{\alpha_m} \mathbf{K}_{(i), \dot{\mathbf{U}}}^p & \mathbf{K}_{(i), \dot{\mathbf{P}}}^p & \mathbf{K}_{(i), \dot{\mathbf{V}}}^p + \frac{\alpha_f \gamma \Delta t_n}{\alpha_m} \mathbf{K}_{(i), \dot{\mathbf{U}}}^p \\ \frac{1}{\alpha_m} \mathbf{K}_{(i), \dot{\mathbf{U}}}^m & \mathbf{K}_{(i), \dot{\mathbf{P}}}^m & \mathbf{K}_{(i), \dot{\mathbf{V}}}^m + \frac{\alpha_f \gamma \Delta t_n}{\alpha_m} \mathbf{K}_{(i), \dot{\mathbf{U}}}^m \end{bmatrix} \begin{bmatrix} \alpha_m \mathbf{I} & \mathbf{0} & -\alpha_f \gamma \Delta t_n \mathbf{I} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix}$$

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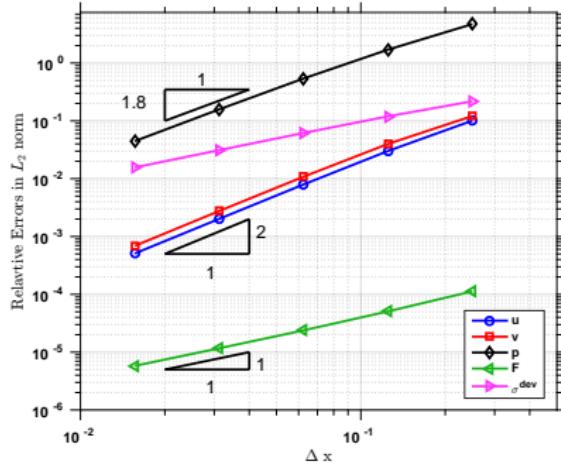
Step 1: Solve for $\Delta \dot{\mathbf{P}}_{n+1,(i)}$ and $\Delta \dot{\mathbf{V}}_{n+1,(i)}$.

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \Delta \dot{\mathbf{P}}_{n+1,(i)} \\ \Delta \dot{\mathbf{V}}_{n+1,(i)} \end{bmatrix} = - \begin{bmatrix} \mathbf{R}_{(i)}^p - \frac{1}{\alpha_m} \mathbf{K}_{(i), \dot{\mathbf{U}}}^p \bar{\mathbf{R}}_{(i)}^k \\ \mathbf{R}_{(i)}^m - \frac{1}{\alpha_m} \mathbf{K}_{(i), \dot{\mathbf{U}}}^m \bar{\mathbf{R}}_{(i)}^k \end{bmatrix}$$

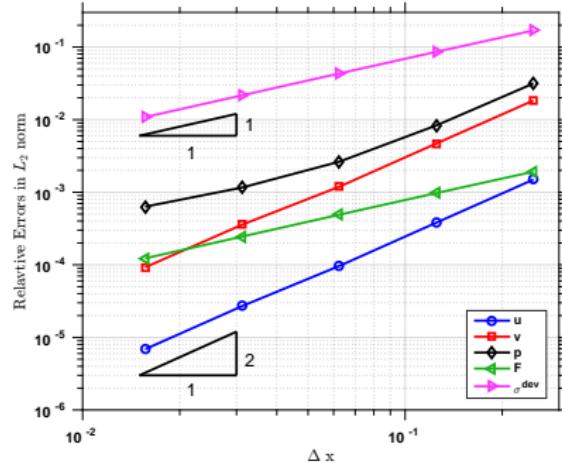
Step 2: Obtain the displacement update $\Delta \dot{\mathbf{U}}_{n+1,(i)}$.

$$\Delta \dot{\mathbf{U}}_{n+1,(i)} = \frac{\alpha_f \gamma \Delta t_n}{\alpha_m} \Delta \dot{\mathbf{V}}_{n+1,(i)} - \frac{1}{\alpha_m} \bar{\mathbf{R}}_{(i)}^k.$$

Verification: manufactured solutions



Compressible material



Incompressible material

A. Masud and K. Xia, A stabilized mixed finite element method for nearly incompressible elasticity. CMAME 2005.

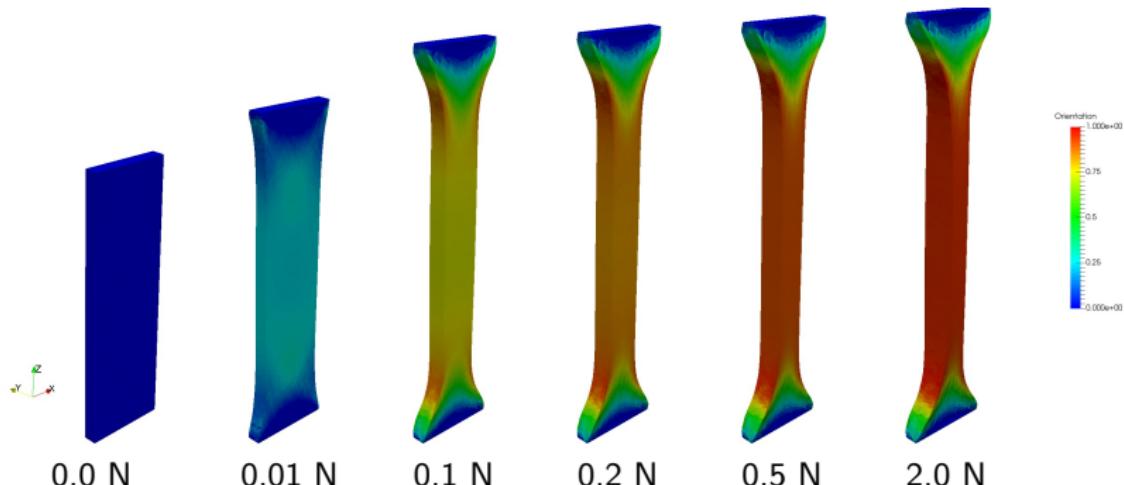
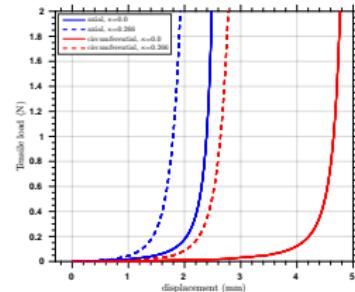
T.J.R. Hughes, et al. A new finite element formulation for computational fluid dynamics: V. Circumventing the Babuska-Brezzi condition. CMAME 1986.

Anisotropic hyperelastic soft tissue model

$$G(\bar{C}, H_i) = G_g(\bar{C}) + \sum_{i=1,2} G_{fi}(\bar{C}, H_i),$$

$$G_g(\bar{C}) = \frac{c}{2} (\text{tr}\bar{C} - 3),$$

$$G_{fi}(\bar{C}, H_i) = \frac{k_1}{2k_2} (\exp(k_2\bar{E}_i^2) - 1).$$



T. Gasser, et al. Hyperelastic modelling of arterial layers with distributed collagen fibre orientations. Journal of the royal society interface. 2005.

Iterative solution method

Block preconditioner based on LDU decomposition:

$$\mathcal{P} := \mathcal{L}DU := \begin{bmatrix} \mathbf{I} & \mathbf{O} \\ \mathbf{C}\mathbf{A}^{-1} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{A} & \mathbf{O} \\ \mathbf{O} & \mathbf{S} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{A}^{-1}\mathbf{B} \\ \mathbf{O} & \mathbf{I} \end{bmatrix},$$

wherein $S := D - CA^{-1}B$ is the **Schur complement**.

Strategy 1: $\mathbf{S} \leftarrow \hat{\mathbf{S}}$ leads to a SIMPLE-type block preconditioner.

Strategy 2: Solve S in a matrix-free manner with \hat{S} as a preconditioner \Rightarrow nested block preconditioner.

M. Benzi, G.H. Golub, and J. Liesen, Numerical solution of saddle point problems. Acta Numerica, 2005.

T.E. Tezduyar, et al., A nested iterative scheme for computation of incompressible flows in long domains, Computational Mechanics, 2008.

Iterative solution method: nested block preconditioner

FGMRES iteration

Initialize the Hessenberg matrix

Solve for $\mathcal{P}\mathbf{x} = \mathbf{r}$

1. Solve $\mathbf{A}\hat{\mathbf{x}}_v = \mathbf{r}_v$ by GMRES preconditioned by AMG(\mathbf{A}).

2. Update the continuity residual: $\mathbf{r}_p \leftarrow \mathbf{r}_p - \mathbf{C}\hat{\mathbf{x}}_v$.

3. Solve $\mathbf{S}\mathbf{x}_p = \mathbf{r}_p$ by GMRES preconditioned by AMG($\hat{\mathbf{S}}$).

Matrix-vector multiplication of \mathbf{S} involves an inner solver for \mathbf{A} .

4. Update the momentum residual: $\mathbf{r}_v \leftarrow \mathbf{r}_v - \mathbf{B}\mathbf{x}_p$.

5. Solve $\mathbf{A}\mathbf{x}_v = \mathbf{r}_v$ by GMRES preconditioned by AMG(\mathbf{A}).

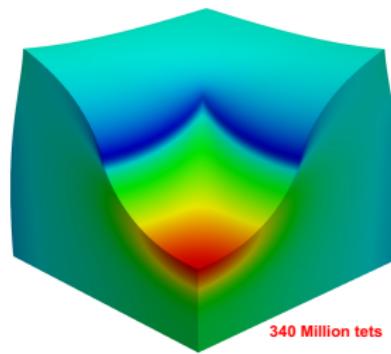
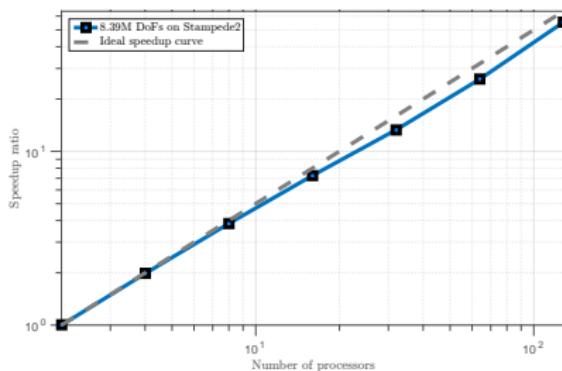
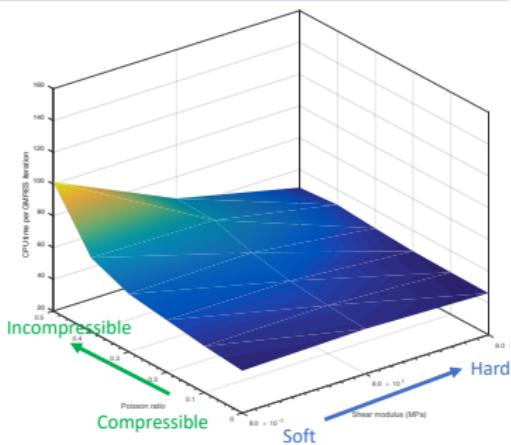
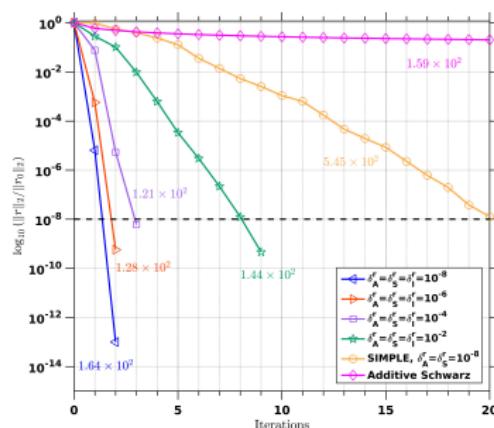
Compute $\mathbf{w} = \mathcal{A}\mathbf{x}$

Update the Hessenberg matrix and solve for solution.

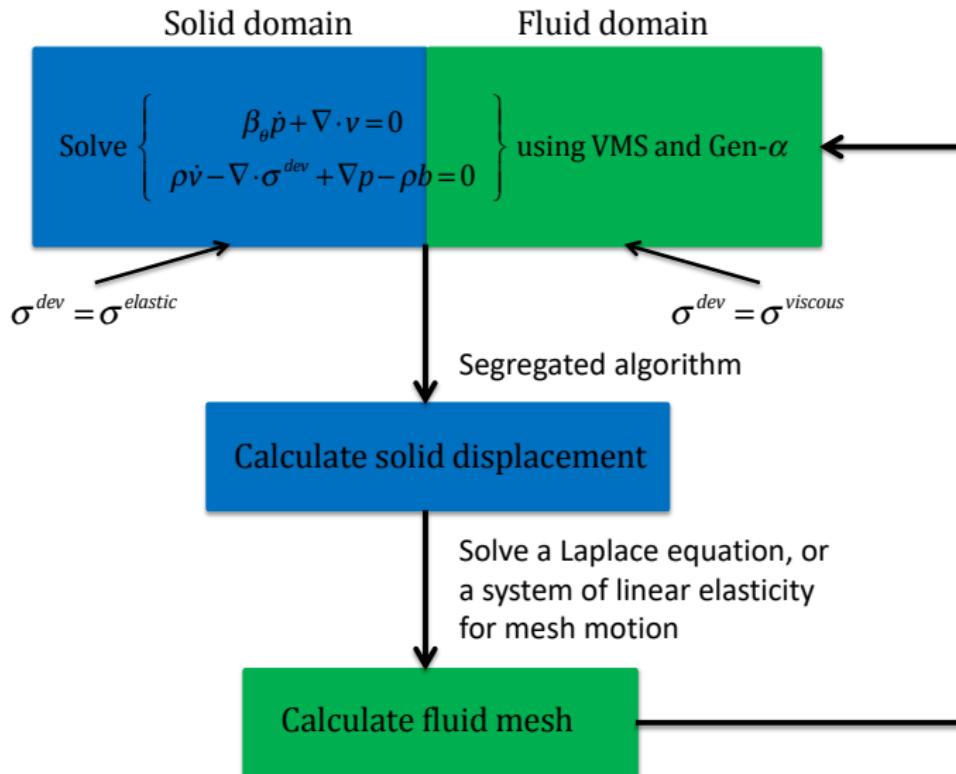
T.E. Tezduyar, et al., A nested iterative scheme for computation of incompressible flows in long domains, Computational Mechanics, 2008.

J. Liu and A.L. Marsden, A robust and efficient iterative solver for hyper-elastodynamics with nested block preconditioning, JCP, 2019.

Iterative solution method: efficiency, scalability and robustness

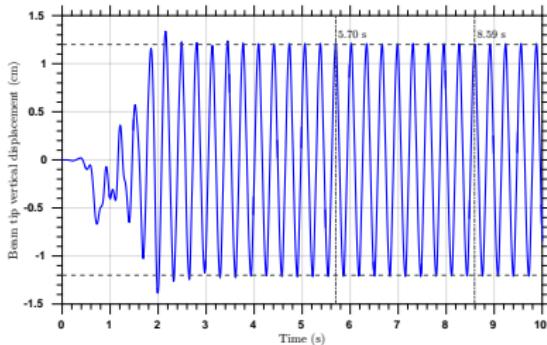


FSI coupling strategy



J. Liu and A.L. Marsden. A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction. CMAME 2018.

Flow over an elastic cantilever



Author	Oscillation period (s)	Tip displacement (cm)
W.A. Wall	0.31 - 0.36	1.12 - 1.32
W.G. Dettmer and D. Perić	0.32 - 0.34	1.1 - 1.4
Y. Bazilevs, et al.	0.33	1.0 - 1.5
C. Wood, et al.	0.32 - 0.36	1.10 - 1.20
Current work	0.32	1.2

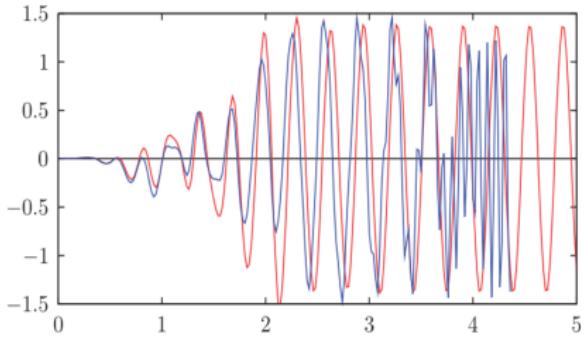
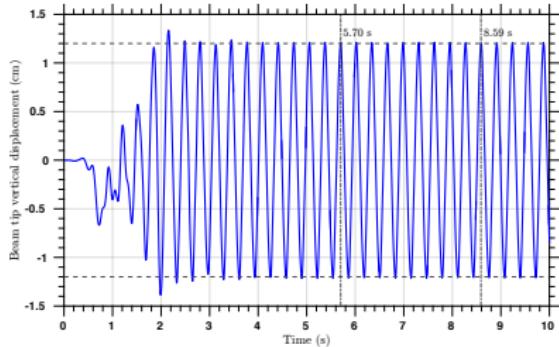
Flow over an elastic cantilever

$$R(d_{n+\alpha_f}, v_{n+\alpha_f}, a_{n+\alpha_m}) = 0$$

$$\alpha_m = \frac{3-\rho_\infty}{2+2\rho_\infty}, \quad \alpha_f = \frac{1}{1+\rho_\infty}$$

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M.M. Joosten, W.G. Dettmer, and D. Perić. On the temporal stability and accuracy of coupled problems with reference to fluid-structure interaction. IJNMF, 2010.

J. Liu and A.L. Marsden. A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction. CMAME 2018.

Conclusion

	New FSI	Traditional FSI
Spatial discretization and material properties	Use stable or stabilized FEM/IGA to handle numerical instabilities	Incompressible is impossible; nearly incompressible is hard.

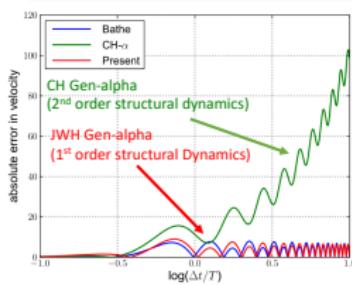
J. Liu and A.L. Marsden. *A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction*. CMAME 2018.

J. Liu and A.L. Marsden, *A robust and efficient iterative solver for hyper-elastodynamics with nested block preconditioning*, JCP, 2019.

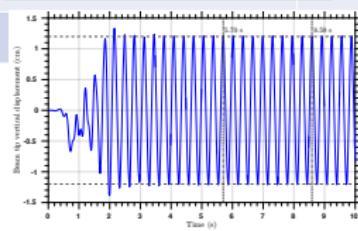
J. Liu, A.L. Marsden, and Z. Tao, *An energy-stable mixed formulation for isogeometric analysis of incompressible hyper-elastodynamics*. IJNME, in review.

Conclusion

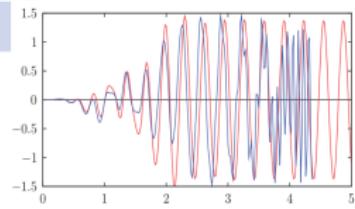
	New FSI	Traditional FSI
Spatial discretization and material properties	Use stable or stabilized FEM/IGA to handle numerical instabilities	Incompressible is impossible; nearly incompressible is hard.
Temporal scheme	No overshoot, better dissipation and dispersion	Overshoot
Coupling	Uniform optimal high-frequency dissipation	Special treatment is needed to handle the coupling between 1 st and 2 nd order ODE systems



$$\alpha_m = \frac{3-\rho_\infty}{2+2\rho_\infty}, \quad \alpha_f = \frac{1}{1+\rho_\infty}$$



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Coupling	Uniform optimal high-frequency dissipation	Special treatment is needed to handle the coupling between 1 st and 2 nd order ODE systems
Linear solver	Robust and efficient linear solution procedure (block PC + AMG)	Complicated
Implementation	As simple (hard) as ALE-CFD	Hard to implement

Two main reasons people reject monolithic FSI

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