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

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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.

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(\mathsf{S}) \begin{cases} \int_{\Omega_{\boldsymbol{x}}} \boldsymbol{w} \cdot \rho \left(\ddot{\boldsymbol{u}} - \boldsymbol{b} \right) + \nabla_{\boldsymbol{x}} \boldsymbol{w} : \boldsymbol{\sigma}^{dev} - \nabla_{\boldsymbol{x}} \cdot \boldsymbol{w} p dV = 0, \\ \int_{\Omega_{\boldsymbol{x}}} \left(\frac{dH_{vol}}{dJ}(J) + \frac{p}{\kappa} \right) q dV = 0. \end{cases}
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$$\Updownarrow \qquad \rho J = \rho_0$$

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

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

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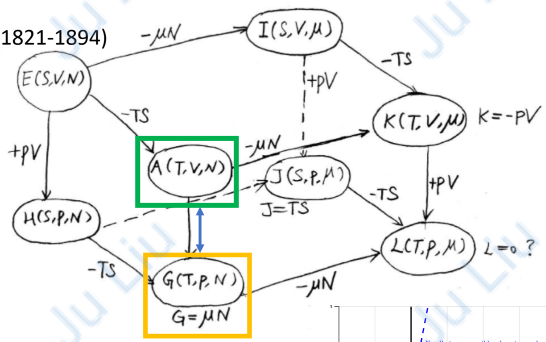
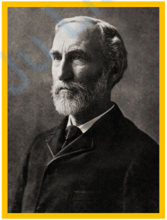
J. Lowengrub and L. Truskinovsky. Quasi-incompressible Cahn-Hilliard fluids and topological transitions. Proceedings of the Royal Society A, 1998.

Constitutive modeling: Gibbs vs. Helmholtz

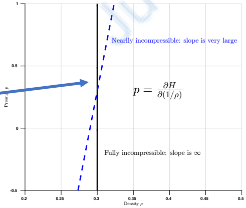
H. Helmholtz (1821-1894)





J.W. Gibbs (1839-1903)

How to take derivative
if the variable is fixed?



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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 $\Rightarrow$

$$
\begin{aligned}
\text{dev}\left[\boldsymbol{\sigma}\right] =& \rho \tilde{\boldsymbol{F}} \left(\mathbb{P} : \tilde{\boldsymbol{S}} \right) \tilde{\boldsymbol{F}}^T + 2\bar{\mu}\text{dev}[\boldsymbol{d}], \\
\frac{1}{3}\text{tr}\left[\boldsymbol{\sigma}\right] =& - p + \left(\frac{2}{3}\bar{\mu} + \bar{\lambda} \right) \nabla_{\boldsymbol{x}} \cdot \boldsymbol{v}, \\
\boldsymbol{q} =& - \kappa \nabla_{\boldsymbol{x}} \theta, \\
s =& - \frac{\partial G}{\partial \theta}, \\
\rho =& \left(\frac{\partial G}{\partial p} \right)^{-1}.
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J. Liu and A.L. Marsden. A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction. CMAME 2018.

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

Proof: $\frac{\partial G\left(\tilde{\boldsymbol{C}}, p, \theta\right)}{\partial p} = \rho^{-1}(p,\theta)$. 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:

$$\begin{aligned}
(?) \qquad & H = \frac{1}{2}\mu\left(\mathrm{tr}\boldsymbol{C} - 3\right) - \mu \log\left(J\right) + H_{vol}(J), \\
(\checkmark) \qquad & H = \frac{1}{2}\mu\left(\mathrm{tr}\tilde{\boldsymbol{C}} - 3\right) + H_{vol}(J).
\end{aligned}$$

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

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 $\Longleftrightarrow$ Soft tissue solver

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

Elasticity:

$$
\boldsymbol{\sigma}^{dev} = \boldsymbol{\sigma}^{ela} = J^{-1} \tilde{\boldsymbol{F}} \left(\mathbb{P} : \tilde{\boldsymbol{S}} \right) \tilde{\boldsymbol{F}}^T, \qquad \tilde{\boldsymbol{S}} = 2 \frac{\partial \tilde{G}(\tilde{\boldsymbol{C}})}{\partial \tilde{\boldsymbol{C}}}.
$$

$$
\rho^{-1} = \rho(p)^{-1} = \frac{d\hat{G}(p)}{dp}, \quad \beta_\theta = \beta_\theta(p) = \frac{1}{\rho} \frac{\partial \rho}{\partial p} = - \frac{d^2 \hat{G}(p)}{dp^2} \Big/ \frac{d\hat{G}(p)}{dp}.
$$

Fluids:

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

Variational multiscale formulation

One (simplest) VMS formulation:

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

$$0 = \int_{\Omega_{\boldsymbol{x}}^t} q\beta_\theta \frac{dp}{dt} + q\nabla_{\boldsymbol{x}} \cdot \boldsymbol{v} d\Omega_{\boldsymbol{x}} + \int_{\Omega_{\boldsymbol{x}}^{t\prime}} \nabla_{\boldsymbol{x}} q \cdot \boldsymbol{\tau}_M \left(\rho \frac{d\boldsymbol{v}}{dt} - \cancelto{0}{\nabla_{\boldsymbol{x}} \cdot \boldsymbol{\sigma}^{dev}} + \nabla_{\boldsymbol{x}} p - \rho \boldsymbol{b} \right) d\Omega_{\boldsymbol{x}},$$

$$\mathbf{0} = \int_{\Omega_{\boldsymbol{x}}^t} \boldsymbol{w}\rho \frac{d\boldsymbol{v}}{dt} + \nabla_{\boldsymbol{x}} \boldsymbol{w} : \boldsymbol{\sigma}^{dev} - \nabla_{\boldsymbol{x}} \cdot \boldsymbol{w} p - \rho \boldsymbol{b} d\Omega_{\boldsymbol{x}} + \int_{\Gamma_{\boldsymbol{x}}^{h\,t}} \boldsymbol{w} \cdot \boldsymbol{h} d\Gamma_{\boldsymbol{x}}$$

$$+ \int_{\Omega_{\boldsymbol{x}}^{t\prime}} \nabla_{\boldsymbol{x}} \cdot \boldsymbol{w} \tau_C \left(\beta_\theta \frac{dp}{dt} + \nabla_{\boldsymbol{x}} \cdot \boldsymbol{v} \right) d\Omega_{\boldsymbol{x}}.$$

$\boldsymbol{\tau}_M = C_M \dfrac{\Delta x}{c\rho} \boldsymbol{I}_3, \quad \tau_C = C_c c \Delta x \rho, \quad c$ 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.
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Dynamic response of the generalized-α method

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

Jansen-Whiting-Hulbert CMAME 2000

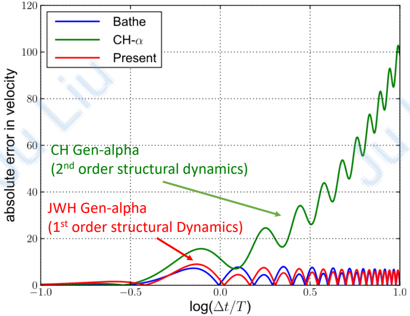
First-order ODE: $\alpha_m = \frac{3-\rho_\infty}{2+2\rho_\infty}$, $\alpha_f = \frac{1}{1+\rho_\infty}$

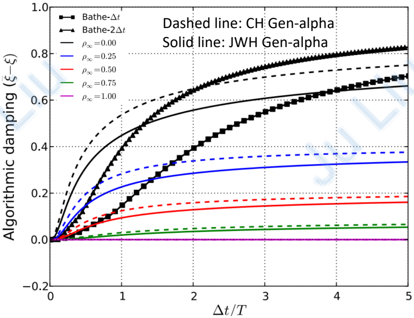
JWH-α does not suffer from `overshoot'.

Chung-Hulbert J. Appl. Mech. 1993

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

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

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

$$\Downarrow$$

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

G. Scovazzi, et al. A simple, stable, and accurate linear tetrahedral finite element for transient, nearly, and fully incompressible solid dynamics: a dynamic variational multiscale approach. IJNME 2016.

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

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

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

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

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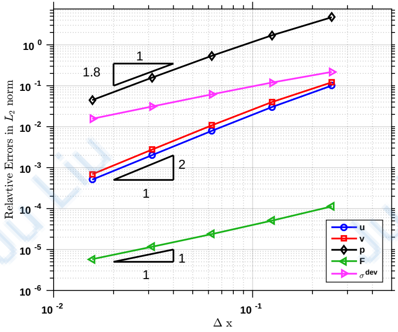
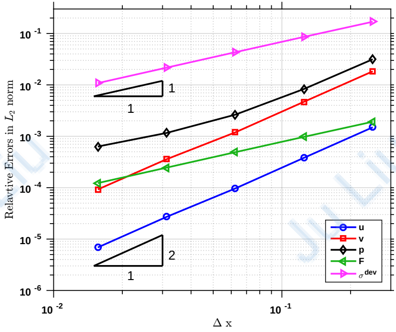
Verification: manufactured solutions



Compressible material



Incompressible material

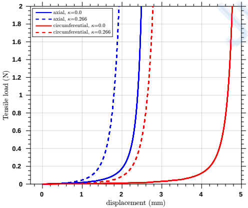
A. Masud and K. Xia, A stabilized mixed finite element method for nearly incompressible elasticity. CMAME 2005.
T.J.R. Hughes, et al. A new finite element formulation for computational fluid dynamics: V. Circumventing the Babuska-Brezzi condition. CMAME 1986.

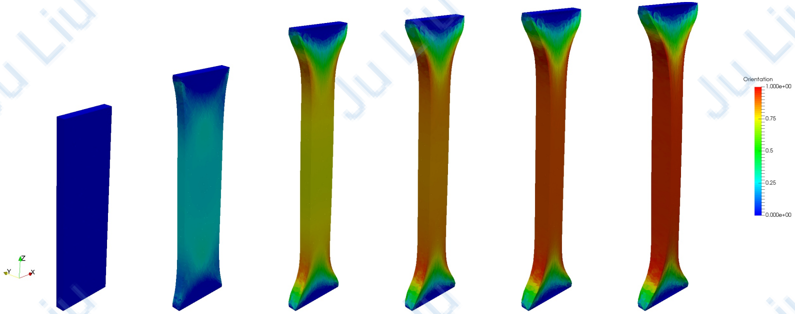
Anisotropic hyperelastic soft tissue model

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

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

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





0.0 N 0.01 N 0.1 N 0.2 N 0.5 N 2.0 N

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

Mass matrix
+ Stiffness matrix + …

Discrete gradient

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \Delta \mathbf{v} \\ \Delta p \end{bmatrix} = - \begin{bmatrix} \mathbf{R}^{p} \\ \mathbf{R}^{m} \end{bmatrix}$$

Discrete divergence

Scaled mass matrix + stabilization

Block preconditioner based on LDU decomposition:

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

wherein $\mathbf{S} := \mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B}$ is the **Schur complement**.

Strategy 1: $\mathbf{S} \longleftarrow \hat{\mathbf{S}}$ leads to a SIMPLE-type block preconditioner.
Strategy 2: Solve $\mathbf{S}$ in a matrix-free manner with $\hat{\mathbf{S}}$ 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 $\mathcal{P}\mathbf{x} = \mathbf{r}$

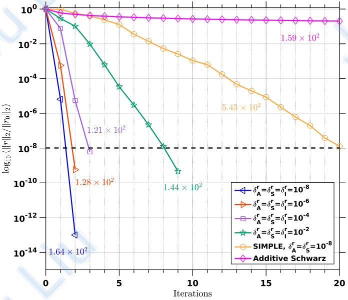
1. Solve $\mathbf{A}\hat{\mathbf{x}}_{v} = \mathbf{r}_{v}$ by GMRES preconditioned by AMG($\mathbf{A}$).
2. Update the continuity residual: $\mathbf{r}_{p} \leftarrow \mathbf{r}_{p} - \mathbf{C}\hat{\mathbf{x}}_{v}$.
3. Solve $\mathbf{S}\mathbf{x}_{p} = \mathbf{r}_{p}$ by GMRES preconditioned by AMG($\hat{\mathbf{S}}$).
   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($\mathbf{A}$).

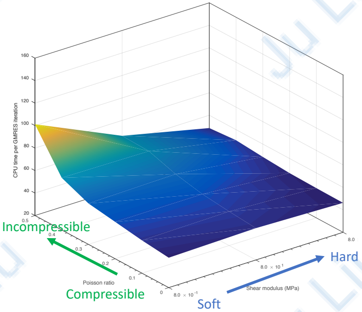
Compute $\mathbf{w} = \mathcal{A}\mathbf{x}$

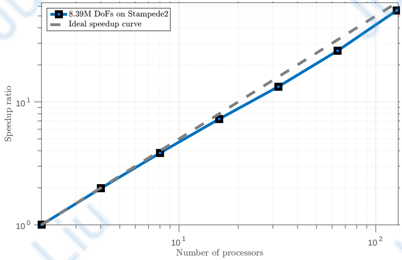
Update the Hessenberg matrix and solve for solution.

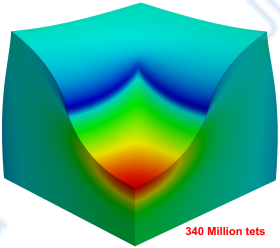
T.E. Tezduyar, et al., A nested iterative scheme for computation of incompressible flows in long domains, Computational Mechanics, 2008.
J. Liu and A.L. Marsden, A robust and efficient iterative solver for hyper-elastodynamics with nested block preconditioning, JCP, 2019.

Iterative solution method: efficiency, scalability and robustness



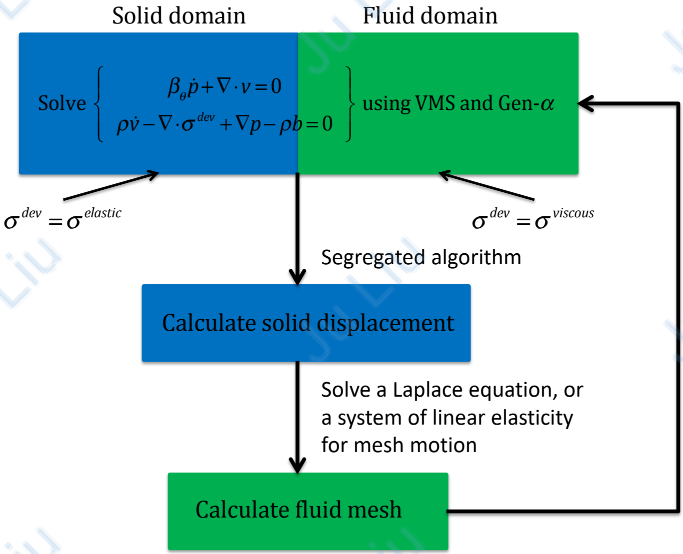






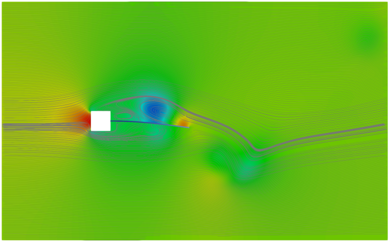
J. Liu and A.L. Marsden, A robust and efficient iterative solver for hyper-elastodynamics with nested block preconditioning, JCP, 2019.

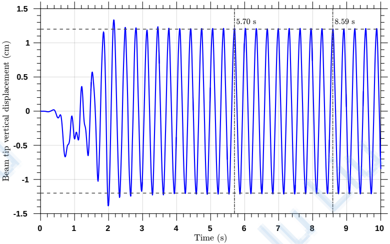
FSI coupling strategy



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

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

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

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

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

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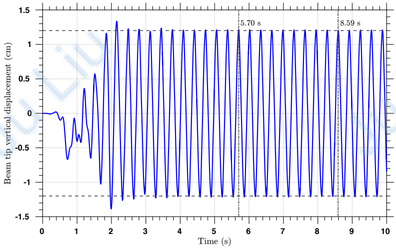

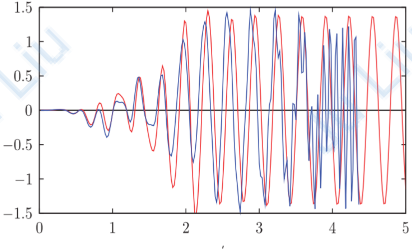

M.M. Joosten, W.G. Dettmer, and D. Perić. On the temporal stability and accuracy of coupled problems with reference to fluid-structure interaction. IJNMF, 2010.
J. Liu and A.L. Marsden. A unified continuum and variational multiscale formulation for fluids, solids, and fluid-structure interaction. CMAME 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.

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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 1st and 2nd order ODE systems

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

$$\alpha_m = \frac{2-\rho_\infty}{1+\rho_\infty}$$

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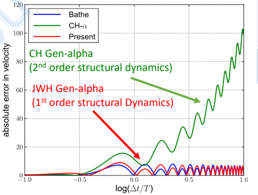

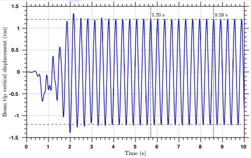

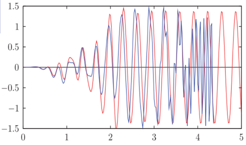

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Temporal scheme	No overshoot, better dissipation and dispersion	Overshoot
Coupling	Uniform optimal high-frequency dissipation	Special treatment is needed to handle the coupling between 1st and 2nd order ODE systems
Linear solver	Robust and efficient 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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