Performance-portable p-multigrid block preconditioning for mixed FE discretizations of nearly incompressible hyperelasticity

Rezgar Shakeri

Jed Brown, Jeremy L Thompson

University of Colorado Boulder

Rezgar.Shakeri@colorado.edu

April 22, 2024

18th Copper Mountain Conference On Iterative Methods

Introduction/Motivation

- Many engineering and biomedical materials exhibit volume-preserving behavior under large deformation.
- Cardiac modeling
- Rubbers with broad range of applications: sealing components, tyres for automobiles and aircraft, soft robotic

Introduction/Motivation

- Many engineering and biomedical materials exhibit volume-preserving behavior under large deformation.
- Cardiac modeling
- Rubbers with broad range of applications: sealing components, tyres for automobiles and aircraft, soft robotic

Challenge

Displacement-based low order FE methods perform poorly in such nearly and fully incompressible scenarios $\nu \to 0.5$

Motivation/Alternative approach

- Using higher order polynomials in $\boldsymbol{u}$-based formulation.

Motivation/Alternative approach

- Using higher order polynomials in $\boldsymbol{u}$-based formulation.

  Heisserer et al. (2007): Compared with analytical solution. With Q_9 element $\|u_r - u_r^h\|/\|u_r\| = 0.00032\%$, $\|\sigma_{rr} - \sigma_{rr}^h\|/\|\sigma_{rr}\| = 6.5\%$

Motivation/Alternative approach

- Using higher order polynomials in $\boldsymbol{u}$-based formulation.

  Heisserer et al. (2007): Compared with analytical solution. With Q_9 element $\|u_r - u_r^h\|/\|u_r\| = 0.00032\%$, $\|\sigma_{rr} - \sigma_{rr}^h\|/\|\sigma_{rr}\| = 6.5\%$

- Introduce a pressure like variable p as an additional unknown to the system and solve mixed $\boldsymbol{u} - p$ formulation.

Motivation/Alternative approach

- Using higher order polynomials in $\boldsymbol{u}$-based formulation.

  Heisserer et al. (2007): Compared with analytical solution. With Q_9 element $\|u_r - u_r^h\|/\|u_r\| = 0.00032\%$, $\|\sigma_{rr} - \sigma_{rr}^h\|/\|\sigma_{rr}\| = 6.5\%$

- Introduce a pressure like variable p as an additional unknown to the system and solve mixed $\boldsymbol{u} - p$ formulation.

  Kadapa et al. (2021): Mixed quadratic elements.
  Karabelas et al. (2022): Used $P_1 P_1$ elements for cardiac problem with different stabilization techniques and solved by GMRES method with a block preconditioner (AMG).
  Barnafi et al. (2023): Performance comparison between the Balancing Domain Decomposition by Constraints (BDDC) and the Algebraic Multigrid (AMG) preconditioners for cardiac mechanics.
  Farrell et al. (2021): $\boldsymbol{\sigma} - \boldsymbol{u} - p$ with GMRES and a new augmented Lagrangian preconditioner (direct solver).

Motivation/What is missing?

***u*-based high order approach**

- Error in stress is still large.
- Cost of single vs mixed fields (Q_3 vs $Q_3 Q_2$) when $\nu \to 0.5$?
- Modeling fully incompressible material ($\nu = 0.5$) is not possible.

Motivation/What is missing?

***u*-based high order approach**

- Error in stress is still large.
- Cost of single vs mixed fields (Q_3 vs Q_3Q_2) when $\nu \to 0.5$?
- Modeling fully incompressible material ($\nu = 0.5$) is not possible.

Mixed $\boldsymbol{u} - p$ formulation

- Low order element, not accurate enough and first-order accuracy for stresses.
- All available mixed formulations are using sparse direct solver and it is expansive for large problem.

Motivation/What is missing?

$\boldsymbol{u}$-based high order approach

- Error in stress is still large.
- Cost of single vs mixed fields (Q_3 vs $Q_3 Q_2$) when $\nu \to 0.5$?
- Modeling fully incompressible material ($\nu = 0.5$) is not possible.

Mixed $\boldsymbol{u} - p$ formulation

- Low order element, not accurate enough and first-order accuracy for stresses.
- All available mixed formulations are using sparse direct solver and it is expansive for large problem.

Proposed work

- High-order mixed element implemented with matrix-free approach.
- Run in parallel on different CPU/GPU architectures.
- Stable, robust, efficient and accurate for for compressible, nearly incompressible and fully incompressible materials.

Incompressibility (small strain)

$$\boldsymbol{\sigma} = \lambda \operatorname{trace} \boldsymbol{\varepsilon} \, \boldsymbol{I} + 2\mu\boldsymbol{\varepsilon},$$

μ is shear modulus and λ is first Lame parameter, ν is Poisson's ratio

$$\lambda = \frac{2\nu\mu}{1-2\nu}$$

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) = \frac{1}{2}\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right).$$

For incompressible material $\nu \to 0.5$ as a result $\lambda \to \infty$ and $\boldsymbol{\sigma} \to \infty$.

Constitutive equations (small strain)

Full strain approach

$$
\begin{aligned}
\boldsymbol{\sigma}(\boldsymbol{u}, p) &= -p\, \boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}, \\
p &= -\lambda\, \mathrm{trace}\, \boldsymbol{\varepsilon}.
\end{aligned}
$$

$\lambda = 2\mu\nu / (1 - 2\nu)$

Incompressible Stokes are similar to this approach, only differences are $\boldsymbol{u}$ is the velocity of the fluid and μ is the dynamic viscosity.

Constitutive equations (small strain)

Full strain approach

$$\boldsymbol{\sigma}(\boldsymbol{u}, p) = -p\, \boldsymbol{I} + 2\mu\boldsymbol{\varepsilon},$$
$$p = -\lambda\, \mathrm{trace}\, \boldsymbol{\varepsilon}.$$

$\lambda = 2\mu\nu / (1 - 2\nu)$

Deviatoric strain approach:

$$\boldsymbol{\sigma}(\boldsymbol{u}, p_{\mathrm{hyd}}) = -p_{\mathrm{hyd}}\, \boldsymbol{I} + 2\mu\boldsymbol{\varepsilon}_{\mathrm{dev}},$$
$$p_{\mathrm{hyd}} = -k\, \mathrm{trace}\, \boldsymbol{\varepsilon}.$$

$k = 2\mu\,(1 + \nu)\,/3\,(1 - 2\nu)$

Mixed hyperelasticity is an extension version fo deviatoric strain.

Constitutive equations (small strain)

Full strain approach

$$\boldsymbol{\sigma}(\boldsymbol{u}, p) = -p\,\boldsymbol{I} + 2\mu\varepsilon,$$
$$p = -\lambda \operatorname{trace} \varepsilon.$$

Deviatoric strain approach:

$$\boldsymbol{\sigma}(\boldsymbol{u}, p_{\text{hyd}}) = -p_{\text{hyd}}\,\boldsymbol{I} + 2\mu\varepsilon_{\text{dev}},$$
$$p_{\text{hyd}} = -k \operatorname{trace} \varepsilon.$$

Genral mixed constitutive equation:

$$\boldsymbol{\sigma}(\boldsymbol{u}, p) = (k_p \operatorname{trace} \varepsilon - p)\,\boldsymbol{I} + 2\mu\varepsilon_{\text{dev}},$$
$$p = -(k - k_p) \operatorname{trace} \varepsilon.$$

where $k_p = 2\mu\,(1+\nu_p)\,/3\,(1-2\nu_p)$ is the primal portion of the bulk modulus, defined in terms of ν_p with $-1 \leq \nu_p < \nu$.

$\nu_p = 0 \equiv$ full strain approach, $\nu_p = -1 \equiv$ deviatoric strain approach

Constitutive equations (finite strain, initial configuration)

Strain energy:

$$\psi = \psi_{\text{vol}}(J) + \psi_{\text{iso}}\left(\bar{\boldsymbol{C}}\right) = k\,U(J) + \psi_{\text{iso}}\left(\bar{\boldsymbol{C}}\right)$$

Standard approach:

$$p_{\text{hyd}} = -\frac{\operatorname{trace}\boldsymbol{\sigma}}{3} = -\frac{\partial \psi_{\text{vol}}}{\partial J} = -k\frac{\partial U(J)}{\partial J},$$

$$\boldsymbol{S} = \frac{\partial \psi}{\partial \boldsymbol{E}} = \frac{\partial \psi_{\text{vol}}}{\partial J}\frac{\partial J}{\partial \boldsymbol{E}} + \frac{\partial \psi_{\text{iso}}}{\partial \boldsymbol{E}} = \boldsymbol{S}_{\text{vol}} + \boldsymbol{S}_{\text{iso}}$$

General constitutive equation:

$$p = -(k - k_p)\frac{\partial U}{\partial J} = p_{\text{hyd}} + k_p U',$$

$$\boldsymbol{S}(\boldsymbol{u}, p) = \boldsymbol{S}_{\text{iso}} + \underbrace{\left(k_p J U' - pJ\right)\boldsymbol{C}^{-1}}_{\boldsymbol{S}_{\text{vol}}},$$

We write our constitutive equations in terms of general function $U(J)$ so user can test with different volumetric energy term.

Strong and weak forms (finite strain, initial configuration)

Strong form:

$$\begin{aligned} -\nabla_X \cdot \boldsymbol{P} - \rho_0 \boldsymbol{g} &= 0. && \text{in } \Omega_0 \\ -U' - \frac{p}{k - k_p} &= 0. && \text{in } \Omega \end{aligned}$$

Weak form:

$$\begin{aligned} R_u(\boldsymbol{u}, p) &\coloneqq \int_{\Omega_0} \nabla_X \boldsymbol{v} : \boldsymbol{P} \, dV - \int_{\Omega_0} \boldsymbol{v} \cdot \rho_0 \boldsymbol{g} \, dV - \int_{\partial \Omega_0^N} \boldsymbol{v} \cdot \bar{\boldsymbol{t}} \, dS = 0, \\ R_p(\boldsymbol{u}, p) &\coloneqq \int_{\Omega_0} q \, L \, J \, dV = 0, \end{aligned}$$

where $\boldsymbol{P} = \boldsymbol{F}\boldsymbol{S}$, and $L = -U' - \frac{p}{k - k_p}$.

Linearization (finite strain, initial configuration)

The linearization can be simplified as

$$\begin{bmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{C} & \mathcal{D} \end{bmatrix} \begin{bmatrix} \mathrm{d}\boldsymbol{u} \\ \mathrm{d}p \end{bmatrix} = - \begin{bmatrix} R_u \\ R_p \end{bmatrix}$$

$$\mathcal{A} \sim \int_{\Omega_0} \nabla_X \boldsymbol{v} : (\mathrm{d}\boldsymbol{F}\boldsymbol{S} + \boldsymbol{F}\,\mathrm{d}\boldsymbol{S}_{\mathrm{iso}} + \boldsymbol{F}\,\mathrm{d}\boldsymbol{S}_{\mathrm{vol}}^{u})\ dV, \quad \mathcal{D} \sim -\int_{\Omega_0} q \frac{J\,\mathrm{d}p}{k - k_p}\, dV,$$

$$\mathcal{B} \sim \int_{\Omega_0} \nabla_X \boldsymbol{v} : \boldsymbol{F}\,\mathrm{d}\boldsymbol{S}_{\mathrm{vol}}^{p}\, dV = -\int_{\Omega_0} \nabla_X \boldsymbol{v} : \mathrm{d}pJ\boldsymbol{F}^{-T}\, dV$$

$$\mathcal{C} \sim -\int_{\Omega_0} q \left(J^2 U'' + JU' + \frac{Jp}{k - k_p} \right) \boldsymbol{C}^{-1} : \mathrm{d}\boldsymbol{E}\, dV \neq \mathcal{B}^T$$

Matrix-free formulation (block structure system)

We use Krylov subspace method at each newton iteration to solve

$$\begin{aligned} \boldsymbol{J}(\boldsymbol{U}^m)\,\mathrm{d}\boldsymbol{U}^m &= -\boldsymbol{R}(\boldsymbol{U}^m) \\ \boldsymbol{U}^{m+1} &= \boldsymbol{U}^m + \mathrm{d}\boldsymbol{U}^m \end{aligned}$$

resulting from discretization at each Newton step m with given initial guess $\boldsymbol{U}^0 = [\boldsymbol{u}^0 \quad p^0]$, where

$$\boldsymbol{J} = \begin{bmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{C} & \mathcal{D} \end{bmatrix}$$

Krylov iteration methods are not necessarily fast on their own, and the iterations count depends on condition number of the operator, therefore we need a preconditioner.

Matrix-free formulation (preconditioner)

To accelerate the solve time and bound the number of iterations, regardless of the system size

$$\boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{P}^{-1}\boldsymbol{b}$$

For the preconditioner to be effective we need

- $\boldsymbol{P}^{-1}\boldsymbol{z}$ is easy to compute for any vector $\boldsymbol{z}$.
- The condition number of the preconditioned problem is smaller than the original problem.

In this study we consider the upper triangular preconditioner of the form

$$\begin{bmatrix} \hat{\mathcal{A}} & \mathcal{B} \\ \mathbf{0} & \hat{\mathcal{D}} \end{bmatrix}^{-1} \begin{bmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{C} & \mathcal{D} \end{bmatrix}$$

$$\begin{bmatrix} \hat{\mathcal{A}} & \mathcal{B} \\ \mathbf{0} & \hat{\mathcal{D}} \end{bmatrix}^{-1} = \begin{bmatrix} \hat{\mathcal{A}}^{-1} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \boldsymbol{I} & \mathcal{B} \\ \mathbf{0} & -\boldsymbol{I} \end{bmatrix} \begin{bmatrix} \boldsymbol{I} & 0 \\ \mathbf{0} & \hat{\mathcal{D}}^{-1} \end{bmatrix}$$

Matrix-free formulation (preconditioner)

$\hat{\mathcal{A}}$, $\hat{\mathcal{D}}$ are related to the original blocks and for instance, in linear elasticity, are defined by

$$\hat{\mathcal{A}} \sim \int_\Omega \nabla \boldsymbol{v} : (2\mu\, \varepsilon_{\text{dev}} + k_{pc}\, \text{trace}(\varepsilon)\boldsymbol{I})\; dv,$$

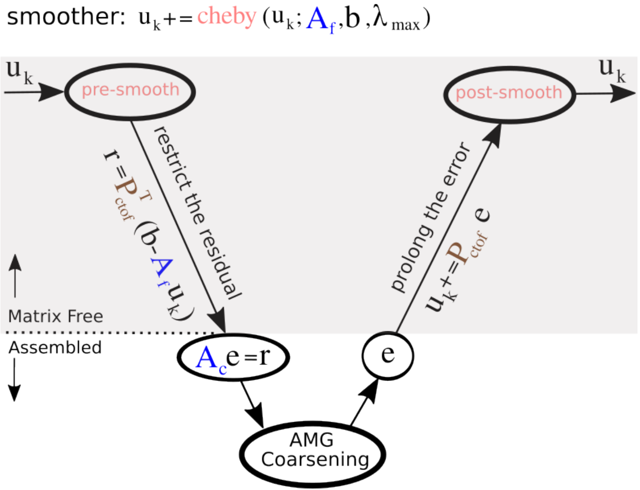
$$\hat{\mathcal{D}} \sim -\int_\Omega q \left(\frac{1}{k - k_{pc}} + \frac{1}{\mu} \right) \mathrm{d}p\, dv,$$

where k_{pc} is bulk modulus defined in terms of ν_{pc} with $-1 \leq \nu_{pc} < \nu$.

if $\nu_p = \nu_{pc} \Longrightarrow \hat{\mathcal{A}} = \mathcal{A}$

We approximate $\hat{\mathcal{A}}^{-1}$, $\hat{\mathcal{D}}^{-1}$, by p-multigrid and Jacobi preconditioners.

Matrix-free formulation (multigrid method)



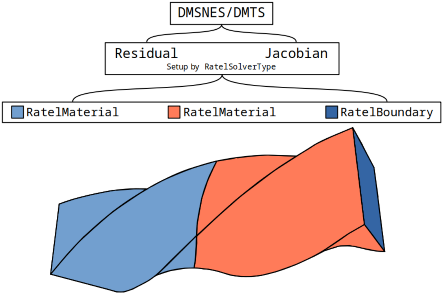
We use *p*-multigrid which is a natural fit for high-order finite elements on unstructured meshes with AMG on the coarse level.

Matrix-free formulation (Ratel)

GitLab-CI passed | License BSD 2-Clause | Documentation latest | coverage 96.05%

Features:

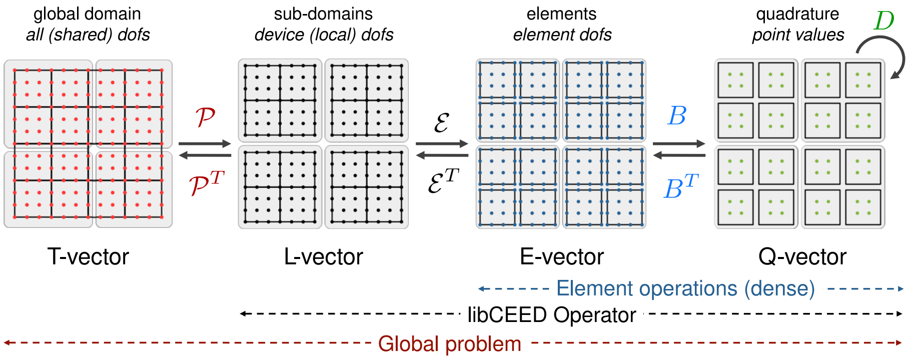
- Mixed/hyperelasticity Neo-Hookean, Mooney-Rivlin, Ogden models in initial and current configurations.
- Multi-material
- Static, Quasistatic, Dynamic
- Pressure and contact boundary conditions.



Ratel is a performance portable solid mechanics library that uses matrix-free operators from **libCEED** and solvers from **PETSc** to provide fast, efficient, and accurate simulations on next-generation architecture.

Matrix-free formulation (libCEED)

$$A = \mathcal{P}^T \mathcal{E}^T B^T D B \mathcal{E} \mathcal{P}$$



- $\mathcal{P}$: Process decomposition,
- $\mathcal{E}$: Element restriction/assembly operator
- B: Basis (DoFs-to-Qpts) evaluator,
- D: Operator at quadrature point- Qfunction $(f_0, f_1, f_{0,0}, \ldots)$

Small strain

$$\begin{bmatrix} \hat{\mathcal{A}} & \mathcal{B} \\ \mathbf{0} & \hat{\mathcal{D}} \end{bmatrix}^{-1} \begin{bmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{C} & \mathcal{D} \end{bmatrix}$$

$\nu_p, \nu_{pc} \in -1, -0.3, 0, 0.3$

if $\nu_p = \nu_{pc} \implies \hat{\mathcal{A}} = \mathcal{A}$

$\nu = 0.49999$

Effect of ν_p (small strain, MMS full Dirichlet BCs)

	$\nu_p = -1.0$	$\nu_p = -0.3$	$\nu_p = 0.0$	$\nu_p = 0.3$
$\nu_{pc} = -1.0$	**20** **9.39** **[0.12, 1]**	29 17.17 [0.12, 1.45]	35 10.05 [0.17, 1.82]	50 63.89 [0.09, 3.12]
$\nu_{pc} = -0.3$	29 13.21 [0.12, 0.99]	19 9.52 [0.11, 1]	29 18.18 [0.11, 1.41]	44 64.32 [0.09, 2.50]
$\nu_{pc} = 0.0$	34 5.0 [0.25, 0.95]	29 13.75 [0.12, 0.99]	**18** **9.85** **[0.11, 1]**	38 25.43 [0.14, 1.98]
$\nu_{pc} = 0.3$	44 22.55 [0.12, 0.99]	41 13.25 [0.12, 0.99]	37 11.19 [0.15, 0.97]	15 11.29 [0.09, 1]

KSP iteration

Con. Number

Eigenvalue's Range

Effect of ν_p (small strain, clamp-traction BCs)

	$\nu_p = -1.0$	$\nu_p = -0.3$	$\nu_p = 0.0$	$\nu_p = 0.3$
$\nu_{pc} = -1.0$	**81** **980.13** **[0.42, 401.92]**	112 1282.02 [0.39, 521.73]	147 1811.23 [0.33, 675.66]	269 6361.95 [0.24, 1290.96]
$\nu_{pc} = -0.3$	43 12.57 [0.36, 1.60]	27 12.57 [0.36, 3.27]	42 15.18 [0.31, 4.73]	73 58.07 [0.21, 10.16]
$\nu_{pc} = 0.0$	57 40.42 [0.18, 0.99]	33 7.12 [0.52, 0.77]	**20** **7.34** **[0.32, 1.47]**	47 39.81 [0.20, 4.34]
$\nu_{pc} = 0.3$	96 20.07 [0.09, 0.92]	55 56.03 [0.19, 0.99]	39 32.48 [0.29, 0.97]	14 5.54 [0.22, 1]

KSP iteration

Con. Number

Eigenvalue's Range

Numerical experiment (finite strain)

Neo-Hookean hyperelastic model with volumetric energy

$$\psi = \psi_{\text{vol}} + \psi_{\text{iso}} = k\,U(J) + \frac{\mu}{2}\left(\bar{\mathbb{I}}_1 - 3\right).$$

Stress

$$\boldsymbol{S} = \boldsymbol{S}_{\text{iso}} + \boldsymbol{S}_{\text{vol}} = 2\mu J^{-2/3}\boldsymbol{C}^{-1}\boldsymbol{E}_{\text{dev}} + \left(k_p J U' - pJ\right)\boldsymbol{C}^{-1},$$

Linearization

$$\begin{aligned} \mathrm{d}\boldsymbol{S}_{\text{iso}} = & -\frac{4}{3}\mu J^{-2/3}(\boldsymbol{C}^{-1}:\mathrm{d}\boldsymbol{E})\boldsymbol{C}^{-1}\boldsymbol{E}_{\text{dev}} \\ & -\frac{1}{3}\mu J^{-2/3}\left(2\,\mathrm{trace}\,\mathrm{d}\boldsymbol{E}\;\boldsymbol{C}^{-1} + \mathbb{I}_1\,\mathrm{d}\boldsymbol{C}^{-1}\right) \end{aligned}$$

and

$$\begin{aligned} \mathrm{d}\boldsymbol{S}_{\text{vol}}^{u} &= \left[k_p J^2 U'' + k_p J U' - pJ\right]\left(\boldsymbol{C}^{-1}:\mathrm{d}\boldsymbol{E}\right)\boldsymbol{C}^{-1} + \left(k_p J U' - pJ\right)\mathrm{d}\boldsymbol{C}^{-1}, \\ \mathrm{d}\boldsymbol{S}_{\text{vol}}^{p} &= -\,\mathrm{d}pJ\boldsymbol{C}^{-1}, \end{aligned}$$

where $U(J) = \frac{1}{2}\left(J-1\right)^2, \qquad U' = J - 1, \qquad U'' = 1.$

Numerical experiment (finite strain)

- **Quasi-Static** method in 10 pseudo time steps for $t \in [0, 1]$.
- Krylov Subspace (KSP) **GMRES**.
- Single field formulation with elements $Q_n,\ n = 1, ..., 4$.
- Mixed formulation with **continuous** and **discontinuous** pressure space i.e., Q_2Q_1, Q_3Q_2 and Q_1P_0, Q_2P_0, Q_2P_1, Q_3Q_1.
- In compressible and nearly incompressible regimes run in parallel using 16 processors.

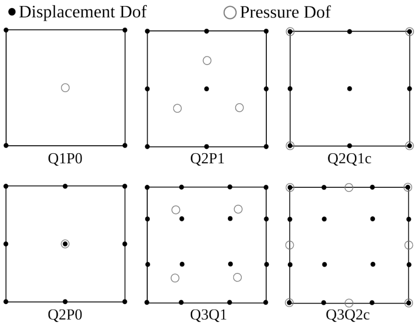
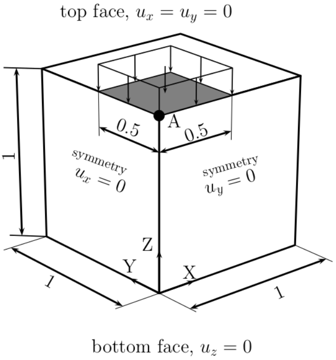


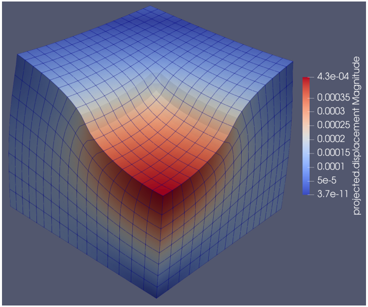
Figure: Mixed element with discontinuous and continuous pressure (2D).

Numerical experiment (finite strain, punch test)

$E = 240.566$ MPa, $(n_x, n_y, n_z) = 2^l(4,4,2)$ with $l \in \{0,1,...,4\}$



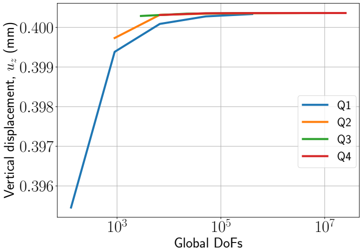
(a) Kadapa et al. (2022)



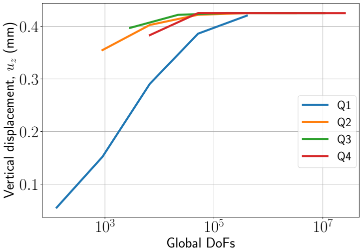
(b)

Figure: 3D block: (a) geometry and boundary conditions and (b) deformed shape under compression load $p_0 = 160$ MPa and $\nu = 0.49999$ at refinement level $l = 2$.

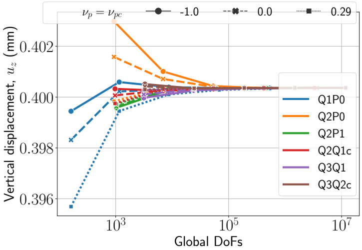
Punch test, displacement convergence study



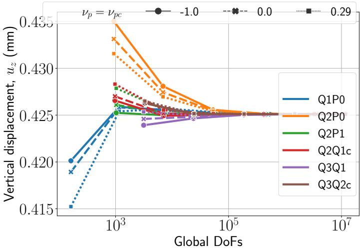
(a) Single field model $\nu = 0.3$.



(b) Single field model $\nu = 0.499$.

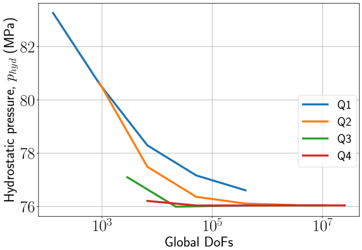


(c) Mixed fields model $\nu = 0.3$.

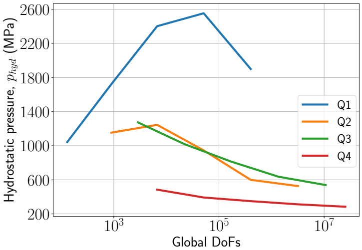


(d) Mixed fields model $\nu = 0.49999$.

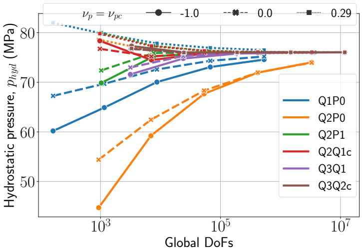
Punch test, pressure convergence study



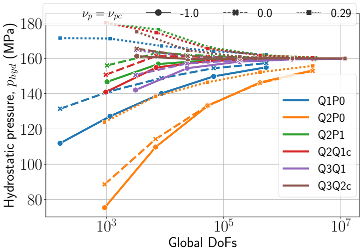
(a) Single field model $\nu = 0.3$.



(b) Single field model $\nu = 0.499$.

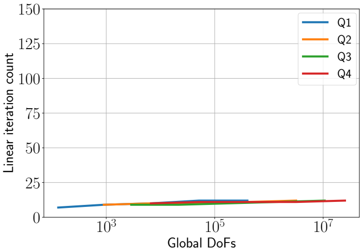


(c) Mixed fields model $\nu = 0.3$.

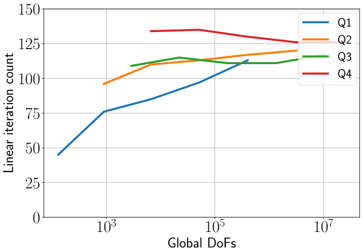


(d) Mixed fields model $\nu = 0.49999$.

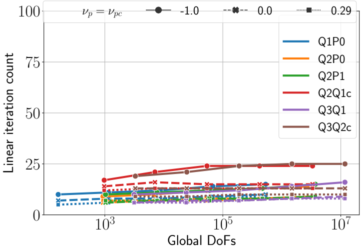
Punch test, KSP iteration



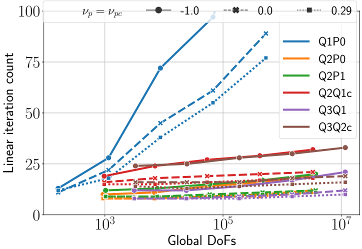
(a) Single field model $\nu = 0.3$.



(b) Single field model $\nu = 0.499$.

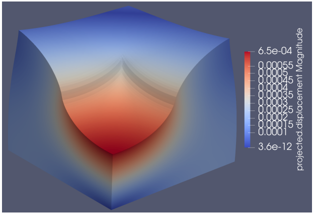


(c) Mixed fields model $\nu = 0.3$.

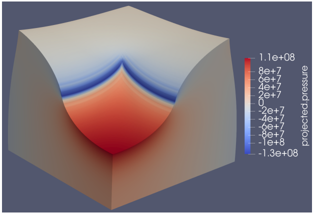


(d) Mixed fields model $\nu = 0.49999$.

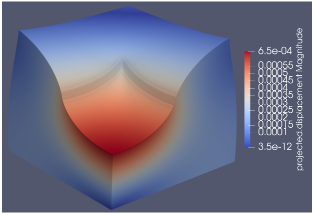
Punch test, displacement and pressure distribution



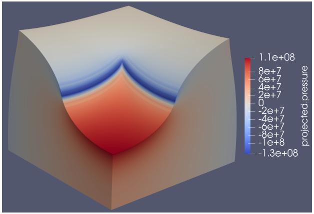
(a) Displacement Q_3.



(b) Pressure Q_3.



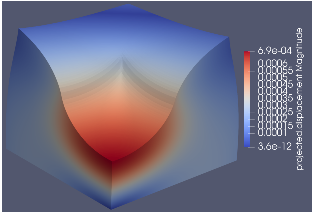
(c) Displacement $Q_3 Q_2$.



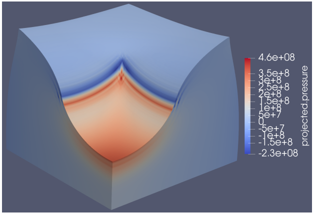
(d) Pressure $Q_3 Q_2$.

$p_0 = 320$ MPa with mesh refinement level $l = 3$, and $\nu = 0.3$.

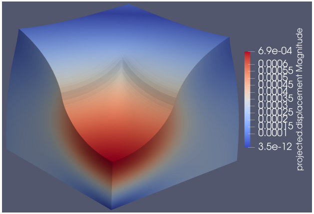
Punch test, displacement and pressure distribution



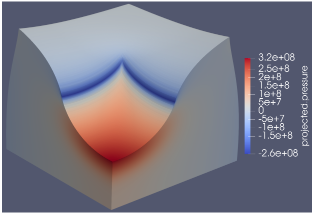
(a) Displacement Q_3.



(b) Pressure Q_3.



(c) Displacement $Q_3 Q_2$.



(d) Pressure $Q_3 Q_2$.

$p_0 = 320$ MPa with mesh refinement level $l = 3$, and $\nu = 0.495$.

Computation cost of $\boldsymbol{u}$-based vs $\boldsymbol{u} - p$ formulations

	Q_3, Total DoFs: 1.35 MDoFs			
ν	SNES Its	KSP Its	Condition number	Solve time (sec)
0.3	5	7	3	175.253
0.495	7	30	67	689.826

Computation cost of $\boldsymbol{u}$-based vs $\boldsymbol{u} - p$ formulations

	Q_3, Total DoFs: 1.35 MDoFs			
ν	SNES Its	KSP Its	Condition number	Solve time (sec)
0.3	5	7	3	175.253
0.495	7	30	67	689.826

	Q_3Q_2, Total DoFs: 1.48 MDoFs			
ν	SNES Its	KSP Its	Condition number	Solve time (sec)
0.3	5	8	9	208.126
0.495	5	13	3	289.666

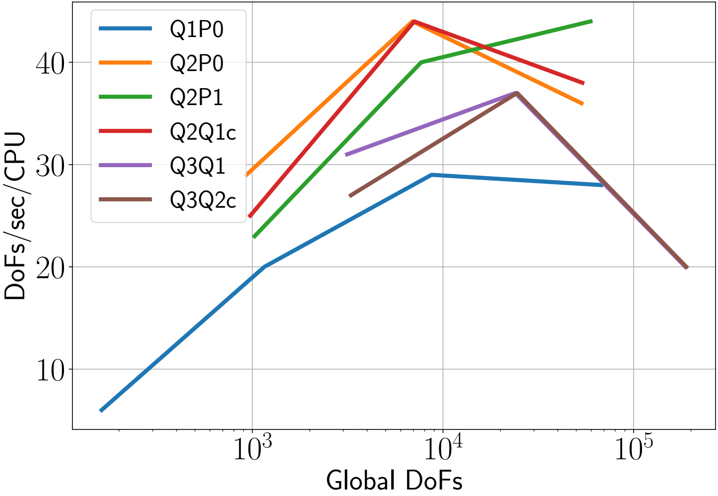
Computation cost of $\boldsymbol{u}$-based vs $\boldsymbol{u} - p$ formulations

	Q_3, Total DoFs: 1.35 MDoFs			
ν	SNES Its	KSP Its	Condition number	Solve time (sec)
0.3	5	7	3	175.253
0.495	7	30	67	689.826

	$Q_3 Q_2$, Total DoFs: 1.48 MDoFs			
ν	SNES Its	KSP Its	Condition number	Solve time (sec)
0.3	5	8	9	208.126
0.495	5	13	3	289.666

Even if we only need displacement results, it is cheaper to run mixed formulation when $\nu \to 0.5$.

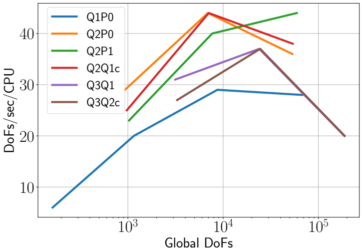
Efficiency of the Sparse direct solver vs Matrix-free



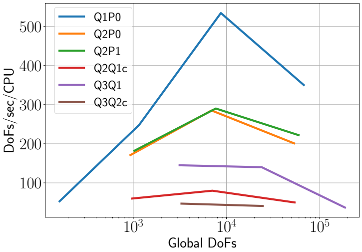
Sparse matrix, Cholesky-Cholesky.

Approximating $\hat{\mathcal{A}}^{-1}, \hat{\mathcal{D}}^{-1}$ by Cholesky factorization.

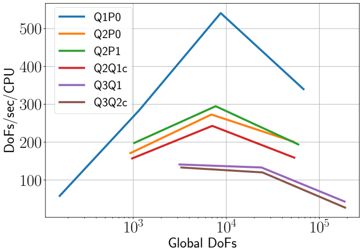
Efficiency of the Sparse matrix vs Matrix-free



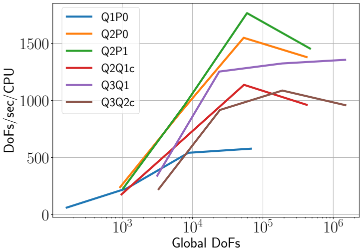
(a) Sparse matrix, Cholesky-Cholesky.



(b) Sparse matrix, AMG-AMG.

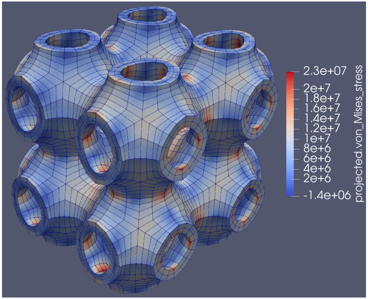


(c) Sparse matrix, AMG-Jacobi.



(d) Matrix-free, pMG-Jacobi.

Element aspect ratio effect on efficiency/robustness



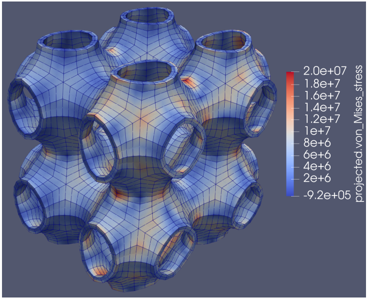
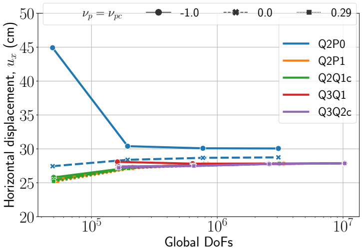
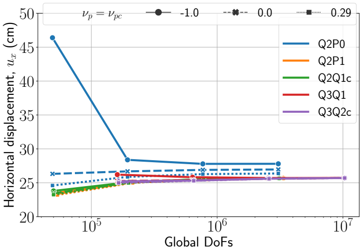


Figure: Displacement distribution for schwarz mesh with refinement level $l = 2$, 2 layers, and extent (2,2,2) using mixed Neo-Hookean model (left) thickness 0.2 under 4 Mpa compression, (right) thickness 0.1 under 2.35 Mpa compression.

Schwarz thickness 0.2, displacement convergence study

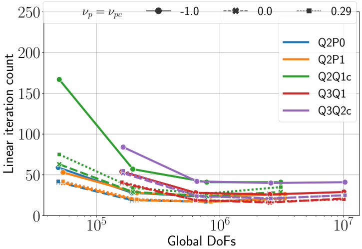


(a) Mixed model $\nu = 0.3$.

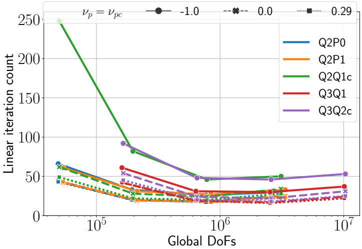


(b) Mixed model $\nu = 0.498$.

Schwarz thickness 0.2, KSP iteration

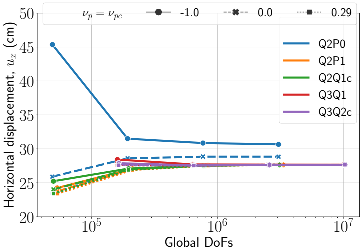


(a) Mixed model $\nu = 0.3$.

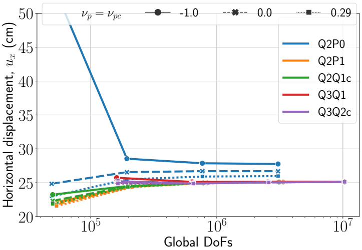


(b) Mixed model $\nu = 0.498$.

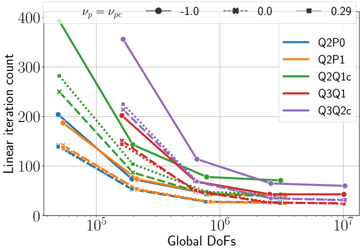
Schwarz thickness 0.1, displacement convergence study



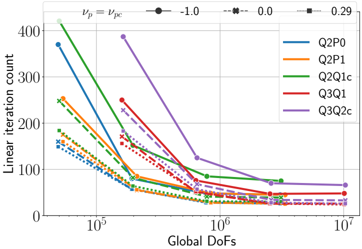
(a) Mixed model $\nu = 0.3$.



(b) Mixed model $\nu = 0.498$.

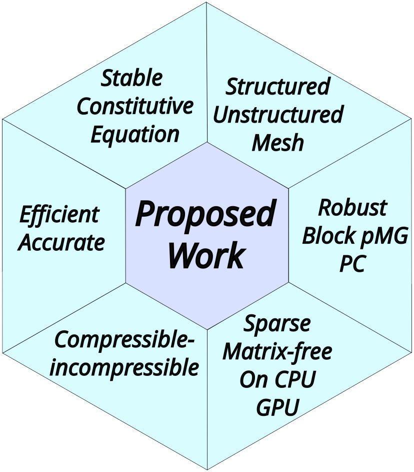


(a) Mixed model $\nu = 0.3$.

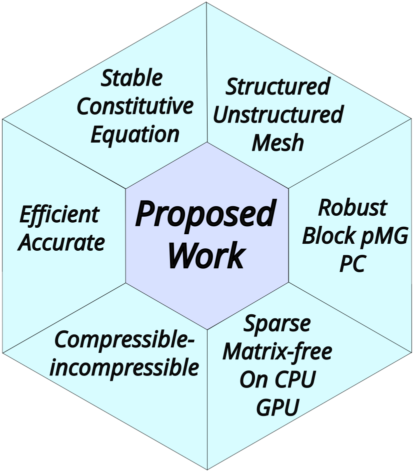


(b) Mixed model $\nu = 0.498$.

Conclusion and future work

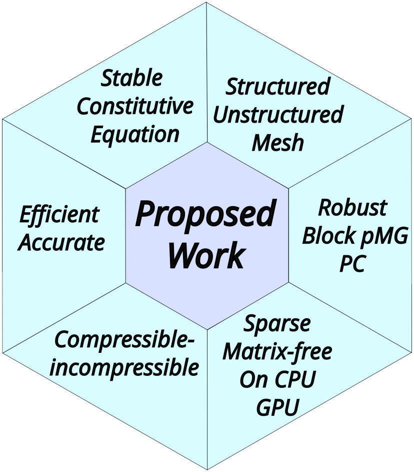


Conclusion and future work



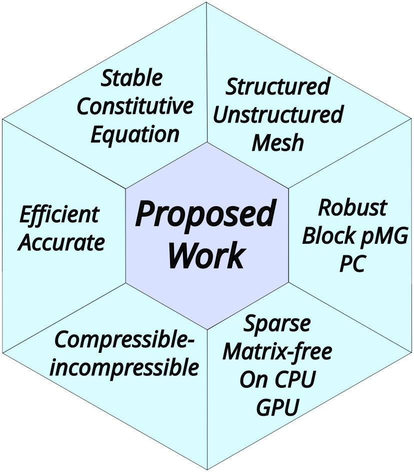
- When $\nu \to 0.5$, $\boldsymbol{u}$-based formulation shows fluctuation in pressure response even with high-order element but almost accurate results in displacement.

Conclusion and future work



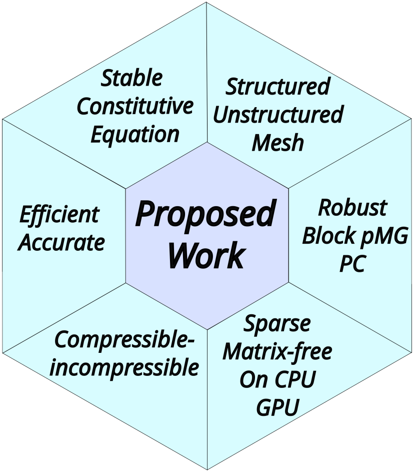
- When $\nu \to 0.5$, $\boldsymbol{u}$-based formulation shows fluctuation in pressure response even with high-order element but almost accurate results in displacement.
- Solve time of $\boldsymbol{u} - p$ simulation is less than single field case when $\nu \to 0.5$.

Conclusion and future work



- When $\nu \to 0.5$, $\boldsymbol{u}$-based formulation shows fluctuation in pressure response even with high-order element but almost accurate results in displacement.
- Solve time of $\boldsymbol{u} - p$ simulation is less than single field case when $\nu \to 0.5$.
- KSP iteration count, and largest eigenvalue are smaller for $\nu_p > 0$

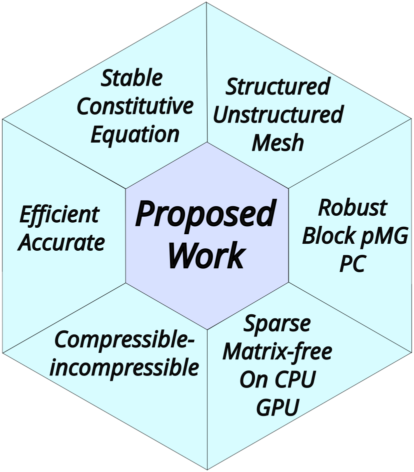
Conclusion and future work



- When $\nu \to 0.5$, $\boldsymbol{u}$-based formulation shows fluctuation in pressure response even with high-order element but almost accurate results in displacement.
- Solve time of $\boldsymbol{u} - p$ simulation is less than single field case when $\nu \to 0.5$.
- KSP iteration count, and largest eigenvalue are smaller for $\nu_p > 0$

- Stable constitutive formulation opens a door for hyperelastic simulation using single or mixed precision.

Conclusion and future work



- When $\nu \to 0.5$, $\boldsymbol{u}$-based formulation shows fluctuation in pressure response even with high-order element but almost accurate results in displacement.
- Solve time of $\boldsymbol{u} - p$ simulation is less than single field case when $\nu \to 0.5$.
- KSP iteration count, and largest eigenvalue are smaller for $\nu_p > 0$

- Stable constitutive formulation opens a door for hyperelastic simulation using single or mixed precision.
- With this implemented mixed formulation in Ratel, we can simulate all other mixed problems like poroelasticity, phase field modeling, ...

More GPU results and stable constitutive formulation

Crusher, Summit, Lassen, Perlmutter

Performance-Portable Solid Mechanics via Matrix-Free p-Multigrid

Jed Brown
University of Colorado, Boulder
jed@jedbrown.org

Valeria Barra
California Institute of Technology
valeria@caltech.edu

Natalie Beams
University of Tennessee
nbeams@icl.utk.edu

Leila Ghaffari
University of Colorado, Boulder
leila.ghaffari@colorado.edu

Matthew Knepley
University of Buffalo
knepley@gmail.com

William Moses
Massachusetts Institute of Technology
wmoses@mit.edu

Rezgar Shakeri
University of Colorado, Boulder
rezgar.shakeri@colorado.edu

Karen Stengel
University of Colorado, Boulder
karen.stengel@colorado.edu

Jeremy L. Thompson
University of Colorado, Boulder
jeremy.thompson@colorado.edu

Junchao Zhang
Argonne National Laboratory
jczhang@mcs.anl.gov

Stable numerics for finite-strain elasticity

Rezgar Shakeri, Leila Ghaffari, Jeremy L. Thompson, Jed Brown

Back-up slides

Stable constitutive modeling

- $\epsilon_{\text{machine}} = \sup_x |\text{fl}(x) - x|/|x|$.
- Elementary math operators $\circledast$ (standing for addition, subtraction, multiplication, or division)

$$x \circledast y = \text{fl}(x * y), \quad |x \circledast y - x * y|/|x * y| \leq \epsilon_{\text{machine}}$$

Remark

Machine epsilon or machine precision is an upper bound on the relative approximation error due to rounding in floating point arithmetic. $\epsilon_{\text{machine}} \approx 10^{-16}$ for double precision and 6×10^{-8} for single precision.

Stable constitutive modeling

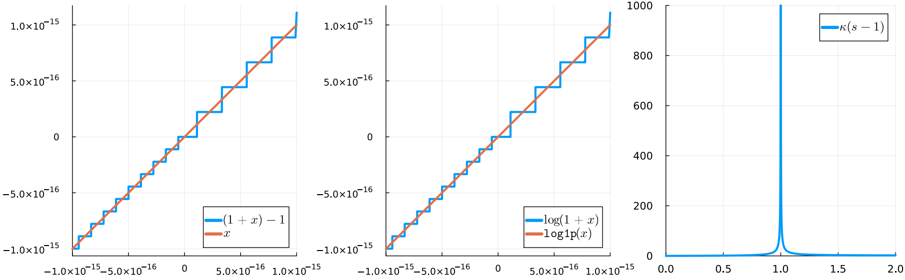
- $\epsilon_{\text{machine}} = \sup_x |\text{fl}(x) - x|/|x|$.
- Elementary math operators $\circledast$ (standing for addition, subtraction, multiplication, or division)

$$x \circledast y = \text{fl}(x * y), \quad |x \circledast y - x * y|/|x * y| \leq \epsilon_{\text{machine}}$$

- How about $(x \circledast y) \circledast z$?

$(x \oplus 1) \ominus 1 = 0$ for $x = 10^{-16}$ has a relative error of 1.

Stable constitutive modeling



$s := 1 + x$, $f(s) = s - 1$ has unbounded condition number as $s \to 1$ (right), despite this operation being computed exactly in floating point arithmetic.

Stable computation of strain

$$\boldsymbol{E} = \frac{1}{2}(\boldsymbol{C} - \boldsymbol{I}) = \frac{1}{2}\left(\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}\right)$$

We substitute $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{H}$, where $\boldsymbol{H} = \nabla_X \boldsymbol{u}$

$$\boldsymbol{E} = \frac{1}{2}\left(\boldsymbol{H} + \boldsymbol{H}^T + \boldsymbol{H}^T\boldsymbol{H}\right)$$

Stable computation of $J = |\boldsymbol{F}|$

Consider the 2-dimensional case

$$\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{H} = \boldsymbol{I} + \nabla_X \boldsymbol{u} = \begin{bmatrix} 1 + u_{1,1} & u_{1,2} \\ u_{2,1} & 1 + u_{2,2} \end{bmatrix},$$

and let compute $\mathrm{J}_{-1} = J - 1$ by

$$\mathrm{J}_{-1} = u_{1,1} + u_{2,2} + u_{1,1}u_{2,2} - u_{1,2}u_{2,1}.$$

then $J = \mathrm{J}_{-1} + 1$.

Stable constitutive modeling

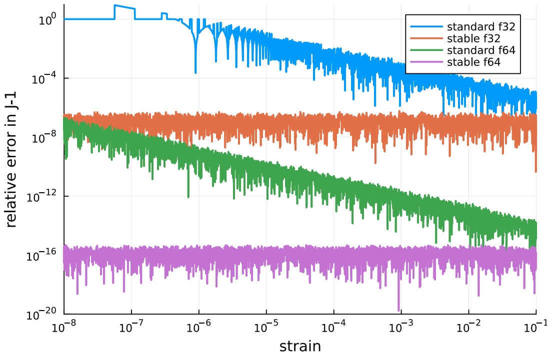


Figure: Relative error of standard computation of $J - 1$ and its stable way $\mathtt{J}_{-1}$

Remark

The standard computation for a strain of order 10^{-m} will result in m digits lost in the computed stress.

Stable constitutive modeling

Software/book	stable strain $\boldsymbol{E}$	stable J	stable $\log J$	stable constitutive equation
FEAP [85]	✓	–	–	–
FEBio [59]	–	–	–	–
Abaqus [82]	–	–	–	–
MOOSE [57]	–	–	–	–
Albany-LCM [77]	–	–	–	–
LifeV [14]	–	–	–	–
MoFEM [50]	–	–	–	–
Ratel [6]	✓	✓	✓	✓
Holzapfel [43]	–	–	–	–
Wriggers [89]	–	–	–	–

We have implemented, Neo-Hookean, Mooney-Rivlin, and Ogden in a stable way in Ratel.

Inf-sup stability

Find $\lambda \in \mathbb{R}$, $0 \neq (\boldsymbol{u}_h, p_h) \in \mathbb{V}_h \times \mathbb{Q}_h$, such that for all $(\boldsymbol{v}, q) \in \mathbb{V}_h^0 \times \mathbb{Q}_h$

$$a(\boldsymbol{v}, \boldsymbol{u}) + b(\boldsymbol{v}, p) + b(q, \boldsymbol{u}) = -\lambda \langle p, q \rangle_{\mathbb{Q}}$$

then, $\lambda \geq 0$ and inf-sup constant is $\beta = \sqrt{\lambda_{\min}}$, $\quad \beta \geq \beta_h > 0$

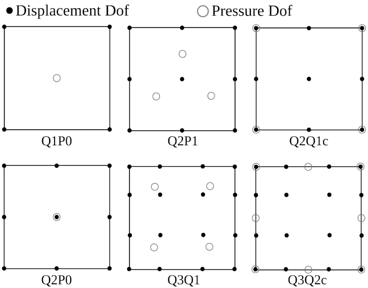
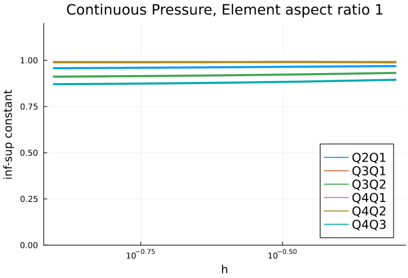
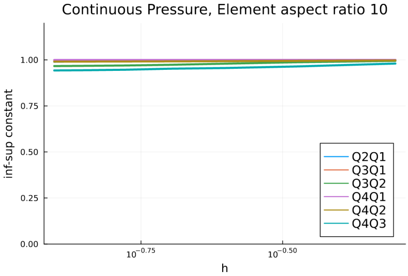


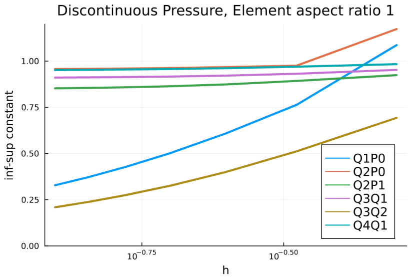
Figure: Mixed element with discontinuous and continuous pressure (2D).

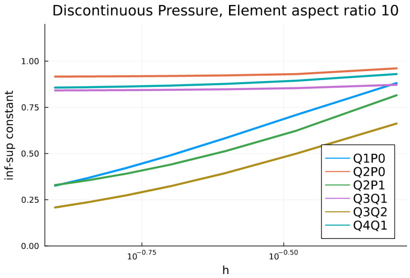
Inf-sup stability- continuous pressure





Inf-sup stability- discontinuous pressure





Convergence study- continuous pressure

Table 4.3: Convergence study for mixed-linear elasticity in incompressibility regime with **continuous** pressure with $n_x \times n_x$ uniform mesh.

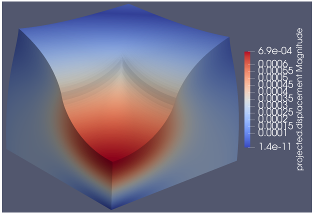
n_x	Q_2Q_{1c}				Q_3Q_{2c}			
	Error $\boldsymbol{u}$	Order $\boldsymbol{u}$	Error p	Order p	Error $\boldsymbol{u}$	Order $\boldsymbol{u}$	Error p	Order p
4	9.467e−05		4.168e−03		6.935e−06		5.669e−04	
8	5.756e−06	4.040	8.953e−04	2.219	6.971e−07	3.314	8.775e−05	2.692
12	1.359e−06	3.559	3.839e−04	2.088	1.584e−07	3.654	2.770e−05	2.844
16	5.231e−07	3.319	2.131e−04	2.046	5.323e−08	3.792	1.201e−05	2.905
n_x	Q_3Q_{1c}				Q_4Q_{2c}			
	Error $\boldsymbol{u}$	Order $\boldsymbol{u}$	Error p	Order p	Error $\boldsymbol{u}$	Order $\boldsymbol{u}$	Error p	Order p
4	1.470e−04		4.150e−03		1.263e−05		5.657e−04	
8	1.381e−05	3.412	8.942e−04	2.214	1.159e−06	3.446	8.772e−05	2.689
12	3.803e−06	3.181	3.837e−04	2.087	2.562e−07	3.723	2.769e−05	2.844
16	1.562e−06	3.095	2.131e−04	2.045	8.510e−08	3.831	1.201e−05	2.905

Convergence study- discontinuous pressure

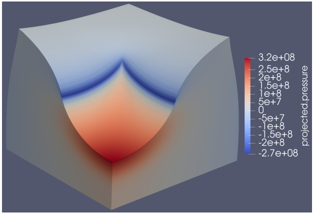
Table 4.2: Convergence study for mixed linear elasticity in the incompressibility regime with **discontinuous** pressure with $n_x \times n_x$ uniform mesh.

n_x	Q_2P_0				Q_2P_1			
	Error $\boldsymbol{u}$	Order $\boldsymbol{u}$	Error p	Order p	Error $\boldsymbol{u}$	Order $\boldsymbol{u}$	Error p	Order p
4	7.331e−04		1.512e−02		1.042e−04		5.774e−03	
8	2.224e−04	1.721	8.085e−03	0.904	7.872e−06	3.727	1.544e−03	1.903
12	1.035e−04	1.886	5.456e−03	0.970	1.765e−06	3.688	6.928e−04	1.976
16	5.932e−05	1.935	4.109e−03	0.986	6.377e−07	3.538	3.907e−04	1.991
n_x	Q_3Q_1				Q_4Q_2			
	Error $\boldsymbol{u}$	Order $\boldsymbol{u}$	Error p	Order p	Error $\boldsymbol{u}$	Order $\boldsymbol{u}$	Error p	Order p
4	8.397e−05		3.228e−03		7.979e−06		4.319e−04	
8	1.156e−05	2.862	8.300e−04	1.960	5.308e−07	3.910	5.519e−05	2.968
12	3.496e−06	2.949	3.707e−04	1.988	1.064e−07	3.963	1.642e−05	2.990
16	1.487e−06	2.971	2.089e−04	1.994	3.388e−08	3.979	6.936e−06	2.995

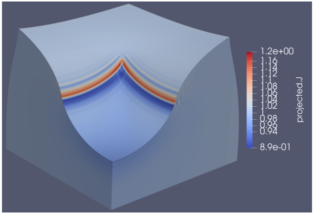
Punch test, displacement and pressure distribution



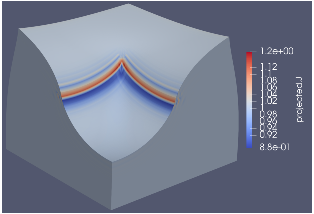
(a) Displacement $Q_3 Q_2$.



(b) Pressure $Q_3 Q_2$.



(c) J, $Q_3 Q_2$, $\nu = 0.495$.



(d) J, $Q_3 Q_2$, $\nu = 0.5$.

$p_0 = 320$ MPa with mesh refinement level $l = 3$, and Poisson's ratio 0.5.

See $\nu = 0.5$ results

	Q_3, Total DoFs: 1345584			
ν	SNES Its	KSP Its	Condition number	Solve time (sec)
0.3	5	7	3	175.253
0.495	7	30	67	689.826
	Q_3Q_2, Total DoFs: 1485009			
ν	SNES Its	KSP Its	Condition number	Solve time (sec)
0.3	5	8	9	208.126
0.495	5	13	3	289.666
0.5	5	13	3	933.915

Only solve time is different