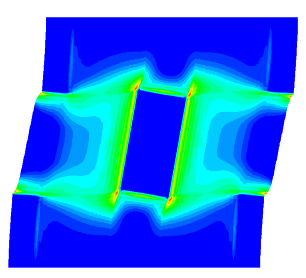
Stability of Multi-field Saddle Point Principles in Irreversible Continuum Thermodynamics

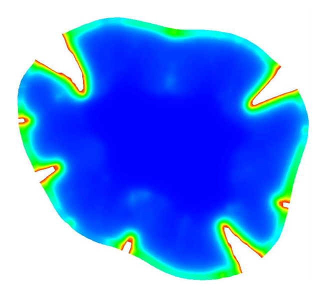
Andreas Krischok & Christian Linder

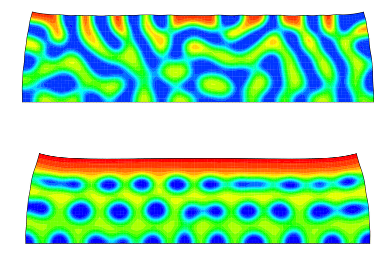
Introduction

Examples of saddle point principles in applied mechanics:


Footing problem in poroelasticity [4].


Shear test in gradient-extended plasticity [3].

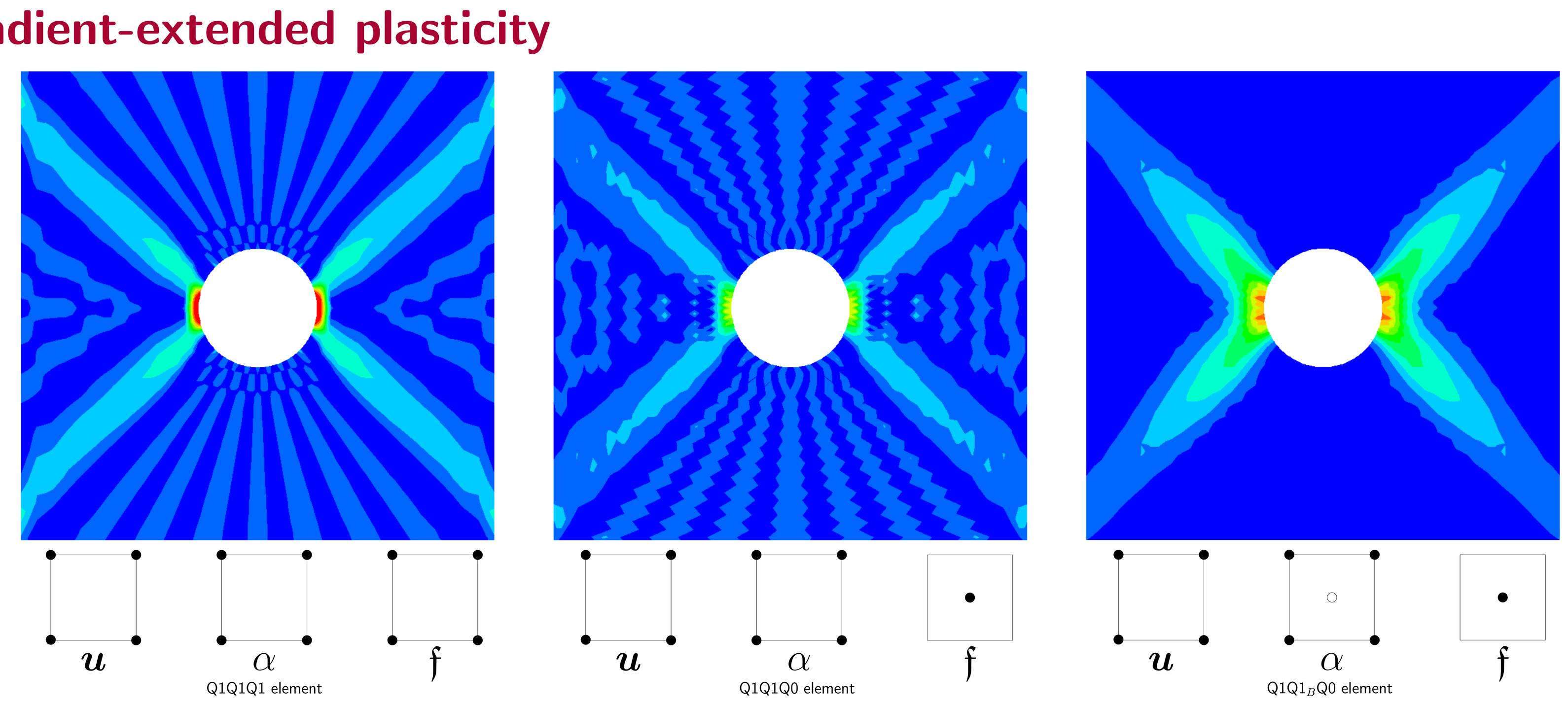

Diffusion-induced fracture in Si-batteries [1].


Manufacturing of blended polymers [3].

Motivation:

- Numerous coupled problems in thermodynamics can be described by a discrete Lagrangian from which the Euler equations follow from a saddle point principle.
- Stability conditions for mixed finite elements for such multi-fold saddle points need to be identified and verified for the element design of new models.
- Phase separation processes such as Cahn-Hilliard type diffusion exhibit physical & numerical instabilities that need to be addressed.

Gradient-extended plasticity



Stability estimate and numerical verification:

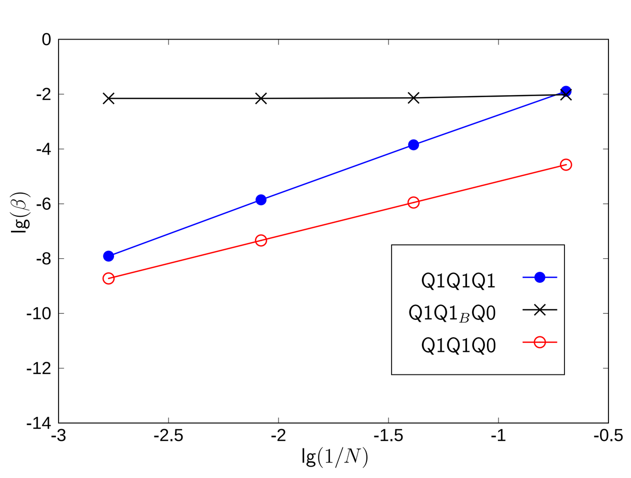
Let the displacements $\boldsymbol{u}$ and equivalent plastic strains $\boldsymbol{\alpha}$ be H^1_0-elliptic and let all fields including the driving forces $\mathfrak{f}$ satisfy for a real constant β that:

$$\{\boldsymbol{u}^*, \boldsymbol{\alpha}^*, \mathfrak{f}^*\} = \text{Arg}\{ \inf_{\boldsymbol{u}\in H^1_0} \inf_{\boldsymbol{\alpha}\in H^1} \sup_{\mathfrak{f}\in L^2} (\Pi^\Delta(\boldsymbol{u}, \boldsymbol{\alpha}, \mathfrak{f}))\} \quad \text{with} \quad \sup_{\boldsymbol{u}_h\in H^1_0} \sup_{\boldsymbol{\alpha}_h\in H^1} \inf_{\mathfrak{f}_h\in L^2} \left[\frac{\int_\Omega \alpha_h \mathfrak{f}_h \, d\Omega - \int_\Omega \sqrt{2/3}\gamma[u_h]\mathfrak{f}_h \, d\Omega}{||\mathfrak{f}_h||_{L^2}(||\boldsymbol{u}_h||_{H^1} + ||\boldsymbol{\alpha}_h||_{H^1})} \right] \geq \beta$$

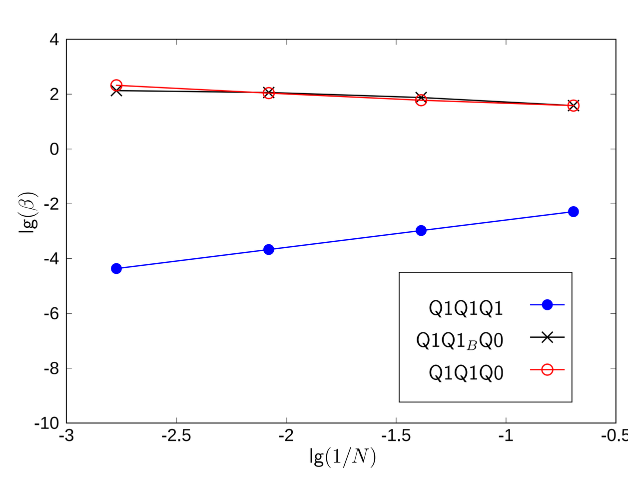
Then for $C > 0$ the estimate for stability (and thus uniqueness)

$$||\boldsymbol{u}^*_h - \boldsymbol{u}^I||_{H^1} + ||\boldsymbol{\alpha}^*_h - \boldsymbol{\alpha}^I||_{H^1} + ||\mathfrak{f}^*_h - \mathfrak{f}^I||_{L^2} \leq C\, (||\boldsymbol{u}^* - \boldsymbol{u}^I||_{H^1} + ||\boldsymbol{\alpha}^* - \boldsymbol{\alpha}^I||_{H^1} + ||\mathfrak{f}^* - \mathfrak{f}^I||_{L^2})$$

holds in a neighborhood around the unique saddle point $\{\boldsymbol{u}^*, \boldsymbol{\alpha}^*, \mathfrak{f}\}$.



Fully elastic case.

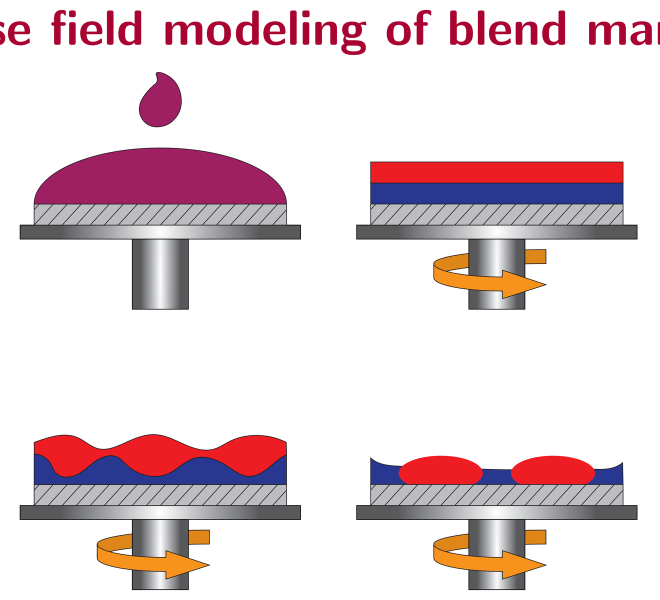


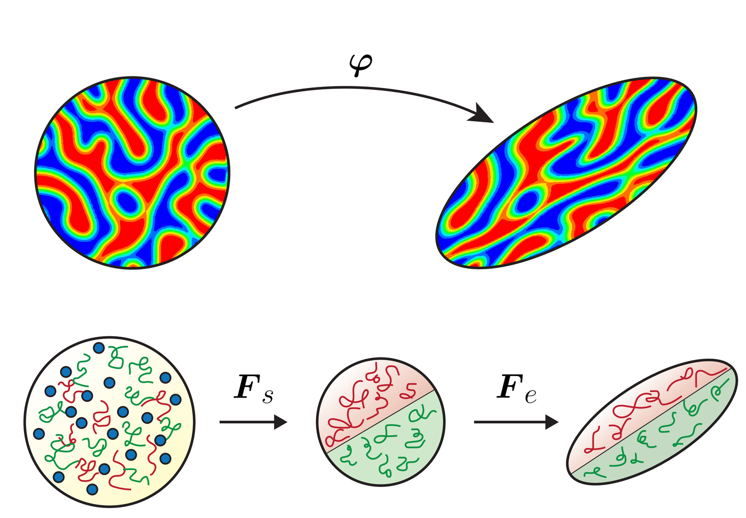
Fully plastic case.

Conclusion:

The previously unknown stability condition was identified and it was shown in a generalized eigenvalue test that the $Q1Q1_BQ0$ element proposed in [3] is always stable.

Phase field modeling of blend manufacturing


Blend formation during spin-coating showing an unstable phase separation.



Displacements can be due to either volumetric evaporation or isochoric chain deformation.

Proposed model:

Consider the motion φ, concentration c and chem. potential in the problem

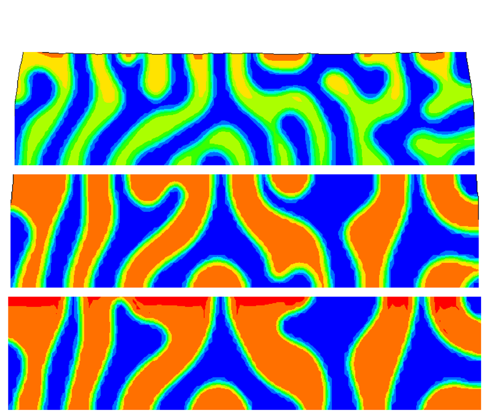
$$\{\boldsymbol{\varphi}^*, c^*_i, \mu^*_i\} = \text{Arg}\{ \inf_{\boldsymbol{u}\in H^1_0} \inf_{c_i\in H^1} \sup_{\mu_i\in H^1} \Pi^\Delta(\boldsymbol{u}, c, \mu)\} \quad \text{where} \quad \Pi^\Delta(\boldsymbol{u}, c, \mu) = \int_\mathcal{B} \psi_{\text{stor}}(\boldsymbol{u}, c) dV + \int_\mathcal{B} \Delta t \phi_{\text{diss}}(c, \mu) dV - \Pi^{\text{ext}}$$

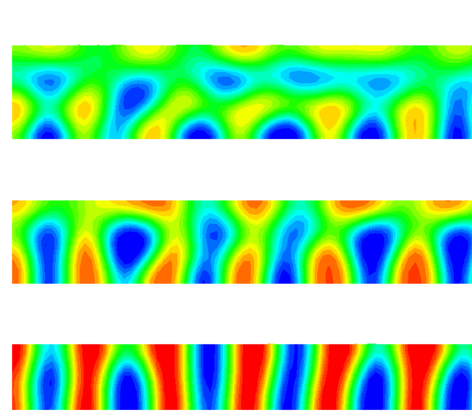
for the phases $i \in \tilde{S} = \{A, B\}$ referring to polymer type A and B satisfying the balance of linear momentum, Cahn-Hilliard diffusion and mass conservation through

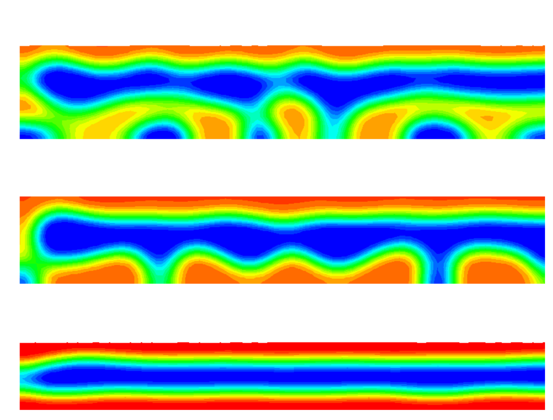
$$\int_\mathcal{B} \boldsymbol{P} : \delta\boldsymbol{F} dV - \mathcal{F}^{\text{ext}}[\delta\boldsymbol{u}^h] = 0 \qquad \text{where } \boldsymbol{P} = \partial_{\boldsymbol{F}}\psi_{\text{stor}}$$

$$\int_\mathcal{B} \{s_i\delta c_i + \epsilon^2_i \nabla c_i \cdot \nabla\delta c_i - \mu_i \delta c_i\} dV = 0 \qquad \text{where } s_i = \partial_c \psi_{\text{stor}}$$

$$\int_\mathcal{B} \{-\delta\mu_i(c_i - c^n_i) + \Delta t \boldsymbol{Q}_i \cdot \nabla\delta\mu_i\} dV = 0 \qquad \text{where } \boldsymbol{Q}_i = \partial_{-\nabla\mu_i}\phi_{\text{diss}} \,.$$


Solidification of a blend.


Solvent dependent interface.


Constant interface.

Conclusion:

The model couples mechanics, Cahn-Hilliard-type phase separation and evaporation in a combined manner and is thus able to predict morphologies in various cases. It supports speculations in [7] that the unfavorable horizontal layer alignment is due to the interface energy being a strong function of the solvent fraction.

Phase field topology optimization

Proposed model:

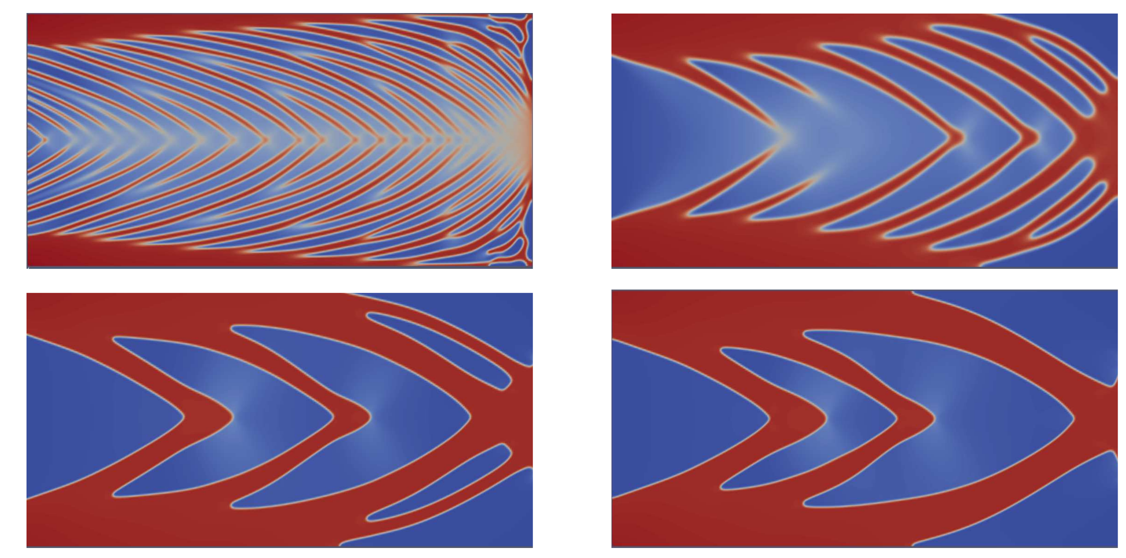
Consider elliptic displacements $\boldsymbol{u}$ and concentration c with a concave potential μ in

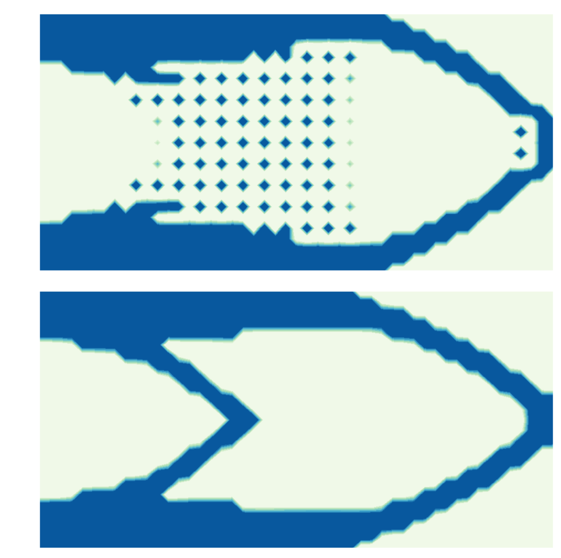
$$\{\boldsymbol{u}^*, c^*, \mu^*\} = \text{Arg}\{ \inf_{\boldsymbol{u}\in H^1_0} \inf_{c\in H^1} \sup_{\mu\in H^1} (\Pi^\Delta(\boldsymbol{u}, c, \mu))\} \quad \text{with} \quad \sup_{\boldsymbol{u}\in H^1_0} \sup_{c\in H^1} \inf_{\mu\in H^1} \left[\frac{\int_\Omega c\psi_{\text{el}}[\boldsymbol{u}] \, d\Omega - \int_\Omega \mu c \, d\Omega}{||\mu||_{L^2}(||\boldsymbol{u}||_{H^1} + ||c||_{H^1})} \right] \geq \beta > 0 \,.$$

Then we have for $C > 0$ the estimate for stability (and thus uniqueness)

$$||\boldsymbol{u}^* - \boldsymbol{u}^I||_{H^1} + ||c^* - c^I||_{H^1} + ||\mu^* - \mu^I||_{H^1} \leq C\, (||\boldsymbol{u}^*_h - \boldsymbol{u}^I||_{H^1} + ||c^*_h - c^I||_{H^1} + ||\mu^*_h - \mu^I||_{H^1})$$

in a neighborhood around the unique saddle point $\{\boldsymbol{u}^*, c^*, \mu^*\}$.

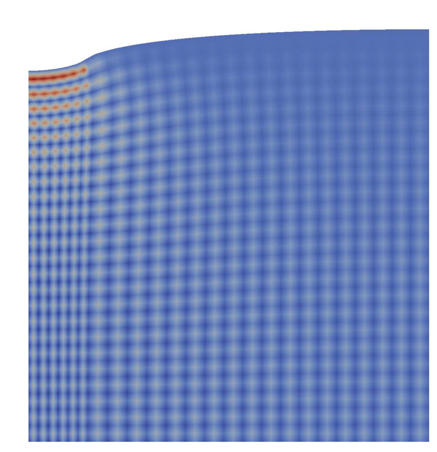

Evolution of phase field to the optimized topology.

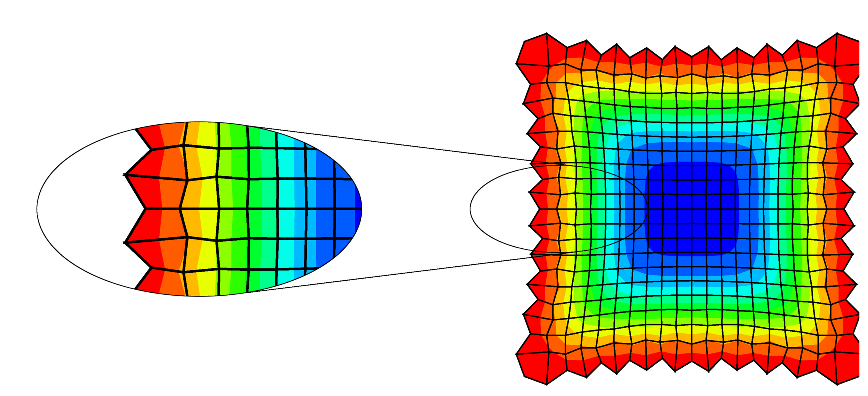

Stable and unstable solution.

Conclusion:

The proposed model provides reliable results with a Q2Q1Q1 interpolation although it can be shown that some minor zero modes remain [3].

Incompatible modes in finite poroelasticity


Footing problem with unstable pressure.


Swelling gel with enhanced modes undergoing hourglassing.

Proposed element formulation and numerical test:

Let the motion φ and the strain enhancement $\tilde{\mathbb{F}}$ be H^1_0-elliptic and let all fields including the (pore) pressure satisfy for a real constant β that:

$$\{\boldsymbol{\varphi}^*, \tilde{\mathbb{F}}^*, p^*\} = \text{Arg}\{ \inf_{\varphi\in H^1_0} \inf_{\tilde{\mathbb{F}}\in L^2} \sup_{p\in H^1} (\Pi(\boldsymbol{u}, \tilde{\mathbb{F}}, p))\} \quad \text{and} \quad \sup_{\varphi_h\in H^1_0} \sup_{\tilde{\mathbb{F}}_h\in L^2} \inf_{p_h\in L^2} \left[\frac{\int_\mathcal{B} p_h \det \boldsymbol{F}(\boldsymbol{\varphi}_h, \tilde{\mathbb{F}}_h) \, dV}{||p_h||_{L^2}(||\boldsymbol{\varphi}_h||_{H^1} + ||\mathbb{F}_h||_{L^2})} \right] \geq \beta > 0$$

The weak equations for balance of linear momentum, the orthogonality constraint and mass conservation are

$$\int_\mathcal{B} \{\boldsymbol{\tau}_{\text{eff}} : \text{sym}(\nabla_{\boldsymbol{x}}\delta\boldsymbol{\varphi}) - Bp\boldsymbol{1}\, DJ[\delta\boldsymbol{\varphi}]\} dV - \mathscr{P}_{\text{ext}}(\delta\boldsymbol{\varphi}) = 0$$

$$\int_\mathcal{B} \{\boldsymbol{\tau}_{\text{eff}} : \text{sym}(\boldsymbol{F}^{-T}\delta\tilde{\boldsymbol{F}}) - Bp\boldsymbol{1}\, DJ[\delta\tilde{\boldsymbol{F}}]\} dV = 0$$

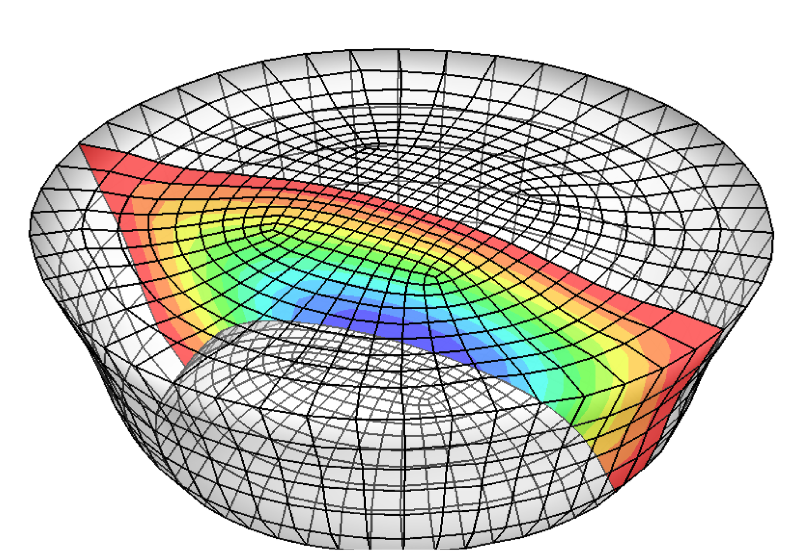
$$\int_\mathcal{B} \{-B(J - J_n)\delta p - \frac{1}{M}(p - p_n)\delta p + \Delta t \boldsymbol{q} \cdot \nabla_{\boldsymbol{x}}\delta p\} dV - \mathscr{P}_{\text{ext}}(\delta p) = 0 \,.$$

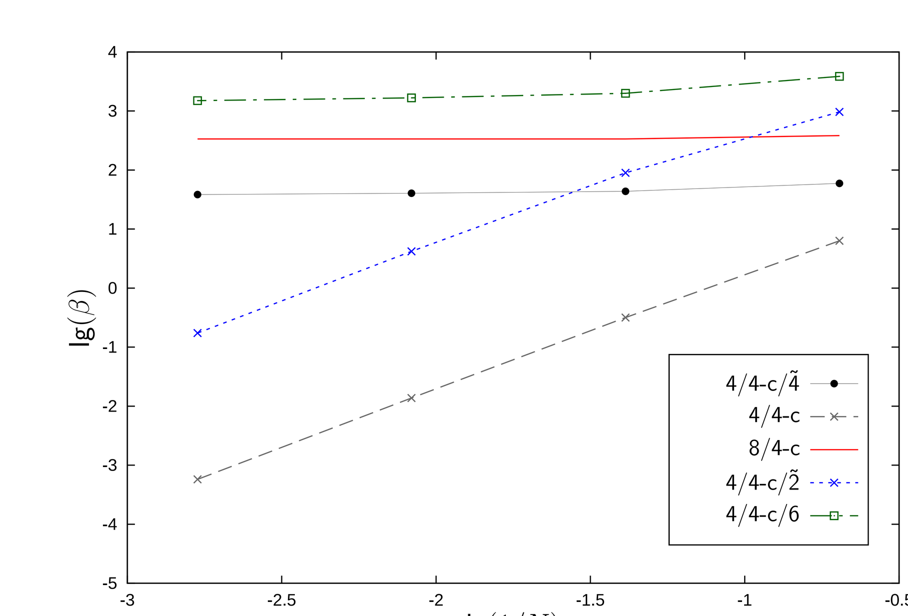
Then we have for $C > 0$ the estimate for stability (and thus uniqueness)

$$||\boldsymbol{u}^*_h - \boldsymbol{u}^I||_{H^1} + ||\tilde{\mathbb{F}}^*_h - \tilde{\mathbb{F}}^I||_{L^2} + ||p^*_h - p^I||_{H^1} \leq C\, (||\boldsymbol{u}^* - \boldsymbol{u}^I||_{H^1} + ||\tilde{\mathbb{F}}^* - \tilde{\mathbb{F}}^I||_{L^2} + ||p^* - p^I||_{H^1}) \,.$$

It can be shown that the classical test and its extension to incompatible modes satisfies uniqueness in poroelasticity [4]. We propose the incompatible enhancement [2]

$$\mathbb{F}_h(\boldsymbol{\xi}) = \begin{bmatrix} \Gamma_1\xi + \tilde{\Gamma}_3\xi\eta & 0 \\ 0 & \Gamma_2\eta + \tilde{\Gamma}_4\xi\eta \end{bmatrix} \quad \text{and} \quad \mathbb{F}(\boldsymbol{\xi}) = \begin{bmatrix} \tilde{\Gamma}_1\xi + \tilde{\Gamma}_4\xi\eta + \tilde{\Gamma}_5\xi\zeta & 0 & 0 \\ 0 & \tilde{\Gamma}_2\eta + \tilde{\Gamma}_6\eta\xi + \tilde{\Gamma}_7\eta\zeta & 0 \\ 0 & 0 & \tilde{\Gamma}_3\zeta + \tilde{\Gamma}_8\zeta\xi + \tilde{\Gamma}_9\zeta\eta \end{bmatrix}$$


Stable swelling of a gel disc with proposed element.



Numerical inf-sup test verifying stability [3].

Conclusion:

The proposed formulation is free from severe hourglassing, locking resistant and inf-sup stable while allowing low-order interpolations and is hence trusted to be a robust alternative to parameter-dependent low-order stabilizations methods in poroelasticity.

References

[1] X. Zhang, A. Krischok & C. Linder (2016). *Comput. Methods Appl. Mech. Eng.* 312(2017):51-77.
[2] A. Krischok & C. Linder (2016). *Int. J. Numer. Meth. Eng.* 106(4):278-297.
[3] A. Krischok & C. Linder (2019). *Comput. Methods Appl. Mech. Eng.* 357:112497.
[4] B. Dortdivanlioglu et al. (2017). *Int. J. Numer. Meth. Eng.* 114(1):28-46.
[5] D. Chapelle & K.J. Bathe (1993). *Comput. Struct.* 47(4-5):537-545.
[6] C. Miehe, F. Aldakheel & S. Mauthe (2013). *Int. J. Numer. Meth. Eng.* 94(11):1037-1074.
[7] S. Heriot & R. Jones (2005). *Nat. Mater.* 4(10):782-768.
[8] P. Mira et al. (2003). *Comput. Methods. Appl. Mech. Eng.* 192(37):4257-4277.
[9] P. Wriggers & S. Reese (1996). *Comput. Methods Appl. Mech. Eng.* 135(3-4):201-209.
[10] D. Pantuso & K.J. Bathe (1997). *Fin. Elem. Anal. Des.* 28(2):83-104.

Stanford | ENGINEERING
Civil & Environmental Engineering

Stanford University

Stanford | DOERR
School of Sustainability