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Abstract: We propose a phase field model to simulate CO₂ fracturing under an isothermal condition. We take advantage of the ability of the phase field approach in predicting fracture initiation and branching, and also to avoid tracking the fracture path. We model the CO₂ as a compressible fluid by modifying Darcy's law. In particular, we assume the permeability is correlated to the phase field value by an exponential function. The dependence of the CO₂ density as a function of the pressure is captured by the Span-Wagner equation of state. The computed breakdown pressure values show good agreement with analytical solutions and experimental results.

Research Data Related to this Submission

There are no linked research data sets for this submission. The following reason is given:

Data will be made available on request

- We propose a phase field model to simulate CO₂ fracturing, where we solve a coupled system consisting of: (i) mass balance with modified Darcy's equation, and (ii) a dissipative potential energy with the phase field.
- CO₂ is treated as a compressible fluid under an isothermal condition in a porous medium by using the Span-Wagner equation of state.
- The implementation is verified through three examples. The predicted breakdown pressure agrees well with analytical solutions and, within 30%, with experiments.

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Numerical modeling of CO₂ fracturing by the phase field approach

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Abstract

We propose a phase field model to simulate CO₂ fracturing under an isothermal condition. We take advantage of the ability of the phase field approach in predicting fracture initiation and branching, and also to avoid tracking the fracture path. We model the CO₂ as a compressible fluid by modifying Darcy's law. In particular, we assume the permeability is correlated to the phase field value by an exponential function. The dependence of the CO₂ density as a function of the pressure is captured by the Span-Wagner equation of state. The computed breakdown pressure values show good agreement with analytical solutions and experimental results.

Keywords: CO₂ fracturing, CO₂ fluid flow, phase field

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1. Introduction

Shale gas is the natural gas trapped within the shale, or mudstone reservoir, the most common sedimentary rock. Shale is a fine-grained, sedimentary rock composed of clay minerals and silt-sized particles. The shale has low permeability so that it significantly inhibits the gas flow from the reservoir rocks to the production wells. As a result, the economic feasibility of shale gas development relies on the effective stimulation of the reservoirs [1]. Shale gas has become an energy source of increasing worldwide interest due to the two technologies that have become mature in industry: horizontal drilling and hydraulic fracturing technique [2].

To date, water-based fluids are the most important fluids regularly used in the commercial shale gas due to their ready availability and low cost. But there are also some disadvantages to use water-based fluids, namely water shortage, contamination of underground water, and low fracturing performance. Also,

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9 15 hydraulic fracturing cannot avoid the clay swelling problem in shale [2]. Due
10 to these problems, researchers actively investigate non-aqueous (see [3]) and
11 non-fluid fracturing techniques such as explosive based method [4].

12 16 Carbon dioxide (CO_2) is one of the non-aqueous fracturing fluids that is
13 considered to be used for fracturing. CO_2 as a fracturing fluid has been success-
14 20 fully applied to fracturing unconventional gas reservoirs decades ago [5]. Since
15 the critical temperature of CO_2 is 31.1°C , once the pressure exceeds its critical
16 pressure of 7.38 MPa, it will change to the supercritical state [6]. It can be
17 injected down-hole either in liquid or supercritical state. The main benefits of
18 CO_2 as a fracturing fluid include reducing consumption of water and water con-
19 tamination, keeping clays (smectite and illite) stabilized, and preventing metal
20 leaching and chemical interactions.

21 22 Brown [7] proposed CO_2 as a fracturing fluid and circulating fluid in geother-
23 mal energy extraction. Middleton *et al.* [8] investigated the potential of using
24 CO_2 as a fracturing fluid for commercial scale of shale production. In the lab-
25 30 oratory scale, Ishida *et al.* [9, 10] conducted fracturing experiments by using
26 supercritical CO_2 . Also, some researchers investigated the effect of different
27 fracturing fluids [11, 12].

28 29 There exist two general approaches for modeling fracture. One is discrete
30 models for fracture where the geometrical discontinuity is modeled by modi-
31 35 fying the geometry of intact structure [13, 14, 15, 16]. The other is smeared
32 crack models where the discontinuity is distributed over a finite width, such as
33 the phase field [17] and the gradient-enhanced damage methods [18]. In this
34 approach, an additional unknown and a length scale are introduced.

35 36 Phase field modeling of fracture has gained popularity since the beginning of
37 this century. The phase field model by Bourdin *et al.* [17] is essentially a regulariza-
38 40 tion of the variational formulation of brittle fracture by Francfort and Marigo
39 [19]. What makes the phase field an attractive approach can be attributed to
40 45 its convenience in simulating complex fracture processes, including crack ini-
41 tiation, propagation, branching and merging. Compared to discrete fracture
42 descriptions, the phase field approaches avoid tracking the complicated crack
43 geometry; instead, the crack evolution is a natural outcome of the numerical
44 solution to a constrained optimization problem. Thus, it significantly decreases
45 the implementation difficulty, especially when dealing with 3D problems.

46 47 Bourdin *et al.* [20] have adopted the phase field approach to model hydraulic
48 fracturing in impermeable media by considering the force that fluid pressure
49 exerts on fracture surfaces. Afterwards, phase field approaches for hydraulic
50 55 fracture in porous media based on Biot's equations and the theory of porous
51 media have been investigated by many researchers.

52 53 Mikelić *et al.* [21] model pressurized fracture in porous media by combining
54 the Biot theory and phase field approach. To minimize code modifications for
55 adopting the phase field approach with an existing reservoir simulator, Yoshioka
56 and Bourdin [22] have proposed an efficient framework by modifying the Darcy
57 law. Wick *et al.* [23] have developed a model to simulate fluid-filled fracture
58 propagation coupled to a reservoir simulator. Also, they have used a single
59 pressure equation for the entire fractured domain by introducing a function to

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distinguish between reservoir and fracture domains. Mauthe and Miehe [24] have coupled the phase field hydraulic fracture and porous media fluid flow by using a permeability decomposition. Ehlers and Luo [25] have combined the theory of porous media (TPM) and the phase field approach to fracture. Also, Culp *et al.* [26] have applied the phase field approach to fracture in CO₂ sequestration. In most cases researchers have supposed the fracturing fluid is incompressible or slightly compressible. Recently, Heider and Markert [27] proposed a method to model the pore fluid which is considered compressible.

The objective of the paper at hand is to propose a phase field model to investigate the effect of CO₂ as a compressible fracturing fluid under the isothermal condition, as the first step towards such modeling. For this purpose, we have adopted the phase field approach to model fracturing in porous media according to Mikelić *et al.* [21]. We model the CO₂ flow as a compressible fluid by modifying Darcy's law. We suppose permeability is correlated to the phase field value by an exponential function. The CO₂ density varies significantly with pressure, which is captured by the Span-Wagner equation of state [28].

In the remaining paper we will proceed as follows: a description of the fracture problem is given in Section 2, including the governing equations of the solid and the fluid flow. Afterwards, the numerical discretization and algorithm are constructed in Section 3. Then Section 4 provides numerical examples and discussions, where we will show that our results for the breakdown pressure agree well with not only widely used analytical solutions but also, within a reasonable error, with experimental results. Finally Section 5 draws conclusions.

2. Mathematical model

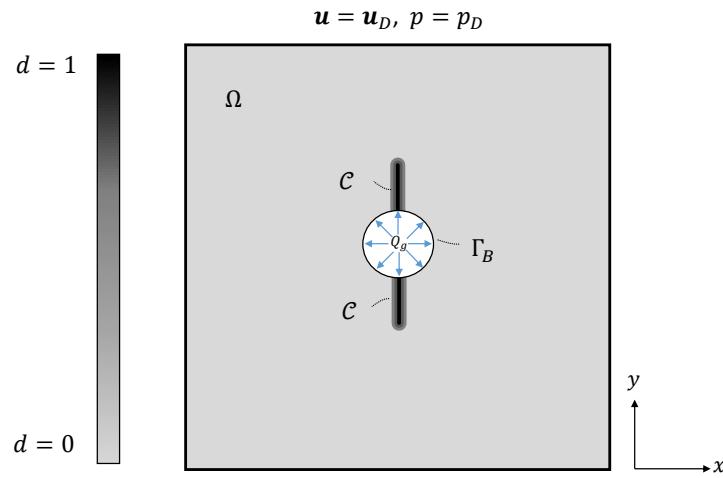
This section describes the mathematical model we will adopt for CO₂ fracturing. For convenience we will confine ourselves to the two-dimensional plane strain case, but the formulation is applicable to three dimensions with minimal changes. During the CO₂ fracturing process, the gas penetrates into the rock around the borehole and the injecting pressure causes the fracture to propagate. Thus, fracture propagation is a coupled phenomenon involving the gas flow inside the fracture and in the entire porous medium, the rock deformation, and the fracture propagation in the rock mass. In the following, in Section 2.1 we introduce the phase field method for fracture and derive the governing equations for the deformation and fracture propagation in the porous medium. Then, in Section 2.2 we present the governing equations for the gas flow within the porous medium. It is worth mentioning that compressible CO₂ exhibits a transport behavior different from that of slightly compressible fluids such as water and oil, due to its large compressibility and possibility of phase change.

2.1. Porous medium deformation and fracture propagation

In this section, we briefly recapitulate the basic notations and the underlying equations of the phase field method for pressurized fractures in brittle materials.

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9 **2.1.1. Variational formulation of brittle fracture**

10 We consider a two-dimensional porous medium under plane strain loading
 11 occupying an open Lipschitz domain $\Omega \subset \mathbb{R}^2$. Let $\Gamma_D, \Gamma_N \subseteq \partial\Omega$ be such that
 12 $\Gamma_D \cup \Gamma_N = \partial\Omega$ and $\Gamma_D \cap \Gamma_N = \emptyset$, and $\mathbf{u}_D : \Gamma_D \rightarrow \mathbb{R}^2$ and $\mathbf{t}_N : \Gamma_N \rightarrow \mathbb{R}^2$ be
 13 prescribed displacement and traction boundary conditions, respectively. Also,
 14 let $\Gamma_B \subset \partial\Omega$ denote the boundary of a borehole. We let $Q_g : \Gamma_B \rightarrow \mathbb{R}$ denote
 15 the fluid source and $\mathbf{b} : \Omega \rightarrow \mathbb{R}^2$ the body force per unit volume exerted to the
 16 solid.



35 Figure 1: Schematic of the computational domain. A square plate with a borehole placed
 36 inside is shown. The *in situ* stress is applied on the external boundary, while the fluid is
 37 injected from the boundary of the borehole. The fracture \mathcal{C} is approximated by a regularized
 38 crack surface $\mathcal{C}_l(d)$ which is a functional of the crack phase field.

39 The variational approach to fracture is built on energy minimization with
 40 respect to the displacement field $\mathbf{u} : \Omega \rightarrow \mathbb{R}^2$ and its jump set, which we denote
 41 as $\mathcal{C} = \mathcal{C}(\mathbf{u}) \subset \Omega$. Let $|\mathcal{C}|$ denote the one-dimensional Hausdorff measure of \mathcal{C} .
 42 Following Griffith's theory, the total potential energy of the fractured poroelastic
 43 solid is written as:

44
 45
$$\Pi_{\mathcal{C}}[\mathbf{u}, \mathcal{C}] := \int_{\Omega \setminus \mathcal{C}} \psi_0[\varepsilon(\mathbf{u})] d\Omega - \int_{\Omega} \mathbf{b} \cdot \mathbf{u} d\Omega - \int_{\Gamma_N} \mathbf{t}_N \cdot \mathbf{u} d\Gamma$$

 46
$$- \int_{\Omega \setminus \mathcal{C}} (\alpha - 1) p \operatorname{div} \mathbf{u} d\Omega + \int_{\Omega \setminus \mathcal{C}} \nabla p \cdot \mathbf{u} d\Omega + g_c |\mathcal{C}|,$$
 (1)
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 48
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 50

51 where p denotes the pore pressure, $\alpha \in [0, 1]$ is the Biot coefficient. Constant
 52 $g_c \in \mathbb{R}^+$ is the strain energy released per unit length of fracture extension. The
 53 strain energy density $\psi_0[\varepsilon(\mathbf{u})]$ is given by

54
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$$\psi_0(\varepsilon) := \frac{\lambda}{2} (\operatorname{tr} \varepsilon)^2 + G \|\varepsilon\|^2,$$

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with λ and G Lamé constants. These constants are related to Young's modulus E and Poisson's ratio ν as $\lambda = E\nu/[(1+\nu)(1-2\nu)]$ and $G = E/[2(1+\nu)]$. The linearized strain tensor takes the form:

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

¹¹⁰ Finally, $\|\cdot\|$ denotes the Frobenius norm of a tensor.

2.1.2. Regularized variational formulation of brittle fracture

To develop a numerical method to approximate (1), the phase field approach replaces the sharp-fracture description \mathcal{C} with a phase field description, where the phase field is denoted as $d : \Omega \rightarrow [0, 1]$. In particular, regions with $d = 0$ and $d = 1$ correspond to the intact and fully broken materials, respectively. Using a phase field approach, the one-dimensional fracture \mathcal{C} is approximated with the help of an elliptic functional [29, 30]:

$$\mathcal{C}_\ell[d] := \frac{1}{4c_w} \int_{\Omega} \left(\frac{w(d)}{\ell} + \ell \nabla d \cdot \nabla d \right) d\Omega, \quad (2)$$

²⁹ where $\ell > 0$ is the regularization length scale, which may also be interpreted
³⁰ as a material property, e.g., the size of the process zone. See Remark 3 for
³¹ comments on the choice of ℓ . Constant $c_w = \int_0^1 \sqrt{w(d)}$ is a normalization
³² constant such that when $\ell \rightarrow 0$, $\mathcal{C}_\ell[d]$ converges to the length of the sharp
³³ fracture, $|\mathcal{C}|$. Classical examples of $w(d)$ and c_w are $w(d) = d^2$ and $c_w = 1/2$
³⁴ for the AT2 model, and $w(d) = d$ and $c_w = 2/3$ for the AT1 model. Interested
³⁵ readers are referred to [31, 32] for more elaborations.

³⁶ On this basis, we replace (1) by a global constitutive dissipation functional
³⁷ for a rate independent fracture process [33]:

$$\begin{aligned} \Pi[\mathbf{u}, d] := & \int_{\Omega} \psi[\boldsymbol{\varepsilon}(\mathbf{u}), d] d\Omega - \int_{\Omega} \mathbf{b} \cdot \mathbf{u} d\Omega - \int_{\Gamma_N} \mathbf{t}_N \cdot \mathbf{u} d\Gamma \\ & - \int_{\Omega} (1-d)^2 (\alpha-1) p \operatorname{div} \mathbf{u} d\Omega + \int_{\Omega} (1-d)^2 \nabla p \cdot \mathbf{u} d\Omega \\ & + \frac{g_c}{4c_w} \int_{\Omega} \left(\frac{w(d)}{\ell} + \ell \nabla d \cdot \nabla d \right) d\Omega, \end{aligned} \quad (3)$$

⁴⁷ where the admissible sets of displacement and phase field can be set as:

$$\mathcal{S}_u := \{ \mathbf{u} \in H^1(\Omega; \mathbb{R}^2) | \mathbf{u} = \mathbf{u}_D \text{ on } \Gamma_D \}, \quad (4a)$$

$$\mathcal{S}_d := \{ d \in H^1(\Omega) | 0 \leq d \leq 1 \}. \quad (4b)$$

⁵² In practice, (4b) will be used in combination with the irreversibility constraint,
⁵³ to be elaborated in Remark 2.

⁵⁵ **Remark 1** (Strain energy degradation). *The solid endures partial loss of stiffness*
⁵⁶ *due to the presence of fractures. In order to model this effect, the strain*

energy density is degraded with respect to the evolution of the phase field. Also note that as the damaged material responds differently to tension and compression, we let only a part of the strain energy density be degraded. For this purpose, we let the degraded strain energy in (3) take the following general form:

$$\psi(\boldsymbol{\varepsilon}, d) = g(d)\psi_+ + \psi_-,$$

where $g(d)$ satisfies $g(0) = 1$, $g(1) = 0$, and $g'(d) < 0$ for all d such that $0 \leq d \leq 1$ [17]. A usual choice is $g(d) = (1-d)^2$. On the other hand, ψ_{\pm} are such that

$$\psi_+(\boldsymbol{\varepsilon}) + \psi_-(\boldsymbol{\varepsilon}) = \psi_0(\boldsymbol{\varepsilon}).$$

Now since $\partial\psi/\partial d = g'(d)\psi_+$, only ψ_+ contributes to fracture propagation.

There are several phase field models that differ in their choice of ψ_{\pm} . In this paper, we adopt the one proposed by Amor *et al.* [34]. This model assumes both volumetric expansion and deviatoric deformation contribute to fracture propagation, but volumetric compression does not. A decomposition of $\boldsymbol{\varepsilon}$ into volumetric and deviatoric parts reads:

$$\text{vol } \boldsymbol{\varepsilon} := \frac{1}{3}(\text{tr } \boldsymbol{\varepsilon})\mathbf{1}, \quad \text{dev } \boldsymbol{\varepsilon} := \boldsymbol{\varepsilon} - \text{vol } \boldsymbol{\varepsilon}.$$

Remark 2 (Irreversibility constraint). *The requirement $g'(d) < 0$ comes from the underlying irreversibility condition (the fracture can never heal) in time:*

$$\partial_t d \geq 0. \tag{5}$$

Consequently, modeling of fracture evolution problems leads to inequality constraints, and sometimes gives rise to a variational inequality formulation.

As an alternative way to model the irreversibility, Miehe *et al.* [35] proposed a phase field model based on a local history field. In this model, the evolution of the phase field d is driven by the historically maximum value of ψ_+ at the point of interest.

Remark 3 (The choice of ℓ). *Based on an analytical solution for the critical tensile strength σ_{cr} that a one-dimensional bar can sustain [32], we use the following equation for the choice of ℓ :*

$$\ell = \frac{3Eg_c}{8\sigma_{cr}^2}, \tag{6}$$

where E and g_c can be obtained from regular experiments, while σ_{cr} can be approximated by the tensile strength σ_t . Assuming all other parameters are known, the formula (6) is able to estimate ℓ , though the accuracy is unknown for more complex cases.

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9 *2.2. Carbon dioxide as a compressible fluid*

10 The governing equations for the fluid flow in a porous medium are given by
11 mass conservation, momentum balance, and the equation of state. The mass
12 conservation equation reads:

13
$$\begin{aligned} \partial_t(\phi\rho) + \nabla \cdot (\rho\mathbf{q}) &= 0 && \text{in } \Omega, \\ -\rho\mathbf{q} \cdot \mathbf{n} &= Q_g && \text{on } \Gamma_B. \end{aligned} \quad (7)$$

17 Here ϕ denotes the porosity of the porous medium (the fraction of volume
18 occupied by the fluid), ρ the density of the fluid, \mathbf{q} the Darcy velocity vector,
19 and Q_g the fluid source. Note that Q_g has the unit of volumetric flow rate per
20 unit volume. Also, we assume the rock is saturated by the fluid so that the fluid
21 content in rock per volume is expressed by $\phi\rho$.
22

23 In addition to (7), we state the momentum balance in the form of Darcy's
24 law. This law indicates a linear relationship between the fluid velocity and the
25 head pressure gradient:

26
$$\mathbf{q} = -\frac{k}{\mu}\nabla p, \quad (8)$$

27 where $k = k(d)$ is the permeability of the rock, and μ is the dynamic fluid viscosity.
28 Note that there could be an additional term $-\rho g \nabla z$ on the right hand
29 side of (8), where g and z are the magnitude of the gravitational acceleration
30 and the depth, respectively. This term is, however, in our case negligible, as we
31 assume an almost horizontal computational domain. Also, we assume the porosity
32 is not dependent on the stress condition. On the other hand, we correlate
33 the permeability to the phase field value by:
34

35
$$k(d) = k_0 \exp(\alpha_k d), \quad (9)$$

36 where k_0 is the permeability of the intact material, and α_k is a coefficient to
37 indicate the effect of phase field evolution on the permeability. We take $\alpha_k =$
38 7.0 (see [36, 37] for more description). Figure 2 illustrates the permeability
39 increasing with respect to the evolution of the phase field variable.
40

41 The first term on the left hand side of (7), the rate of change of fluid content,
42 can be written as:

43
$$\partial_t(\phi\rho) = \rho \partial_t \phi + \phi \partial_t \rho = \rho \partial_t \varepsilon_v + \phi \partial_t \rho, \quad (10)$$

44 where we have assumed the rate of change of pore volume is equal to that of
45 the volumetric strain, which is given by $\varepsilon_v = \nabla \cdot \mathbf{u}$.

46 Under isothermal conditions, the gas density varies significantly with pressure.
47 This is captured by an equation of state (EOS). One applicable EOS for
48 CO₂ is known as the Span-Wagner (S-W) equation [28] defined in terms of the
49 Helmholtz free energy. The CO₂ density and pressure are related by:

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$$p = (1 + \delta\varphi_\delta^r) \rho RT, \quad (11)$$

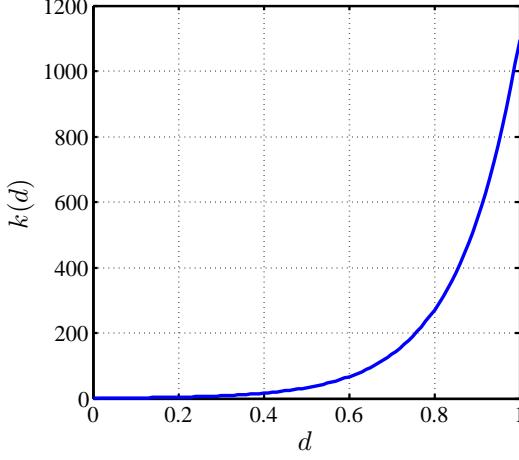


Figure 2: Plot of $k(d) = \exp(7.0d)$, permeability, as a function of the phase field variable d .

where R is the universal gas constant, and φ_δ^r is the derivative of the residual part of the full expression of Helmholtz energy φ^r with respect to the reduced density δ , with

$$\begin{aligned} \varphi^r(\delta, \tau) = & \sum_{i=1}^7 n_i \delta^{d_i} \tau^{t_i} + \sum_{i=8}^{34} n_i \delta^{d_i} \tau^{t_i} e^{-\delta^{c_i}} + \sum_{i=35}^{39} n_i \delta^{d_i} \tau^{t_i} e^{-\alpha_i(\delta-\varepsilon_i)^2 - \beta_i(\tau-\gamma_i)^2} \\ & + \sum_{i=40}^{42} n_i \Delta^{b_i} \delta e^{C_i(\delta-1)^2 - D_i(\tau-1)^2}, \end{aligned} \quad (12)$$

in which

$$\Delta = \left\{ (1-\tau) + A_i \left[(\delta-1)^2 \right] \frac{1}{2\beta_i} \right\}^2 + B_i \left[(\delta-1)^2 \right]^{a_i}.$$

In (12), ρ_c and T_c are the critical density and temperature, respectively, and $\delta = \rho/\rho_c$ and $\tau = T/T_c$ are the reduced ones. For the sake of brevity, here we do not provide the definitions and values of other parameters in (12), but refer the readers to [28].

By substituting (8),(9), (10), and (11) in (7), the governing equation for CO₂ flow is written as follows:

$$\begin{aligned} \phi \partial_t \rho + \rho \partial_t \varepsilon_v - \nabla \cdot \left(\rho \frac{k(d)}{\mu} \nabla p \right) &= 0, \quad \text{in } \Omega, \\ \rho \mathbf{q} \cdot \mathbf{n} &= -Q_g, \quad \text{on } \Gamma_B, \\ p &= p_D, \quad \text{on } \Gamma_P, \end{aligned} \quad (13)$$

where $\Gamma_P = \partial\Omega \setminus \Gamma_B$.

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 9 *Summary of governing equations.* The governing equations for modeling the
 10 CO₂ fracturing are summarized as follow: for the porous medium deformation,
 11 the functional defined in (3) is minimized among $(\mathbf{u}, d) \in \mathcal{S}_u \times \mathcal{S}_d$ under the
 12 constraint (5), while for the compressible fluid the boundary value problem (13)
 13 is used to solve for the pressure p .
 14

3. Numerical solution

155 In this section we present an algorithm that adopts standard procedures to
 15 obtain a numerical method to solve the initial boundary value problem presented
 16 in Section 2. In this algorithm, a staggered approach is employed to solve the
 17 underlying equations, i.e., the solution is obtained via iteration between the
 18 variables [17, 38]. This idea is based on the fact that by fixing two variables, the
 19 problem becomes convex in the remaining unknown. However, one drawback for
 20 such an approach is that it might need many iterations to achieve convergence
 21 among the three fields.
 22

23 For the problem at hand, we need to solve a coupled system consisting of
 24 mass balance for the compressible fluid and a dissipative potential energy with
 25 the phase field. We provide a fully iterative approach in which at each stage we
 26 solve for one unknown while the other two variables are fixed to their values at
 27 the last iteration. Readers are referred to Algorithm 1 for complete elaboration.
 28

Algorithm 1: Algorithm for modeling the CO₂ by phase field.

```

34      Input:  $p_0$ ,  $d_0$ ,  $\mathbf{u}_0$ ,  $\rho_0$ , and  $\varepsilon_{tol}$ 
35      Output:  $p_n$ ,  $d_n$ , and  $\mathbf{u}_n$ ,  $n = 1, \dots, N$ 
36      1 Set flow and mechanical boundary conditions  $\sigma_1$ ,  $\sigma_3$ , and  $Q_g$ ;
37      2 for  $n = 1$  to  $N$ ; do
38        3    Set  $t = n\Delta t$  and  $k = 0$ ; /*  $k$  is an iteration counter      */
39        4    repeat
40            5     $m = 0$ ; /*  $m$  is another iteration counter      */
41            6    repeat
42              7    Step - P: compute  $p_n$  with (B.3);
43              8    Step - U: compute  $\mathbf{u}_n$  with (B.1);
44              9    Update  $\rho_n^{(k+1)} \leftarrow \rho(p_n^{(k)})$  with (11);
45              10    $k + 1 \leftarrow k$ 
46              11   until  $\|p_n^{(k)} - p_n^{(k-1)}\|_2 < \varepsilon_{tol}$  and  $\|\mathbf{u}_n^{(k)} - \mathbf{u}_n^{(k-1)}\|_2 < \varepsilon_{tol}$ ;
47              12   Step - d: compute  $d_n$  with (B.1);
48              13    $m + 1 \leftarrow m$ 
49              14   until  $\varepsilon_d = \|d_n^{(m)} - d_n^{(m-1)}\|_2 < \varepsilon_{tol}$ ;
50              15    $\mathbf{u}_{n-1} \leftarrow \mathbf{u}_n$ ;
51              16    $p_{n-1} \leftarrow p_n$ ;
52              17    $\rho_{n-1} \leftarrow \rho_n$ ;
53      18 end
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We implement our method on FEniCS, an open-source finite element software [39, pp. 173–225]. Therein, the user merely needs to provide the variational form of the problem as well as the geometry and mesh information. Then, a big advantage of FEniCS is that the software itself completes all steps toward generating the global stiffness matrix.

Below we show an excerpt of the used FEniCS code. This piece of code performs some calculations for line 8 in Algorithm 1 wherein \mathbf{u} is solved for while the other two unknowns are fixed. It first defines $\boldsymbol{\varepsilon}$, ψ_0 , and $\psi(\boldsymbol{\varepsilon}, d)$ in lines 1, 3, and 5, respectively. Then, the standard finite element shape functions are defined in line 8, and the admissible function space (`TrialFunction`), the test function space (`TestFunction`), and the unknown function \mathbf{u} (`Function`) are defined in line 9. Afterwards, the elastic energy is introduced as a variational form in line 11. Finally, in lines 12 and 13, the code takes the first variation $\delta\Pi[(\mathbf{u}, d); \bar{\mathbf{u}}]$ (B.1a) and the second variation $\delta^2\Pi[(\mathbf{u}, d); \bar{\mathbf{u}}; \delta\mathbf{u}]$ (B.2a) and builds the nodal residual vector as `Residual_u` and the tangent stiffness matrix as `Jacobian_u`.

```

185 def eps(u_):
186     return sym(grad(u_))
187 def psi_0(u_):
188     return 0.5 * lmbda * tr(eps(u_))**2 + mu * eps(u_)**2
189 def psi_(u_, d_):
190     return ((1 - d_)**2 + k_ell) * psi_0(u_)
191
192 V_u = VectorFunctionSpace(mesh, "CG", 1)
193 u_, u, u_t = Function(V_u), TrialFunction(V_u), TestFunction(V_u)
194
195 energy_elastic = psi_(u_, d_) * dx
196 Residual_u = derivative(energy_elastic, u, u_t)
197 Jacobian_u = derivative(Residual, u_, u_t)

```

To solve the three unknowns, we select for \mathbf{u} and p the linear solver MUMPS which is convenient for solving large linear systems [40], and for d the TAO optimization solver integrated into the PETSc library [41, 42], which has the capability of solving inequality constrained optimization problems as the one at hand. Interested readers are referred to [43] for more information about the applied solvers.

4. Numerical examples

In this section, we present a numerical example to demonstrate the capability of the proposed model. To verify the implementation, we performed several other numerical experiments in Appendix A.

In this example, we investigate the fracture propagation in a square plate with a pressurized CO₂ flow, with [10, 11] as the benchmarks. The specimen has edge lengths of $L = 170$ mm. The geometric setup and boundary conditions are depicted in Figure 3. The sample is discretized into 4,832 three-noded triangular

elements so that the mesh size $h \approx 5.68$ mm is obtained. Also, we set $\ell = 1.6$ mm. Table 1 shows the remaining parameters to be input.

$$\mathbf{u} = \mathbf{u}_D, p = p_D$$

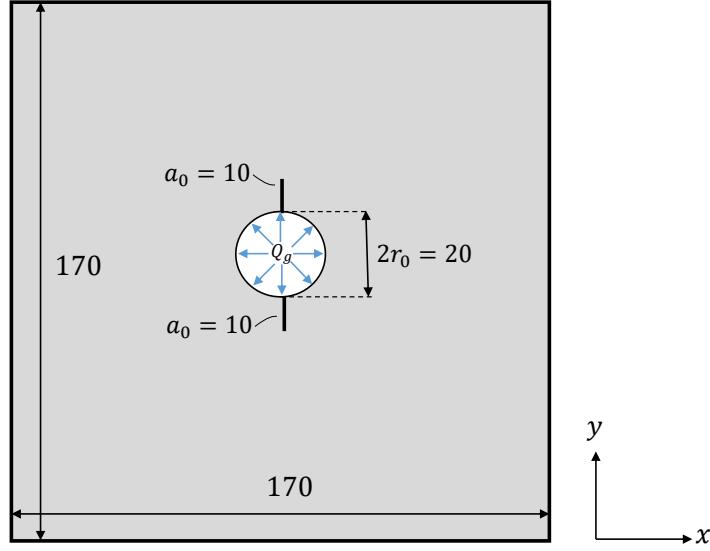


Figure 3: Schematic of a cracked square plate (unit: mm) with pressurized CO₂ flow.

As in Figure 3, there exist two preexisting fractures representing the perforations. We set $d = 1$ for both fractures and set the Dirichlet boundary condition $d = 0$ on the external boundary. The fluid is continuously injected into the central borehole with diameter $2r_0 = 20$ mm, until after the fractures propagate. Note that in this problem, the isothermal condition is adopted so that CO₂ is in the supercritical phase ($T = 45^\circ\text{C}$).

For the sake of simplicity, the *in situ* stress is imposed on the boundary by means of its “equivalent” prescribed displacement. More precisely, the displacement of the same specimen with no crack under the same *in situ* stress is first computed, then used as the Dirichlet boundary condition for the problem at hand. On the external boundary, we set $p = p_D$ where $p_D = 0$. Moreover, $\Gamma_P = \Gamma_D$ in this example.

Figure 4 shows the evolution of phase field diagram (left) and pressure profile (right) at different time steps. As seen, the fractures propagate along a straight line, and the pressure profile is accordingly distributed with the highest gradient around the borehole.

Next, we aim to calculate the breakdown pressure p_b , the pressure value when the fractures start to propagate. Figure 5 illustrates the pressure evolution at the top of the borehole and the fracture length function. To estimate the breakdown pressure, first we output the fracture length with regard to (2). Then, we obtain the time when the slope suddenly changes in the fracture length function (\mathcal{C}_ℓ),

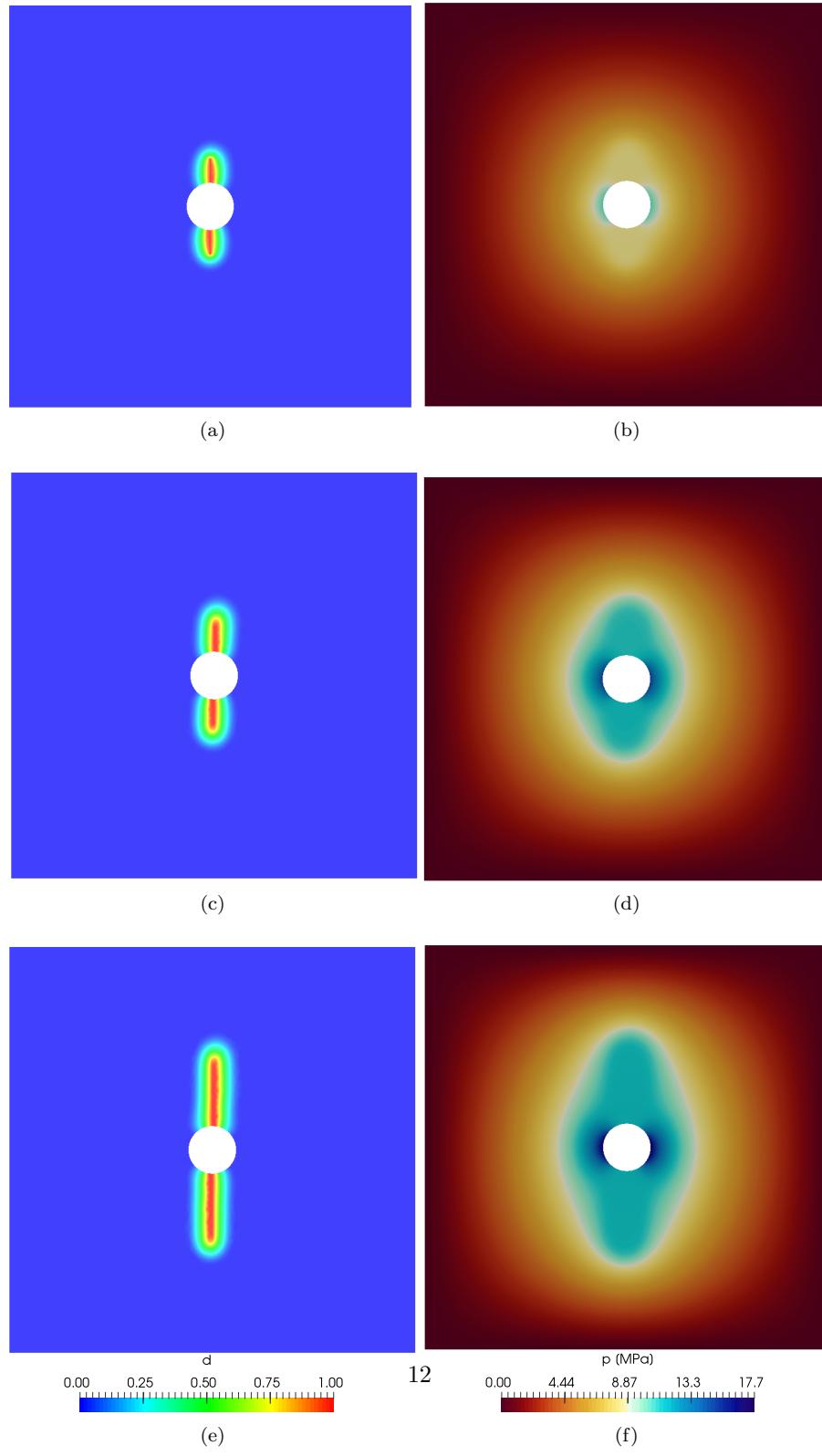


Figure 4: Left: Phase field diagram at different stages (4a) $t = 0.5t_f$, (4c) $t = 0.74t_f$, and (4e) $t = t_f$. Right: Pressure profile at (4b) $t = 0.5t_f$, (4d) $t = 0.74t_f$, and (4f) $t = t_f$.

Table 1: Default parameter values for the example. These values are taken from [11] except g_c , which is from (6).

| Parameters | symbol | unit | value |
|--------------------------------------|------------|-----------------|------------------------|
| Young's modulus | E | MPa | 6×10^3 |
| Poisson's ratio | ν | — | 0.34 |
| Critical energy release rate | g_c | MPa·mm | 0.306 |
| Biot coefficient | α | — | 0.85 |
| Porosity | ϕ | — | 0.01 |
| Initial permeability | k_0 | mm ² | 1×10^{-12} |
| Dynamic viscosity of CO ₂ | μ | MPa·s | 4.04×10^{-11} |
| Initial pressure | p_0 | MPa | 0.1 |
| Rock's tensile strength | σ_T | MPa | 11 |

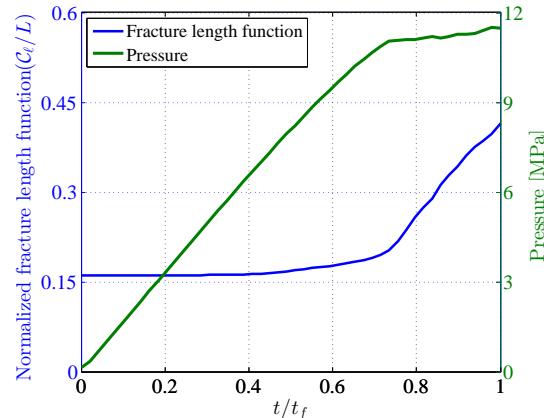


Figure 5: The pressure at the top of the borehole (green line), and the fracture length function (blue line) as functions of time. The time when there is a sudden change of slope in C_ℓ assumes the time corresponding to the breakdown pressure ($t = 0.72t_f$) and the corresponding breakdown pressure is $p_b = 10.9$ MPa. This is in agreement with H-F and H-W analytical solutions.

which is the time corresponding to the breakdown pressure (here $t \approx 0.72t_f$).
 Hence the breakdown pressure reads $p_b = 10.9$ MPa. This value for p_b is in
 agreement with H-F and H-W analytical solutions. Also, our results agree with
 experiments results of Ishida *et al.* [9] within 30%, see Table 2 and the next
 paragraph for more elaborations.

Table 2: Breakdown pressure of numerical test and analytical solutions for $\sigma_1 = \sigma_3 = 1$ MPa.

| | Numerical | H-F solution | H-W solution | Experimental [9] |
|-------------|-----------|--------------|--------------|------------------|
| p_b (MPa) | 10.9 | 11 | 9.1 | 8.44 |

Classical solutions of breakdown pressure. There exist two classical expressions
 to calculate the breakdown pressure. In the case without poroelastic effect the
 rock deformation does not penetrate into the pressurized fracture, the Hubbert-
 Willis (H-W) solution applies [44]:

$$p_b = 3\sigma_3 - \sigma_1 + \sigma_T,$$

in which the rock is assumed to be an elastic medium. When the porous medium
 is set, the Haimson-Fairhurst (H-F) solution is preferred [45]:

$$p_b = \frac{3\sigma_3 - \sigma_1 + \sigma_T + p_0}{1 + \frac{\nu}{1-\nu}\alpha},$$

where we denote by p_b the breakdown fluid pressure, σ_3 , and σ_1 are the mini-
 mum and maximum principal stresses, respectively, and σ_T is the rock's tensile
 strength.

Effect of N , h , and ℓ on the breakdown pressure. Here we aim to study how the
 number of time steps N , the mesh size h , and the regularization length scale
 ℓ affect the value of breakdown pressure. As seen in Figure 6, the plots show
 similar numerical results for the pressure evolution.

Breakdown pressure result of an anisotropic in situ stress. In this example we
 set the maximum ($\sigma_1 = 3$ MPa) and minimum ($\sigma_3 = 2$ MPa) *in situ* stress.
 The other input data and boundary conditions are the same as aforementioned.

The pressure at the top of the borehole and the fracture length function, (2),
 at different stages are illustrated in Figure 7. The breakdown time ($t \approx 0.77t_f$)
 and the corresponding breakdown pressure is $p_b = 11.9$ MPa, see Table 3.

Table 3: Breakdown pressure of numerical test and analytical solutions for $\sigma_1 = 3$ MPa and
 $\sigma_3 = 2$ MPa.

| | Numerical | H-F solution | H-W solution |
|-------------|-----------|--------------|--------------|
| p_b (MPa) | 11.9 | 14 | 9.8 |

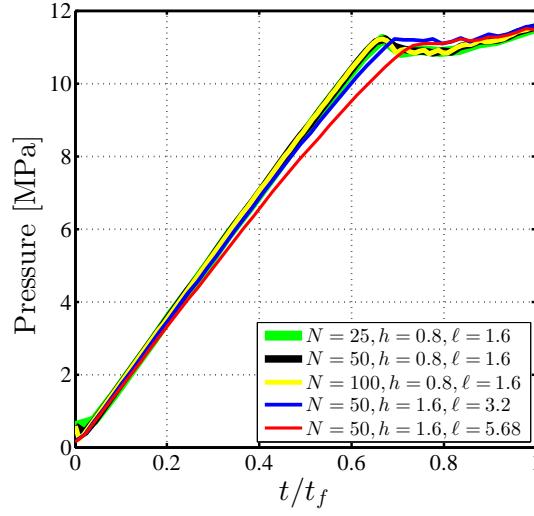


Figure 6: Evolution of the pressure at the top of the borehole for different numbers of time steps N , mesh size h , and ℓ .

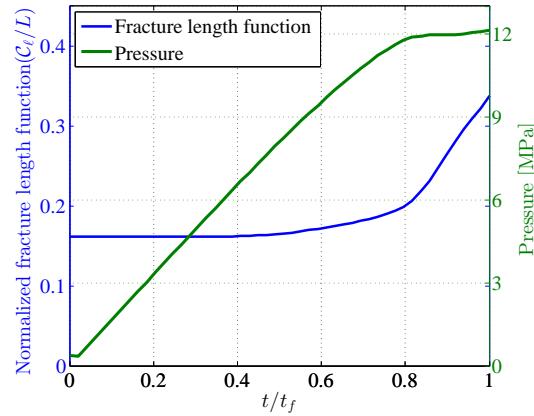
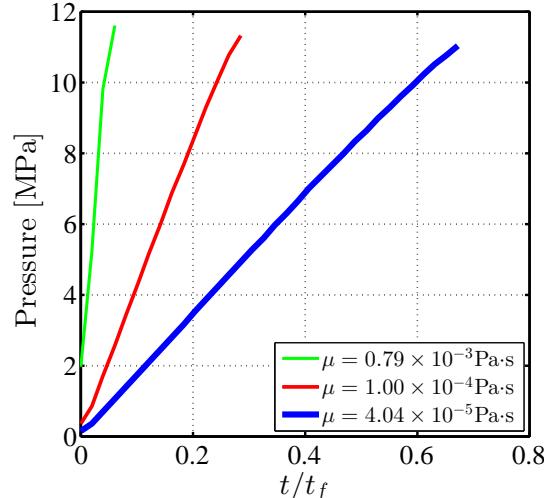


Figure 7: The pressure at the top of the borehole (green line) and the fracture length function (blue line) versus time for deviatoric *in situ* stress are shown. The time ($t \approx 0.8t_f$) when there is a change of slope in the fracture length function (C_ℓ) should correspond to the breakdown pressure ($p_b = 11.9$ MPa).

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 9 *Effect of dynamic viscosity on breakdown pressure.* We conduct several numerical
 10 examples to investigate the effect of dynamic viscosity μ on the breakdown
 11 pressure p_b . In this set of examples an effective mesh size, the mesh size near the
 12 borehole or the fractures, $h \approx 1.6$ mm is adopted. Also, we set $\ell = 2h$. In Figure
 13 8 we plot the pressure evolution up to the time when $\mathcal{C}_\ell(t)$ changes slope, so that
 14 the end points correspond to the breakdown pressures. The results indicate that
 15 p_b is approximately the same for different fluid viscosities, but the time when
 16 breakdown pressure reaches is different. Figure 8 demonstrates that the rock
 17 will break earlier for the fluid with bigger dynamic viscosity. Also it shows that
 18 regardless of the fracturing fluid, the breakdown pressure is slightly the same for
 19 all cases. This is in accordance with the physics that the breakdown pressure
 20 normally reflects the strength of the solid. However, Wang *et al.* [11] reported
 21 different breakdown pressures for different fluids which also agrees with some
 22 experiments [9, 10]. We believe this discrepancy demands further research.
 23



42 Figure 8: Evolution of the pressure at the top of the borehole for different μ 's. As seen, even
 43 though p_b is the same for different fracturing fluids, by increasing μ , the breakdown pressure
 44 is reached earlier.

47 5. Conclusions

49 We have proposed a phase field approach to simulate CO₂ fracturing, with
 50 CO₂ treated as a compressible fluid. The breakdown pressure agrees well with
 51 widely used analytical solutions. Also, the results agree with experimental re-
 52 sults within 30%. While this work represents the first of its kind, potentially
 53 the phase field approach allows complicated modeling of fracture initiation and
 54 branching.

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275 Appendix A. Verification of the method

This appendix devotes to a verification of our implementation of the present phase field method for CO₂ fracturing. To this end, we present three examples with exact or otherwise trusted solutions to study how our outputs are in accordance with the analytical solutions and other works.

280 *Appendix A.1. Single-edge-notched tension test*

We first investigate a square plate with a horizontal initial crack at the middle height starting from the left end and ending at the plate center. The geometric setup is depicted in Figure A.9. To capture the crack pattern properly, the mesh is refined in areas where the crack is expected to propagate, i.e., in the center strip of the specimen. In effect, for a discretization with 105,352 standard P_1 elements, an effective element size of $h \approx 5 \times 10^{-3}$ mm is obtained in the critical zone. The specimen is under a direct tension test, in which a monotonically increasing displacement with constant increments $\Delta\mathbf{u} = 6 \times 10^{-5}$ mm is imposed on the top edge while the bottom edge is fixed. In this example, the evolution is simulated for 100 uniform time steps so that a final deformation of 6×10^{-3} mm is reached. We will adopt the values of the material parameters given in Table A.4. Note that all our models are implemented with the AT1 model.

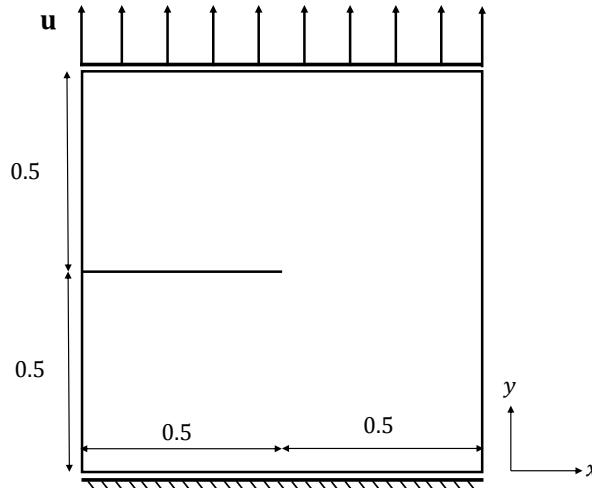


Figure A.9: Schematic of a cracked square plate (unit: mm) under a single-edge-notched tension test. A monotonically increasing displacement with constant increments $\Delta\mathbf{u} = 6 \times 10^{-5}$ mm is applied on the top edge while the bottom edge is fixed.

The resulting crack patterns at different stages of the deformation for two fixed regularization length scales $\ell = \ell_1 = 1 \times 10^{-2}$ mm and $\ell = \ell_2 = 2 \times 10^{-2}$ mm are illustrated in Figure A.10. As expected, in both simulations, the fracture propagates straightforward to the end. This straight crack topology agrees well

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9 Table A.4: Cracked square plate under a tension test: Material parameters [46]

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| Parameters | symbol | unit | value |
|------------------------------|--------|--------|-------------------|
| Young's modulus | E | MPa | 210×10^3 |
| Poisson's ratio | ν | — | 0.3 |
| Critical energy release rate | g_c | MPa·mm | 2.7 |

15
16 with the results in [47]. Also as seen, the resulting crack pattern with the smaller
17 ℓ looks sharper.

18 We also output the load-deflection curves for the two setups of Figure A.11.
19 As seen, both models will result in similar trends. Hence, the effect of ℓ on the
20 response is small in this range.

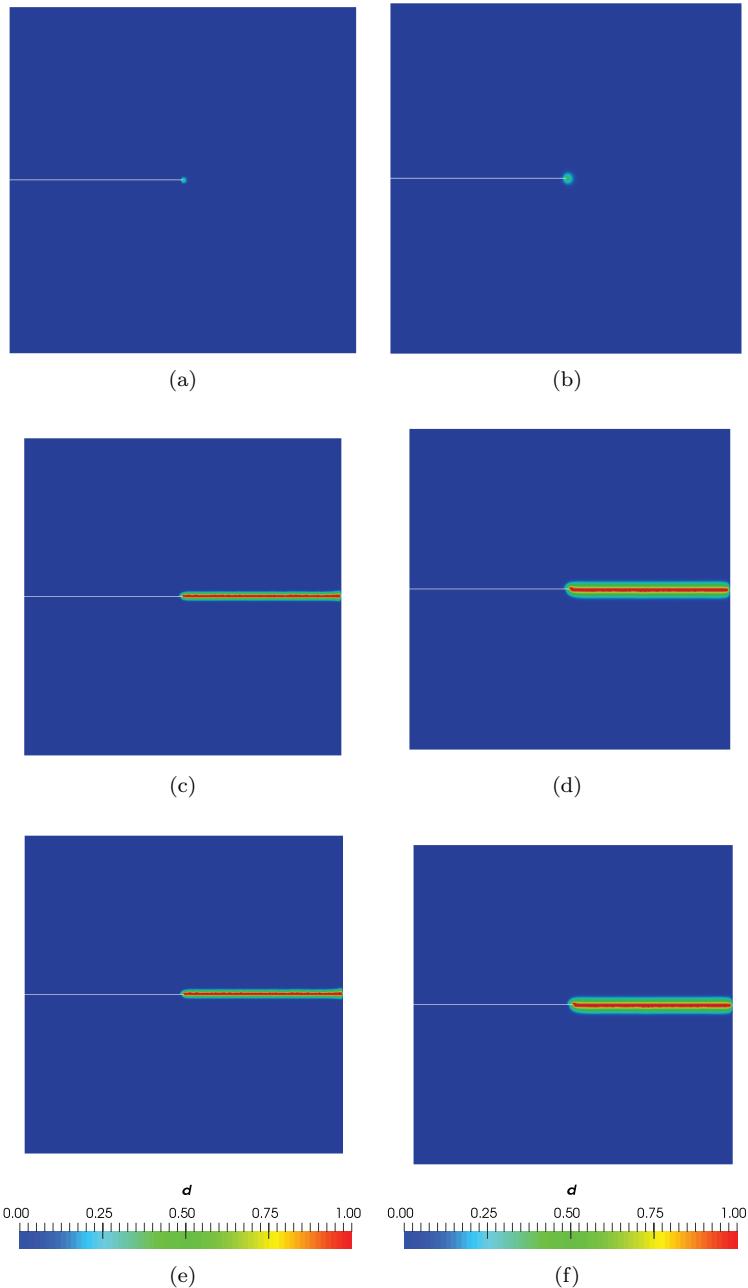


Figure A.10: Cracked square plate under a tension test with two different regularization length scales $\ell = \ell_1 = 10^{-2}$ mm $\approx 2h$ (left) and $\ell = \ell_2 = 2 \times 10^{-2}$ mm $\approx 4h$ (right). Both simulations are done with 100 uniform time steps with $\Delta\mathbf{u} = 6 \times 10^{-5}$ mm (See also Table A.4 for the input values). Phase field contours at three different stages $\mathbf{u} = 5.52 \times 10^{-3}$ mm (A.10a,A.10b), $\mathbf{u} = 5.58 \times 10^{-3}$ mm (A.10c,A.10d), and $\mathbf{u} = 6 \times 10^{-3}$ mm (A.10e,A.10f) are shown in deformed configurations with the deformations scaled. The initial cracks are explicitly imposed, so in the deformed configuration it appears as a white line. As expected, we observe a straight crack pattern in both cases.

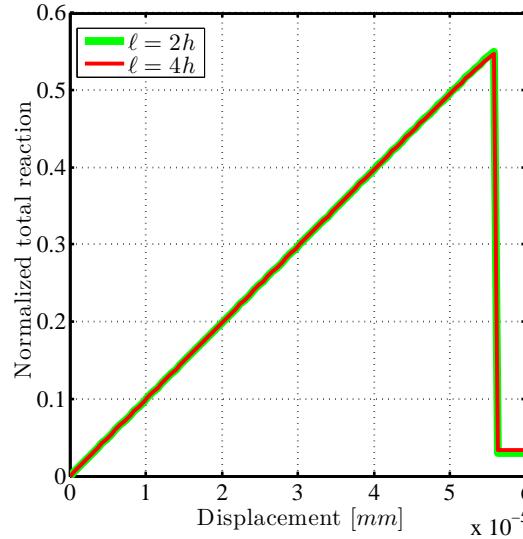


Figure A.11: Cracked square plate under a tension test with two different regularization length scales $\ell = \ell_1 = 10^{-2}$ mm $\approx 2h$ (red) and $\ell = \ell_2 = 2 \times 10^{-2}$ mm $\approx 4h$ (green). Load-deflection curves for both ℓ_1 and ℓ_2 are obtained. Both simulations are done with 100 load steps with $\Delta u = 6 \times 10^{-5}$ mm. The total reaction is normalized by the one in the case without any crack or phase field evolution. Both models give rise to similar trends so the effect of changes in ℓ is small within this range. Note that the reaction highly decreases at the 93rd time step where the crack starts to propagate.

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9 *Appendix A.2. Poroelastic response of a borehole*

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11 This example aims to study the effect of fluid pressurization on the poroelastic
12 response around the borehole. It was first studied by Detourney and Cheng
13 [48] (see also [11, 49]). Consider a plane strain hydraulic fracturing problem
14 where there is a square plate containing a central borehole. The geometry and
15 the loading conditions in this example are the same as Figure 3. The far-field
16 *in situ* stress is set to zero in this example. Note also that $d \equiv 0$, i.e., there is
17 no preexisting crack in the specimen and we do not allow for any nucleation of
18 the fracture as the rock strength is assigned a very large value. A discretization
19 with 28,140 standard P_1 elements is applied to the problem. To capture the
20 high gradient of pressure near the borehole, the mesh is refined in that area so
21 that an effective mesh size of $h \approx 0.15$ mm is adopted. The fluid is slightly
22 compressible, and we set the fluid pressure in the borehole to 1 MPa. The other
23 material properties are prescribed according to Table A.5.
24

25 Here, the governing equation for the slightly compressible flow is written as
26 follows [48]:
27

$$\partial_t p + M \nabla \cdot \left(\frac{k_0}{\mu} \nabla p \right) = 0$$

28 where $M = E(1-\nu)/[(1+\nu)(1-2\nu)]$ is called the constrained modulus.
29

30 Table A.5: Poroelastic response of a borehole: Material parameters
31

| Parameters | symbol | unit | value |
|------------------|----------|---------------|---------------------|
| Young's modulus | E | MPa | 6000 |
| Poisson's ratio | ν | — | 0.34 |
| Biot coefficient | α | — | 1. |
| Permeability | k_0 | mm^2 | 1×10^{-12} |

32 Figure A.12 shows the distribution of pore pressure around the borehole
33 for three values of dynamic viscosity μ at early time $t = 0.1$ s. Note that
34 the horizontal axis is $(r - r_0)/r_0$, ranging from 0 to 0.25 in the direction of
35 $\theta = \pi/2$. The simulation results are then compared to the analytical solution
36 by Detourney and Cheng [48].
37

38 Figure A.13 depicts the effect of dynamic viscosity on the effective tangential
39 stress in the vicinity of the borehole at early time $t = 0.1$ s.
40

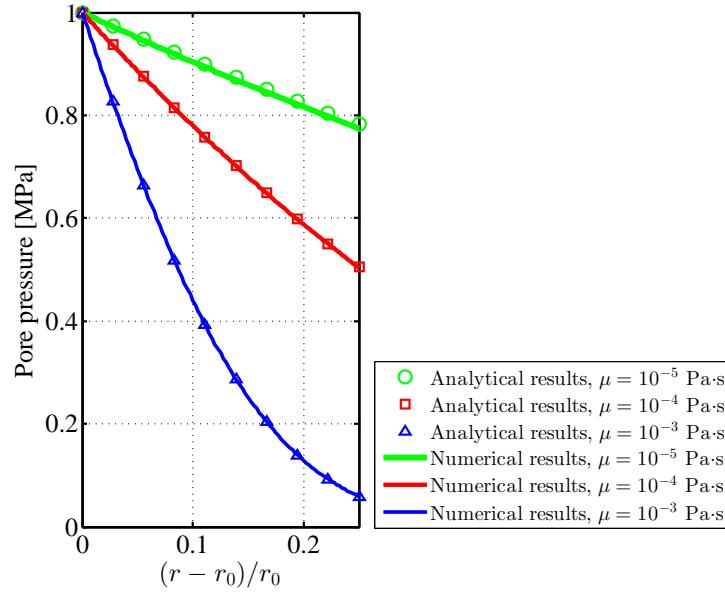


Figure A.12: Poroelastic response of a borehole. The distribution of pore pressure caused by fluid pressurization is shown around the borehole for three different dynamic viscosities μ at early time $t = 0.1$ s. As seen, the results are in good accordance with the analytical in [48].

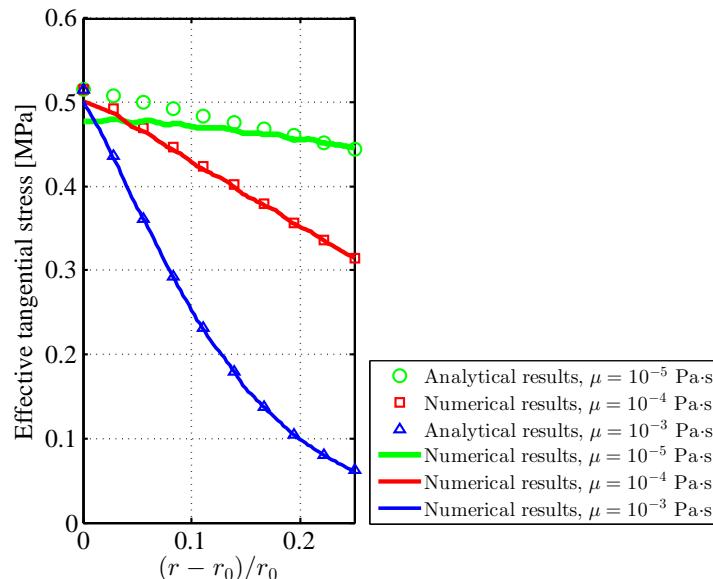


Figure A.13: Poroelastic response of a borehole. The effective tangential stress is plotted near the borehole for three different dynamic viscosities μ at early time $t = 0.1$ s.

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10 325 *Appendix A.3. Computation of the crack opening displacement*

11 We now focus on a classical problem first solved by Sneddon and Lowengrouo
12 [50] (see also [20]) that solves the opening displacement of a static line crack.

13 Consider a computational domain of $\Omega = 4 \text{ m} \times 4 \text{ m}$ with a preexisting line
14 fracture of length $2a_0 = 0.4 \text{ m}$, i.e., $\mathcal{C} = [1.8, 2.2] \times \{0\}$. To minimize the effect
15 of the boundary conditions on the results, the domain size is much larger than
16 the crack length ($L \gg 2a_0$).

17 The mechanical properties of the material are the Young's modulus $E = 1000$
18 MPa, the Poisson's ratio $\nu = 0$, and the fracture toughness $g_c = 1 \text{ MPa}\cdot\text{s}$.

19 We impose zero displacements on the external boundary of Ω . Also we set
20 $d = 1$ on prescribed (initial) fracture and $d = 0$ on the external boundary of Ω .
21 A monotonically increasing pressure is applied on the upper and lower faces of
22 fracture with the magnitude $p = 1 \text{ MPa}$. Figure A.14 depicts the geometry and
23 boundary conditions.

24 Bourdin *et al.* [33] proposed a formula to compute the fracture aperture as:

$$w = \mathbf{u} \cdot \mathbf{n}_\Gamma \simeq \int_s \mathbf{u} \cdot \nabla d \, dx.$$

25
26 Then, the fracture volume is calculated by integrating the fracture aperture
27 along the fracture's path:

$$V_f = \int_\Gamma w \, ds \simeq \int_\Omega \mathbf{u} \cdot \nabla d \, d\Omega.$$

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32 Figure A.15 shows the aperture profile for different h and ℓ . The dash
33 line in black represents the Sneddon's analytical solution [50]. Also, the crack
34 volume computed by Sneddon's analytical solution and our numerical tests are
35 summarized in Table A.6.

52 Table A.6: Crack volumes for different ℓ for numerical tests and analytical solution ($h = 4\text{mm}$).

| ℓ (mm) | 1.4×10^2 | 1.2×10^2 | 1.0×10^2 |
|---|--------------------|--------------------|--------------------|
| Numerical fracture volume (mm ²) | 2.89×10^2 | 2.75×10^2 | 2.60×10^2 |
| Analytical fracture volume (mm ²) | 2.51×10^2 | | |

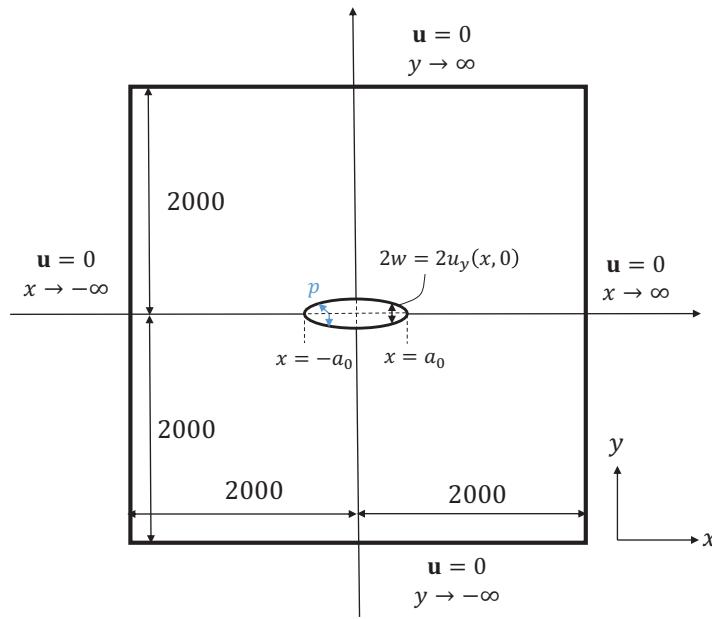


Figure A.14: Computation of the crack opening displacement. Schematic view of the deformed line crack in a two dimensional domain.

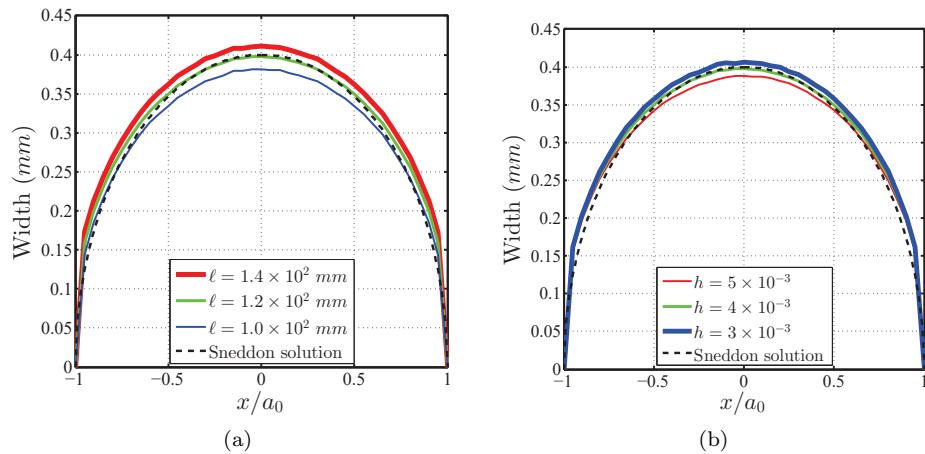


Figure A.15: Computation of the crack opening displacement. We output the results for (A.15a) various ℓ with $h = 4 \text{ mm}$ and (A.15b) various h with $\ell = 1.2 \times 10^2 \text{ mm}$, and compare them with Sneddon's analytical solution [50].

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9 **Appendix B. Weak forms**

10 Here we provide weak forms useful for FEniCS implementation.

11
12 *Appendix B.1. Porous medium*

13 To proceed, let the test function spaces be

$$16 \quad \mathcal{V}_u := \{\bar{\mathbf{u}} \in H^1(\Omega; \mathbb{R}^2) \mid \bar{\mathbf{u}} = \mathbf{0} \text{ on } \Gamma_D\}, \\ 17 \quad \mathcal{V}_d := H^1(\Omega).$$

18
19 Then we derive the first variations of the energy functional (3), which will be
20 needed for stating the weak form:

$$22 \quad \delta\Pi_\ell [(\mathbf{u}, d); \bar{\mathbf{u}}] := \int_{\Omega} \boldsymbol{\sigma}[\boldsymbol{\varepsilon}(\mathbf{u}), d] : \boldsymbol{\varepsilon}(\bar{\mathbf{u}}) d\Omega - \int_{\Gamma_N} \mathbf{t}_N \cdot \bar{\mathbf{u}} d\Gamma - \int_{\Omega} \mathbf{b} \cdot \bar{\mathbf{u}} d\Omega \\ 23 \quad + \int_{\Omega} (\alpha - 1) \nabla ((1 - d)^2 p) \cdot \bar{\mathbf{u}} d\Omega + \int_{\Omega} (1 - d)^2 \nabla p \cdot \bar{\mathbf{u}} d\Omega \quad (B.1a)$$

$$24 \quad \delta\Pi_\ell [(\mathbf{u}, d); \bar{d}] := \int_{\Omega} (\alpha - 1) g'(d) \bar{d} p \operatorname{div} \mathbf{u} d\Omega + \int_{\Omega} g'(d) \bar{d} \nabla p \cdot \mathbf{u} d\Omega \\ 25 \quad + \int_{\Omega} g'(d) \psi_+(\boldsymbol{\varepsilon}) \bar{d} d\Omega + \frac{g_c}{4c_w} \int_{\Omega} \left(\frac{\omega'(d) \bar{d}}{\ell} + 2\ell \nabla d \cdot \nabla \bar{d} \right) d\Omega. \quad (B.1b)$$

32 The weak form can thus be stated as: Find $(\mathbf{u} \times d) \in \mathcal{S}_{\mathbf{u}} \times \mathcal{S}_d$, such that for all
33 admissible functions $(\bar{\mathbf{u}} \times \bar{d}) \in \mathcal{V}_{\mathbf{u}} \times \mathcal{V}_d$, $\delta\Pi_\ell [(\mathbf{u}, d); \bar{\mathbf{u}}] = 0$ and $\delta\Pi_\ell [(\mathbf{u}, d); \bar{d}] = 0$.

34 Also we take another variation from (3) which will be needed for the dis-
35 cretized formulation:

$$36 \quad \delta^2\Pi_\ell [(\mathbf{u}, d); \bar{\mathbf{u}}, \delta\mathbf{u}] = \int_{\Omega} \boldsymbol{\varepsilon}(\delta\mathbf{u}) : \mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}), d] : \boldsymbol{\varepsilon}(\bar{\mathbf{u}}) d\Omega, \quad (B.2a)$$

$$37 \quad \delta^2\Pi_\ell [(\mathbf{u}, d); \bar{d}, \delta d] = \int_{\Omega} \delta d g''(d) \psi_+(\boldsymbol{\varepsilon}) \bar{d} d\Omega \\ 38 \quad + \int_{\Omega} (\alpha - 1) g''(d) \bar{d} \delta d p \operatorname{div} \mathbf{u} d\Omega + \int_{\Omega} g''(d) \bar{d} \delta d \nabla p \cdot \mathbf{u} d\Omega \\ 39 \quad + \frac{g_c}{4c_w} \int_{\Omega} \left[\frac{\delta d w''(d) \bar{d}}{\ell} + 2\ell \nabla(\delta d) \cdot \nabla \bar{d} \right] d\Omega, \quad (B.2b)$$

40 where the fourth-order tensor $\mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}), d] = \frac{\partial \boldsymbol{\sigma}(\boldsymbol{\varepsilon}, d)}{\partial \boldsymbol{\varepsilon}} \Big|_{\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}(\mathbf{u})}$ is the tangent elastic-
41 ity tensor.

42
43 *Appendix B.2. Compressible (CO₂) fluid flow discretization*

44 The compressible fluid flow discretization is also done via the finite element
45 method. We first discretize in time and then in space. We will adopt the
46 backward Euler method for time discretization.

To proceed, let the admissible set of pressure be:

$$\mathcal{S}_p := \{p \in H^1(\Omega) \mid p = p_D \text{ on } \Gamma_P\}.$$

The test function space can be defined as:

$$\mathcal{V}_p = \{\bar{p} \in H^1(\Omega) \mid \bar{p} = 0 \text{ on } \Gamma_P\}.$$

The weak form can be stated as: find $p \in \mathcal{S}_p$ such that for all admissible functions $\bar{p} \in \mathcal{V}_p$,

$$\begin{aligned} & \frac{1}{\Delta t} \int_{\Omega} \phi(\rho - \rho^{n-1}) \bar{p} \, d\Omega + \frac{1}{\Delta t} \int_{\Omega} \rho(\varepsilon_v - \varepsilon_v^{n-1}) \bar{p} \, d\Omega \\ & + \int_{\Omega} \rho \frac{k(d)}{\mu} \nabla p \cdot \nabla \bar{p} \, d\Omega - \int_{\Gamma_B} Q_g \bar{p} \, d\Gamma = 0, \end{aligned} \quad (\text{B.3})$$

where ρ^{n-1} and ε_v^{n-1} denote solutions at the previous time step.

Acknowledgments

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