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Abstract

We construct a formal gradient flow structure for phase-field evolution coupled to mechanics in Lagrangian coordinates, present common ways to couple the evolution and provide an incremental minimization strategy. While the usual presentation of continuum mechanics is intentionally very brief, the focus of this paper is on an extensible functional analytical framework and a discretization approach that preserves an appropriate variational structure as much as possible. As examples, we first present phase separation and swelling of gels and then the approach of stationary states of multiphase systems with surface tension and show the robustness of the general approach.

1 Introduction

Beyond the continuum mechanical description of Newtonian fluids or of linear elastic solids, which is considered simple nowadays, complex material behavior often arises through the use of nonlinear material laws or through the consideration of additional order parameters. For the latter, the additional complexity of material behavior emerges from the interplay of the various time and length scales of the processes involved, *i.e.*, material flow and displacement, diffusion, phase separation, damage, chemical reactions, and heat transport. In addition to the mechanics, whose mathematical description is based on displacement and momentum as primary variables, the complex dynamics in the volume and at the surface of such materials can usually be described by scalar order parameters and systems thereof. For these mathematical descriptions, energetic-variational principles are a valuable tool to ensure the validity of the laws of thermodynamics, in particular the *second law*.

Mathematical descriptions of nonlinear diffusion, phase separation and phase transitions for a scalar order parameter $\psi : \Omega \to \mathbb{R}$ in a domain $\Omega \subset \mathbb{R}^d$ are usually based either on the Cahn-Hilliard equation [19] or on the Allen-Cahn equation [3] or variations thereof, i.e., the evolution $\partial_t \psi = \nabla \cdot m\nabla\eta - n\eta$ is based on the free energy

$$\mathscr{F}(\psi) = \int_\Omega W(\psi, \nabla\psi)\,\mathrm{d}x, \qquad W(\psi, z) = \frac{\varepsilon}{2}|z|^2 + \frac{1}{4\varepsilon}(1-\psi^2)^2, \tag{1}$$

such that a solution $\psi(t) : \Omega \to \mathbb{R}$ satisfies equality of energy descent and dissipation $2R$, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}(\psi(t)) = -2R = -\int_\Omega m|\nabla\eta|^2 + n\eta^2\,\mathrm{d}x \le 0, \qquad \eta = \frac{\delta W}{\delta\psi} = -\varepsilon\Delta\psi + \varepsilon^{-1}(\psi^3 - \psi). \tag{2}$$

The stability of corresponding discretizations of the Cahn-Hilliard or the Allen-Cahn equations is related to numerical schemes that guarantee this energy descent [31, 77]. When coupling this dynamics of systems of order parameters to the mechanics of fluids and solids one covers a wide range of phenomena in soft matter physics.

Phase-field models modeling diffuse interfaces include capillary stresses using gradients of the phase-field in the driving energy as introduced by Rayleigh, van der Waals and Korteweg, cf. [6] and references therein. For a binary mixture of incompressible fluids with surface tension, the phase-field evolution is described by the so-called *model H* [47]. Based on the rational mechanics by Truesdell and others [87], Gurtin [42, 43] proposed a generalized model for phase-field evolutions and mechanical stresses based on micro- and macrostresses. This model was later extended to a thermodynamic consistent formulations with different viscosities by Lowengrub

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and Truskinovsky [57]. Extensions to different mass densities where proposed by Boyer [15] for incompressible constituents. Such models are used to model suspension flows, e.g., [69], and are motivated by microscopic averaging [29]. Abels et al. [1] further extended the model with different densities to soluble species and studied the sharp-interface limit using formal asymptotics. For incompressible fluids, the system of conservation laws for momentum $\boldsymbol{p} = \varrho \boldsymbol{u}$ with velocity $\boldsymbol{u}$, mass, and phase-field reads

$$\begin{aligned} \varrho(\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}) - \nabla \cdot \boldsymbol{\sigma} &= -\varepsilon \nabla \cdot (\nabla \psi \otimes \nabla \psi) \\ \nabla \cdot \boldsymbol{u} &= 0 \\ \partial_t \psi + \boldsymbol{u} \cdot \nabla \psi &= \nabla \cdot (m \nabla \eta), \end{aligned} \tag{3}$$

with Newtonian viscous stress $\boldsymbol{\sigma} = -p\mathbb{I} + \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$ and the chemical potential η of (2). In many of the cases the main function of the order parameter/phase-field is to track the transport of microscopic consituents in an Eulerian continuum approach.

However, for complex materials such as hydrogels, colloidal suspensions or polymer solutions, viscoelastic properties, diffusion, swelling, shrinking, and transformation of properties by phase separation and phase transition play a major role in a mathematical description. A two-fluid model coupling solid viscoelastic behavior and Darcy flow was proposed by Tanaka [82] and later improved with respect to thermodynamical consistency by Zhou et al. [94]. Also for these models the (energy) stability is associated with the descent of the free energy of the system, now consisting of kinetic energy, phase-field energy, conformational entropy and elastic energy [80], i.e.,

$$\mathscr{F}(\psi, p, \boldsymbol{u}, \boldsymbol{\sigma}_{\text{elast}}) = \int_\Omega \tfrac{1}{2}|\boldsymbol{u}|^2 + W(\psi, \nabla\psi) + \tfrac{1}{2}p^2 + \tfrac{1}{2}\mathrm{tr}(\boldsymbol{\sigma}_{\text{elast}})\,\mathrm{d}x \tag{4}$$

with scalar bulk stress p and elastic shear stress $\boldsymbol{\sigma}_{\text{elast}}$. This implies that, as for the simple Cahn-Hilliard or Allen-Cahn model, we have a balance of energy descent and dissipation according to $\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F} = -2R \leq 0$. For hydrogel models, this can be guaranteed using incremental schemes based on minimization procedures [13]. Also phase-field models for damage and crack propagation fall into this class of models that couple elasticity and order parameters, but they are often more complex due to the rate-independent nature of some of the underlying dissipative processes and their coupling to finite strain, e.g., cf. [60, 86].

For the discussion of well-posedness and existence for such elliptic-parabolic systems, i.e., fourth-order diffusion equation via Cahn-Hilliard coupled with elasticity, one may use techniques from the calculus of variations [38, 36, 44, 86] going back to the Italian school [23, 40]. Therein, one main concept is the direct method in the calculus of variations which relays on coercivity and weakly lower semi-continuity assumptions. For the finite strain elasticity case one employs the concept of polyconvex energy functionals introduced in [8].

While many of these models describe entirely different physical processes and phenomena, the underlying commonality is that they are based on coupling of scalar order parameters and mechanical displacements. Their thermodynamical consistency relies on a balance of energy descent and dissipation, which is usually also reflected on the choice of discretization scheme. Therefore, the goal of this paper is to provide a concise mathematical introduction into the relevant construction of evolution laws for those systems in terms of *gradient flow evolution* defined in the Lagrangian frame using quadratic dissipation. While the restriction to gradient flows does not allow to consider inertial effects and waves and the restriction to Lagrangian frames somehow restricts the practical usability to fluid-mechanical applications[1], the class of phenomena accessible with such an approach based on finite strain is considerable.

2 Gradient flows for phase-fields and mechanics

Starting with a free energy functional $\mathscr{F} : \mathcal{Q} \to \mathbb{R}$ mapping from a state space $\mathcal{Q}$ of (vectors of) functions, energetic variational methods are a common tool for multiphase systems. Depending on the choice of model

[1] The fluid displacement might be difficult to track in the Lagrangian configuration for turbulent flows and for large times and require sophisticated ALE techniques.

parameters and coupling, one can treat a wide class of phenomena within one class of models.

2.1 General gradient flow structure

In this section we are going to lay the foundation for a formal construction of dissipation and energy balances, which are the main ingredients for gradient flows. A gradient flow structure is a tuple $(\mathcal{Q}, \mathscr{F}, R)$ of a state space $\mathcal{Q}$, a (free) energy $\mathscr{F} : \mathcal{Q} \to \mathbb{R}$, and for any $q \in \mathcal{Q}$ a positive convex dissipation potential $R(q, \cdot) : \mathcal{V} \to \mathbb{R}$ with $R(q, 0) = 0$ and $\mathcal{V} = T_q\mathcal{Q}$. Morally, in particular in finite dimensions, $\mathcal{Q}$ and $\mathcal{V}$ need to be understood as a manifold and its corresponding tangent space at a point q respectively, e.g., cf. [66, 62, 33]. However, we will keep the notation simple and consider these spaces as subsets of Banach or Hilbert spaces. Throughout this paper we restrict to spaces, where the components are functions from subsets of the Hilbert space $H^1(\Omega; \mathbb{R}^\ell)$ for some material domain $\Omega \subset \mathbb{R}^d$.

We restrict to cases where the dissipation potential $R(q, \cdot)$ is a quadratic functional in the velocity and is generated by a positive-symmetric operator $G(q) : \mathcal{V} \to \mathcal{V}^*$ such that

$$R(q, v) = \tfrac{1}{2}\langle G(q)v, v\rangle_{\mathcal{V}}, \tag{5}$$

with the canonical dual pairing $\langle\cdot,\cdot\rangle_{\mathcal{V}} : \mathcal{V}^* \times \mathcal{V} \to \mathbb{R}$. Due to the general dependence of G on q this applies to a rather general class of nonlinear problems. An element $v \in \mathcal{V}$ is called *the gradient of $\mathscr{F}$ with respect to G at q* if $\langle G(q)v, w\rangle_{\mathcal{V}} = \langle \mathrm{D}\mathscr{F}(q), w\rangle_{\mathcal{V}}$ for all $w \in \mathcal{V}$, where $\mathrm{D}\mathscr{F}(q) \in \mathcal{V}^*$ is the Fréchet derivative[2] of $\mathscr{F}$ at q, i.e.,

$$\langle \mathrm{D}\mathscr{F}(q), w\rangle_{\mathcal{V}} \equiv \mathrm{D}\mathscr{F}(q)\{w\} = \lim_{h\to 0} \frac{\mathscr{F}(q + hw) - \mathscr{F}(q)}{h}, \tag{6}$$

and one usually writes $v = \nabla_G \mathscr{F}(q)$. The *gradient flow* $q : [0, T] \to \mathcal{Q}$ is defined by the equation

$$\partial_t q = -\nabla_G \mathscr{F}(q) \qquad \text{in } \mathcal{V}, \tag{7}$$

or equivalently by $G(q)\partial_t q = -\mathrm{D}\mathscr{F}(q)$ in $\mathcal{V}^*$ or the Helmholtz minimum dissipation theorem [90]

$$\partial_t q = \operatorname*{arg\,min}_{w\in\mathcal{V}} \big(R(q, w) + \langle \mathrm{D}\mathscr{F}(q), w\rangle_{\mathcal{V}}\big). \tag{8}$$

The dynamics (7) gives the energy descent by construction

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}\big(q(t)\big) = \langle \mathrm{D}\mathscr{F}(q), \partial_t q\rangle_{\mathcal{V}} = -\langle G(q)\partial_t q, \partial_t q\rangle_{\mathcal{V}} = -2R(q, \dot q) \le 0. \tag{9}$$

Alternative formulations of (7) and instructive examples can be found in [66, 72, 28, 62, 84]. In [18] the authors present a model allowing for various effects such as force balance at a three phase contact line, a rising bubble through a fluid-fluid interface (via density increase) and a sliding particle into a binary fluid with slip conditions at certain interfaces. An expanded discussion on modelling aspects including discussions on the choice of the state space, the driving energy and possible dissipation potentials in the variational frame we refer to [67, 39]. In what follows, we narrow down the class of dissipation potentials to a practical definition and point out avenues for extending this definition.

2.2 Cahn-Hilliard/Allen-Cahn-type gradient flows

It is common to model phase separation through Cahn-Hilliard (interpreted as H^{-1} flows) or Allen-Cahn (interpreted as L^2 flows) equations or by combining their conserved and non-conserved evolution. Theses models can be coupled with linear [45] or nonlinear [86] elasticity.

[2] In finite dimensions $\mathcal{Q} \subset \mathbb{R}^k$, the Fréchet derivative is the usual differential of a function $\mathrm{D}\mathscr{F}(q) \equiv \mathrm{d}\mathscr{F}(q) \in \mathbb{R}^k$.

For a given $q \in \mathcal{Q}$, we want to construct a general quadratic dissipation potential $R(q,\cdot) : \mathcal{V} \to \mathbb{R}$ for the Hilbert space $\mathcal{V} = H^1(\Omega;\mathbb{R}^\ell)$. Note that the construction below formally applies even to $\mathcal{V} = L^2(\Omega;\mathbb{R}^\ell)$ and then will be be restricted to $H^1(\Omega;\mathbb{R}^\ell)$. Therefore, let $\mathcal{U} = H^1(\Omega;\mathbb{R}^\ell)$ and we have a symmetric positive bilinear form $a : \mathcal{U} \times \mathcal{U} \to \mathbb{R}$

$$a(u,v) = \int_\Omega \sum_{i,j=1}^{\ell} m_{ij} \nabla u_i \cdot \nabla v_j + n_{ij} u_i v_j \,\mathrm{d}x, \tag{10}$$

which for given positive matrices $m_{ij}, n_{ij} \in L^\infty(\Omega)$ for $i,j = 1 \dots \ell$ is invertible. For $n = 0$ one usually requires functions in U to have zero average or homogeneous Dirichlet boundary conditions on all or parts of the boundary. The dependence of R on q will enter this construction by assuming $m = m(x,q)$ and $n = n(x,q)$, which we avoid to write explicitly for clarity of the presentation. We have a corresponding symmetric, positive, invertible operator $A(q) : \mathcal{U} \to \mathcal{U}^*$ such that $a(u,v) = \langle A(q)u, v\rangle_{\mathcal{U}}$.

The inverse of A induces a bilinear form $a^*(\eta,\mu) = \langle \eta, A^{-1}(q)\mu\rangle_{\mathcal{U}}$ and is generated by the corresponding operator $A^*(q) = A^{-1}(q)$ via $a^*(\eta,\mu) = \langle \eta, A^*(q)\mu\rangle_{\mathcal{U}}$. The final ingredient is a linear map $M : \mathcal{V} \to U^*$ defined, for example[3], by

$$\langle Mv, u\rangle_{\mathcal{U}} = (u,v)_{L^2(\Omega)}, \tag{11}$$

where we have by definition $\langle Mv,u\rangle_{\mathcal{U}} \equiv \langle M^*u, v\rangle_{\mathcal{V}}$ and where everything is well-defined for $\mathcal{U} = H^1(\Omega)$ and $\mathcal{V} = L^2(\Omega)$. With all the ingredients above, let us define the dissipation potential $R(q,\cdot) : \mathcal{V} \to \mathbb{R}$ by

$$R(q,v) = \tfrac{1}{2} a^*(Mv, Mv) = \tfrac{1}{2}\langle G(q)v, v\rangle_{\mathcal{V}}, \qquad G(q) = M^* A^{-1}(q) M, \tag{12}$$

for all $v \in \mathcal{V}$. Let us shortly investigate the properties of the dissipation potential R introduced above. Frequently we have to compute the Legendre transformation $R^*(q,\cdot) : \mathcal{V}^* \to \mathbb{R}$

$$R^*(q,\xi) = \sup_{v\in\mathcal{V}} \big(\langle \xi, v\rangle - R(q,v)\big), \tag{13}$$

which for the given quadratic and differentiable R produces the weak formulation

$$a^*(Mv, Mw) = \langle Mw, A^{-1}(q)Mv\rangle_{\mathcal{U}} = \langle \xi, w\rangle_{\mathcal{V}} \qquad \forall w \in \mathcal{V} \tag{14}$$

for the minimizer $v \in \mathcal{V}$. If we denote $\eta = A^{-1}(q)Mv$, then (14) becomes a saddle point problem

$$\begin{aligned} A\eta - Mv &= 0 \\ M^*\eta &= \xi \end{aligned} \quad \text{in} \quad \mathcal{U}^* \times \mathcal{V}^*. \tag{15}$$

Since M, M^* from (11) has a trivial kernel, any solution of (15) is unique and insertion into (13) gives $R^*(q,\xi) = \frac{1}{2}a(\eta,\eta)$. In general, the main issue in showing the solvability of (15) is the potential lack of coercivity of R, which can be *repaired* by adding a regularization $R_\varepsilon(q,\dot q) = R(q,\dot q) + \varepsilon\|\dot q\|_{\mathcal{V}}^2$, resulting in the modified saddle point problem

$$\begin{aligned} A\eta - Mv &= 0 \\ M^*\eta + Sv &= \xi \end{aligned} \quad \text{in} \quad U^* \times \mathcal{V}^*, \tag{16}$$

where $S : \mathcal{V} \to \mathcal{V}^*$ is the Riez isomorphism $\langle Sv, w\rangle := \varepsilon(v,w)_{\mathcal{V}}$. The evolution equation of (7) is then given by replacing $v \to \partial_t q$ and $\xi \to -\mathrm{D}\mathscr{F}(q)$ in (15) or (16). In general we are going to consider free energy functionals of the form

$$\mathscr{F}(q) = \int_\Omega W(x,q,\nabla q)\,\mathrm{d}x, \qquad \langle \mathrm{D}\mathscr{F}(q), v\rangle = \int_\Omega (\partial_q W)v + (\partial_{\nabla q} W)\cdot\nabla q \,\mathrm{d}x. \tag{17}$$

where $\mathrm{D}\mathscr{F}$ is the Fréchet derivative defined in (6). Then, assuming sufficient regularity, the dynamics of (7) with the functionals R and $\mathscr{F}$ defined above gives rise to the evolution

$$\partial_t q = \nabla\cdot(m\nabla\eta) - n\eta, \qquad \eta = \frac{\delta W}{\delta q} = -\nabla\cdot(\partial_{\nabla q} W) + \partial_q W. \tag{18}$$

[3] Alternative choices for M that include boundary dynamics are discussed in [68] and [70].

2.3 Natural extensions of gradient flow framework

Note that the restriction to this class of dissipation potentials R is purely to keep the presentation concise. Common material frame-indifferent potentials for mechanical problems, e.g., viscous dissipation of the Brinkman (Darcy-Stokes) problem, are of the form

$$R_{\text{Brinkman}}(q,\dot{q}) = \int_\Omega \frac{1}{2} \sum_{i,j=1}^{\ell} \nabla\dot{q}_i \cdot \mu_{ij}(q,\nabla q)\nabla\dot{q}_j + \dot{q}_i \cdot \nu_{ij}(q,\nabla q)\dot{q}_j \,\mathrm{d}x, \tag{19}$$

which is a straight-forward extension of the concepts presented here. In the context of phase-field variables and mechanical variables, one would use Cahn-Hilliard/Allen-Cahn type dissipation for phase-field and concentration variables and Brinkman/Stokes/Darcy-type dissipation for mechanical variables. The off-diagonal coupling terms between phase-field evolution and mechanics need to be chosen such that they maintain positivity of $R(q,\cdot)$.

While in this work we focus on quadratic dissipation functions $R(q,\cdot)$, in the context of damage models also rate-independent phase-field evolution [71, 60] and in the context of Bingham flows rate-independent viscosity is considered [25], i.e.,

$$R_{\text{Bingham}}(q,\dot{q}) = \int_\Omega \tfrac{1}{2}\mu|\nabla\dot{q}|^2 + \mu_0|\nabla\dot{q}| \,\mathrm{d}x, \tag{20}$$

so that the system of partial-differential equations turns into a system of variational inequalities and specific numerical methods are necessary to solve these systems [74]. Such extensions of gradient flows with nonquadratic dissipation $R(q,\cdot)$ are also called *generalized gradient flows* [53].

In many cases, one might be interested to add further conditions. While essential and natural boundary conditions are usually directly imposed by the space $\mathcal{V}$ or $\mathcal{Q}$ or the functionals R and $\mathscr{F}$, alternatively one might enforce conditions approximately by penalty, e.g. cf. [7], or by Lagrange multipliers, e.g. cf. [48]. From a discretization and analysis point of view the latter approach usually leads to saddle-point problems, whose solvability requires a Ladyzhenskaya–Babuška–Brezzi (LBB or inf-sup) condition to be valid [12]. In the context of the coupling of order-parameters and mechanics we will use multipliers to satisfy solvability conditions on translation and rotation in the absence of Dirichlet boundary conditions in the mechanical problem and to enforce incompressibility of materials in certain cases. For example, a given condition $C(q,\nabla q) = 0$ can be enforced by a functional

$$\mathcal{C}(q,\lambda) = \int_\Omega C(q,\nabla q)\cdot\lambda \,\mathrm{d}\boldsymbol{x} = 0, \qquad \forall\lambda\in\mathcal{V}_\lambda,$$

by extending $q_\lambda = (q,\lambda) \in \mathcal{Q}_\lambda = \mathcal{Q}\times\mathcal{V}_\lambda$ and by defining the Lagrangian

$$\mathscr{L}(q_\lambda) = \mathscr{F}(q) + C(q,\lambda).$$

In this case the saddle-point problem (15) becomes

$$\begin{aligned} A\eta - M\partial_t q &= 0 \\ M^*\eta &= -\mathrm{D}_q\mathscr{L} \qquad \text{in } \mathcal{U}^*\times\mathcal{V}^*\times\mathcal{V}_\lambda^*. \\ 0 &= -\mathrm{D}_\lambda\mathscr{L} \end{aligned} \tag{21}$$

This structure can be directly obtained by extending $M^* : \mathcal{U} \to (\mathcal{V}\times\mathcal{V}_\lambda)^*$ via $\langle M_\lambda^*\eta_\lambda, v_\lambda\rangle_{\mathcal{V}\times\mathcal{V}_\lambda} = \langle M^*\eta, v\rangle_{\mathcal{V}}$ trivially and using $\mathscr{L}$ as the driving functional.

2.4 Incremental minimization schemes

One of the major problems of any discretization of transient problems is maintaining numerical stability, which for dissipative problems is usually associated with a provable discrete energy-decay. This is particularly important for ill-conditioned problems with large scale separation, as it is usually the case in phase-separation problems with a small parameter, e.g., the interfacial thickness. A simple first-order in time discretization scheme of the gradient structures introduced before is the well-known incremental scheme.

Definition 1 (Incremental minimization scheme) *Let $R(q,\cdot) : \mathcal{V} \to \mathbb{R}$ a convex and positive dissipation potential and $\mathscr{F} : \mathcal{Q} \to \mathbb{R}$ an energy. For given initial data $q_0 = q(t=0)$ and time-step size $\tau = T/N$ we consider the sequence of functions $q^k = q(k\tau)$ being successive solutions of the minimization problem*

$$q^k = \arg\min_q \mathscr{R}(q^{k-1}, v = \tfrac{1}{\tau}(q - q^{k-1})) \qquad \mathscr{R}(q,v) = \tau R(q,v) + \mathscr{F}(q+\tau v) \tag{22}$$

where in particular non-affine constraints need to be handeled with care. ⋆

Due to the property $R(q,0) = 0$ and $R(q,v) \geq 0$ we have for $v_{\text{min}} = (q^k - q^{k-1})/\tau$ that

$$\mathscr{R}(q^{k-1}, v_{\text{min}}) = \tau R(q^{k-1}, v_{\text{min}}) + \mathscr{F}(q^k) \leq \mathscr{R}(q^{k-1}, 0) = \mathscr{F}(q^{k-1}),$$

and thus the discrete energy inequality $\mathscr{F}(q^k) - \mathscr{F}(q^{k-1}) \leq -\tau R(q^{k-1}, v_{\text{min}})$. Since $\mathscr{R}$ is convex and (assumed) smooth in the second argument, we can classify the first-order conditions, based on which we will devise the weak formulation of this smooth incremental minimization problem.

Based on time-incremental minimization and employing additional regularization terms, the authors in [45, 38] prove existence of weak solutions for a coupled phase separation damage model at small strains. In [86] the authors use a staggered time-discrete scheme, i.e. two separate minimization problems, to show an existence result. An abstract formulation and detailed description of the strategy to prove existence of minimizer in the energetic form, for linear and nonlinear elasticity, is given in [36, 61].

Differentiation of $\mathscr{R}$ in the direction of an arbitrary direction $\phi \in \mathcal{V}$ gives

$$\begin{aligned} \langle \mathrm{D}\mathscr{R}(q^{k-1}, v_{\text{min}}), \phi\rangle &= a^*\left(M(\tfrac{q^k - q^{k-1}}{\tau}), M\phi\right) + \langle \mathrm{D}\mathscr{F}(q^k), \phi\rangle \\ &= \langle M\phi, A^{-1}(q^{k-1}) M(\tfrac{q^k - q^{k-1}}{\tau})\rangle_{\mathcal{U}} + \langle \mathrm{D}\mathscr{F}(q^k), \phi\rangle \stackrel{!}{=} 0. \end{aligned} \tag{23a}$$

As before in the construction of the Legendre transformation R^* of R in (15), we introduce a new variable $\eta = A^{-1}(q^{k-1}) M v_{\text{min}}$ are therefore get

$$\begin{aligned} A\eta - M(\tfrac{q^k - q^{k-1}}{\tau}) &= 0 \\ M^*\eta &= \mathrm{D}\mathscr{F}(q^k), \end{aligned} \qquad \text{in } \mathcal{U}^* \times \mathcal{V}^*, \tag{23b}$$

as a nonlinear system of partial differential equations for q^k and η. Using the explicit form of the bilinear form a and the operator M we get the weak formulation

$$\begin{aligned} a(\eta, \phi_u) - (\tfrac{q^{k+1} - q^k}{\tau}, \phi_u)_{L^2(\Omega)} &= 0, \\ (\eta, \phi_v)_{L^2(\Omega)} &= \langle \mathrm{D}\mathscr{F}(q^{k+1}), \phi_v\rangle, \end{aligned} \tag{23c}$$

with the bilinear form a as defined in (10) and for all $(\phi_u, \phi_v) \in \mathcal{U} \times \mathcal{V}$.

Remark 1 (Alternative time discretizations) *In the (formal) sense of Riemanian manifolds, the gradient flows we consider here are generated by a metric tensor $g_q : \mathcal{V} \times \mathcal{V} \to \mathbb{R}$ with $g_q(v,v) = 2R(q,v) = \langle G(q)v, v\rangle_{\mathcal{V}}$ for given $q \in \mathcal{Q}$. However, there are also gradient flows which are rather written in terms of a distance $d : \mathcal{Q} \times \mathcal{Q} \to \mathbb{R}$, e.g. most prominently Wasserstein gradient flows [49, 4]. In such cases, the steepest decent with cost/dissipation/distance can be generated by minimizing movements as introduced by De Giorgi [24]. Discrete Lagrangian approaches are also relevant in this case [20]. For suitably generalized solution concepts, e.g. see [63] for alternative balances of energy and dissipation, minimization is performed over solutions that are interpolated in time.* ⋆

In the remainder of the manuscript we discuss different choices of dissipation R through definitions of a and M and choices of energy $\mathscr{F}$ through choices of the density W. Correspondingly, we discuss the proper choice of $\mathcal{Q}$ by defining tuples of functions for a setting, where a phase-field evolution is coupled to finite-strain elastodynamics. As it was noted before, the extension of this Cahn-Hilliard/Allen-Cahn type dynamics to Stokes/Darcy evolution is a straight-forward extension of the dissipation R.

3 Lagrangian finite-strain hyperelasticity and phase-field evolution

3.1 Continuum mechanical setup

We start by giving a short introduction to continuum mechanics to motivate the considered model class. In this branch of mechanics, one investigates the dynamics of solid bodies, liquids and gases by describing them via their occupied domain and physical quantities such as mass, momentum and energy are expressed through density functions [41, 87, 76]. Thereby one neglects the discrete, atomistic structure of nature and assumes the regarded material as continuous matter [88]. The mathematical description through partial differential equations of such a system is gained by applying conservation laws for mass, momentum, energy density and constitutive equations.

Let $\Omega \subset \mathbb{R}^d$ be so-called *Lagrangian reference configuration* or *material configuration*, i.e., the set of points described to label material points of the physical body. The physical body undergoes deformations due the application of forces which, for example, can be of mechanical, chemical or thermodynamical nature. The dynamics of displaced material points is described using a displacement $\boldsymbol{u}$ defined such that

$$\boldsymbol{u} : \Omega \to \mathbb{R}^d, \quad (t, \boldsymbol{X}) \mapsto \tilde{\boldsymbol{x}} = \chi(t, \boldsymbol{X}) = \boldsymbol{X} + \boldsymbol{u}(t, \boldsymbol{X}) \in \mathbb{R}^d,$$

i.e., a material point $\boldsymbol{X} \in \Omega$ in the material configuration is mapped to a point $\boldsymbol{x} \in \tilde{\Omega}(t)$ in the time-dependent *deformed* or *Eulerian current configuration*. The description of variables as functions defined in Ω is usually called a *Lagrangian description*, the one in $\tilde{\Omega}$ is called *Eulerian description*. In this work we focus on Lagrangian descriptions of the coupled dynamics of displacements $\boldsymbol{u}$ and systems of scalar order parameters $\boldsymbol{\psi}$.

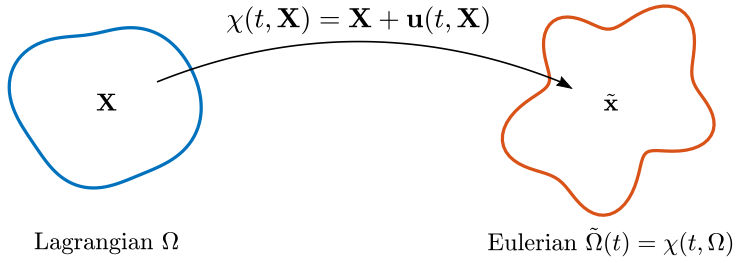

Figure 1: Deformation of Lagrangian reference configuation Ω into Eulerian current configuration Ω

Therefore, additionally to a displacement we introduce the N-component field $\boldsymbol{\psi} : \Omega \to \mathbb{R}^N$ to describe the state of the material. The role of $\boldsymbol{\psi}$ can be, for example, a concentration in a model for diffusion and phase separation, the phase-field serving as an indicator function in a model with free boundaries, a volume fraction in a mixture model, or a damage variable in a damage model.

3.2 State space and free energy density

In accordance with the previous section, we summarize the components as an element q of the state space $\mathcal{Q}$ as

$$q = \begin{pmatrix} \boldsymbol{u} : \Omega \to \mathbb{R}^d \\ \boldsymbol{\psi} : \Omega \to \mathbb{R}^N \end{pmatrix} \in \mathcal{Q}, \tag{24}$$

and construct models that describe the dynamics of states $q : [0, T] \to \mathcal{Q}$. In the following we use $\mathcal{Q} = H^1(\Omega, \mathbb{R}^d) \times H^1(\Omega, \mathbb{R}^N)$ for the state space and whenever necessary highlight the dependence on the components $(\boldsymbol{u}, \boldsymbol{\psi}) = q$. The most general form of the free energy $\mathscr{F} : \mathcal{Q} \to \mathbb{R}$ that we use here is

$$\mathscr{F}(q) = \int_\Omega W_{\text{elast}}(F F_{\text{p}}^{-1}(\boldsymbol{\psi}), \boldsymbol{\psi}) + W_{\text{phase}}(\boldsymbol{\psi}, \nabla \boldsymbol{\psi}, F) \mathrm{d}\boldsymbol{X} \tag{25}$$

with the deformation gradient $F = \mathbb{I}_d + \nabla \boldsymbol{u}$, $J = \det F$, and $\mathbb{I}_d$ the $d \times d$ identity matrix. The free energy density $W(q, \nabla q) = W_{\text{elast}} + W_{\text{phase}}$ consists of a mechanical contribution in form of a hyperelastic energy W_{elast} and a remaining contribution W_{phase} which covers all remaining thermal, chemical, entropic contributions to the free energy of the system.

The restriction to this type of free energy density presents a considerable simplification of the general energy density $W(q, \nabla q)$ and is steered to allow for multiple relevant coupling mechanisms of mechanics and phase-field evolution:

i) The dependence of the elastic energy on the product FF_{p}^{-1} is the *multiplicative decomposition*, which for finite-strains is common in description for inelastic phenomena where multiple reference configurations are viable, e.g. cf. [32, 52, 50, 73, 5, 58, 21, 92].

ii) Additionally, the direct dependence of the elastic energy on $\boldsymbol{\psi}$ allows for the elastic material parameters to depend on the order parameter as common for damage phase-field models or in phase-field approaches to topology optimization, e.g. cf. [60, 81].

iii) The dependence of the energy W_{free} on $\boldsymbol{\psi}$ and its gradients allows the inclusion of diffusion and phase separation using logarithmic entropic terms. The dependence of this energy density on F allows the inclusion of diffusion in the deformed configuration, which naturally creates Korteweg stresses in the momentum balance, e.g. cf. [47, 1].

For a free energy of the general form $\mathscr{F}(q) = \int_\Omega W(q, \nabla q)\,\mathrm{d}\boldsymbol{X}$ we denote the Frechet derivative $\mathrm{D}\mathscr{F}(q) \in \mathcal{V}^*$ by its action on an element $\boldsymbol{v} = (v_{\boldsymbol{u}}, v_{\boldsymbol{\psi}}) \in \mathcal{V} = V_{\boldsymbol{u}} \times V_{\boldsymbol{\psi}}$ as

$$\begin{aligned}
\langle \mathrm{D}\mathscr{F}(q), \boldsymbol{v}\rangle_{\mathcal{V}} &= \int_\Omega \partial_q W \cdot \boldsymbol{v} + \partial_{\nabla q} W \cdot \nabla \boldsymbol{v}\,\mathrm{d}\boldsymbol{X} = \langle \mathrm{D}_{\boldsymbol{u}}\mathscr{F}(q), v_{\boldsymbol{u}}\rangle_{V_{\boldsymbol{u}}} + \langle \mathrm{D}_{\boldsymbol{\psi}}\mathscr{F}(q), v_{\boldsymbol{\psi}}\rangle_{V_{\boldsymbol{\psi}}},\\
\langle \mathrm{D}_{\boldsymbol{u}}\mathscr{F}(q), v_{\boldsymbol{u}}\rangle_{V_{\boldsymbol{u}}} &= \int_\Omega \partial_{\boldsymbol{u}} W \cdot v_{\boldsymbol{u}} + \partial_{\nabla \boldsymbol{u}} W : \nabla v_{\boldsymbol{u}}\,\mathrm{d}\boldsymbol{X},\\
\langle \mathrm{D}_{\boldsymbol{\psi}}\mathscr{F}(q), v_{\boldsymbol{\psi}}\rangle_{V_{\boldsymbol{\psi}}} &= \int_\Omega \partial_{\boldsymbol{\psi}} W \cdot v_{\boldsymbol{\psi}} + \partial_{\nabla \boldsymbol{\psi}} W \cdot \nabla v_{\boldsymbol{\psi}}\,\mathrm{d}\boldsymbol{X},
\end{aligned} \tag{26}$$

and using these derivatives $\mathrm{D}\mathscr{F} \simeq (\mathrm{D}_{\boldsymbol{u}}\mathscr{F}, \mathrm{D}_{\boldsymbol{\psi}}\mathscr{F}) \in V_{\boldsymbol{u}}^* \times V_{\boldsymbol{\psi}}^*$ as driving forces for the gradient evolution for the specific free energy constructed in (25) is the cornerstone of a structure-preserving energy-based variational formulation. With $A : B$ we denote the Frobenius inner product defined $A : B = \mathrm{tr}(A^T B)$ for matrices/tensors $A, B \in \mathbb{R}^{d\times d}$.

3.3 Discretization in time and space

For the time discretization we use the incremental minimization scheme introduced in (1). We consider an equidistant decomposition of the time interval $[0, T] = \{0 = t^0 < t^1 < \ldots < t^N\}$ with time step size $t^k - t^{k-1} =: \tau$. Finite difference methods are used to approximate time derivatives. The space discretization is based on the finite element method where we use a decomposition of the (polygonal) domain into non-overlapping simplicial elements, i.e.,

$$\partial_t q \approx \frac{q^k - q^{k-1}}{\tau} \qquad \text{and} \qquad \Omega = \bigcup_{e=1}^{n_e} \Omega_e.$$

By employing a Galerkin approximation, we approximate solutions and test functions in the finite dimensional function spaces $V_{\boldsymbol{u},h} \times V_{\boldsymbol{\psi},h} = \mathcal{Q}_h \subset \mathcal{Q}$ with vectorial basis $\{\boldsymbol{w}_{i_{\boldsymbol{u}}}\}$ for $i_{\boldsymbol{u}} \in \{1, ..., N_{\boldsymbol{u}}\}$, $N_{\boldsymbol{u}} = \dim V_{\boldsymbol{u},h}$ and basis $\{\boldsymbol{\varphi}_{i_{\boldsymbol{\psi}}}\}$ for $i_{\boldsymbol{\psi}} \in \{1, ..., N_{\boldsymbol{\psi}}\}$ with $N_{\boldsymbol{\psi}} = \dim V_{\boldsymbol{\psi},h}$. We write solutions as

$$\boldsymbol{u}^h(t, \boldsymbol{X}) = \sum_{i=1}^{N_{\boldsymbol{u}}} \hat{u}_h^i(t)\boldsymbol{w}_i(\boldsymbol{X}), \qquad \boldsymbol{\psi}^h(t, \boldsymbol{X}) = \sum_{i=1}^{N_{\boldsymbol{\psi}}} \hat{\psi}_h^i(t)\boldsymbol{\varphi}_i(\boldsymbol{X}),$$

with basis functions $\boldsymbol{w}_i \in \boldsymbol{V}_h^2$, $\boldsymbol{\varphi}_i \in \boldsymbol{V}_h^1$ and coefficients $\hat{u}_h^i, \hat{\psi}^i \in \mathbb{R}$. The functions $\boldsymbol{u}(t) : \Omega \to \mathbb{R}^d$ and $\boldsymbol{\psi}(t) : \Omega \to \mathbb{R}^N$ are approximated using the basis functions $\boldsymbol{w}_i \in \boldsymbol{V}_{\boldsymbol{u},h}$ and $\boldsymbol{\varphi}_i \in \boldsymbol{V}_{\psi,h}$ with Ω a domain with polygonal boundaries and a corresponding triangulation $\{\mathcal{T}_h\}_{h>0}$ with

$$\begin{aligned}\boldsymbol{V}_{\boldsymbol{u},h} &= \{\boldsymbol{v} \in C^1(\bar{\Omega}, \mathbb{R}^d) : \boldsymbol{v}|_T \in P_{k_u}(T, \mathbb{R}^d), T \in \mathcal{T}_h\},\\ V_{\psi,h} &= \{v \in C^1(\bar{\Omega}) : v|_T \in P_{k_\psi}(T, \mathbb{R}^N), T \in \mathcal{T}_h\}.\end{aligned}$$

and $P_k(T, \mathbb{R}^r)$ being $\mathbb{R}^r$-valued polynomials of degree k on triangles $T \in \mathcal{T}_h$. We will usually use $k_\psi = 1$ and $k_u = 1$ or $k_u = 2$. The Eulerian density $\tilde{\boldsymbol{\psi}}^h(t, \boldsymbol{x})$ is then defined by

$$\tilde{\boldsymbol{\psi}}^h(t, \boldsymbol{\chi}^h(t, \boldsymbol{X})) = \boldsymbol{\psi}^h(t, \boldsymbol{X}). \tag{27}$$

at the deformed coordinates[4] $\boldsymbol{\chi}^h(t, \boldsymbol{X}) = \boldsymbol{X} + \boldsymbol{u}^h(t, \boldsymbol{X})$.

3.4 Fully discrete and nonlinear incremental minimization

Let $\boldsymbol{u} : \Omega \to \mathbb{R}^d$ be the displacement field, $F = \mathbb{I}_d + \nabla \boldsymbol{u}$ the deformation gradient and $\boldsymbol{\psi} : \Omega \to \mathbb{R}^N$ the N-component order parameter. To solve the incremental minimization scheme in (1) numerically, let us seek minimizers of $\mathscr{R}$ via $\partial_q \mathscr{R}(q^{k-1}, v(q)) = 0$ with $v(q) = \tau^{-1}(q - q^{k-1})$, which similar to (23) gives a time discrete residual $\mathcal{R} : \mathcal{V} \times \mathcal{U} \to \mathbb{R}^{N_{\mathcal{V}\times\mathcal{U}}}$ with components $\mathcal{R} = (\mathcal{R}^{(\boldsymbol{u})}, \mathcal{R}^{(\boldsymbol{\psi})}, \mathcal{R}^{(\boldsymbol{\eta}_u)}, \mathcal{R}^{(\boldsymbol{\eta}_\psi)})$ defined as

$$\mathcal{R}_{i_\alpha}^{(\alpha)}(q, \boldsymbol{\eta}) = \begin{cases} (\boldsymbol{\eta}_{\boldsymbol{u}}, \boldsymbol{w}_{i_\alpha}) + \langle \mathrm{D}_{\boldsymbol{u}} \mathscr{F}(q), \boldsymbol{w}_{i_\alpha} \rangle & \text{if} \quad \alpha = \boldsymbol{\eta}_{\boldsymbol{u}} \\ (\boldsymbol{\eta}_{\boldsymbol{\psi}}, \boldsymbol{\varphi}_{i_\alpha}) + \langle \mathrm{D}_{\boldsymbol{\psi}} \mathscr{F}(q), \boldsymbol{\varphi}_{i_\alpha} \rangle & \text{if} \quad \alpha = \boldsymbol{\eta}_{\boldsymbol{\psi}} \\ \frac{1}{\tau}(\boldsymbol{u} - \boldsymbol{u}^{k-1}, \boldsymbol{w}_{i_\alpha}) - a_{\boldsymbol{u}}(\boldsymbol{\eta}_{\boldsymbol{u}}, \boldsymbol{w}_{i_\alpha}) & \text{if} \quad \alpha = \boldsymbol{u} \\ \frac{1}{\tau}(\boldsymbol{\psi} - \boldsymbol{\psi}^{k-1}, \boldsymbol{\varphi}_{i_\alpha}) - a_{\boldsymbol{\psi}}(\boldsymbol{\eta}_{\boldsymbol{\psi}}, \boldsymbol{\varphi}_{i_\alpha}) & \text{if} \quad \alpha = \boldsymbol{\psi} \end{cases} \tag{28}$$

with $i_\alpha \in \{1, ..., N_\alpha\}$ and index set $\alpha \in \{\boldsymbol{u}, \boldsymbol{\psi}, \boldsymbol{\eta}_{\boldsymbol{u}}, \boldsymbol{\eta}_{\boldsymbol{\psi}}\}$. The incremental minimization Def. 1 is then equivalent to seek at each time step k for q^k such that $\mathcal{R}(q^k, \boldsymbol{\eta}^k) = 0$ for all α_i. The nonlinear problem is solved using a Newton method. Let $\hat{q}_0 = q^{k-1}, \hat{\boldsymbol{\eta}}_0 = \boldsymbol{\eta}^{k-1}$ be an initial guess for the Newton iteration $(\hat{q}_{l-1}, \hat{\boldsymbol{\eta}}_{l-1}) \mapsto (\hat{q}_l, \hat{\boldsymbol{\eta}}_l)$ and repeat the iteration

$$\begin{pmatrix} \hat{q}_l \\ \hat{\boldsymbol{\eta}}_l \end{pmatrix} = \begin{pmatrix} \hat{q}_{l-1} \\ \hat{\boldsymbol{\eta}}_{l-1} \end{pmatrix} - \left(\partial_{(q,\eta)} \mathcal{R}(\hat{q}_{l-1}, \boldsymbol{\eta}_{l-1})\right)^{-1} \mathcal{R}\left(\hat{q}_{l-1}, \boldsymbol{\eta}_{l-1}\right), \tag{29}$$

until a certain tolerance goal (e.g. $\|\mathcal{R}((q_l, \boldsymbol{\eta}_l)\| < r_{\mathrm{tol}}$ is met or a certain maximal number of iteration $l_{\max}$) is reached and set $(q^k, \boldsymbol{\eta}^k) = (\hat{q}_l, \hat{\boldsymbol{\eta}}_l)$ or reject the iteration.

Before we specify the energy densities let us have a closer look at the structure of the Jacobian $\partial_q \mathcal{R}$. On can understand $\mathcal{R}$ as four component vector, precisely $\mathcal{R}^{\boldsymbol{u}}(q) \in \mathbb{R}^{N_{\boldsymbol{u}}}$, $\mathcal{R}^{\boldsymbol{\psi}}(q) \in \mathbb{R}^{N_{\boldsymbol{\psi}}}$, $\mathcal{R}^{\boldsymbol{\eta}_u}(q) \in \mathbb{R}^{N_{\boldsymbol{u}}}$ and $\mathcal{R}^{\boldsymbol{\eta}_\psi}(q) \in \mathbb{R}^{N_{\boldsymbol{\psi}}}$. The Jacobi matrix has the dimension $N_{\mathcal{V}\times\mathcal{U}} \times N_{\mathcal{V}\times\mathcal{U}}$ and can be understood as a four by four block structure of the form

$$(\partial_{q_j} \mathcal{R}_i)_{i,j=1}^{N_{\mathcal{V}\times\mathcal{U}}}(q, \boldsymbol{\eta}) = \begin{pmatrix} \mathrm{D}^2_{\boldsymbol{u}\boldsymbol{u}} \mathscr{F}(q)\{\boldsymbol{w}_{i_\alpha}, \boldsymbol{w}_{j_\alpha}\} & \mathrm{D}^2_{\boldsymbol{\psi}\boldsymbol{v}} \mathscr{F}(q)\{\boldsymbol{\varphi}_{i_\alpha}, \boldsymbol{w}_{j_\alpha}\} & \frac{1}{\tau}(\boldsymbol{w}_{i_\alpha}, \boldsymbol{w}_{j_\alpha})_{L^2} & 0 \\ \mathrm{D}^2_{\boldsymbol{u}\boldsymbol{\psi}} \mathscr{F}(q)\{\boldsymbol{w}_{i_\alpha}, \boldsymbol{\varphi}_{j_\alpha}\} & \mathrm{D}_{\boldsymbol{\psi}\boldsymbol{\psi}} \mathscr{F}(q)\{\boldsymbol{\varphi}_{i_\alpha}, \boldsymbol{\varphi}_{j_\alpha}\} & 0 & \frac{1}{\tau}(\boldsymbol{\varphi}_{i_\alpha}, \boldsymbol{\varphi}_{j_\alpha})_{L^2} \\ -(\boldsymbol{w}_{i_\alpha}, \boldsymbol{w}_{i_\alpha})_{L^2} & 0 & a_{\boldsymbol{u}}(\boldsymbol{w}_{i_\alpha}, \boldsymbol{w}_{i_\alpha}) & 0 \\ 0 & -(\boldsymbol{\varphi}_{i_\alpha}, \boldsymbol{\varphi}_{j_\alpha})_{L^2} & 0 & a_\psi(\boldsymbol{\varphi}_{i_\alpha}, \boldsymbol{\varphi}_{j_\alpha}) \end{pmatrix}.$$

The entries of $\partial_{q_j} \mathcal{R}_i$ are obtained by differentiating each component of the residual in (28) with respect to $\boldsymbol{u}, \boldsymbol{\psi}, \boldsymbol{\eta}_{\boldsymbol{u}}, \boldsymbol{\eta}_{\boldsymbol{\psi}}$. We understand the indexing as $i, j \mapsto i_\alpha, j_\alpha$ with the same meaning as above, such that $i_\alpha \in \{1, \ldots, N_\alpha\}$. Corresponding to (6) we denote the second-order Fréchet derivative of $\mathscr{F}$ at q by

$$\mathrm{D}^2_{qq} \mathscr{F}(q)\{v, w\} = \mathrm{D}_q(\langle \mathrm{D}_a \mathscr{F}, v\rangle)\{w\} = \lim_{h\to 0} \frac{\langle \mathrm{D}_q \mathscr{F}(q + hw), v\rangle - \langle \mathrm{D}_q \mathscr{F}(q), v\rangle}{h}$$

with test functions $v, w \in \mathcal{V}$.

[4] Sometimes $\boldsymbol{\chi}$ is also called flow map.

4 Continuum mechanics and order-parameter evolution

In continuum mechanics, internal variables are used to model materials with multiple phases such as fluid structure/solid (-air) interaction [89, 9, 78, 65] or complex fluids (mixtures of two or three component) [54, 17, 16, 93, 18, 1]. These models are used to describe effects like damage/fracture in solid mechanics [64, 37], swelling of hydrogels [10, 46, 21] and phase separation [82, 43]. Due to possible large deformations in these situations one is especially interested in models allowing for finite strain elasticity. An other challenge when modelling multiple component materials is that one needs to take into account different length scales (molecular ones inside each component, mesoscopic interfacial morphology and macroscopic hydrodynamics) [93]. To bring together fluid flows, given in Euleraian coordinates, and a solid structure in the Lagrangian frame by accomplishing interface conditions one may use the *Arbitrary Lagrangian-Eulerian* (ALE) approach [91, 34]. Fully Lagrangian descriptions may prove advantageous for problems involving singularities, sharp interface limits and free boundaries. Moreover, the authors in [55] discuss different dissipation functionals in a variational Lagrangian frame addressing physical and numerical aspects. They compare numerical results for diffuse interface models within the Lagrangian and the Eulerian frame indicating that the first method has advantages in capturing thin diffuse interface, while the latter one is favourable for to approximate the solution in the bulk region. In a fully Eulerian approaches one overcomes re-meshing and interpolations to reconnect the different grids [65].

In the following, we present examples of coupled mechanical (elastic and fluid-like) dynamics, coupled to the evolution of scalar order-parameters, i.e., phase-fields, concentrations, volume fractions. For this we consider the concrete state variable $q = (\boldsymbol{u}, \psi)$ with displacement $\boldsymbol{u} : \Omega \to \mathbb{R}^d$ and multicomponent phase-field $\boldsymbol{\psi} : \Omega \to \mathbb{R}^N$ and the following free energy

$$\mathscr{F}(q) = \int_\Omega W_{\text{elast}}(F_{\text{e}}, \boldsymbol{\psi}) \mathrm{d}\boldsymbol{X} + \int_\Omega W_{\text{phase}}(\boldsymbol{\psi}, \nabla\boldsymbol{\psi}, F) \mathrm{d}\boldsymbol{X}, \tag{30}$$

for deformation gradient $F = \mathbb{I}_d + \nabla\boldsymbol{u} = F_{\text{e}}F_{\text{p}}$ with a given plastic (swelling) strain $F_{\text{p}} = F_{\text{p}}(\psi)$ and thus $F_{\text{e}} = FF_{\text{p}}^{-1}$, e.g. cf. [56]. We consider a Neo-Hookean elastic energy density

$$W_{\text{elast}}(F_{\text{e}}, \boldsymbol{\psi}) = \frac{G}{2}\Big(\text{tr}(F_{\text{e}}^T F_{\text{e}} - \mathbb{I}_d) - 2\log(\det(F_{\text{e}}))\Big) + \frac{K}{2}\big(\det(F_{\text{e}}) - H\big)^2, \tag{31}$$

with bulk modulus $G = G(\psi)$ and phase volume $H = H(\psi)$ and inverse compressibility $K \in \mathbb{R}$. The remaining part of the free energy is

$$W_{\text{phase}}(\boldsymbol{\psi}, \nabla\boldsymbol{\psi}, F) = \left[\frac{1}{2}\nabla\boldsymbol{\psi} \cdot \sigma\nabla\boldsymbol{\psi} + W_{\text{entropy}}(\boldsymbol{\psi}, F)\right] \det(F), \tag{32}$$

with second-order tensor $\sigma = \sigma(F) \in \mathbb{R}^{d\times d}$. Together with a given dissipation potential $R(q, \dot{q})$, different parameters, double-well or Flory-Huggins-type entropy W_{entropy} and possible constraints $C(q, \nabla q) = 0 \in \mathbb{R}^M$ added through the Lagrangian in terms of $q_\lambda = (q, \lambda)$ with the optional Lagrange multiplier $\lambda : \Omega \to \mathbb{R}^M$

$$\mathscr{L}(q_\lambda) = \mathscr{F}(q) + \int_\Omega C(q, \nabla q) \cdot \lambda \, \mathrm{d}\boldsymbol{X} \tag{33}$$

we consider the formal gradient flow evolution $\partial_t q = -\nabla_R \mathscr{F}(q)$, which we solve by a saddle-point problem generated by the minimization problem

$$\min_{v_\lambda = (v, \hat{\lambda})} \Big[R(q, v) + \langle \mathrm{D}\mathscr{L}(q_\lambda), v_\lambda\rangle\Big] \tag{34}$$

solved by incremental minimization, as described in more detail in Def. 1. In the following, we introduce different physically relevant examples that fit into this framework, present details of the coupling and the choice of $R(q, \dot{q})$ and provide a corresponding discussion.

The approach presented here has the general advantage of generating all coupling terms in the evolution equation automatically and, thus, ensuring thermodynamic consistency, i.e., decrease of the free energy (30) of (9),

by construction. The resulting systems of PDEs are highly nonlinear and usually require linearisation and Newtons method (29) for efficient solving. We employ the automatic-differentiation functionality provided by the FEniCS toolbox [51] and concentrate our considerations on properties specifically related to the energetic-variational formulation (34) of the complex nonlinearly-coupled problem.

For each example we provide the setup, the physical context and relevance, show explicit solutions, discuss accuracy and stability of the incremental minimization strategy. The examples differ in the coupling of order-parameter evolution by the coupling in the free energy $\mathscr{F}$, by the constraints C, and by the construction of the dissipation $R(q,\dot{q})$ that involves the bilinear form a, the operator M and S, see Sec. 2.

The sources and data for all the following examples can be viewed, run and downloaded at [75] (for the data a link to Zenodo is provided).

4.1 Multiplicative coupling with quasistatic elasticity

Physical background and setup of the problem The first example described nonlinear diffusion and phase separation in a solid, where the inelastic strain F_p in $F_\mathrm{e} = FF_\mathrm{p}^{-1}$ in the elastic energy density $W_\mathrm{elast}(F_\mathrm{e})$ of (30) couples to the phase-field $\psi : \Omega \to \mathbb{R}$ via $F_\mathrm{p} = (1+\alpha\psi)\mathbb{I}_d$ and generates and swelling and contraction for $\psi = \pm 1$ depending on the sign of α. For hydrogels such a coupling is one possibility to model the swelling when the dry gel absorbs a fluid and expands considerably [27]. Phase separation is described by a double-well energy $W_\mathrm{entropy}(\psi) = \frac{1}{4\varepsilon}(1-\psi^2)^2$ and $\sigma = \varepsilon F^{-1}F^{-T}$, such that the phase-field contribution to the energy can be written

$$W_\mathsf{phase}(\psi, \nabla\psi, F) = \left[\frac{\varepsilon}{2}|F^{-T}\nabla\psi|^2 + \frac{1}{4\varepsilon}(1-\psi^2)^2\right]\det(F). \tag{35}$$

For this example we use Cahn-Hilliard-type dissipation of (12) defined through the bilinear form (10) with $\ell = 1$, $m = 1$ and $n = 0$ and stationary elasticity, i.e., $R(q,v) = \frac{1}{2}a_\psi^*(M_\psi v, M_\psi v)$. Then, incorporating stationary elasticity is achieved by using the space $\mathcal{U}_\psi \equiv V_\psi$ and for any $\eta_\psi, w_\psi \in \mathcal{U}$ and $v = (v_u, v_\psi) \in \mathcal{V}$ by defining the bilinear form a_ψ and operator M_ψ

$$a_\psi(\eta_\psi, w_\psi) = (\nabla\eta_\psi, \nabla w_\psi)_{L^2(\Omega)} \equiv \int_\Omega \nabla\eta_\psi \cdot \nabla w_\psi \,\mathrm{d}\boldsymbol{X}, \tag{36a}$$

$$\langle M_\psi v, \eta_\psi\rangle_\mathcal{U} \equiv \langle M_\psi^*\eta_\psi, v\rangle_\mathcal{V} = (\eta_\psi, v_\psi)_{L^2(\Omega)}. \tag{36b}$$

While the stationarity of the elastic problem could also be set using a Lagrange multiplier, the approach by setting $\mathcal{U} \equiv \mathcal{U}_\psi = V_\psi$ appears more elegant, since the stationarity follows directly from the definition of the elastic energy. Hence, no further constraints C are required for this problem. On the boundary we employ natural boundary conditions for ψ and essential boundary conditions $\boldsymbol{u} = 0$ (no displacement).

Weak and strong form of gradient flow evolution As in (12), M_ψ and a_ψ define the dissipation $R_\psi(q,\dot{q})$ and therefore also the corresponding gradient flow evolution $q : [0,T] \to \mathcal{Q}$. The weak formulation of this gradient flow evolution is to find $\dot{q} \in \mathcal{V}$ and $\eta_{\boldsymbol{\psi}} \in \mathcal{U}_{\boldsymbol{\psi}}$ such that

$$\begin{aligned} a_{\boldsymbol{\psi}}(\eta_{\boldsymbol{\psi}}, w_{\boldsymbol{\psi}}) - \langle M_{\boldsymbol{\psi}}^* w_{\boldsymbol{\psi}}, \dot{q}\rangle_\mathcal{V} &= 0 \\ \langle M_{\boldsymbol{\psi}}^*\eta_{\boldsymbol{\psi}}, \boldsymbol{v}\rangle_\mathcal{V} &= -\langle \mathrm{D}\mathscr{F}(q), \boldsymbol{v}\rangle_\mathcal{V} \end{aligned}$$

for all $w_{\boldsymbol{\psi}} \in \mathcal{U}_{\boldsymbol{\psi}}$ and $\boldsymbol{v} \in \mathcal{V}$. Using the definition of $M_{\boldsymbol{\psi}}^*$, this can be expanded to

$$\begin{aligned} (\partial_t\psi, w_\psi)_{L^2} &= a_\psi(\eta_\psi, w_\psi), \\ (\eta_\psi, v_\psi)_{L^2} &= -\langle \mathrm{D}_\psi\mathscr{F}(q), v_\psi\rangle_{V_\psi}, \\ 0 &= -\langle \mathrm{D}_{\boldsymbol{u}}\mathscr{F}(q), v_{\boldsymbol{u}}\rangle_{V_{\boldsymbol{u}}}, \end{aligned} \tag{37}$$

where the last two equations can be equivalently written as the single equation $(\eta_{\boldsymbol{\psi}}, v_{\boldsymbol{\psi}})_{L^2} = \langle \mathrm{D}\mathscr{F}(q), \boldsymbol{v}\rangle_{\mathcal{V}}$. Assuming sufficient regularity, this weak formulation is equivalent to the strong form

$$\begin{aligned} \partial_t \psi - \nabla\cdot(\nabla\eta_\psi) &= 0, \\ \eta_\psi &= \frac{\delta W}{\delta \psi} \equiv \frac{\partial W}{\partial \psi} - \nabla\cdot\frac{\partial W}{\partial \nabla\psi}, \\ 0 &= \frac{\delta W}{\delta \boldsymbol{u}} \equiv \frac{\partial W}{\partial \boldsymbol{u}} - \nabla\cdot\frac{\partial W}{\partial \nabla\boldsymbol{u}}, \end{aligned} \tag{38}$$

with appropriate essential or natural boundary conditions $\bar{\boldsymbol{\nu}}\cdot m\nabla\eta_{\boldsymbol{\psi}} = 0$ and $\boldsymbol{u} = 0$. This evolution is useful if the existence of solutions for the elastic problem is guaranteed and viscoelastic effects can be neglected, e.g. cf. [11, 27, 85, 46, 59]. While terms in this formulation are rather abstract and do not necessarily promote physical interpretation but mathematical (variational) structure, we will later provide examples for this evolution where the concrete free energy, coupling mechanisms and physical interpretation will be discussed.

Remark 2 (Derivatives of the free energy $\mathscr{F}$) *In the weak formulation* (37) *or the corresponding strong form* (38) *we require the derivatives of the free energy $\mathscr{F}$. Let $J = \det(F)$ the Jacobian determinant, $\boldsymbol{w} \in V_{\boldsymbol{u}}$ and $\boldsymbol{\varphi} \in V_{\psi}$ arbitrary vectorial test functions. We consider again the general N-component phase-field $\boldsymbol{\psi} : \Omega \to \mathbb{R}^N$. Then the first variation of the free energy with respect to the displacement $\boldsymbol{u}$ is*

$$\langle \mathrm{D}_{\boldsymbol{u}}\mathscr{F}, \boldsymbol{w}\rangle = \int_\Omega \partial_{F_\mathrm{e}} W_\mathrm{elastic}(F_\mathrm{e}) : F_\mathrm{p}^{-1}\nabla\boldsymbol{w} + \partial_F\left[\left(\tfrac{1}{2}\nabla\boldsymbol{\psi}\cdot\sigma\nabla\boldsymbol{\psi} + W_\mathrm{entropy}(\boldsymbol{\psi}, F)\right)J\right]\{\boldsymbol{w}\}\,\mathrm{d}X. \tag{39}$$

with $\sigma = \sigma(F)$. Correspondingly, the first variation of $\mathscr{F}$ with respect to the order parameter $\boldsymbol{\psi}$ is

$$\langle \mathrm{D}_{\boldsymbol{\psi}}\mathscr{F}, \boldsymbol{\varphi}\rangle = \int_\Omega \left[\partial_{\boldsymbol{\psi}} W_\mathrm{elastic}(FF_\mathrm{p}^{-1}(\boldsymbol{\psi}))\boldsymbol{\varphi} + (\sigma\nabla\boldsymbol{\psi}\cdot\nabla\boldsymbol{\varphi} + W'_\mathrm{entropy}(\boldsymbol{\psi})\boldsymbol{\varphi})J\right]\mathrm{d}X \tag{40}$$

and is usually identified with the chemical potential $\boldsymbol{\eta}_{\boldsymbol{\psi}}$ via $\langle \mathrm{D}_{\boldsymbol{\psi}}\mathscr{F}, \boldsymbol{\varphi}\rangle = (\boldsymbol{\eta}_{\boldsymbol{\psi}}, \boldsymbol{\varphi})_{L^2(\Omega)}$. Note that the identification of driving forces in this manner requires integration by parts, which then imposes natural boundary conditions. Denote by $\Sigma_\mathrm{e} = \partial_{F_\mathrm{e}} W_\mathrm{elastic}$ the (elastic) first Piola Kirchhoff stress tensor. ⋆

Remark 3 (Transformation into the Eulerian frame) *Based on* (39) *and* (40) *we calculate the derivatives of the free energy $\mathscr{F}$ in the Eulerian frame. Quantities in the current configuration are labeled by $\tilde{\cdot}$, e.g. $\tilde{\Omega}$. To write down the weak form in the form of* (37) *one would redefine the bilinear form $a_{\boldsymbol{\psi}}$ as*

$$\tilde{a}_{\boldsymbol{\psi}}(\boldsymbol{\eta}_{\boldsymbol{\psi}}, \boldsymbol{w}_{\boldsymbol{\psi}}) = \int_\Omega \left(mF^{-T}\nabla\boldsymbol{\eta}_{\boldsymbol{\psi}}\cdot F^{-T}\nabla\boldsymbol{w}_{\boldsymbol{\psi}} + n\eta_{\boldsymbol{\psi}}w_{\boldsymbol{\psi}}\right)(\det F)\,\mathrm{d}\boldsymbol{X}$$

as in [55]. The (Lagrangian) deformation gradient is $F = \mathbb{I}_d + \nabla\boldsymbol{u} = F_\mathrm{e}F_\mathrm{p}(\psi)$ and $J = \det F$ with Lagrangian gradient ∇ as compared to the Eulerian one denoted by $\tilde{\nabla}$. For a scalar function $f : \Omega \to \mathbb{R}$ and $\tilde{f} : \tilde{\Omega} \to \mathbb{R}$ with $\tilde{f}(x) = f(\boldsymbol{\chi}^{-1}(x))$ it is $\nabla f = F^T\tilde{\nabla}\tilde{f}$, for a vector-field $\boldsymbol{f} : \Omega \to \mathbb{R}^d$ and $\tilde{\boldsymbol{f}} : \tilde{\Omega} \to \mathbb{R}^d$ with $\tilde{\boldsymbol{f}}(x) = \boldsymbol{f}(\boldsymbol{\chi}^{-1}(x))$ it is $\nabla\boldsymbol{f} = (\tilde{\nabla}\tilde{\boldsymbol{f}})F$, and $\int_{\tilde{\Omega}}\mathrm{d}x = \int_\Omega J\,\mathrm{d}X$, cf.[34]. We unravel (39) *and perform the passage to the Eulerian space. The first term on the left hand side in* (39) *emerges as*

$$\int_\Omega \Sigma_e F_\mathrm{p}^{-T} : \nabla\bar{\boldsymbol{w}}\,\mathrm{d}X = \int_\Omega \frac{1}{J}\Sigma F_\mathrm{p}^{-T}F^T : \nabla\bar{\boldsymbol{w}}F^{-1}J\,\mathrm{d}X = \int_{\tilde{\Omega}} \boldsymbol{\sigma}_e : \tilde{\nabla}\boldsymbol{w}\,\mathrm{d}x$$

with elastic Cauchy stress $\boldsymbol{\sigma}_e = \frac{1}{J}\Sigma_e F_\mathrm{e}^T$ in the current configuration, similar to [79]. Let $\nabla\boldsymbol{\psi}\cdot\sigma\nabla\boldsymbol{\psi} = \varepsilon|F^{-T}\nabla\boldsymbol{\psi}|^2$ such that the second term in (39) *becomes*

$$\int_\Omega \varepsilon F^{-T}\nabla\boldsymbol{\psi}\cdot(-F^{-T}\nabla\boldsymbol{w}F^{-T})\nabla\boldsymbol{\psi}J\,\mathrm{d}X = \int_{\tilde{\Omega}} \varepsilon\tilde{\nabla}\boldsymbol{\psi}\cdot(-\tilde{\nabla}\boldsymbol{w})\tilde{\nabla}\boldsymbol{\psi}\,\mathrm{d}x = \int_{\tilde{\Omega}} \varepsilon\nabla\boldsymbol{\psi}\otimes\tilde{\nabla}\boldsymbol{\psi} : (-\tilde{\nabla}\boldsymbol{w})\,\mathrm{d}x.$$

The last term in (39) *can be transformed as*

$$\int_\Omega \left(\frac{1}{2}|F^{-T}\nabla\boldsymbol{\psi}|^2 + W_\mathrm{entropy}(\boldsymbol{\psi})\right)JF^{-T}\cdot\nabla\boldsymbol{w}_i\,\mathrm{d}X = \int_{\tilde{\Omega}} \left(\frac{1}{2}|\tilde{\nabla}\boldsymbol{\psi}|^2 + W_\mathrm{entropy}(\boldsymbol{\psi})\right)\mathbb{I}_d\cdot\tilde{\nabla}\boldsymbol{w}_i\,\mathrm{d}x.$$

Summarizing, after a partial integration one obtains

$$-\nabla\cdot\Big(\boldsymbol{\sigma}_e+\frac{\varepsilon}{2}|\tilde{\nabla}\boldsymbol{\psi}|^2\mathbb{I}_d-\varepsilon\tilde{\nabla}\boldsymbol{\psi}\otimes\tilde{\nabla}\boldsymbol{\psi}+W_{\text{entropy}}(\boldsymbol{\psi})\mathbb{I}_d\Big)=0\quad \text{in }\tilde{\Omega}. \tag{41}$$

Moreover, the last term $-\nabla\cdot W_{\text{entropy}}(\boldsymbol{\psi})\mathbb{I}_d$ can be included to the Lagrange multiplier (pressure) in the incompressible case. Next we calculate the contributions from the $\boldsymbol{\psi}$ derivative of $\mathscr{F}$ starting from (40)*. Using the chain rule we obtain for the first term*

$$\int_\Omega \partial_{\bar{\psi}} W_{\text{elastic}}(FF_{\text{p}}(\boldsymbol{\psi})^{-1})\boldsymbol{\varphi}_i\,\mathrm{d}X=\int_\Omega \frac{1}{J}\boldsymbol{\Sigma}_e\cdot FF_{\text{p}}^{-1}(\bar{\boldsymbol{\psi}})\frac{-g'(\boldsymbol{\psi})}{g(\boldsymbol{\psi})}\bar{\boldsymbol{\varphi}}_i J\,\mathrm{d}X=\int_{\tilde{\Omega}}\boldsymbol{\sigma}_e\cdot\mathbb{I}_d\frac{-g'(\boldsymbol{\psi})}{g(\boldsymbol{\psi})}\boldsymbol{\varphi}_i\,\mathrm{d}x.$$

The second and third term can be transformed into the Eulerian configuration as

$$\int_\Omega J\sigma\nabla\boldsymbol{\psi}\cdot\nabla\boldsymbol{\varphi}_i+JW'_{\text{entropy}}(\boldsymbol{\psi})\boldsymbol{\varphi}_i\,\mathrm{d}X=\int_{\tilde{\Omega}}\varepsilon\tilde{\nabla}\boldsymbol{\varphi}_i\cdot\tilde{\nabla}\boldsymbol{\psi}+W'_{\text{entropy}}(\boldsymbol{\psi})\boldsymbol{\varphi}_i\,\mathrm{d}x.$$

After an integration by parts can identify the chemical potential η in the current configuration

$$-\tilde{\nabla}(\varepsilon\nabla\boldsymbol{\psi})+W'_{\text{entropy}}(\boldsymbol{\psi})-\operatorname{tr}(\boldsymbol{\sigma}_e)\frac{g'(\boldsymbol{\psi})}{g(\boldsymbol{\psi})}=\eta_{\boldsymbol{\psi}}.$$

The last term occurs due to the multiplicative coupling. The Cahn-Hilliard type evolution equation in $\boldsymbol{\psi}$ has the form

$$\partial_t\boldsymbol{\psi}=\tilde{\nabla}\cdot(m\tilde{\nabla}\boldsymbol{\eta}_{\boldsymbol{\psi}})$$

with mobility m. ⋆

Parameters, results and discussion For this introductory example we examine some general aspects of the gradient flow discretization. More details concerning the discretization using the *Unified Form Language* (UFL) and FEniCS can be found in the Appendix A. There it is shown, in particular, that the incremental scheme from Definition (1) can be written very naturally using the UFL and solved in a compact Python program conveniently using FEniCS. For this and all following examples we provide a well-documented FEniCS code example in an open GitHub repository, cf. [75], that can also be run directly using Goole Colab[5] from the GitHub page.

parameter	G	K	H	ε	α	Ω	$\psi(t=0)$
value	10	10	1	1/25	1/2	$[0,1]\times[0,1]$	$\frac{1}{2}\left(\sin(6x)\cos(5y)+\cos(3x)\sin(7y)\right)$

Table 1: Parameters for the introductory example.

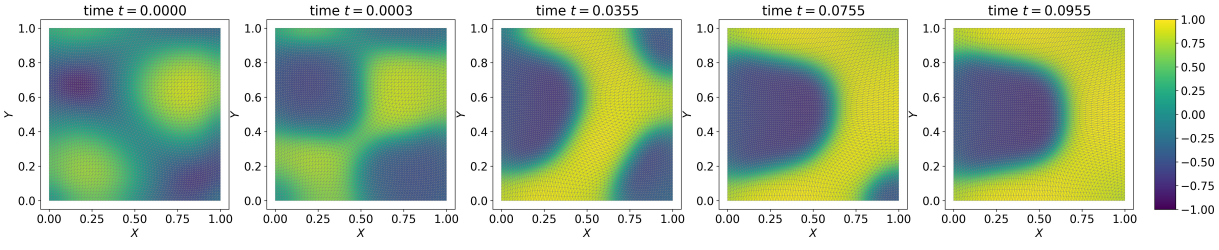

Figure 2: Evolution of phase-field ψ (shading) on mesh displaced with $\boldsymbol{u}$ (fine gray mesh) for increasing time t from left to right.

[5] see `https://colab.research.google.com`

The set of parameters for the introductory examples are given in Table 1. Figure 3 shows the energy descent of free energy as a function of time for the evoling phase-field and displacements shown in Figure 2. The free energy is composed of a decreasing contribution from the phase-field energy W_{phase} and a mostly increasing elastic energy W_{elast}.

After an initial step descent for $0 < t < 0.01$ for the phase-fields approaches the values $\phi = \pm 1$, the energy usually decents through topological transitions, i.e., when areas with $\psi = -1$ vanish (diffuse) between panel 3 & 4 and panel 4 & 5 of Figure 2. Note that the order-parameter in the Cahn-Hilliard evolution is conserved, i.e., $\frac{\mathrm{d}}{\mathrm{d}t} \int \psi(t) \mathrm{d}X = 0$. For $t = 0.09$ the domain consists of two connected areas with $\psi = +1$ and $\psi = -1$ and the energy $\mathscr{F}(q(t))$ has reached a flat plateau. From the deformation of the mesh in Figure 2 it is clearly visible that we have swelling where $\psi > 0$ and contraction where $\psi < 0$ for $\alpha = 1/2 > 0$. This effect will be more visible in the next examples, which have freely movable interfaces. As with all the following examples, the decrease of free energy is guaranteed, which makes this methods very stable, assuming that a solution of the nonlinear system can be found using Newton iterations. For finite strain elasticity this can be a restriction if forces acting on the hyperelastic material are too large or not very smooth, which is why for this example with quasistatic elasticity smooth initial $\psi(t = 0)$ were used. Alternatively, the Newton iteration can be stabilized using underrelaxation, e.g. cf. [26]. In order to deal with nonsmooth (or random) initial data, in the next example we regularize the evolution by adding Darcy-type dissipation for the elastic relaxation.

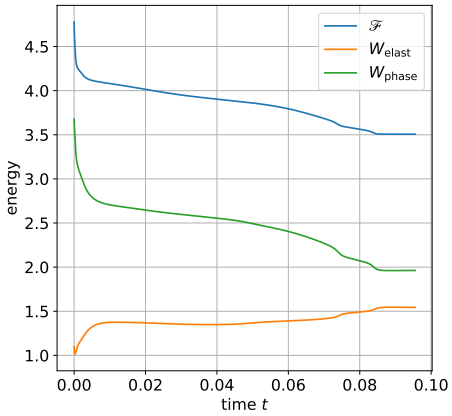

Figure 3: Energy descent of free energy as a function of time.

4.2 Phase separation and gels with Darcy-type dissipation (Example 2)

Physical background and setup of the problem One application of multiphase models undergoing large deformations are hydrogels. They are crosslinked networks of (hydrophilic) polymers swollen in water. During swelling and squeezing processes, hydrogels undergo enormously volume changes and phase transitions [10], which make finite strain approaches imperative for realistic applications. The total free energy to model this phenomena is a composition of an elastic part of the polymer network, a mixing term, of Flory-Huggins type, and an interfacial contribution [35, 27, 30, 46, 59, 22].

The phase-field parameter couples to the elastic problem via the compressibility condition, precisely, we impose $\det(F) = 1 + \alpha\psi$ such that the compressibility condition becomes $\frac{K}{2}(\det(F) - (1 + \alpha\psi))^2$. We consider again a Neo-Hookean elastic contribution as in (31) but without the multiplicative coupling, i.e. $F_{\text{p}} = \mathbb{I}_d$.

Depending on the evolution of the phase-fields, it might turn out that the general nonlinear elasticity prbolem $\langle \mathrm{D}_{\boldsymbol{u}} \mathscr{F}(q), v_{\boldsymbol{u}} \rangle_{V_{\boldsymbol{u}}} = 0$ might not have a sensible or a unique solution that can be found using standard methods, e.g., Newton-type fixed-point iterations. Then it makes sense to define a new dissipation $R_\psi(q, \dot{q}) + \frac{\nu}{2} \|\dot{\boldsymbol{u}}\|^2_{L^2}$ to provide coercivity to the dissipation. Equivalently we can choose a Darcy type dissipation (D) via $\boldsymbol{\eta} =$

$(\eta_{\boldsymbol{u}}, \eta_\psi) \in \mathcal{U}_\mathsf{D} = V_{\boldsymbol{u}} \times V_\psi$ and define $M^*_\mathsf{D} : \mathcal{U} \to \mathcal{V}^*$ as the sum

$$\langle M^*_\mathsf{D} \boldsymbol{\eta}, \boldsymbol{v}\rangle_\mathcal{V} = \langle M^*_\psi \eta_\psi, \boldsymbol{v}\rangle_\mathcal{V} + \langle M^*_{\boldsymbol{u}} \boldsymbol{\eta}_{\boldsymbol{u}}, \boldsymbol{v}\rangle_\mathcal{V} \quad \text{where} \quad \langle M^*_{\boldsymbol{u}} \boldsymbol{\eta}_{\boldsymbol{u}}, \boldsymbol{v}\rangle_\mathcal{V} = \int_\Omega \boldsymbol{\eta}_{\boldsymbol{u}} \cdot \boldsymbol{v}_{\boldsymbol{u}} \,\mathrm{d}\boldsymbol{X}. \tag{42}$$

for any $\boldsymbol{v} = (v_{\boldsymbol{u}}, v_\psi) \in \mathcal{V}$. The corresponding bilinear form $a_\mathsf{D} : \mathcal{U}_\mathsf{D} \times \mathcal{U}_\mathsf{D} \to \mathbb{R}$ is the sum

$$a_\mathsf{D}(\boldsymbol{\eta}, \boldsymbol{w}) = a_\psi(\eta_\psi, w_\psi) + a_{\boldsymbol{u}}(\eta_{\boldsymbol{u}}, w_{\boldsymbol{u}}) \quad \text{where} \quad a_{\boldsymbol{u}}(\boldsymbol{\eta}_{\boldsymbol{u}}, \boldsymbol{w}_{\boldsymbol{u}}) = \int_\Omega \sum_{i,j=1}^{d} \nu_{ij}^{-1} \boldsymbol{\eta}_{\boldsymbol{u}_i} \boldsymbol{w}_{\boldsymbol{u}_j} \,\mathrm{d}\boldsymbol{X} \tag{43}$$

where the matrix ν_{ij}^{-1} is an invertible symmetric positive matrix and potentially depends on the state q. The general weak formulation of this gradient flow evolution is to find $\dot{q} \in \mathcal{V}$ and $\boldsymbol{\eta} \in \mathcal{U}_\mathsf{D}$ such that

$$\begin{aligned} a_\mathsf{D}(\boldsymbol{\eta}, \boldsymbol{w}) - \langle M^*_\mathsf{D} \boldsymbol{w}, \dot{q}\rangle_\mathcal{V} &= 0 \\ \langle M^*_\mathsf{D} \boldsymbol{\eta}, \boldsymbol{v}\rangle_\mathcal{V} &= -\langle \mathrm{D}\mathscr{F}(q), \boldsymbol{v}\rangle_\mathcal{V} \end{aligned}$$

for all $\boldsymbol{w} \in \mathcal{U}_\mathsf{D}$ and all $\boldsymbol{v} \in \mathcal{V}$. Using again the definition of M^*_D and a_D, this can be rewritten into

$$\begin{aligned} a_{\boldsymbol{u}}(\boldsymbol{\eta}_{\boldsymbol{u}}, \boldsymbol{w}_{\boldsymbol{u}}) - (\partial_t \boldsymbol{u}, \boldsymbol{w}_{\boldsymbol{u}})_{L^2} &= 0, \\ a_\psi(\eta_\psi, w_\psi) - (\partial_t \psi, w_\psi)_{L^2} &= 0, \\ (\eta_{\boldsymbol{u}}, v_{\boldsymbol{u}})_{L^2} &= -\langle \mathrm{D}_{\boldsymbol{u}} \mathscr{F}(q), \boldsymbol{v}_{\boldsymbol{u}}\rangle_{V_{\boldsymbol{u}}}. \\ (\eta_\psi, v_\psi)_{L^2} &= -\langle \mathrm{D}_\psi \mathscr{F}(q), v_\psi\rangle_{V_\psi}, \end{aligned} \tag{44}$$

Using the invertibility of the matrix ν the first and the third equation of (45) can also be written simultaneously as

$$(\nu_{ij} \partial_t \boldsymbol{u}_i, v_{\boldsymbol{u}_j})_{L^2} = \langle \mathrm{D}_{\boldsymbol{u}} \mathscr{F}(q), v_{\boldsymbol{u}}\rangle_{V_{\boldsymbol{u}}}. \tag{45}$$

Note that it is straightforward to modify the bilinear form a_D to also include cross-coupling terms between order-parameter evolution and mechanics by coupling $\eta_{\boldsymbol{u}}$ and $\eta_{\boldsymbol{\psi}}$ in a symmetric-positive bilinear form. We already take into account cross-diffusion by allowing for non-diagonal diffusion matrix m_{ij}. For a discussion of cross-coupling effects, e.g. cf. [14]. Note that the corresponding dissipation related to displacements encoded in $a_{\boldsymbol{u}}$ is, with the exception of Darcy flow in a porous medium, purely artificial.

parameter	G	K	H	ε	Ω	$\psi(t=0)$	ν	μ	χ_{FH}	β	α
value	10	10	1+ψ	1/200	$B_{r=1}((0,0))$	$0.1 + 0.8\,\mathtt{rand}()$	1	1	3	20	1

Table 2: Parameters for the example phase separation and gels.

Parameters, results and discussion We use uniformly distributed random initial data in the interval $[0.1, 0.9]$ for the coefficients of $\boldsymbol{\psi}^h$. The Flory-Huggins entropy density is

$$W_{\mathrm{entropy}}(\psi) = \beta\big[\psi \ln(\psi) + \chi_{\mathrm{FH}} \psi(1-\psi) + (1-\psi)\ln(1-\psi)\big],$$

with χ_{FH} the Flory-Huggins parameter [35] which controls the (non-)convexity of the potential. When modeling gels this contribution has the role of a mixing energy between solvent and the polymer network. The phase-field energy reads

$$W_{\mathsf{phase}}(\psi, \nabla\psi, F) = \Big[\frac{\varepsilon}{2}|F^{-T}\nabla\psi|^2 + W_{\mathrm{entropy}}(\boldsymbol{\psi})\Big] \det(F). \tag{46}$$

We use a Cahn-Hilliard-type dissipation, precisely $m = 1$, $n = 0$, $\ell = 1$ in (12).

In this example we consider a free body, i.e., a problem without Dirichlet boundary conditions for the displacement $\boldsymbol{u}$. In the quasistatic case this means that rotations and translations of deformations $\boldsymbol{u}$ are also solutions such that the uniqueness of minimizers $\boldsymbol{u}$ is not guaranteed without further conditions in this case. To fix this one introduces, for $d = 2$, three conditions (two translation, one rotation) to ensure the uniqueness of solutions. Hence, the residual in (28) is extended by the component $\mathcal{R}^{(\lambda)}$. Precisely, we define $C(q, \nabla q) \in \mathbb{R}^3$ with coordinate vector $\boldsymbol{X} = (X, Y)$ through

$$C(q, \nabla q) = \begin{pmatrix} \int u_x \,\mathrm{d}\boldsymbol{X} \\ \int u_y \,\mathrm{d}\boldsymbol{X} \\ \int (-Yu_x + Xu_y) \,\mathrm{d}\boldsymbol{X} \end{pmatrix} \text{ with } \boldsymbol{u} = (u_x, u_y). \tag{47}$$

Nevertheless, in the current case with Darcy-dissipation in the solid these conditions are not necessary. The sum of $\mathscr{L}(q_\lambda) = \mathscr{F}(q) + \mathcal{C}(q, \lambda)$ with the constraint $\mathcal{C}(q, \lambda) = C \cdot \lambda$ with the Lagrange multiplier $\boldsymbol{\lambda} \in \mathbb{R}^3$ defines the Lagrangian (33) with $q_\lambda = (q, \boldsymbol{\lambda})$. We provide some further examples for relevant constraints in Remark 4.

The parameters for the second example are given in (2). Figure 5 shows the energy decrease of the free energy over time. The phase-field density becomes negative due to the $\log$ term in the Flory-Huggins potential for small values of ψ. The energy reaches a constant value $t = 0.08$ and the step decent after the disappearance of a isolated domain is clearly visible in W_{phase} looking at the evolution of the phase-field in Figure 4. One can also see the deformation of the mesh, in particular of the free boundary, subject to the evolution of the phase-field.

The initial data for this example is equilibrated, i.e. the two phases are evenly present and conserved due to the Cahn-Hilliard evolution. In the case of a Allen-Cahn type dissipation, i.e. with $m = 0$ and $n = 1$ in (10) the system seeks for an equilibrium state with one remaining phase. The current system can be extended by an influx to model the swelling process of a dry gel immersed in water leading to the discussion of pattern formation [10, 83].

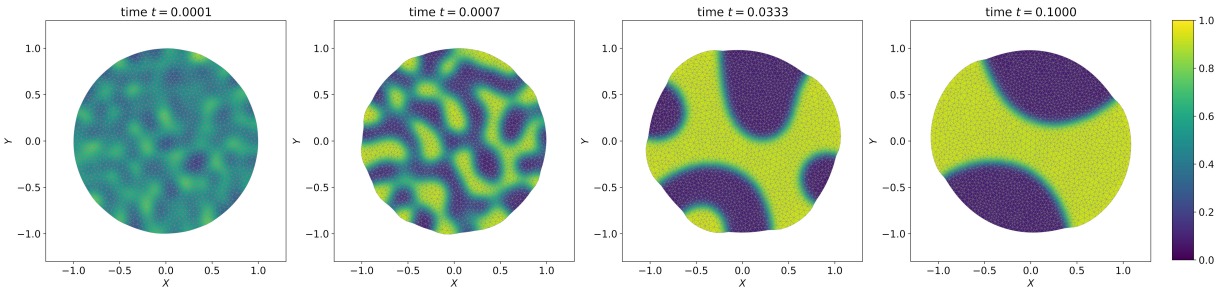

Figure 4: Evolution of the phase-field ψ on a freely moving mesh (no Dirichlet BC for $\boldsymbol{u}$) displaced with $\boldsymbol{u}$ (fine gray mesh) for increasing time t from left to right.

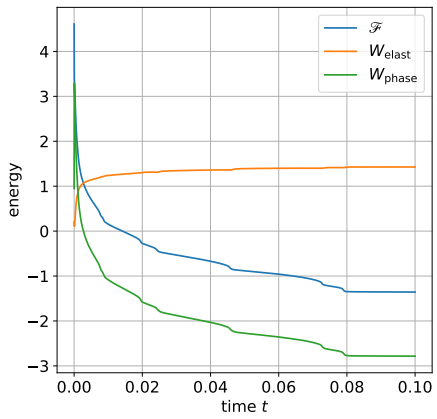

Figure 5: Energy descent of free energy as a function of time with the elastic and the phase-field contribution separately.

Remark 4 (Enforcing constraints) *The possibility to enforce constraints such as* (47) *naturally in the gradient flow evolution by penalization or by Lagrange multipliers as in* (34) *presents a powerful tool for mechanical problems. Typical relevant cases are elimination of symmetries as in* (47)*, nonlocal conservation of mass*

$$\int_\Omega \lambda \cdot (\psi - \psi_0)\,\mathrm{d}\boldsymbol{X}, \tag{48a}$$

for nonconserved dynamics. Essential boundary conditions $\boldsymbol{u} = \boldsymbol{g}$ *on* $\Gamma_{\mathrm{D}} \subset \partial\Omega$ *can be enforced by*

$$\int_{\Gamma_{\mathrm{D}}} \lambda \cdot (\boldsymbol{u} - \boldsymbol{g})\,\mathrm{d}\boldsymbol{S}, \tag{48b}$$

and easily differentiated. One of the most-studied constraints for mechanical systems is incompressibility

$$\int_\Omega \lambda(\det(F) - 1)\,\mathrm{d}\boldsymbol{X}, \tag{48c}$$

which translates into the condition of vanishing divergence of the Eulerian velocity. Then, LBB conditions are satisfied for inf-sup stable velocity and multiplier, e.g., Taylor-Hood elements $\boldsymbol{P}_2$-P_1*. Assuming the polymer network in a gel to be incompressible requires a slightly more general condition of the form* $J = 1 + \alpha\psi$ *via* C*, cf.[46]. This would be imposed using*

$$\int_\Omega \lambda(\det(F) - H(\boldsymbol{\psi}))\,\mathrm{d}\boldsymbol{X}, \tag{48d}$$

for the function $H = 1 + \alpha\psi$*.* ⋆

4.3 Multiphase systems with dynamic elasticity (Example 3)

In the following example we consider a three phase system introducing a second phase-field and implicitly such that $\boldsymbol{\psi} = (\psi_1, \psi_2) : \Omega \to \mathbb{R}^2$ with $\psi_3 = 1 - \psi_1 - \psi_2$. In concrete we model a liquid (2) droplet placed on an elastic substrate (1), modeled with the Neo-Hookean type elastic energy (31) with $F_{\mathrm{p}} = \mathbb{I}_d$ and $G = G(\boldsymbol{\psi})$, and surrounded by an air (3) phase, cf. [89, 65, 16]. Consider the reference configuration $\Omega = \Omega_{\text{solid}} \cup \Omega_{\text{liquid}} \cup \Omega_{\text{air}}$ with three domains. The order parameters $\psi_i : \Omega \to \mathbb{R}$ indicate the phase via

$$\begin{cases} \psi_1(x) & = 1 \text{ in } \Omega_{\text{solid}} \text{ and } \psi_1(x) = -1 \text{ otherwise} \\ \psi_2(x) & = 1 \text{ in } \Omega_{\text{liquid}} \text{ and } \psi_2(x) = -1 \text{ otherwise.} \end{cases}$$

such that $\psi_3(x) = 1$ in Ω_{air} and $\psi_3(x) = -1$ otherwise. The elastic problem couples to the phase indicators via the shear modulus $G(\boldsymbol{\psi})$ with $G_1 \gg G_2 = G_3$, $G_i = G(\psi_i)$ based on the physical assumption of elasticity in the solid opposed to *nearly* no elasticity in the liquid and air phases. This is realized through a function $G(\boldsymbol{\psi}) \equiv \texttt{GshearF}(\psi_1, \psi_2)$ with

$$\texttt{GshearF}(\psi_1, \psi_2) = G_1 \left(\frac{1+\psi_1}{2}\right) + G_2 \left(\frac{1+\psi_2}{2}\right) + G_3 \left(\frac{1+\psi_3}{2}\right).$$

All phases are assumed to be compressible. This condition is expressed through the constraint $C(q, \nabla q) = (J-1)$ and the Lagrange multiplier $\lambda \in L^2(\Omega)$. We consider a double-well potential (35) in $\boldsymbol{\psi}$ such that

$$W_{\text{phase}}(\boldsymbol{\psi}, \nabla\boldsymbol{\psi}, F) = \sum_{i=1}^{3} \sigma_i \left[\frac{\varepsilon}{2}|F^{-T}\nabla\psi_i|^2 + \frac{1}{4\varepsilon}(1-\psi_i^2)^2\right] \det(F) \tag{49}$$

for the small parameter $\varepsilon > 0$ measuring the interface size and surface tensions σ_i. Precisely, to bring it into a physical context, $\sigma_1 + \sigma_2$ equals the surface tension between the solid and the liquid phase, $\sigma_1 + \sigma_3$ is the surface tension at the solid-air interface and $\sigma_2 + \sigma_3$ at the liquid-air interface. For the phase-fields we consider again a Cahn-Hilliard dissipation as in the previous example.

In situations where viscous (Newtonian) dissipation as in the Stokes equation or a drag-term as in the Darcy equation should be included, we need to find a weak formulation for $R = R_{\boldsymbol{\psi}} + R_{\text{Stokes}}$ using (19). For the reformulation of the Darcy flow in (45) we use $M^*_{\boldsymbol{\psi}}, \mathcal{W}_{\boldsymbol{\psi}}$ as before and find the general weak formulation

$$\begin{aligned} &a_{\boldsymbol{\psi}}(\eta_{\boldsymbol{\psi}}, w_{\boldsymbol{\psi}}) - \langle M^*_{\boldsymbol{\psi}} w_{\boldsymbol{\psi}}, \partial_t q\rangle_{\mathcal{V}} = 0 \\ &\langle M^*_{\boldsymbol{\psi}} \eta_{\boldsymbol{\psi}}, \boldsymbol{v}\rangle_{\mathcal{V}} + k_{\text{Stokes}}(\partial_t q, \boldsymbol{v}) = -\langle \mathrm{D}\mathscr{F}(q), \boldsymbol{v}\rangle_{\mathcal{V}} \end{aligned} \tag{50}$$

for some $z, v \in \mathcal{V}$. As before, using the specific definition of the bilinear forms and $M^*_{\boldsymbol{\psi}}$ this can be rewritten in more detail. Note that for $\mu_{ij} = 0$, the weak formulation of (50) agrees with the one in (44), which can be readily seen using (45). Also, the weak formulation is a saddle-point problem similar to the one in (16), if we replaced εS by the corresponding Stokes operator.

Parameters, results and discussion We consider a domain with three subdomains as mentioned above. Therefore we introduce the height of the substrate h_0, the radius of the liquid droplet h_1 and the size of the domain. Note that we present a non dimensional version of the problem here, i.e. without physical units. One can re-dimensionalise the problem such that the length scales are given in meters m and G, σ in their corresponding SI units. The values used are motivated by a comparison with simulations and experimental results in a paper by [89].

parameter	G_1	$G_{2,3}$	σ_1	σ_2	σ_3	ε	Ω	h_0	h_1	ν	μ
value	1	0.3	0.21	0.51	0.41	0.02	$[0,10]\times[0,10]$	1.0	3.53	0.5	0.01

Table 3: Parameters for multiphase system example.

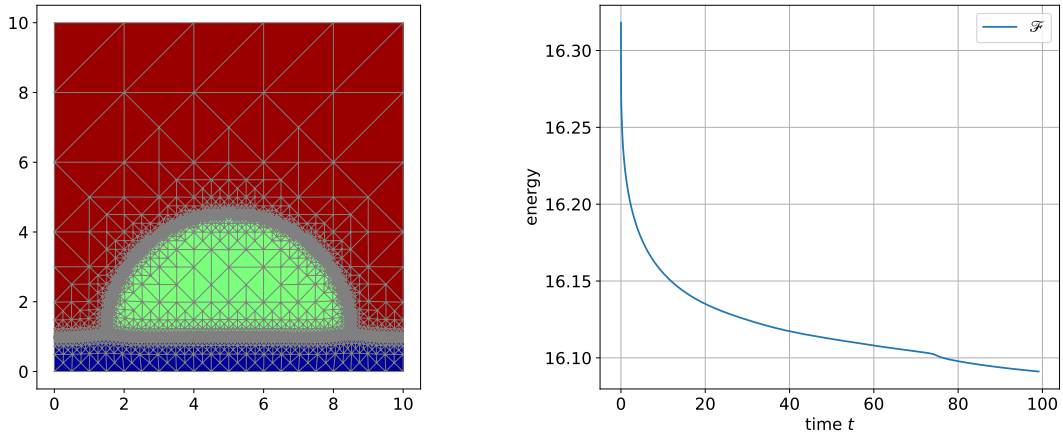

Figure 6: (**Left**) Evolution of the phase-fields ψ_i with air phase (red) fluid phase (green) and solid phase (blue) on the current configuration at larger times. The locally refined mesh is displaced with $\boldsymbol{u}$ (fine gray mesh). (**Right**) Descent of the free energy over time.

We use the initial data $\boldsymbol{\psi}(t=0) = (\psi_1(0), \psi_2(0))$ for

$$\psi_1(0) = \tanh\left(i_f(h_0 - Y)\right),$$
$$\psi_2(0) = -1 + \tfrac{1}{2}\left(1 + \tanh\left[i_f(\tfrac{Y}{h_0} - h_0)\right]\right)\left(1 + \tanh\left[i_f\,(h_1 - r)\right]\right),$$
$$\text{where} \quad r = \sqrt{\left(\tfrac{X}{h_0} - \tfrac{H_1}{2}\right)^2 + \left(\tfrac{Y}{h_0} - h_0\right)^2},$$

and with an interfacial scaling factor $i_f = \frac{1}{\sqrt{2}\varepsilon}$ consistent with a Cahn-Hilliard solution, cf. [2].

For the evolution of the three phase system we use the adaptive mesh refinement method `meshspace` to provide a high resolution at the interfaces. Thanks to this function we can start with a coarse mesh and refine it only were it is needed such that the computational coast stays manageable. This is shown for in the left panel of Figure 6. One main focus lies in the observation of the three phase contact line, i.e. were the three phases meet, shown in Figure 7. We also see the energy decrease over time in the right panel of Figure 6.

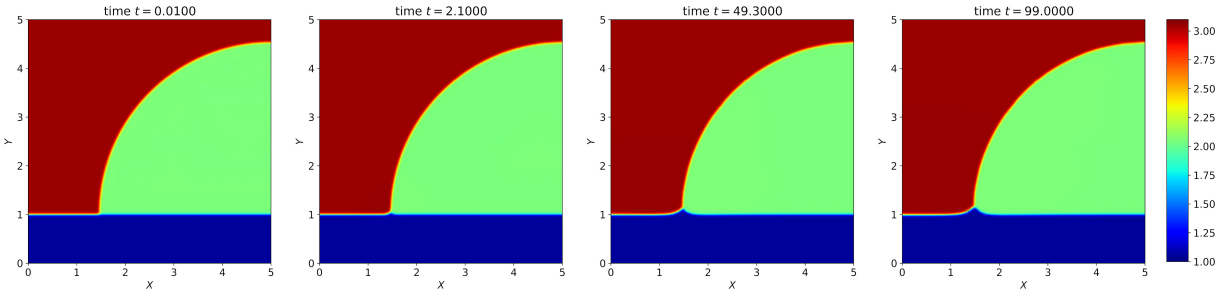

Figure 7: Evolution of the phase-fields ψ_i on a moving mesh.

5 Summary and conclusion

In this paper we presented a general approach to gradient dynamics based on the coupling of scalar or multicomponent order-parameters $\boldsymbol{\psi}$ with displacements $\boldsymbol{u}$. We provided a general introduction to gradient flows and a

specific formulation, which is well-suited for direct numerical implementation using variational FE-based space-discretization and incremental minimization as the time-discretization. We discussed different variants, which give Cahn-Hilliard or Allen-Cahn equations for the phase-field dissipation and Darcy or Stokes dissipation for the solid dissipation. We also showed how quasistatic elasticity can be easily included in the formal description. Then we discussed several variants of this coupling, which can take into account diffusion, phase-separation and phase-transitions, swelling, porous medium flow, viscoelasticity and capillarity phenomena.

All these effects are relevant for the description of hydrogels with free capillary interfaces. Due to the different coupling mechanisms and the difficulty of having free boundaries, discretization of the highly nonlinear PDEs for gel dynamics with *finite strain* can be challenging. We presented a Lagrangian phase-field approach for this coupled evolution which we believe can simplify modeling and simulation of such systems by ensuring the thermodynamic consistency by construction. In this respect, FEniCS is a useful platform since the automated differentiation of functionals and residua simplifies the setup of the variational formulation drastically.

A Appendix: UFL implementation of incremental minimization

For the introductory example in Sec. 4.1 we examine some particular aspects of the FEniCS open-source computing platform [51] with respect to our implementation of the formal gradient structure and how it is discretized in saddle-point form. FEniCS uses the *Unified Form Language* (UFL) to declare finite element discretizations of variational forms (see `http://www.fenicsproject.org`).

A.1 Tensor spaces for saddle-point problem

One essential ingredient to this problem is the structure of spaces used in the saddle point problem, i.e., $\mathcal{V} = V_u \times V_\psi$ and the space $\mathcal{U} \equiv V_\psi$ for this example. The corresponding tensor space $\texttt{VxU} = \mathcal{V} \times \mathcal{U}$ for the full problem is attached to a rectangular mesh in the Python UFL syntax below:

```
# mesh parameters of tensorial Nx x Nx x 2 triangular elements mesh
Nx    = 64
mesh  = RectangleMesh(Point(0,0),Point(1,1),Nx,Nx)
# define the function spaces
Vu    = VectorElement("P", mesh.ufl_cell(), 1) # V_u   = displacements
Vpsi  = FiniteElement("P", mesh.ufl_cell(), 1) # V_psi = order-parameter(s)
U     = FiniteElement("P", mesh.ufl_cell(), 1) # U     = forces
VxU   = FunctionSpace(mesh, MixedElement([Vu,Vpsi,U])) # tensor space of V x U
# homogeneous Dirichlet boundary conditions
bc    = DirichletBC(VxU.sub(0), Constant((0, 0)), 'on_boundary')
```

A.2 Incremental minimization

At the core of the gradient flow discretization, the incremental scheme solves for given $q^{k-1} = \texttt{old\_q}$ and given $\tau = \texttt{tau}$ the minimization problem from Definition 1. The implementation below shows that the UFL-syntax for the definition of the energy is very natural, such that the minimization problem $\mathrm{D}_q \mathscr{R}(q^{k-1}, v) = 0$ for $v = \frac{1}{\tau}(q - q^{k-1})$ reads:

```
# incremental minimization for coupled finite strain elasticity + phase field
def incremental_minimization(old_q, tau):

    q  = Function(VxU)
    dq = TestFunction(VxU)

    # current solution
    u, psi, eta_psi = split(q)
    # old solution
    old_u,old_psi,old_eta_psi = split(old_q)
    # test functions
```

```
    du,dpsi,deta_psi  = TestFunctions(VxU)

    # define continuum mechanics / plasticity variables
    d       = psi.geometric_dimension()
    I       = Identity(d)
    F       = I + grad(u)        # deformation gradient
    iFp     = 1/(1+alpha*psi)    # inverse of plastic strain
    Fe      = F*iFp              # strain = elastic strain * plastic strain
    Je      = det(Fe)            # Jacobian elastic strain
    J       = det(F)             # Jacobian strain
    gradpsi = inv(F).T*grad(psi)

    # define free energy F_free
    W_elastic = (G/2)*(tr(Fe.T*Fe - I) - 2*ln(Je)) + (K/2)*(Je-1)**2
    W_phase   = ((eps/2)*inner(gradpsi,gradpsi) + 1/(4*eps)*((1-psi**2)**2))*J
    F_free    = (W_elastic + W_phase)*dx

    # backward Euler time derivative
    dot_psi = (psi-old_psi)/tau

    # add energy and M_psi operator
    Res  = derivative(F_free, q, dq) - inner(eta_psi,dpsi)*dx

    # add bilinear form a_psi and M_psi*
    Res += inner(dot_psi, deta_psi)*dx + inner(mu*grad(eta_psi), grad(deta_psi))*dx

    # solve nonlinear problem using old solution as initial guess
    q.assign(old_q)

    solve(Res == 0, q, bc)
    return q
```

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