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THERMODYNAMICALLY CONSISTENT HIGHER ORDER PHASE FIELD NAVIER-STOKES MODELS WITH APPLICATIONS TO BIOLOGICAL MEMBRANES

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Abstract. In this paper we derive thermodynamically consistent higher order phase field models for the dynamics of vesicle membranes in incompressible viscous fluids. We start with basic conservation laws and an appropriate version of the second law of thermodynamics and obtain generalizations of models introduced by Du, Li and Liu [5] and Jamet and Misbah [13]. In particular we derive a stress tensor involving higher order derivatives of the phase field and generalize the classical Korteweg capillarity tensor.

1. **Introduction.** The study of the dynamics of vesicle membranes in fluids is of general interest in many biological applications. The equilibrium shapes of the vesicle membranes are characterized with the help of the bending elastic energy of the membrane [11, 19], see also the references in [5]:

$$\mathcal{E}_{\text{ben}} = \int_\Gamma \left(a_1 + a_2(\mathcal{H} - c_0)^2 + a_3\mathcal{G}\right) dS, \tag{1}$$

where $\mathcal{H}$ is the mean curvature of the membrane surface Γ, c_0 is the spontaneous curvature, $\mathcal{G}$ is the Gaussian curvature, a_1 is the surface tension, a_2 is the bending rigidity and a_3 is the Gaussian rigidity. For vesicle membranes one has to take volume and area constraints into account, i.e. globally stationary states are minimizers of $\mathcal{E}_{\text{ben}}$ subject to the constraints

$$\text{Vol}(\Gamma) = \alpha, \quad \int_\Gamma 1\, dS = \hat{\beta},$$

where $\text{Vol}(\Gamma)$ denotes the volume enclosed by Γ. In recent years the phase field framework has been used successfully in many applications, see overview and references in [4]. For biological membranes, this approach has been introduced by Du et al. [5], Jamet and Misbah [12, 13] and Lowengrub, Rätz and Voigt [16]. For further information on the mathematics of biological membranes we refer to [7] and

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the references therein. In particular we refer to Arroyo and DeSimone [1] for a new modeling approach for the dynamics of liquid membranes within the context of sharp interface models.

In this paper, we consider a higher order phase field Navier-Stokes model for the vesicle shape dynamics, which is governed by the coupling of the hydrodynamic fluid flow and the bending elastic properties of the vesicle membrane. In recent works of Du et al., see [5, 6], phase field models have been developed on a general energetic framework using the above bending elastic energy. In particular, for the simplified energy

$$\mathcal{E}(\Gamma) = \int_\Gamma (\mathcal{H} - c_0)^2 dS, \tag{2}$$

its corresponding form in the phase field model is given by

$$\mathcal{E}^\epsilon(\phi) = \int_\Omega \frac{k}{2\epsilon} \left(\epsilon \Delta \phi + (\frac{1}{\epsilon}\phi + c_0\sqrt{2})(1-\phi^2) \right)^2 dx, \tag{3}$$

where k is a multiple of the bending rigidity a_2. Here $\epsilon > 0$ is a small interfacial parameter, $\Omega \subset \mathbb{R}^3$ is an open and bounded domain and as this is needed later we assume throughout the paper that Ω has a C^2-boundary. The phase field ϕ is defined on the physical domain Ω and is used to label the inside and the outside of the vesicle Γ. The level set $\{x : \phi(x) = 0\}$ approximates the membrane, while $\{x : \phi(x) > 0\}$ approximates the interior of the membrane and $\{x : \phi(x) < 0\}$ the exterior. The thickness of the regularized diffuse interface is proportional to ϵ. In a phase field model the surface area and volume constraints can be approximated by

$$A(\phi) = \int_\Omega \phi \, dx = \alpha, \quad B(\phi) = \int_\Omega \left(\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2 \right) dx = \beta,$$

where β is a multiple of $\hat{\beta}$. The expression $B(\phi)$ models the total surface energy and in fact it can be shown that $B(\phi)$ converges to a term proportional to $\int_\Gamma 1 \, dS$, see [17]. The phase field framework can be extended to include additional contributions to the energy modelling e.g. the Gaussian curvature energy. An ansatz of Du et al. [5, 6] is given by

$$\mathcal{G}_{\text{pha}}(\phi) = \frac{1}{|\nabla\phi|} \Lambda \left(D^2\phi - \frac{\nabla\phi \cdot D^2\phi \cdot \nabla\phi}{|\nabla\phi|^4} \nabla\phi \otimes \nabla\phi \right), \tag{4}$$

where $\Lambda(M)$, for a 3×3 matrix M, denotes the sum of the determinants of its three principal minors. The vesicle deformation and the fluid velocity field are then regarded as the result of the competition between vesicle membrane bending energy and fluid kinetic energy, subject to the constraints that the volume and surface area of the vesicle are preserved. To enforce the two constraints one can use a penalty formulation as in [5]. For convenience, let us denote for $c, c_0 \in \mathbb{R}$ the operators

$$f_c(\phi) = -\epsilon\Delta\phi + (\frac{1}{\epsilon}\phi + c\sqrt{2})(\phi^2 - 1), \quad g(\phi) = -\Delta f_{c_0}(\phi) + \frac{1}{\epsilon^2}(3\phi^2 - 1) f_{c_0}(\phi).$$

Then the corresponding modified bending energy $E(\phi)$ is given by

$$E(\phi) = \frac{k}{2\epsilon} \int_\Omega |f_{c_0}(\phi)|^2 dx + \frac{1}{2} M_1 (A(\phi) - \alpha)^2 + \frac{1}{2} M_2 (B(\phi) - \beta)^2. \tag{5}$$

For the variational derivative we obtain

$$\frac{\delta E}{\delta \phi} = k g(\phi) + M_1(A(\phi) - \alpha) + M_2(B(\phi) - \beta) f_0(\phi).$$

Du et al. [6] define an action functional and by the least action principle they obtain the following coupled phase field Euler system for functions $\mathbf{v}$ and ϕ defined on a time-space cylinder $[0,T]\times\Omega$:

$$\begin{cases} \mathbf{v}_t + \mathbf{v}\cdot\nabla\mathbf{v} = -\nabla p + \frac{\delta E}{\delta\phi}\nabla\phi & \text{in} \quad [0,T]\times\Omega, \\ \nabla\cdot\mathbf{v} = 0 & \text{in} \quad [0,T]\times\Omega, \\ \phi_t + \mathbf{v}\cdot\nabla\phi = 0 & \text{in} \quad [0,T]\times\Omega, \\ \mathbf{v}(0,x) = \mathbf{v}_0(x) & \text{in} \quad \Omega, \\ \phi(0,x) = \phi_0(x) & \text{in} \quad \Omega. \end{cases} \tag{6}$$

We remark that here and in what follows we rescale such that the constant mass density fulfils $\rho\equiv 1$. The authors in [6] also postulate a phase field Navier-Stokes system by carefully adding regularization terms $\mu\Delta\mathbf{v}$ and $-\gamma\frac{\delta E}{\delta\phi}$ to (6) which guarantee that the new system satisfies a global dissipation inequality:

$$\begin{cases} \mathbf{v}_t + \mathbf{v}\cdot\nabla\mathbf{v} = -\nabla p + \mu\Delta\mathbf{v} + \frac{\delta E}{\delta\phi}\nabla\phi & \text{in} \quad [0,T]\times\Omega, \\ \nabla\cdot\mathbf{v} = 0 & \text{in} \quad [0,T]\times\Omega, \\ \phi_t + \mathbf{v}\cdot\nabla\phi = -\gamma\frac{\delta E}{\delta\phi} & \text{in} \quad [0,T]\times\Omega, \\ \mathbf{v}(0,x) = \mathbf{v}_0(x) & \text{in} \quad \Omega, \\ \phi(0,x) = \phi_0(x) & \text{in} \quad \Omega. \end{cases} \tag{7}$$

The above system is complemented by boundary conditions for the phase field ϕ

$$\phi = -1,\ \Delta\phi = 0 \qquad \text{on} \quad \partial\Omega \tag{8}$$

and a no-slip condition for the velocity field $\mathbf{v}$

$$\mathbf{v} = 0 \qquad \text{on} \quad \partial\Omega. \tag{9}$$

The main objective of this paper is to provide a thermodynamically consistent higher order phase field Navier-Stokes model, which in particular gives a derivation of a modified stress tensor in the Navier-Stokes equation. Knowing the stress tensor then makes it possible to formulate classical dissipation inequalities as well as slip boundary conditions which both involve the stress tensor. Furthermore, we also discuss how the phase field description of the Gaussian bending energy enters the model. The derivation of our model is as follows: In Section 2 we formulate the basic balance laws for mass

$$\nabla\cdot\mathbf{v} = 0$$

and momentum

$$\frac{d}{dt}\int_\Omega \mathbf{v}dx = \int_{\partial\Omega}\mathbb{T}\mathbf{n}dS,$$

where $\mathbb{T}$ denotes the stress tensor and $\mathbf{n}$ is the outer unit normal to $\partial\Omega$. In an isothermal situation a *dissipation inequality*

$$\frac{d}{dt}\left\{\int_\Omega\left(\frac{|\mathbf{v}|^2}{2} + G^0(Y)\right)dx + \sum_{k=1}^{s}\frac{M_k}{2}\left(\int_\Omega G^k(Y)\,dx\right)^2\right\} + \int_{\partial\Omega}\mathbf{n}\cdot\mathbf{J}_D\,dS \le 0,$$

where $\mathbf{J}_D$ is the energy flux, is the appropriate version of the second law of thermodynamics. The second term in the dissipation inequality is motivated by the penalization terms in (5) involving volume and area constraints. Without these penalization terms we would obtain the following local form of the dissipation inequality

$$D_t\left(\frac{|\mathbf{v}|^2}{2}+G^0(Y)\right)-\nabla\cdot\left(\mathbb{T}^\top\mathbf{v}+\left[G'^0_{\nabla\phi}-\nabla\cdot G'^0_{D^2\phi}\right]D_t\phi+G'^0_{D^2\phi}D_t\nabla\phi\right)\leq 0,$$

where $D_t:=\partial_t+\mathbf{v}\cdot\nabla$ denotes the material derivative. Exploiting the dissipation inequality we derive restrictions on the constitutive relations and we obtain fourth order phase field models

$$\gamma D_t\phi=-\left(G'^I_{\phi}-\nabla\cdot\left[G'^I_{\nabla\phi}-\nabla\cdot G'^I_{D^2\phi}\right]\right), \tag{10}$$

which generalize the model in [5] and provide an explicit representation formula for the stress tensor $\mathbb{T}$. The resulting constitutive equation yields the macroscopic stress $\mathbb{T}$ as a classical Newtonian stress $\mathbb{S}-p\mathbb{I}$ minus an additional possibly nonsymmetric term

$$\mathbb{U}^I=\nabla\phi\otimes[G'^I_{\nabla\phi}-\nabla\cdot G'^I_{D^2\phi}]+D^2\phi\, G'^I_{D^2\phi}, \tag{11}$$

representing stresses stemming from the bending energy and non-local contributions resulting from the penalty terms in (5). We observe that the constitutive law consists of a dissipative part $\mathbb{S}$ (for a Newtonian fluid) and a nondissipative elastic part $\mathbb{U}^I$ (arising from the elastic membrane forces).

Furthermore we also discuss several boundary conditions leading to a global energy decay. Here in particular generalized boundary conditions for fourth order operators and new slip conditions involving higher order derivatives of the phase field variable will be stated.

In the local case, i.e. without penalization terms, a similar expression for $\mathbb{U}^I$ has already been derived by Jamet and Misbah in a thermodynamically consistent manner, see [13]. In [13] the starting point is a bending energy (Helfrich energy), which is written in the phase-field approach in terms of a density

$$E_{\text{Mis}}(\nabla\phi,\nabla\nabla\phi)=E\left[|\nabla\phi|,\mathcal{C}(\nabla\phi,\nabla\nabla\phi)\right]=\frac{\alpha}{2}\left[\mathcal{C}(\nabla\phi,\nabla\nabla\phi)-\mathcal{C}_0\right]|\nabla\phi|, \tag{12}$$

where α is the rigidity of the membrane, $\mathcal{C}$ is the mean curvature of the membrane, and $\mathcal{C}_0$ represents the spontaneous curvature and is considered to be a constant. In (12) the term $|\nabla\phi|$ is a smeared Dirac function and allows one to pass from an energy per unit area (as is treated in the sharp interface limit) to an energy per unit volume (as is treated in phase field approximation). This model differs from a classical phase field model where the energy depends on ϕ and $\nabla\phi$ only. In [13] the three expressions in (12) correspond to the three hierarchies of models. The upper hierarchy, i.e. the expression on the left-hand side, refered as model 1, allows for any general expression that depends on the two arguments. The other hierarchies are called model 2 and model 3. The general derivation procedure is done for model 1 and does not induce any complication in the derivation. For the general model the material derivative of (12) reads

$$D_tE_{\text{Mis}}=\Phi\cdot D_t\nabla\phi+\mathcal{T}:D_t\nabla\nabla\phi, \tag{13}$$

where the vector Φ and the tensor $\mathcal{T}$ are defined by

$$\Phi=\frac{\partial E}{\partial\nabla\phi},\quad \mathcal{T}=\frac{\partial E}{\partial\nabla\nabla\phi}. \tag{14}$$

To determine the form of the evolution equations Jamet and Misbah, see [13], use besides the mass and the momentum balance law a local version of a balance law for the energy containing terms accounting for energy dissipation. By exploiting the second law of thermodynamics they get after some algebra the following expression for the evolution equation and the constitutive law that relates the stress tensor to the velocity field and the phase field

$$D_t\phi = \kappa\nabla\cdot(\Phi - \nabla\cdot\mathcal{T}), \tag{15}$$

$$\boldsymbol{\tau}^\top = -(\boldsymbol{\tau}^c)^\top + (\boldsymbol{\tau}^D)^\top, \tag{16}$$

where $\boldsymbol{\tau}^D = \eta[\nabla\mathbf{v}+\nabla\mathbf{v}^T]$ is the dissipative stress tensor, η is the dynamical viscosity of the ambient fluid and $(\boldsymbol{\tau}^c)^\top = \nabla\phi\otimes(\Phi - \nabla\cdot\mathcal{T}) + \nabla\nabla\phi\cdot\mathcal{T}$ is the nondissipative part of the stress tensor. We immediately observe the equality of our derived extra stress $\mathbb{U}^I$ and the extra stress $(\boldsymbol{\tau}^c)^\top$, which is derived by Jamet and Misbah, see [13]. Taking into account (14) and considering for a moment that our energy does not depend on ϕ one can observe the equality of (10) and (15). So we conclude that the model of Jamet and Misbah is a special case of our model and does not contain penalization terms which account for additional volume or area constraints, i.e. in general nonlocal constraints. The special theory of Jamet and Misbah is based on model 3, i.e on the explicit expression (the third expression in (12)) for the bending energy. In Section 4 we will discuss this in detail.

The outline of the paper is as follows. In Section 2 we formulate the balance laws and the dissipation inequality and derive several conclusions which then allows it to state thermodynamically consistent evolution equations for the velocity and the phase field together with appropriate boundary conditions. In Section 3 we state the complete model and discuss weak formulations. Finally in Section 4 we compare the model we derived with other models in the literature.

2. Balance laws and the dissipation inequality.

2.1. **Notation.** Tensors are linear transformations of $\mathbb{R}^3$ into $\mathbb{R}^3$ and are denoted by letters like $\mathbb{A}, \mathbb{B}, ...$. Vectors may be viewed as 3×1 column vectors and are denoted by boldface letters. Tensors may be represented as 3×3 matrices. $\mathbb{I}$ denotes the unit tensor and for $\mathbb{A}$ the tensor $\mathbb{A}^\top$ denotes its transpose; $\mathbf{a}\otimes\mathbf{b}$ is the tensor product of vectors $\mathbf{a}$ and $\mathbf{b}$ and is defined via $(\mathbf{a}\otimes\mathbf{b})\mathbf{u} = (\mathbf{b}\cdot\mathbf{u})\mathbf{a}$ for all vectors $\mathbf{u}$; the inner product of tensors $\mathbb{A}$ and $\mathbb{B}$ is defined by $\mathbb{A}:\mathbb{B} = \sum_{i,j=1}^{N} A_{ij}B_{ij}$. The partial derivative of a function $\Phi(a,b,c,...)$ (of scalar, vector or tensor variables) with respect to b, say, is written as $\partial_b\Phi(a,b,c,...)$.

2.2. **Constitutive relations.** First of all we fix the list of constitutive variables we base our *constitutive theory* on. Classical phase field theories are derived from *free energies*. So motivated by (4) and (5) we assume an energy functional as a sum of the kinetic and the free energy

$$\mathbf{G}_E = \int_\Omega \left(\frac{|\mathbf{v}|^2}{2} + G^0(Y)\right)\,dx + \sum_{k=1}^{s}\frac{M_k}{2}\left(\int_\Omega G^k(Y)\,dx\right)^2, \tag{17}$$

where

$$Y = (y_1, \mathbf{y}_2, \mathbb{Y}_3, y_4, \mathbb{Y}_5) = (\phi, \nabla\phi, D^2\phi, D_t\phi, \nabla\mathbf{v})$$

denotes the vector of the constitutive variables and the M_k, $k\in\{1,...,s\}$, are some non-negative constants. Here ϕ and $\mathbf{v}$ denote respectively the phase field variable and the velocity field. To allow for general functionals like in (4) we have to choose $D^2\phi$, the Hessian of ϕ, as a constitutive variable. In (17) the term $G^0(Y)$ is the density of the local part of the free energy. The sum $\sum_{k=1}^{s}\frac{M_k}{2}\left(\int_\Omega G^k(Y)\,dx\right)^2$ takes nonlocal energy contributions like the second and third summand of (5) into account.

In the sequel we will deal with derivatives of G^k, $k\in\{0,1,...,s\}$, with respect to the constitutive variables $(\phi,\nabla\phi,D^2\phi,D_t\phi,\nabla\mathbf{v})$. To fix notations we mean by $G^k_{\prime\nabla\phi}$ respectively $G^k_{\prime D^2\phi}$ the vector respectively the matrix with the entries $G^k_{\prime\partial_i\phi}$, $i\in\{1,...N\}$ and $G^k_{\prime\partial_{ij}\phi}$, $i,j\in\{1,...N\}$. With a slight abuse of notation we always denote by $G^k_{\prime\partial_i\phi}$, $G^k_{\prime\partial_{ij}\phi}$, ... the partial derivative with respect to the variable corresponding to $\partial_i\phi$, $\partial_{ij}\phi$, ... We make the assumption that G^k, $k\in\{0,1,...,s\}$, only depends on the symmetric part of the variable $\mathbb{Y}_3$ representing $D^2\phi$ in the vector Y. Denoting by $\mathbb{Y}_3^\top$ the transpose of $\mathbb{Y}_3$ we require

$$G^k(...,\mathbb{Y}_3,...)=G^k(...,\mathbb{Y}_3^\top,...)\qquad\text{for}\quad k\in\{0,1,...,s\}.$$

Since $D^2\phi$ is symmetric, this assumption does not lead to any restriction in the choice of G^k, $k\in\{0,1,...,s\}$. Otherwise one can define

$$G^k_{\text{new}}(...,\mathbb{Y}_3,...)=\frac{1}{2}\left(G^k(...,\mathbb{Y}_3,...)+G^k(...,\mathbb{Y}_3^\top,...)\right),\quad k\in\{0,1,...,s\},\tag{18}$$

in order to fulfil the requirement.

2.3. **Balance laws.** To formulate the balance laws we consider a material volume $\Omega\subset\mathbb{R}^3$ filled by an incompressible fluid. The balance equations for an incompressible fluid are the mass balance equation in local form, see Gurtin [9],

$$\nabla\cdot\mathbf{v}=0\tag{19}$$

and the balance law for the *linear momentum* which we state in integral form, see [9],

$$\frac{d}{dt}\int_V\mathbf{v}dx=\int_{\partial V}\mathbb{T}\mathbf{n}dS,$$

where $V\subset\Omega$ is a control volume, see [9], $\mathbb{T}$ is the stress tensor and $\mathbf{n}$ denotes the outer unit normal on ∂V. Using *Reynold's transport theorem*, the definition of the material derivative $D_t=\partial_t+(\mathbf{v}\cdot\nabla)$ and the divergence theorem we obtain

$$\int_V(D_t\mathbf{v}-\nabla\cdot\mathbb{T})\,dx=0.\tag{20}$$

and since the control volume is arbitrary we obtain the local form of the balance equations as $D_t\mathbf{v}-\nabla\cdot\mathbb{T}=0$.

2.4. **Dissipation inequality.** Furthermore we take, as the appropriate version of the second law in an isothermal situation, the *dissipation inequality*

$$\frac{d}{dt}\left\{\int_\Omega\left(\frac{|\mathbf{v}|^2}{2}+G^0(Y)\right)dx+\sum_{k=1}^{s}\frac{M_k}{2}\left(\int_\Omega G^k(Y)\,dx\right)^2\right\}+\int_{\partial\Omega}\mathbf{n}\cdot\mathbf{J}_D\,dS\le 0,$$

where $\mathbf{J}_D$ is the energy flux. We now use *Reynold's transport theorem* and the mass balance (19) in order to obtain

$$\int_\Omega D_t\left(\frac{|\mathbf{v}|^2}{2}+G^0(Y)\right)dx+\sum_{k=1}^{s}M_k\left(\int_\Omega G^k(Y)\,dx\right)\int_\Omega D_t\,G^k(Y)\,dx+\int_{\partial\Omega}\mathbf{n}\cdot\mathbf{J}_D\,dS\le 0.$$

Introducing the abbreviations

$$I^0 := 1, \quad I^k := M_k\left(\int_\Omega G^k(Y)\,dx\right), \quad k \in \{1,\ldots,s\},$$

we can rewrite the above inequality as follows

$$\int_\Omega \mathbf{v}\cdot D_t\mathbf{v}\,dx + \sum_{k=0}^{s} I^k \int_\Omega D_t G^k(Y)\,dx + \int_{\partial\Omega} \mathbf{n}\cdot\mathbf{J}_D\,dS \le 0.$$

Remark 1. The above dissipation inequality holds for all control volumes $V \subset \Omega$ if no nonlocal terms are present, i.e. in the case $s = 0$.

Similar as Liu and Müller [15] we now use the method of *Lagrange multipliers* to derive restrictions on the constitutive relations which are enforced by the *dissipation inequality*. Introducing *Lagrange multipliers* λ_ρ for the mass balance and $\lambda_\mathbf{v}$ for the momentum equation we obtain for solutions fulfilling the balance laws and the dissipation inequality

$$\int_\Omega \left[\mathbf{v}\cdot D_t\mathbf{v} + \sum_{k=0}^{s} I^k\left(D_t G^k(Y)\right) - \lambda_\rho \nabla\cdot\mathbf{v} - \lambda_\mathbf{v}(D_t\mathbf{v} - \nabla\cdot\mathbb{T})\right]dx + \int_{\partial\Omega}\mathbf{n}\cdot\mathbf{J}_D\,dS \le 0. \tag{21}$$

Choosing the classical *Lagrange multipliers* $\lambda_\rho := p$ and $\lambda_\mathbf{v} := \mathbf{v}$, see [15], we get after standard calculations

$$\int_\Omega \sum_{k=0}^{s} I^k\left(D_t G^k(Y)\right)dx - \int_\Omega (\mathbb{T} + p\mathbb{I}) : \nabla\mathbf{v}dx + \int_\Omega \nabla\cdot(\mathbf{J}_D + \mathbb{T}^\top\mathbf{v})dx \le 0, \tag{22}$$

where p denotes the pressure and $\mathbb{I}$ the identity matrix. Calculating the first summand of (22) gives

$$D_t G^k = G'^k_\phi D_t\phi + \sum_{i=1}^{N} G'^k_{\partial_i\phi} D_t\partial_i\phi + \sum_{i,j=1}^{N} G'^k_{\partial_{ij}\phi} D_t\partial_{ij}\phi + G'^k_{D_t\phi} D_t^2\phi + G'^k_{\nabla\mathbf{v}} D_t\nabla\mathbf{v}. \tag{23}$$

The commutator rule

$$D_t\partial_i\phi = \partial_i D_t\phi - \partial_i\mathbf{v}\cdot\nabla\phi$$

then gives

$$\sum_{i=1}^{N} G'^k_{\partial_i\phi} D_t\partial_i\phi = \sum_{i=1}^{N}\partial_i[G'^k_{\partial_i\phi} D_t\phi] - \sum_{i=1}^{N}\partial_i G'^k_{\partial_i\phi} D_t\phi - \sum_{i,l=1}^{N}\partial_l\phi\, G'^k_{\partial_i\phi}\partial_i v_l. \tag{24}$$

Standard calculations involving the product and the commutator rules give

$$
\begin{aligned}
\sum_{i,j=1}^{N} G'^{k}_{\partial_{ij}\phi} D_t \partial_{ij}\phi &= \sum_{i,j=1}^{N} G'^{k}_{\partial_{ij}\phi} \left[\partial_j D_t \partial_i \phi - \partial_j \mathbf{v} \cdot \nabla(\partial_i \phi)\right] \\
&= \sum_{i,j=1}^{N} \partial_j [G'^{k}_{\partial_{ij}\phi} D_t \partial_i \phi] - \sum_{i,j=1}^{N} \partial_j G'^{k}_{\partial_{ij}\phi} D_t \partial_i \phi - \sum_{i,j,l=1}^{N} G'^{k}_{\partial_{ij}\phi} \partial_j v_l \partial_{li}\phi \\
&= \sum_{i,j=1}^{N} \partial_j [G'^{k}_{\partial_{ij}\phi} D_t \partial_i \phi - \partial_i G'^{k}_{\partial_{ij}\phi} D_t \phi] + \sum_{i,j=1}^{N} \partial_{ij} G'^{k}_{\partial_{ij}\phi} D_t \phi \\
&\quad + \sum_{i,l=1}^{N} \left(\partial_l \phi \sum_{j=1}^{N} \partial_j G'^{k}_{\partial_{ij}\phi} - \sum_{j=1}^{N} \partial_{lj}\phi G'^{k}_{\partial_{ij}\phi} \right) \partial_i v_l. \qquad (25)
\end{aligned}
$$

Making use of the identities

$$
\begin{aligned}
& G'^{k}_{\nabla\phi} = (G'^{k}_{\partial_i \phi})_{i=1}^{N}, \quad \nabla \cdot G'^{k}_{\nabla\phi} = \sum_{i=1}^{N} \partial_i G'^{k}_{\partial_i \phi}, \\
& \nabla \cdot [G'^{k}_{\nabla\phi} D_t \phi] = \sum_{i=1}^{N} \partial_i [G'^{k}_{\partial_i \phi} D_t \phi], \\
& \nabla \cdot [G'^{k}_{D^2\phi} D_t \nabla\phi - \nabla \cdot G'^{k}_{D^2\phi} \, D_t \phi] = \sum_{i,j=1}^{N} \partial_j [G'^{k}_{\partial_{ij}\phi} D_t \partial_i \phi - \partial_i G'^{k}_{\partial_{ij}\phi} D_t \phi], \\
& \nabla \cdot (\nabla \cdot G'^{k}_{D^2\phi}) = \sum_{i,j=1}^{N} \partial_{ij} G'^{k}_{\partial_{ij}\phi}, \\
& (\nabla\phi \otimes G'^{k}_{\nabla\phi}) : \nabla \mathbf{v} = \sum_{i,l=1}^{N} \partial_l \phi \, G'^{k}_{\partial_i \phi} \partial_i v_l, \\
& Q^k = G'^{k}_{\phi} - \nabla \cdot \left[G'^{k}_{\nabla\phi} - \nabla \cdot G'^{k}_{D^2\phi} \right], \\
& \mathbb{U}^k = \nabla\phi \otimes \left[G'^{k}_{\nabla\phi} - \nabla \cdot G'^{k}_{D^2\phi} \right] + D^2\phi \, G'^{k}_{D^2\phi}, \\
& \mathbf{B}^k = \left[G'^{k}_{\nabla\phi} - \nabla \cdot G'^{k}_{D^2\phi} \right] D_t \phi + G'^{k}_{D^2\phi} D_t \nabla\phi,
\end{aligned}
$$

we can rewrite (23) as

$$
D_t G^k = Q^k D_t \phi - \mathbb{U}^k : \nabla \mathbf{v} + \nabla \cdot \mathbf{B}^k + G'^{k}_{D_t\phi} D_t^2 \phi + G'^{k}_{\nabla \mathbf{v}} D_t \nabla \mathbf{v}. \qquad (26)
$$

With the following notations

$$
\begin{aligned}
& G'^{I}_{\partial_i \phi} = \sum_{k=0}^{s} I^k G'^{k}_{\partial_i \phi}, \quad \partial_j G'^{I}_{\partial_{ij}\phi} = \partial_j \sum_{k=0}^{s} I^k G'^{k}_{\partial_{ij}\phi}, \\
& G'^{I}_{D_t\phi} = \sum_{k=0}^{s} I^k G'^{k}_{D_t\phi}, \quad G'^{I}_{\nabla \mathbf{v}} = \sum_{k=0}^{s} I^k G'^{k}_{\nabla \mathbf{v}}, \\
& Q^I = \sum_{k=0}^{s} I^k Q^k = G'^{I}_{\phi} - \nabla \cdot \left[G'^{I}_{\nabla\phi} - \nabla \cdot G'^{I}_{D^2\phi} \right], \qquad (27) \\
& \mathbb{U}^I = \sum_{k=0}^{s} I^k \mathbb{U}^k = \nabla\phi \otimes \left[G'^{I}_{\nabla\phi} - \nabla \cdot G'^{I}_{D^2\phi} \right] + D^2\phi \, G'^{I}_{D^2\phi}, \\
& \mathbf{B}^I = \sum_{k=0}^{s} I^k \mathbf{B}^k = \left[G'^{I}_{\nabla\phi} - \nabla \cdot G'^{I}_{D^2\phi} \right] D_t \phi + G'^{I}_{D^2\phi} D_t \nabla\phi,
\end{aligned}
$$

we obtain, using (22) and (26),

$$\int_\Omega Q^I\, D_t\phi\, dx - \int_\Omega \mathbb{S} : \nabla \mathbf{v}\, dx + \int_\Omega \nabla\cdot(\mathbf{J}_D + \mathbb{T}^\top \mathbf{v} + \mathbf{B}^I)\, dx + \int_\Omega G^I_{,D_t\phi} D_t^2\phi\, dx + \int_\Omega G^I_{,\nabla\mathbf{v}} D_t \nabla\mathbf{v}\, dx \le 0, \quad (28)$$

where

$$\mathbb{S} = \mathbb{T} + p\mathbb{I} + \mathbb{U}^I \quad (29)$$

is the extra stress, see also [10] for the case where $\mathbf{G}_E$ does not depend on second derivatives. We will later derive a constitutive equation giving the macroscopic stress $\mathbb{T}$ as a classical Newtonian stress $\mathbb{S} - p\mathbb{I}$ minus the additional term

$$\mathbb{U}^I = \nabla\phi \otimes \left[G^I_{,\nabla\phi} - \nabla\cdot G^I_{,D^2\phi}\right] + D^2\phi\, G^I_{,D^2\phi} \quad (30)$$

taking stresses resulting from the phase field into account.

Remark 2. Note that in $\mathbb{U}^I$ the expression $G^I_{,\phi}$ does not appear. The nonsymmetric term $\mathbb{U}^I$ stems from the elastic bending forces and is furthermore responsible for the coupling of the phase field to the velocity field.

2.5. **Exploiting the dissipation inequality for local models.** In this subsection we assume that $s = 0$ and therefore computations as in Subsection 2.4 show that the inequality (28) holds for all control volumes $V \subset \Omega$ (compare also Remark 1). Using the fact that V can be chosen arbitrarily we can derive a local form of (28) as follows

$$Q^0\, D_t\phi - \mathbb{S} : \nabla\mathbf{v} + \nabla\cdot(\mathbf{J}_D + \mathbb{T}^\top\mathbf{v} + \mathbf{B}^0) + G^0_{,D_t\phi} D_t^2\phi + G^0_{,\nabla\mathbf{v}} D_t\nabla\mathbf{v} \le 0, \quad (31)$$

where Q^0 and B^0 denote respectively the quantities Q^I and B^I for $s = 0$. We now use a Coleman-Noll procedure similar as in [10], Section III, to derive restrictions on the constitutive relations. Arguing similar as in [10] it is possible to find fields ϕ and $\mathbf{v}$ such that at some chosen point and time ϕ and $\mathbf{v}$ together with all derivatives that appear in (31) take prescribed values. Hence all terms appearing linear in (31) will vanish and we obtain

$$G^0_{,D_t\phi} = 0 \qquad \text{and} \qquad G^0_{,\nabla\mathbf{v}} = 0.$$

This implies that the free energy density cannot depend on $D_t\phi$ and $\nabla\mathbf{v}$. We do not aim to derive the most general models and hence choose $\mathbf{J}_D$ such that it reduces to the standard form $-\mathbb{T}^\top\mathbf{v}$, i.e. it is given by the working of the macroscopic stresses, when $D_t\phi$ and $D_t\nabla\phi$ vanish and is affine linear with respect to $D_t\phi$ and $D_t\nabla\phi$. With the choice

$$\mathbf{J}_D = -\mathbb{T}^\top\mathbf{v} - \mathbf{B}^0, \quad (32)$$

the inequality (31) now reduces to

$$Q^0\, D_t\phi - \mathbb{S} : \nabla\mathbf{v} \le 0. \quad (33)$$

This inequality is fulfilled if

$$-\left(G^0_{,\phi} - \nabla\cdot\left[G^0_{,\nabla\phi} - \nabla\cdot G^0_{,D^2\phi}\right]\right) = A_1 D_t\phi + A_2\nabla\mathbf{v}, \quad (34)$$

$$\mathbb{S} = B_2 D_t\phi + B_1\nabla\mathbf{v}, \quad (35)$$

where

$$\begin{array}{llll} A_1(Y) & : \mathbb{R} & \to & \mathbb{R}, \\ A_2(Y) & : \mathbb{R}^{d\times d} & \to & \mathbb{R}, \\ B_2(Y) & : \mathbb{R} & \to & \mathbb{R}^{d\times d}, \\ B_1(Y) & : \mathbb{R}^{d\times d} & \to & \mathbb{R}^{d\times d}, \end{array}$$

are such that the matrix

$$\begin{pmatrix} A_1 & A_2 \\ B_2 & B_1 \end{pmatrix} \tag{36}$$

is positive semi-definite, see also [8]. Using a lemma of Liu, see [14] and [15], it can be shown that this form is in fact necessary to fulfil the dissipation inequality (33) for all fields.

Taking into account the computations of Subsection 2.4 we now obtain a local form of the dissipation inequality:

$$\begin{aligned} D_t\left(\frac{|\mathbf{v}|^2}{2} + G^0(Y)\right) - \nabla\cdot\left(\mathbb{T}^\top\mathbf{v} + \left[G'^0_{\nabla\phi} - \nabla\cdot G'^0_{D^2\phi}\right] D_t\phi + G'^0_{D^2\phi} D_t\nabla\phi\right) \\ = Q^0\, D_t\phi - \mathbb{S} : \nabla\mathbf{v} \le 0, \end{aligned} \tag{37}$$

where the inequality holds since the matrix in (36) is positive semi-definite. The term $-(Q^0\, D_t\phi - \mathbb{S} : \nabla\mathbf{v})$ is the non-negative energy dissipation.
In the following we will neglect cross effects in (34), i.e. we consider

$$-\left(G'^0_{\phi} - \nabla\cdot\left[G'^0_{\nabla\phi} - \nabla\cdot G'^0_{D^2\phi}\right]\right) = A_1 D_t\phi \text{ in } \Omega, \tag{38}$$

$$\mathbb{S} = B_1\nabla\mathbf{v} \text{ in } \Omega. \tag{39}$$

It turns out that (38) is a generalized phase field equation of fourth order, where $A_1(Y) \in \mathbb{R}_0^+$. Equation (39) gives a general form of the stress tensor $\mathbb{S}$ in terms of $\nabla\mathbf{v}$ where the tensor $B_1(Y) : \mathbb{R}^{d\times d} \to \mathbb{R}^{d\times d}$ may depend on Y and is symmetric and positive semi-definite. If we assume that the fluid is Newtonian, i.e. in particular that $\mathbb{S}$ depends linearly on $\nabla\mathbf{v}$ we obtain the standard relation, see [9],

$$\mathbb{S} = 2\mu\mathbb{D}, \tag{40}$$

where $\mathbb{D} = \mathbb{D}(\nabla\mathbf{v}) = \frac{1}{2}(\nabla\mathbf{v} + \nabla\mathbf{v}^\top)$ is the rate-of-strain tensor and the scalar μ is the viscosity of the fluid and might depend on $\phi, \nabla\phi$ and $D^2\phi$. In this case we obtain

$$\begin{aligned} D_t\left(\frac{|\mathbf{v}|^2}{2} + G^0(Y)\right) - \nabla\cdot\left(\mathbb{T}^\top\mathbf{v} + \left[G'^0_{\nabla\phi} - \nabla\cdot G'^0_{D^2\phi}\right] D_t\phi + G'^0_{D^2\phi} D_t\nabla\phi\right) \\ = -A_1|D_t\phi|^2 - 2\mu|\mathbb{D}(\nabla\mathbf{v})|^2 \le 0, \end{aligned} \tag{41}$$

where $|\mathbb{D}|^2 = \mathbb{D} : \mathbb{D}$. Hence the energy dissipation is given by the standard energy dissipation due to friction, given by $2\mu|\mathbb{D}(\nabla\mathbf{v})|^2$, and a term stemming from the energy dissipation due to interface motion, given by $A_1|D_t\phi|^2$.

2.6. **Thermodynamical consistent non-local models.** Due to non-local interactions we cannot expect that a local dissipation inequality holds for the non-local model. We hence only require that a global dissipation inequality holds. Motivated from the derivation of the local model in Subsection 2.5 we set

$$G'^I_{D_t\phi} = 0 \qquad \text{and} \qquad G'^I_{\nabla\mathbf{v}} = 0,$$

and

$$\mathbf{J}_D = -\mathbb{T}^\top \mathbf{v} - \mathbf{B}^I, \tag{42}$$

where the term $\mathbf{B}^I$ contains non-local contributions, compare (27). In what follows we will demonstrate that the choice (42) leads to a model fulfilling a global dissipation inequality. Furthermore, we consider a model without cross effects between the stresses in the fluid and the interface velocity given by $D_t\phi$ and set

$$-\left(G^I_{,\phi} - \nabla\cdot\left[G^I_{,\nabla\phi} - \nabla\cdot G^I_{,D^2\phi}\right]\right) = A_1 D_t\phi \text{ in } \Omega, \tag{43}$$

$$\mathbb{S} = B_1\nabla\mathbf{v} \text{ in } \Omega, \tag{44}$$

where $A_1(Y) \in \mathbb{R}^+_0$ and $B_1(Y) : \mathbb{R}^{d\times d} \to \mathbb{R}^{d\times d}$ is symmetric and positive semidefinite. Taking the results of Subsection 2.4 into account we obtain

$$\frac{d}{dt}\left\{\int_\Omega \left(\frac{|\mathbf{v}|^2}{2} + G^0(Y)\right) dx + \sum_{k=1}^s \frac{M_k}{2}\left(\int_\Omega G^k(Y)\, dx\right)^2\right\} + \int_{\partial\Omega} \mathbf{n}\cdot\mathbf{J}_D\, dS$$
$$= -\int_\Omega \left[A_1|D_t\phi|^2 + (B_1\nabla\mathbf{v}) : \nabla\mathbf{v}\right]\, dx \le 0.$$

From now on we assume that the fluid is Newtonian and hence the second dissipative term is given as $\int_\Omega 2\mu|\mathbb{D}(\nabla\mathbf{v})|^2\, dx$. We now want to discuss boundary conditions which guarantee that the total energy in Ω always decreases. This is a thermodynamical requirement on a closed system. To proceed we need to discuss the boundary integral $\int_{\partial\Omega} \mathbf{n}\cdot\mathbf{J}_D\, dS$ in more detail. Using the fact that $D_t\nabla\phi = \partial_t\nabla\phi + D^2\phi\,\mathbf{v}$ we have

$$\mathbf{J}_D = -\mathbb{T}^\top\mathbf{v} - \left[G^I_{,\nabla\phi} - \nabla\cdot G^I_{,D^2\phi}\right] D_t\phi - G^I_{,D^2\phi}\partial_t\nabla\phi - \mathbf{v}D^2\phi G^I_{,D^2\phi}.$$

Introducing

$$\widehat{\mathbf{B}}^I = \left[G^I_{,\nabla\phi} - \nabla\cdot G^I_{,D^2\phi}\right]$$

we now obtain using

$$\mathbf{J}_D = -\left[\mathbb{T} + \mathbb{U}^I\right]^\top \mathbf{v} - \partial_t\phi\widehat{\mathbf{B}}^I - G^I_{,D^2\phi}\partial_t\nabla\phi$$

that the global energy always decreases if and only if

$$-\int_\Omega \left(A_1|D_t\phi|^2 + 2\mu|\mathbb{D}(\nabla\mathbf{v})|^2\right) dx + \int_{\partial\Omega} (\widehat{\mathbf{B}}^I\partial_t\phi + G^I_{,D^2\phi}\nabla\partial_t\phi)\cdot\mathbf{n}dS$$
$$+ \int_{\partial\Omega} \left(\left[\mathbb{T} + \mathbb{U}^I\right]\mathbf{n}\right)\cdot\mathbf{v}dS \le 0.$$

By $\nabla\partial_t\phi = (\mathbf{n}\otimes\mathbf{n})\nabla\partial_t\phi + \nabla_S\partial_t\phi$, where $\nabla_S = (\mathbb{I} - \mathbf{n}\otimes\mathbf{n})\nabla$ denotes the surface-gradient, we obtain, using the divergence theorem on surfaces, see [2], the following inequality

$$-\int_\Omega \left(A_1|D_t\phi|^2 + 2\mu|\mathbb{D}(\nabla\mathbf{v})|^2\right) dx + \int_{\partial\Omega} \left[\mathbf{n}\cdot\widehat{\mathbf{B}}^I - \nabla_S\cdot(G^I_{,D^2\phi}\mathbf{n}) - \boldsymbol{\kappa}\cdot G^I_{,D^2\phi}\mathbf{n}\right]\partial_t\phi dS$$
$$+ \int_{\partial\Omega} (\mathbf{n}\cdot G^I_{,D^2\phi}\mathbf{n})(\nabla\partial_t\phi\cdot\mathbf{n})dS$$
$$+ \int_{\partial\Omega} \left(\left[\mathbb{T} + \mathbb{U}^I\right]\mathbf{n}\right)\cdot\mathbf{v}dS \le 0, \tag{45}$$

where $\boldsymbol{\kappa}$ denotes the mean curvature vector of $\partial\Omega$. We remark that $\boldsymbol{\kappa} = \kappa\mathbf{n}$ where κ is the sum of the principal curvatures of $\partial\Omega$. Energy decrease is hence guaranteed if we prescribe on the boundary $\partial\Omega$

$$0 = \mathbf{n} \cdot \widehat{\mathbf{B}}^I - \nabla_S \cdot (G^I_{\prime D^2\phi}\mathbf{n}) - \boldsymbol{\kappa} \cdot G^I_{\prime D^2\phi}\mathbf{n}, \tag{46}$$

$$0 = \mathbf{n} \cdot G^I_{\prime D^2\phi}\mathbf{n}, \tag{47}$$

$$0 = \mathbf{v}. \tag{48}$$

Using (47) and the identity $\boldsymbol{\kappa} = \kappa\mathbf{n}$ the boundary condition in (46) can be simplified to $\mathbf{n} \cdot \widehat{\mathbf{B}}^I - \nabla_S \cdot (G^I_{\prime D^2\phi}\mathbf{n}) = 0$. But of course also boundary conditions taking dissipation at the boundary are possible. Examples are slip conditions which we will discuss later or dynamic boundary conditions of the form

$$\partial_t\phi = -\omega\left(\mathbf{n} \cdot \widehat{\mathbf{B}}^I - \nabla_S \cdot (G^I_{\prime D^2\phi}\mathbf{n}) - \boldsymbol{\kappa} \cdot G^I_{\prime D^2\phi}\mathbf{n}\right), \tag{49}$$

where ω is a non-negative constant.

Remark 3. The boundary conditions (46)-(48) and also the boundary condition (49) are also possible boundary conditions in the local case. In this case we set $s = 0$ in the definition of $\mathbf{B}^I$ and G^I.

3. Higher order phase field Navier-Stokes model and its weak formulation.

3.1. The model.

To get the incompressible phase field Navier-Stokes model we need the balance of momentum (20) in its local form

$$D_t\mathbf{v} - \nabla \cdot \mathbb{T} = 0. \tag{50}$$

By (19), (29), (43), (40), (50) and $\gamma := A_1(Y)$ we finally get the following **general higher order phase field Navier-Stokes model**

$$\begin{cases} \mathbf{v}_t + \mathbf{v}\cdot\nabla\mathbf{v} = \nabla\cdot\mathbb{T} & \text{in} \quad [0,T]\times\Omega, \\ \mathbb{T} + p\mathbb{I} = \mathbb{S} - \mathbb{U}^I & \text{in} \quad [0,T]\times\Omega, \\ \mathbb{S} = 2\mu\mathbb{D} & \text{in} \quad [0,T]\times\Omega, \\ \mathbb{U}^I = \nabla\phi\otimes\left[G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}\right] + D^2\phi\, G^I_{\prime D^2\phi} & \text{in} \quad [0,T]\times\Omega, \\ \nabla\cdot\mathbf{v} = 0 & \text{in} \quad [0,T]\times\Omega, \\ \gamma\phi_t + \gamma\mathbf{v}\cdot\nabla\phi = -\left(G^I_{\prime\phi} - \nabla\cdot\left[G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}\right]\right) & \text{in} \quad [0,T]\times\Omega, \\ \mathbf{v}(0,x) = \mathbf{v}_0(x) & \text{in} \quad \Omega, \\ \phi(0,x) = \phi_0(x) & \text{in} \quad \Omega, \end{cases} \tag{51}$$

complemented by the boundary conditions, which will be discussed in the next subsection.

Remark 4. It is possible to choose $\gamma = 0$ which leads to a quasi-stationary model which is in instantaneous equilibrium with respect to ϕ.

Besides we can write (51) in a different form. A straightforward calculation gives

$$-\nabla\cdot\mathbb{U}^I = \nabla\phi\left(G^I_{\prime\phi} - \nabla\cdot\left[G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}\right]\right) - \nabla G^I,$$

where $G^I := \left(\sum\limits_{k=0}^{s} I^k G^k\right)$. If we now as in [10] replace the pressure p by a modified pressure $\hat{p} = p + G^I$ we obtain for $\nabla\cdot\mathbb{T}$ the following expression

$$\nabla\cdot\mathbb{T} = -\nabla\hat{p} + \mu\Delta\mathbf{v} + \nabla\phi\left(G^I_{\prime\phi} - \nabla\cdot\left[G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}\right]\right), \tag{52}$$

which leads to the system

$$
\begin{cases}
\mathbf{v}_t + \mathbf{v}\cdot\nabla\mathbf{v} = -\nabla\hat{p} + \mu\Delta\mathbf{v} + \nabla\phi\left(G^I_{\prime\phi} - \nabla\cdot\left[G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}\right]\right) & \text{in} \quad [0,T]\times\Omega,\\
\nabla\cdot\mathbf{v} = 0 & \text{in} \quad [0,T]\times\Omega,\\
\gamma\phi_t + \gamma\mathbf{v}\cdot\nabla\phi = -\left(G^I_{\prime\phi} - \nabla\cdot\left[G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}\right]\right) & \text{in} \quad [0,T]\times\Omega,\\
\mathbf{v}(0,x) = \mathbf{v}_0(x) & \text{in} \quad \Omega,\\
\phi(0,x) = \phi_0(x) & \text{in} \quad \Omega.
\end{cases}
\tag{53}
$$

Later we will exploit (53) in order to derive (7). We will see that by choosing $\mathbf{G}_E := E(\phi)$ the expression $G^I_{\prime\phi} - \nabla\cdot[G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}]$ is nothing else than the variational derivative of $E(\phi)$ and this will provide (7).

3.2. **Boundary conditions.** Now we postulate several boundary conditions which guarantee energy decrease, that means they fulfil (45) and fall in two categories. Boundary conditions of the first category $(\mathbf{BC})_1$, $(\mathbf{BC})_3$ and $(\mathbf{BC})_5$ take into account no slip conditions, where boundary conditions of the second category $(\mathbf{BC})_2$, $(\mathbf{BC})_4$ and $(\mathbf{BC})_6$ allow for non zero tangential velocities, which depend on the tangential component of the stress tensor and the additional tensor (30) we derived in this paper. These two categories will affect the choice of the test function spaces and consequently the weak form of the derived equations, see Section 3.3. As for some other fourth order equations we furthermore obtain boundary conditions which take into account the mean curvature of the domain boundary and also provide conditions on the second and third order derivatives of the energy functional with respect to the phase field. The set of boundary conditions involve second and third spatial derivatives of ϕ.

$$
(\mathbf{BC})_1 \quad \begin{cases}
0 = \mathbf{v},\\
0 = \mathbf{n}\cdot(G^I_{\prime D^2\phi}\mathbf{n}),\\
0 = \mathbf{n}\cdot\left(G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}\right) - \nabla_S\cdot(G^I_{\prime D^2\phi}\mathbf{n}).
\end{cases}
$$

A variant which allows for slip is given as

$$
(\mathbf{BC})_2 \quad \begin{cases}
\mathbf{v}_n = 0,\\
-\sigma\mathbf{v}_\tau = [\mathbb{S}\mathbf{n}]_\tau,\\
0 = \mathbf{n}\cdot(G^I_{\prime D^2\phi}\mathbf{n}),\\
0 = \mathbf{n}\cdot\left(G^I_{\prime\nabla\phi} - \nabla\cdot G^I_{\prime D^2\phi}\right) - \nabla_S\cdot(G^I_{\prime D^2\phi}\mathbf{n}),
\end{cases}
$$

where $\sigma \geq 0$ and $[\cdot]_\tau, [\cdot]_n$ denote the tangential and normal component of a vector $[\cdot]$. If we specify a Dirichlet boundary condition for a general fourth order elliptic operator we necessarily obtain an additional boundary condition involving second derivatives. In our context this is given by

$$
(\mathbf{BC})_3 \quad \begin{cases}
0 = \mathbf{v},\\
0 = \mathbf{n}\cdot(G^I_{\prime D^2\phi}\mathbf{n}),\\
\phi = \phi_0(x),
\end{cases}
$$

and the slip analogue

$$
(\mathbf{BC})_4 \quad \begin{cases}
\mathbf{v}_n = 0,\\
-\sigma\mathbf{v}_\tau = [\mathbb{S}\mathbf{n}]_\tau,\\
0 = \mathbf{n}\cdot(G^I_{\prime D^2\phi}\mathbf{n}),\\
\phi = \phi_0(x),
\end{cases}
$$

where again $\sigma \geq 0$. A third possibility is given as

$$(\mathbf{BC})_5 \quad \begin{cases} 0 &= \mathbf{v}, \\ 0 &= \mathbf{n} \cdot \nabla\phi, \\ 0 &= \mathbf{n} \cdot \left(G^I_{\prime\nabla\phi} - \nabla \cdot G^I_{\prime D^2\phi} \right) - \nabla_S \cdot (G^I_{\prime D^2\phi}\mathbf{n}) - \boldsymbol{\kappa} \cdot G^I_{\prime D^2\phi}\mathbf{n}, \end{cases}$$

which has the slip analogue

$$(\mathbf{BC})_6 \quad \begin{cases} \mathbf{v}_n &= 0, \\ -\sigma\mathbf{v}_\tau &= [\mathbb{S}\mathbf{n}]_\tau, \\ 0 &= \mathbf{n} \cdot \nabla\phi, \\ 0 &= \mathbf{n} \cdot \left(G^I_{\prime\nabla\phi} - \nabla \cdot G^I_{\prime D^2\phi} \right) - \nabla_S \cdot (G^I_{\prime D^2\phi}n) - \boldsymbol{\kappa} \cdot G^I_{\prime D^2\phi}\mathbf{n}, \end{cases}$$

with $\sigma \geq 0$. A further possibility is to prescribe $\phi = \mathbf{n} \cdot \nabla\phi = 0$ together with a slip or a no-slip boundary condition on the boundary. We derive from (45) that in the cases $(\mathbf{BC})_1$, $(\mathbf{BC})_3$ and $(\mathbf{BC})_5$ the total dissipation has no boundary contributions and is given as

$$\int_\Omega \left(\gamma |D_t\phi|^2 + 2\mu |\mathbb{D}(\nabla\mathbf{v})|^2 \right) dx \geq 0 \tag{54}$$

and in the cases $(\mathbf{BC})_2$, $(\mathbf{BC})_4$ and $(\mathbf{BC})_6$ we obtain an additional dissipation term on the boundary and the total dissipation is

$$\int_\Omega \left(\gamma |D_t\phi|^2 + 2\mu |\mathbb{D}(\nabla\mathbf{v})|^2 \right) dx + \sigma \int_{\partial\Omega} |\mathbf{v}|^2 dS \geq 0. \tag{55}$$

Thus the *dissipation inequality* holds for all boundary conditions stated above.

3.3. **Weak formulation and energy identities.** To get weak formulations of (51) subject to the different boundary conditions $(\mathbf{BC})_1$-$(\mathbf{BC})_6$ we multiply the first equation (momentum equation) in (51) by a vector-valued smooth test function $\boldsymbol{\varphi}$ and the phase field equation by a smooth scalar test function ζ. These test functions will be specified later taking the different boundary conditions into account. We obtain for almost all $t \in (0,T)$ after integration over Ω

$$\begin{aligned} &\int_\Omega \mathbf{v}_t \cdot \boldsymbol{\varphi}\, dx + \int_\Omega (\mathbf{v}\cdot\nabla)\mathbf{v} \cdot \boldsymbol{\varphi}\, dx - \int_\Omega (\nabla \cdot \mathbb{T}) \cdot \boldsymbol{\varphi}\, dx = 0, \\ &\int_\Omega \gamma\phi_t\zeta\, dx + \int_\Omega \gamma(\mathbf{v}\cdot\nabla)\phi\zeta\, dx + \int_\Omega \left(G^I_{\prime\phi} - \nabla \cdot \left[G^I_{\prime\nabla\phi} - \nabla \cdot G^I_{\prime D^2\phi} \right] \right) \zeta\, dx = 0. \end{aligned}$$

Integration by parts gives

$$\begin{aligned} &\int_\Omega \mathbf{v}_t \cdot \boldsymbol{\varphi}\, dx + \int_\Omega (\mathbf{v}\cdot\nabla)\mathbf{v} \cdot \boldsymbol{\varphi}\, dx - \int_{\partial\Omega} (\mathbb{T}\mathbf{n}) \cdot \boldsymbol{\varphi} + \int_\Omega \mathbb{T} : \nabla\boldsymbol{\varphi}\, dx = 0, \\ &\int_\Omega \gamma\phi_t\zeta\, dx + \int_\Omega \gamma(\mathbf{v}\cdot\nabla)\phi\zeta\, dx + \int_\Omega G^I_{\prime\phi}\zeta\, dx + \int_\Omega G^I_{\prime\nabla\phi} \cdot \nabla\zeta\, dx + \\ &+ \int_\Omega G^I_{\prime D^2\phi} : D^2\zeta\, dx - \int_{\partial\Omega} \mathbf{n} \cdot (G_{\prime D^2\phi}\mathbf{n})(\mathbf{n}\cdot\nabla\zeta) dS - \\ &- \int_{\partial\Omega} \left(\mathbf{n} \cdot \left(G^I_{\prime\nabla\phi} - \nabla \cdot G^I_{\prime D^2\phi} \right) - \nabla_S \cdot (G^I_{\prime D^2\phi}\mathbf{n}) - \boldsymbol{\kappa} \cdot G^I_{\prime D^2\phi}\mathbf{n} \right) \zeta\, dS = 0. \end{aligned}$$

Now we have to choose the corresponding test function spaces associated to the different boundary condition.

In the case of a no-slip boundary condition we obtain the following weak formulation.

3.3.1. *Weak formulation of (51) associated to* $(\boldsymbol{BC})_1$, $(\boldsymbol{BC})_3$ *and* $(\boldsymbol{BC})_5$. For the test function $\boldsymbol{\varphi}$ corresponding to the momentum equation we choose divergence-free test functions with compact support. The space for the test functions ζ depends on the boundary conditions as follows: In case $(\mathbf{BC})_1$ we choose $C^\infty(\overline{\Omega})$, in case $(\mathbf{BC})_3$ we choose $\{\zeta \in C^\infty(\overline{\Omega}) \,:\, \zeta|_{\partial\Omega} = 0\}$ and in case $(\mathbf{BC})_5$ we choose $\{\zeta \in C^\infty(\overline{\Omega}) \,:\, \mathbf{n}\cdot\nabla\zeta|_{\partial\Omega} = 0\}$.

Theorem 3.1. *Assume that* $\phi : \overline{\Omega} \to \mathbb{R}$ *and* $\boldsymbol{v} : \overline{\Omega} \to \mathbb{R}^3$ *are smooth functions. Then* $(\phi, \boldsymbol{v})$ *is a solution of (51) with boundary conditions* $(\boldsymbol{BC})_1$, $(\boldsymbol{BC})_3$ *or* $(\boldsymbol{BC})_5$ *if and only if* $(\phi, \boldsymbol{v})$ *fulfils:*

i) for all test functions $(\zeta, \boldsymbol{\varphi})$ *chosen according to the boundary conditions stated above the identities*

$$\int_\Omega \boldsymbol{v}_t \cdot \boldsymbol{\varphi}\, dx + \int_\Omega (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\cdot\boldsymbol{\varphi}\, dx + \int_\Omega (\mathbb{S} - \mathbb{U}^I) : \nabla\boldsymbol{\varphi}\, dx = 0, \tag{56}$$

$$\int_\Omega \gamma\phi_t\zeta\, dx + \int_\Omega \gamma(\boldsymbol{v}\cdot\nabla)\phi\zeta\, dx + \int_\Omega {G^I}'_\phi \zeta\, dx + \int_\Omega {G^I}'_{\nabla\phi}\cdot\nabla\zeta\, dx + \\ + \int_\Omega {G^I}'_{D^2\phi} : D^2\zeta\, dx = 0, \tag{57}$$

holds for almost all $t \in (0, T)$,

ii) $\nabla\cdot\boldsymbol{v} = 0$ *in* $[0, T]\times\Omega$,

iii) the initial conditions in $\{0\}\times\Omega$ *and the no-slip boundary condition* $\boldsymbol{v} = 0$ *on* $[0, T]\times\partial\Omega$ *holds and in case* $(\boldsymbol{BC})_3$ *we require* $\phi = \phi_0$ *on* $[0, T]\times\partial\Omega$ *and in case* $(\boldsymbol{BC})_5$ *we require* $\boldsymbol{n}\cdot\nabla\phi = 0$ *on* $[0, T]\times\partial\Omega$.

Besides for all solutions of (51) with boundary conditions $(\boldsymbol{BC})_1$, $(\boldsymbol{BC})_3$ *and* $(\boldsymbol{BC})_5$ *the energy identity*

$$\frac{d}{dt}\boldsymbol{G}_E = -\int_\Omega \left(\gamma|D_t\phi|^2 + 2\mu|\mathbb{D}(\nabla\boldsymbol{v})|^2\right) dx \tag{58}$$

holds.

Remark 5. The energy identity is derived by using the test function $\mathbf{v}$ in (56) and $Q^I = \left({G^I}'_\phi - \nabla\cdot\left[{G^I}'_{\nabla\phi} - \nabla\cdot {G^I}'_{D^2\phi}\right]\right)$ in (57). Using integration by parts, exploiting the boundary conditions $(\mathbf{BC})_1$, $(\mathbf{BC})_3$, $(\mathbf{BC})_5$ and taking into account $Q^I = -\gamma D_t\phi$ we finally get (58).

In the case of a slip boundary condition we obtain the following weak formulation.

3.3.2. *Weak formulation of (51) associated to* $(\boldsymbol{BC})_2$, $(\boldsymbol{BC})_4$ *and* $(\boldsymbol{BC})_6$. For the test function $\boldsymbol{\varphi}$ corresponding to the momentum equation we choose divergence-free test functions $\boldsymbol{\varphi} \in \{C^\infty(\overline{\Omega}; \mathbb{R}^3) \,:\, n\cdot\boldsymbol{\varphi}|_{\partial\Omega} = 0\}$. The space for the test functions ζ depends on the boundary conditions as follows: In case $(\mathbf{BC})_2$ we choose $C^\infty(\overline{\Omega})$, in case $(\mathbf{BC})_4$ we choose $\{\zeta \in C^\infty(\overline{\Omega}) \,:\, \zeta|_{\partial\Omega} = 0\}$ and in case $(\mathbf{BC})_6$ we choose $\{\zeta \in C^\infty(\overline{\Omega}) \,:\, \mathbf{n}\cdot\nabla\zeta|_{\partial\Omega} = 0\}$. Exploiting (52) and arguing similar as in **Remark 5** we obtain

Theorem 3.2. *Assume that* $\phi : \overline{\Omega} \to \mathbb{R}$ *and* $\boldsymbol{v} : \overline{\Omega} \to \mathbb{R}^3$ *are smooth functions. Then* $(\phi, \boldsymbol{v})$ *is a solution of (51) with boundary conditions* $(\boldsymbol{BC})_2$, $(\boldsymbol{BC})_4$ *or* $(\boldsymbol{BC})_6$ *if and only if* $(\phi, \boldsymbol{v})$ *fulfils:*

i) for all test functions $(\zeta, \boldsymbol{\varphi})$ chosen according to the boundary conditions stated above the identities

$$\int_\Omega \boldsymbol{v}_t \cdot \boldsymbol{\varphi}\, dx + \int_\Omega (\boldsymbol{v}\cdot\nabla)\boldsymbol{v}\cdot\boldsymbol{\varphi}\, dx + \int_\Omega \mathbb{S} : \nabla\boldsymbol{\varphi}\, dx -$$

$$- \int_\Omega \nabla\phi \left(G^I{}'_\phi - \nabla\cdot\left[G^I{}'_{\nabla\phi} - \nabla\cdot G^I{}'_{D^2\phi}\right]\right)\cdot\boldsymbol{\varphi}\, dx + \sigma\int_{\partial\Omega} \boldsymbol{v}\cdot\boldsymbol{\varphi}\, dS = 0, \qquad (59)$$

$$\int_\Omega \gamma\phi_t\zeta\, dx + \int_\Omega \gamma(\boldsymbol{v}\cdot\nabla)\phi\zeta\, dx + \int_\Omega G^I{}'_\phi\zeta\, dx + \int_\Omega G^I{}'_{\nabla\phi}\cdot\nabla\zeta\, dx +$$

$$+ \int_\Omega G^I{}'_{D^2\phi} : D^2\zeta\, dx = 0, \qquad (60)$$

holds for almost all $t \in (0,T)$,

ii) $\nabla\cdot\boldsymbol{v} = 0$ in $[0,T]\times\Omega$,

iii) the initial conditions in $\{0\}\times\Omega$ and the boundary condition $\boldsymbol{v}_n = 0$ on $[0,T]\times\partial\Omega$ holds and in case $(\boldsymbol{BC})_4$ we require $\phi = \phi_0$ on $[0,T]\times\partial\Omega$ and in case $(\boldsymbol{BC})_6$ we require $\boldsymbol{n}\cdot\nabla\phi = 0$ on $[0,T]\times\partial\Omega$.

Besides for all solutions of (51) with boundary conditions $(\boldsymbol{BC})_2$, $(\boldsymbol{BC})_4$ and $(\boldsymbol{BC})_6$ the energy identity

$$\frac{d}{dt}\boldsymbol{G}_E = -\int_\Omega \left(\gamma|D_t\phi|^2 + 2\mu|\mathbb{D}(\nabla\boldsymbol{v})|^2\right) dx - \sigma\int_{\partial\Omega} |\boldsymbol{v}|^2 dS$$

holds.

4. Relation to other models.

4.1. Relation to Korteweg's theory of capillarity. In section 3 we derived

$$\mathbb{T} + p\mathbb{I} = f(\mathbb{D}, \nabla\phi, D^2\phi, D^3\phi),$$

where

$$f(\mathbb{D}, \nabla\phi, D^2\phi, D^3\phi) = \mathbb{S}(\mathbb{D}) - \nabla\phi\otimes[G^I{}'_{\nabla\phi} - \nabla\cdot G^I{}'_{D^2\phi}] - D^2\phi\, G^I{}'_{D^2\phi}. \qquad (61)$$

In our model we observe a dependence of f on the derivatives of order three, i.e. the term $\nabla\cdot G^I{}'_{D^2\phi}$, appearing in the stress tensor. In Korteweg's theory of capillarity, see [20] Section 124, the general constitutive relation

$$\mathbb{T} + p\mathbb{I} = f(\mathbb{D}, \nabla\phi\otimes\nabla\phi, D^2\phi), \qquad (62)$$

was stated and the specific form

$$\mathbb{T} + p\mathbb{I} = \mathbb{S}(\mathbb{D}) - \lambda_1|\nabla\phi|^2\mathbb{I} - \lambda_2\nabla\phi\otimes\nabla\phi + \lambda_3(\Delta\phi)\mathbb{I} + \lambda_4 D^2\phi, \qquad (63)$$

where $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ are functions of ϕ or constants, was discussed.

Comparing (61) with (63) we observe that in Korteweg's theory a dependence on third derivatives is neglected.

If furthermore our constitutive variable Y does not contain $D^2\phi$ then our model would lead to

$$\mathbb{T} + p\mathbb{I} = \mathbb{S}(\mathbb{D}) - \nabla\phi\otimes G^I{}'_{\nabla\phi},$$

which reduces to a classical Korteweg stress tensor if $G^I(\nabla\phi) = \frac{1}{2}|\nabla\phi|^2$.

4.2. **Relation to the model of Du et al., see [5, 6].** To derive the model of Du et al., see (7), we choose $\mathbf{G}_E := E(\phi)$. For this special case we have $s = 2$ and

$$\begin{aligned} &G^0 := \frac{k}{2\epsilon}|f(\phi)|^2, \quad G^1 := \phi - \frac{\alpha}{|\Omega|}, \\ &G^2 := \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2 - \frac{\beta}{|\Omega|}, \\ &I^0 := 1, \quad I^1 := M_1(A(\phi)-\alpha), \quad I^2 := M_2(B(\phi)-\beta). \end{aligned}$$

Standard calculations give

$$G'^I_\phi - \nabla\cdot(G'^I_{\nabla\phi} - \nabla\cdot G'^I_{D^2\phi}) = \frac{\delta E}{\delta\phi},$$

so that exploiting **Remark 4** we finally get (7). So we note that starting directly from the first principles of thermodynamics we get by exploiting the dissipation inequality a specific expression for the stress tensor and finally the model of Du et al., see [5].

4.3. **Relation to the model by Jamet and Misbah [13].** Model 3 of Jamet and Misbah is based on the phase field bending energy

$$E_{\mathrm{Mis}} = \frac{\alpha}{2}\left[\mathcal{C}(\nabla\phi, \nabla\nabla\phi) - \mathcal{C}_0\right]|\nabla\phi|.$$

This energy is a different phase field approximation of the Helfrich bending energy than the approximation (3) which was chosen in Du et al., see [5]. For the energy (3) at least for $c_0 = 0$ it was already shown that one obtains the elastic energy (1) in the sharp interface limit, see Röger and Schätzle [18], and therefore we prefer this choice as the suitable phase field energy for (1). By taking into account (14) one finds after lengthy algebra the following phase field equation

$$D_t\phi = \frac{\kappa\alpha}{2}(\mathcal{C}-\mathcal{C}_0)[-\mathcal{C}(\mathcal{C}+\mathcal{C}_0) + 4H] - \alpha\nabla_s\cdot(\nabla_s\mathcal{C}),$$

where H is the Gauss curvature defined by

$$H = \frac{1}{2}[(\nabla_s\cdot\mathbf{n})^2 - \nabla_s\mathbf{n} : \nabla_s\mathbf{n}].$$

Our approach leads to the same phase field equation if we would choose $\mathbf{G}_E := E_{\mathrm{Mis}}$.

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