A new thermodynamic framework for active polar fluids

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Polar active fluids are an important topic in theoretical and applied physics, particularly in biophysics and the modeling of active materials such as living tissues. There are currently many continuum hydrodynamic frameworks for liquid crystals and active gels in the literature, which we would like to propose unifying here. In this paper, we propose a new thermodynamic framework for continuous mechanical modelling of active polar fluids. This framework is designed to take into account the most complex situations, combining activity, polarity, and nonlinear rheology. It unifies the skew-symmetric couple-stress theory with a general thermodynamic formalism recently developed by one of us, providing a more complete and rigorous description of active polar fluids. We show that, starting from a free energy and a dissipation potential, it is possible to derive constitutive equations that automatically satisfy the second law of thermodynamics. By construction, our framework allows a thermodynamically-consistent coupling of the different variables, in particular the density through the Hencky strain tensor. In addition, the use of a dissipation potential and of the Hencky strain tensor allows us to generalize Onsager's relations to nonlinear rheologies in large deformations, such as plasticity. Finally, a major advantage of our approach is its ability to naturally provide an energy estimate in the general case, for any free energy and any dissipation potential. Our theoretical framework paves the way for better modeling of active gels and could also be applied to other complex systems. In particular, we propose an application to the modeling of collective cell motion, where a rigorous treatment of energy and dissipation is crucial for understanding the underlying physical mechanisms.

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1. Introduction

1.1. Context

Epithelial cells proliferate and expand during the formation of embryos, heal wounds by filling the vacant space or invade neighbouring tissues if they themselves form tumour aggregates. In all cases, these phenomena largely involve the collective migration of cells. The cells interact with each other, attracting and repelling each other, and therefore display closely correlated movements [Dup03; TCJ12; Xi+19; Dur20].

Among the systems that exhibit collective behaviour, biological tissues belong to the family of active materials, i.e. those made up of self-propelled units, here the cells, capable of converting energy (previously stored or immediately available in their environment) into movement, thus taking the system out of thermodynamic equilibrium [Mar+13].

The transition from a disordered system to a collective motion results in a symmetry breaking in the system, which is similar to a phase change in a material [VZ12; Mar+13]. Just as phase changes occur as a function of the value of one or more so-called order or control parameters (e.g. temperature for a solid-liquid transition), the degree of symmetry of a system subject to collective behaviour must be quantifiable. This is the case for cells, which have the ability to reorganise their internal structure asymmetrically in response to external stimuli, whether chemical or physical. This asymmetry is called polarity and gives the cell a front-to-back direction, in which it can exert forces [LMT16]. To describe collective cell migration, the literature mainly considers polarity as a vector with variable norm [KP13; Not+16; BC17; CR17; HS17; Cza+18; AT19; BM19; Pér+19; Boo+21], which is denoted $\boldsymbol{p}$ in the following; symmetry breaking then results in a polar order. In other situations, it may be more appropriate to describe polarity as a tensor [LMT16; Pop+17; Saw+17]; symmetry breaking then leads to a nematic order.

The nature and physical characterisation of this polarity, its role in the emergence of collective movements and its coupling with the other physical quantities involved therefore constitute a major challenge and an open question in the modelling of the collective movement of epithelia. Given the arbitrary complexity of the coupling between mechanics and polarity, it is important to have thermodynamic guarantees for the resulting equations. Indeed, the now classical hydrodynamic theory [Kru+05; Mar+13; AT19] omits an important term in the expression of the stress tensor. This term is called the Ericksen stress tensor in the theory of liquid crystals [GP93, equation (3.100)], from which the theory of active gels is inspired. Here, we show that omitting this term can lead to solutions violating the second principle of thermodynamics. Moreover, this classical hydrodynamic theory uses the Onsager relations to construct its constitutive equations, which limits force-flux relations to linear cases only, and therefore does not allow the introduction of nonlinear rheologies such as plasticity. In this paper, we propose a rigorous mathematical framework that guarantees by construction the second principle of thermodynamics and the generalized Onsager-Edelen symmetry, an extension of the linear Onsager relations to the nonlinear case [Sar24, section 4.3].

1.2. State of the art of physical models of collective cell migration

There are broadly two approaches to modelling collective motion. The first approaches the problem from the point of view of discrete mechanics and focuses on modelling the individual behaviour of cells and their interactions [CR17; HS17; AT19; Xi+19; Bea+22]. It allows collective effects to emerge and links ingredients at the cellular level with emerging behaviour at the tissue level. The second approach is based on continuum mechanics, and is the one adopted in this paper. It is relevant insofar as, experimentally, it is possible to extract descriptive mechanical quantities at a mesoscopic scale, i.e. that are statistically homogeneous and continuous. In other words, it is possible to neglect the effect of fluctuations intrinsic to the microstructure of the epithelium with respect to variables that have been averaged over a small representative group of cells, assumed much bigger than a cell but much smaller than the complete tissue [Tli+18]. It is therefore possible to describe the tissue locally, at the level of these cell groups, using tensorial variables that are regular in space and time, which justifies the approach [CD07; Gra+08] – this approach is already widely used in the literature to describe this type of system [Sto84; GP93; Fun93; Eri99; Eri01; Hum03; CD07; Mar+13; Tli+15; HS17; JGS18; AT19; Xi+19].

The vast majority of continuous models of collective movement in epithelia in the literature, also called hydrodynamic models, are based on a common set of assumptions:

(i) tissues under consideration can be likened to shallow incompressible isothermal fluids: they are continuum undergoing large deformations, the thickness of which is assumed to be negligible compared with the characteristic length, so that migration can be considered to be two-dimensional;

(ii) migration takes place under conditions that do not allow cells to be observed growing, dividing or dying;

(iii) the system respects the basic principles of continuum mechanics and is at mechanical equilibrium: migration is slow, of the order of a micron per minute, so inertia can be neglected;

(iv) migration takes place on timescales that prevent genetics from modifying the mechanical properties of cells;

(v) the activity of cells is sufficient for them to change their neighbours without a yield strain, so the contribution of plasticity to rheology can be neglected.

Several reviews of cell migration models (discrete and/or continuous) exist in the literature; for instance, [HS17; AT19; BM19] can be consulted.

More generally, in mathematical modelling for biology, a broad consensus has been established in favour of viscoelastic mechanical models [Fun93; Cia03; Hum03; CD07; CV07; Bre+09; Éti+15; Clé+17; VCL20], and the modelling of collective cell motion is no exception to the rule, as shown by the three reviews cited above. In cases where the arrangement of cells within the tissue remains unchanged, for example in arterial walls, muscles or skin, the tissue behaves like an elastic or viscoelastic solid, and can therefore be described using, among others, the Kelvin-Voigt [BM19] or Burger models. Conversely, if the arrangement evolves in response to tissue deformation or strong cell motility, then the tissue is subjected to large unbounded deformations over relatively long times, and acts more like a viscoelastic fluid [Tli+20]: it can be more accurately described with, for example, Maxwell [AT19] or Oldroyd [Old50] models.

However, a viscoelastic model alone is not sufficient to describe the active dynamics of cell migration, and it needs to be supplemented with an evolution equation for the polarity. This can be obtained from the global Helmholtz free energy $\mathscr{F}$ of the system as follows [AT19]:

$$\overset{\square}{\boldsymbol{p}} = -\frac{1}{\gamma}\frac{\partial \mathscr{F}}{\partial \boldsymbol{p}}, \tag{1}$$

where γ is a rotational viscosity. The notation $\overset{\square}{\boldsymbol{p}} \coloneqq \partial_t \boldsymbol{p} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{p} - (\boldsymbol{W}(\boldsymbol{v}) + a\boldsymbol{D}(\boldsymbol{v}))\cdot\boldsymbol{p}$ stands for the Gordon-Schowalter objective rate, where $\boldsymbol{v}$ is the velocity field, $\boldsymbol{W}(\boldsymbol{v}) = (\nabla\boldsymbol{v} - \nabla\boldsymbol{v}^{\mathsf{T}})/2$ is the vorticity tensor, $\boldsymbol{D}(\boldsymbol{v}) = (\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^{\mathsf{T}})/2$ is the deformation rate tensor and $a \in \mathbb{R}$ is a parameter. The operator $\square \cdot \square$ refers to the contracted product and its associated norm is noted $|\cdot|$. Here, we adopt the convention $\nabla\boldsymbol{v} = (\frac{\partial v_i}{\partial x_j})_{i,j}$ for the gradient of a vector field. Thanks to this formulation, it is possible to propose a coupling between polarity and other physical fields such as cell density ρ [AT19], elastic deformation [Mar14; Tli+18], the anisotropy of cell shape [Cza+18] or the concentration of a chemical signal [Not+16] or of one or more proteins [IM23], such as actomyosin [BM19].

A final ingredient characterising continuous models of cell migration is the presence of an active stress $\boldsymbol{\sigma}_a$ often defined as a function of the polarity [Mar+13; AT19]:

$$\boldsymbol{\sigma}_a \coloneqq -\zeta\Delta\mu\, \boldsymbol{p}\otimes\boldsymbol{p}, \tag{2}$$

where $\zeta\Delta\mu$ is the active stress coefficient and $\Delta\mu$ can be seen for instance as the energy gain per ATP molecule. For instance, it can be interpreted as the result of the contraction of actin filaments induced by molecular motors. The characteristic of this term is that it can a priori adopt any sign, reflecting both contraction ($\zeta < 0$) and extension ($\zeta > 0$), which tends to put the system out of equilibrium. In practice, the sign of ζ is fixed in advance, and the coefficient $\zeta \Delta\mu$ is mostly taken to be positive [Mar+13]. Note that generalisations of this definition have been proposed, in particular by introducing a dependence on the concentration of a given chemical agent [Not+16; BM19].

1.3. State of the art of frameworks to derive hydrodynamics models

1.3.1. Tissues as active gels

The protein filaments (such as actin) that make up the cytoskeleton are elongated objects immersed in the cytoplasm. When the cell polarises, the fibres contract and, more importantly, align. In addition, the cell is an active material and can regulate its mechanical properties and microstructure, in particular by consuming ATP. Such a material is generally referred to as an active gel [Mar+13].

The average orientation of the active gels filaments is represented by the vector $\boldsymbol{p}$, called the director and, unlike continuous models of collective cell migration, assumed to be unitary, i.e. $|\boldsymbol{p}| = 1$. Through this constraint, the theory implicitly considers filaments as rigid rods: the distinction between the ends of molecules is irrelevant, so the roles played by $-\boldsymbol{p}$ and $-\boldsymbol{p}$ are identical. Mathematically, this translates into an evolution equation invariant to the $\boldsymbol{p} \mapsto -\boldsymbol{p}$ transformation. In our context, this is suitable for the axial part of the anisotropy of the cells, in this case their shape, but not for the polar part represented by the vector $\boldsymbol{p}$, which distinguishes the front and back of the cell and vanishes when the cell is not polarized.

If a tissue is equated with its underlying protein network, then it can be treated as an active gel, but at the cost of several simplifications: we do not take into account the fact that $\boldsymbol{p}$ is a vector whose modulus can vary, the fact that $\boldsymbol{p}$ and $-\boldsymbol{p}$ are different vectors, and the fact that cellular materials can have plasticity due to cellular rearrangements.

With or without these simplifications, most models of collective cell migration in the literature are in fact adaptations of the theory of active gel [Mar+13; JGS18; AT19; BM19]. The latter extends the nematic liquid crystal formalism to active gels, mainly by introducing an active stress tensor as in (2). The theory of nematic liquid crystals provides a theoretical thermodynamic framework that makes it possible to construct continuum mechanics equations from Onsager's principle, coupling an order parameter describing the level of symmetry of the system, as explained previously, with the usual mechanical fields (velocity, deformation, etc.), while guaranteeing the second principle of thermodynamics and the objectivity of the equations obtained [GP93]. The result is the equation (1) and a Cauchy stress tensor which is also derived from the free energy.

Although the theory of active gels has already envisaged the coupling of polarity with the Maxwell model [Mar+13; AT19], it does not a priori allow the systematic introduction of any rheology, nor does it facilitate the coupling of different physical fields with elastic deformation in the context of large deformations.

1.3.2. Micromechanical generalisations of the liquid crystal theory

Since the introduction of the theory of liquid crystals, many other theoretical frameworks have emerged in the literature. Although they have not been considered in the construction of equations for the theory of active gels or models of collective cell migration, they are nonetheless relevant.

These theoretical frameworks are based on the following observation (which we restrict here to cells, but the reasoning is the same): cells have the capacity to align their polarities locally, in the same way as sardines orient themselves in the same direction as their neighbours in a shoal. The distance over which neighboring polarities maintain a certain alignment before it is gradually reduced is called the coherence length. To create this alignment, the cells can be induced to exert torques, using rotations that occur on a microscopic scale, relative to the size of the tissue, called microrotations. From this point of view, tissues are continuum whose microscopic scale can have a significant influence on the macroscopic behaviour. A priori, classical continuum mechanics does not allow these length scales to be taken into account.

The first attempt to put the concept of microrotation into a mathematical formalism probably dates back to the beginning of the 20th century with the publication of [CC09], which developed the beginnings of the theory of so-called micropolar media, in which a new kinematic variable is introduced, microrotation, assumed to be independent of macroscopic rotation. This theory has since been generalized by the theory of microcontinuum, which applies to both solids [Eri99] and fluids [Eri01]. For example, it has been used in the mechanical modelling of esophageal tissue [San+14].

A microcontinuum is a continuum whose microscopic constituents are themselves considered to be deformable and contribute to the macroscopic behaviour of the material. The intrinsic deformability and orientation of a microscopic constituent are described using a so-called microdeformation tensor, which generalises the concept of microrotation and is assumed to be representable by a continuous tensor field at the macroscopic level. It therefore adds a certain number of additional degrees of freedom to the kinematic level, depending on the material under consideration. In particular, the theory of micropolar media adds three more. As a result, the conservation laws derived from this theory of microcontinuum are much more voluminous than in the framework of classical continuum mechanics: in the most general framework, in addition to the conservation equations for mass and momentum, we have to add a conservation equation known as the microinertia equation (6 equations) and the angular momentum equation (9 equations), which involves a tensor of order 3. In addition to the complexity of such a theory, the concept of microstrain is not necessarily legitimate as pointed out in [HD11].

Couple stress theory, on the other hand, seeks to describe the influence of microstructure on macroscopic behaviour solely on the basis of purely kinematic continuous fields. It also introduces the concept of the couple stress tensor, which is the analogue of the Cauchy stress tensor for rotations. A first version of this theory applied to solids appeared in the early 1960s, before being adapted to fluids in 1966 [Sto66]. Although it provides a solid mechanical basis for the theory of liquid crystals, and a fortiori for models of collective cell migration, it suffers from the same defects as the classical theory of liquid crystals presented in [GP93], given at the end of the previous section. The original couple stress theory suffers from some indeterminacies [HHD15], which two papers in the literature have attempted to remove [Yan+02; HHD15], making it a self-consistent size-dependent theory within the context of classical continuum mechanics. In the first one, the couple stress is proven to be deviatoric and symmetric by assuming the couple moment must vanish; we will refer to it as the deviatoric-symmetric couple stress theory. The second yields a diametrically opposed conclusion, proving that the couple stress is skew-symmetric; we will refer to it as the skew-symmetric couple stress theory. There seems to be no consensus on the question, even though according to [HD11], the formulation in [Yan+02] « is not consistent with proper boundary condition specifications and energy conjugacy within the principle of virtual work ».

1.3.3. Hydrodynamics with a dissipation potential

Alternatively, in a preceding paper, some of us have proposed to apply the dissipation potential formalism to tissue dynamics [Tli+15]. This formalism relies on the dissipation potential, a function that describes the dissipative phenomena (i.e. non-equilibrium thermodynamic) occurring in the dynamics under consideration and allows the introduction of nonlinear rheologies (unlike Maxwell's), such as plasticity for example, thus generalizing Onsager's linear relations. Like the theory of active gels, this theoretical framework uses the free energy in addition to the dissipation potential, making it possible to derive a large number of constitutive equations, which are guaranteed to satisfy the second principle of thermodynamics.

The concept of dissipation potential was introduced independently by Ziegler in 1968 [Zie68], by Verhás in 1972 [Ver72], by Edelen in 1973 [Ede73; Ede74] and by Moreau in 1974 [Mor74]. In 1975, Halphen and Son Nguyen proposed the formalism of generalized standard materials [HS75] which, although it applies only to the case of small deformations, relaxes the hypothesis of differentiability of the dissipation potential. More recently, one of us has updated the dissipation potential formalism and proposed a unified framework for it [Sar24]. However, this framework does not allow higher-order derivatives to be introduced into the constitutive equations, and thus the equations of the theory of nematic liquid crystals and its derivatives to be obtained. For example, to take into account the alignment of polarities, it is common to introduce the Laplacian of the polarity field into the equations, something the framework does not allow.

Conceptually similar, the use of a Rayleigh potential allows similar results to be obtained, in particular by generalizing Onsager's linear relations. For example, it has been used to obtain the hydrodynamic equations for nematic liquid crystals [SV01; SMV04] and, more recently, for active nematic gels [Mir+25].

1.4. Scope of this article

In this paper, we propose a unified framework of all these theories allowing at least to obtain the equations of the theory of active gels and furthermore to couple it with more complex rheology. For this purpose, we combine the skew-symmetric couple stress theory [HHD15] and the unified formalism of dissipation potential developed in [Sar24].

Like the others, this new theoretical framework allows to obtain objective constitutive equations that satisfy the second principle of thermodynamics, based solely on free energy and dissipation potential. As in active gel theory and contrary to the framework in [Sar24], the free energy here can depend, among other things, on the polarity gradient, allowing a Laplacian of the polarity field to be incorporated into the equations. In addition, the use of a dissipation potential makes it possible to generalize Onsager's relations to the nonlinear case, and thus to introduce a wide variety of different rheologies, such as plasticity. On the other hand, the introduction of viscoelastic ingredients is not discussed in this paper, but is possible by considering the so-called intermediate configuration, developed for example in [Sar24, section 3.6]. Such ingredients could be used to describe nonlinear elasticity, which is crucial in morphogenesis for instance.

We also show how our framework enables us to obtain a rigorous coupling of the various physical fields with the density of the continuous medium under consideration and an energy estimate of the equations from the theory of active gels, a result which had not been envisaged by the other formalisms and which is the gateway to results of the mathematical existence of solutions to the equations. Importantly, by construction our framework includes the term called Ericksen tensor in the theory of liquid crystals [GP93, equation (3.100)], which we show to be indispensable for energy estimate. In the literature of active gel theory, this contribution to the stress tensor is mentioned in some reference articles [JGS18; ACJ22] but is absent from others [Mar+13; AT19]. In simple cases, the absence of this term has no detectable impact on equation solutions. However, we argue that in the general case the absence of this term can have crucial effects in relation with the second principle of thermodynamics. We discuss its consequence on the solution stability.

Unlike [Mir+25], our approach is based on more recent developments in microrotation theory, bases its argument on the Clausius-Duhem inequality, and uses more general tools to deal with large deformations, such as the Hencky strain tensor. In particular, this last consideration allows a rigorous coupling with the density field and paves the way for a greater variety of rheologies under large deformations, as shown in [Sar24].

An outline of the paper is as follows. Section 2 gives a brief presentation of the skew-symmetric couple stress theory of Hadjesfandiari, Hajesfandiari, and Dargush [HHD15] and of the unified thermodynamic framework developed in [Sar24]. Then, section 3 combines them in a new theory of constitutive equations within the couple stress theory. In section 4, this new framework is applied to active gels and collective cell migration. Finally, in section 5, the resulting system of equations is solved numerically on a simple geometry to illustrate the effect of active stress.

2. Conservation laws and constitutive equations

In this section, we first give the conservation laws in the skew-symmetric couple stress theory, then recall the main ingredients to build thermodynamically consistent constitutive equations in classical continuum mechanics, based on the framework developed in [Sar24].

2.1. Conservation laws in the skew-symmetric couple stress theory

Within a size-dependent continuum, the extension of the classical continuum in the skew-symmetric couple stress theory, boundaries of elementary volumes are subject to both a normal force-traction vector and a normal moment-traction vector. The Cauchy's theorem then gives the existence of the Cauchy stress tensor $\boldsymbol{\sigma}$ and the couple stress tensor $\boldsymbol{\mu}$, which has been proven to be skew-symmetric [HHD15]. They represent respectively the surface forces and couples. The linear momentum and angular momentum conservation laws in the domain $\Omega \subset \mathbb{R}^3$ write respectively [HHD15, equation (53) and (54)]

$$\rho\dot{\boldsymbol{v}} - \mathbf{div}\,\boldsymbol{\sigma}^{\mathsf{T}} = \rho\boldsymbol{b} \quad \text{in} \quad \Omega \times \,]0,+\infty[, \tag{3a}$$

$$-\mathbf{div}\,\boldsymbol{\mu}^{\mathsf{T}} = \boldsymbol{\epsilon} : \boldsymbol{\sigma} \ \text{in} \quad \Omega \times \,]0,+\infty[, \tag{3b}$$

where $\boldsymbol{v}$ is the velocity field, $\dot{\varphi} := \partial_t\varphi + (\boldsymbol{v}\cdot\nabla)\varphi$ is the Lagrangian rate, $\boldsymbol{b}$ represents the volume forces and $\boldsymbol{\epsilon}$ is the Levi-Civita third order pseudo-tensor. Here, $\boldsymbol{\sigma}$ is not necessarily a symmetric tensor, but note that if $\boldsymbol{\mu} = \mathbf{0}$, then it is. The divergence of a tensor field $\boldsymbol{\tau}$ is defined as $\mathbf{div}\,\boldsymbol{\tau} = \tau_{ij,j}$, with the Einstein summation convention. The operator $\Box : \Box$ refers to the double contracted product and its associated norm is noted $|\cdot|$. Those equations are complemented with the law of conservation of mass:

$$\frac{\partial\rho}{\partial t} + \operatorname{div}(\rho\boldsymbol{v}) = 0 \ \text{in} \quad \Omega \times \,]0,+\infty[. \tag{3c}$$

In practice, constitutive equations satisfying the second principle are determined from the Clausius-Duhem inequality. This inequality links the Lagrangian rate of the local free energy Ψ (hence $\mathscr{F} := \int_\Omega \rho\Psi\,\mathrm{d}\boldsymbol{x}$ is the global free energy) to energetically conjugated pairs coupling deformation rates and stress tensors. For an isothermal size-dependent fluid, the Clausius-Duhem inequality is [HHD15, equation (90)]

$$-\rho\dot{\Psi} + \mathbf{sym}\,\boldsymbol{\sigma} : \boldsymbol{D}(\boldsymbol{v}) + \boldsymbol{\mu} : \boldsymbol{K}^{\mathsf{T}} \geqslant 0 \ \text{in} \quad \Omega \times \,]0,+\infty[, \tag{3d}$$

where $\mathbf{sym}$ gives the symmetric part of a tensor. The tensor $\boldsymbol{K} := \boldsymbol{W}(\boldsymbol{\omega})$, where $\boldsymbol{\omega} := \frac{1}{2}\nabla \times \boldsymbol{v}$ is the vorticity, is the mean curvature rate tensor and is energetically conjugated to the couple stress tensor. Because both $\boldsymbol{\mu}$ and $\boldsymbol{K}$ are skew-symmetric, they can be better represented by only a vector, respectively $\boldsymbol{l}$ and $\boldsymbol{k} = \frac{1}{2}\nabla \times \boldsymbol{\omega}$, so that

$$\boldsymbol{\mu} = -\boldsymbol{\epsilon} \cdot \boldsymbol{l} = \begin{pmatrix} 0 & -l_3 & l_2 \\ l_3 & 0 & -l_1 \\ -l_2 & l_1 & 0 \end{pmatrix}, \quad \boldsymbol{K} = -\boldsymbol{\epsilon} \cdot \boldsymbol{k} = \begin{pmatrix} 0 & -k_3 & k_2 \\ k_3 & 0 & -k_1 \\ -k_2 & k_1 & 0 \end{pmatrix}. \tag{3e}$$

Then, (3d) writes equivalently

$$-\rho\dot{\Psi} + \mathbf{sym}\,\boldsymbol{\sigma} : \boldsymbol{D}(\boldsymbol{v}) - 2\boldsymbol{l} \cdot \boldsymbol{k} \geqslant 0 \text{ in } \ \Omega \times]0, +\infty[. \tag{3f}$$

2.2. Building constitutive equations

Here, we recall the thermodynamic framework proposed in [Sar24, Remark 4.3]. It applies in three steps:

1. Choose a set of objective thermodynamic variables $\mathbb{A}$ and corresponding objective rates $\mathbb{D}$, expressed as corotational rates of the former. In our case, $\mathbb{A}$ could contain the polarity field, the elastic strain tensor, etc.

2. Define an objective Helmholtz free energy Ψ with respect to $\mathbb{A}$. If $\mathbb{A}$ contains a vector, then Ψ should only depend on its norm. If it contains a tensor, then Ψ should only depend on its corresponding sets of invariants (see for instance [Eri80, Appendix B]). In that case, Ψ is said to be objective-isotropic [Sar24, definition 2.38].

3. Define an objective dissipation potential Φ with respect to $\mathbb{D}$; it is allowed to depend on $\mathbb{A}$. It should be positive and satisfy $\Phi(\mathbb{D} = 0; \mathbb{A}) = 0$ and the inequality

$$\left(\frac{\partial \Phi}{\partial \mathbb{D}}(\mathbb{D}; \mathbb{A}) \,\middle|\, \mathbb{D} \right) \geqslant 0. \tag{4}$$

The operator $(\cdot \mid \cdot)$ refers to the canonical inner product, obtained by integrating over Ω the pointwise inner product of two fields of matching nature (scalar, vector or tensor). The associated norm is denoted by $\|\cdot\|$. If Φ is convex, then inequality (4) is automatically satisfied.

Applying those three steps and assuming the gyroscopic terms vanish, we obtain the following thermodynamically-consistent constitutive equations:

$$\boldsymbol{\sigma} \in \rho \frac{\partial \Psi}{\partial \boldsymbol{h}} + \frac{\partial \Phi}{\partial \boldsymbol{D}(\boldsymbol{v})}, \tag{5a}$$

$$0 \in \rho \frac{\partial \Psi}{\partial \mathbb{A}_i} + \frac{\partial \Phi}{\partial \mathbb{D}_i}, \tag{5b}$$

where $\mathbb{A}_i$ represents the i-th thermodynamic variable and $\mathbb{D}_i$ its corresponding rate. The tensor $\boldsymbol{h}$ is the Hencky strain, representing the true strain in the large deformations context. It can be proven that $\boldsymbol{D}(\boldsymbol{v})$ expresses actually as a corotational rate of the Hencky strain. When Φ is differentiable, then the symbol $\in$ can be replaced by a simple equality. When it is not but is convex, its partial derivative actually refers to its subdifferential with respect to the considered variable.

As we previously said, this framework does not allow higher-order derivatives in the constitutive equations (5b) and thus excludes the polarity equation from the active gel theory. From now, we are going to show how it is possible to extend it thanks to the skew-symmetric couple stress theory so it becomes possible.

3. Our framework

3.1. Introduction

To build our framework, we follow a rather classic approach, as presented for instance in [Eri01; Sar24]. We start off from the Clausius-Duhem inequality (3f), by integrating it over the whole domain then expanding the Lagrangian rate of the free energy with respect to the thermodynamic variables $\mathbb{A}$, using the chain rule. Then, we can write the inequality under a big inner product between generalized thermodynamic forces (the stress tensor $\boldsymbol{\sigma}$, the couple stress vector $\boldsymbol{l}$ and the partial derivatives of Ψ with respect to $\mathbb{A}$) and generalized thermodynamic fluxes (the rates $\mathbb{D}$). We conclude with the convexity and the positivity of the dissipation potential Φ.

The main difficulty lies in finding an appropriate kinematic measure of the rotational deformation, a corotational derivative of which gives the mean curvature rate vector $\boldsymbol{k}$. We denote by $\boldsymbol{r}$ this deformation vector, defined as the unique solution to the Cauchy's problem

$$\overset{\circ}{\boldsymbol{r}} = \boldsymbol{k}, \quad \text{in } \Omega \times]0, +\infty[, \tag{6a}$$
$$\boldsymbol{k}(t=0) = \boldsymbol{k}_0, \text{ in } \Omega, \tag{6b}$$

where $\overset{\circ}{\boldsymbol{r}} := \partial_t \boldsymbol{r} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{r} - \boldsymbol{W}(\boldsymbol{v}) \cdot \boldsymbol{r}$ denotes the corotational rate of a vector. We could also introduce the mean curvatue rate tensor $\boldsymbol{R} = -\boldsymbol{\epsilon} \cdot \boldsymbol{r}$. The kinematic definition of $\boldsymbol{R}$ using the deformation gradient is beyond the scope of this paper. Note that by construction, $\boldsymbol{R}$ is skew-symmetric.

Just as the Cauchy stress tensor $\boldsymbol{\sigma}$ is the conjugate of the Hencky strain $\boldsymbol{h}$ via the free energy Ψ, the couple stress vector $\boldsymbol{l}$ will be that of the mean curvature vector $\boldsymbol{r}$ we have just introduced.

Now we assume the local free energy Ψ to be a function of the thermodynamic variables $\mathbb{A} = (\boldsymbol{h}, \boldsymbol{r}, c, \boldsymbol{g}, \boldsymbol{p}, \boldsymbol{\tau})$, where $\boldsymbol{g}$ (resp. $\boldsymbol{\tau}$) is a vector (resp. a second order tensor) representing the spatial variations of the concentration c (resp. the polarity $\boldsymbol{p}$). We then define the global free energy $\mathscr{F}$ by

$$\mathscr{F}(\boldsymbol{h}(t), \boldsymbol{r}(t), c(t), \boldsymbol{p}(t)) = \int_{\Omega(t)} \rho(t)\Psi(\boldsymbol{h}(t), \boldsymbol{r}(t), c(t), \boldsymbol{g}(t), \boldsymbol{p}(t), \nabla\boldsymbol{p}(t))\, \mathrm{d}\boldsymbol{x}. \tag{7}$$

Note that we do not need to precise the dependence of $\mathscr{F}$ with respect to ρ, despite the presence of the latter in its expression, because the density is linked to the Hencky strain tensor through the relation [Sar24, equation (3.18)]

$$\rho = \rho_0 \exp(-\operatorname{tr} \boldsymbol{h}), \tag{8}$$

where ρ_0 is the density in the reference frame.

Similarly, let us assume the dissipation potential Φ is a function of the thermodynamic rates $\mathbb{D} = (\boldsymbol{D}(\boldsymbol{v}), \boldsymbol{k}, \dot{c}, \overset{\square}{\boldsymbol{p}})$, where we recall that $\overset{\square}{\boldsymbol{p}} := \partial_t \boldsymbol{p} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{p} - (\boldsymbol{W}(\boldsymbol{v}) + a\boldsymbol{D}(\boldsymbol{v})) \cdot \boldsymbol{p}$.

In the following, we use the abusive but widely used notation

$$\frac{\partial \Psi}{\partial \nabla c} = \left.\frac{\partial \Psi}{\partial \boldsymbol{g}}\right|_{\boldsymbol{g}=\nabla c}, \quad \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} = \left.\frac{\partial \Psi}{\partial \boldsymbol{\tau}}\right|_{\boldsymbol{\tau}=\nabla \boldsymbol{p}}. \tag{9}$$

3.2. Constitutive equations

If the boundary conditions

$$\boldsymbol{l} \times \boldsymbol{n} = \boldsymbol{0}, \; \frac{\partial \Psi}{\partial \boldsymbol{r}} \times \boldsymbol{n} = \boldsymbol{0}, \; \frac{\partial \Psi}{\partial \nabla c} \cdot \boldsymbol{n} = 0, \; \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} \cdot \boldsymbol{n} = \boldsymbol{0}, \tag{10}$$

hold in $\partial\Omega \times]0, +\infty[$, then the constitutive equations are given by

$$\mathbf{sym}\,\boldsymbol{\sigma} \in \frac{\partial(\rho\Psi)}{\partial \boldsymbol{h}} + \frac{\partial \Phi}{\partial \boldsymbol{D}(\boldsymbol{v})} - \nabla c \otimes \rho \frac{\partial \Psi}{\partial \nabla c} + a\,\mathbf{sym}\left(\boldsymbol{p} \otimes \frac{\partial \mathscr{F}}{\partial \boldsymbol{p}}\right) - \rho \nabla \boldsymbol{p}^{\mathsf{T}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} \tag{11a}$$

$$\mathbf{skw}\,\boldsymbol{\sigma} = -\frac{1}{2}\boldsymbol{W}\left(\rho \frac{\partial \Psi}{\partial \boldsymbol{r}}\right) + \mathbf{skw}\left(\boldsymbol{p} \otimes \frac{\partial \mathscr{F}}{\partial \boldsymbol{p}}\right) \tag{11b}$$

$$0 \in \frac{\partial \mathscr{F}}{\partial c} + \frac{\partial \Phi}{\partial \dot{c}}, \tag{11c}$$

$$\mathbf{0} \in \frac{\partial \mathscr{F}}{\partial \boldsymbol{p}} + \frac{\partial \Phi}{\partial \overset{\square}{\boldsymbol{p}}}, \tag{11d}$$

where $\mathbf{skw}$ gives the skew-symmetric part of a tensor and $\frac{\partial \mathscr{F}}{\partial c}$ (resp. $\frac{\partial \mathscr{F}}{\partial \boldsymbol{p}}$) is the Gâteaux derivative of $\mathscr{F}$ with respect to c (resp. $\boldsymbol{p}$), that is

$$\frac{\partial \mathscr{F}}{\partial c} = \rho \frac{\partial \Psi}{\partial c} - \operatorname{div}\left(\rho \frac{\partial \Psi}{\partial \nabla c}\right), \quad \frac{\partial \mathscr{F}}{\partial \boldsymbol{p}} = \rho \frac{\partial \Psi}{\partial \boldsymbol{p}} - \mathbf{div}\left(\rho \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}}\right). \tag{12}$$

Note there is not any constitutive equation for the couple stress tensor $\boldsymbol{\mu}$ (nor its vector counterpart $\boldsymbol{l}$), rather a constitutive relation is directly given for the skew-symmetric part of the stress tensor $\boldsymbol{\sigma}$. An expression for the couple stress vector can still be retrieved through lemma 8 and the use of the identities $\boldsymbol{\epsilon} : (\boldsymbol{y} \otimes \boldsymbol{z}) = \boldsymbol{y} \times \boldsymbol{z}$ and $\boldsymbol{\epsilon} : \boldsymbol{W}(\boldsymbol{q}) = -\nabla \times \boldsymbol{q}$:

$$\nabla \times \boldsymbol{l} = -\frac{1}{2}\nabla \times \left(\rho \frac{\partial \Psi}{\partial \boldsymbol{r}}\right) + \frac{\partial \mathscr{F}}{\partial \boldsymbol{p}} \times \boldsymbol{p}. \tag{13}$$

However, when $\frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} = \mathbf{0}$, a constitutive equation for the couple stress vector can be obtained, involving the (sub)differential of Φ with respect to the mean curvature rate vector $\boldsymbol{k}$, if the boundary condition

$$\frac{\partial \Psi}{\partial \nabla c} \cdot \boldsymbol{n} = 0 \tag{14}$$

holds in $\partial\Omega \times]0, +\infty[$:

$$\mathbf{sym}\,\boldsymbol{\sigma} \in \frac{\partial(\rho\Psi)}{\partial \boldsymbol{h}} + \frac{\partial \Phi}{\partial \boldsymbol{D}(\boldsymbol{v})} - \nabla c \otimes \rho \frac{\partial \Psi}{\partial \nabla c} + a\boldsymbol{p} \otimes \rho \frac{\partial \Psi}{\partial \boldsymbol{p}} \tag{15a}$$

$$\boldsymbol{l} \in -\frac{1}{2}\rho \frac{\partial \Psi}{\partial \boldsymbol{r}} - -\frac{1}{2}\frac{\partial \Phi}{\partial \boldsymbol{k}} \tag{15b}$$

$$0 \in \frac{\partial \mathscr{F}}{\partial c} + \frac{\partial \Phi}{\partial \dot{c}}, \tag{15c}$$

$$\mathbf{0} \in \rho \frac{\partial \Psi}{\partial \boldsymbol{p}} + \frac{\partial \Phi}{\partial \overset{\square}{\boldsymbol{p}}}. \tag{15d}$$

Note the term $\boldsymbol{p} \otimes \rho \frac{\partial \Psi}{\partial \boldsymbol{p}}$ does not present the $\mathbf{sym}$ operator in the expression of the stress tensor (15a). Indeed, when the free energy does not depend on the polarity gradient, $\frac{\partial \Psi}{\partial \boldsymbol{p}}$ is necessary colinear to the polarity field, by objective-isotropy. In this case, the skew-symmetric part of the stress tensor can be obtained from lemma 8:

$$\mathbf{skw}\,\boldsymbol{\sigma} = \boldsymbol{W}(\boldsymbol{l}). \tag{16}$$

Thus, if $\frac{\partial \Phi}{\partial \boldsymbol{k}} = \mathbf{0}$, constitutive equations (15) lead to (11) when $\frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} = \mathbf{0}$.

Theorem 1 – Second law of thermodynamics

If the dissipation potential Φ is convex and positive, and satisfies $\Phi(\mathbb{D}=0;\mathbb{A})=0$ for any $\mathbb{A}$, then the Clausius-Duhem inequality (3d) (or equivalently (3f)) is satisfied when equations (11) (or (15) when $\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}=\boldsymbol{0}$) are chosen as constitutive equations.

Proof. See appendix B.2. ■

Remark I – *Converse of the theorem*: The convexity of the dissipation function is a sufficient condition to obtain the second principle of the thermodynamics, but is not necessary according to [Sar24, remark 4.4]. The Edelen's theorem is more general because it gives in addition a necessary condition, but to our knowledge is not applicable in this context, since it only applies when thermodynamic variables are defined in finite-dimensional spaces.

Remark II – *Boundary conditions*: See remark VII in appendix B.2.

Remark III – *Viscoelasticity*: The introduction of viscoelastic ingredients, not discussed here, is entirely possible and requires the introduction of a new thermodynamic variable $\boldsymbol{h}_e$, the reversible part of the Hencky strain tensor, whose existence can be established by considering the so-called intermediate configuration, as explained in section 3.6 in [Sar24]. Several examples are also developed in sections 5.11 to 5.15 in [Sar24].

3.3. Resulting equations

The derived equations (11) can be gathered with the conservation laws from section 2.1 to become the

Problem 1. Find $\boldsymbol{v}$, ρ, c and $\boldsymbol{p}$ defined in $\Omega\times]0,+\infty[$ such that

$$\rho\dot{\boldsymbol{v}}-\mathbf{div}\,\boldsymbol{\sigma}^{\mathsf{T}}=\rho\boldsymbol{b} \text{ in } \Omega\times]0,+\infty[, \tag{17a}$$

$$\frac{\partial\rho}{\partial t}+\operatorname{div}(\rho\boldsymbol{v})=0 \quad\text{in}\quad \Omega\times]0,+\infty[, \tag{17b}$$

$$\frac{\partial\Phi}{\partial\dot{c}}+\rho\frac{\partial\Psi}{\partial c}-\operatorname{div}\left(\rho\frac{\partial\Psi}{\partial\nabla c}\right)\ni 0 \quad\text{in}\quad \Omega\times]0,+\infty[, \tag{17c}$$

$$\frac{\partial\Phi}{\partial\overset{\square}{\boldsymbol{p}}}+\rho\frac{\partial\Psi}{\partial\boldsymbol{p}}-\mathbf{div}\left(\rho\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}\right)\ni\boldsymbol{0} \quad\text{in}\quad \Omega\times]0,+\infty[, \tag{17d}$$

where the stress tensor $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma}\in\frac{\partial(\rho\Psi)}{\partial\boldsymbol{h}}+\frac{\partial\Phi}{\partial\boldsymbol{D}(\boldsymbol{v})}-\frac{1}{2}\boldsymbol{W}\left(\rho\frac{\partial\Psi}{\partial\boldsymbol{r}}\right)-\nabla c\otimes\rho\frac{\partial\Psi}{\partial\nabla c}-\rho\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}$$
$$+\frac{a+1}{2}\boldsymbol{p}\otimes\frac{\partial\mathscr{F}}{\partial\boldsymbol{p}}+\frac{a-1}{2}\frac{\partial\mathscr{F}}{\partial\boldsymbol{p}}\otimes\boldsymbol{p}. \tag{17e}$$

The variables $\boldsymbol{h}$ and $\boldsymbol{r}$ are obtained as time-primitive of respectively the deformation rate tensor $\boldsymbol{D}(\boldsymbol{v})$ and the curvature rate vector $\boldsymbol{k}$ (see Cauchy's problem (6)), both of them depending on the velocity field.

When $\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}=\boldsymbol{0}$, the constitutive equations (15) gathered with the conservation laws from section 2.1 present an additional source of dissipation from the term $\boldsymbol{W}(\frac{\partial\Phi}{\partial\boldsymbol{k}})$, absent in the previous problem.

Problem 2. Find $\boldsymbol{v}$, ρ, c and $\boldsymbol{p}$ defined in $\Omega \times]0, +\infty[$ such that

$$\rho\dot{\boldsymbol{v}} - \mathbf{div}\boldsymbol{\sigma}^{\mathsf{T}} = \rho\boldsymbol{b} \text{ in } \Omega \times]0, +\infty[, \tag{18a}$$

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho\boldsymbol{v}) = 0 \quad \text{in} \quad \Omega \times]0, +\infty[, \tag{18b}$$

$$\frac{\partial \Phi}{\partial \dot{c}} + \rho\frac{\partial \Psi}{\partial c} - \operatorname{div}\left(\rho\frac{\partial \Psi}{\partial \nabla c}\right) \ni 0 \quad \text{in} \quad \Omega \times]0, +\infty[, \tag{18c}$$

$$\frac{\partial \Phi}{\partial \overset{\square}{\boldsymbol{p}}} + \rho\frac{\partial \Psi}{\partial \boldsymbol{p}} \ni \boldsymbol{0} \quad \text{in} \quad \Omega \times]0, +\infty[, \tag{18d}$$

where the stress tensor $\boldsymbol{\sigma}$ is given by

$$\boldsymbol{\sigma} \in \frac{\partial(\rho\Psi)}{\partial \boldsymbol{h}} + \frac{\partial \Phi}{\partial \boldsymbol{D}(\boldsymbol{v})} - \frac{1}{2}\boldsymbol{W}\left(\rho\frac{\partial \Psi}{\partial \boldsymbol{r}}\right) - \frac{1}{2}\boldsymbol{W}\left(\frac{\partial \Phi}{\partial \boldsymbol{k}}\right) - \nabla c \otimes \rho\frac{\partial \Psi}{\partial \nabla c} + a\boldsymbol{p} \otimes \rho\frac{\partial \Psi}{\partial \boldsymbol{p}}. \tag{18e}$$

3.4. Energy estimate

Energy estimates are useful for establishing existence results for solutions. A definite advantage of introducing our abstract framework is the ability of proving an energy estimate in the general case, that is for any free energy Ψ and any dissipation potential Φ.

Theorem 2 – Energy estimate

Assume constitutive equations (11) (or (15) when $\frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} = \boldsymbol{0}$) are satisfied with a dissipation potential Φ convex and positive, which satisfies $\Phi(\mathbb{D} = 0; \mathbb{A}) = 0$ for any $\mathbb{A}$. Then, the energy estimate writes

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathscr{E}_k(\boldsymbol{v}) + \mathscr{F}(\boldsymbol{h}, \boldsymbol{r}, c, \boldsymbol{p})] + \mathscr{D} = (\rho\boldsymbol{b} \mid \boldsymbol{v}) + \int_{\partial\Omega(t)} (\boldsymbol{\sigma} \cdot \boldsymbol{v} + \boldsymbol{l} \times \boldsymbol{\omega}) \cdot \boldsymbol{n} \, \mathrm{d}s. \tag{19}$$

The notation $\mathscr{E}_k(\boldsymbol{v})$ stands for the kinetic energy, defined by

$$\mathscr{E}_k(\boldsymbol{v}) := \int_{\Omega(t)} \frac{1}{2}\rho|\boldsymbol{v}|^2 \, \mathrm{d}\boldsymbol{x}. \tag{20}$$

The quantity $\mathscr{D}$ is called the dissipation and is positive. It is defined by

$$\mathscr{D} := (\boldsymbol{\sigma}_p \mid \boldsymbol{D}(\boldsymbol{v})) - 2(\boldsymbol{l}_p \mid \boldsymbol{k}) + (c_p \mid \dot{c}) + \left(\boldsymbol{p}_p \,\middle|\, \overset{\square}{\boldsymbol{p}}\right), \tag{21}$$

where $\boldsymbol{\sigma}_p \in \frac{\partial \Phi}{\partial \boldsymbol{D}(\boldsymbol{v})}$, $\boldsymbol{l}_p \in -\frac{1}{2}\frac{\partial \Phi}{\partial \boldsymbol{k}}$, $c_p \in \frac{\partial \Phi}{\partial \dot{c}}$ and $\boldsymbol{p}_p \in \frac{\partial \Phi}{\partial \overset{\square}{\boldsymbol{p}}}$. When $\frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} \neq \boldsymbol{0}$, the boundary term $(\boldsymbol{l} \times \boldsymbol{\omega}) \cdot \boldsymbol{n}$ in (19) and the second term in (21) vanish.

Proof. See appendix B.3. ■

Here, $\mathscr{E}_k(\boldsymbol{v}) + \mathscr{F}(\boldsymbol{h}, \boldsymbol{r}, c, \boldsymbol{p})$ represents the total mechanical energy of the system. The dissipation $\mathscr{D}$ tends to decrease it while the right hand side of equation (19) can decrease the energy as well as increase it. In some cases, therefore, this right hand side may be a source of energy that tends to put the system out of equilibrium, and this source of energy may be injected either in the bulk or across the boundary.

3.5. Discussion

To recap, we have proposed a new thermodynamic framework to derive constitutive equations (11) and (15) for general polar fluids. This framework combines the unified dissipation potential formalism developed in [Sar24] (section 2.2) and the skew-symmetric couple stress theory (section 2.1) [HHD15]. From the free energy of the system Ψ (7) – which is allowed to depend on gradients of thermodynamic variables, such as the polarity, unlike continuum mechanics – and the dissipation potential Φ, our formalism makes it possible to obtain objective constitutive equations that satisfy the second principle of thermodynamics (theorem 1) and a rigorous cloupling of the various physical fields involved, such as polarity, density, concentration of a chemical agent... In particular, equation (17d) shows that choosing Ψ quadratic in $\nabla \boldsymbol{p}$ leads to a Laplacian of the polarity field in the polarity equation. Also, the dissipation function makes it possible to generalize Onsager's relations to the nonlinear case, and thus to describe many nonlinear rheologies such as plasticity. For this, we can refer, for example, to sections 2.6 and 3.1 in [Sar16], which give examples of dissipation potentials adapted to Quasi-Newtonian and viscoplastic fluids.

Furthermore, our framework differs from that of active gels in that it adds an explicit dependence of the stress tensor on two measures of strain (17e): the Hencky strain tensor $\boldsymbol{h}$ and the mean curvature vector $\boldsymbol{r}$. The dependence on $\boldsymbol{h}$ allows to consider rigourous coupling with the density ρ, thanks to the formula (8). When the free energy is independ from the polarity gradient, the stress tensor has an additional dependence on the mean curvature rate vector $\boldsymbol{k}$ (18e): this terms adds another dissipation source but cannot appear in equations if the free energy has this dependence.

Finally, our approach naturally results in a general energy estimate (theorem 2), i.e. one that can be expressed for any free energy and any dissipation potential. It could be useful for establishing existence results for solutions or for analyzing the stability of our equations, for instance.

3.6. Examples

In this section, we give some examples of the application of our framework, with the aim of demonstrating its ability to derive models already known in the literature and to determine their energy estimates. We start off with an incompressible viscous couple-stress fluid to highlight the fact our framework is indeed a generalization of the nonpolar skew-symmetric couple stress theory. Then, we present the coupling of Allen–Cahn and incompressible Navier-Stokes equations to show a case where the free energy depends on the gradient of a given field. Nonlinear rheologies such as plasticity are not discussed here but some relevant examples can be found in sections 2.6 and 3.1 in [Sar16], as mentioned in the previous discussion section.

3.6.1. Incompressible viscous couple-stress fluid

To illustrate the impact of the couple stress theory on the classical incompressible Navier-Stokes equations, let us consider the example of an incompressible viscous couple-stress fluid, as discussed in section 7 in [HHD15]. In contrast to the classical approach using the Navier-Stokes equations, such a description makes it possible to explain flow phenomena in microchannels, for instance. Indeed, when the size of the molecules making up the fluid under study is comparable to that of the channel, their spinning significantly affects the macroscopic dynamics [CLL10], a phenomenon that can be captured by the couple-stress theory.

We assume no dependence of the system on any concentration field c nor polarity field $\boldsymbol{p}$, thus the couple stress tensor $\boldsymbol{\mu}$ can present a dissipative part whatever the chosen couple stress theory. Then, we choose a zero free energy Ψ and a quasi-quadratic dissipation potential Φ in

$\boldsymbol{D}(\boldsymbol{v})$ and in $\boldsymbol{k}$, under the form

$$\Phi(\boldsymbol{D}(\boldsymbol{v}), \boldsymbol{k}) = \mathcal{I}_{\ker(\mathrm{tr})}(\boldsymbol{D}(\boldsymbol{v})) + \eta|\boldsymbol{D}(\boldsymbol{v})|^2 + 8\nu|\boldsymbol{k}|^2, \tag{22}$$

where η is the shear viscosity and ν is a viscosity-like coefficient, specific to couple-stress fluids. Note that the ratio $\nu/\eta = \ell^2$ highlights the presence of a length scale ℓ, absent in classical fluid dynamics. The notation $\mathcal{I}_{\ker(\mathrm{tr})}(\boldsymbol{D}(\boldsymbol{v}))$ stands for the indicator of the convex set $\ker(\mathrm{tr}) = \{\boldsymbol{\tau} \mid \mathrm{tr}\,\boldsymbol{\tau} = 0\}$, which takes the value 0 when $\operatorname{div}\boldsymbol{v} = 0$ and $+\infty$ otherwise. This term does not admit a differential with respect to $\boldsymbol{D}(\boldsymbol{v})$ but a subdifferential, which will lead to the existence of the pressure field Π, here seen as a Lagrangian multiplier to the free-divergence constraint [Sar16, section 5.3.3].

By remarking that $\boldsymbol{k} = -\frac{1}{4}\Delta\boldsymbol{v}$ from the incompressibility condition and by the relation (18e), the stress tensor writes

$$\boldsymbol{\sigma} = -\Pi\boldsymbol{\delta} + 2\eta\boldsymbol{D}(\boldsymbol{v}) + 2\nu\Delta\boldsymbol{W}(\boldsymbol{v}), \tag{23}$$

where $\boldsymbol{\delta}$ is the identity matrix. Injecting this expression into the conservation of momentum (18a), we finally get the

Problem 3. Find $\boldsymbol{v}$ and Π defined in $\Omega \times]0, +\infty[$ such that

$$\rho\dot{\boldsymbol{v}} - \eta\Delta\boldsymbol{v} + \nu\Delta^2\boldsymbol{v} + \nabla\Pi = \rho\boldsymbol{b} \text{ in } \Omega \times]0, +\infty[, \tag{24a}$$

$$\operatorname{div}(\boldsymbol{v}) = 0 \quad \text{in } \Omega \times]0, +\infty[, \tag{24b}$$

where $\Delta^2 = \Delta\Delta$ is the bilaplacian operator.

Using theorem 2, the energy estimate associated to this problem writes

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathscr{E}_k(\boldsymbol{v})] + 2\eta\|\boldsymbol{D}(\boldsymbol{v})\|^2 + 16\nu\|\boldsymbol{k}\|^2 = (\rho\boldsymbol{b} \mid \boldsymbol{v}) + \int_{\partial\Omega(t)} \boldsymbol{n}\cdot\boldsymbol{\sigma}\cdot\boldsymbol{v}\,\mathrm{d}s. \tag{25}$$

3.6.2. Coupling of Allen–Cahn and incompressible Navier-Stokes equations

Let us consider the example of the coupling of the Allen–Cahn equation [AC79] with the previous incompressible couple-stress Navier-Stokes equations. Compared to the previous case, we assume in addition a dependence of the system on a dimensionless order parameter c, to take into account a possible phase separation: the free energy is given by

$$\rho\Psi(c, \nabla c) = m\beta W(c) + m\beta\frac{\varepsilon^2}{2}|\nabla c|^2, \tag{26}$$

where W is the so-called double-well potential (see figure 1) defined for any real number u by

$$W(u) = \frac{1}{4}(u^2 - 1)^2, \tag{27}$$

while the dissipation potential is simply quadratic in $\dot{c}$:

$$\Phi(\boldsymbol{D}(\boldsymbol{v}), \boldsymbol{k}, \dot{c}) = \mathcal{I}_{\ker(\mathrm{tr})}(\boldsymbol{D}(\boldsymbol{v})) + \eta|\boldsymbol{D}(\boldsymbol{v})|^2 + 8\nu|\boldsymbol{k}|^2 + \frac{\beta}{2}|\dot{c}|^2, \tag{28}$$

where β is a given coefficient, m is the mobility (which has the dimension of the inverse of a time) and ε is a correlation length. As in the previous case, the absence of dependence of the system on the gradient of the polarity field allows us to consider a dissipative part in the expression of the couple stress tensor $\boldsymbol{\mu}$, whatever the chosen couple stress theory.

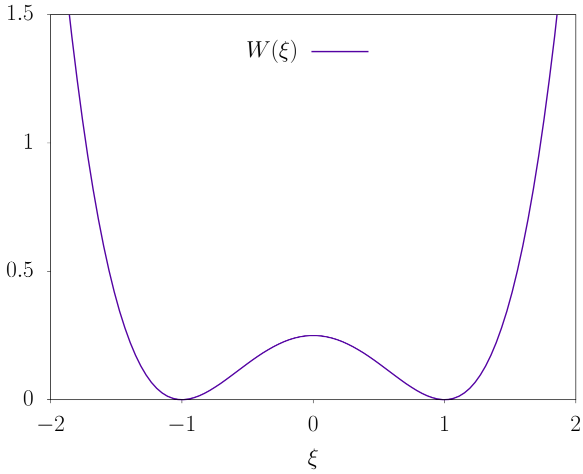

Figure 1: Double-well potential.

By remarking that $\boldsymbol{k} = -\frac{1}{4}\Delta \boldsymbol{v}$ from the incompressibility condition and by the relation (18e), the stress tensor writes

$$\boldsymbol{\sigma} = -\Pi\boldsymbol{\delta} + 2\eta\boldsymbol{D}(\boldsymbol{v}) + 2\eta l^2 \Delta \boldsymbol{W}(\boldsymbol{v}) - m\beta\varepsilon^2 \nabla c \otimes \nabla c. \tag{29}$$

Injecting this expression into the conservation of momentum (18a), we finally get the

Problem 4. Find $\boldsymbol{v}$, Π and c defined in $\Omega \times]0, +\infty[$ such that

$$\rho\dot{\boldsymbol{v}} - \eta\Delta\boldsymbol{v} + \eta l^2 \Delta^2 \boldsymbol{v} + \nabla\Pi + m\beta\varepsilon^2 \mathbf{div}(\nabla c \otimes \nabla c) = \rho\boldsymbol{b} \text{ in } \Omega \times]0, +\infty[, \tag{30a}$$

$$\operatorname{div} \boldsymbol{v} = 0 \quad \text{in} \quad \Omega \times]0, +\infty[, \tag{30b}$$

$$\frac{\partial c}{\partial t} + (\boldsymbol{v} \cdot \nabla)c + m(c^2 - 1)c - m\varepsilon^2 \Delta c = 0 \quad \text{in} \quad \Omega \times]0, +\infty[. \tag{30c}$$

Using theorem 2, the energy estimate associated to this problem writes

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathscr{E}_k(\boldsymbol{v}) + \mathscr{F}(c)] + 2\eta\|\boldsymbol{D}(\boldsymbol{v})\|^2 + 16\nu\|\boldsymbol{k}\|^2 + \beta\left\|m(c^2-1)c - m\varepsilon^2\Delta c\right\|^2 = (\rho\boldsymbol{b} \mid \boldsymbol{v}) + \int_{\partial\Omega(t)} \boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{v} \,\mathrm{d}s, \tag{31}$$

where

$$\mathscr{F}(c) := \int_{\Omega(t)} \rho\Psi(c, \nabla c)\,\mathrm{d}\boldsymbol{x}. \tag{32}$$

4. A new framework for active gel theory. Application to collective cell migration

In this section, we describe a new method for constructing hydrodynamic equations from the theory of active gels (nematic or polar), as defined in section 1.3.1, based on the framework presented in the section 3. The resulting equations satisfy, by construction, the second principle of thermodynamics. As shown at the end of this section, in Corollary 2, this is major improvement with respect to former active gels theories [Kru+04; Mar+13; JGS18].

4.1. Conservation laws

Here, we adopt the assumptions given in section 1.2. From this point of view, tools from continuum mechanics, and in particular the framework developed in the section 3, can be used to build a continuous model of the collective cell migration.

From points (i) and (ii), the mass conservation (3c) reduces to

$$\operatorname{div}(\boldsymbol{v}) = 0 \text{ in } \Omega \times]0, +\infty[. \tag{33}$$

From point (iii), the momentum conservation (3a) reduces to

$$-\mathbf{div}\left(\boldsymbol{\sigma}^{\mathsf{T}}\right) = \rho \boldsymbol{b} \text{ in } \Omega \times]0, +\infty[. \tag{34}$$

The couples exerted by the cells to align their polarities with each other are represented by the couple stress tensor $\boldsymbol{\mu}$, which satisfies the conservation of angular momentum (3b)

$$-\mathbf{div}\left(\boldsymbol{\mu}^{\mathsf{T}}\right) = \boldsymbol{\epsilon} : \boldsymbol{\sigma} \text{ in } \Omega \times]0, +\infty[. \tag{35}$$

4.2. Constitutive equations

Following [Mar+13], we assume the bulk active behavior of the active gels filaments comes from a nonequilibrium chemical reaction such as the consumption of ATP. Formally, it means the free energy $\mathscr{F}$ can depend on the advancement ξ of this reaction, that is the number of ATP molecules consumed per unit volume, in addition to the polarity field $\boldsymbol{p}$ (we assume no dependence on $\boldsymbol{h}$ nor $\boldsymbol{r}$):

$$\mathscr{F}(\boldsymbol{p}, \xi) = \int_{\Omega(t)} \rho \Psi(\boldsymbol{p}, \nabla \boldsymbol{p}, \xi) \, \mathrm{d}\boldsymbol{x}. \tag{36}$$

As for the choice of Ψ, we synthesize the classical approaches developed for example in [ZSA12; Mar14; Not+16; Cza+18; AT19]. We essentially introduce three physical ingredients:

(i) In order to ensure motion, we consider a double-well energy generalizing to the vector case the one used by the Allen-Cahn model (27):

$$W(\boldsymbol{p}) = \frac{1}{4}\left(|\boldsymbol{p}|^2 - 1\right)^2. \tag{37}$$

It defines the polarized $|\boldsymbol{p}| = 1$ state as stable (the energy is minimal for this state), in contrast to the $|\boldsymbol{p}| = 0$ state, which is unstable (see figure 1).

(ii) Spatial variations in polarity are penalized, so that polarity vectors in the same neighborhood tend to align.

(iii) Advancement of the reaction and polarity are not coupled.

Thus, the free energy Ψ is given by

$$\rho \Psi(\boldsymbol{p}, \nabla \boldsymbol{p}, \xi) = \alpha W(\boldsymbol{p}) + \frac{K_F}{2} |\nabla \boldsymbol{p}|^2 + \rho \Psi_a(\xi), \tag{38}$$

where $|\boldsymbol{\tau}|^2 = \boldsymbol{\tau} : \boldsymbol{\tau}$, α is the modulus of the polar restoring force, K_F is the so-called Frank constant and Ψ_a is the free energy stored by the consumption of ATP molecules. The ratio of K_F and α defines the polar correlation length $L_p = \sqrt{K_F/\alpha}$, a characteristic scale of spatial variations of the polarity. It also can be seen as a characteristic scale of alignment between polarities.

Let

$$\Phi(\boldsymbol{D}(\boldsymbol{v}),\overset{\square}{\boldsymbol{p}},\dot{\xi};\boldsymbol{p}) = \mathcal{I}_{\ker(\mathrm{tr})}(\boldsymbol{D}(\boldsymbol{v})) + \eta|\boldsymbol{D}(\boldsymbol{v})|^2 + \frac{\gamma}{2}|\overset{\square}{\boldsymbol{p}}|^2 + \frac{1}{2\Lambda}\Big[\zeta\boldsymbol{p}\otimes\boldsymbol{p}:\boldsymbol{D}(\boldsymbol{v}) - \dot{\xi}\Big]^2 \tag{39}$$

be the dissipation potential, where γ is the rotational viscosity, ζ has the same dimension as the inverse of a volume and Λ is an ad-hoc coefficient. Then, the constitutive equations write

$$\begin{aligned}\boldsymbol{\sigma} = & -\Pi\boldsymbol{\delta} + 2\eta\boldsymbol{D}(\boldsymbol{v}) - K_F\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\nabla\boldsymbol{p} & \text{(40a)}\\ & + \frac{a+1}{2}\boldsymbol{p}\otimes\boldsymbol{m}(\boldsymbol{p}) + \frac{a-1}{2}\boldsymbol{m}(\boldsymbol{p})\otimes\boldsymbol{p} + \boldsymbol{\sigma}_a, & \\ \gamma\overset{\square}{\boldsymbol{p}} + \boldsymbol{m}(\boldsymbol{p}) = \boldsymbol{0}, & & \text{(40b)}\end{aligned}$$

where Π is the pressure field, $\boldsymbol{\delta}$ is the identity matrix,

$$\boldsymbol{m}(\boldsymbol{p}) = \frac{\partial\mathscr{F}}{\partial\boldsymbol{p}} = \alpha\big(|\boldsymbol{p}|^2 - 1\big)\boldsymbol{p} - K_F\Delta\boldsymbol{p} \tag{41}$$

is the so-called molecular field (up to a minus sign) and $\boldsymbol{\sigma}_a$ is the active stress tensor defined by (2), that is

$$\boldsymbol{\sigma}_a = -\zeta\Delta\mu\,\boldsymbol{p}\otimes\boldsymbol{p}, \tag{42a}$$

with

$$\Delta\mu = -\rho\frac{\partial\Psi}{\partial\xi}. \tag{42b}$$

In this context, we have in addition the following relation:

$$\dot{\xi} = \Lambda\Delta\mu + \zeta\boldsymbol{p}\otimes\boldsymbol{p}:\boldsymbol{D}(\boldsymbol{v}). \tag{43}$$

With these constitutive equations, the second principle of thermodynamics is satisfied according to theorem 1. However, in practice, the energy term $\Delta\mu$ is assumed known and uniform in space and time, so that equation (43) is not necessary to solve the model, and ξ can be computed during a post-processing step. With this assumption, the second principle of thermodynamics is not satisfied anymore, and the active stress should act as a nonequilibrium term. Thus, this active stress could have been equivalently introduced as an exterior force, through the relation

$$\rho\boldsymbol{b} = \mathbf{div}\boldsymbol{\sigma}_a, \tag{44}$$

for instance.

Remark IV: Because of the incompressibility condition $\operatorname{div}\boldsymbol{v} = 0$, the last term in the definition of the dissipation potential (39) could be replaced by $\frac{1}{2\Lambda}\Big[\zeta\boldsymbol{Q}:\boldsymbol{D}(\boldsymbol{v}) - \dot{\xi}\Big]^2$ so that $\boldsymbol{\sigma}_a = -\zeta\Delta\mu\boldsymbol{Q}$, where $\boldsymbol{Q} = \mathbf{dev}(\boldsymbol{p}\otimes\boldsymbol{p}) = \boldsymbol{p}\otimes\boldsymbol{p} - \frac{1}{d}|\boldsymbol{p}|^2\boldsymbol{\delta}$, and $d = 2$ or 3 is the space dimension. In practice, this does not change the nature of the equations, as the pressure adjusts accordingly, Π being a Lagrange multiplier to the constraint of incompressibility. Similarly, the dissipation potential can be modified to make appear the isotropic parts of the various tensors present in the stress tensor expression (40a), so that the pressure corresponds exactly to the isotropic part of the stress tensor. In other words, we could equivalently have

$$\begin{aligned}\boldsymbol{\sigma} = -\Pi\boldsymbol{\delta} + 2\eta\boldsymbol{D}(\boldsymbol{v}) + \boldsymbol{\sigma}_a - K_F\,\mathbf{dev}\big(\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\nabla\boldsymbol{p}\big)&\\ + \frac{a+1}{2}\boldsymbol{p}\otimes\boldsymbol{m}(\boldsymbol{p}) + \frac{a-1}{2}\boldsymbol{m}(\boldsymbol{p})\otimes\boldsymbol{p} - \frac{a}{d}\boldsymbol{p}\cdot\boldsymbol{m}(\boldsymbol{p})\boldsymbol{\delta},&\end{aligned} \tag{45}$$

with $\boldsymbol{\sigma}_a = -\zeta\Delta\mu\,\boldsymbol{Q}$ and $\Pi = -\frac{1}{d}\operatorname{tr}\boldsymbol{\sigma}$.

4.3. Application to collective cell migration

Let us consider a monolayer epithelium freely spreading on a substrate, whose geometry is described at time t by the set $\Omega(t) \subset \mathbb{R}^2$. Following [Bla+17], we assume the migration occurs at time scales longer than the relaxation time scales of intracellular and intercellular kinetics, so that the effects of the cells elasticity can be neglected: the tissue spreading can be described on a macroscopic scale as an active viscopolar material. Cells are in particular able to exert active tractions on the substrate in order to spread, in the direction of their polarity.

As discussed in section 1.3.1, hydrodynamics equations of collective cell migration can be obtained from the theory of polar active gels. Thus, we assume the tissue spreading can be described by conservation laws (33), (34) and (35), and constitutive equations (40).

Let us assume the external forces are composed of a passive friction $k\boldsymbol{v}$ of the tissue with the substrate, of an active traction $f_a\boldsymbol{p}$ exerted by the cells on the substrate to move and of the active stress introduced previously in (42a), that is

$$\rho\boldsymbol{b} = f_a\boldsymbol{p} - k\boldsymbol{v} + \mathbf{div}\boldsymbol{\sigma}_a, \tag{46}$$

where f_a is the modulus of the active force and k is the friction coefficient, as considered for instance in [BC17; AT19]; see figure 2. The ratio of the viscosity η and the friction coefficient k defines another length, the friction length $L_F = \sqrt{\eta/k}$, in addition to the polar correlation length L_p. Similarly, it can be seen as a characteristic scale of spatial variations of the velocity.

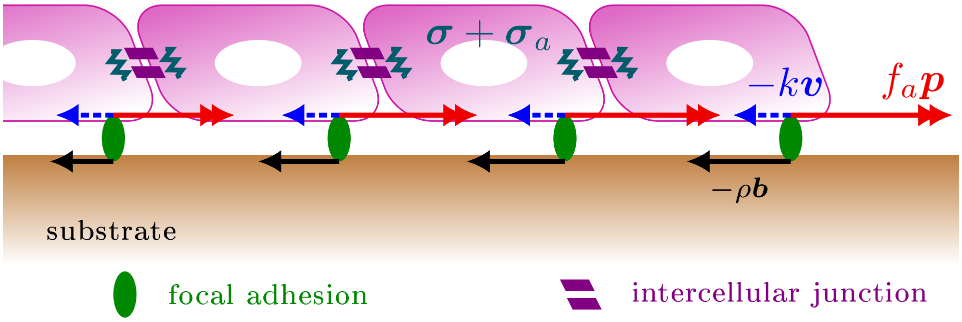

Figure 2: Forces and stress in a spreading epithelium. As defined in equation (46), the traction $-\rho\boldsymbol{b}$ exerted by the cells on the substrate (black arrows) is composed of an active force $f_a\boldsymbol{p}$ due to cell polarization (two headed red arrows), the divergence of the active stress $\boldsymbol{\sigma}_a$ defined by (42a) and a viscous friction term $k\boldsymbol{v}$ (dashed blue arrows). It is balanced locally by the divergence of the stress: $\mathbf{div}\boldsymbol{\sigma}^\mathsf{T} = -\rho\boldsymbol{b}$ (see equation (34)). Adapted from [BM19, figure 1].

To close the system, we consider the following natural boundary conditions:

$$(\boldsymbol{\sigma}^\mathsf{T})_{\boldsymbol{nt}} = \mathbf{0} \text{ on } \partial\Omega \times]0, +\infty[, \tag{47a}$$

$$\boldsymbol{v} \cdot \boldsymbol{n} = 0 \text{ on } \partial\Omega \times]0, +\infty[, \tag{47b}$$

$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{n}} = \mathbf{0} \text{ on } \partial\Omega \times]0, +\infty[, \tag{47c}$$

where $\boldsymbol{\chi}_{\boldsymbol{nt}} = \boldsymbol{\chi} \cdot \boldsymbol{n} - (\boldsymbol{n} \cdot \boldsymbol{\chi} \cdot \boldsymbol{n})\boldsymbol{n}$. The first boundary condition accounts for zero tangential traction force, the second one to slip boundary condition and the last one to homogeneous Neumann condition for the polarity.

This leads to

Problem 5 – Coherent active gel model applied to collective cell migration. Given the initial polarity $\boldsymbol{p}_0$, find $\boldsymbol{v}$, Π and $\boldsymbol{p}$ defined in $\Omega \times]0,+\infty[$ such that

$$\begin{aligned} -\mathbf{div}\big(\boldsymbol{\sigma}^{\mathsf{T}}\big) + k\boldsymbol{v} &= f_a\boldsymbol{p} + \mathbf{div}\boldsymbol{\sigma}_a \quad \text{in } \Omega \times]0,+\infty[, && (48a)\\ \operatorname{div}\boldsymbol{v} &= 0 \quad \text{in } \Omega \times]0,+\infty[, && (48b)\\ \lambda_p\overset{\square}{\boldsymbol{p}} + (|\boldsymbol{p}|^2-1)\boldsymbol{p} - L_p^2\Delta\boldsymbol{p} &= \boldsymbol{0} \quad \text{in } \Omega \times]0,+\infty[, && (48c)\end{aligned}$$

where $\lambda_p = \gamma/\alpha$ is the polar time relaxation, and satisfying the boundary conditions (47). The Cauchy stress tensor is given by

$$\boldsymbol{\sigma} = -\Pi\boldsymbol{\delta} + 2\eta\boldsymbol{D}(\boldsymbol{v}) - K_F\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\nabla\boldsymbol{p} + \frac{a+1}{2}\boldsymbol{p}\otimes\boldsymbol{m}(\boldsymbol{p}) + \frac{a-1}{2}\boldsymbol{m}(\boldsymbol{p})\otimes\boldsymbol{p} \tag{48d}$$

and

$$\begin{aligned} \overset{\square}{\boldsymbol{p}} &= \partial_t\boldsymbol{p} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{p} - (\boldsymbol{W}(\boldsymbol{v}) + a\boldsymbol{D}(\boldsymbol{v}))\cdot\boldsymbol{p}, && (48e)\\ \boldsymbol{m}(\boldsymbol{p}) &= \alpha\big(|\boldsymbol{p}|^2-1\big)\boldsymbol{p} - K_F\Delta\boldsymbol{p}, && (48f)\\ \boldsymbol{\sigma}_a &= -\zeta\Delta\mu\boldsymbol{p}\otimes\boldsymbol{p}. && (48g)\end{aligned}$$

The physical ingredients introduced in section 4.2 and repeated here can be exactly found in [Not+16; BC17]. In the most general case, up to five ingredients can be found if we add a dependence on cell density [AT19, equation (11)], or even more if we introduce new fields to describe other physico-chemical quantities, such as myosin concentration [Not+16; BM19], cell shape anisotropy [Cza+18] or the activity of ERK (*Extracellular signal-Regulated Kinases*), an enzyme influencing the actomyosin complex, and thus active force [Boo+21].

Finally, a major advantage of our framework, as already pointed out in section 3.4, is its ability to naturally lead to an energy estimate of the proposed model, which is crucial to obtain more advanced theoretical results such as the existence of a solution to problem 5.

Corollary 1 – Coherent model 5 in its passive form satisfies the 2nd principle

Let Δ be the dissipation-like term defined for any vector fields $\boldsymbol{w}$ and $\boldsymbol{q}$ by

$$\Delta(\boldsymbol{w},\boldsymbol{q}) = \frac{k}{2}\|\boldsymbol{w}\|^2 + \eta\|\boldsymbol{D}(\boldsymbol{w})\|^2 + \frac{1}{\gamma}\|\boldsymbol{m}(\boldsymbol{q})\|^2. \tag{49}$$

If $\boldsymbol{v}$, Π and $\boldsymbol{p}$ are solution of problem 5, then

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{p})) + \Delta(\boldsymbol{v},\boldsymbol{p}) \leqslant \frac{f_a^2}{2k}\|\boldsymbol{p}\|^2 + \frac{|\zeta\Delta\mu|^2}{4\eta}\int_\Omega |\boldsymbol{p}|^4. \tag{50}$$

The dissipation-like term $\Delta(\boldsymbol{v},\boldsymbol{p})$ is nonnegative. In consequence, coherent model 5 of collective cell migration, without activity ($f_a = 0$ and $\zeta = 0$), satisfies the second principle of thermodynamics.

Proof. See appendix B.3. ■

Remark V – *Dissipation*: The dissipation obtained from (21) writes

$$\mathscr{D} = 2\eta\|\boldsymbol{D}(\boldsymbol{v})\|^2 + \frac{1}{\gamma}\|\boldsymbol{m}(\boldsymbol{p})\|^2. \tag{51}$$

Adding the damping term results in the dissipation associated to model 5:

$$\hat{\mathscr{D}} = \mathscr{D} + k\|\boldsymbol{v}\|^2. \tag{52}$$

It is different from (49) because the equality resulting from equation (19) has been transformed into an inequality (see the proof above).

4.4. On former active gel theories

Compared to models found in active gel theory [Mar+13] or in collective cell migration [BC17; AT19], our stress tensor (48d) has in addition the symmetric term $K_F \nabla \boldsymbol{p}^\intercal \cdot \nabla \boldsymbol{p}$, which looks like the Ericksen stress tensor introduced in the liquid crystal theory [GP93]. In this section, we show why it is necessary to guarantee the second principle of thermodynamics in the passive case.

Problem 6 – Former active gel model applied to collective cell migration. This problem is obtained from problem 5 by dropping the third term in the expression (48d) of the Cauchy stress tensor $\boldsymbol{\sigma}$.

Corollary 2 – Former model 6 in its passive form violates the 2nd principle

Let $\tilde{\Delta}$ be the dissipation-like term defined for any vector fields $\boldsymbol{w}$ and $\boldsymbol{q}$ by

$$\tilde{\Delta}(\boldsymbol{w}, \boldsymbol{q}) = \frac{k}{2}\|\boldsymbol{w}\|^2 + \eta\|\boldsymbol{D}(\boldsymbol{w})\|^2 + \frac{1}{\gamma}\|\boldsymbol{m}(\boldsymbol{q})\|^2 + K_F\big(\nabla \boldsymbol{q}^\intercal \cdot \nabla \boldsymbol{q} \,\big|\, \boldsymbol{D}(\boldsymbol{w})\big). \tag{53}$$

If $\boldsymbol{v}$, Π and $\boldsymbol{p}$ are solution of problem 6, then

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{p})) + \tilde{\Delta}(\boldsymbol{v}, \boldsymbol{p}) \leqslant \frac{f_a^2}{2k}\|\boldsymbol{p}\|^2 + \frac{|\zeta\Delta\mu|^2}{4\eta}\int_\Omega |\boldsymbol{p}|^4. \tag{54}$$

There exists a velocity field $\boldsymbol{v}$ and a polarity field $\boldsymbol{p}$ such that $\tilde{\Delta}(\boldsymbol{v}, \boldsymbol{p}) < 0$. In consequence, former model of collective cell migration 6, violates the second principle of thermodynamics, even in a purely passive case ($f_a = 0$ and $\zeta = 0$).

Proof. See appendix B.3. ■

Remark VI – *Coherent vs former active gel models applied to collective cell migration*: Introducing the stress term $K_F \nabla \boldsymbol{p}^\intercal \cdot \nabla \boldsymbol{p}$ into (48d) as in problem 5 constitutes a major improvement of former active gel model 6: the coherent model fully satisfies the second principle of thermodynamics and leads to an energy estimate (corollary 1), while the former violates it (corollary 2).

5. Numerical illustration: resolution of the model on a disk

5.1. Problem specifications

Let us consider a monolayer epithelium swarming on a fixed disk $\Omega \subset \mathbb{R}^2$ of radius R. In other words, Ω does not evolve over time. The tissue is assumed to be confined on this substrate, so that $\boldsymbol{v} \cdot \boldsymbol{n} = 0$ and $(\boldsymbol{\sigma}^\intercal)_{\boldsymbol{nt}} = \boldsymbol{0}$ on $\partial\Omega \times]0, +\infty[$. Here, we completely neglect the third space dimension.

With this problem, we aim to demonstrate our ability to solve numerically the 2D problem 5, and to interpret the evolution of the free energy (38) in relation to the energy estimate (50). We also aim to show the ability of this model to create collective motion spontaneously. To do so, we start from a randomly distributed polarity, close to zero. Specifically, we build the initial polarity $\boldsymbol{p}_0$ as a unit vector of angle drawn uniformly between 0 and 2π, and of norm weighted by a number following a normal distribution of mean zero and standard deviation equal to 0.1.

In practice, we solve a dimensionless version of problem 5. Let V, $T = R/V$ and $\Sigma = \eta V/R$ be the characteristic cell velocity, swarming time and stress, respectively. Keeping the notations of problem 5 for the dimensionless problem, for the sake of economy of notations, we obtain the

Problem 7. Given the initial polarity $\boldsymbol{p}_0$, find $\boldsymbol{v}$, Π and $\boldsymbol{p}$ defined in $\Omega \times]0, +\infty[$ such that

$$\begin{aligned}
-\mathbf{div}\big(\boldsymbol{\sigma}^{\mathsf{T}}\big) + C_F \boldsymbol{v} &= T_a \boldsymbol{p} + \mathbf{div}\boldsymbol{\sigma}_a && \text{in } \Omega \times]0, +\infty[, && \text{(55a)}\\
\operatorname{div} \boldsymbol{v} &= 0 && \text{in } \Omega \times]0, +\infty[, && \text{(55b)}\\
\mathrm{Pe}\,\overset{\square}{\boldsymbol{p}} + (|\boldsymbol{p}|^2 - 1)\boldsymbol{p} - \kappa^2 \Delta \boldsymbol{p} &= \boldsymbol{0} && \text{in } \Omega \times]0, +\infty[, && \text{(55c)}
\end{aligned}$$

where $\Omega = \{\boldsymbol{x} \in \mathbb{R}^2 \mid |\boldsymbol{x}| < 1\}$ is the open unit disk in this context, and satisfying the boundary conditions (47). The Cauchy stress tensor is given by

$$\boldsymbol{\sigma} = -\Pi \boldsymbol{\delta} + 2\boldsymbol{D}(\boldsymbol{v}) - \kappa^2 B \nabla \boldsymbol{p}^{\mathsf{T}} \cdot \nabla \boldsymbol{p} + \frac{a+1}{2} \boldsymbol{p} \otimes \boldsymbol{m}(\boldsymbol{p}) + \frac{a-1}{2} \boldsymbol{m}(\boldsymbol{p}) \otimes \boldsymbol{p} \qquad \text{(55d)}$$

and

$$\begin{aligned}
\overset{\square}{\boldsymbol{p}} &= \partial_t \boldsymbol{p} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{p} - (\boldsymbol{W}(\boldsymbol{v}) + a\boldsymbol{D}(\boldsymbol{v})) \cdot \boldsymbol{p}, && \text{(55e)}\\
\boldsymbol{m}(\boldsymbol{p}) &= B\big(|\boldsymbol{p}|^2 - 1\big)\boldsymbol{p} - \kappa^2 B \Delta \boldsymbol{p}, && \text{(55f)}\\
\boldsymbol{\sigma}_a &= -S_a \boldsymbol{p} \otimes \boldsymbol{p}. && \text{(55g)}
\end{aligned}$$

In total, problem 7 has seven dimensionless numbers, whose definitions we give in order of appearance below.

- $\mathrm{Pe} = \lambda_p V/R$: in accordance with current nomenclature, this is the Péclet number, but it can be interpreted more as a polar or vector Weissenberg number, by analogy with viscoelastic fluids. It's the ratio of the polar relaxation time to the characteristic swarming time. Multiplying up and down by α, we obtain $\mathrm{Pe} = (\gamma V/L)/\alpha$, which is then interpreted as the ratio between rotational viscous forces and polar restoring forces

- $\kappa = L_p/R$: alignement coefficient, or relative size of fluctuations in the polarity field.

- a: parameter of the objective Gordon-Schowalter time rate (55e).

- $B = \alpha R/(\eta V)$: ratio between polar restoring forces and viscous forces. An alternative parameter is the Ericksen number, defined by $\mathrm{Er} = (\eta V R)/K_F$, so that $B = 1/(\kappa^2\,\mathrm{Er})$. For practical reasons, we prefer to use B directly. When B is large, i.e. when the viscous forces are small compared with the polar restoring forces, the polarity has a strong resistance to variations in tissue deformation. In short, the parameter B characterizes the polarity's resistance to viscous forces.

- $C_F = kR^2/\eta$: the coefficient of friction compares the relative contributions of viscosity and friction to dissipation.

- $S_a = \zeta \Delta\mu R/(\eta V)$: the dimensionless active stress coefficient.
- $T_a = f_a R/(\eta V)$: active traction materializes the competition between active and viscous forces.

Note that two non-polar quantities play a dissipative role, tending to slow down the movement of the tissue: the characteristic stress Σ and the characteristic friction stress kV. Instead, we could have introduced the total dissipation $\Sigma + kVR$ and defined the dimensionless number $\beta = kVR/(\Sigma + kVR) = R^2/(L_F^2 + R^2) \in]0,1[$, which represents the proportion of friction in the total dissipation. Scaling using Σ or $\Sigma + kVR$ as the characteristic stress are equivalent, and it is possible to switch from one to the other by noting that $C_F = \beta/(1-\beta)$ or $\beta = C_F/(1+C_F)$. In the same way, we could have equivalently considered $\kappa_F = L_F/R$, the relative size of fluctuations in the velocity field, instead of C_F, as $C_F = 1/\kappa_F^2$; in this case, $\beta = 1/(1+\kappa_F^2)$. Continuing this reasoning, $\tilde{\beta} = 1/(1+\kappa_F) = \sqrt{\beta}/(\sqrt{1-\beta} + \sqrt{\beta})$ could have been used.

For this study, we retain the following set of parameters:

$$C_F = T_a = 19, \quad \mathrm{Pe} = 0.5, \quad \kappa = 0.03, \quad B = 0.1, \quad a = 1. \tag{56}$$

Here, we take $\beta = 0.95$ and $\kappa = 0.03$ to create significant size effects. Indeed, the closer β is to 1, i.e. $C_F \to +\infty$, the smaller the friction length L_F, corresponding to a case where the size of the domain dominates that of the velocity structures; the same reasoning applies to κ. From a certain point of view, our aim is to model the collective motion of a large number of cells confined on a disk, if we interpret correlation lengths as effective interaction distances between cells.

In the following, we study the influence of the active stress coefficient S_a, taking it successively equal to 0, 1 and 3.

5.2. Resolution method

The problem 7 is a strongly coupled nonlinear problem, whose polarity evolution equation involves a transport term, a Laplacian and the nonlinear double-well term. It also includes an incompressibility constraint and a nonlinear and nonsymmetric stress tensor, which contains higher-order derivatives of polarity. To solve it on any bidimensional geometry, we use an semi-implicit time scheme, made fully implicit via the fixed-point method, and the discontinuous Galerkin method to solve the polarity evolution equation. The full numerical resolution method is out of the scope of this article and will be discussed in another publication [SCS].

To accurately capture the effective size of the structures represented by κ_F and κ, we need to mesh the computation domain Ω sufficiently finely. Ideally, these lengths cover 3 to 4 elements of the mesh, which means imposing a relationship of the form

$$h \leqslant \frac{1}{3} \min(\kappa_F, \kappa), \tag{57}$$

where h is the meshsize. For a first study and to avoid too fine meshes, we relax this constraint slightly by asking only

$$h \approx \min(\kappa_F, \kappa). \tag{58}$$

The mesh of the disk Ω is built as a N-sided polygon using `BAMG` [Hec06]. The meshsize is therefore of the order of $h \approx 2\pi/N$. In our case, the relation (58) then gives $N \approx 2\pi/\kappa$, i.e. $N = 210$. The result is shown on the figure 3.

Finally, we set the timestep to $\Delta t = 10^{-2}$, the maximum number of iterations of the fixed-point method to 10 and its tolerance threshold to 10^{-5}.

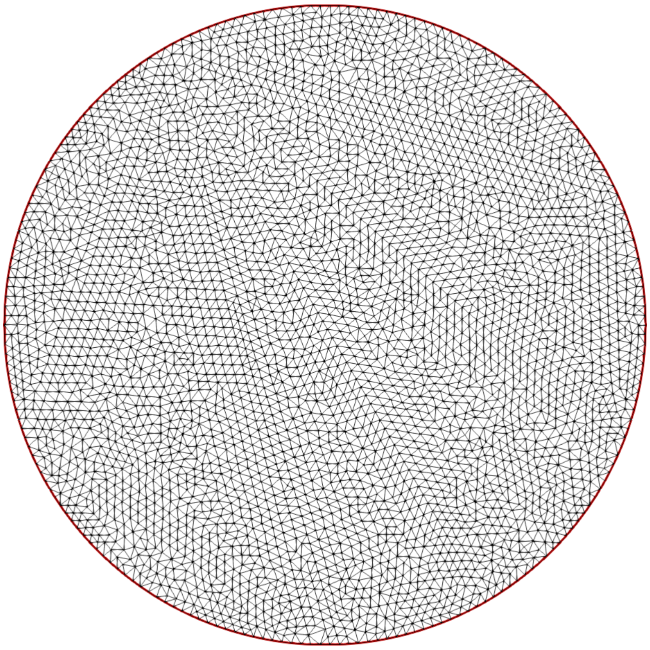

Figure 3: Mesh of the computation domain Ω, built as a regular polygon with $N = 210$ sides. It is made up of 7554 triangles.

5.3. Results

5.3.1. Maps of velocity and polarity fields

The absence of active stress ($S_a = 0$) does not mean the total absence of activity: remember that the active force $T_a \boldsymbol{p}$ is always present. However, without active stress, if the system creates a semblance of spontaneous motion, it does not last, and velocity tends towards 0 (figure 4, left-hand column). Indeed, if we look at the structure of the energy estimate (50), we notice that the term derived from the active force is only in $O(|\boldsymbol{p}|^2)$, whereas the term derived from the active stress is in $O(|\boldsymbol{p}|^4)$, hence its lesser capacity to push the system out of equilibrium.

Still when $S_a = 0$, polarity tends to stabilize in an isotropic configuration (figure 5, left-hand column). It is globally of norm 1, and its changes in direction create boundary layers (white filaments), similar to the topological defects found in liquid crystals and active gels [Mar+13; TS17; Lin+18], although these are more likely to be punctual and not filamentary. We should point out that what we are observing is only similar to topological defects: they are not really, since in our case the polarity is of variable norm and can vanish. When $S_a = 0$, these boundary layers gradually merge (figure 5, left-hand column), leaving only two singular points. We have not taken the calculation any further, but we conjecture that these two points will eventually merge into a single singular point that will stabilize at the center of the disk and from which the polarity will radiate.

On the contrary, the presence of active stress ($S_a \in \{1, 3\}$) does create spontaneous movement, and even sustains it (figure 4, center and right columns). It also maintains or shapes those filaments that look like topological defects, all the more so as S_a is large (figure 5, center and right columns).

5.3.2. Evolution of the free energy as a function of S_a

These calculations are prone to many fluctuations, so quantitative representations using cross-sections along specific axes are not relevant, especially in the prospect of comparisons with experimental data. Statistical physics tools could undoubtedly prove useful here, especially for future comparisons with experimental data. We propose here to compare effective quantities

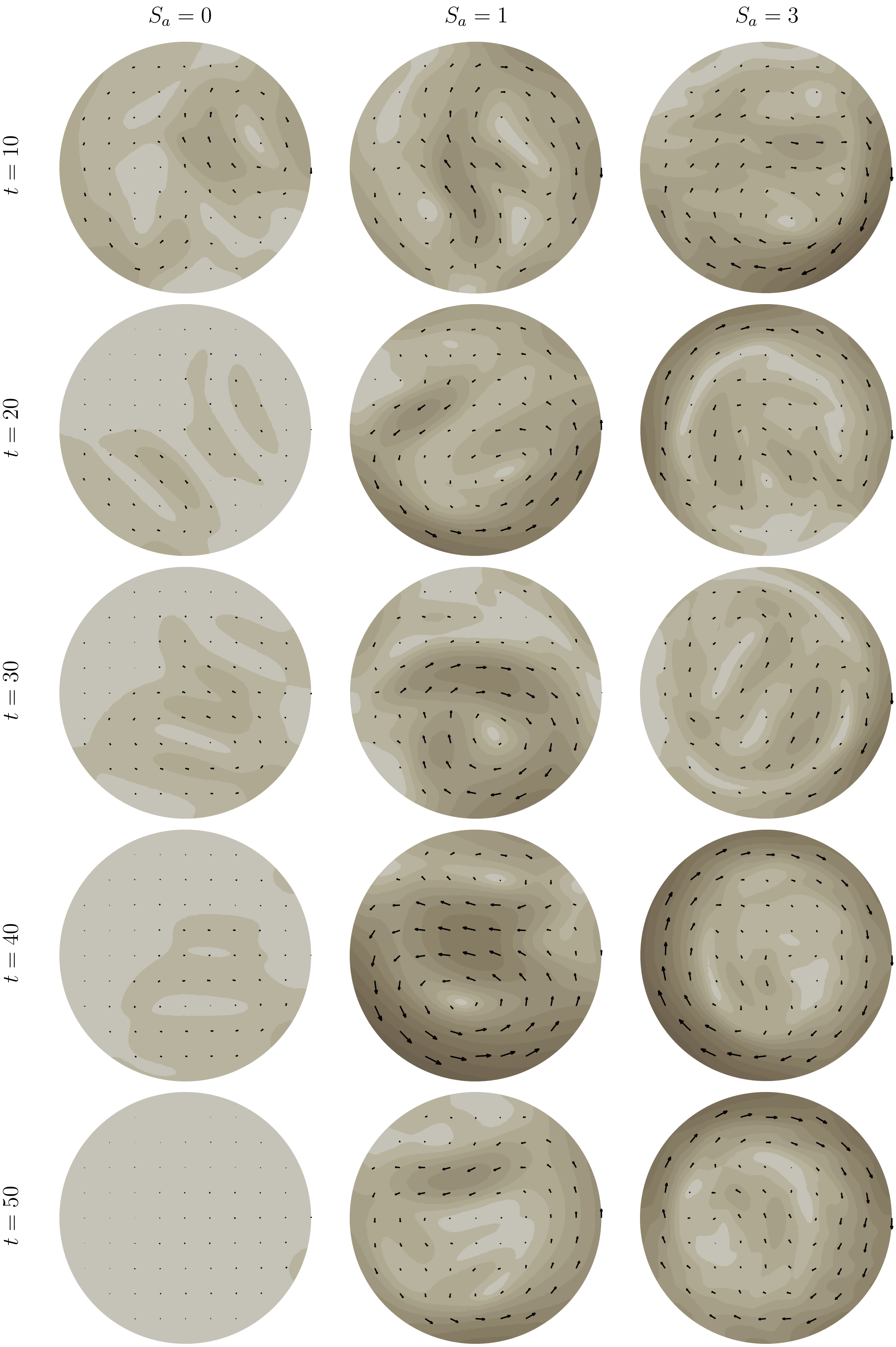

Figure 4: Velocity maps at different times, depending on the active stress coefficient S_a. Other parameters are given by (56).

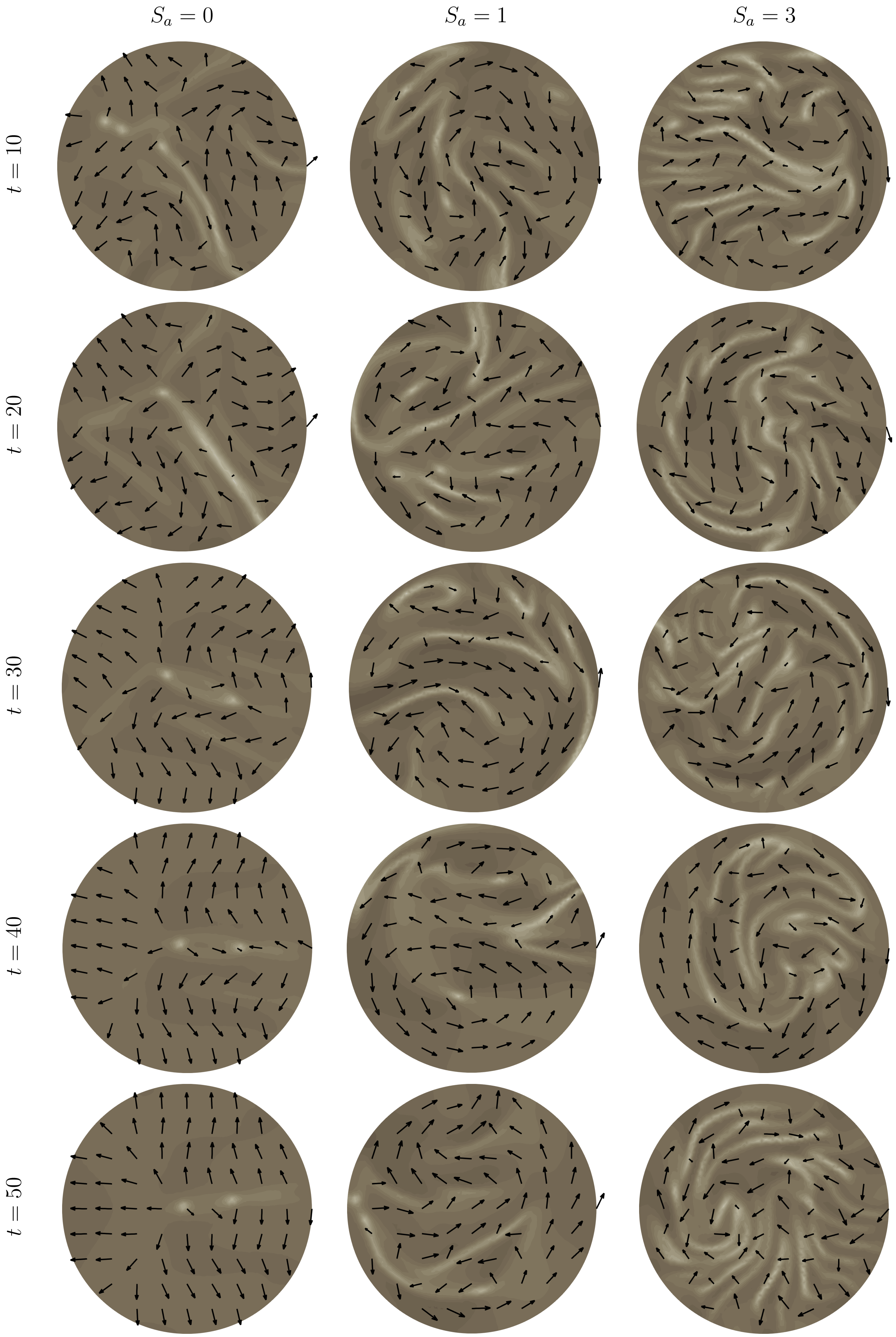

Figure 5: Polarity maps at different times, depending on the active stress coefficient S_a. Other parameters are given by (56).

over the whole domain, and in particular the influence of the active stress coefficient S_a on the time evolution of the free energy.

Note that theorem 1 still holds in our study, even if Ω does not evolve over time, because the tissue is assumed confined; we still have

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \int_\Omega \rho \frac{\partial \Psi}{\partial t}\,\mathrm{d}\boldsymbol{x} = \int_\Omega \Big(\rho\dot{\Psi} - \operatorname{div}(\rho\Psi\boldsymbol{v})\Big)\,\mathrm{d}\boldsymbol{x} = \int_\Omega \rho\dot{\Psi}\,\mathrm{d}\boldsymbol{x} - \int_{\partial\Omega} \rho(\boldsymbol{v}\cdot\boldsymbol{n})\Psi\,\mathrm{d}s = \int_\Omega \rho\dot{\Psi}\,\mathrm{d}\boldsymbol{x},$$

from the incompressibility condition and the boundary condition $\boldsymbol{v}\cdot\boldsymbol{n} = 0$. In this energy estimate, the active stress plays a crucial role and, in particular, competes with the deformation rate tensor $\boldsymbol{D}(\boldsymbol{v})$, one tending to destabilize the system (i.e. increase energy), the other to stabilize it (i.e. decrease energy). The figure 6 actually shows that the free energy tends towards a constant (probably zero) for $S_a = 0$, meaning that the system is tending towards a state of equilibrium, while it oscillates for $S_a > 0$, indicating that the system is constantly being kept out of equilibrium. It confirms the visual impression from figures 4 and 5 where fluctuations increase with S_a.

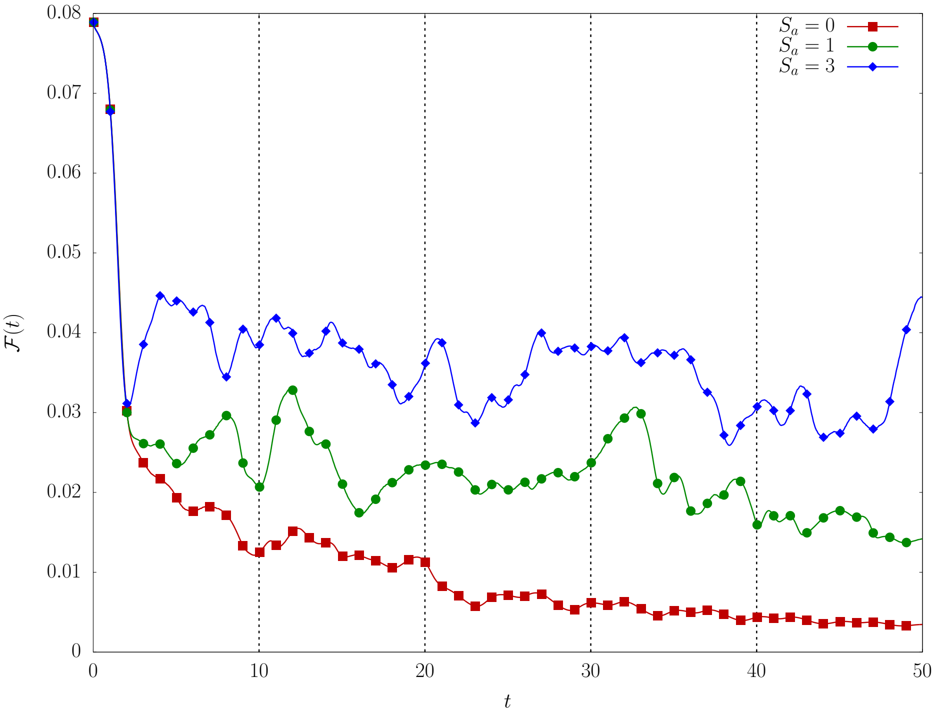

Figure 6: Variations over time of the free energy $\mathscr{F}$ as a function of the dimensionless active stress coefficient S_a. Other parameters are given by (56). The dotted vertical bars correspond to the instants from which the figure maps 4 and 5 were extracted.

5.4. Discussion

The influence of the active stress has long been known in the literature [Mar+13]. Numerous computations have already been carried out showing the same type of complex structures [Saw+17; TS17; Lin+18], similar to topological defects, that are obtained here. The numerical resolutions we carry out in this section are, however, to our knowledge, the first to have been carried out with a continuous model, using the finite element method. As a result, we can easily imagine similar calculations on more complex geometries.

6. Conclusion

In this paper, we have proposed a new thermodynamic framework to derive objective constitutive equations (11) and (15) for general active polar fluids. It combines the unified dissipation potential formalism developed in [Sar24] (section 2.2) and the skew-symmetric couple stress theory (section 2.1) [HHD15]. It takes as input only a free energy Ψ and a convex and positive dissipation potential Φ, reaching its minimum in 0. By construction, the resulting equations satisfy the second principle of thermodynamics (theorem 1), which is a crucial requirement for the equations of continuum mechanics.

As in active gel theory and contrary to the framework in [Sar24], the free energy (7) here can depend on gradients of thermodynamic variables, such as the polarity, allowing its Laplacian to be incorporated into the equations (see equations (17d) and (48c)). In addition, the use of a dissipation potential makes it possible to generalize Onsager's relations to the nonlinear case, and thus to introduce a wide variety of different rheologies, such as plasticity. On the other hand, the introduction of viscoelastic ingredients was not discussed in this paper, but is possible as pointed out by remark III. Such ingredients could be used to describe nonlinear elasticity, which is crucial in morphogenesis for instance. We have also shown how to rigorously couple the physical fields with density ρ, through the Hencky strain tensor $\boldsymbol{h}$ (8). The dependence of the free energy on the Hencky strain tensor, in addition to allowing this coupling with the density, paves the way for a greater variety of rheologies under large deformations, as shown in [Sar24], which represents a significant improvement with respect to the pioneering approach of [Mir+25]. A last but definite advantage of introducing our abstract framework is the ability of proving an energy estimate in the general case (theorem 2), that is for any free energy Ψ and any dissipation potential Φ. It could be useful for establishing existence results for solutions or for analyzing the stability of our equations, for instance.

Then, we have demonstrated the ability of our framework to retrieve the equations from the active gel theory [Mar+13, equations (42) to (46)], adapted to collective cell migration. To achieve this result, we have considered three classical physical ingredients: a double-well potential to ensure motion, the penalization of spatial variations of the polarity field and the decoupling of reaction advancement and polarization. By construction, our formalism includes the stress term $K_F \nabla \boldsymbol{p}^{\mathsf{T}} \cdot \nabla \boldsymbol{p}$, known as the Ericksen stress in the liquid crystal theory, up to the pressure contribution [GP93, equation (3.100) p. 153]. Like the other polar terms, this polar stress tends to realign polarities to minimize energy, thus helping to establish a spatial correlation between neighboring polarities. It is a kind of reversible distorsion: it does not contribute to dissipation. Our framework also leads to the energy estimate (50), which predicts the decrease of the free energy in the absence of activity, as might be expected. Corollaries 1 and 2 pointed out the necessity of the term $K_F \nabla \boldsymbol{p}^{\mathsf{T}} \cdot \nabla \boldsymbol{p}$ to be present in the expression of the Cauchy stress tensor: when present, the second principle of thermodynamics is satisfied, when absent, it is violated. Several active gel theory articles omit this term [Kru+05; Mar+13; BC17; AT19], probably because in simple cases this term barely affects the equation solutions; we strongly recommend to reintroduce it.

Finally, we have solved the model on a simple geometry, illustrating the model's ability to spontaneously create collective motion, in this case taking the form of a swarm-like behavior, all the more important as the active stress is.

Acknowledgements

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A. Functional framework for thermodynamics

In the following, functions are defined in Ω, an open subset of $\mathbb{R}^d$, where $d \in \mathbb{N}^*$, and are assumed to be sufficiently smooth to allow differentiation and integration operations to be formally applied to them, without regard to the functional spaces to which they belong. Thus, a functional is said differentiable if it is Gâteaux-differentiable.

A.1. Scalar case

In this section, $\mathscr{E}$ is the functional defined for any $\rho \in L^\infty(\Omega)$ and for any sufficiently smooth scalar field $c\colon \Omega \to \mathbb{R}$ by

$$\mathscr{E}(\rho, c) := \int_\Omega \rho e(c, \nabla c) \,\mathrm{d}\boldsymbol{x}, \tag{59}$$

where $e\colon (c, \boldsymbol{g}) \longmapsto e(c, \boldsymbol{g})$ is a real-valued function defined in $\mathbb{R} \times \mathbb{R}^d$, differentiable with respect to each of its variables.

Lemma 1 – Differential of a gradient-dependent functional

The differential $\frac{\partial \mathscr{E}}{\partial c}$ is the linear form defined for any sufficiently smooth test function $\theta\colon \Omega \to \mathbb{R}$ by

$$\left\langle \frac{\partial \mathscr{E}}{\partial c}, \theta \right\rangle = (w(\rho, c) \mid \theta) + \int_{\partial\Omega} \rho\theta \left(\frac{\partial e}{\partial \boldsymbol{g}}(c, \nabla c) \cdot \boldsymbol{n} \right) \mathrm{d}s, \tag{60}$$

where

$$w(\rho, c) := \rho \frac{\partial e}{\partial c}(c, \nabla c) - \operatorname{div}\left(\rho \frac{\partial e}{\partial \boldsymbol{g}}(c, \nabla c) \right). \tag{61}$$

The differential $\frac{\partial \mathscr{E}}{\partial \rho}$ is the linear form defined for any $z \in L^\infty(\Omega)$ by

$$\left\langle \frac{\partial \mathscr{E}}{\partial \rho}, z \right\rangle = (e(c, \nabla c) \mid z). \tag{62}$$

If the surface integral vanishes, we also note $\frac{\partial \mathscr{E}}{\partial c} = w(\rho, c)$ by the Riesz representation theorem. By virtue of the same theorem, we note $\frac{\partial \mathscr{E}}{\partial \rho} = e(c, \nabla c)$.

Proof. The function e is differentiable with respect to each of its variables so by definition of the differential, for any sufficiently smooth scalar fields c and θ and $\varepsilon > 0$, we have

$$e(c + \varepsilon\theta, \nabla c + \varepsilon \nabla\theta) - e(c, \nabla c) = \varepsilon \left(\frac{\partial e}{\partial c}\theta + \frac{\partial e}{\partial \boldsymbol{g}}(c, \nabla c) \cdot \nabla\theta \right) + O(\varepsilon^2). \tag{*.1}$$

Thus,

$$\begin{aligned} \mathscr{E}(\rho, c + \varepsilon\theta) - \mathscr{E}(\rho, c) &= \int_\Omega \rho e(c + \varepsilon\theta, \nabla c + \varepsilon\nabla\theta) \,\mathrm{d}\boldsymbol{x} - \int_\Omega \rho e(c, \nabla c) \,\mathrm{d}\boldsymbol{x} \\ &= \varepsilon \int_\Omega \rho \left(\frac{\partial e}{\partial c}\theta + \frac{\partial e}{\partial \boldsymbol{g}}(c, \nabla c) \cdot \nabla\theta \right) \mathrm{d}\boldsymbol{x} + O(\varepsilon^2). \end{aligned} \tag{*.2}$$

Then we integrate by parts and get formula (60) by taking the limit $\varepsilon \to 0$:

$$\begin{aligned} \frac{\mathscr{E}(\rho, c + \varepsilon\theta) - \mathscr{E}(\rho, c)}{\varepsilon} = \int_\Omega \left(\rho \frac{\partial e}{\partial c}(c, \nabla c) - \operatorname{div}\left(\rho \frac{\partial e}{\partial \boldsymbol{g}}(c, \nabla c) \right) \right) \theta \,\mathrm{d}\boldsymbol{x} \\ + \int_{\partial\Omega} \rho\theta \left(\frac{\partial e}{\partial \boldsymbol{g}}(c, \nabla c) \cdot \boldsymbol{n} \right) \mathrm{d}s + O(\varepsilon). \end{aligned} \tag{*.3}$$

Equation (62) is automatically obtained from the linearity of $\mathscr{E}$ with respect to ρ. ■

Lemma 2 – Integration by parts with a gradient-dependent functional

The following relation holds:

$$-\left(e(c,\nabla c)\mid \operatorname{div}(\rho\boldsymbol{v})\right)=\left\langle\frac{\partial\mathscr{E}}{\partial c},(\boldsymbol{v}\cdot\nabla)c\right\rangle-\int_\Omega\rho\left(\nabla c\otimes\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\right):\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}\\-\int_{\partial\Omega}\rho(\boldsymbol{v}\cdot\boldsymbol{n})e(c,\nabla c)\,\mathrm{d}s,\quad(63)$$

where $\frac{\partial\mathscr{E}}{\partial c}$ is defined by (60).

Proof. By integration by parts,

$$\begin{aligned}\int_\Omega -e(c,\nabla c)\operatorname{div}(\rho\boldsymbol{v})\,\mathrm{d}\boldsymbol{x}&=\int_\Omega\rho(\boldsymbol{v}\cdot\nabla)[e(c,\nabla c)]\,\mathrm{d}\boldsymbol{x}-\int_{\partial\Omega}\rho(\boldsymbol{v}\cdot\boldsymbol{n})e(c,\nabla c)\,\mathrm{d}s\\&=\int_\Omega\rho\frac{\partial e}{\partial c}(c,\nabla c)\cdot[(\boldsymbol{v}\cdot\nabla)c]\,\mathrm{d}\boldsymbol{x}\\&\qquad+\int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\cdot\{(\boldsymbol{v}\cdot\nabla)[\nabla c]\}\,\mathrm{d}\boldsymbol{x}\\&\qquad-\int_{\partial\Omega}\rho(\boldsymbol{v}\cdot\boldsymbol{n})e(c,\nabla c)\,\mathrm{d}s.\end{aligned}\quad(*.1)$$

But $\nabla[(\boldsymbol{v}\cdot\nabla)c]=(\boldsymbol{v}\cdot\nabla)[\nabla c]+\nabla c\cdot\nabla\boldsymbol{v}$, therefore

$$\begin{aligned}\int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\cdot\{(\boldsymbol{v}\cdot\nabla)[\nabla c]\}\,\mathrm{d}\boldsymbol{x}&=\int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\cdot\nabla[(\boldsymbol{v}\cdot\nabla)c]\,\mathrm{d}\boldsymbol{x}\\&\qquad-\int_\Omega\rho(\nabla c\cdot\nabla\boldsymbol{v})\cdot\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\,\mathrm{d}\boldsymbol{x}\\&=\int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\cdot\nabla[(\boldsymbol{v}\cdot\nabla)c]\,\mathrm{d}\boldsymbol{x}-\int_\Omega\rho\left(\nabla c\otimes\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\right):\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}.\end{aligned}$$

Then, an integration by parts gives

$$\begin{aligned}\int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\cdot\{(\boldsymbol{v}\cdot\nabla)[\nabla c]\}\,\mathrm{d}\boldsymbol{x}&=\int_{\partial\Omega}\rho\left(\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\cdot\boldsymbol{n}\right)[(\boldsymbol{v}\cdot\nabla)c]\,\mathrm{d}s\\&\qquad-\int_\Omega\operatorname{div}\left(\rho\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\right)\cdot[(\boldsymbol{v}\cdot\nabla)c]\,\mathrm{d}\boldsymbol{x}\\&\qquad-\int_\Omega\rho\left(\nabla c\otimes\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\right):\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}\end{aligned}\quad(*.2)$$

Combining this result, (*.1) and (60), we finally get the desired result. ■

Lemma 3 – Time rate of a gradient-dependent functional

Let us assume that Ω is a volume transported by the velocity field $\boldsymbol{v}$ and that ρ is the density. For any sufficiently smooth time-dependent scalar field $c\colon\Omega\times]0,+\infty[\to\mathbb{R}$, the following relation holds:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{E}(\rho,c))=\left\langle\frac{\partial\mathscr{E}}{\partial c}(\rho,c),\dot{c}\right\rangle-\int_{\Omega(t)}\rho\left(\nabla c\otimes\frac{\partial e}{\partial\boldsymbol{g}}(c,\nabla c)\right):\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}.\qquad(64)$$

Proof. By the Reynolds formula and integration by parts,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{E}(\rho,c)) &= \int_{\Omega(t)} \left(\frac{\partial}{\partial t}(\rho e(c,\nabla c)) + \operatorname{div}(\rho e(c,\nabla c)\boldsymbol{v})\right)\mathrm{d}\boldsymbol{x} \\ &= \int_{\Omega(t)} \left(\rho\frac{\partial}{\partial t}(e(c,\nabla c)) + e(c,\nabla c)\frac{\partial \rho}{\partial t}\right)\mathrm{d}\boldsymbol{x} + \int_{\partial\Omega(t)} \rho(\boldsymbol{v}\cdot\boldsymbol{n})e(c,\nabla c)\,\mathrm{d}s. \qquad (*.1)\end{aligned}$$

By applying the mass conservation (3c) and remarking that

$$\int_{\Omega(t)} \rho\frac{\partial}{\partial t}(e(c,\nabla c))\,\mathrm{d}\boldsymbol{x} = \left\langle \frac{\partial \mathscr{E}}{\partial c}(\rho,c), \frac{\partial c}{\partial t}\right\rangle, \qquad (*.2)$$

we get

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{E}(\rho,c)) = \left\langle \frac{\partial \mathscr{E}}{\partial c}(\rho,c), \frac{\partial c}{\partial t}\right\rangle - (e(c,\nabla c) \mid \operatorname{div}(\rho\boldsymbol{v})) + \int_{\partial\Omega(t)} \rho(\boldsymbol{v}\cdot\boldsymbol{n})e(c,\nabla c)\,\mathrm{d}s. \qquad (*.3)$$

We can apply the lemma 2 and conclude. ■

A.2. Vector case

In this section, $\mathscr{E}$ is the functional defined for any $\rho \in L^\infty(\Omega)$ and for any sufficiently smooth vector field $\boldsymbol{p}\colon \Omega \to \mathbb{R}^d$ by

$$\mathscr{E}(\rho,\boldsymbol{p}) := \int_\Omega \rho e(\boldsymbol{p},\nabla\boldsymbol{p})\,\mathrm{d}\boldsymbol{x}, \qquad (65)$$

where $e\colon (\boldsymbol{p},\boldsymbol{\tau}) \longmapsto e(\boldsymbol{p},\boldsymbol{\tau})$ is a real-valued function defined in $\mathbb{R}^d \times \mathbb{R}^{d\times d}$, differentiable with respect to each of its variables.

Lemma 4 – Differential of a gradient-dependent functional

The differential $\frac{\partial \mathscr{E}}{\partial \boldsymbol{p}}$ is the linear form defined for any sufficiently smooth test function $\boldsymbol{q}\colon \Omega \to \mathbb{R}^d$ by

$$\left\langle \frac{\partial \mathscr{E}}{\partial \boldsymbol{p}}, \boldsymbol{q}\right\rangle = (\boldsymbol{m}(\rho,\boldsymbol{p}) \mid \boldsymbol{q}) + \int_{\partial\Omega} \rho\boldsymbol{q}\cdot\frac{\partial e}{\partial \boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p})\cdot\boldsymbol{n}\,\mathrm{d}s, \qquad (66)$$

where

$$\boldsymbol{m}(\rho,\boldsymbol{p}) := \rho\frac{\partial e}{\partial \boldsymbol{p}}(\boldsymbol{p},\nabla\boldsymbol{p}) - \mathbf{div}\left(\rho\frac{\partial e}{\partial \boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p})\right). \qquad (67)$$

The differential $\frac{\partial \mathscr{E}}{\partial \rho}$ is the linear form defined for any $z \in L^\infty(\Omega)$ by

$$\left\langle \frac{\partial \mathscr{E}}{\partial \rho}, z\right\rangle = (e(\boldsymbol{p},\nabla\boldsymbol{p}) \mid z). \qquad (68)$$

If the surface integral vanishes, we also note $\frac{\partial \mathscr{E}}{\partial \boldsymbol{p}} = \boldsymbol{m}(\rho,\boldsymbol{p})$ by the Riesz representation theorem. By virtue of the same theorem, we note $\frac{\partial \mathscr{E}}{\partial \rho} = e(\boldsymbol{p},\nabla\boldsymbol{p})$.

Proof. The function e is differentiable with respect to each of its variables so by definition of the differential, for any sufficiently smooth vector fields $\boldsymbol{p}$ and $\boldsymbol{q}$ and $\varepsilon > 0$, we have

$$e(\boldsymbol{p}+\varepsilon\boldsymbol{q}, \nabla\boldsymbol{p}+\varepsilon\nabla\boldsymbol{q}) - e(\boldsymbol{p},\nabla\boldsymbol{p}) = \varepsilon\left(\frac{\partial e}{\partial \boldsymbol{p}}\cdot\boldsymbol{q} + \frac{\partial e}{\partial \boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p}) : \nabla\boldsymbol{q}\right) + O(\varepsilon^2). \qquad (*.1)$$

Thus,

$$\begin{aligned}\mathscr{E}(\rho,\boldsymbol{p}+\varepsilon\boldsymbol{q})-\mathscr{E}(\rho,\boldsymbol{p}) &= \int_\Omega \rho e(\boldsymbol{p}+\varepsilon\boldsymbol{q},\nabla\boldsymbol{p}+\varepsilon\nabla\boldsymbol{q})\,\mathrm{d}\boldsymbol{x} - \int_\Omega \rho e(\boldsymbol{p},\nabla\boldsymbol{p})\,\mathrm{d}\boldsymbol{x}\\ &= \varepsilon\int_\Omega \rho\left(\frac{\partial e}{\partial\boldsymbol{p}}\cdot\boldsymbol{q}+\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p}):\nabla\boldsymbol{q}\right)\mathrm{d}\boldsymbol{x}+O(\varepsilon^2). \qquad (*.2)\end{aligned}$$

Then we integrate by parts and get formula (66) by taking the limit $\varepsilon\to 0$:

$$\begin{aligned}\frac{\mathscr{E}(\rho,\boldsymbol{p}+\varepsilon\boldsymbol{q})-\mathscr{E}(\rho,\boldsymbol{p})}{\varepsilon} &= \int_\Omega\left(\rho\frac{\partial e}{\partial\boldsymbol{p}}-\mathbf{div}\left(\rho\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p})\right)\right)\cdot\boldsymbol{q}\,\mathrm{d}\boldsymbol{x}\\ &\quad+\int_{\partial\Omega}\rho\boldsymbol{q}\cdot\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p})\cdot\boldsymbol{n}\,\mathrm{d}s+O(\varepsilon). \qquad (*.3)\end{aligned}$$

Equation (68) is automatically obtained from the linearity of $\mathscr{E}$ with respect to ρ. ■

Lemma 5 – Integration by parts with a gradient-dependent functional

The following relation holds

$$\begin{aligned}-\left(e(\boldsymbol{p},\nabla\boldsymbol{p})\mid \operatorname{div}(\rho\boldsymbol{v})\right) &= \left\langle\frac{\partial\mathscr{E}}{\partial\boldsymbol{p}},(\boldsymbol{v}\cdot\nabla)\boldsymbol{p}\right\rangle-\int_\Omega\rho\left(\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p})\right):\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}\\ &\quad-\int_{\partial\Omega}\rho(\boldsymbol{v}\cdot\boldsymbol{n})e(\boldsymbol{p},\nabla\boldsymbol{p})\,\mathrm{d}s, \qquad (69)\end{aligned}$$

where $\frac{\partial\mathscr{E}}{\partial\boldsymbol{p}}$ is defined by (66).

Proof. By integration by parts,

$$\begin{aligned}\int_\Omega -e(\boldsymbol{p},\nabla\boldsymbol{p})\operatorname{div}(\rho\boldsymbol{v})\,\mathrm{d}\boldsymbol{x} &= \int_\Omega\rho(\boldsymbol{v}\cdot\nabla)[e(\boldsymbol{p},\nabla\boldsymbol{p})]\,\mathrm{d}\boldsymbol{x}-\int_{\partial\Omega}\rho(\boldsymbol{v}\cdot\boldsymbol{n})e(\boldsymbol{p},\nabla\boldsymbol{p})\,\mathrm{d}s\\ &= \int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{p}}(\boldsymbol{p},\nabla\boldsymbol{p})\cdot[(\boldsymbol{v}\cdot\nabla)\boldsymbol{p}]\,\mathrm{d}\boldsymbol{x} \qquad (*.1)\\ &\quad+\int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p}):\{(\boldsymbol{v}\cdot\nabla)[\nabla\boldsymbol{p}]\}\,\mathrm{d}\boldsymbol{x}\\ &\quad-\int_{\partial\Omega}\rho(\boldsymbol{v}\cdot\boldsymbol{n})e(\boldsymbol{p},\nabla\boldsymbol{p})\,\mathrm{d}s.\end{aligned}$$

But $\nabla[(\boldsymbol{v}\cdot\nabla)\boldsymbol{p}]=(\boldsymbol{v}\cdot\nabla)[\nabla\boldsymbol{p}]+\nabla\boldsymbol{p}\cdot\nabla\boldsymbol{v}$, therefore

$$\begin{aligned}\int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p}):\{(\boldsymbol{v}\cdot\nabla)[\nabla\boldsymbol{p}]\}\,\mathrm{d}\boldsymbol{x} &= \int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p}):\nabla[(\boldsymbol{v}\cdot\nabla)\boldsymbol{p}]\,\mathrm{d}\boldsymbol{x}\\ &\quad-\int_\Omega\rho(\nabla\boldsymbol{p}\cdot\nabla\boldsymbol{v}):\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p})\,\mathrm{d}\boldsymbol{x}\\ &= \int_\Omega\rho\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p}):\nabla[(\boldsymbol{v}\cdot\nabla)\boldsymbol{p}]\,\mathrm{d}\boldsymbol{x}-\int_\Omega\rho\left(\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\frac{\partial e}{\partial\boldsymbol{\tau}}(\boldsymbol{p},\nabla\boldsymbol{p})\right):\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}.\end{aligned}$$

Then, an integration by parts gives

$$\int_\Omega \rho \frac{\partial e}{\partial \boldsymbol{\tau}}(\boldsymbol{p}, \nabla \boldsymbol{p}) : \{(\boldsymbol{v}\cdot\nabla)[\nabla \boldsymbol{p}]\} \,\mathrm{d}\boldsymbol{x} = \int_{\partial\Omega} \rho \left(\frac{\partial e}{\partial \boldsymbol{\tau}}(\boldsymbol{p}, \nabla \boldsymbol{p}) \cdot \boldsymbol{n}\right) \cdot [(\boldsymbol{v}\cdot\nabla)\boldsymbol{p}] \,\mathrm{d}s$$
$$- \int_\Omega \mathbf{div}\left(\rho \frac{\partial e}{\partial \boldsymbol{\tau}}(\boldsymbol{p}, \nabla \boldsymbol{p})\right) \cdot [(\boldsymbol{v}\cdot\nabla)\boldsymbol{p}] \,\mathrm{d}\boldsymbol{x}$$
$$- \int_\Omega \rho \left(\nabla \boldsymbol{p}^\mathsf{T} \cdot \frac{\partial e}{\partial \boldsymbol{\tau}}(\boldsymbol{p}, \nabla \boldsymbol{p})\right) : \nabla \boldsymbol{v} \,\mathrm{d}\boldsymbol{x} \qquad (*.2)$$

By combining this result, (*.1) and (66), we finally get the desired result. ■

Lemma 6 – Time rate of a gradient-dependent functional

Let us assume that Ω is a volume transported by the velocity field $\boldsymbol{v}$ and that ρ is the density. For any sufficiently smooth time-dependent vector field $\boldsymbol{p}\colon \Omega \times]0, +\infty[\to \mathbb{R}^d$, the following relation holds

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{E}(\rho, \boldsymbol{p})) = \left\langle \frac{\partial \mathscr{E}}{\partial \boldsymbol{p}}(\rho, \boldsymbol{p}), \dot{\boldsymbol{p}} \right\rangle - \int_{\Omega(t)} \rho \left(\nabla \boldsymbol{p}^\mathsf{T} \cdot \frac{\partial e}{\partial \boldsymbol{\tau}}(\boldsymbol{p}, \nabla \boldsymbol{p})\right) : \nabla \boldsymbol{v} \,\mathrm{d}\boldsymbol{x}. \qquad (70)$$

Proof. By the Reynolds formula and integration by parts,

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{E}(\rho, \boldsymbol{p})) = \int_{\Omega(t)} \left(\frac{\partial}{\partial t}(\rho e(\boldsymbol{p}, \nabla \boldsymbol{p})) + \mathrm{div}(\rho e(\boldsymbol{p}, \nabla \boldsymbol{p})\boldsymbol{v})\right) \mathrm{d}\boldsymbol{x}$$
$$= \int_{\Omega(t)} \left(\rho \frac{\partial}{\partial t}(e(\boldsymbol{p}, \nabla \boldsymbol{p})) + e(\boldsymbol{p}, \nabla \boldsymbol{p}) \frac{\partial \rho}{\partial t}\right) \mathrm{d}\boldsymbol{x} + \int_{\partial\Omega(t)} \rho(\boldsymbol{v}\cdot\boldsymbol{n}) e(\boldsymbol{p}, \nabla \boldsymbol{p}) \,\mathrm{d}s. \qquad (*.1)$$

By applying the mass conservation (3c) and remarking that

$$\int_{\Omega(t)} \rho \frac{\partial}{\partial t}(e(\boldsymbol{p}, \nabla \boldsymbol{p})) \,\mathrm{d}\boldsymbol{x} = \left\langle \frac{\partial \mathscr{E}}{\partial \boldsymbol{p}}(\rho, \boldsymbol{p}), \frac{\partial \boldsymbol{p}}{\partial t} \right\rangle, \qquad (*.2)$$

we get

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{E}(\rho, \boldsymbol{p})) = \left\langle \frac{\partial \mathscr{E}}{\partial \boldsymbol{p}}(\rho, \boldsymbol{p}), \frac{\partial \boldsymbol{p}}{\partial t} \right\rangle - (e(\boldsymbol{p}, \nabla \boldsymbol{p}) \mid \mathrm{div}(\rho \boldsymbol{v})) + \int_{\partial\Omega(t)} \rho(\boldsymbol{v}\cdot\boldsymbol{n}) e(\boldsymbol{p}, \nabla \boldsymbol{p}) \,\mathrm{d}s. \qquad (*.3)$$

We can apply the lemma 5 and conclude. ■

A.3. Solving functional inequalities

Proposition 1

Let $\mathbb{D} = (\mathbb{D}_1, \ldots, \mathbb{D}_m)$ be a set of tensor fields of arbitrary order defined in Ω, an open subset of $\mathbb{R}^d$, where $d \in \mathbb{N}^*$, and Φ be a given real-valued function of $\mathbb{D}$, non necessarily differentiable. If Φ is convex and positive, and satisfies $\Phi(\mathbb{D} = 0) = 0$, then inequality

$$\sum_{i=1}^{m} \langle \mathbb{J}_i, \mathbb{D}_i \rangle \geqslant 0 \tag{71}$$

is satisfied for any $\mathbb{J} = (\mathbb{J}_1, \ldots, \mathbb{J}_m)$ such that $\mathbb{J}_i \in \partial_{\mathbb{D}_i}\Phi(\mathbb{D})$, where $\partial_{\mathbb{D}_i}\Phi(\mathbb{D})$ is the subdifferential of Φ with respect to $\mathbb{D}_i$, for any $i = 1, \ldots, m$.

Proof. The proof is adapted from [Sar16, Theorem 5.5]. Let $\mathbb{J} = (\mathbb{J}_1, \ldots, \mathbb{J}_m)$ such that $\mathbb{J}_i \in \partial_{\mathbb{D}_i}\Phi(\mathbb{D})$, for any $i = 1, \ldots, m$. In that case, we also have $\mathbb{J} \in \partial\Phi(\mathbb{D})$. By definition of the subdifferential for a convex function, inequality

$$\Phi(\mathbb{D}) + \langle \mathbb{J}, \tilde{\mathbb{D}} - \mathbb{D} \rangle \leqslant \Phi(\tilde{\mathbb{D}}) \tag{*.1}$$

holds for any $\tilde{\mathbb{D}}$. In particular, for $\tilde{\mathbb{D}} = 0$ and by hypothesis, $\Phi(\mathbb{D}) \leqslant \langle \mathbb{J}, \mathbb{D} \rangle$, but Φ is a positive function, hence the result (71). ■

B. Proofs of theorems 1 and 2

As explained at the beginning of the section 3.1, we start off by expanding the Lagrangian rate of the global free energy $\mathscr{F}$ with respect to the thermodynamic variables $\mathbb{A}$, then we inject the resulting expression in the Clausius-Duhem inequality (3d) integrated over the whole domaine Ω, which is dependent on time, and we finally deduce the constitutive equations.

B.1. Time rate of the global free energy

Let us start off by integrating the Clausius-Duhem inequality (3f) over the domain Ω. From the Reynolds formula and the continuity equation (3c), we get

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} = \int_{\Omega(t)} \left(\frac{\partial}{\partial t}(\rho\Psi) + \operatorname{div}(\rho\Psi\boldsymbol{v}) \right) \mathrm{d}\boldsymbol{x} = \int_{\Omega(t)} \rho\dot{\Psi}\, \mathrm{d}\boldsymbol{x}. \tag{72}$$

Hence this reformulation of the Clausius-Duhem inequality:

$$-\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} + (\mathbf{sym}\,\boldsymbol{\sigma} \mid \boldsymbol{D}(\boldsymbol{v})) - 2(\boldsymbol{l} \mid \boldsymbol{k}) \geqslant 0. \tag{73}$$

Now, we shall expand the time rate of the free energy $\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t}$.

Lemma 7 – Time rate of the global free energy $\mathscr{F}$

If the free energy Ψ is objective-isotropic with respect to each of its variables, then

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{h},\boldsymbol{r},c,\boldsymbol{p})) = {}&\\
&\left(\frac{\partial(\rho\Psi)}{\partial\boldsymbol{h}} - \nabla c\otimes\rho\frac{\partial\Psi}{\partial\nabla c} - \rho\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}} + a\,\mathbf{sym}(\boldsymbol{p}\otimes\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p}))\,\middle|\,\boldsymbol{D}(\boldsymbol{v})\right)\\
&+\left(\frac{1}{2}\boldsymbol{W}\left(\rho\frac{\partial\Psi}{\partial\boldsymbol{r}}\right) + \mathbf{skw}(\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p})\otimes\boldsymbol{p})\,\middle|\,\boldsymbol{W}(\boldsymbol{v})\right)\\
&+(w(\boldsymbol{h},c)\mid\dot{c}) + \left(\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p})\,\middle|\,\overset{\square}{\boldsymbol{p}}\right) + \int_{\partial\Omega(t)}\rho\left\{\frac{1}{2}\boldsymbol{\omega}\times\frac{\partial\Psi}{\partial\boldsymbol{r}} + \dot{c}\frac{\partial\Psi}{\partial\nabla c} + \dot{\boldsymbol{p}}\cdot\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}\right\}\cdot\boldsymbol{n}\,\mathrm{d}s,
\end{aligned} \tag{74a}$$

or if $\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}} = \mathbf{0}$,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{h},\boldsymbol{r},c,\boldsymbol{p})) = {}&\left(\frac{\partial(\rho\Psi)}{\partial\boldsymbol{h}} - \nabla c\otimes\rho\frac{\partial\Psi}{\partial\nabla c} + a\boldsymbol{p}\otimes\rho\frac{\partial\Psi}{\partial\boldsymbol{p}}\,\middle|\,\boldsymbol{D}(\boldsymbol{v})\right)\\
&+\left(\rho\frac{\partial\Psi}{\partial\boldsymbol{r}}\,\middle|\,\boldsymbol{k}\right) + (w(\boldsymbol{h},c)\mid\dot{c}) + \left(\rho\frac{\partial\Psi}{\partial\boldsymbol{p}}\,\middle|\,\overset{\square}{\boldsymbol{p}}\right) + \int_{\partial\Omega(t)}\rho\dot{c}\frac{\partial\Psi}{\partial\nabla c}\cdot\boldsymbol{n}\,\mathrm{d}s,
\end{aligned} \tag{74b}$$

where

$$w(\boldsymbol{h},c) := \rho\frac{\partial\Psi}{\partial c} - \operatorname{div}\left(\rho\frac{\partial\Psi}{\partial\nabla c}\right), \quad \boldsymbol{m}(\boldsymbol{h},\boldsymbol{p}) := \rho\frac{\partial\Psi}{\partial\boldsymbol{p}} - \mathbf{div}\left(\rho\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}\right). \tag{75}$$

Proof. From the chain rule and lemmas 3 and 6, we get

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{h},\boldsymbol{r},c,\boldsymbol{p})) = {}&\left\langle\frac{\partial\mathscr{F}}{\partial\boldsymbol{h}},\dot{\boldsymbol{h}}\right\rangle + \left\langle\frac{\partial\mathscr{F}}{\partial\boldsymbol{r}},\dot{\boldsymbol{r}}\right\rangle + \left\langle\frac{\partial\mathscr{F}}{\partial c},\dot{c}\right\rangle + \left\langle\frac{\partial\mathscr{F}}{\partial\boldsymbol{p}},\dot{\boldsymbol{p}}\right\rangle\\
&-\int_{\Omega(t)}\rho\left(\nabla c\otimes\frac{\partial\Psi}{\partial\nabla c}\right):\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x} - \int_{\Omega(t)}\rho\left(\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}\right):\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}
\end{aligned} \tag{*.1}$$

where, according to lemmas 1 and 4,

$$\left\langle\frac{\partial\mathscr{F}}{\partial\boldsymbol{h}},\boldsymbol{\chi}\right\rangle = \left(\frac{\partial(\rho\Psi)}{\partial\boldsymbol{h}}\,\middle|\,\boldsymbol{\chi}\right) \tag{*.2a}$$

$$\left\langle\frac{\partial\mathscr{F}}{\partial\boldsymbol{r}},\boldsymbol{q}\right\rangle = \left(\rho\frac{\partial\Psi}{\partial\boldsymbol{r}}\,\middle|\,\boldsymbol{q}\right) \tag{*.2b}$$

$$\left\langle\frac{\partial\mathscr{F}}{\partial c},\theta\right\rangle = (w(\boldsymbol{h},c)\mid\theta) + \int_{\partial\Omega(t)}\rho\theta\frac{\partial\Psi}{\partial\nabla c}\cdot\boldsymbol{n}\,\mathrm{d}s, \tag{*.2c}$$

$$\left\langle\frac{\partial\mathscr{F}}{\partial\boldsymbol{p}},\boldsymbol{q}\right\rangle = (\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p})\mid\boldsymbol{q}) + \int_{\partial\Omega(t)}\rho\boldsymbol{q}\cdot\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}\cdot\boldsymbol{n}\,\mathrm{d}s, \tag{*.2d}$$

with $w(\boldsymbol{h},c)$ and $\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p})$ being defined by (75). From the objective-isotropy of Ψ with respect to each of its variables, we have necessarily the following consequences:

- $\frac{\partial\Psi}{\partial\boldsymbol{h}}$ commutes with $\boldsymbol{h}$ and $\frac{\partial\Psi}{\partial\boldsymbol{h}}:\dot{\boldsymbol{h}} = \frac{\partial\Psi}{\partial\boldsymbol{h}}:\boldsymbol{D}(\boldsymbol{v})$, according to [Sar24, corollary 3.27];
- $\frac{\partial\Psi}{\partial\boldsymbol{r}}$ is colinear to $\boldsymbol{r}$ and $\frac{\partial\Psi}{\partial\boldsymbol{r}}\cdot\dot{\boldsymbol{r}} = \frac{\partial\Psi}{\partial\boldsymbol{r}}\cdot\overset{\circ}{\boldsymbol{r}}$, then $\frac{\partial\Psi}{\partial\boldsymbol{r}}\cdot\dot{\boldsymbol{r}} = \frac{\partial\Psi}{\partial\boldsymbol{r}}\cdot\boldsymbol{k}$, by definition of $\boldsymbol{r}$ (6);

- $\frac{\partial \Psi}{\partial \nabla c}$ is colinear to ∇c, therefore $\nabla c \otimes \frac{\partial \Psi}{\partial \nabla c}$ is symmetric;
- $\frac{\partial \Psi}{\partial \nabla \boldsymbol{p}}$ commutes with $\nabla \boldsymbol{p}$, therefore $\nabla \boldsymbol{p}^{\mathsf{T}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}}$ is symmetric.

Thus,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{h}, \boldsymbol{r}, c, \boldsymbol{p})) = &\left(\frac{\partial(\rho\Psi)}{\partial \boldsymbol{h}} - \nabla c \otimes \rho \frac{\partial \Psi}{\partial \nabla c} - \rho \nabla \boldsymbol{p}^{\mathsf{T}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} \,\middle|\, \boldsymbol{D}(\boldsymbol{v})\right) \\ &+ \left(\rho \frac{\partial \Psi}{\partial \boldsymbol{r}} \,\middle|\, \boldsymbol{k}\right) + (w(\boldsymbol{h}, c) \mid \dot{c}) + (\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) \mid \dot{p}) \\ &+ \int_{\partial\Omega(t)} \rho \dot{c} \frac{\partial \Psi}{\partial \nabla c} \cdot \boldsymbol{n} \, \mathrm{d}s + \int_{\partial\Omega(t)} \rho \dot{\boldsymbol{p}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} \cdot \boldsymbol{n} \, \mathrm{d}s. \quad (*.3)\end{aligned}$$

Then, from the definition of the Gordon-Schowalter objective rate

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{h}, \boldsymbol{r}, c, \boldsymbol{p})) = &\\ &\left(\frac{\partial(\rho\Psi)}{\partial \boldsymbol{h}} - \nabla c \otimes \rho \frac{\partial \Psi}{\partial \nabla c} - \rho \nabla \boldsymbol{p}^{\mathsf{T}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} + a \, \mathbf{sym}(\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) \otimes \boldsymbol{p}) \,\middle|\, \boldsymbol{D}(\boldsymbol{v})\right) \\ &+ \left(\rho \frac{\partial \Psi}{\partial \boldsymbol{r}} \,\middle|\, \boldsymbol{k}\right) + (\mathbf{skw}(\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) \otimes \boldsymbol{p}) \mid \boldsymbol{W}(\boldsymbol{v})) + (w(\boldsymbol{h}, c) \mid \dot{c}) + \left(\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) \,\middle|\, \overset{\square}{\boldsymbol{p}}\right) \\ &+ \int_{\partial\Omega(t)} \rho \dot{c} \frac{\partial \Psi}{\partial \nabla c} \cdot \boldsymbol{n} \, \mathrm{d}s + \int_{\partial\Omega(t)} \rho \dot{\boldsymbol{p}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} \cdot \boldsymbol{n} \, \mathrm{d}s. \quad (*.4)\end{aligned}$$

When $\frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} = \boldsymbol{0}$, we directly obtain relation (74b). Otherwise, to get (74a), all that remains is to transform the term $(\rho \frac{\partial \Psi}{\partial \boldsymbol{r}} \mid \boldsymbol{k}) + (\mathbf{skw}(\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) \otimes \boldsymbol{p}) \mid \boldsymbol{W}(\boldsymbol{v}))$ to conclude.
It turns out that integration by parts leads directly to the desired result (74a), since

$$\begin{aligned}\left(\rho \frac{\partial \Psi}{\partial \boldsymbol{r}} \,\middle|\, \boldsymbol{k}\right) &= \int_{\Omega(t)} \frac{1}{2} \rho \frac{\partial \Psi}{\partial \boldsymbol{r}} \cdot \nabla \times \boldsymbol{\omega} \, \mathrm{d}\boldsymbol{x} = \int_{\Omega(t)} \frac{1}{2} \rho \frac{\partial \Psi}{\partial r_i} \epsilon_{ijk} \omega_{k,j} \, \mathrm{d}\boldsymbol{x} \\ &= \int_{\Omega(t)} -\frac{1}{2} \left(\rho \frac{\partial \Psi}{\partial r_i}\right)_{,j} \epsilon_{ijk} \omega_k \, \mathrm{d}\boldsymbol{x} + \int_{\partial\Omega(t)} \frac{1}{2} \rho \frac{\partial \Psi}{\partial r_i} \epsilon_{ijk} \omega_k n_j \, \mathrm{d}s \\ &= \int_{\Omega(t)} -\frac{1}{2} \nabla \left(\rho \frac{\partial \Psi}{\partial \boldsymbol{r}}\right) : \boldsymbol{\epsilon} \cdot \boldsymbol{\omega} \, \mathrm{d}\boldsymbol{x} + \int_{\partial\Omega(t)} \frac{1}{2} \rho \frac{\partial \Psi}{\partial r_i} \epsilon_{ijk} \omega_k n_j \, \mathrm{d}s \\ &= \int_{\Omega(t)} \frac{1}{2} \boldsymbol{W} \left(\rho \frac{\partial \Psi}{\partial \boldsymbol{r}}\right) : \boldsymbol{W}(\boldsymbol{v}) \, \mathrm{d}\boldsymbol{x} + \int_{\partial\Omega(t)} \left(\boldsymbol{\omega} \times \frac{1}{2} \rho \frac{\partial \Psi}{\partial \boldsymbol{r}}\right) \cdot \boldsymbol{n} \, \mathrm{d}s,\end{aligned}$$

where Einstein summation convention has been adopted. We have also used the relation $\boldsymbol{W}(\boldsymbol{v}) = -\boldsymbol{\epsilon} \cdot \boldsymbol{\omega}$. ■

B.2. Proof of theorem 1

Lemma 8 – Skew-symmetric part of the stress tensor

In the skew-symmetric couple stress theory, the skew-symmetric part of the stress tensor satisfies

$$\mathbf{skw}\, \boldsymbol{\sigma} = \boldsymbol{W}(\boldsymbol{l}). \quad (76)$$

Proof. This proof is an adaptation of the calculations performed in [HHD15, page 12].

By definition of the couple stress vector $\boldsymbol{l}$, we have

$$\boldsymbol{\mu} = -\boldsymbol{\epsilon} \cdot \boldsymbol{l}. \tag{*.1}$$

Then, from the conservation law of angular momentum (3b), we get

$$\boldsymbol{\epsilon} : \left(\nabla \boldsymbol{l}^{\mathsf{T}} + \boldsymbol{\sigma}\right) = \boldsymbol{0}. \tag{*.2}$$

Thus, $\nabla \boldsymbol{l}^{\mathsf{T}} + \boldsymbol{\sigma}$ is symmetric, therefore its skew-symmetric part $-\boldsymbol{W}(\boldsymbol{l}) + \mathbf{skw}\,\boldsymbol{\sigma}$ vanishes, hence (76). ■

Lemma 9

$$-2(\boldsymbol{l} \mid \boldsymbol{k}) = -(\mathbf{skw}\,\boldsymbol{\sigma} \mid \boldsymbol{W}(\boldsymbol{v})) + \int_{\partial\Omega(t)} (\boldsymbol{l} \times \boldsymbol{\omega}) \cdot \boldsymbol{n} \,\mathrm{d}s. \tag{77}$$

Proof. From $\boldsymbol{k} = \frac{1}{2}\nabla \times \boldsymbol{\omega}$, we first get

$$-2(\boldsymbol{l} \mid \boldsymbol{k}) = -\int_{\Omega(t)} \boldsymbol{l} \cdot \nabla \times \boldsymbol{\omega} \,\mathrm{d}\boldsymbol{x} = -\int_{\Omega(t)} \epsilon_{ijk} l_i \omega_{k,j} \,\mathrm{d}\boldsymbol{x}, \tag{*.1}$$

where Einstein summation convention is adopted. Then an integration by parts gives

$$-2(\boldsymbol{l} \mid \boldsymbol{k}) = \int_{\Omega(t)} \epsilon_{ijk} l_{i,j} \omega_k \,\mathrm{d}\boldsymbol{x} - \int_{\partial\Omega(t)} \epsilon_{ijk} l_i n_j \omega_k \,\mathrm{d}s. \tag{*.2}$$

We conclude with the relation $\boldsymbol{W}(\boldsymbol{v}) = -\boldsymbol{\epsilon} \cdot \boldsymbol{\omega}$ and lemma 8. ■

Proof of theorem 1. Injecting the first version of the time rate of the global free energy (74a) in the global Clausius-Duhem inequality (73) and using the lemma 9 leads to

$$\begin{aligned}
&\left(\mathbf{sym}\,\boldsymbol{\sigma} - \frac{\partial(\rho\Psi)}{\partial \boldsymbol{h}} + \nabla c \otimes \rho\frac{\partial \Psi}{\partial \nabla c} + \rho\nabla \boldsymbol{p}^{\mathsf{T}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} - a\,\mathbf{sym}(\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p}) \otimes \boldsymbol{p}) \,\middle|\, \boldsymbol{D}(\boldsymbol{v})\right) \\
&\quad - \left(\mathbf{skw}\,\boldsymbol{\sigma} + \frac{1}{2}\boldsymbol{W}\left(\rho\frac{\partial \Psi}{\partial \boldsymbol{r}}\right) + \mathbf{skw}(\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p}) \otimes \boldsymbol{p}) \,\middle|\, \boldsymbol{W}(\boldsymbol{v})\right) \\
&\quad - (w(\boldsymbol{h},c) \mid \dot{c}) - \left(\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p}) \,\middle|\, \overset{\square}{\boldsymbol{p}}\right) \\
&\quad + \int_{\partial\Omega(t)} \left\{\boldsymbol{l} \times \boldsymbol{\omega} - \rho\left[\frac{1}{2}\boldsymbol{\omega} \times \frac{\partial \Psi}{\partial \boldsymbol{r}} + \dot{c} \cdot \frac{\partial \Psi}{\partial \nabla c} + \dot{\boldsymbol{p}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}}\right]\right\} \cdot \boldsymbol{n} \,\mathrm{d}s \geqslant 0.
\end{aligned} \tag{*.1}$$

Because $\boldsymbol{W}(\boldsymbol{v})$ cannot be expressed as the corotational rate of a tensor, the terms involving it must vanish [CN63], hence equation (11b).
Taking into account the boundary conditions (10), inequality (*.1) writes equivalently

$$\begin{aligned}
&\left(\mathbf{sym}\,\boldsymbol{\sigma} - \frac{\partial(\rho\Psi)}{\partial \boldsymbol{h}} + \nabla c \otimes \rho\frac{\partial \Psi}{\partial \nabla c} + \rho\nabla \boldsymbol{p}^{\mathsf{T}} \cdot \frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} - a\,\mathbf{sym}(\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p}) \otimes \boldsymbol{p}) \,\middle|\, \boldsymbol{D}(\boldsymbol{v})\right) \\
&\quad - (w(\boldsymbol{h},c) \mid \dot{c}) - \left(\boldsymbol{m}(\boldsymbol{h},\boldsymbol{p}) \,\middle|\, \overset{\square}{\boldsymbol{p}}\right) \geqslant 0.
\end{aligned} \tag{*.2}$$

If constitutive equations (11) are satisfied, then by hypothesis on Φ, the Clausius-Duhem inequality is satisfied, according to proposition 1. ■

Proof of theorem 1 when $\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}} = \boldsymbol{0}$. When $\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}} = \boldsymbol{0}$, injecting the second version of the time rate of the global free energy (74b) in the global Clausius-Duhem inequality (73) and taking into account the boundary condition (14) leads to

$$\left(\mathbf{sym}\,\boldsymbol{\sigma} - \frac{\partial(\rho\Psi)}{\partial\boldsymbol{h}} + \nabla c \otimes \rho\frac{\partial\Psi}{\partial\nabla c} - a\boldsymbol{p} \otimes \rho\frac{\partial\Psi}{\partial\boldsymbol{p}} \,\middle|\, \boldsymbol{D}(\boldsymbol{v})\right) - 2\left(\boldsymbol{l} + \frac{1}{2}\rho\frac{\partial\Psi}{\partial\boldsymbol{r}} \,\middle|\, \boldsymbol{k}\right) \\ - (w(\boldsymbol{h}, c) \mid \dot{c}) - \left(\rho\frac{\partial\Psi}{\partial\boldsymbol{p}} \,\middle|\, \overset{\square}{\boldsymbol{p}}\right) \geqslant 0. \quad (*.1)$$

If constitutive equations (15) are satisfied, then by hypothesis on Φ, the Clausius-Duhem inequality is satisfied, according to proposition 1. ■

Remark VII – *Boundary conditions*: If the boundary conditions (10) (respectively (14)) are not imposed, surface integrals remain in inequality (*.1) (respectively (*.1)), but because $\boldsymbol{\omega}$, $\dot{c}$ and $\dot{\boldsymbol{p}}$ are arbitrary and independent, the positivity of the inequality is not guaranteed anymore.

B.3. Energy estimates

Proof of theorem 2. Let us introduce the elastic stress $\boldsymbol{\sigma}_e$ defined by

$$\boldsymbol{\sigma}_e := \frac{\partial(\rho\Psi)}{\partial\boldsymbol{h}} - \nabla c \otimes \rho\frac{\partial\Psi}{\partial\nabla c} + a\,\mathbf{sym}\left(\boldsymbol{p} \otimes \frac{\partial\mathscr{F}}{\partial\boldsymbol{p}}\right) - \rho\nabla\boldsymbol{p}^{\mathsf{T}} \cdot \frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}. \quad (*.1)$$

By hypothesis, constitutive equations (11) are satisfied, and with this newly introduced variable, they write

$$\begin{aligned} \mathbf{sym}\,\boldsymbol{\sigma} - \boldsymbol{\sigma}_e &\in \frac{\partial\Phi}{\partial\boldsymbol{D}(\boldsymbol{v})}, && (*.2\text{a}) \\ \mathbf{skw}\,\boldsymbol{\sigma} &= -\frac{1}{2}\boldsymbol{W}\left(\rho\frac{\partial\Psi}{\partial\boldsymbol{r}}\right) + \mathbf{skw}(\boldsymbol{p} \otimes \boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p})), && (*.2\text{b}) \\ -w(\boldsymbol{h}, c) &\in \frac{\partial\Phi}{\partial\dot{c}}, && (*.2\text{c}) \\ -\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) &\in \frac{\partial\Phi}{\partial\overset{\square}{\boldsymbol{p}}}, && (*.2\text{d}) \end{aligned}$$

where $w(\boldsymbol{h}, c)$ and $\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p})$ are defined by (75). By definition of the subdifferential, there exists $\boldsymbol{\sigma}_p \in \frac{\partial\Phi}{\partial\boldsymbol{D}(\boldsymbol{v})}$, $c_p \in \frac{\partial\Phi}{\partial\dot{c}}$ and $\boldsymbol{p}_p \in \frac{\partial\Phi}{\partial\overset{\square}{\boldsymbol{p}}}$ such that

$$\begin{aligned} \mathbf{sym}\,\boldsymbol{\sigma} - \boldsymbol{\sigma}_e &= \boldsymbol{\sigma}_p, && (*.3\text{a}) \\ \mathbf{skw}\,\boldsymbol{\sigma} &= -\frac{1}{2}\boldsymbol{W}\left(\rho\frac{\partial\Psi}{\partial\boldsymbol{r}}\right) + \mathbf{skw}(\boldsymbol{p} \otimes \boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p})), && (*.3\text{b}) \\ -w(\boldsymbol{h}, c) &= c_p, && (*.3\text{c}) \\ -\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) &= \boldsymbol{p}_p. && (*.3\text{d}) \end{aligned}$$

Injecting these relations into the first version of the time rate of the global free energy (74a) leads to

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} + \mathscr{D} = (\mathbf{sym}\,\boldsymbol{\sigma} \mid \boldsymbol{D}(\boldsymbol{v})) - (\mathbf{skw}\,\boldsymbol{\sigma} \mid \boldsymbol{W}(\boldsymbol{v})) = \left(\boldsymbol{\sigma}^{\mathsf{T}} \,\middle|\, \nabla\boldsymbol{v}\right), \quad (*.4)$$

where $\mathscr{D}$ is defined by (21), but without the second term. The last term is transformed thanks to an integration by parts and the conservation of momentum (3a):

$$\begin{aligned}(\boldsymbol{\sigma}^{\mathsf{T}} \mid \nabla \boldsymbol{v}) &= -(\mathbf{div}(\boldsymbol{\sigma}^{\mathsf{T}}) \mid \boldsymbol{v}) + \int_{\partial\Omega(t)} \boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{v} \, \mathrm{d}s \\ &= -(\rho \dot{\boldsymbol{v}} \mid \boldsymbol{v}) + (\rho \boldsymbol{b} \mid \boldsymbol{v}) + \int_{\partial\Omega(t)} \boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{v} \, \mathrm{d}s.\end{aligned}$$

Finally, the term $(\rho \dot{\boldsymbol{v}} | \boldsymbol{v})$ is classically changed into $\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{E}_k(\boldsymbol{v}))$ using the conservation of mass (3c), where $\mathscr{E}_k(\boldsymbol{v})$ is the kinetic energy defined by (20), hence the result.
To conclude, by construction of $\mathscr{D}$ and according to proposition 1, we have $\mathscr{D} \geqslant 0$. ■

Proof of theorem 2 when $\frac{\partial \Psi}{\partial \nabla \boldsymbol{p}} = \mathbf{0}$. Let us introduce the elastic stress $\boldsymbol{\sigma}_e$ and the elastic couple stress $\boldsymbol{l}_e$, respectively defined by

$$\boldsymbol{\sigma}_e \coloneqq \frac{\partial(\rho\Psi)}{\partial \boldsymbol{h}} - \nabla c \otimes \rho \frac{\partial \Psi}{\partial \nabla c} + a \boldsymbol{p} \otimes \rho \frac{\partial \Psi}{\partial \boldsymbol{p}}, \tag{*.1a}$$

$$\boldsymbol{l}_e \coloneqq -\frac{1}{2} \rho \frac{\partial \Psi}{\partial \boldsymbol{r}}. \tag{*.1b}$$

By hypothesis, constitutive equations (15) are satisfied, and with those newly introduced variables, they write

$$\mathbf{sym}\, \boldsymbol{\sigma} - \boldsymbol{\sigma}_e \in \frac{\partial \Phi}{\partial \boldsymbol{D}(\boldsymbol{v})}, \tag{*.2a}$$

$$\boldsymbol{l} - \boldsymbol{l}_e \in -\frac{1}{2} \frac{\partial \Phi}{\partial \boldsymbol{k}}, \tag{*.2b}$$

$$-w(\boldsymbol{h}, c) \in \frac{\partial \Phi}{\partial \dot{c}}, \tag{*.2c}$$

$$-\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) \in \frac{\partial \Phi}{\partial \overset{\square}{\boldsymbol{p}}}, \tag{*.2d}$$

where $w(\boldsymbol{h}, c)$ and $\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p})$ are defined by (75). By definition of the subdifferential, there exists $\boldsymbol{\sigma}_p \in \frac{\partial \Phi}{\partial \boldsymbol{D}(\boldsymbol{v})}$, $\boldsymbol{l}_p \in -\frac{1}{2} \frac{\partial \Phi}{\partial \boldsymbol{k}}$, $c_p \in \frac{\partial \Phi}{\partial \dot{c}}$ and $\boldsymbol{p}_p \in \frac{\partial \Phi}{\partial \overset{\square}{\boldsymbol{p}}}$ such that

$$\mathbf{sym}\, \boldsymbol{\sigma} - \boldsymbol{\sigma}_e = \boldsymbol{\sigma}_p, \tag{*.3a}$$

$$\boldsymbol{l} - \boldsymbol{l}_e = \boldsymbol{l}_p, \tag{*.3b}$$

$$-w(\boldsymbol{h}, c) = c_p, \tag{*.3c}$$

$$-\boldsymbol{m}(\boldsymbol{h}, \boldsymbol{p}) = \boldsymbol{p}_p. \tag{*.3d}$$

Injecting these relations into the second version of the time rate of the global free energy (74b) leads to

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} + \mathscr{D} = (\mathbf{sym}\, \boldsymbol{\sigma} \mid \boldsymbol{D}(\boldsymbol{v})) - 2(\boldsymbol{l} \mid \boldsymbol{k}), \tag{*.4}$$

where $\mathscr{D}$ is defined by (21). Then, using lemma 9 and the boundary condition (14), we get

$$\frac{\mathrm{d}\mathscr{F}}{\mathrm{d}t} + \mathscr{D} = (\mathbf{sym}\, \boldsymbol{\sigma} \mid \boldsymbol{D}(\boldsymbol{v})) - (\mathbf{skw}\, \boldsymbol{\sigma} \mid \boldsymbol{W}(\boldsymbol{v})) + \int_{\partial\Omega(t)} (\boldsymbol{l} \times \boldsymbol{\omega}) \cdot \boldsymbol{n} \, \mathrm{d}s. \tag{*.5}$$

We conclude in the same way as in the previous proof. ■

Proof of corollary 1. From theorem (2), we have by hypothesis

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{p})) - (\Pi \mid \operatorname{div} \boldsymbol{v}) + 2\eta\|\boldsymbol{D}(\boldsymbol{v})\|^2 + \gamma\|\overset{\square}{\boldsymbol{p}}\|^2 + k\|\boldsymbol{v}\|^2 + (\boldsymbol{\sigma}_a \mid \boldsymbol{D}(\boldsymbol{v})) \\ = f_a(\boldsymbol{p} \mid \boldsymbol{v}) + \int_{\partial\Omega(t)} \boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{v}\, \mathrm{d}s. \quad (*.1)$$

Then, we apply the incompressibility condition (48b), the constitutive equation (40b), the boundary condition (47) and the Cauchy-Schwarz inequality, which gives

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{p})) + 2\eta\|\boldsymbol{D}(\boldsymbol{v})\|^2 + \frac{1}{\gamma}\|\boldsymbol{m}(\boldsymbol{p})\|^2 + k\|\boldsymbol{v}\|^2 \leqslant f_a\|\boldsymbol{p}\|\|\boldsymbol{v}\| + |\zeta\Delta\mu|\|\boldsymbol{p}\otimes\boldsymbol{p}\|\|\boldsymbol{D}(\boldsymbol{v})\|. \quad (*.2)$$

Finally, applying two times the Young inequality

$$ab \leqslant \frac{a^2}{2\varepsilon} + \frac{\varepsilon b^2}{2}, \quad (*.3)$$

valid for any real numbers a and b and any strictly positive real number ε leads to the result (50), since $\|\boldsymbol{p}\otimes\boldsymbol{p}\|^2 = \int_\Omega |\boldsymbol{p}|^4$. ■

Lemma 10

There exists a polarity field $\boldsymbol{p}$ such that

$$\|\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})\|^4 - \frac{2}{\gamma}\left(2\eta\|\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})\|^2 + k\|\boldsymbol{w}_{\boldsymbol{p}}\|^2\right)\|\boldsymbol{m}(\boldsymbol{p})\|^2 > 0, \quad (78)$$

where $\boldsymbol{w}_{\boldsymbol{p}}$ is the unique solution to the following problem:
$(S_{\boldsymbol{p}})$: find $\boldsymbol{w}$ and ϖ such that

$$\begin{aligned} -\mathbf{div}(\boldsymbol{D}(\boldsymbol{w})) + \nabla\varpi &= -\mathbf{div}(\boldsymbol{Q}(\boldsymbol{p})) && \text{in } \Omega, && (79a)\\ \operatorname{div} \boldsymbol{w} &= 0 && \text{on } \Omega, && (79b)\\ \boldsymbol{w} &= \mathbf{0} && \text{on } \partial\Omega, && (79c) \end{aligned}$$

where $\boldsymbol{Q}(\boldsymbol{p}) = K_F \nabla\boldsymbol{p}^{\mathsf{T}} \cdot \nabla\boldsymbol{p}$.

Proof. Assume that $|\boldsymbol{p}| = P$, where P is a positive real number. Thus there exists $\theta\colon \Omega \to \mathbb{R}$ such that $\boldsymbol{p} = P\boldsymbol{n}_\theta$, where $\boldsymbol{n}_\theta = (\cos\theta, \sin\theta)$. With this choice, the molecular field writes

$$\begin{aligned} \boldsymbol{m}(\boldsymbol{p}) &= \alpha\left(|\boldsymbol{p}|^2 - 1\right)\boldsymbol{p} - K_F\Delta\boldsymbol{p} \\ &= \alpha P^3\boldsymbol{n}_\theta - P(\alpha\boldsymbol{n}_\theta + K_F\Delta\boldsymbol{n}_\theta) \\ &= P^3\boldsymbol{y}_\theta - P\boldsymbol{z}_\theta, \end{aligned} \quad (*.1)$$

where

$$\begin{aligned} \boldsymbol{y}_\theta &= \alpha\boldsymbol{n}_\theta, && (*.2a)\\ \boldsymbol{z}_\theta &= \alpha\boldsymbol{n}_\theta + K_F\Delta\boldsymbol{n}_\theta. && (*.2b) \end{aligned}$$

As a consequence, its functional norm reads

$$\|\boldsymbol{m}(\boldsymbol{p})\|^2 = \|\boldsymbol{y}_\theta\|^2P^6 - 2(\boldsymbol{y}_\theta \mid \boldsymbol{z}_\theta)P^4 + \|\boldsymbol{z}_\theta\|^2P^2. \quad (*.3)$$

Let $\boldsymbol{w}_\theta$ be the unique solution to problem $(S_{\boldsymbol{n}_\theta})$, so that

$$\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}}) = P^2\boldsymbol{D}(\boldsymbol{w}_\theta). \quad (*.4)$$

Note that from the linearity and unicity of the solution of problem $(S_{\boldsymbol{p}})$, we also have $\boldsymbol{w_p} = P^2\boldsymbol{w}_\theta$. Then

$$\begin{aligned} & \|\boldsymbol{D}(\boldsymbol{w_p})\|^4 - \frac{2}{\gamma}\big(2\eta\|\boldsymbol{D}(\boldsymbol{w_p})\|^2 + k\|\boldsymbol{w_p}\|^2\big)\|\boldsymbol{m}(\boldsymbol{p})\|^2 > 0, \\ \iff\ & A_\theta\|\boldsymbol{y}_\theta\|^2P^4 - \big[\|\boldsymbol{D}(\boldsymbol{w}_\theta)\|^4 + 2A_\theta(\boldsymbol{y}_\theta \mid \boldsymbol{z}_\theta)\big]P^2 + A_\theta\|\boldsymbol{z}_\theta\|^2 < 0, \end{aligned} \tag{*.5}$$

where, for convenience,

$$A_\theta = \frac{2}{\gamma}\big(2\eta\|\boldsymbol{D}(\boldsymbol{w}_\theta)\|^2 + k\|\boldsymbol{w}_\theta\|^2\big) \geqslant 0. \tag{*.6}$$

When $A_\theta = 0$, it means both $\boldsymbol{D}(\boldsymbol{w}_\theta) = \boldsymbol{0}$ and $\boldsymbol{w}_\theta = \boldsymbol{0}$, and inequality (78) is not satisfied: it corresponds to $\nabla\theta = \boldsymbol{0}$. So let us assume the function θ is chosen such that $A_\theta > 0$. Introducing $B_\theta = 1/A_\theta$, the previous inequality writes equivalently

$$\|\boldsymbol{y}_\theta\|^2P^4 - \big[B_\theta\|\boldsymbol{D}(\boldsymbol{w}_\theta)\|^4 + 2(\boldsymbol{y}_\theta \mid \boldsymbol{z}_\theta)\big]P^2 + \|\boldsymbol{z}_\theta\|^2 < 0. \tag{*.7}$$

This is a biquadratic equation in P. Its discriminant Δ_θ is given by

$$\Delta_\theta = B_\theta\|\boldsymbol{D}(\boldsymbol{w}_\theta)\|^4 + 2(\boldsymbol{y}_\theta \mid \boldsymbol{z}_\theta) - 4\|\boldsymbol{y}_\theta\|^2\|\boldsymbol{z}_\theta\|^2. \tag{*.8}$$

With fixed viscosity η, it is possible to choose friction k such that $\Delta_\theta = 0$, as A_θ is linear in k. In that case, the unique root P^2 to this biquadratic equation is given by

$$P^2 = \frac{B_\theta}{\|\boldsymbol{y}_\theta\|^2}\|\boldsymbol{D}(\boldsymbol{w}_\theta)\|^4 + \frac{(\boldsymbol{y}_\theta \mid \boldsymbol{z}_\theta)}{\|\boldsymbol{y}_\theta\|^2}. \tag{*.9}$$

Note that $\|\boldsymbol{y}_\theta\|^2 = \alpha^2 \neq 0$. We finally choose η and k sufficiently small so that B_θ is sufficiently large to make the root P^2 positive. Thus, there exists a real value P for which inequality (78) is satisfied. In other words, the polarity field defined by $\boldsymbol{p} = P\boldsymbol{n}_\theta$ satisfied this inequality. ■

Proof of corollary 2. By hypothesis, the stress term $K_F\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\nabla\boldsymbol{p}$ is absent from the elastic stress $\boldsymbol{\sigma}_e$ (*.1) as defined in the proof of theorem 2. Applying the same procedure as in this proof and taking into account the absence of inertia and the boundary conditions (47) leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathscr{F}(\boldsymbol{p})) + \mathscr{D} + \left(\rho\nabla\boldsymbol{p}^{\mathsf{T}}\cdot\frac{\partial\Psi}{\partial\nabla\boldsymbol{p}}\,\middle|\,\boldsymbol{D}(\boldsymbol{v})\right) = (\rho\boldsymbol{b} \mid \boldsymbol{v}), \tag{*.1}$$

where $\mathscr{D}$ is defined by (21) and $\rho\boldsymbol{b}$ by (46). Then, the explicit form of the dissipation can be calculated, resulting in (51). Finally applying the same procedure as in the proof of corollary 1 leads to inequality (54).

The dissipation-like term $\tilde{\Delta}$ (53) involved in the energy estimate (54) is obviously not quadratic nor convex: its additional last term is linear with respect to $\boldsymbol{D}(\boldsymbol{v})$. Clearly, there is some possibilities for this term to be negative and to dominate all the other positive terms in absolute value, causing $\tilde{\Delta}(\boldsymbol{v},\boldsymbol{p}) < 0$, which is a violation of the second principle. Let us show that such a possibility exists.

Following the classical Coleman and Noll argument [CN63, p. 171], at any time $t \geqslant 0$ and any position $\boldsymbol{x}$ in Ω, we assume to be able to independently impose some arbitrarily values to $\boldsymbol{D}(\boldsymbol{v})$ without changing neither $\boldsymbol{p}$ nor $\nabla\boldsymbol{p}$ nor $\Delta\boldsymbol{p}$. Thus, $\boldsymbol{D}(\boldsymbol{v})$ can be considered thermodynamically independent from $\boldsymbol{p}$. Then, it is sufficient to choose $\boldsymbol{D}(\boldsymbol{v})$ such that the last term becomes negative and arbitrarily large in absolute value, in order to finally show that $\tilde{\Delta}(\boldsymbol{v},\boldsymbol{p}) < 0$. Note that due to the presence of the non-local energy term with $\nabla\boldsymbol{p}$, the dissipation involves a sum over Ω: the notation $\|\cdot\|$ is a functional norm, and inequality (54) is not pointwise but global over Ω. As a consequence, $\boldsymbol{p}$, $\nabla\boldsymbol{p}$ and $\Delta\boldsymbol{p}$ can not be considered as independent variables.

Let us define

$$\boldsymbol{Q}(\boldsymbol{p}) = K_F \nabla \boldsymbol{p}^{\mathsf{T}} \cdot \nabla \boldsymbol{p} \tag{*.2}$$

and let us consider the following generic Stokes-like linear and elliptic problem:

$(S_{\boldsymbol{q}})$: find $\boldsymbol{w}$ and ϖ such that

$$-\mathbf{div}(\boldsymbol{D}(\boldsymbol{w})) + \nabla\varpi = -\mathbf{div}(\boldsymbol{Q}(\boldsymbol{q})) \text{ in } \Omega, \tag{*.3a}$$

$$\operatorname{div} \boldsymbol{w} = 0 \quad \text{on } \Omega, \tag{*.3b}$$

$$\boldsymbol{w} = \mathbf{0} \quad \text{on } \partial\Omega. \tag{*.3c}$$

The unique solution to problem $(S_{\boldsymbol{p}})$ is denoted by $(\boldsymbol{w}_{\boldsymbol{p}}, \varpi_{\boldsymbol{p}})$; the subscript $\boldsymbol{p}$ emphasizes their dependence on $\boldsymbol{p}$. The vector field $\boldsymbol{w}_{\boldsymbol{p}}$ satisfies

$$(\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}}) - \boldsymbol{Q}(\boldsymbol{p}) \mid \boldsymbol{D}(\boldsymbol{w})) = 0 \tag{*.4}$$

for all divergence-free vector field $\boldsymbol{w}$ with $\boldsymbol{w} = \mathbf{0}$ on $\partial\Omega$. In particular, choosing $\boldsymbol{w} = \boldsymbol{w}_{\boldsymbol{p}}$ gives

$$\|\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})\|^2 = (\boldsymbol{Q}(\boldsymbol{p}) \mid \boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})). \tag{*.5}$$

As the system is linear, its solution depends linearly on its right-hand-side. Thus, when replacing $\boldsymbol{Q}(\boldsymbol{p})$ by $\xi\boldsymbol{Q}(\boldsymbol{p})$ in $(S_{\boldsymbol{p}})$, ξ being any real number, the solution becomes

$$\boldsymbol{v}_{\boldsymbol{p}} = \xi \boldsymbol{w}_{\boldsymbol{p}} \tag{*.6}$$

and satisfies

$$\|\boldsymbol{D}(\boldsymbol{v}_{\boldsymbol{p}})\|^2 = \xi(\boldsymbol{Q}(\boldsymbol{p}) \mid \boldsymbol{D}(\boldsymbol{v}_{\boldsymbol{p}})) = \xi^2 \|\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})\|^2. \tag{*.7}$$

The factor ξ will be chosen later.
Choosing $\boldsymbol{v}_{\boldsymbol{p}}$ as the velocity field allows to write $\tilde{\Delta}$ as

$$\begin{aligned}\tilde{\Delta}(\boldsymbol{v}_{\boldsymbol{p}}, \boldsymbol{p}) &= \frac{k}{2}\|\boldsymbol{v}_{\boldsymbol{p}}\|^2 + \eta\|\boldsymbol{D}(\boldsymbol{v}_{\boldsymbol{p}})\|^2 + \frac{1}{\gamma}\|\boldsymbol{m}(\boldsymbol{p})\|^2 + (\boldsymbol{Q}(\boldsymbol{p}) \mid \boldsymbol{D}(\boldsymbol{v}_{\boldsymbol{p}})) \\ &= \frac{1}{2}\big(2\eta\|\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})\|^2 + k\|\boldsymbol{w}_{\boldsymbol{p}}\|^2\big)\xi^2 + \|\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})\|^2\xi + \frac{1}{\gamma}\|\boldsymbol{m}(\boldsymbol{p})\|^2.\end{aligned} \tag{*.8}$$

Then $\tilde{\Delta}$ appears as a second order polynomial expression in terms of ξ. Its discriminant is nonnegative if, and only if,

$$\|\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})\|^4 - \frac{2}{\gamma}\big(2\eta\|\boldsymbol{D}(\boldsymbol{w}_{\boldsymbol{p}})\|^2 + k\|\boldsymbol{w}_{\boldsymbol{p}}\|^2\big)\|\boldsymbol{m}(\boldsymbol{p})\|^2 > 0. \tag{*.9}$$

Lemma 10 above shows that it is possible to choose the thermodynamic variable $\boldsymbol{p}$ such that this inequality is satisfied. Then the second order polynomial equation $\tilde{\Delta}(\boldsymbol{v}_{\boldsymbol{p}}, \boldsymbol{p}) = 0$ admits two distinct real roots $\xi_1 < \xi_2$, such that for any $\xi \in]\xi_1, \xi_2[$, $\tilde{\Delta}(\boldsymbol{v}_{\boldsymbol{p}}, \boldsymbol{p}) < 0$. In consequence, this model violates the second principle of thermodynamics. ■

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