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Variational derivation for higher gradient Van der Waals fluids equilibria and bifurcating phenomena

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Abstract. The equilibrium equations for a higher gradient van der Waals fluid is obtained in this paper from a variationally consistent formulation. An initial instability analysis for a fluid in a cubic-shaped hard device with sliding walls is then performed. In particular, the uniform contraction of a cubic block of fluid governed by the van der Waals free energy is analyzed. A finite perturbation about a homogeneous state is considered and a consistent linearization of such perturbation is shown to yield the possibility of bifurcation. This happens whenever the local volume ratio lies within the spinodal region of the energy and in the presence of sufficiently small capillarity.

Keywords: higher gradient, van der Waals fluids, bifurcation, bifurcating phenomena

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1 Introduction

In his seminal paper of 1893 [9], van der Waals proposed a free energy density for compressible fluids exhibiting capillarity as the sum of a non-convex function of the density and a term proportional to the spatial gradient of the density. Sixty-five years later a similar approach was rediscovered by Cahn and Hilliard [3]. In any case, starting with van der Waals himself, most, if not all, analyses of the theory have been restricted to one-dimensional settings, viz., the the density variation across a "flat" interface is a function of one spatial variable, e.g., [3–5, 9]. Indeed, the difficulty in analyzing van der Waals' model in space-dimensions larger than one has been acknowledged by Gurtin [6].

In this work we tackle a class of such problems in three spatial dimensions, while adopting the same point of view as that in [8]. That is, in seeking energy minima, we choose variations in the density that are kinematically induced by variations in the deformation (with respect to a Lagrangian description). Nonetheless, we develop the Euler-Lagrange equations of equilibrium in the spatial or Eulerian description. Although the derivation is complex, the final form of the equilibrium equations have a decided advantage over that obtained from a purely Lagrangian description—the main governing equation is a pde in the density (or equivalently in the local volume ratio) alone. In contrast, the Euler-Lagrange equations from a purely Lagrangian description directly reflect the coupling between the density and the deformation, the latter of which is hopefully indeterminate for a fluid. In addition, we present an initial instability analysis for a fluid in a cubic-shaped hard device with sliding walls.

The outline of the paper is as follows. In Section 1 we formulate the problem. There we consistently employ the change-of-variables theorem for integrals to realize the appropriate variations within the spatial description in order to compute the first variation. With the later in hand, integration by parts then delivers the strong form of the Euler-Lagrange equilibrium equations along with the natural boundary conditions. Many of the surprisingly detailed and tedious calculations are relegated to the appendices. In Section 2 we first consider the uniform compression of a cubic block of fluid governed by the van der Waals free energy. A homogeneous solution is readily written down, and we then recast our formulation in terms of a finite perturbation about the homogeneous state. Next we obtain the consistent linearization of the former—about the homogeneous state. Finally, we demonstrate the possibility of bifurcation from the homogeneous state when the local volume ratio of the later lies within the so-called spinodal region of the energy and in the presence of sufficiently small capillarity. Section 3 comprises several appendices, giving the detailed calculations leading to the summary presented within the main body of the paper.

1.1 Preliminaries

Let $\mathcal{B} \subset \mathbb{R}^3$ be a Lipschitz open bounded region with finite perimeter[1] representing the current configuration occupied by a (hyperelastic) fluid[2]. Let $\mathcal{B}_0 \subset \mathbb{R}^3$ be the underlying reference configuration and let $\mathbf{y} : \mathcal{B}_0 \to \mathbb{R}^3$ be the deformation from $\mathcal{B}_0$. We assume that $\mathbf{y}(\circ)$ is an orientation preserving C^1 diffeomorphism, although different regularity requirements may be imposed in the sequel.

Let $\mathbf{x} \in \mathcal{B}$ be a place in the current configuration and let $\mathbf{X} \in \mathcal{B}_0$ the corresponding material point in $\mathcal{B}_0$, i.e. $\mathbf{X} := \mathbf{y}^{-1}(\mathbf{x})$. If

$$\mathbf{F}(\mathbf{X}) := \nabla_X \mathbf{y}(\mathbf{X}) \tag{1}$$

[1]We then have that $\mathcal{H}^2(\partial\mathcal{B}) < \infty$, where is the Hausdorff measure of dimension two.

[2]The constitutive equation for such a fluid will be introduced in the next section.

denotes the (material) deformation gradient at $\mathbf{X}$, the change in volume J at $\mathbf{x} \in \mathcal{B}$ may be defined as follows:

$$J := \tilde{J}(\mathbf{x}) := \hat{J}\left(\mathbf{y}^{-1}(\mathbf{x})\right), \tag{2}$$

$$\hat{J}(\mathbf{X}) := \det(\mathbf{F}(\mathbf{X}))\,; \tag{3}$$

we also introduce the following notation:

$$\{J\}_m := \hat{J}(\mathbf{X}) = \tilde{J}(\mathbf{y}(\mathbf{X}))\,, \tag{4}$$

where $\{\circ\}_m$ denotes the material description of "$\circ$".

The local form for the mass continuity equation reads

$$\rho(\mathbf{x})J(\mathbf{x}) = \rho_0(\mathbf{y}^{-1}(\mathbf{x}))\,, \tag{5}$$

where $\rho(\mathbf{x})$ is the mass density of the fluid at $\mathbf{x}$ and $\rho_0(\mathbf{y}^{-1}(\mathbf{x}))$ is the referential density at $\mathbf{X} := \mathbf{y}^{-1}(\mathbf{x}) \in \mathcal{B}_0$.

Let us consider the equilibrium configurations that a Van Der Waals elastic fluid may experience; by this name we mean a hyperelastic fluid whose energy E_ϵ takes the form

$$E_\epsilon(J) = \int_{\mathcal{B}} \rho \left(W(J) + \epsilon \frac{|\nabla J|^2}{2} \right) \, d\mathcal{L}^3, \tag{6}$$

where W is a double well potential[3][4] and $\mathcal{L}^3$ denotes the Lebesgue measure of dimension three[5].

The energy can also be expressed in terms of material quantities:

$$\hat{E}_\epsilon(\boldsymbol{y}) := E_\epsilon(\{J\}_m) \tag{7}$$

$$= \int_{\mathcal{B}_0} \rho_0 \left\{ W(J) + \epsilon \frac{|\nabla J|^2}{2} \right\}_m d\mathcal{L}_0^3$$

$$= \int_{\mathcal{B}_0} \rho_0 \left(W(\hat{J}(\mathbf{X})) + \epsilon \frac{|\mathbf{F}^{-T}(\mathbf{X})\nabla_X \hat{J}(\mathbf{X})|^2}{2} \right) d\mathcal{L}_{0\mathbf{X}}^3\,, \tag{8}$$

where $\mathcal{L}_0^3$ is the Lebesgue measure of dimension three for the reference region $\mathcal{B}_0$[6], $\mathbf{F}(\mathbf{X})$ and $\hat{J}(\mathbf{X})$ are related to $\boldsymbol{y}$ through (1) and (3) respectively.

[3]For now the function $W(\circ)$ is assumed to be sufficiently smooth.

[4]Here ∇ denotes the spatial gradient.

[5]The assumed boundedness of $\mathcal{B}$ may be stated as $\mathcal{L}^3(\mathcal{B}) = \int_{\mathcal{B}} d\mathcal{L}_{\mathbf{x}}^3 < \infty$; from now on the dependence upon the place $\mathbf{x}$ will be omitted unless required for the sake of clarity.

[6]Obviously $\mathcal{L}_0^3(\mathcal{B}_0) = \int_{\mathcal{B}_0} d\mathcal{L}_{0\mathbf{X}}^3 < \infty$: form now on the dependence upon the material point $\mathbf{X}$ will be omitted unless required from the specific context.

1.2 Description of the problem

Here we want to study the equilibrium configurations of a fluid in a hard device. In particular, we study the case in which the boundary $\partial\mathcal{B}_0$ undergoes a prescribed follower normal displacement[7]:

$$\frac{(\nabla_X \mathbf{y})^{-T}\hat{\mathbf{n}}(\mathbf{X})}{|(\nabla_X \mathbf{y})^{-T}\hat{\mathbf{n}}(\mathbf{X})|}\cdot(\mathbf{y}(\mathbf{X})-\mathbf{X})=\bar{\lambda}\,\bar{\ell}\quad\forall\mathbf{X}\in\partial\mathcal{B}_0\,, \tag{9}$$

where $\bar{\ell}$ is a characteristic length of the domain $\mathcal{B}_0$.

Admissible variations $\mathbf{y}(\mathbf{X})+\varepsilon\eta(\mathbf{X})$ of the deformation have to be such that this constraint is not violated, and hence $\mathbf{X}\mapsto\mathbf{y}(\mathbf{X})+\varepsilon\eta(\mathbf{X})$ must verify (9), i.e.

$$\frac{(\nabla_X \mathbf{y})^{-T}\hat{\mathbf{n}}(\mathbf{X})}{|(\nabla_X \mathbf{y})^{-T}\hat{\mathbf{n}}(\mathbf{X})|}\cdot\eta(\mathbf{X})=0\quad\forall\mathbf{X}\in\partial\mathcal{B}_0\,. \tag{10}$$

Appendix A give equations (109, 110, 111) which allow for deriving the relationship between the material description of the variation η of the deformation $\mathbf{y}$ and the spatial description ζ of the variation itself; this is such that

$$\eta(\mathbf{X})=\zeta(\mathbf{y}(\mathbf{X}))\,, \tag{11}$$

or equivalently

$$\eta(\mathbf{y}^{-1}(\mathbf{x}))=\zeta(\mathbf{x})\,. \tag{12}$$

From now on we shall use the following notation for the spatial variation ζ:

$$\delta\mathbf{x}:=\zeta(\mathbf{x})\,. \tag{13}$$

We now note that the vector $\frac{(\nabla_X \mathbf{y})^{-T}\hat{\mathbf{n}}(\mathbf{X})}{|(\nabla_X \mathbf{y})^{-T}\hat{\mathbf{n}}(\mathbf{X})|}$ appearing in (9) represents the unit vector $\mathbf{n}(\mathbf{x})$ of the current normal at $\mathbf{x}=\mathbf{y}(\mathbf{X})$. Hence, such a boundary condition and the compatibility equation (10) for the variation $\delta\mathbf{x}$ may be rewritten in their spatial description as follows:

$$\mathbf{n}(\mathbf{x})\cdot(\mathbf{x}-\mathbf{y}^{-1}(\mathbf{x}))=\bar{\lambda}\bar{\ell}\quad\forall\mathbf{x}\in\partial\mathcal{B} \tag{14}$$

$$\mathbf{n}(\mathbf{x})\cdot\delta\mathbf{x}=0\quad\forall\mathbf{x}\in\partial\mathcal{B}\,. \tag{15}$$

The problem, which we denote by P_ϵ, may be stated as follows[8]:

$$P_\epsilon:=\mathrm{stat}_{\{J\in\mathcal{A}\}}\,E_\epsilon(J)\,, \tag{16}$$

[7]From now on we occasionally shall make an abuse of notation by denoting a function and its values with the same symbol.

[8]Here *stat* stands for "stationarity of".

i.e., we seek stationary points of E_ϵ in the set $\mathcal{A}$ of admissible J, which is defined as follows:

$$\mathcal{A} := \{\, J > 0 \mid\ J = \widehat{J}(\mathbf{y}^{-1}(\mathbf{x})),\ \mathbf{y} \in \mathcal{S}\,(\mathcal{B}_0)\,,\ \mathbf{n}(\mathbf{x}) \cdot (\mathbf{x} - \mathbf{y}^{-1}(\mathbf{x}))|_{\partial\mathcal{B}} = \bar{\lambda}\bar{\ell} \text{ and (5) hold}\,\}\,, \tag{17}$$

where $\mathcal{S}\,(\mathcal{B}_0)$ denotes the set of of all C^1 diffeomorphisms, $\mathcal{B}_0 \to \mathcal{B}$, such that the inverse of each element, $\mathbf{y}^{-1}$, also belongs to the function space $W^{2,2}\left(\mathcal{B}, \mathbb{R}^3\right)$.

In Appendix D (Sec. A.3) we shall see why the mass continuity (5) does not actually constraint the variations of the energy E_ϵ.

In order to solve (P_ϵ), we remark that if we take the first variation of E_ϵ in its material description, the variation goes inside the integral term. Indeed, the arbitrariness of the choice of reference configuration enables us to choose $\rho_0 = const$, which leads to the following expression for the first variation of the energy:

$$\delta E_\epsilon(\{J\}_m) = \int_{\mathcal{B}_0} \rho_0 \delta \left\{ W(J) + \epsilon \frac{|\nabla J|^2}{2} \right\}_m d\mathcal{L}_0^3\,. \tag{18}$$

Making use of (5), relation (18) is equivalent to the following expression in the spatial description:

$$\delta E_\epsilon(J) = \int_{\mathcal{B}} \rho \delta \left(W(J) + \epsilon \frac{|\nabla J|^2}{2} \right)\ d\mathcal{L}^3\,. \tag{19}$$

In the Appendix B (Sect. A.3) we provide derivations for the following variations induced by the material variation $\mathbf{y}(\mathbf{X}) \to \mathbf{y}(\mathbf{X}) + \varepsilon\eta(\mathbf{X})$:

$$\delta J = J \operatorname{div} \delta\mathbf{x}\,, \tag{20}$$

and

$$\delta(\nabla J) = \nabla(\delta J) - [\nabla(\delta\mathbf{x})]^T \nabla J \tag{21}$$

(see 113 and 114 respectively) where $\operatorname{div}\mathbf{v} = \nabla\mathbf{v}\cdot\mathbf{I}$ denotes the spatial divergence. Substitution of (20), (21) in (19) now yields

$$\delta E_\epsilon(J) = \int_{\mathcal{B}} \rho \left[W'(J) J \operatorname{div}\delta\mathbf{x} + \epsilon\nabla J \cdot (\nabla(J \operatorname{div}\delta\mathbf{x}) - [\nabla(\delta\mathbf{x})]^T \nabla J) \right]\ d\mathcal{L}^3.$$

Integration by parts (the details of which are carried out in (85), Section 1 and (101), Sect. A.2 of Appendix A) leads to the final form:

$$\delta\, E_\epsilon(J) = \int_{\mathcal{B}} \delta\,\mathbf{x}\,\cdot\,\operatorname{div}\,\mathbf{T}\ d\mathcal{L}^3 + \int_{\partial\mathcal{B}} \delta\,\mathbf{x}\,\cdot [\mathbf{Tn} - \epsilon\nabla_\Sigma(\rho J \nabla J\cdot\mathbf{n})]\ d\mathcal{H}^2 + \left\langle \int_{\bigcup_i \gamma_i} \delta\mathbf{x}\cdot\ \rfloor_i(\boldsymbol{t}_i)\ d\mathcal{H}^1 \right\rangle = 0 \quad \forall \text{ admissible } \delta\mathbf{x} \text{ such that (15) holds} \tag{22}$$

where

$$\mathbf{T} := \rho J \left\{ \left[W'(J) - \frac{\epsilon}{J} \left(\Delta J - \frac{|\nabla J|^2}{J} \right) \right] \mathbf{I} - \epsilon \frac{\nabla J \otimes \nabla J}{J} \right\} \tag{23}$$

is the Cauchy stress, $\nabla_\Sigma(\cdot)$ denotes the surface gradient (of the restriction of the argument function to $\partial\mathcal{B}$); if

$$\partial\mathcal{B} = \bigcup_j \partial\mathcal{B}_j, \quad \bigcap_k \partial\mathcal{B}_k = \bigcup_i \gamma_i$$

with $\{\gamma_i\}_{i\in\mathbb{N}}$ a countable (finite or infinite) set of closed contours γ_i,[9] the quantity $\rfloor_i(\boldsymbol{t}_i)$ represents the jump of an "edge-traction field" $\boldsymbol{t}_i$, whose precise definition is given in (100) (see Appendix A, Section 3.2), across the ith closed line γ_i. It is worth noting that, roughly speaking, from (95, 98) it follows that the third term in (22) is identically zero whenever no edges are present on the boundary $\partial\mathcal{B}$.

The surface-boundary condition resulting from (22) can be deduced by considering normal and tangential variations to the boundary $\partial\mathcal{B}$, i.e.

$$\delta\mathbf{x} = (\delta\mathbf{x}\cdot\mathbf{n})\mathbf{n} + (\delta\mathbf{x}\cdot\tau)\tau\,, \tag{24}$$

where $\tau := (\mathbf{I} - \mathbf{n}\otimes\mathbf{n})[\mathbf{e}]$, where $\mathbf{e}$ is any vector. In view of (15), the boundary variation reduces to

$$\delta\mathbf{x} = (\delta\mathbf{x}\cdot\tau)\tau\,. \tag{25}$$

An alternative boundary condition with respect to (9) could be deduced by (22) by dropping (15), in which case the following natural boundary condition would hold:

$$0 = \mathbf{n}\cdot[\mathbf{Tn} - \epsilon\nabla_\Sigma(\rho J \nabla J\cdot\mathbf{n})]\,; \tag{26}$$

this case will not be treated in this paper, although we keep record of it for future reference. In this case, the set of admissible deformations $\mathcal{A}$ should be obviously re-defined by replacing (14) with (26).

Returning to our case, substitution of (23) and (25) into the surface-boundary integral of (22) and subsequent localization lead to the following relationship[10]:

$$0 = \rho(\tau\cdot\nabla J)(\mathbf{n}\cdot\nabla J) + \rho J\tau\cdot\nabla_\Sigma(\mathbf{n}\cdot\nabla J)\,. \tag{27}$$

We note that the second term in the previous equation may be rewritten as follows:

$$\tau\cdot\nabla_\Sigma(\mathbf{n}\cdot\nabla J) = \mathbf{n}\cdot\nabla_\Sigma(\nabla J)[\tau] + \nabla J\cdot\nabla_\Sigma\mathbf{n}[\tau]. \tag{28}$$

[9]Technical issues relative to the boundedness of those sets are discussed in Appendix A, Section A.2.

[10]See e.g. the surface term in (102) for inspection.

Hence the boundary condition (27) takes the form:

$$0 = \mathbf{n} \cdot \left(\frac{\nabla J \otimes \nabla J}{J} + \nabla_\Sigma (\nabla J) \right) [\tau] + \nabla J \cdot \nabla_\Sigma \mathbf{n}[\tau], \quad \mathbf{x} \in \partial \mathcal{B}. \tag{29}$$

It is worth noting that, in the presence of a flat boundary, the latter term on the right-hand side of the previous equation drops out.

The Euler-Lagrange equation can be deduced by the first term in (22) and (23) and reads as follows[11][12]:

$$\operatorname{div} \left\{ \rho J \left\{ \left[W'(J) - \frac{\epsilon}{J} (\Delta J - \frac{|\nabla J|^2}{J}) \right] \mathbf{I} - \epsilon \frac{\nabla J \otimes \nabla J}{J} \right\} \right\} = \mathbf{0} \text{ in } \mathcal{B}\,. \tag{30}$$

The local form of (P_ϵ) is formed by the latter equation, together with (29) and (99), the surface and edge boundary conditions respectively, relation (118) (which may be deuced by the second term in (22)), the hard-device condition

$$\bar{\lambda} \bar{\ell} = \mathbf{n}(\mathbf{x}) \cdot (\mathbf{x} - \mathbf{y}^{-1}(\mathbf{x})), \quad \mathbf{x} \in \partial \mathcal{B}\,, \tag{31}$$

and

$$J = \tilde{J}(\mathbf{x})\,, \tag{32}$$

where (32) is defined in (2).

These last relations determine the deformations whose determinant of the gradient solves (30), (29) and (118).

2 The onset of bifurcation

In this section we presume that the reference configuration $\mathcal{B}_0$ is a cube of edge length $\bar{\ell}$. Consider a reference frame with origin at the center of mass of $\mathcal{B}_0$.

A homogeneous solution of the problem (P_ϵ), characterized by the homogeneous deformation $\bar{\boldsymbol{y}}$ from the reference configuration, may constructed as follows. First, observe that the constant $\bar{J}$ given by

$$\bar{J} := \frac{\int_{\mathcal{B}} \rho_0 \, d^3 \mathcal{L}}{\bar{m}} \tag{33}$$

[11]The Euler-Lagrange equation (30) may be viewed in the sense of distributions, as well as the boundary condition (29).

[12]For further developments we record that the second term in (30) may be rewritten as follows:

$$\rho \left(\Delta J - \frac{|\nabla J|^2}{J} \right) = \operatorname{div}(\rho \nabla J).$$

verifies the mass constraint (118). Furthermore, seek for an affine deformation map in the following form

$$\bar{\boldsymbol{y}}(\mathbf{X}) := \bar{\alpha}\mathbf{X}, \tag{34}$$

with $\bar{\alpha} \in \mathbb{R}$ to be determined in such a way that:

(1)

$$\frac{(\nabla_X \bar{\boldsymbol{y}})^{-T}\hat{\mathbf{n}}(\mathbf{X})}{|(\nabla_X \bar{\boldsymbol{y}})^{-T}\hat{\mathbf{n}}(\mathbf{X})|} \cdot (\bar{\boldsymbol{y}}(\mathbf{X}) - \mathbf{X}) = (\bar{\alpha} - 1)\hat{\mathbf{n}}(\mathbf{X}) \cdot \mathbf{X} = (\bar{\alpha} - 1)\frac{\bar{\ell}}{2}\,, \tag{35}$$

after using the fact that $\hat{\mathbf{n}}(\mathbf{X}) \cdot \mathbf{X} = \frac{\bar{\ell}}{2}$, i.e.

$$\bar{\alpha} = 1 + 2\bar{\lambda} \tag{36}$$

(2) and also the following relation is satisfied:

$$\det \nabla_X \bar{\boldsymbol{y}} = \bar{J}\,.$$

Hence, because of (36)

$$\bar{J} = (1 + 2\bar{\lambda})^3. \tag{37}$$

In spatial description the homogeneous solution reads as follows:

$$\bar{\boldsymbol{y}}^{-1}(\mathbf{x}) = \frac{\mathbf{x}}{(1 + 2\bar{\lambda})}\,; \tag{38}$$

Hence both (34) and (38) represent the material and the spatial form of the homogeneous solution of (P_ϵ) respectively.

In anticipation of our bifurcation analysis, we introduce:

$$J := \bar{J} + \tilde{J}\,. \tag{39}$$

The corresponding deformation $\boldsymbol{y}$ may be written in the following form

$$\boldsymbol{y}(\mathbf{X}) := \bar{\boldsymbol{y}}(\mathbf{X}) + \tilde{\boldsymbol{y}}(\mathbf{X})\,, \tag{40}$$

where the relationship between $\tilde{J}$ and $\tilde{\boldsymbol{y}}$ reads as follows:

$$\tilde{J} = \bar{J}\left[\det(\mathbf{I} + \bar{J}^{-\frac{1}{3}}\nabla_X\, \tilde{\boldsymbol{y}}) - 1\right]. \tag{41}$$

The spatial description of such relation may be easily obtained:

$$\tilde{J} = \bar{J}\left[\det\left(\mathbf{I} + \bar{J}^{-\frac{1}{3}}(\nabla\tilde{\boldsymbol{y}}^{-1})^{-1}\right) - 1\right]. \tag{42}$$

The spatial description of the decomposition (40) may be obtained by appealing to (109) (see Appendix A); indeed, by making the following identifications in (109)

$$\bar{\mathbf{x}} := \bar{\boldsymbol{y}}(\mathbf{X}) \,, \tag{43}$$

$$\tilde{\mathbf{x}} := \zeta(\bar{\mathbf{x}}) \,, \tag{44}$$

$$\zeta(\bar{\mathbf{x}}) = \zeta(\bar{\boldsymbol{y}}(\mathbf{X})) = \tilde{\boldsymbol{y}}(\mathbf{X}) \,, \tag{45}$$

$$\eta(\mathbf{X}) := \tilde{\boldsymbol{y}}(\mathbf{X}) \tag{46}$$

so that

$$\tilde{\mathbf{x}} = \tilde{\boldsymbol{y}}(\mathbf{X}) \,. \tag{47}$$

Hence, the spatial description of (40) reads as follows:

$$\mathbf{x} := \bar{\mathbf{x}} + \tilde{\mathbf{x}}. \tag{48}$$

It is straightforward to show that the field equations (30, 29, 31, 42, 118) are equivalent to the following relations:

$$\begin{cases} \operatorname{div}\left\{\rho(\bar{J}+\tilde{J})\left\{\left[W'(\bar{J}+\tilde{J}) - \dfrac{\epsilon}{\bar{J}+\tilde{J}}(\Delta\tilde{J} - \dfrac{|\nabla\tilde{J}|^2}{\bar{J}+\tilde{J}})\right]\mathbf{I} \right.\right. \\ \qquad\left.\left. -\epsilon\dfrac{\nabla\tilde{J}\otimes\nabla\tilde{J}}{\bar{J}+\tilde{J}}\right\}\right\} = \mathbf{0} \text{ in } \mathcal{B}\,, \\ \mathbf{n}\cdot\left(\dfrac{\nabla\tilde{J}\otimes\nabla\tilde{J}}{\bar{J}+\tilde{J}} + \nabla_\Sigma(\nabla\tilde{J})\right)[\tau] + \nabla\tilde{J}\cdot\nabla_\Sigma\mathbf{n}[\tau] = 0 \text{ on } \partial\mathcal{B}\,, \\ \bar{m} = \displaystyle\int_{\mathcal{B}} \frac{\rho_0}{(\bar{J}+\tilde{J})}\, d\mathcal{L}^3\,, \\ \tilde{J} = \bar{J}\left(\det\left(\mathbf{I} + \bar{J}^{-\frac{1}{3}}\left(\nabla\tilde{\boldsymbol{y}}^{-1}\right)^{-1}\right) - 1\right) \text{ in } \mathcal{B}\,, \\ \mathbf{n}(\mathbf{x})\cdot(\mathbf{x} - (\bar{\boldsymbol{y}}+\tilde{\boldsymbol{y}})^{-1}(\mathbf{x})) = \bar{\lambda}\bar{\ell} \text{ on } \partial\mathcal{B}\,, \\ \langle \rfloor_i\,(\mathbf{m}_i\otimes\mathbf{n}\nabla J)\rangle_{\gamma_i} = 0, \quad i = 1 \div 6\,, \end{cases} \tag{49}$$

after making use of (120), $(8)_1$ and (48) and where $\{\gamma_i\}_{i=1\div 6}$ are the six closed circuits obtained by “walking” (for example counterclockwise) on the edges of the cube.[13]

Obviously the material form of both $(49)_4$ and $(49)_5$ are

$$\left(\det(\mathbf{I} + \bar{J}^{-\frac{1}{3}}\nabla_X\tilde{\boldsymbol{y}}) - 1\right)\tilde{J} = \bar{J} \tag{50}$$

$$\mathbf{n}\left((\bar{\boldsymbol{y}}+\tilde{\boldsymbol{y}})(\mathbf{X})\right)\cdot\left((\bar{\boldsymbol{y}}+\tilde{\boldsymbol{y}})(\mathbf{X}) - \mathbf{X}\right) = \bar{\lambda}\bar{\ell}, \quad \mathbf{X}\in\partial\mathcal{B}_0\,. \tag{51}$$

[13] It is worth noting that no contributions come from the vertexes, which are indeed transversed an even number of times.

Let $\bar{\mathcal{B}}$ be current configuration corresponding to the trivial solution. Linearization of (49) results in the following eigenvalue problem

$$
\begin{cases}
\nabla \left\{ W''(\bar{J})\widehat{J} - \epsilon \Delta \widehat{J} \right\} = \mathbf{0} \text{ in } \bar{\mathcal{B}}\,, \\
\mathbf{n} \cdot \left(\nabla_\Sigma (\nabla \widehat{J}) + \nabla \widehat{J} \cdot \nabla_\Sigma \mathbf{n} \right) [\tau] = 0 \text{ on } \partial \bar{\mathcal{B}}\,, \\
\int_{\bar{\mathcal{B}}} \rho_0 \widehat{J}\, d\mathcal{L}^3 = 0\,, \\
\widehat{J} = \bar{J}^{\frac{2}{3}}\, Div\, \widehat{\boldsymbol{y}}(\mathbf{X}), \quad \mathbf{X} = \dfrac{\mathbf{x}}{1+2\bar{\lambda}}, \quad \mathbf{x} \in \bar{\mathcal{B}}\,, \\
\mathbf{n}((1+2\bar{\lambda})\mathbf{X}) \cdot \left(\mathbf{I} + \nabla_{\Sigma_X} \mathbf{n}((1+\bar{\lambda})\mathbf{X}) \right) [\widehat{\boldsymbol{y}}(\mathbf{X})] = 0\,, \\
\qquad \mathbf{X} = \dfrac{\mathbf{x}}{1+2\bar{\lambda}}\,, \quad \mathbf{x} \in \partial \bar{\mathcal{B}}\,, \\
\left\langle \rfloor_i \left(\mathbf{m}_i((1+2\bar{\lambda})\mathbf{X}) \otimes \mathbf{n}((1+2\bar{\lambda})\mathbf{X}) \nabla_X \widehat{J} \right) \right\rangle_{\gamma_i} = 0, \quad i = 1 \div 6\,,
\end{cases}
\tag{52}
$$

where $Div := tr, \nabla_X$ and, from $(49)_4$ and $(52)_4$, it is clear that $\widehat{J}$ represents the linear part of $\tilde{J}$.

It is worth noting that if the curvature tensor $\nabla_\Sigma\, \mathbf{n}(\mathbf{x})|_{\mathbf{x} \in \partial \bar{\mathcal{B}}} \neq \mathbf{O}$ at the boundary[14] $\partial \bar{\mathcal{B}}$, this contributes to the boundary condition $(52)_5$. Whenever this tensor vanishes, for example on a flat portion of $\partial \bar{\mathcal{B}}$, relation $(52)_5$ reduces to the following condition:

$$
\mathbf{n}((1+\bar{\lambda})\mathbf{X}) \cdot \widehat{\boldsymbol{y}}(\mathbf{X}) = 0\,, \quad \mathbf{X} = \frac{\mathbf{x}}{1+2\bar{\lambda}}\,, \quad \mathbf{x} \in \partial \bar{\mathcal{B}}\,, \tag{53}
$$

From equation $((52)_1)$ it is clear that bifurcation may arise whenever

$$
W''(\bar{J}) < 0\,, \tag{54}
$$

i.e. whenever $\bar{J}$ lies in the spinodal region of the double well potential W.

It is worth noting that in order for $(52)_4$ to be satisfied it is necessary and sufficient that $\widehat{y}$ derives from a scalar potential, i.e. there exists $\widehat{\chi} : \mathcal{B} \to \mathbb{R}$ such that

$$
\widehat{y} = \nabla_X \widehat{\chi}\,.
$$

Hence, $(52)_4$ may be rewritten as follows:

$$
\widehat{J} = \bar{J}^{\frac{2}{3}} \Delta_X \widehat{\chi}. \tag{55}
$$

[14]Because $X = x/(1+2\bar{\lambda})$, the relationship between the surface gradient in the current configuration and the surface gradient in the reference reads as follows: $\nabla_\Sigma = \nabla_{\Sigma_X} \nabla_\Sigma X = \nabla_{\Sigma_X}/(1+2\bar{\lambda})$.

The bifurcation problem may then be summarized as follows:

$$
\begin{cases}
\nabla\left\{W''(\bar{J})\widehat{J}-\epsilon\Delta\widehat{J}\right\}=\mathbf{0} \text{ on } \bar{\mathcal{B}} \\
\mathbf{n}\cdot\left(\nabla_\Sigma(\nabla\widehat{J})+\nabla\widehat{J}\cdot\nabla_\Sigma\mathbf{n}\right)[\tau]=0 \text{ on } \partial\bar{\mathcal{B}} \\
\int_{\bar{\mathcal{B}}}\rho_0\widehat{J}d\mathcal{L}^3=0 \\
\widehat{J}=\bar{J}^{\frac{2}{3}}\Delta_X\widehat{\chi}, \quad \mathbf{X}=\dfrac{\mathbf{x}}{1+2\bar{\lambda}}\,, \quad \mathbf{x}\in\bar{\mathcal{B}} \\
n(x)\cdot(I+\nabla_\Sigma n(x))\,[\nabla\widehat{\chi}(\dfrac{x}{1+\bar{\lambda}})]=0\,, \quad x\in\partial\bar{\mathcal{B}} \\
\left\langle \rfloor_i\left(\mathbf{m}_i\otimes\mathbf{n}\nabla\widehat{J}\right)\right\rangle_{\gamma_i}=0, \quad i=1\div 6\,.
\end{cases}
\tag{56}
$$

The first equation in (56) implies that

$$
-\epsilon\Delta\widehat{J}+W''(\bar{J})\widehat{J}=c\,, \tag{57}
$$

But $(56)_3$ immediately shows that the constant $c=0$. Thus, bifurcation may arise only if the quantity $-W''(\bar{J})\,/\epsilon$ is an eigenvalue of the Laplacian (subject to the boundary condition $(56)_2$), i.e., $\bar{J}$ must be in the so-called spinodal region of the energy W.

The problem of determining the onset of bifurcation for a given vessel with flat boundary is left to the next section.

2.1 The onset of bifurcation for a cubic container with sliding walls

In this this section we focus exclusively on the case when $\mathcal{B}$ is a cube. According to (36) the edges of the cube have magnitude $\ell=\bar{\alpha}\ell=(1+2\bar{\lambda})\bar{\ell}$. Since boundary of the cube is "flat", we have $\nabla_\Sigma\mathbf{n}=\mathbf{0}$, and the second terms in both $(56)_2$ and $(56)_5$ vanish. We introduce a right-handed coordinate system $\{\,O,\mathbf{e}_i\,\}_{i=1,\,2,\,3}$ with O at the centroid of the cube and set

$$
\mathbf{x}:=x_i\,\mathbf{e}_i,
$$

where $-\frac{\ell}{2}\le x_i\le\frac{\ell}{2}$, $i=1,2,3$. It is easy to show that the eigenfunctions

$$
\widehat{J}_{m_1m_2m_3}(\mathbf{z})=\prod_{i=1}^{3}\cos\left(\frac{\pi m_i x_i}{\ell}\right), \quad m_i\in\mathbb{N}\,, \tag{58}
$$

satisfy (57) (with $c=0$) and $(56)_{2,3}$, provided that the following characteristic equation holds:

$$
-\epsilon W''(\bar{J})+\sum_{k=1}^{3}\left(\frac{\pi m_k}{\ell}\right)^2=0\,. \tag{59}
$$

Relations $(56)_{4,5}$ are then easily satisfied via:

$$\widehat{\chi}_{m_1 m_2 m_3}(\mathbf{X}) = -\bar{J}^{-\frac{2}{3}} \left(\sum_{k=1}^{3} \left(\frac{\pi m_k}{2} \right)^2 \right)^{-1} \prod_{i=1}^{3} \cos \left(\frac{\pi m_i X_i}{2} \right) , \tag{60}$$

where $X_i := x_i/(1+2\overline{\lambda})$, $i = 1, 2, 3$, and $\overline{J}^{\frac{1}{3}} = (1+2\overline{\lambda})$.

We may note that the edge conditions

$$\left\langle \rfloor_i \left(\mathbf{m}_i \otimes \mathbf{n}_i \nabla \widehat{J} \right) \right\rangle_{\gamma_i} = \left\langle \rfloor_i \left(\mathbf{m}_i \ \mathbf{n}_i \cdot \nabla \widehat{J} \right) \right\rangle_{\gamma_i} = 0 \,, \quad i = 1 \div 6 \tag{61}$$

in (56) are automatically satisfied. Indeed

$$\nabla \widehat{J}_{m_1\, m_2\, m_3}(\mathbf{z}) = \sum_{i=1}^{3} \prod_{\substack{j=1,\\ j \neq i}}^{3} \cos \left(\frac{\pi m_j x_j}{\ell} \right) \sin \left(\frac{\pi m_i x_i}{\ell} \right) \boldsymbol{e}_i, \ m_i, \, m_j \ \in \mathbb{N} \,,$$

hence

$$\begin{aligned} (\mathbf{n}_i \cdot \nabla \widehat{J})_{\gamma_i} &= \boldsymbol{e}_i \cdot \nabla \widehat{J}_{m_1\, m_2\, m_3} |_{\{x_k\}_{k=\{1,\,2,\,3\}} = \frac{\ell}{2}} \\ &= \pm \prod_{\substack{j=1,\\ j \neq i}}^{3} \cos \left(\frac{\pi m_j x_j}{\ell} \right) |_{x_j = \frac{\ell}{2}} \,, \quad m_j = 2k_j + 1, \, k_j \in \mathbb{N} \,; \end{aligned} \tag{62}$$

actually $\cos \left(\frac{\pi m_j x_j}{\ell} \right) |_{x_j = \frac{\ell}{2}} = 0$ so that (61) is identically verified.

We denote by $(J_*, \, J^*)$ the interval in which $W''(J) < 0$.

Then, from the characteristic equation (59), we see that necessary condition for bifurcation is that

$$\bar{J} \in (J_*, \, J^*).$$

Whenever this is the case, for a fixed $\epsilon > 0$, the characteristic equation has two solutions, which will be denoted by $\left\{ \bar{J}^{(I)}_{m_1,\, m_2,\, m_3}(\epsilon), \, \bar{J}^{(II)}_{m_1,\, m_2,\, m_3}(\epsilon) \right\}$, ordered in such a way that $\bar{J}^{(I)}_{m_1,\, m_2,\, m_3}(\epsilon) < \bar{J}^{(II)}_{m_1,\, m_2,\, m_3}(\epsilon)$.

Hence, the least value of J for which there may be bifurcation from the trivial solution is $\bar{J}^{(I)}_{1,\,1,\,1}(\epsilon)$, i.e. the least root of (59) which is achieved for $m_i = 1$, $i = 1, 2, 3$.

Sufficient conditions for bifurcation—both local and global—will be investigated in a future work.

Appendix A: Explicit calculation of the first variation of E_ϵ

We want to obtain (22) starting from (19).

The first term in (19) reads as follows:

$$\int_{\mathcal{B}} \rho\delta W(J)\, d\mathcal{L}^3 = \int_{\mathcal{B}} \rho(\delta J)W'(J)\, d\mathcal{L}^3 = \int_{\mathcal{B}} \rho \operatorname{div}(\delta \mathbf{x})W'(J)\, d\mathcal{L}^3, \tag{63}$$

because, after making use of (113) in Appendix B (Sect. A.3) we get:

$$\delta J = J\left(I \cdot \nabla(\delta \mathbf{x})\right). \tag{64}$$

The first variation of the second term, i.e.

$$\frac{\epsilon}{2}\int_{\mathcal{B}} \rho\delta|\nabla J|^2\ d\mathcal{L}^3, \tag{65}$$

is more involved and it requires a few more steps. First of all we observe that

$$\frac{\epsilon}{2}\int_{\mathcal{B}} \rho\delta|\nabla J|^2\ d\mathcal{L}^3 = \epsilon\int_{\mathcal{B}} \rho\nabla J \cdot \delta(\nabla J)\, d\mathcal{L}^3. \tag{66}$$

We now recall relation (114), obtained in Appendix C, to calculate $\delta(\nabla J)$. By replacing φ with $\tilde{J}$ and, as in Appendix B (Sect. A.3), by identifying $\boldsymbol{\zeta}$ with $\delta\mathbf{x}$ from (114) we get

$$\delta(\nabla J) = \nabla(\delta J) - \nabla(\delta \mathbf{x})^T \nabla J\,. \tag{67}$$

Relation (67) into (66) yields two integrals, i.e.

$$\int_{\mathcal{B}} \rho\ \nabla J\ \cdot \delta(\nabla\, J)\, d\mathcal{L}^3 = I_1 - I_2$$

where

$$I_1 := \int_{\mathcal{B}} \rho\ \nabla J\ \cdot\ \nabla(\delta\, J)\ d\mathcal{L}^3, \tag{68}$$

$$I_2 := \int_{\mathcal{B}} \rho \nabla J\ \cdot\ (\nabla(\delta\, x))^T\, \nabla J\ d\mathcal{L}^3. \tag{69}$$

Let us first explore I_1. First of all we note that because of the identity

$$\mathbf{v} \cdot \nabla\varphi = \operatorname{div}(\varphi\, \mathbf{v}) - \varphi \operatorname{div} \mathbf{v}, \tag{70}$$

which holds for all scalar field φ and vector field $\mathbf{v}$, the integrand in (68) may be easily rewritten as follows

$$\rho\ \nabla J\ \cdot\ \nabla(\delta\, J) = \operatorname{div}(\delta J\, \rho\, \nabla J) - \delta J\ \operatorname{div}(\rho\, \nabla J)$$

after identifying $\mathbf{v}$ with ∇J and φ with δJ.

Hence, substitution of the latter relation into (68) and divergence theorem yield:

$$I_1 = \int_{\partial\mathcal{B}} \delta J \ \rho \ \nabla J \ \cdot \ \mathbf{n} \ d\mathcal{H}^2 \ - \ \int_{\mathcal{B}} \delta \, J \ \operatorname{div}(\rho \, \nabla J) \ d\mathcal{L}^3. \tag{71}$$

In order to evaluate I_2 we first note that the following relation holds[15]:

$$I_2 = I_2^{(1)} - I_2^{(2)} \tag{72}$$

where

$$I_2^{(1)} := \int_{\mathcal{B}} \rho \ \nabla J \ \cdot \ \nabla(\delta\mathbf{x} \cdot \nabla J) \ d\mathcal{L}^3, \tag{73}$$

$$I_2^{(2)} := \int_{\mathcal{B}} \rho \, \nabla(\nabla J) \, \nabla \, J \ \cdot \ \delta \, \mathbf{x} \ d\mathcal{L}^3. \tag{74}$$

Another application of (70) and divergence theorem lead to the following expression for (73)

$$I_2^{(1)} = \int_{\partial\mathcal{B}} (\delta\mathbf{x} \ \cdot \ \nabla \, J) \rho \, \nabla \, J \ \cdot \ \mathbf{n} \ d\mathcal{H}^2 - \int_{\mathcal{B}} \delta\mathbf{x} \ \cdot \ \nabla J \ \operatorname{div}(\rho \, \nabla J) \ d\mathcal{L}^3 \tag{75}$$

and hence substituting this expression into (72) yields

$$\begin{aligned} I_2 = \int_{\partial\mathcal{B}} & (\delta\mathbf{x} \ \cdot \ \nabla \, J) \rho \, \nabla \, J \ \cdot \ \mathbf{n} \ d\mathcal{H}^2 \\ & - \int_{\mathcal{B}} \delta\mathbf{x} \ \cdot \ (\nabla J \ \operatorname{div}(\rho \, \nabla J) + \rho \, \nabla(\nabla \, J) \, \nabla \, J) \ d\mathcal{L}^3. \end{aligned} \tag{76}$$

The substitution of (76) and (71) into (66) lead to the following expression for (19):

$$\begin{aligned} \delta E_\epsilon = \epsilon \int_{\partial\mathcal{B}} & (\delta \, J - \delta\mathbf{x} \ \cdot \ \nabla \, J) \ \rho \, \nabla \, J \ \cdot \ \mathbf{n} \ d\mathcal{H}^2 \\ & + \int_{\mathcal{B}} \big(\rho \, W'(J) \ - \ \epsilon \ \operatorname{div}(\rho \, \nabla \, J)\big) \ \delta \, J \ d\mathcal{L}^3 \\ & + \epsilon \int_{\mathcal{B}} \delta\mathbf{x} \ \cdot \ (\nabla J \ \operatorname{div}(\rho \, \nabla J) + \rho \, \nabla(\nabla \, J) \, \nabla \, J) \ d\mathcal{L}^3. \end{aligned} \tag{77}$$

[15]It is worth noting that the following identity holds:

$$\nabla\mathbf{u}^T\mathbf{v} = \nabla(\mathbf{u} \cdot \mathbf{v}) - \nabla\mathbf{v}^T\mathbf{u}$$

for any vector fields $\mathbf{u}$, $\mathbf{v}$.

The first and second term in the latter relation may be further investigated.

For the second term

$$\int_{\mathcal{B}} \big(\rho\, W'(J) - \epsilon\ \mathrm{div}(\rho\,\nabla\, J)\big)\, \delta J\ d\mathcal{L}^3 \tag{78}$$

we note that, because (64) holds and by virtue of (70), the integrand of (78) term takes the form:

$$\begin{aligned}\big(\rho\, W'(J)\ -\ \epsilon\ \mathrm{div}(\rho\,\nabla\, J)\big)\ J\ \mathrm{div}(\delta\,\mathbf{x})&\\ = \mathrm{div}\{J[\rho W'(J) - \epsilon\, \mathrm{div}(\rho\nabla J)]\ \delta\,\mathbf{x}\}&\\ -\,\delta\,\mathbf{x}\ \cdot\ \nabla\{J[\rho W'(J) - \epsilon\, \mathrm{div}(\rho\nabla J)]\}\,.&\end{aligned} \tag{79}$$

By integrating the latter relation over $\mathcal{B}$ and divergence theorem yield

$$\begin{aligned}\int_{\mathcal{B}} \big(\rho\, W'(J)\ -\ \epsilon\ \mathrm{div}(\rho\,\nabla\, J)\big)\ \delta\, J\ d\mathcal{L}^3&\\ = \int_{\partial\mathcal{B}} \delta\mathbf{x}\ \cdot\mathbf{n}\ \big[J\,\big(\rho\, W'(J) - \epsilon\ \mathrm{div}(\rho\,\nabla\, J)\big)\big]\ d\mathcal{H}^2&\\ -\int_{\mathcal{B}} \delta\mathbf{x}\ \cdot\ \nabla\,\big[J\,\big(\rho\, W'(J) - \epsilon\ \mathrm{div}(\rho\,\nabla\, J)\big)\big]\ d\mathcal{L}^3,&\end{aligned} \tag{80}$$

and hence equation (77) takes the form

$$\begin{aligned}\delta E_\epsilon = \int_{\partial\mathcal{B}} \mathbf{n}\cdot\big\{\delta\mathbf{x}J\,\big(\rho W'(J) - \epsilon\,\mathrm{div}(\rho\nabla J)\big) + \epsilon(\delta J - \delta\mathbf{x}\cdot\nabla J)\rho\nabla J\big\}\ d\mathcal{H}^2&\\ + \int_{\mathcal{B}} \delta\mathbf{x}\cdot\big\{-\nabla\,\big[J\,\big(\rho W'(J) - \epsilon\,\mathrm{div}(\rho\nabla J)\big)\big]&\\ +\epsilon\,(\nabla J\,\mathrm{div}(\rho\nabla J) + \rho\nabla(\nabla J)\nabla J)\}\ d\mathcal{L}^3;&\end{aligned} \tag{81}$$

In the sequel we shall refer the the first integral as *the surface term* and to the second one as *the bulk term*.

A.1 The bulk term

We may remark that the item multiplying the variation $\delta\mathbf{x}$ in the integrand of the second term in (81) may be trivially rewritten as follows:

$$-\,\mathrm{div}\,\big(J\rho W'(J)\mathbf{I}\big) + \epsilon\,(J\nabla(\mathrm{div}(\rho\nabla J)) + 2\nabla J\,\mathrm{div}(\rho\nabla J) + \rho\nabla(\nabla J)[\nabla J])\,. \tag{82}$$

The second and the third term in (82) may also be manipulated by taking into account the following relations:

(1)
$$\nabla\rho = -\frac{\rho}{J}\,\nabla J\,, \tag{83}$$

by (5);

(2)
$$\mathrm{div}(\rho\,\nabla J) = \rho\;\mathrm{div}(\nabla J)\;+\;\nabla J\cdot\nabla\rho\;=\rho\left(\Delta J-\frac{|\nabla J|^2}{J}\right), \tag{84}$$

after making use of (83);

(3)
$$\begin{aligned}\nabla(J(\mathrm{div}(\rho\,\nabla J))) &= J\,\nabla(\mathrm{div}(\rho\,\nabla J))\;+\nabla J\;\mathrm{div}(\rho\,\nabla J)\,,\\ \nabla(J(\mathrm{div}(\rho\,\nabla J))) &= \mathrm{div}(J(\mathrm{div}(\rho\,\nabla J)\,\mathbf{I}))\;=\;\mathrm{div}\left(\rho\left(\Delta J-\frac{|\nabla J|^2}{J}\right)\mathbf{I}\right),\end{aligned}$$

after making use of (84);

(4) we note that, for any constant vector $\mathbf{a}$ the following relation holds:

$$\begin{aligned}&\mathbf{a}\cdot\nabla J\,\mathrm{div}(\rho\nabla J)+\rho\nabla J\cdot\nabla(\mathbf{a}\cdot\nabla J)\\ &\qquad=\mathrm{div}\left((\mathbf{a}\cdot\nabla J)\rho\nabla J\right)=\mathrm{div}\left(\rho\nabla J\otimes\nabla J\right)\mathbf{a}.\end{aligned}$$

By virtue of items 3 and 4 relation (82) yields[16]

$$\begin{aligned}&-\mathrm{div}\left(J\rho W'(J)\mathbf{I}\right)+\epsilon\left(J\nabla(\mathrm{div}(\rho\nabla J))+2\nabla J\,\mathrm{div}(\rho\nabla J)+\rho\nabla(\nabla J)[\nabla J]\right)\\ &\qquad=-\,\mathrm{div}\left\{\rho J\left\{\left[W'(J)-\frac{\epsilon}{J}\left(\Delta J-\frac{|\nabla J|^2}{J}\right)\mathbf{I}\right]-\epsilon\frac{\nabla J\otimes\nabla J}{J}\right\}\right\}.\end{aligned} \tag{85}$$

A.2 The surface term

For the integral over the boundary $\partial\mathcal{B}$ in (80), which is called the surface term, only the third term has to be made explicitly dependent upon the variation $\delta\mathbf{x}$. To this end, by virtue of (113), we may write:

$$\int_{\partial\mathcal{B}}\mathbf{n}\cdot\nabla J\,\rho\;\;\delta\,J\,d\mathcal{H}^2\;=\;\int_{\partial\mathcal{B}}\mathbf{n}\;\cdot\;\nabla J\,\rho\,J\;\mathrm{div}(\delta\mathbf{x})\,d\mathcal{H}^2. \tag{86}$$

We note that
$$\mathrm{div}(\delta\mathbf{x})\;=\;\mathrm{div}_\Sigma(\delta\mathbf{x})\;+\;(\delta\mathbf{x})_{,n}\,, \tag{87}$$

[16]This relation holds up to sets of Lebesgue measure zero.

where

$$(\delta\mathbf{x})_{,n} := \nabla(\delta\mathbf{x})\mathbf{n} \cdot \mathbf{n}$$

and

$$\mathrm{div}_\Sigma(\delta\mathbf{x}) := I_\Sigma \cdot \nabla_\Sigma \delta\mathbf{x}\,,$$

where

$$I_\Sigma := \mathbf{a}_\alpha \otimes \mathbf{a}^\alpha,$$

where $\{\,\mathbf{a}_\alpha\,\}_{\{\alpha=1,\,2\}}$ is a covariant basis of the tangent space at a generic point of the boundary $\partial\mathcal{B}$ and $\{\mathbf{a}^\alpha\}_{\{\alpha=1,\,2\}}$ is the corresponding dual basis, $\nabla_\Sigma(\circ) := \circ_{,\alpha} \otimes \mathbf{a}^\alpha$ is the surface gradient operator.

Hence, (87) into (86) and the divergence theorem yield

$$\begin{aligned}\int_{\partial\mathcal{B}} \mathbf{n}\cdot\nabla J\,\rho\;\;\delta J\,d\mathcal{H}^2 &= \int_{\partial\mathcal{B}} \mathbf{n}\cdot\nabla J\,\rho\, J\;\;\mathrm{div}_\Sigma(\delta\mathbf{x}) + \int_{\partial\mathcal{B}} \rho\, J\,(\delta\mathbf{x})_{,n}\;d\mathcal{H}^2\\ &= \int_{\partial\mathcal{B}} \mathrm{div}_\Sigma\left(\delta\mathbf{x}\quad \mathbf{n}\cdot\nabla J\,\rho\, J\right)\,d\mathcal{H}^2 - \int_{\partial\mathcal{B}} \delta\mathbf{x}\;\cdot\;\nabla_\Sigma\left(\rho\, J\;\mathbf{n}\cdot\nabla J\right)\,d\mathcal{H}^2\,;\end{aligned} \tag{88}$$

indeed the term

$$\int_{\partial\mathcal{B}} \rho\, J\,(\delta\mathbf{x})_{,n}\,d\mathcal{H}^2 \equiv 0.$$

In order to evaluate the term

$$\int_{\partial\mathcal{B}} \mathrm{div}_\Sigma\left(\delta\mathbf{x}\quad \mathbf{n}\cdot\nabla J\,\rho\, J\right)\,d\mathcal{H}^2 \tag{89}$$

in (88) we may note that if $\partial\mathcal{B} = \bigcup_j \partial\mathcal{B}_j$, with $\mathcal{H}^2(\bigcup_j \partial\mathcal{B}_j) < \infty$, and if $\bigcap_k \partial\mathcal{B}_k = \{\,\gamma_i\,\}_{i\in\mathbb{N}}$ is a countable (finite or infinite) set of closed lines γ_i such that $\mathcal{H}^2\left(\bigcap_k \partial\mathcal{B}_k\right) < \infty$, by virtue of the divergence theorem the first term in (88) may be rewritten as follows

$$\begin{aligned}&\sum_j \int_{\partial\mathcal{B}_j} \mathrm{div}_\Sigma\Big(\delta\mathbf{x}(\boldsymbol{z})\quad \mathbf{n}_i(\boldsymbol{z})\cdot\nabla\tilde{J}(\boldsymbol{z})\,\rho(\boldsymbol{z})\,\tilde{J}(\boldsymbol{z})\Big)\;d\mathcal{H}^2(\boldsymbol{z})\\ &\quad= \sum_i \int_{\gamma_i} \rfloor_i\Big(\mathbf{m}_i(\boldsymbol{z})\cdot\delta\mathbf{x}(\boldsymbol{z})\quad \rho(\boldsymbol{z})\,\tilde{J}(\boldsymbol{z})\,\nabla\tilde{J}(\boldsymbol{z})\cdot\mathbf{n}_i(\boldsymbol{z})\Big)\;d\mathcal{H}^1(\boldsymbol{z})\\ &\quad= \sum_i \int_{\gamma_i} \rho(\boldsymbol{z})\,\tilde{J}(\boldsymbol{z})\,\rfloor_i\Big(\mathbf{m}_i(\boldsymbol{z})\cdot\delta\mathbf{x}(\boldsymbol{z})\;\;\nabla\tilde{J}(\boldsymbol{z})\cdot\mathbf{n}_i(\boldsymbol{z})\Big)\;d\mathcal{H}^1(\boldsymbol{z})\\ &\quad= \sum_i \int_{\gamma_i} \rho(\boldsymbol{z})\,\tilde{J}(\boldsymbol{z})\,\rfloor_i\Big(\mathbf{m}_i(\boldsymbol{z})\otimes\mathbf{n}_i(\boldsymbol{z})\;\nabla\tilde{J}(\boldsymbol{z})\cdot\delta\mathbf{x}(\boldsymbol{z})\Big)\;d\mathcal{H}^1(\boldsymbol{z})\\ &\quad= \sum_i \int_{\gamma_i} \rho(\boldsymbol{z})\,\tilde{J}(\boldsymbol{z})\;\;\delta\mathbf{x}(\boldsymbol{z})\cdot\;\rfloor_i\Big(\mathbf{m}_i(\boldsymbol{z})\otimes\mathbf{n}_i(\boldsymbol{z})\;\nabla\tilde{J}(\boldsymbol{z})\Big)\;d\mathcal{H}^1(\boldsymbol{z})\end{aligned} \tag{90}$$

where $\mathbf{n}_i$ denotes the normal to points on the ith closed contour γ_i and the quantity $\rfloor_i(\circ(\boldsymbol{z}))$ represents the jump at $\boldsymbol{z} \in \gamma_i$ of the field $\circ$ across γ_i; the precise mathematical definition of this jump is

$$\rfloor_i(\circ(\boldsymbol{z})) := \lim_{\varepsilon \to 0} \frac{\circ(\boldsymbol{z} + \varepsilon \mathbf{n}(\boldsymbol{z}) \wedge \tau(\boldsymbol{z})) - \circ(\boldsymbol{z} - \varepsilon \mathbf{n}(\boldsymbol{z}) \wedge \tau(\boldsymbol{z}))}{\varepsilon}, \tag{91}$$

where $\mathbf{n}(\boldsymbol{z})$ is the normal to $\partial\mathcal{B}_j$ at $\boldsymbol{z}$ and $\tau(\boldsymbol{z})$ is the unit tangent vector to γ_i at the same point $\boldsymbol{z}$.[17]

Obviously each γ_i comes from the intersection of elements of the list $\{\, \partial\mathcal{B}_k \,\}$.

Hence, the normal field $\mathbf{n}$ to the boundary $\partial\mathcal{B} = \bigcup_j \partial\mathcal{B}_j$ does jump across γ_i, as well as the vector $\mathbf{m}_i(\boldsymbol{z})$, which is normal to γ_i at $\boldsymbol{z}$ and such that $\mathbf{m}_i(\boldsymbol{z}) \cdot \mathbf{n}_i(\boldsymbol{z}) = 0$, where $\mathbf{n}_i = \mathbf{n}$.

It is worth noting that in the last step of (90) we used the continuity of $\delta\mathbf{x}$.

This term (90) may be interpreted as the virtual work exerted by the jump of edge tractions $\rfloor_i \left(\rho(\boldsymbol{z})\, \tilde{J}(\boldsymbol{z})\ \mathbf{m}_i(\boldsymbol{z}) \otimes \mathbf{n}_i(\boldsymbol{z})\ \nabla \tilde{J}(\boldsymbol{z})\right)$ at $\boldsymbol{z} \in \gamma_i$ across γ_i at $\boldsymbol{z} \in \gamma_i$ against the virtual displacement $\delta\mathbf{x}(\boldsymbol{z})$ of that point. Hence, the nullity of (90) either yields the condition of balance of the jump of the edge tractions[18]

$$0 = \rfloor_i \left(\epsilon\, \rho(\boldsymbol{z})\, \tilde{J}(\boldsymbol{z})\ \mathbf{m}_i(\boldsymbol{z}) \otimes \mathbf{n}_i(\boldsymbol{z})\ \nabla \tilde{J}(\boldsymbol{z})\right) \quad \text{on } \gamma_i \subset \partial\mathcal{B}\,, \tag{92}$$

or boundary conditions are such that

$$\rfloor_i(\mathbf{m}_i) \cdot \delta\mathbf{x} \,=\, 0\,. \tag{93}$$

Only (92) is meaningful. Indeed, the latter condition would mean no discontinuity in the normals to γ_i, hence no discontinuity of the normal $\mathbf{n} = \mathbf{n}_i$ to the boundary $\partial\mathcal{B}$ at points on γ_i, so that $\partial\mathcal{B}$ would be smooth across γ_i.

Actually, because $\rho(\boldsymbol{z})\, \tilde{J}(\boldsymbol{z})$ does not jump, relation (92) reduces to

$$0 = \rfloor_i \left(\mathbf{m}_i(\boldsymbol{z}) \otimes \mathbf{n}_i(\boldsymbol{z})\ \nabla \tilde{J}(\boldsymbol{z})\right) \quad \text{on } \gamma_i \subset \partial\mathcal{B},\ \forall\ i\,, \tag{94}$$

Finally, we may summarize (89, 90) to saying that if

$$\partial\mathcal{B} = \bigcup_j \partial\mathcal{B}_j\,,\ \text{with } \mathcal{H}^1\left(\bigcup_j \partial\mathcal{B}_j\right) < \infty$$

and if

$$\bigcap_k \partial\mathcal{B}_k \,=\, \bigcup_i \gamma_i \text{ such that } \mathcal{H}^1\left(\bigcap_k \partial\mathcal{B}_k\right) < \infty,$$

[17] The tangent vector is well defined since $\mathcal{H}^1(\gamma_i) \leq \mathcal{H}^1\left(\bigcap_k \partial\mathcal{B}_k\right) < \infty$.

[18] See the third term in the boundary integral of equation (81).

with $\{\gamma_i\}_{i\in\mathbb{N}}$ a countable (finite or infinite) set closed contours γ_i, we have the following result for (88):

$$\int_{\partial\mathcal{B}} \mathrm{div}_\Sigma\left(\delta\mathbf{x} \quad \mathbf{n}\cdot\nabla J\,\rho\,J\right)\,d\mathcal{H}^2 = \sum_j \int_{\partial\mathcal{B}_j} \mathrm{div}_\Sigma\left(\delta\mathbf{x} \quad \mathbf{n}\cdot\nabla J\,\rho\,J\right)\,d\mathcal{H}^2$$
$$= \begin{cases} 0 & \text{if } \mathcal{H}^1\left(\bigcap_k \partial\mathcal{B}_k\right) = 0, \\ \sum_i \int_{\gamma_i} \rho\,J \;\; \delta\mathbf{x}\cdot\; \rfloor_i\left(\mathbf{m}_i \otimes \mathbf{n}_i\;\nabla J\right)\;d\mathcal{H}^1 & \text{if } \mathcal{H}^1\left(\bigcap_k \partial\mathcal{B}_k\right) \neq 0\,. \end{cases} \tag{95}$$

Since

$$\mathcal{H}^1\left(\bigcap_k \partial\mathcal{B}_k\right) = \mathcal{H}^1\left(\bigcup_i \gamma_i\right) = \sum_i \mathcal{H}^1\left(\gamma_i\right), \tag{96}$$

by countable additivity of (Hausdorff)[19] measures allows for rewriting relation (95) as follows

$$\int_{\partial\mathcal{B}} \mathrm{div}_\Sigma\left(\delta\mathbf{x} \quad \mathbf{n}\cdot\nabla J\,\rho\,J\right)\,d\mathcal{H}^2$$
$$= \left\langle \int_{\bigcup_i \gamma_i} \rho\,J \;\; \delta\mathbf{x}\cdot\; \rfloor_i\left(\mathbf{m}_i \otimes \mathbf{n}_i\;\nabla J\right)\;d\mathcal{H}^1 \right\rangle \tag{97}$$

where

$$\left\langle \int_{\bigcup_i \gamma_i} \rho\,J \;\; \delta\mathbf{x}\cdot\; \rfloor_i\left(\mathbf{m}_i \otimes \mathbf{n}_i\;\nabla J\right)\;d\mathcal{H}^1 \right\rangle$$
$$:= \begin{cases} 0 & \text{if } \sum_i \mathcal{H}^1\left(\gamma_i\right) = 0, \\ \sum_i \int_{\gamma_i} \rho\,J \;\; \delta\mathbf{x}\cdot\; \rfloor_i\left(\mathbf{m}_i \otimes \mathbf{n}_i\;\nabla J\right)\;d\mathcal{H}^1 & \text{if } \sum_i \mathcal{H}^1\left(\gamma_i\right) \neq 0, \end{cases} \tag{98}$$

after using (96).

For further developments we may define the following local form of (98)[20]

$$\left\langle \rho\,J \;\; \delta\mathbf{x}\cdot\; \rfloor_i\left(\mathbf{m}_i \otimes \mathbf{n}_i\;\nabla J\right)\right\rangle_{\gamma_i}$$
$$:= \begin{cases} \rho\,J \;\; \delta\mathbf{x}\cdot\; \rfloor_i\left(\mathbf{m}_i \otimes \mathbf{n}_i\;\nabla J\right) & \text{on } \gamma_i \text{ if } \mathcal{H}^1(\gamma_i) \neq 0 \\ 0 & \text{otherwise} \end{cases} \tag{99}$$

It may be of use to single out the field

$$\rfloor_i(\boldsymbol{t}_i) := \rfloor_i(\epsilon\,\rho\,J\;\mathbf{m}_i \otimes \mathbf{n}_i\,\nabla J) \tag{100}$$

[19] This property, often called σ-additivity, holds for any measure.

[20] This holds up to set of Hausdorff measure zero, i.e. sets formed by points.

representing the jump of the "edge-tractions" $\boldsymbol{t}_i$ acting at a point of the contour γ_i.

Hence, relation (88) then becomes

$$\epsilon \int_{\partial\mathcal{B}} \mathbf{n} \cdot \nabla J \, \rho \;\; \delta\, J \, d\mathcal{H}^2 = \left\langle \int_{\bigcup_i \gamma_i} \delta\mathbf{x} \cdot \; \rfloor_i(\boldsymbol{t}_i) \; d\mathcal{H}^1 \right\rangle - \epsilon \int_{\partial\mathcal{B}} \delta\mathbf{x} \;\cdot\; \nabla_\Sigma \, (\rho \, J \; \mathbf{n} \;\cdot\; \nabla J) \; d\mathcal{H}^2. \quad (101)$$

A.3 The final form of δE_ϵ

We are now back to the first variation δE_ϵ of the energy (81).

Relations (85, 101) into (81) yield

$$\begin{aligned}
\delta E_\epsilon &= \left\langle \int_{\bigcup_i \gamma_i} \delta\mathbf{x} \cdot \; \rfloor_i(\boldsymbol{t}_i) \; d\mathcal{H}^1 \right\rangle \\
&+ \int_{\partial\mathcal{B}} \big\{ \delta\mathbf{x} \cdot \big[\rho \, J \; W'(J) - \epsilon \;\; (J \; \mathrm{div}(\rho \, \nabla \, J) \, \mathbf{n} \, + \, \nabla \, J \; \cdot \; \mathbf{n} \, \rho \, \nabla \, J) \big] \\
&- \epsilon \; \delta\mathbf{x} \; \cdot \; \nabla_\Sigma (\rho J \, \mathbf{n} \; \cdot \; \nabla J) \big\} \; d\mathcal{H}^2 \\
&+ \int_{\mathcal{B}} \delta\mathbf{x} \; \cdot \; \big\{ -\nabla \left[J \left(\rho \, W'(J) - \epsilon \; \mathrm{div}(\rho \, \nabla \, J) \right) \right] \\
&+ \; \epsilon \; (\nabla J \;\; \mathrm{div}(\rho \, \nabla J) + \rho \, \nabla (\nabla \, J) \, \nabla \, J) \big\} \;\; d\mathcal{L}^3 \, ; \qquad (102) \\
&= \left\langle \int_{\bigcup_i \gamma_i} \delta\mathbf{x} \cdot \; \rfloor_i(\boldsymbol{t}_i) \; d\mathcal{H}^1 \right\rangle \\
&+ \int_{\partial\mathcal{B}} \delta\mathbf{x} \; \cdot \;\; [\mathbf{T} \, \mathbf{n} - \; \epsilon \; \nabla_\Sigma (\rho J \, \mathbf{n} \; \cdot \; \nabla J)] \, d\mathcal{H}^2 - \int_{\mathcal{B}} \delta\mathbf{x} \; \cdot \; \mathrm{div} \, \mathbf{T} \; d\mathcal{L}^3, \qquad (103)
\end{aligned}$$

after setting $\mathbf{T}$ as in (23).

Appendix B: Variation of the determinant

Because

$$J = (\det \mathbf{F}^T \mathbf{F})^{\frac{1}{2}} = \det \left[(\nabla_X \, \boldsymbol{y})^T (\nabla_X \, \boldsymbol{y}) \right]^{\frac{1}{2}} \qquad (104)$$

the variation of J can be calculated as follows.

We first introduce the following change of the deformation mapping: $y \mapsto \boldsymbol{y} + \varepsilon \, \eta$; consequently, the (material) deformation gradient takes the following form: $\nabla_X \, \boldsymbol{y} \mapsto \; \nabla_X \, \boldsymbol{y} + \varepsilon \nabla_X \, \eta$. Hence, the determinant of the consequent (material) gradient reads as follows:

$$J_\varepsilon = (\det \mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)^{\frac{1}{2}} = \left[\det \left[(\nabla_X \boldsymbol{y} + \varepsilon \nabla_X \eta)^T (\nabla_X \boldsymbol{y} + \varepsilon \nabla_X \eta) \right] \right]^{\frac{1}{2}}$$

The material description of the variation of the determinant, here denoted by $\{\delta J\}_m$, is then the variational derivative of J_ε evaluated at $J_\varepsilon = 0$, i.e.

$$\{\,\delta J\,\}_m \;:=\; \frac{d}{d\varepsilon}\left(\det \mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon\right)^{\frac{1}{2}}|_{\varepsilon=0} \tag{105}$$

$$\begin{aligned}
\frac{d}{d\varepsilon}(\det \mathbf{F}^T \mathbf{F}_\varepsilon)^{\frac{1}{2}}|_{\varepsilon=0} &= \frac{1}{2}\left(\det \mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon\right)^{-\frac{1}{2}} \frac{d(\det \mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)}{d(\mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)} \cdot \frac{d(\mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)}{d\varepsilon}|_{\varepsilon=0} \\
&= \frac{1}{2}(\det \mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)^{-\frac{1}{2}}\left[(\det \mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)\mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon^{-T}\right] \\
&\quad \cdot \left[(\nabla_S \boldsymbol{y})^T(\nabla_S \eta) + (\nabla_S \eta)^T(\nabla_S \boldsymbol{y}) + o(\varepsilon)\right]|_{\varepsilon=0} \\
&= \frac{1}{2} J_\varepsilon (F_\varepsilon^T F_\varepsilon)^{-T} \cdot \left[(\nabla_S \boldsymbol{y})^T(\nabla_S \eta) + (\nabla_S \eta)^T(\nabla_S \boldsymbol{y}) + o(\varepsilon)\right]|_{\varepsilon=0} \\
&= J_\varepsilon\ \left((\mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)^{-T}|_{\varepsilon=0} \cdot \left[(\nabla_X \boldsymbol{y})^T(\nabla_X \eta)\right]\right);
\end{aligned} \tag{106}$$

indeed, because $(\mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)^{-T}|_{\varepsilon=0} \in Sym$ it results that

$$\begin{aligned}
(\mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)^{-T}|_{\varepsilon=0} &\cdot \frac{1}{2}((\nabla_X \boldsymbol{y})^T(\nabla_X \eta) + ((\nabla_X \boldsymbol{y})^T(\nabla_X \eta))^T) \\
&= 2\ (\mathbf{F}_\varepsilon^T \mathbf{F}_\varepsilon)^{-T}|_{\varepsilon=0} \cdot \left[(\nabla_X \boldsymbol{y})^T(\nabla_X \eta)\right].
\end{aligned}$$

Hence, (106) implies:

$$\begin{aligned}
\{\delta J\}_m \;&=\; J\ \nabla_X \boldsymbol{y}^{-T}(\nabla_X \boldsymbol{y})^{-1} \cdot \left[(\nabla_X \boldsymbol{y})^T(\nabla_X \eta)\right] \\
&= J\ \left(I\ \cdot\ \nabla_X \eta\ (\nabla_X\, \boldsymbol{y})^{-1}\right).
\end{aligned} \tag{107}$$

In order to get the spatial description of such variation we recall that the variation

$$\mathbf{x}_\varepsilon := \mathbf{x} + \varepsilon\zeta(\mathbf{x}) \tag{108}$$

of points $\mathbf{x} = \boldsymbol{y}(\mathbf{X})$ of the current configuration $\mathcal{B}$ is related to the variation $\boldsymbol{y}(\mathbf{X}) + \varepsilon\eta(\mathbf{X})$ of the deformation $\boldsymbol{y}$ as follows

$$\mathbf{x} + \varepsilon\zeta(\mathbf{x}) = \boldsymbol{y}(\mathbf{X}) + \varepsilon\eta(\mathbf{X}), \tag{109}$$

hence

$$\boldsymbol{y}(X) + \varepsilon\zeta(\boldsymbol{y}(\mathbf{X})) = \boldsymbol{y}(\mathbf{X}) + \varepsilon\eta(\mathbf{X}), \tag{110}$$

so that

$$\eta(\mathbf{X}) = \zeta(\boldsymbol{y}(\mathbf{X})). \tag{111}$$

Differentiation of (111) yields

$$\begin{aligned}
\nabla_x \zeta \nabla_X \boldsymbol{y} &= \nabla_X\, \eta \\
\nabla_x \zeta &= \nabla_X\, \eta\ (\nabla_X \boldsymbol{y})^{-1}.
\end{aligned} \tag{112}$$

From now on and in the main text of the paper we shall drop the $\mathbf{x}$-dependence on writing the spatial gradient, hence

$$\nabla := \nabla_x.$$

The spatial description δJ of the variation of the determinant can then be deduced by substituting (A.3) into (107) to get:

$$\delta J = J \ (I \cdot \nabla\zeta) = J \ \operatorname{div}\zeta\,, \tag{113}$$

where $\operatorname{div}\zeta := I\cdot\zeta$ denotes the spatial divergence of $\zeta(\circ)$, i.e. the trace of the spatial gradient of the spatial field ζ inherited from the material field $\eta(\circ)$ characterizing the variation of the deformation.

In the main text of the paper, i.e. from equation (19) on, such ζ is denoted by δx.

Appendix C: variation of the spatial gradient of J

This section has been essentially worked out in [10]. We first wish to prove the following identity

$$\nabla(\delta\varphi) = \delta(\nabla\varphi) + (\nabla\boldsymbol{\zeta})^T(\nabla\varphi) \tag{114}$$

where φ is any spatial scalar-valued field, as in the previous section, $\boldsymbol{\zeta}$ a perturbation of the positions $\mathbf{x}$ of points of the current configuration. Let

$$\nabla_\varepsilon := \nabla_{\mathbf{x}_\varepsilon},$$

where $\mathbf{x}_\varepsilon$ is defined by (108), and recall that $\nabla := \nabla_s$. Let us consider the following change in the scalar field φ:

$$\varphi_\varepsilon := \varphi(\mathbf{x}_\varepsilon).$$

Thus, the variational derivative of φ reads as follows

$$\delta\varphi = \left[\frac{d\varphi_\varepsilon}{d\varepsilon}\right]_{\varepsilon=0} = [\nabla_\varepsilon\varphi\cdot\boldsymbol{\zeta}]_{\varepsilon=0} = \nabla\varphi\cdot\boldsymbol{\zeta}\,.$$

Differentiating this last relation we obtain

$$\nabla(\delta\varphi) = \nabla(\nabla\varphi)^T\boldsymbol{\zeta} + \nabla\boldsymbol{\zeta}^T\nabla\varphi = \nabla(\nabla\varphi)\boldsymbol{\zeta} + \nabla\boldsymbol{\zeta}^T\nabla\varphi\,, \tag{115}$$

because $\nabla(\nabla\varphi)$ is symmetric. Let us now consider the vector field

$$\boldsymbol{h}(\mathbf{x}) := \nabla\varphi(\mathbf{x}),$$

and let us compute the variational derivative of $\boldsymbol{h}$. It follows that

$$\delta \boldsymbol{h} = \left[\frac{d\boldsymbol{h}_\varepsilon}{d\varepsilon}\right]_{\varepsilon=0} = [(\nabla_\varepsilon \boldsymbol{h})\boldsymbol{\zeta}]_{\varepsilon=0} = (\nabla \boldsymbol{h})\boldsymbol{\zeta}\,.$$

Hence, the following relation holds:

$$\delta(\nabla\varphi) = \nabla(\nabla\varphi)\boldsymbol{\zeta}\,. \tag{116}$$

Substitution of (116) in (115) yields (114).

Finally, by replacing φ with $\tilde{J}$, the spatial description of the determinant J of the of the deformation gradient, relation (67) easily follows.

Appendix D: The mass constraint does not influence the variations

If $\bar{m}$ denotes the total mass of the fluid, which here is assumed to be constant at at all times, the continuity equation (5) implies that the following relation has to hold:

$$\bar{m} = \int_{\mathcal{B}} \rho\, d\mathcal{L}^3, \tag{117}$$

which in turn may be recasted as follows

$$\bar{m} = \int_{\mathcal{B}} \frac{\rho_0}{J}\, d\mathcal{L}^3, \tag{118}$$

where here ρ_0 means $\rho_0(y^{-1}(x))$.

The same equation written in material form implies that

$$\bar{m} = \int_{\mathcal{B}_0} \rho_0\, d\mathcal{L}_0^3\,. \tag{119}$$

At first sight relation (118) seems to impose an integral constraint on the functional E_ϵ defined by (6); if so, this constraint could be easily incorporated in the following modified functional

$$G_\epsilon(J) := E_\epsilon(J) - \bar{\mu}\left(\int_{\mathcal{B}} \frac{\rho_0}{J}\, d\mathcal{L}^3 - \bar{m}\right), \tag{120}$$

where $\bar{\mu}$ would be the constant multiplier which would allow for keeping the constraint itself. However, this would be required only if we were to take free variations in J. In the next section we show that the mass constraint equation (118) is identically satisfied whenever the variations in J are induced by free variations in the placement y (via the material description and (3)), i.e., by consistently carrying out the latter, we may work directly with the functional (6).

If we were to evaluate the first variation of G_ϵ, we would consider its expression in terms of the material description via the change-of-variables formula:

$$G_\epsilon(\{J\}_m) := E_\epsilon(\{J\}_m) - \bar{\mu}\left(\int_{\mathcal{B}_0} \rho_0 \left\{\frac{1}{J}\right\}_m \hat{J}\, d\mathcal{L}_0^3 - \bar{m}\right). \tag{121}$$

Note that the latter term in (121) is identically zero by (119). Hence,

$$G_\epsilon(\{J\}_m) = E_\epsilon(\{J\}_m). \tag{122}$$

Thus in the material formulation of the problem, based on (8),the multiplier is not required. The spatial formulation (6) corresponding to (121) may then be obtained by the change-of-variables formula. That is, the mass-preserving constraint is automatically satisfied when working in the admissible set $\mathcal{A}$. Without loss of generality we henceforth modify (16) accordingly:

$$P_\epsilon := stat_{\{J\in\mathcal{A}\}}\ E_\epsilon(J). \tag{123}$$

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