Structured Deformations: Part Two

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1 Refinements of Balance Laws

The aim in this lecture is to propose a method for refining balance laws that takes into account the presence of non-classical deformations. The key idea in obtaining refinements of balance laws is that passing from classical to structured deformations provides a broader choice of reference configurations relative to which one may write balance laws. In the case of a classical deformation $g \in Cld(\mathcal{A})$, we may think in the usual way of $\mathcal{A}$ as the region occupied by a body in a chosen reference configuration and of $g(\mathcal{A})$ as the region occupied by the body in the deformed cofiguration associated with g. If one assumes that the standard equations of balance of forces and moments, written in terms of the Cauchy stress, hold in the region $g(\mathcal{A})$, then one deduces easily that equivalent balance equations hold in the region $\mathcal{A}$, written in terms of the Piola-Kirchhoff stress.

Suppose now that a body undergoes a structured deformation of the form $(\emptyset, g, G) \in Std(\mathcal{A})$ with the special property that the triple $(\emptyset, g, \nabla g)$ represents a classical deformation. In this case, we may again associate with $g(\mathcal{A})$ the deformed configuration of the body, but $\mathcal{A}$ now must be a fit region; in addition, the factorization (4.4), Part One takes the special form

$$(\emptyset, g, G) = (\emptyset, g, \nabla g) \circ (\emptyset, i, K) \tag{1.1}$$

where i is the identity mapping on $\mathcal{A}$ and $K = (\nabla g)^{-1} G$. Although the purely microscopic deformation $(\emptyset, i, K)$ in (**??**) maps the region $\mathcal{A}$ onto itself without changing the position of points, when $\nabla g \neq G$ this deformation causes disarrangements at the microlevel. The classical deformation $(\emptyset, g, \nabla g)$ then maps $\mathcal{A}$ onto $g(\mathcal{A})$ without causing any further disarrangements. Thus, we may use (**??**) to associate the region $\mathcal{A}$ before undergoing $(\emptyset, g, G)$ with a *virgin configuration of the body*, free from any of the disarrangements caused by $(\emptyset, g, G)$, and to associate the same region $\mathcal{A}$ after undergoing $(\emptyset, i, K)$ with a *microscopically deformed configuration of the body*. Because the second deformation $(\emptyset, g, \nabla g)$ on the right-hand side of (**??**) is a classical deformation, balance laws written in the deformed configuration and in the microscopically deformed configuration would bear the usual relation, the first containing the Cauchy stress and the second the Piola-Kirchhoff stress. The main question that we address here is: what forms should the balance laws attain when written in the virgin configuration? These forms will contain the refinements referred to in the title of this lecture.

1.1 Decomposition of fluxes

The first ingredient in the process of refining balance laws is a simple vector identity that involves a structured deformation $(\emptyset, g, G)$ of the special type introduced above and a continuously differentiable vector field $w : \mathcal{A} \to \mathcal{V}$. Here, $\mathcal{V}$ is the translation space of the underlying Euclidean space $\mathcal{E}$, and, for brevity, we drop the first entry $\emptyset$ in the structured deformation as well as in the other deformations appearing in (**??**). We also assume that the tensor field $K : \mathcal{A} \to Lin\mathcal{V}$ is continuously differentiable. It is helpful (1) to identify the set $\mathcal{A}$ with the microscopically deformed configuration of the body, when $\mathcal{A}$ is viewed as the domain of the vector field w, and (2) to identify the set $\mathcal{A}$ with the virgin configuration, when $\mathcal{A}$ is viewed as the domain of the tensor field K. The *decomposition of fluxes* (**??**) will reflect the effects of disarrangements occuring when the purely microscopic deformation (i, K) takes the body from the virgin configuration into the microscopically deformed configuration:

$$\det K \, div \, w = div(K^{*T} w) - div K^* \cdot w + [(\det K) I - K^*] \cdot \nabla w. \qquad (1.2)$$

This relation is an immediate consequence of the product rule

$$div(K^{*T} w) = div K^* \cdot w + K^* \cdot \nabla w$$

and the identity

$$I \cdot \nabla w = div \, w.$$

(In these relations, $A \cdot B := tr(A^T B)$ for all $A, B \in Lin\mathcal{V}$, and $K^* := \det K \, K^{-T}$ is the adjugate of K.) In the next section, we use the Approximation Theorem (Section 4, Part One) to identify the expressions $\det K \, div \, w$, $div(K^{*T} w)$, and $-div K^* \cdot w + [(\det K) I - K^*] \cdot \nabla w$ in (**??**) as refined measures of the volume density of fluxes due to the vector field w.

1.2 Identification relations

The proof of the Approximation Lemma (Lemma 5.7, [11, Part One]) provides a sequence $m \longmapsto (\lambda_m, h_m)$ of simple deformations that converges to (i, K) and, for each m, a finite set $\mathbf{C}_m$ of non-overlapping closed cubes $\mathcal{C}$ for which we can verify the *identification relations* (**??**), (**??**), and (**??**) below. (The identification relations as well as the decomposition of fluxes were stated without proof in the article [**?**].) In each identification relation, x is an arbitrary point in $\mathcal{A}$, $\mathcal{C}_r(x)$ is the closed cube centered at x of edge length $r > 0$ all of whose faces are disjoint from all of the disarrangement sites λ_m, and the disarrangement sites λ_m and cubes $\mathcal{C} \in \mathbf{C}_m$ may be chosen so that $\lambda_m \subset \bigcup_{\mathcal{C} \in \mathbf{C}_m} bdy\, \mathcal{C}$ for all m.

Figure 1: Surfaces contributing to the total flux

$$\det K \; div\, w \;|_x = \lim_{r \to 0} \lim_{m \to \infty} r^{-3} \sum_{\mathcal{C} \in \mathbf{C}_m} \int_{h_m\,(\,bdy(\mathcal{C}_r(x) \cap \mathcal{C})\,)} w(y) \cdot N(y)\, dA_y. \tag{1.3}$$

As one sees in Figure 1, the simple deformation (λ_m, h_m) takes the cube $\mathcal{C}_r(x)$ and breaks it into pieces of the form $\mathcal{C}_r(x) \cap \mathcal{C}$ with $\mathcal{C} \in \mathbf{C}_m$ such that the restriction of h_m to each piece is an affine deformation. Therefore, the surface integral over $h_m\,(\,bdy(\mathcal{C}_r(x)\cap\mathcal{C})\,) = \; bdy(h_m(\mathcal{C}_r(x)\cap\mathcal{C})\,)$ in the first identification relation (**??**) represents the flux of the vector field w out of all of the faces of the deformed parallelepiped $h_m\,(\,(\mathcal{C}_r(x)\cap\mathcal{C})\,)$. Hence, the sum of the surface integrals in (**??**) represents the flux of w out of all the faces of all the image parallelepipeds $h_m(\mathcal{C}_r(x)\cap\mathcal{C})$ for $\mathcal{C}\in\mathbf{C}_m$. Because r^3 is the volume of the cube $\mathcal{C}_r(x)$, the double limit in (**??**) is a volume density of flux. Therefore, we call $\det K\; div\, w\;|_x$ *the volume density (at the point x) of the total flux of w*. The word "total" is appropriate, because the identification relation takes into account the flux across all of the faces of the image parallelepipeds.

Figure 2: Surfaces contributing to the flux without disarrangements

$$div\,(K^{*T}w)\quad|\quad_x = \lim_{r\to 0}\lim_{m\to\infty} r^{-3}\sum_{\mathcal{C}\in\mathbf{C}_m}\;\int_{h_m\,(\,(bdy\mathcal{C}_r(x))\cap\mathcal{C}\,)} w(y)\cdot N(y)\,dA_y. \quad (1.4)$$

The darkened lines in Figure 2 represent the surfaces appearing in the surface integrals in the second identification relation (**??**). In particular, because all of the faces of $\mathcal{C}_r(x)$ are disjoint from all of the disarrangement sites λ_m, the surfaces represented in the sum of surface integrals in (??) all are disjoint from the disarrangement sites, and we may call $div\,(K^{*T}w)\mid_x$ *the volume density (at the point x) of the flux of w without disarrangements.*

Figure 3: Surfaces contributing to the flux due to disarrangements

$$(-divK^* \cdot w + [(\det K)I - K^*] \cdot \nabla w)\mid_x =$$
$$\lim_{r\to 0}\lim_{m\to\infty} r^{-3} \sum_{\mathcal{C}\in\mathbf{C}_m} \int_{h_m(\,bdy(\mathcal{C}_r(x)\cap\mathcal{C})\,\setminus\,((bdy\mathcal{C}_r(x))\cap\mathcal{C}\,)\,)} w(y)\cdot N(y)\,dA_y. \tag{1.5}$$

We observe in Figure 3 that the sum of surface integrals in (??) takes into account only the flux of w across those faces of parallelepipeds that are images under h_m of disarrangement sites within $\mathcal{C}_r(x)$. Therefore, we may call $(-divK^* \cdot w + [(\det K)I - K^*] \cdot \nabla w)\mid_x$ *the volume density (at the point x) of the flux of w due to disarrangements.*

In the next subsection, we derive the identification relations. We remark before doing so that, *in light of the identification relations (??), (??), and (??), the decomposition of fluxes (??) establishes a representation for the volume density of the total flux of a vector field as the sum of the volume density of flux without disarrangements and of the volume density of flux due to disarrangements.*

1.3 Derivation of the identification relations

To derive (??), we let a positive number r, a positive integer m, and cube $\mathcal{C} \in \mathbf{C}_m$ be given, and we use the relation $h_m\,(\,bdy(\mathcal{C}_r(x) \cap \mathcal{C})\,) = \,bdy(h_m(\mathcal{C}_r(x) \cap \mathcal{C})\,)$, the Divergence Theorem, and the Change of Variables Formula for volume integrals to write

$$\begin{aligned}
\int_{h_m\,(\,bdy(\mathcal{C}_r(x)\cap\mathcal{C})\,)} w(y)\cdot N(y)\,dA_y &= \int_{bdy(\,h_m\,(\mathcal{C}_r(x)\cap\mathcal{C})\,)} w(y)\cdot N(y)\,dA_y \\
&= \int_{h_m\,(\mathcal{C}_r(x)\cap\mathcal{C})} (div\,w)(y)\,dV_y \\
&= \int_{\mathcal{C}_r(x)\cap\mathcal{C}} (div\,w)(h_m(z))\,\det\nabla h_m(z)\,dV_z.
\end{aligned}$$

Summing over all cubes $\mathcal{C} \in \mathbf{C}_m$, dividing by r^3, and letting $m \to \infty$ yields

$$\begin{aligned}
&\lim_{m\to\infty} r^{-3} \sum_{\mathcal{C}\in\mathbf{C}_m} \int_{h_m\,(\,bdy(\mathcal{C}_r(x)\cap\mathcal{C}\,)\,)} w(y)\cdot N(y)\,dA_y \\
=\; &\lim_{m\to\infty} r^{-3} \sum_{\mathcal{C}\in\mathbf{C}_m} \int_{\mathcal{C}_r(x)\cap\mathcal{C}} (div\,w)(h_m(z))\,\det\nabla h_m(z)\,dV_z \\
=\; &\lim_{m\to\infty} r^{-3} \int_{\mathcal{C}_r(x)} (div\,w)(h_m(z))\,\det\nabla h_m(z)\,dV_z \\
=\; &r^{-3} \int_{\mathcal{C}_r(x)} \lim_{m\to\infty} [(div\,w)(h_m(z))\,\det\nabla h_m(z)]\,dV_z
\end{aligned}$$

$$
\begin{aligned}
&= r^{-3} \int_{\mathcal{C}_r(x)} (div\, w)(z) \det K(z)\, dV_z \\
&\longrightarrow (div\, w)(x) \det K(x)
\end{aligned}
$$

as $r \to 0$, and this establishes the identification relation (**??**) for $(div\, w)(x) \det K(x)$ as the volume density of the total flux of w.

To derive the second identification relation (**??**), we first use the Change of Variables Formula for surface integrals to write

$$
\begin{aligned}
\int_{h_m(\,(bdy\mathcal{C}_r(x)) \cap \mathcal{C}\,)} w(y) \cdot N(y)\, dA_y &= \int_{(bdy\mathcal{C}_r(x)) \cap \mathcal{C}} w(h_m(z)) \cdot \nabla h_m(z)^* \nu(z)\, dA_z \\
&= \int_{(bdy\mathcal{C}_r(x)) \cap \mathcal{C}} \nabla h_m(z)^{*T}\, w(h_m(z)) \cdot \nu(z)\, dA_z.
\end{aligned}
$$

Summing over $\mathcal{C} \in \mathbf{C}_m$, letting $m \to \infty$, and applying the Divergence Theorem, we conclude that

$$
\begin{aligned}
&\lim_{m\to\infty} \sum_{\mathcal{C}\in\mathbf{C}_m} \int_{h_m(\,(bdy\mathcal{C}_r(x)) \cap \mathcal{C}\,)} w(y) \cdot N(y)\, dA_y \\
&= \lim_{m\to\infty} \sum_{\mathcal{C}\in\mathbf{C}_m} \int_{(bdy\mathcal{C}_r(x)) \cap \mathcal{C}} \nabla h_m(z)^{*T}\, w(h_m(z)) \cdot \nu(z)\, dA_z \\
&= \lim_{m\to\infty} \int_{bdy\mathcal{C}_r(x)} \nabla h_m(z)^{*T}\, w(h_m(z)) \cdot \nu(z)\, dA_z \\
&= \int_{bdy\mathcal{C}_r(x)} \lim_{m\to\infty} [\nabla h_m(z)^{*T}\, w(h_m(z))] \cdot \nu(z)\, dA_z \\
&= \int_{bdy\mathcal{C}_r(x)} K(z)^{*T}\, w(z) \cdot \nu(z)\, dA_z \\
&= \int_{\mathcal{C}_r(x)} div(K^{*T}\, w)(z)\, dV_z.
\end{aligned}
$$

The identification relation (**??**) for the volume density of the flux of w without disarrangements follows upon division of the last relation by r^3 and letting $r \to 0$.

The last identification relation (**??**) follows immediately from the first two identification relations, the decomposition of fluxes (**??**), and the relation:

$$\int_{h_m(\,bdy(\mathcal{C}_r(x)\cap\mathcal{C})\setminus((bdy\mathcal{C}_r(x))\cap\mathcal{C})\,)} w(y)\cdot N(y)\,dA_y \;=$$

$$\int_{h_m(\,bdy(\mathcal{C}_r(x)\cap\mathcal{C})\,)} w(y)\cdot N(y)\,dA_y - \int_{h_m(\,(bdy\mathcal{C}_r(x))\cap\mathcal{C}\,)} w(y)\cdot N(y)\,dA_y.$$

1.4 Examples of refinements of balance laws

1.4.1 Balance of energy in a macroscopically rigid heat conductor

We consider a body that can conduct heat but that can only deform at the microlevel. Accordingly, only purely microscopic structured deformations (i, K) are studied here. (We continue to omit the first entry $\emptyset$ in the triples in (**??**).) Moreover, of the three configurations discussed in the paragraph below (**??**), the virigin configuration and the microscopically deformed configuration will differ if $K \neq I$, but the current configuration and the microscopically deformed configuration necessarily coincide. Letting ρ denote the mass density and q the heat flux vector field in the microscopically deformed configuration, and letting r denote the heat supply per unit mass, the balance of energy at steady state takes the form

$$-div\, q + \rho r = 0. \tag{1.6}$$

Multiplication by $\det K$ and use of the decomposition of fluxes yields the equivalent *refinement of the balance of energy*

$$-div(K^{*T}q) + divK^{*}\cdot q - [(\det K)I - K^{*}]\cdot\nabla q + \rho_v r = 0 \tag{1.7}$$

where $\rho_v := \rho\det K$. We use the identification relations to justify the terminology *volume density of heat flux without disarrangements* for $div(K^{*T}q)$ and the terminology *volume density of heat flux due to disarrangements* for $-divK^{*}\cdot q + [(\det K)I - K^{*}]\cdot\nabla q$. Just as (**??**) is the balance of energy in the microscopically deformed configuration, (**??**) is the balance of energy in the virgin configuration, and we may call the vector field $K^{*T}q$ the *heat flux in the virgin configuration* and the scalar field ρ_v the *density in the virgin configuration.* While the scalar field $div(K^{*T}q)$ describes the volume density of thermal contact interactions within intact microscopic pieces of the body, the scalar field $-divK^* \cdot q + [(\det K)I - K^*] \cdot \nabla q$ describes the rate at which heat must be supplied per unit volume in order to maintain geometrical changes at the microlevel such as microslip and creation of voids; unlike $div(K^{*T}q)$, it need not be the divergence of a vector field. The distinction between these mechanisms of heat conduction is significant, for example, when a substance undergoes an incoherent phase transition. In this specific physical context, one may think of the original phase as incorporating voids at the microlevel that are filled by creation of a new phase: the scalar field $div(K^{*T}q)$ here represents the volume density of heat flux within the original phase, away from sites where the new phase is forming, and $-divK^* \cdot q + [(\det K)I - K^*] \cdot \nabla q$ represents the volume density of heat flux out of the original phase into the new phase.

1.4.2 Balance of forces and moments in a deformable body

The balance of forces referred to a given, microscopically deformed configuration of the body have the classical form

$$divS + \rho_m b = 0 \tag{1.8}$$

with S the Piola-Kirchhoff stress, ρ_m the density in the microscopically deformed configuration, and b the body force per unit mass. The factorization (**??**) leads us again to the problem of determining the form of the balance of forces in the virgin configuration, using the fact that the microscopically deformed configuration is obtained from the virgin configuration by the purely microscopic structured deformation (i, K). (As before, we omit the initial entry $\emptyset$ in the triples appearing in (**??**).) After using the definition of the divergence of a tensor field, we apply the decomposition of fluxes for the vector field $w := S^T a$, where $a \in \mathcal{V}$ is a fixed but arbitrary vector, to obtain

$$\begin{aligned}
\det K\,(divS) \cdot a &= \det K\, div(S^T a) = \det K\, div\, w \\
&= div(K^{*T} w) - divK^* \cdot w + [(\det K)I - K^*] \cdot \nabla w \\
&= div(K^{*T} S^T a) - divK^* \cdot S^T a + [(\det K)I - K^*] \cdot \nabla(S^T a)
\end{aligned}$$

$$
\begin{aligned}
&= div(SK^*) \cdot a - (S\, divK^*) \cdot a + (\nabla S\, [(\det K)I - K^*]) \cdot a \\
&= (div(SK^*) - S\, divK^* + \nabla S\, [(\det K)I - K^*]) \cdot a.
\end{aligned}
$$

Here, for each $x \in \mathcal{A}$, $(\nabla S)(x) \in Lin(Lin\mathcal{V}, \mathcal{V})$ is defined by means of the relation

$$((\nabla S)(x)A) \cdot b = \nabla(S^T b) \mid_x \cdot A$$

for all $A \in Lin\mathcal{V}$ and $b \in \mathcal{V}$, and the previous relation and the arbitrariness of a tell us that

$$\det K\, divS = div(SK^*) - S\, divK^* + \nabla S\, [(\det K)I - K^*]. \tag{1.9}$$

Based on the identification relations, we may describe this relation as the decomposition of the *volume density of total contact forces* $\det K\, divS$ into the sum of the *volume density of contact forces without disarrangements* $div(SK^*)$ and the *volume density of contact forces due to disarrangements* $-S\, divK^* + \nabla S\, [(\det K)I - K^*]$. While the first and third densities need not be the divergence of a tensor field, the volume density of contact forces without disarrangements is the divergence of the tensor field SK^*. Therefore, we may call SK^* the *stress without disarrangments.* The terminology *stress in the virgin configuraion* also may be used and is justified by the fact that the Cauchy stress T, which is the stress in the current configuration, is related to the Piola-Kirchoff stress S, which here is the stress in the microscopically deformed configuration, by the equation $S = (T \circ g)(\nabla g)^*$. If we write $S_\backslash := SK^*$ for the stress in the virgin configuration, then we have both

$$S_\backslash = (S \circ i)K^* \text{ and } S = (T \circ g)(\nabla g)^*, \tag{1.10}$$

and the interpretation of SK^* as a stress relative to a new configuration, the virgin configuration, is completely evident.

In [**?**], a special instance of the stress in the virgin configuration and of the decomposition (**??**) was obtained when the purely microscopic deformation (i, K) involved only slips. In this situation, $\det K = 1$ and the decomposition (**??**) can be written

$$
\begin{aligned}
divS &= div(SK^*) + (divS - div(SK^*)) \\
&= div(SK^*) + div(S - (SK^*)).
\end{aligned}
$$

Thus, when $\det K = 1$ (even when some other mechanism than slips leads to this relation), all three volume densities of contact forces appearing in the decomposition (**??**) can be written as the divergence of a tensor field, and this leads to the *decompostion of stresses:*

$$\det K = 1 \Longrightarrow S = SK^* + (S - SK^*) \tag{1.11}$$

in which we are justified in calling $S - SK^*$ the *stress due to disarrangements* and (as in the case where $\det K$ need not equal the constant field 1) calling SK^* the *stress without disarrangments.*

Returning to the balance of forces (**??**), we multiply both sides by $\det K$ and use the decomposition (**??**) to obtain the *refined balance of forces*

$$div(SK^*) - S\,divK^* + \nabla S\,[(\det K)I - K^*] + \rho_v b = 0 \tag{1.12}$$

in which $\rho_v := \rho_m \det K$ is the density in the virgin configuration. This relation is a refinement of (**??**), because the original volume density of contact forces in the microscopically deformed configuration now is written in more precise form, based on the information contained in the purely microscopic deformation (i, K). We also may call (**??**) the *balance of forces in the virgin configuration.* In it, the volume density of contact forces without disarrangements $div(SK^*)$ represent contact forces inside microscopically intact pieces of the body; the volume density of contact forces due to disarrangements $-S\,divK^* + \nabla S\,[(\det K)I - K^*]$ represent forces needed to maintain the deformations at the microlevel and need not take the form of the divergence of a tensor field. Not only is the refined balance of forces equivalent to the balance of forces in the microscopically deformed configuration, but it reduces identically to it in the special case when $K = I$, i.e., when the virgin configuration and the microscopically deformed configuration differ neither at the macrolevel nor at the microlevel.

A procedure analogous to the one used above (see [**?**] for details) permits one to derive a *refined balance of moments, i.e.,* a *balance of moments in the virgin configuration*:

$$0 = Sk(\det K\ S(\nabla g)^T) = Sk(\,SK^*(\nabla g)^T) + Sk(\,S((\det K)I - K^*)(\nabla g)^T). \tag{1.13}$$

Here, for each $A \in Lin\mathcal{V}$, $SkA := (A - A^T)/2$ is the skew part of A, and the refined balance of moments shows that, while the moments associated with the total contact forces must be self-equilibrated, the separate moments due to disarrangements and without disarrangements must balance one another, without the necessity that either be self-equilibrated.

2 Free Energies for Structured Deformations

In this lecture we discuss some issues central to the development in the context of structured deformations of an analogue of the subject of elastostatics for classical deformations. Recall that under isothermal conditions the Helmholtz free energy $\Psi_{Cld}(\mathcal{P}, f)$ of a part $\mathcal{P}$ of a homogeneous elastic body that undergoes a classical deformation f is given by

$$\Psi_{Cld}(\mathcal{P}, f) = \int_{\mathcal{P}} \hat{\psi}(\nabla f(x)) dV_x.$$

Here, $\hat{\psi} : Lin\mathcal{V}^+ \to \mathbb{R}$ is a constitutive function characterizing the particular elastic material under consideration, and $\hat{\psi}(\nabla f(x))$ is the volume density of (Helmholtz) free energy at the point $x \in \mathcal{P}$. We wish to study the question: what form should the right-hand side of this relation assume if the classical deformation $f \in Cld(\mathcal{A})$ is replaced by a structured deformation $(\kappa, g, G) \in Std(\mathcal{A})$?

This question was first studied by Choksi & Fonseca [**?**] within a broader notion of structured deformation based on "special functions of bounded variation". Leaving aside this technical difference, they answered the following question: *if one has a formula for the free energy $\Psi_{Sid}(\mathcal{P}, (\kappa, f))$ of a part $\mathcal{P}$ that is valid for all parts and for all simple deformations (κ, f), what should be the formula for the free energy when (κ, f) is replaced by a structured deformation (κ, g, G)*? Here are two key points in the answer supplied by Choksi & Fonseca:

1. the free energy $\Psi_{Std}(\mathcal{P}, (\kappa, g, G))$ for a structured deformation should be determined by the free energies $\Psi_{Sid}(\mathcal{P}, (\kappa_m, f_m))$ of approximating simple deformations in a manner that does not depend upon the particular choice of sequence $m \to (\kappa_m, f_m)$ converging to a given structured deformation (κ, g, G);

2. $\Psi_{Sid}(\mathcal{P},(\kappa_m, f_m))$ should be given in terms of both a bulk contribution and an interfacial contribution, and it is to be proved (or disproved) that the expression $\Psi_{Std}(\mathcal{P},(\kappa, g, G))$ has both bulk and interfacial terms. If so, the manner in which the bulk and surface terms for $\Psi_{Sid}(\mathcal{P},(\kappa_m, f_m))$ affect the corresponding terms for $\Psi_{Std}(\mathcal{P},(\kappa, g, G))$ should be made explicit.

In what follows, we present some of Choksi and Fonseca's ideas in the one-dimensional context of $Std((0,1))$ and within the context of structured deformations used throughout these lectures. We derive an explicit, surprisingly simple formula for $\Psi_{Std}(\mathcal{P},(\kappa, g, G))$, and we give an alternative starting formula for $\Psi_{Sid}(\mathcal{P},(\kappa_m, f_m))$ that leads by means of a similar analysis to a broader set of possibilities for $\Psi_{Std}(\mathcal{P},(\kappa, g, G))$.

2.1 Free energy for simple deformations

We note that for each $(\kappa, f) \in Sid((0,1))$, κ is a finite subset of $(0,1)$ and f is an injective, piecewise continuously differentiable real-valued function. Moreover, because the interval $(0,1)$ is a fit region, the jump set $\Gamma(f)$ is a subset of the disarrangement site κ and also is a finite set. We fix $\mathcal{P} := (0,1)$ and define

$$\Psi_{Sid}((\kappa, f)) := \int_0^1 W(\nabla f(x))\, dx + \sum_{z\in\Gamma(f)} h([f](z)), \tag{2.1}$$

where $[f](z) := f(z+) - f(z-) = Jf(z)$. We assume that the functions $W : [0,\infty) \to [0,\infty)$ and $h : \mathbb{R} \to [0,\infty)$ are continuous and that h satisfies

$$h(0) = 0 \text{ and } 0 \leq L := \liminf_{\zeta\to 0+} \frac{h(\zeta)}{\zeta} < +\infty. \tag{2.2}$$

We call W the *bulk energy density for simple deformations* and h the *interfacial energy density for simple deformations.*

2.2 Behavior of the bulk energy density in the limit

Let $(\kappa, g, G) \in Std((0,1))$ and $m \mapsto (\kappa_m, f_m) \in Sid((0,1))$ be given such that

$$\lim_{m\to\infty} \sup_{x\in (0,1)\setminus(\kappa\cup\kappa_m)} (|f_m(x) - g(x)| + |\nabla f_m(x) - G(x)|) = 0. \tag{2.3}$$

In particular, we follow Choksi & Fonseca [?] in not requiring here that $\liminf_{m\to\infty} \kappa_m = \kappa$. To distinguish this weaker convergence (??), we write here $(f_m, \nabla f_m) \to (g, G)$ in place of the notation $(\kappa_m, f_m) \to (\kappa, g, G)$ used in Part One for the convergence that includes the requirement $\liminf_{m\to\infty} \kappa_m = \kappa$. From the definition of Std, we may choose positive constants $\bar{m}, \bar{M}$ such that $0 < \bar{m} < G(x) < \bar{M}$ for all $x \in (0,1)\backslash\kappa$. Because $(f_m, \nabla f_m) \to (g, G)$, we may choose a positive integer N such that $\frac{\bar{m}}{2} \leq \nabla f_m(x) \leq 2\bar{M}$ for all $x \in (0,1) \setminus (\kappa \cup \kappa_m)$ and for all $m > N$. Since W is continuous, its restriction $W\mid_{[\frac{\bar{m}}{2}, 2\bar{M}]}$ is uniformly continuous, and we conclude that

$$\lim_{m\to\infty} \int_0^1 W(\nabla f_m(x))\, dx = \int_0^1 W(G(x))\, dx. \tag{2.4}$$

Thus, *the bulk energies for the approximating simple deformations form a convergent sequence whose limit is independent of the choice of sequence* $(\kappa_m, f_m) \to (g, G)$; *in particular, the limiting bulk energy depends only upon G, the deformation without disarrangements.*

2.3 Limiting behavior of the interfacial energy associated with $\Gamma(g)$

With (κ, g, G) and $m \mapsto (\kappa_m, f_m)$ as above, we recall from Subsection 2.1 that the jump sets $\Gamma(g)$ and $\Gamma(f_m)$ must be finite sets. By the Trace Theorem (Part One, Section 6), for each $z \in \Gamma(g)$ we may choose a positive integer $m(z)$ such that $z \in \Gamma(f_p)$ for all $p \geq m(z)$. Because the set $\{m(z) \mid z \in \Gamma(g)\}$ is a finite set of positive integers, it has a maximum $m(g)$, and $z \in \Gamma(f_m)$ for all $m \geq m(g)$. Since the point $z \in \Gamma(g)$ is arbitrary, the jump set $\Gamma(g)$ is a subset of the jump set $\Gamma(f_m)$ for all $m \geq m(g)$, and we assume $m \geq m(g)$ from now on in this argument. Of course, we may write

$$\sum_{z\in\Gamma(f_m)} h([f_m](z)) = \sum_{z\in\Gamma(g)} h([f_m](z)) + \sum_{z\in\Gamma(f_m)\setminus\Gamma(g)} h([f_m](z)),$$

and, by the Trace Theorem, $\lim_{m\to\infty}[f_m](z)=[g](z)$ for every $z\in\Gamma(g)$. The continuity of h and the finiteness of $\Gamma(g)$ then yield immediately

$$\lim_{m\to\infty}\sum_{z\in\Gamma(f_m)\cap\Gamma(g)}h([f_m](z))=\sum_{z\in\Gamma(g)}h([g](z)).$$

Thus, *the portion of the interfacial energy of the approximating simple deformations f_m that is associated with the jump points of g converges to the interfacial energy of the simple deformation (κ,g).*

2.4 Limiting behavior of the interfacial energy not associated with $\Gamma(g)$

We begin by listing the points of $\Gamma(g)$ in increasing order

$$0=x_0<x_1<x_2<\cdots<x_k<\cdots<x_K<x_{K+1}=1,$$

and we consider for each positive integer m as above and $k\in\{0,\ldots,K\}$ the pair

$$(\kappa_m^{(k)},f_m^{(k)}):=(\kappa_m\cap(x_k,x_{k+1})\,,\,f_m\,|_{(x_k,x_{k+1})})$$

and the triple

$$(\emptyset,g^{(k)},G^{(k)}):=(\emptyset,g\,|_{(x_k,x_{k+1})},G\,|_{(x_k,x_{k+1})}).$$

It is easy to see that $(\kappa_m^{(k)},f_m^{(k)})\to(\emptyset,g^{(k)},G^{(k)})$, that

$$(\kappa_m^{(k)},f_m^{(k)})\in Sid((x_k,x_{k+1})),\quad(\emptyset,g^{(k)},G^{(k)})\in Std((x_k,x_{k+1})),\quad\Gamma(g^{(k)})=\emptyset,$$

and

$$\sum_{z\in\Gamma(f_m)\setminus\Gamma(g)}h([f_m](z))=\sum_{k=0}^{K}\sum_{z\in\Gamma(f_m^{(k)})}h([f_m^{(k)}](z)).\tag{2.5}$$

Therefore, to find the behavior of the left hand side of (**??**) as $m\to\infty$, it suffices to determine the behavior of $\sum_{z\in\Gamma(f_m^{(k)})}h([f_m^{(k)}](z))$ as $m\to\infty$ for each $k\in\{0,\ldots,K\}$. Thus, without loss of generality, we may now replace $(\kappa,g,G)\in Std((0,1))$ by $(\emptyset,g,G)\in Std((0,1))$.

Proposition 2.1 *Let $(\emptyset, g, G) \in Std((0,1))$ be given and let $m \mapsto (\kappa_m, f_m)$ be a sequence of simple deformations such that $(f_m, \nabla f_m) \to (g, G)$ and, for all positive integers m and $z \in \Gamma(f_m)$, there holds $[f_m](z) > 0$. It follows that*

$$\liminf_{m\to\infty} \sum_{z\in\Gamma(f_m)} h([f_m](z)) \geq L \int_0^1 (\nabla g(x) - G(x))dx \tag{2.6}$$

*with L the non-negative number defined in (**??**).*

Proof. Because $\kappa = \emptyset$, the function g is continuous, so that $[g](z) = 0$ for all $z \in (0,1)$. By the Trace Theorem and the continuity of g, we may conclude that $\lim_{m\to\infty} \max\{[f_m](z) \mid z \in \Gamma(f_m)\} = 0$. The definition of "lim inf" and the assumed positivity of $[f_m(z)]$ tell us that, for each $\varepsilon > 0$, we may choose a positive integer M_ε such that

$$\frac{h([f_m](z))}{[f_m](z)} \geq (1-\varepsilon)L$$

for all $m > M_\varepsilon$ and $z \in \Gamma(f_m)$. Multiplying both members of this inequality by $[f_m](z)$ and summing over $z \in \Gamma(f_m)$ we find

$$\begin{aligned}
\sum_{z\in\Gamma(f_m)} h([f_m](z)) &\geq (1-\varepsilon)L \sum_{z\in\Gamma(f_m)} [f_m](z) \\
&= (1-\varepsilon)L\{f_m(1-) - f_m(0+) - \int_0^1 \nabla f_m(x)\,dx\} \\
&\longrightarrow (1-\varepsilon)L\{g(1-) - g(0+) - \int_0^1 G(x)\,dx\} \\
&= (1-\varepsilon)L \int_0^1 (\nabla g(x) - G(x))\,dx,
\end{aligned}$$

and this yields the desired conclusion. ■

The next result gives us full information about the limiting behavior of the interfacial energy not associated with the jumps of g.

Proposition 2.2 *For every $(\emptyset, g, G) \in Std((0,1))$,*

$$\inf\left(\liminf_{m\to\infty}\sum_{z\in\Gamma(f_m)} h([f_m](z))\right) = L\int_0^1 (\nabla g(x) - G(x))dx \tag{2.7}$$

with L the non-negative number defined in (??) and with the infimum taken over the sequences of simple deformations satisfying (i) $(f_m, \nabla f_m) \to (g, G)$ and (ii) $[f_m](z) > 0$ for all positive integers m and for all $z \in \Gamma(f_m)$.

Before we prove this proposition, we discuss the important and immediate conclusion that we may draw from it and the results in Subsections 2.2 and 2.3:

$$\begin{aligned}\inf\left(\liminf_{m\to\infty}\Psi_{Sid}((\kappa_m, f_m))\right) \;=\; & \int_0^1 \left(W(G(x)) + L(\nabla g(x) - G(x))\right)dx \\ & + \sum_{z\in\Gamma(g)} h([g](z)),\end{aligned} \tag{2.8}$$

with again L the non-negative number defined in (??) and with the infimum taken over the sequences of simple deformations satisfying (i) $(f_m, \nabla f_m) \to (g, G)$ and (ii) $[f_m](z) > 0$ for all positive integers m and for all $z \in \Gamma(f_m)$. This result captures the flavor of the conclusions obtained by Choksi & Fonseca [?]: (1) it involves the double limit operation "inf lim inf" to yield a quantity depending only upon (g, G) and not on a particular choice of sequence satisfying (i) and (ii); (2) the bulk term $\int_0^1 (W(G(x)) + L(\nabla g(x) - G(x)))\,dx$ on the right-hand side of (??) contains two terms in the integrand: one comes from the bulk energy density W and the other comes from the interfacial energy density h for simple deformations. Thus, the diffusion of disarrangements occurring as m tends to infinity causes the interfacial energy for simple deformations to contribute to the limiting bulk energy, while the persistent disarrangements associated with $\Gamma(g)$ cause the initial interfacial energy for simple deformations to contribute to the limiting interfacial energy. If we followed Choksi & Fonseca one step further, we would define

$$\Psi_{Std}((g,G)) := \int_0^1 (W(G(x)) + L(\nabla g(x) - G(x)))\,dx + \sum_{z\in\Gamma(g)} h([g](z)).$$

Instead, we give at the end of this lecture an alternative method for calculating an energy for structured deformation that leads to terms in the integral that can depend non-linearly on $\nabla g(x) - G(x)$, the deformation due to microdisarrangements.

2.5 Proof of Proposition 2.2

From the analysis in Subsection 2.4, it suffices to consider the case $\kappa = \emptyset$, and Proposition 2.1 reduces our task to veryfying: for each $(\emptyset, g, G) \in Std((0,1))$, there exists a sequence of simple deformations satisfying $(f_m, \nabla f_m) \to (g, G)$ and

$$\lim_{m\to\infty} \sum_{z\in\Gamma(f_m)} h([f_m](z)) = L \int_0^1 (\nabla g(x) - G(x))dx. \tag{2.9}$$

Our first step in constructing such a sequence is to consider the case $\nabla g(x) = G(x)$ for all $x \in (0,1)$. In this case, $(\emptyset, g, \nabla g) = (\emptyset, g, G) \in Std((0,1))$, and we may put $\kappa_m := \emptyset$ and $f_m := g$ for every positive integer m. Thus, $\Gamma(f_m) = \emptyset$ and $\sum\limits_{z\in\Gamma(f_m)} h([f_m](z)) = 0 = \int_0^1 (\nabla g(x) - G(x))\,dx$ for all m, so that (**??**) is evident.

The remaining case to consider is when there exists $x_0 \in (0,1)$ for which $\nabla g(x_0) \neq G(x_0)$. The continuity of ∇g and of G and the relations $\nabla g(x) = \det \nabla g(x) \geq \det G(x) = G(x)$ for all $x \in (0,1)$ imply that

$$I := \int_0^1 (\nabla g(x) - G(x))dx > 0. \tag{2.10}$$

By the definition $L := \liminf_{\zeta\to 0+} \frac{h(\zeta)}{\zeta}$, we may choose $m \mapsto \zeta_m > 0$ such that $\lim_{m\to\infty} \zeta_m = 0$ and $\lim_{m\to\infty} \frac{h(\zeta_m)}{\zeta_m} = L$. Moreover, we may assume that $m \mapsto \zeta_m$

is strictly decreasing and, because $I > 0$, that $\zeta_m < I$ for all m. Let m now be given, and note that, because the function $y \mapsto \int_0^y (\nabla g(x) - G(x))\, dx$ is continuous, we may choose a number $x_{q_1} \in (0,1)$ such that

$$\int_0^{x_{q_1}} (\nabla g(x) - G(x))\, dx = \zeta_m. \tag{2.11}$$

For x in the interval $(0, x_{q_1})$, put

$$f_m(x) := g(0+) + \int_0^x G(\xi) d\xi \tag{2.12}$$

and note that $\nabla f_m(x) = G(x)$ and

$$\begin{aligned} 0 \ \leq \ g(x) - f_m(x) &= \left(g(0+) + \int_0^x \nabla g(\xi) d\xi \right) - \left(g(0+) + \int_0^x G(\xi) d\xi \right) \\ &= \int_0^x (\nabla g(\xi) - G(\xi)) d\xi \leq \int_0^{x_{q_1}} (\nabla g(\xi) - G(\xi)) d\xi = \zeta_m. \end{aligned}$$

To define f_m on $(x_{q_1}, 1)$, we first consider the case

$$\int_{x_{q_1}}^1 (\nabla g(x) - G(x))\, dx \leq \zeta_m.$$

For $x \in (x_{q_1}, 1)$ we define

$$f_m(x) := g(x_{q_1}) + \int_{x_{q_1}}^x G(\xi) d\xi \tag{2.13}$$

and we note as above that $\nabla f_m(x) = G(x)$ and $0 \leq g(x) - f_m(x) \leq \zeta_m$. Relations (**??**) and (**??**) tell us that

$$f_m(x_{q_1}+) - f_m(x_{q_1}-) \ = \ g(x_{q_1}) - \left(g(0+) + \int_0^{x_{q_1}} G(\xi) d\xi \right)$$

$$= \quad (g(x_{q_1}) - g(0+)) - \int_0^{x_{q_1}} G(\xi)d\xi$$
$$= \quad \int_0^{x_{q_1}} (\nabla g(\xi) - G(\xi))d\xi = \zeta_m > 0,$$

and it follows that $\Gamma(f_m) = \{x_{q_1}\}$ and $[f_m](x_{q_1}) = \zeta_m > 0$. Consequently, $(\{x_{q_1}\}, f_m) \in Sid((0,1))$, the condition (ii) in Proposition 2.2 is satisfied, and

$$|f_m(x) - g(x)| \leq \zeta_m \text{ and } |\nabla f_m(x) - G(x)| = 0 \tag{2.14}$$

for all $x \in (0,1) \setminus \{x_{q_1}\}$.

In the remaining case

$$\int_{x_{q_1}}^{1} (\nabla g(x) - G(x))\, dx > \zeta_m,$$

we may choose $x_{q_2} \in (x_{q_1}, 1)$ such that

$$\int_{x_{q_1}}^{x_{q_2}} (\nabla g(x) - G(x))\, dx = \zeta_m,$$

and for x in the interval (x_{q_1}, x_{q_2}) we define $f_m(x)$ again using the formula (**??**), so that the relations (**??**) are satisfied for all $x \in (x_{q_1}, x_{q_2})$ and $[f_m](x_{q_1}) = \zeta_m > 0$. If we now put $M_m := \lfloor \frac{I}{\zeta_m}$, i.e., the greatest integer less than or equal to the number $\frac{I}{\zeta_m} > 1$, then we may choose for each $k \in \{1, 2, \dots, M_m\}$ a point $x_{q_k} \in (0,1)$ such that

$$x_{q_1} < \cdots < x_{q_k} < x_{q_{k+1}} < \cdots < x_{q_{M_m}}, \tag{2.15}$$

$$\begin{aligned} \int_0^{x_{q_1}} (\nabla g(x) - G(x))\, dx &= \int_{x_{q_1}}^{x_{q_2}} (\nabla g(x) - G(x))\, dx \\ &= \cdots = \int_{x_{q_{M_m - 1}}}^{x_{q_{M_m}}} (\nabla g(x) - G(x))\, dx = \zeta_m, \end{aligned} \tag{2.16}$$

and

$$\int_{x_{q_{M_m}}}^{1} (\nabla g(x) - G(x))\, dx \leq \zeta_m. \tag{2.17}$$

We now define $\kappa_m := \left\{x_{q_1}, \cdots, x_{q_k}, x_{q_{k+1}}, \cdots, x_{q_{M_m}}\right\}$ and, setting $x_{q_0} := 0$ and $x_{q_{M_m+1}} := 1$, we put

$$f_m(x) := g(x_{q_k}) + \int_{x_{q_k}}^{x_{q_{k+1}}} G(\xi)\, d\xi \text{ if } x \in (x_{q_k}, x_{q_{k+1}}) \text{ and } k \in \{0, 1, 2, \ldots, M_m\}. \tag{2.18}$$

This definition yields a simple deformation $(\kappa_m, f_m) \in Sid((0,1))$ with $\Gamma(f_m) = \kappa_m$, $[f_m](z) = \zeta_m$ for all $z \in \Gamma(f_m)$, and satisfying (**??**) for all $x \in (0,1)\backslash\kappa_m$. We now may write

$$\begin{aligned} \sum_{z\in\Gamma(f_m)} h([f_m](z)) &= \sum_{z\in\Gamma(f_m)} h(\zeta_m) \\ &= M_m h(\zeta_m) \in \left[\frac{I\, h(\zeta_m)}{\zeta_m}, (\frac{I}{\zeta_m} + 1)h(\zeta_m)\right). \end{aligned}$$

In other words, for all positive integers m,

$$\begin{aligned} &\tfrac{h(\zeta_m)}{\zeta_m} \int_0^1 (\nabla g(x) - G(x))dx \leq \\ &\sum_{z\in\Gamma(f_m)} h([f_m](z)) < \tfrac{h(\zeta_m)}{\zeta_m}(\int_0^1 (\nabla g(x) - G(x))dx + \zeta_m) \end{aligned}$$

and, letting $m \to \infty$, we obtain the desired relation(**??**). ■

2.6 Another choice for Ψ_{Sid} and its limiting behavior

The choice $\Psi_{Sid}(\kappa, f) = \int_0^1 W(\nabla f(x))\, dx + \sum_{z\in\Gamma(f)} h([f](z))$ made in (**??**) has led in Subsection 2.3 to the "relaxed" energy

$$\int_0^1 (W(G(x)) + L(\nabla g(x) - G(x)))\, dx + \sum_{z\in\Gamma(g)} h([g](z))$$

as a reasonable candidate for the free energy $\Psi_{Std}(\kappa, g, G)$ for a structured deformation. Note however that the dependence of the relaxed energy upon $\nabla g - G$, the deformation due to disarrangements, necessarily is linear, and this outcome may be viewed as a limitation from the point of view of eventual applications. As an alternative, for each $r > 0$ we put:

$$\Psi^r_{Sid}(\kappa, f) := \Psi_{Sid}(\kappa, f) + \int_0^1 \psi\Big(\sum_{z\in\Gamma(f)\cap(x-r,x+r)} [f](z)\,/\,2r\Big)\,dx, \tag{2.19}$$

where $\psi : \mathbb{R} \to \mathbb{R}$ is a bounded, uniformly continuous function. Note that the spatial distribution of the disarrangements affects the integral in (**??**) but not the original energy $\Psi_{Sid}(\kappa, f)$ in (**??**).

The last result of this lecture shows that the added term in (**??**) allows for a more general albeit entirely local dependence of the relaxed energy on the deformation due to disarrangements.

Proposition 2.3 *For each $(\kappa, g, G) \in Std((0,1))$ and sequence of simple deformations $m \mapsto (\kappa_m, f_m)$ satisfying $(f_m, \nabla f_m) \to (g, G)$, there holds*

$$\lim_{r\to 0}\lim_{m\to\infty} \int_0^1 \psi\Big(\sum_{z\in\Gamma(f_m)\cap(x-r,x+r)} [f_m](z)\,/\,2r\Big)\,dx = \int_0^1 \psi(\nabla g(x) - G(x))\,dx. \tag{2.20}$$

*Consequently, the relaxed energy associated with (**??**) is given by the formula*

$$\begin{aligned}
&\lim_{r\to 0}\lim_{m\to\infty} \Psi^r_{Sid}(\kappa_m, f_m)\\
= \;& \int_0^1 (W(G(x)) + L(\nabla g(x) - G(x)))\,dx \,+ \\
& \sum_{z\in\Gamma(g)} h([g](z)) + \int_0^1 \psi(\nabla g(x) - G(x))\,dx,
\end{aligned} \tag{2.21}$$

with the infimum taken over the sequences of simple deformations satisfying (i) $(f_m, \nabla f_m) \to (g, G)$ and (ii) $[f_m](z) > 0$ for all positive integers m and for all $z \in \Gamma(f_m)$.

Before proving this proposition, we note that the definition

$$\Psi_{Std}(\kappa, g, G) := \lim_{r\to 0}\lim_{m\to\infty} \Psi^r_{Sid}(\kappa_m, f_m) \tag{2.22}$$

yields the desired, possibly non-linear dependance $W(G(x)) + L(\nabla g(x) - G(x)) + \psi(\nabla g(x) - G(x))$ of the bulk energy density on the deformation due to disarrangements $\nabla g(x) - G(x)$. Moreover, evaluation of Ψ_{Std} at the simple deformation (κ, f), when identified with the structured deformation $(\kappa, f, \nabla f)$ (so that $g := f$, $G := \nabla f$ and, therefore, $\nabla g = G$), yields the formula

$$\Psi_{Std}(\kappa, f, \nabla f) = \int_0^1 (W(\nabla f(x)) + \psi(0))\, dx + \sum_{z\in\Gamma(f)} h([f](z)).$$

When $\psi(0) = 0$, we find that Ψ_{Std} defined in (**??**) reduces to the original energy Ψ_{Sid} defined in (**??**) when evaluated on simple deformations.

Proof of Proposition 2.1: From the Trace Theorem and Integral-Gradient Formula (Part One, Sections 6 and 7), we have

$$\begin{aligned}
&\lim_{m\to\infty} \sum_{z\in\Gamma(f_m)\cap(x-r,x+r)} [f_m](z) \\
&= \lim_{m\to\infty}\left(f_m((x+r)-) - f_m((x-r)+) - \int_{x-r}^{x+r} \nabla f_m(\xi) d\xi \right) \\
&= g((x+r)-) - g((x-r)+) - \int_{x-r}^{x+r} G(\xi) d\xi \\
&= \sum_{z\in\Gamma(g)\cap(x-r,x+r)} [g](z) + \int_{x-r}^{x+r} (\nabla g(\xi) - G(\xi))\, d\xi,
\end{aligned}$$

where the convergence as $m \to \infty$ is uniform in x. The uniform continuity of ψ then allows us to write

$$\lim_{m\to\infty} \psi\left(\sum_{z\in\Gamma(f_m)\cap(x-r,x+r)} [f_m](z) \,/\, 2r \right)$$

$$= \psi\left(\Big(\sum_{z\in\Gamma(g)\cap(x-r,x+r)} [g](z) + \int_{x-r}^{x+r} (\nabla g(\xi) - G(\xi))\, d\xi \Big) \,/\, 2r \right), \qquad (2.23)$$

for each $r > 0$. Now, put

$$\mathcal{I}(\Gamma(g), r) := \{ y \in (0,1) \mid \text{ there exists } z \in \Gamma(g) \text{ for which } |y - z| < r \},$$

note that $\mathcal{I}(\Gamma(g), r)$ is a finite union of open intervals, and denote by $n(g)$ the number of such open intervals. The measure of $\mathcal{I}(\Gamma(g), r)$ is bounded above by $2rn(g)$. Moreover, we have from (**??**)

$$\begin{aligned}
&\lim_{m\to\infty} \int_0^1 \psi\left(\sum_{z\in\Gamma(f_m)\cap(x-r,x+r)} [f_m](z) \,/\, 2r \right) dx \\
= &\int_0^1 \lim_{m\to\infty} \psi\left(\sum_{z\in\Gamma(f_m)\cap(x-r,x+r)} [f_m](z) \,/\, 2r \right) dx \\
= &\int_0^1 \psi\left(\Big(\sum_{z\in\Gamma(g)\cap(x-r,x+r)} [g](z) + \int_{x-r}^{x+r} (\nabla g(\xi) - G(\xi))\, d\xi \Big) \,/\, 2r \right) dx. \qquad (2.24)
\end{aligned}$$

In the last expression, we may write the integral as a sum of the integral over the set $\mathcal{I}(\Gamma(g), r)$ and the integral over its complement $(0,1)\backslash\mathcal{I}(\Gamma(g), r)$. If M denotes the maximum of the function ψ, then

$$\left| \int_{\mathcal{I}(\Gamma(g),r)} \psi\left(\Big(\sum_{z\in\Gamma(g)\cap(x-r,x+r)} [g](z) + \int_{x-r}^{x+r} (\nabla g(\xi) - G(\xi))\, d\xi \Big) \,/\, 2r \right) dx \right| \le 2rn(g)M. \qquad (2.25)$$

Because $\Gamma(g) \cap (x - r, x + r) = \emptyset$ for every $x \in (0,1)\backslash\mathcal{I}(\Gamma(g), r)$, we also have

$$\int_{(0,1)\,\backslash\,\mathcal{I}(\Gamma(g),r)} \psi\left(\Big(\sum_{z\in\Gamma(g)\cap(x-r,x+r)} [g](z) + \int_{x-r}^{x+r} (\nabla g(\xi) - G(\xi))\, d\xi \Big) \,/\, 2r \right) dx$$

$$= \int\limits_{(0,1)\setminus \mathcal{I}(\Gamma(g),r)} \psi \left((\int\limits_{x-r}^{x+r} (\nabla g(\xi) - G(\xi))\, d\xi) \,/\, 2r \right) dx, \tag{2.26}$$

and, as $r \to 0$, relations (**??**) - (**??**) yield the desired formula (**??**). ■

3 Constitutive Equations

Our study of structured deformations has led to the following refined measures of deformation and of contact interactions, together with precise mathematical results that justify our interpretations of these quantities:

G	$\cdots$ deformation without disarrangements
$M := \nabla g - G$	$\cdots$ deformation due to disarrangements at the microlevel
$K := (\nabla g)^{-1} G$	$\cdots$ deformation without disarrangements in a purely microscopic deformation
SK^*	$\cdots$ stress without disarrangements
$\det K\, divS - div(SK^*)$	$\cdots$ volume density of contact forces due to disarrangments.

This list can be augmented in various ways by other refined measures of stress and deformation (for example, the "continuum stress" and the "stress due to change in internal structure" introduced in reference [8, Part One]). Nevertheless, we already are in a position to give some specific results and proposals for constitutive equations in the setting of bodies undergoing structured deformations. One example emerged through relations (**??**) and (**??**) as a formula for the free energy in a structured deformation. Our aim in this lecture is to consider further proposals for constitutive relations and to give some elementary applications of these and previous proposals. Our examples deal both with constitutive relations that do not involve the concept of free energy (Section 3.2) and constitutive relations associated with a formula for the free energy (Section 3.3).

3.1 Change of observer and of reference configuration

We begin with a general issue concerning constitutive relations: constitutive equations should be independent of the choice of observer (frame-indifferent) and should be capable of reflecting independence of the choice of reference configuration to an extent appropriate for a given material (material symmetry). For our purposes, a *change of observer* is specified by an orthogonal tensor $Q \in Orth\mathcal{V}$ (so that $QQ^T = Q^TQ = I$) and the following transformation laws for macroscopic deformation ∇g (with g the transplacement of an arbitrary structured deformation), free energy Ψ, and Caucy stress T:

$$\nabla g \to Q\nabla g, \qquad \Psi \to \Psi, \quad \text{and} \quad T \to QTQ^T. \tag{3.1}$$

A *change of (virgin) configuration* is specified by a unimodular tensor $H \in Unim(\mathcal{V})$ (so that $|\det H| = 1$) along with the transformation laws

$$\nabla g \to (\nabla g)H, \qquad \Psi \to \Psi, \quad \text{and} \quad T \to T. \tag{3.2}$$

Because simple deformations are structured deformations, these transformation laws apply to the deformation gradients ∇f_m associated with simple deformations $(\kappa_m,\, f_m)$ that approximate a structured deformation $(\kappa, g, G) \in Std(\mathcal{A})$. The Approximation Theorem tells us that for every $x \in \mathcal{A}\backslash\kappa$ we may write $G(x) = \lim_{m\to\infty} \nabla f_m(x)$, and we conclude from (**??**) and (**??**) that G transforms in the same way as ∇g. This fact and the relation $S := (T \circ g)(\nabla g)^*$ between Piola-Kirchhoff stress S and Cauchy stress T permit one to deduce immediately the following transformation laws for the quantities identified at the beginning of this lecture:

$$
\begin{array}{cc}
\textbf{Change of observer} & \textbf{Change of virgin configuration} \\
G \to QG & G \to GH \\
M \to QM & M \to MH \\
K \to K & K \to H^{-1}KH \\
S \to QS & S \to SH^* \\
SK^* \to QSK^* & SK^* \to SK^*H^* \\
divS \to QdivS & divS \to \nabla S\,[H^*] \\
div(SK^*) \to Qdiv(SK^*) & div(SK^*) \to \nabla(SK^*)[H^*]
\end{array}
\tag{3.3}
$$

and, for the volume density of contact forces due to disarrangements, the transformation laws

$$
\begin{aligned}
\det K divS - div(SK^*) &\to Q\,(\det K divS - div(SK^*)) \\
\det K divS - div(SK^*) &\to (\det K\,\nabla S - \nabla(SK^*))\,[H^*].
\end{aligned}
\tag{3.4}
$$

Note that no arbitrary choices enter into the transformation laws (**??**) and (**??**): the refined measures of deformation G, M, and K and of contact forces SK^* and $\det K divS - div(SK^*)$ associated with structured deformations transform in a predetermined way. Moreover, it is a convenient outcome that both the deformation without disarrangements G and the deformation due to microdisarrangements M transform in the same way as the macroscopic deformation ∇g.

3.2 Some stress-strain relations for single slip in crystals

Let $(\emptyset, g, G) \in Std(\mathcal{A})$ be given, and assume there is given a unit vector $\nu \in \mathcal{V}$ and a sequence $m \mapsto (\kappa_m, f_m)$ of simple deformations such that $(\kappa_m, f_m) \to (\emptyset, g, G)$ and the following "slip conditions" are satisfied:

s1) for every positive integer m, the jump set $\Gamma(f_m)$ is a family of planes perpendicular to ν;

s2) $\det G(x) = \det \nabla g(x)$ for every $x \in \mathcal{A}$;

Condition s1) tells us that approximating simple deformations can be chosen so that their jumps only occur across planes in a given family all having normal the given unit vector ν. Relation s2) is the assertion that no volume changes occur due to the jumps. We refer to the deformations associated with $(\emptyset, g, G)$ and $m \mapsto (\kappa_m, f_m)$ as *single slip*; the word "single' refers to the existence of a single family of parallel planes that govern the changes in geometry due to disarrangements. These disarrangements will be called *microslips*. Note that the definition of single slip employed in [**?**] imposed the condition: for every m and $y \in \Gamma(f_m)$, the jump in f_m at y is perpendicular to ν:

$$((f_m)_\nu(y) - (f_m)_{-\nu}(y)) \cdot \nu = 0.$$

While this condition is consistent with s1) and s2), it renders the example of single slip more restrictive, and we choose not to impose it here.

The following are consequences of the conditions s1), s2) and earlier results:

SS1) For every $x \in \mathcal{A}$, the deformation due to microdisarrangements $M(x) := \nabla g(x) - G(x)$ is given by the formula

$$M(x) = s(x) \otimes \nu, \tag{3.5}$$

where the *slip vector* $s(x)$ is defined by the relation:

$$s(x) := \lim_{r\to 0}\lim_{m\to\infty} r^{-3} \int\limits_{\Gamma(f_m)\cap\mathcal{C}(x,r)} ((f_m)_\nu(y) - (f_m)_{-\nu}(y))\, dA_y; \tag{3.6}$$

and where $\mathcal{C}(x,r)$ is the cube centered at x of edge length r.

SS2) For every $x \in \mathcal{A}$, $s(x) \cdot G(x)^*\nu = 0$.

In the present context of single slip, we call $M = s \otimes \nu$ the *deformation due to microslip* and G the *deformation without slip*. Because $(\kappa_m, f_m) \to (\emptyset, g, G)$ we may write $G(x) = \lim_{m\to\infty} \nabla f_m(x)$, so that $G(x)^*\nu = \lim_{m\to\infty}(\nabla f_m(x))^*\nu$. Therefore, we may interpret the vector $G(x)^*\nu$ in SS2) as the normal to the image, under the deformation without slip, of the given family planes in the virgin configuration, and SS2) asserts that the direction of slip is perpendicular to $G(x)^*\nu$. In case one knows, in addition, that the unit vector $\nu_\backslash := G(x)^*\nu \,/\, |G(x)^*\nu|$ is independent of x, then we conclude that for every $x \in \mathcal{A}$, the slip vector $s(x)$ is perpendicular to the unit vector $\nu_\backslash$. This condition on $G(x)^*\nu$ often can be met for single crystals under tensile or compressive loadings.

Verification of SS1): From the relations (7.7) and (6.14) of Part One, we may write

$$M(x) = \lim_{r\to 0}\lim_{m\to\infty} r^{-3} \int\limits_{\Gamma(f_m)\cap\mathcal{C}(x,r)} ((f_m)_\nu(y) - (f_m)_{-\nu}(y)) \otimes \nu \, dA_y,$$

and the fact that ν is independent of y in the surface integral immediately yields the relations in SS1).
Verification of SS2*)*: Because of s2), the identity

$$\det(I + a\otimes b) = 1 + a\cdot b,$$

and SS1) we may write

$$\begin{aligned}\det G &= \det(G+M) = \det(G(I + G^{-1}(s\otimes\nu)))\\ &= \det G\ \det(I + G^{-1}(s\otimes\nu)) = \det G\ \det(I + (G^{-1}s)\otimes\nu)\\ &= \det G\,(1 + (G^{-1}s)\cdot\nu),\end{aligned}$$

and it follows that $(G^{-1}s)\cdot\nu = 0$. Thus, for every $x\in\mathcal{A}$

$$\begin{aligned}s(x)\cdot G^*(x)\nu &= s(x)\cdot\det G(x)\,(G^{-1}(x))^T\nu = \det G(x)G^{-1}(x)s(x)\cdot\nu\\ &= \det G(x)0 = 0.\end{aligned}$$

■

We note by s2) that $\det K = \det\left((\nabla g)^{-1}G\right) = 1$ in the case of single slip, and the discussion preceding (**??**) justifies our here calling SK^* the *stress without slip* and $S - SK^*$ the *stress due to microslip*. We can further use SS1) to write

$$\begin{aligned}K^* &= K^{-T} = \left((\nabla g)^{-1}G\right)^{-T} = \left(G^{-1}\nabla g\right)^T\\ &= \left(G^{-1}(G+M)\right)^T = (I + G^{-1}(s\otimes\nu))^T\\ &= \left(I + (G^{-1}s)\otimes\nu\right)^T = I + \nu\otimes(G^{-1}s),\end{aligned} \tag{3.7}$$

and this yields the following formulae for the stress without slip and the stress due to microslip:

$$SK^* = S + (S\nu)\otimes(G^{-1}s) \tag{3.8}$$

$$S - SK^* = -(S\nu) \otimes (G^{-1}s). \tag{3.9}$$

If a surface in the virgin configuration passes through a given point x and has normal n, then the portion of the total traction $S(x)n$ that is due to microslip is given by

$$\begin{aligned}(S - SK^*)(x)n &= -\left((G(x)^{-1}s(x)) \cdot n\right)\ S(x)\nu \\ &= -\left(s(x) \cdot G(x)^{-T}n\right)\ S(x)\nu \\ &= -\frac{1}{\det G(x)}\left(s(x) \cdot G(x)^* n\right) S(x)\nu. \end{aligned}\tag{3.10}$$

Therefore, the traction due to microslip $(S-SK^*)(x)n$ is colinear with the traction $S(x)\nu$ on each plane introduced in the condition s1) and, by SS2), must vanish when $n = \nu$, i.e., must vanish when the given surface with normal n is parallel to such a plane. Moreover, the magnitude of $(S - SK^*)(x)n$ is maximized when $G(x)^*n$ has the same direction as the slip vector $s(x)$.

The laws of balance of forces and moments (see (**??**) and (**??**))

$$div S + \rho_m b = 0 \tag{3.11}$$

$$Sk(S(\nabla g)^T) = 0 \tag{3.12}$$

amount to 6 scalar equations to determine the unknown fields g, G, s, and S, amounting to 3+9+3+9=24 scalar unknowns, for single slip. There are 9 additional scalar equations due to the relation

$$\nabla g = G + M = G + s \otimes \nu, \tag{3.13}$$

and one additional scalar relation due to SS2)

$$s \cdot G^* \nu = 0. \tag{3.14}$$

Assuming that the unit vector ν is given, for example, as a crystallographically preferred direction for slip in a single crystal in a given loading device, we then have 6+9+1=16 equations to determine 24 scalar unknowns. This leads us to consider the problem of specifying constitutive equations, amounting to 24-16=8 additional scalar equations, for a body undergoing single slip. To this end we recall that G measures deformation not affected by slip, e.g., the distortion of the crystalline lattice of a single crystal between the slip bands that support microslip, and that SK^* measures contact forces not associated with the presence of slips. These observations suggest that the mechanical response of the material away from slip bands be described by a relation between G and SK^*:

$$S(x)K^*(x) = S_\backslash(G(x)) \text{ for all } x \in \mathcal{A}, \tag{3.15}$$

with the function $S_\backslash$ called the *response without microslip.* This relation requires that pure distortion of the lattice is governed by an elastic stress-strain law, and it yields (in view of the balance of moments) 6 of the required 8 additional scalar equations. Note that when the single slip $(\emptyset, g, G)$ happens to be a classical deformation, then $G = \nabla g$ and $K = I$, and (**??**) reduces to

$$S(x) = S_\backslash(\nabla g(x)),$$

which is the classical constitutive equation for an elastic body. Thus, (**??**) is an extension of the classical constitutive equation for an elastic body to the case of a body undergoing single slip.

To summarize: *when the orientation ν of the distinguished family of planes is specified in advance, relations (**??**)-(**??**) represent a system of 22 scalar equations in 24 scalar unknowns for the determination of the stress S and the fields g, G, and s associated with single slip.*

There remain to be specified two additional scalar constitutitve relations. These additional relations would fully determine how the macroscopic deformation $\nabla g(x)$ distributes between deformation without slip $G(x)$ and deformation due to slip $M(x) = s(x) \otimes \nu$. Although this problem awaits further analysis in the present context, the discussion of free energy presented in Section 2 leads to the required additional relations in the more special geometrical context of two-level shears as described in the next subsection.

3.3 Constitutive equations via a minimization of energy: the example of a two-level shear and a generalization

Here we consider a structured deformation $(\emptyset, g, G) \in Std((0,1)^2)$ defined in terms of the Cartesian coordinates (x, y) of a point in the unit square $(0,1)^2$ by the relations

$$g(x,y) = (x+\mu y, y) \tag{3.16}$$

$$G(x,y) = \begin{pmatrix} 1 & \gamma \\ 0 & 1 \end{pmatrix} \tag{3.17}$$

with μ and γ arbitrary real numbers. This deformation is an example of the two-level shears discussed in Section 9.2 of Part I, where we have here put $h = l = 1$, $\mu = \delta/h$, and $\gamma = (1-\alpha)\delta/h$. The determining sequence (κ_m, f_m) shown in Figure 9.3, Part I satisfies the condition s1) in the previous subsection with $\nu = (0,1)$, the unit vector in the y-direction, and the formula

$$\nabla g(x,y) = \begin{pmatrix} 1 & \mu \\ 0 & 1 \end{pmatrix} \tag{3.18}$$

together with (**??**) shows that the condition s2) also is satisfied. Therefore, this two-level shear also illustrates the notion of single slip discussed above, and we may write relation (**??**) in the particular form

$$M(x,y) = \begin{pmatrix} 0 & \mu-\gamma \\ 0 & 0 \end{pmatrix} = (\mu-\gamma, 0) \otimes (0,1). \tag{3.19}$$

Therefore, the slip vector s at each point is the vector $(\mu-\gamma, 0)$. Following the terminology of the previous section, we call the numbers γ and $\mu-\gamma$ the *shear without slip* and the *shear due to (micro)slip*, respectively. Because the mapping g represents the macroscopic shearing of the body, we call the number μ the *macroshear.*

The two scalar constitutive relations that were left unspecified at the end of the previous subsection here should tell us how the macroshear μ is to be distributed between shear without slip γ and shear due to slip $\mu-\gamma$, and we devote the remainder of this subsection to the determination of such relations via energetic arguments. To this end, we specialize the formulas (**??**) and (**??**) for the Helmholtz free energy per unit volume in a general structured deformation to the case of a two-level shear to obtain the relation

$$\Psi(\mu,\gamma) = \varphi(\gamma) + \psi(\mu-\gamma). \tag{3.20}$$

A physical example covered by the present discussion is that of a single crystal undergoing both slip along slip bands and lattice distortion between the slip bands. In this physical context, the term $\varphi(\gamma)$ represents the free energy due to distortion of the lattice, and the term $\psi(\mu - \gamma)$ represents the free energy associated with relative tangential motion along slip bands of the intact portions of the crystal on either side of a slip band. Motivated by these interpretations, we assume that φ is non-negative, smooth and strictly convex, whereas we take ψ to be non-negative, smooth, and periodic. Detailed versions of these mathematical assumptions are presented in [**?**], and it is shown there that the period p of ψ, the free energy density due to slip, is of the order 10^{-4} in many crystals. (See Figures 4 and 5.)

Figure 4: Free energy density due to lattice distortion

Figure 5: Free energy density due to slip

Following the analysis in [?], we seek to relate a given shear stress $\sigma \in \mathbb{R}$ applied on the boundary of the unit square $(0,1)^2$ to the macroshear μ by seeking pairs (μ, γ) that are local minimizers of the Gibbs free energy

$$\mathcal{E}(\mu, \gamma) = \varphi(\gamma) + \psi(\mu - \gamma) - \sigma\mu. \tag{3.21}$$

Thus, we seek pairs (μ, γ) that satisfy not only the stationarity conditions on $\mathcal{E}$

$$\frac{\partial \mathcal{E}}{\partial \mu} = \psi'(\mu - \gamma) - \sigma = 0 \tag{3.22}$$

$$\frac{\partial \mathcal{E}}{\partial \gamma} = \varphi'(\gamma) - \psi'(\mu - \gamma) = 0, \tag{3.23}$$

but also the condition for local minimizers of positive definiteness of the Hessian of $\mathcal{E}$

$$\varphi''(\gamma)\psi''(\mu - \gamma) > 0 \text{ and } \psi''(\mu - \gamma) > 0. \tag{3.24}$$

These relationships among μ, γ and σ are, in the present context, the additional scalar constitutive equations required to complete the system of equilibrium equations and constitutive equations developed in the previous subsection. The pairs (μ, γ) that satisfy (**??**) will be called stationary pairs, and the collection of stationary pairs in the $\mu - \gamma$ plane is illustrated in Figure 6.

Figure 6: Stable and unstable branches of stationary pairs

The stationary pairs that violate the conditions (**??**) for local minimizers form the collection of unstable branches in Figure 6, and these pairs yield values $\mu - \gamma$ of the shear due to slip for which $\psi''(\mu - \gamma) \leq 0$, i.e., they correspond to the concave portions of the graph of the free energy density due to slip in Figure 5. The fact that transition between stable and unstable branches of the stationary locus occurs when $\psi''(\mu - \gamma) = 0$, together with the relation

$$\frac{d\gamma}{d\mu} = \frac{\psi''(\mu - \gamma)}{\varphi''(\gamma) + \psi''(\mu - \gamma)}, \tag{3.25}$$

shows that the transition points between stable and unstable branches occur at points where the tangent line is horizontal (e.g., the points labelled 1- 6 in Figure 6). Consecutive transition points have a horizontal separation equal to p, the period of ψ. Horizontal jumps in the directions shown in Figure 6 between transition points (e.g., $1 \to 2 \to 3$ or $4 \to 5 \to 6$) do not change the Helmholtz free energy density Ψ but do decrease the energy $\mathcal{E}$. Such energetically favorable jumps between stable branches of the stationary locus are compatible with the Second Law of thermodynamics, because the work done is positive while the change in Helmholtz free energy is zero:

$$\sigma\, \Delta\mu > \Delta\Psi. \tag{3.26}$$

The strict inequality in this relation shows that these jumps in μ are dissipative; moreover, their magnitudes are integral multiples of the period $p \approx 10^{-4}$. On the other hand, when the point (μ, γ) moves along a metastable branch of the stationary locus we have

$$\begin{aligned} \int \sigma\, d\mu &= \int \sigma\, d\mu + 0 d\gamma \\ &= \int \psi'(\mu - \gamma)\, d\mu + (\varphi'(\gamma) - \psi'(\mu - \gamma))\, d\gamma \\ &= \int \frac{\partial\Psi}{\partial\mu} d\mu + \frac{\partial\Psi}{\partial\gamma} d\gamma = \Delta\Psi, \end{aligned} \tag{3.27}$$

so that no dissipation occurs. Thus, *smooth changes in $\mu - \gamma$ along metastable branches entail no dissipation, whereas jumps in $\mu - \gamma$ between metastable branches* *are dissipative*. For single crystals, the dissipative mechanism described here can be viewed as an onset of instabilities at a smaller length scale, because the smallest jumps between metastable branches correspond to relative tangential displacements of two portions of the crystal equal to one atomic unit ($\approx 10^{-9}m$). (See [**?**] for details.) The source of this instability is the fact that the tractions $\psi'(\mu-\gamma)$ supplied through microslip cannot exceed $|\max\psi'|$, the maximum of the absolute value of the bounded function ψ'.

A generalization of this method for determining constitutive relations by means of a finite-dimensional minimization problem would read as follows: *given* $S \in Lin\mathcal{V}$, *find* $F, G \in Lin\mathcal{V}^+$ *satisfying the relation* $\det G \leq \det F$ *and for which*

$$\mathcal{E}(F,G) = \Psi(F,G) - S \cdot F \tag{3.28}$$

has a local minimum. Here, we associate the pair (F,G) with $(\nabla g, G)$ for a *homogeneous* structured deformation $(\emptyset, g, G)$, and the number $\Psi(F,G)$ represents the volume density of Helmholtz free energy. For example, the balance relations (**??**) and (**??**) would be augmented by the restriction that at each point x of the body the pair $(\nabla g(x), G(x))$ would be a local minimizer with S replaced by $S(x)$. Such a procedure would yield all candidates for equilibrium configurations of the body corresponding to structured deformations of the specified type.

4 Plasticity

In this section, we indicate some points of contact and contrast between theories of plasticity and our development of structured deformations, and we comment on some issues in plasticity that can be clarified by employing structured deformations. Our discussion covers single slip in crystals, various measures of elastic and plastic deformation in phenomenological theories of plasticity, and the use of structured deformations in the description of crystals with defects.

4.1 Single slip in crystals

In Section 3, we described single slip by specifying a unit vector ν, a structured deformation $(\emptyset, g, G)$, and a vector field $s : \mathcal{A} \to \mathcal{V}$ (the slip) satisfying

$$G^*\nu \cdot s = 0 \text{ and } \nabla g = G + s \otimes \nu. \tag{4.1}$$

Assuming that the unit vector ν is given in advance, one must know $3+9+3+9=24$ scalar fields in order to know g, G, s,and the Piola-Kirchhoff stress S. In the context of the statics of single slip, the balance of forces and moments provide 6 scalar equations in addition to the 10 scalar equations provided by (**??**), leaving $24-16=8$ more unknowns than equations. However, the energetic approach embodied in relation (**??**) yields in this context additional relations required for determining the fields g, G, s,and S, leading us to a field theory of the statics of single slip in crystals. The example of the two-level shear analyzed in Section 3 suggests that, in contrast to the situation in elastostatics, the statics of single slip outlined here will provide a large number of narrowly separated metastable branches of the constitutive relation and, correspondingly, a large number of neighboring solutions of the field equations. The multitude of solutions will be reduced, but not always significantly, through the specification of boundary conditions. This situation is in agreement with the behavior of real crystals in which, for example, a variety of closely neighboring stress-free states are observed. Again, the example of the two-level shear suggests the possibility of identifying admissible jumps between metastable branches of the constitutive relation; these, in turn, should permit one to identify admissible families of equilibrated single-slip fields g, G, s, and S for the crystal corresponding to prescribed families of contact forces and displacements on the boundary of the body.

The present, proposed scenario for using structured deformations to describe geometrical changes in single crystals under prescribed loading programs must be contrasted with the standard modelling of deformations of crystals such as "physically based", phenomenological theories of crystal plasticity. First of all, the proposed use of structured deformations is in its infancy, whereas the standard, physically based models have been developed in much depth. (See, for example, the book of Havner [**?**].) Beyond this obvious remark, the phenomenolgical theories of crystal plasticity employ, in place of the energetic constitutive approach (**??**) proposed here, yield conditions and flow rules that are specially refined and adapted to the description of slip systems in crystals. These "incremental" constitutive relations follow the evolution in time of the internal variables chosen to describe slip and lattice distortion. Flow rules play the role of the evolution equation for internal variables in phenomenological constitutive relations, and they complete the system of balance laws and constitutive relations, often leading to well-posed boundary-value problems. For the proposed analysis of single slip based on structured deformations, the possibilty arises that specification of a family of loads and displacements on complementary portions of the boundary of a crystal together with the specification of an initial structured deformation will select, from the multitude of solutions available at each single stage of loading, a single structured deformation satisfying the balance laws and the energetically-based constitutive relation (**??**) at that stage of the loading. This would correspond to the situation in non-linear elasticity theory: in elastostatics, non-uniqueness of solutions is to be expected, while in elastodynamics, uniqueness of solutions is to be expected. It should be noted nere that direct counterparts for structured deformations of flow rules have yet to be studied, but they could be based on the notion of "structured motion", to be discussed in Section 6.

4.2 Measures of elastic and plastic deformation in phenomenological theories of plasticity

Many phenomenological theories of plasticity, including the "physically based" plasticity theories described in Havner's book [**?**] and the more classical theories of engineering plasticity, share the feature that the total deformation is assumed at the outset to decompose into "elastic" and "plastic" parts. Although sound physical or geometrical motivation for such decompositions sometimes can be provided, these phenomenological theories leave the "elastic" part and the "plastic" part of the deformation as primitive quantities in the theory. Until one formulates and solves a full set of constitutive equations to obtain further information about them, one can only assert that these quantities are intended to capture certain physical aspects of the deformation of single or polycrystalline metals. For example, in polycrystalline metals, the "plastic"deformation often is asserted to be the residual deformation obtained when the forces on a material element are removed in a specified way. In crystalline metals, the "plastic" deformation often is asserted to be deformation of a material element that rearranges through slips small parts of the crystal relative to other parts, without shearing the associated pieces of the crystal. These assertions are rules of interpretation for plastic deformation; plastic deformation remains a primitive quantity in these phenomenological theories. (It is worth noting, however, that one category of phenomenological theories of plasticity, "theories of materials with elastic range", e.g., [**?**], provides a setting in which "elastic" and "plastic" deformations and a decomposition of total deformation need not be specified at the outset. Instead, at the outset, the stress is assumed to depend upon the past history of deformation in such a way that each history determines a set of further deformations inside of which continuations of the history produce a path-independent stress response. Plastic and elastic deformation can then be defined in terms of the given constitutive information about the stress response functional.)

Phenomenological theories of plasticity often contain the additional requirements that "plastic deformation is dissipative" and that "plastic deformation produces no volume change". The first property of plastic deformation usually is imposed as an additional condition, or is deduced from the other constitutive relations together with the second law of thermodynamics; the second is imposed directly as a condition on the quantity in the given phenomenological theory representing plastic deformation.

Structured deformations can provide clarification of the concepts of "elastic" and "plastic" deformation in two ways. The first clarification appears at the outset, before any constitutive relations are assumed, and rests on the fact that the relations (7.6) and (7.7) of Part I permit us for a given structured deformation (κ, g, G) to identify G as the deformation occuring away from sites of slip or separation and to identify $\nabla g - G$ as the volume density of deformation due to slips and separation at smaller length scales. In the context of crystal plasticity, G and $\nabla g - G$ capture the properties asserted of elastic deformation and plastic deformation, respectively; moreover, the macroscopic deformation ∇g immediately relates to these quantities through the decomposition

$$\nabla g = G + (\nabla g - G). \tag{4.2}$$

Thus, choosing the geometrical setting of structured deformations offers at the outset specific and appropriate geometrical quantities that already are identified within the theory and that decompose in a natural way. Moreover, the standard assumption in crystal plasticity, that plastic deformation does not change the volume of the crystal, immediately can be stated here: the volume changes at the macrolevel and the volume changes without disarrangements are the same, i.e.,

$$\det \nabla g = \det G. \tag{4.3}$$

In addition, if one excludes disarrangements at the macrolevel such as macroscopic cracks, then $\kappa = \emptyset$, and (**??**) tells us that $(\emptyset, g, G)$ is an invertible structured deformation (see Figure 4.1 and Excercise 4.1, Part I). For these reasons, *the set of invertible structured deformations is an appropriate starting point for formulating theories of plasticity.*

Although an additive decomposition of deformation gradient is not customary, the validity of (**??**) and the interpretation given here of each term are firmly established within the theory of structured deformation. Nevertheless, the more customary multiplicative decompositions of deformation gradient used in phenomenological plasticity theories do have counterparts for structured deformations:

$$\nabla g = G(G^{-1}\nabla g) \tag{4.4}$$

$$\nabla g = (\nabla g\, G^{-1})G. \tag{4.5}$$

The first relation (**??**) depicts the local macroscopic deformation as the tensor field $G^{-1}\nabla g$ preceding G: first all the disarrangements are introduced and then only deformation without disarrangements occurs. The second relation (**??**) reverses this: first no disarrangements are introduced and then all the disarrangements occur; the local macroscopic deformation is now the tensor field G followed by $\nabla g\, G^{-1}$. Note that the tensor field $(\nabla g)^{-1}G$ already occured in Part I, relation (4.4), where it was shown that an arbitrary structured deformation can be factored into a purely microscopic deformation followed by a simple deformation.

Relation (**??**) is the counterpart for structured deformations of the multiplicative decomposition "$F = F_e F_p$" of Lee & Liu [**?**], whereas (**??**) is the counterpart of the multiplicative decompositon "$F = \bar{F}_p \bar{F}_e$" of Clifton [**?**]. We note that decompositions of Lee & Liu and of Clifton, as introduced by these authors, are not consequences of any geometrical theory such as that of structured deformations, but are part of the constitutive prescription of the material in their theories; similarly, $\bar{F}_p, \bar{F}_e, F_e$, and F_p are primitive quantities in the theories of Lee & Liu and of Clifton and are not directly identifiable within the theories themselves. Consequently, transformation properties of these quantities under change of observer and change of reference configuration have to be supplied as additional conditions consistent with the know transformation properties of F. In contrast, the decompositions (**??**), (**??**), and (**??**) are immediate results within the theory of structured deformations, all of the quantities appearing in them have direct interpretations within that theory, and the discussion in Section 3, Part II yields immediately their transformation properties.

A second clarification provided by structured deformations with respect to choices of "elastic" and "plastic" deformation relates to the remaining requirement mentioned above: "plastic deformation is dissipative". This requirement is not solely geometrical, as were those such as the absence of plastic volume change already treated in this section. In fact, a constitutive structure for the material must be specified in order that the work done in a process can be compared with the change in Helmholtz free energy, thereby to determine whether or not dissipative changes occur. We may illustrate this point by means of the energetic analysis of two-level shears provided in Section 3.3. There, the constitutive structure is specified in the assumed form (**??**) for the Helmholtz free energy, and relations (**??**) and (**??**) determine that dissipation occurs only when the shear due to slip $\mu-\gamma$ changes discontinuously as the point (μ,γ) jumps horizontally from the end of one metastable branch to the end of another. By means of relations (**??**), (**??**), and the assumption that $\psi' \mid_{[-\frac{p}{4},\frac{p}{4}]}$ is invertible, we may write

$$\mu-\gamma=\left(\psi' \mid_{[-\frac{p}{4},\frac{p}{4}]}\right)^{-1}(\sigma)+kp \tag{4.6}$$

for values of the applied shear stress σ satisfying $|\sigma| \leq \max\psi'$ and where k is an integer that can change only when a horizontal jump between metastable branches occurs. Changes in $\mu-\gamma$ that occur when σ varies in the interval $(-\max\psi',\max\psi')$ cause the pair (μ,γ) to vary continuously along a single metastable branch and, according to (**??**), without dissipation. These dissipationless changes give rise to the term $\left(\psi' \mid_{[-\frac{p}{4},\frac{p}{4}]}\right)^{-1}(\sigma)$ in (**??**). The remaining possible changes, when (μ,γ) jumps horizontally from the end of one metastable branch to the end of another, correspond to the values $\sigma=\pm\max\psi'$ and give rise to the term kp. Thus, the shear due to slip is decomposed via (**??**) into a portion that arises without dissipation and a portion that is purely dissipative. The portion of $\mu-\gamma$ arising without dissipation has magnitude no greater than $\frac{1}{4}p$, whereas the portion that is dissipative, kp, is not restricted in magnitude. As we remarked just above Figure 4, the number p in these expressions is of the order 10^{-4}; for typical single crystal specimens, the integer k can be of the order 10^4.

These considerations lead us to define :

$$\text{plastic deformation}: \ =kp=\mu-\gamma-\left(\psi' \mid_{[-\frac{p}{4},\frac{p}{4}]}\right)^{-1}(\sigma). \tag{4.7}$$

(Here, of course, we restrict our attention to a two-level shear (μ, γ) lying on or at an end of a metastable branch). Relations (**??**) and (**??**) permit us to write the plastic deformation in the form

$$kp = \mu - \gamma - \left(\psi' \mid_{[-\frac{p}{4},\frac{p}{4}]}\right)^{-1} (\varphi'(\gamma)), \tag{4.8}$$

so that the plastic deformation is determined completely by the two-level shear. The last term on the right-hand side of (**??**) is bounded above in absolute value by $\frac{p}{4} \approx .25 \times 10^{-4}$, and we may conclude from (**??**) that the shear due to slip $\mu - \gamma$ is a good approximation to the plastic deformation for sizes of strains usually encountered in deformations of single crystals [**?**].

4.3 Lattice basis fields for crystals with defects

Physicists and material scientists have established that geometrical changes in single crystals at length scales on the order of ten atomic units depend upon the presence of defects in the crystalline structure. In this section we describe briefly how structured deformations can be employed to provide as the outcome of an elementary analysis *lattice basis fields* $x \mapsto (e_1(x), e_2(x), e_3(x))$, principal ingredients in continuum theories of crystals with defects.

To this end, we consider a purely microscopic structured deformation $(\emptyset, i, K)$, satisfying the condition $\det K = 1$, and a given orthonormal basis (u_1, u_2, u_3) of $\mathcal{V}$ that will remain fixed throughout this discussion. By the Approximation Lemma, we may choose a sequence $m \mapsto (\kappa_m,\ f_m)$ of piecewise affine, simple deformations converging to $(\emptyset, i, K)$. The invertibility of $\nabla f_m(x)$ for each m and each $x \in A \backslash \kappa_m$ implies that the triple $(\nabla f_m(x)u_1, \nabla f_m(x)u_2, \nabla f_m(x)u_3)$ is a basis of $\mathcal{V}$. For each integer m, because f_m is piecewise affine, its gradient $\nabla f_m(x)$ takes on only finitely many values as x varies through A/κ_m, so that the triples $(\nabla f_m(x)u_1, \nabla f_m(x)u_2, \nabla f_m(x)u_3)$ as x varies through A/κ_m form a finite set of bases of $\mathcal{V}$. We interpret each of these triples of directions as being obtained by connection of a single atom to each of its immediate neighbors in the deformed configuration associated with $(\kappa_m,\ f_m)$. Equivalently, we may regard the triple of directions $(\nabla f_m(x)u_1, \nabla f_m(x)u_2, \nabla f_m(x)u_3)$ as three edges of an atomic cell in the deformed configuration and call $(\nabla f_m(x)u_1,\ \nabla f_m(x)u_2, \nabla f_m(x)u_3)$ a *discrete lattice basis* at x. The nature of the convergence of $m \mapsto (\kappa_m,\ f_m)$ to $(\emptyset, i, K)$

permits us, for each $x \in \mathcal{A}$, to choose a subsequence $m' \mapsto (\kappa_{m'}, f_{m'})$ of $m \mapsto (\kappa_m, f_m)$ such that the pointwise limit $\lim_{m' \to \infty} \nabla f_{m'}(x)$ exists and equals the invertible tensor $K(x)$. Therefore, $(K(x)u_1, K(x)u_2, K(x)u_3)$ is also a basis of $\mathcal{V}$ called the *continuum lattice basis at* x, and $x \mapsto (K(x)u_1, K(x)u_2, K(x)u_3)$ is the desired *lattice basis field* for the purely microscopic deformation $(\emptyset, i, K)$.

Alternatively, one can prove ([11, Part One]): for every $x \in \mathcal{A}$ and $l \in \{1, 2, 3\}$,

$$\lim_{m \to \infty} \frac{\int\limits_{\mathcal{B}(x,1/m) \cap \mathcal{A}} \nabla f_m(y) u_l dV_y}{vol(\mathcal{B}(x, 1/m) \cap \mathcal{A})} = K(x)u_l,$$

i.e., *the continuum lattice basis at* x, $(K(x)u_1, K(x)u_2, K(x)u_3)$, *is a limit of averages of discrete lattice bases.* Here, $\mathcal{B}(x, 1/m)$ is the ball centered at x of radius $1/m$. The italicized statement, which is a proven result for structured deformations, is given without proof as a "rule of interpretation" in other continuum theories of crystals with defects.

Another useful feature of structured deformations as a basis for describing crystals with defects arises from the compositional factorization

$$(\emptyset, f, \nabla f) = (\emptyset, f, I) \circ (\emptyset, i, \nabla f), \tag{4.9}$$

valid for every classical deformation f, viewed as the structured deformation $(\emptyset, f, \nabla f)$, for which $\det \nabla f = 1$. The factor $(\emptyset, f, I)$ can be approximated by piecewise-affine deformations each of whose gradients is close to the identity I, so that the macroscopic transplacement f can be viewed as being accomplished by breaking the body into pieces and translating the pieces relative to one another without interpenetration, with a limit then taken as the number of pieces goes to infinity and the sizes go to zero. In the study of crystals with defects [**?**], such a deformation is called a *rearrangement.* When $\nabla f \neq \nabla i = I$, the second factor $(\emptyset, i, \nabla f)$ in (**??**) is such that the deformation due to disarrangements $M = \nabla f - \nabla i = \nabla f - I$, although non-zero, is the gradient of $f - i$. Therefore, the Burgers vector $\int_c M(x)dx = \int_c \nabla(f - i)(x)dx$ vanishes for every smooth, closed curve c in the region $\mathcal{A}$. This situation is described by saying that the purely microscopic deformation $(\emptyset, i, \nabla f)$ introduces no new defects in a crystal. Measures of defectiveness for crystals are defined and a characterization of changes of state that preserve defects is established in the article [**?**]. Our structured deformations of the form $(\emptyset, i, \nabla f)$, with $\det \nabla f = 1$, correspond to a special class of "neutral deformations" in [?].

5 Internal Friction, Liquid Crystals, and Mixtures

The continuum modelling of materials exhibiting internal friction, of liquid crystals, and of intermingling constituents in mixtures form three major areas of continuum mechanics. In this section, we indicate how structured deformations can contribute to these areas. The ideas chosen for presentation here may serve to reinforce the notion that the language of structured deformations is meaningful and useful in a variety of applications as well as to illustrate further some of the methodologies presented in previous sections.

5.1 Internal friction

Materials such as soils exhibit internal friction caused by the interactions of tiny particles that comprise the material. Our goal here is to show that an energetic analysis of a class of structured deformations called "translation-induced shear/dilatations" [?] leads directly to a macroscopic material response that can be identified with Coulumb friction.

5.1.1 Translation-induced shear/dilatations

To specify a translation-induced shear/dilatation, we need only specify a continuously differentiable, even, periodic function $w : \mathbb{R} \to \mathbb{R}$ with period p. The function w is intended to describe the shapes of rigid pieces of a body that are visible in a magnifying glass or microscope. In terms of w we define a second, even, p-periodic function θ through the relation

$$\theta(s) := w(\frac{p}{4} + \frac{s}{2}) - w(\frac{p}{4} - \frac{s}{2}) \text{ for } s \in [0, \frac{p}{2}]. \tag{5.1}$$

Figure 7: Wave and separation functions

We call w the wave function and θ the separation function. Let us imagine that the $s-w$ plane in Figure 7 is cut into two pieces along the graph of the wave function w, and the two pieces undergo a relative horizontal translation and a relative vertical translation. The non-negative number $\theta(s)$ is then the magnitude of the relative vertical translation needed if the magnitude of the relative horizontal translation is s and if the pieces are required to be touching but not interpenetrating after the two translations. We note that the smoothness of the wave function need not be preserved in the separation function at the points $s = kp$, with k an integer, where θ' can jump by an amount $2w'(\frac{p}{4})$, as shown in Figure 7. A translation-induced shear/dilatation can now be specified in terms of the separation function θ by giving a positive number s and defining

$$g(x, y) := (x + sy, y + \theta(s)y), \quad G(x, y) := \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{5.2}$$

for each (x, y) in the unit square $[0, 1] \times [0, 1]$. It is evident that the triple $(\emptyset, g, G)$ is a structured deformation and that the deformation due to microdisarrangements M is given by

$$M(x, y) := \nabla g(x, y) - G(x, y) = \begin{bmatrix} 0 & s \\ 0 & \theta(s) \end{bmatrix}. \tag{5.3}$$

Figure 8: Macroview of a translation-induced shear/dilatation

As indicated in Figure 8, the transplacement g maps the unit square into a parallelogram via a shear of amount s and an increase in vertical height of amount $\theta(s) \times 1$ unit of length. The fact that $G(x, y)$ is the identity at every point indicates that the shearing and increase in volume at the macrolevel are induced by translations alone at the microlevel. This indication is confirmed by the fact that a determining sequence for the translation-induced shear/dilatation can be found in which the transplacements f_m are given by

$$f_m(x, y) = (x, y) + \frac{\lfloor (my - w(mx))}{m}(s, \theta(s)). \tag{5.4}$$

Here, the symbol $\lfloor$ denotes the greatest integer function, so that the factor multiplying the pair $(s, \theta(s))$ is a piecewise constant function of x and y. Hence, relation (**??**) shows that f_m differs from the identity map by a step function that describes translations in the direction $(s, \theta(s))$ of wavy regions as shown in Figure 9.

Figure 9: Microview of a translation-induced shear/dilation

Each pair of adjacent wavy regions translate relative to one another by $(s, \theta(s))/m$ but remain in contact after the translation. This fact justifies the term "translation-induced" as an indicator of the geometrical mechanism at a smaller length scale that produces the macroscopic shear and dilatation of the body.

5.1.2 Macroscopic response to translation-induced shear/dilatations

We follow the ideas in Section 3.3 for deducing properties of the macroscopic response of a body undergoing particular structured deformations by seeking local minima of the total energy assigned to the structured deformations. Here, the considerations are simplified by the following assumption: the relative translations of the wavy rigid pieces appearing at a smaller length scale (see Figure 9) do not change the Helmholtz free energy of the body. Because the pieces are assumed to be rigid, we may assume that the Helmholtz free energy density in the body is constant (which we take to be zero). These assumptions lead us to the following minimization problem: *given constant normal and tangential tractions* $-N$ *and* F (measured in force per unit length) *acting on the top of the unit square, determine the macroscopic shear* s *so that the Gibbs free energy*

$$\mathcal{E}_{F,N}\left(s\right) := N\theta(s) - Fs \tag{5.5}$$

for the shear induced dilatation $(\emptyset, g, I)$ *in* (**??**) *has a local minimum.* The right-hand side of (**??**) represents the work done (per unit area) by the material in the unit square on its environment during the transplacement g. According to our assumptions above, the Helmholtz free energy does not contribute to the right-hand side of (**??**).

Figure 10: Energy versus F and s

Figure 10 displays the graph of $\mathcal{E}_{F,N}\left(s\right)$ (vertical axis in page) versus F (out of page axis) and s (horizontal axis in page) for a fixed positive value of N. In that figure we note that when F is zero, the graph of the energy is the same as the graph of $s \mapsto N\theta(s)$ with local minima occuring when the amount of macroshear s is an integral multiple of the period p of the separation function θ. These local minima correspond to corners on the graph that are bisected by the vertical direction, and they represent values of the macroshear for which the corresponding translation-induced shear/dilatation is metastable. When the tangential force F is fixed at a positive but sufficiently small value, subtraction of the linear function $s \mapsto Fs$ from $s \mapsto N\theta(s)$ preserves the location of the local minima but tilts the graph downward so that the corners are no longer bisected by the vertical. When F is fixed at the value $Nw'(\frac{p}{4})$, the graph is tilted just enough that the local minima at $s = kp$, with k an integer, all disappear, because one leg of each corner becomes becomes horizontal; when F is fixed at a value greater than $Nw'(\frac{p}{4})$, the absence of local minima persists. Thus, the number $w'(\frac{p}{4})$ represents a critical value for $\frac{F}{N}$: it is the least upper bound for the set of ratios $\frac{F}{N}$ for which metastable values of the macroshear s for translation-induced shear/dilatations exist. A similar analysis when F is negative shows that $-w'(\frac{p}{4})$ is the greatest lower bound for the set of values $\frac{F}{N}$ for which metastable values translation-induced shear/dilatations exist. Thus, we have the result:

- If $0 \leq \left|\frac{F}{N}\right| < w'(\frac{p}{4})$, then $\mathcal{E}_{F,N}$ has a local minimum at $s = 0, \pm p, \pm 2p, \cdots$.
- If $w'(\frac{p}{4}) \leq \left|\frac{F}{N}\right|$, then $\mathcal{E}_{F,N}$ has no local minima.

We call a pair $(s, \frac{F}{N})$ a *metastable state for translation-induced shear/dilatations* if $\mathcal{E}_{F,N}$ has a local minimum at $s = 0, \pm p, \pm 2p, \cdots$. The result just established describes all of the metastable states $(s, \frac{F}{N})$, and these pairs are displayed in Figure 11.

Figure 11: Metastable states

As the figure illustrates, when s is fixed at an integral multiple of the period p of the separation function, the ratio $\frac{F}{N}$ can be increased from 0 to $w'(\frac{p}{4})$ and the state $(s, \frac{F}{N})$ remains metastable until $\frac{F}{N} = w'(\frac{p}{4})$. At that value of the ratio, s may jump to *larger* integral multiples of p while lowering the energy $\mathcal{E}_{F,N}$, and the decrease in energy represents the amount of dissipation in the jump. Similarly, $\frac{F}{N}$ can be decreased from 0 to $-w'(\frac{p}{4})$ and the state $(s, \frac{F}{N})$ remains metastable untill $\frac{F}{N} = -w'(\frac{p}{4})$. At that value of the ratio, s may jump to *smaller* integral multiples of p while lowering the energy $\mathcal{E}_{F,N}$, and the decrease in energy represents the amount of dissipation in the jump. When the state lies on one of the vertical line segments in Figure 11, the rigid wavy pieces comprising the body are "locked" in a configuration corresponding to the given amount of shear $s = kp$. If $\frac{F}{N}$ is increased to $w'(\frac{p}{4})$ or decreased to $-w'(\frac{p}{4})$, the pieces may "unlock" and s may in the first case jump to a larger multiple of p and in the second case jump to a smaller value, corresponding to the wavy pieces sliding relative to one another in one direction. Thus, we may say that the macroscopic response of the body exhibits internal friction due to the occurence of material instabilities at a smaller length scale.

5.2 Liquid Crystals

Many liquid crystals consist of nearly rigid, rod-like molecules that tend to align within small regions of the liquid crystal and whose alignment can be influenced by the environment. Continuum theories replace the large number of small, nearly linear molecules by a "director field" n whose value $n(x)$ at a point x is a unit vector that is interpreted to be the average of the orientations of molecules near x. In addition, the global state of the liquid crystal is delimited further by providing a scalar field S whose value $S(x)$, called the "degree of orientation at x," is interpreted to be the deviation of the orientations of molecules near x from the orientation associated with the unit vector $n(x)$.

To identify the director field n for a liquid crystal in the context of a body undergoing a structured deformation, we let $(\emptyset, i, K) \in Std(\mathcal{A})$ be a purely microscopic structured deformation and let $k \in \mathcal{V}$ be a unit vector. We assume that for each $x \in \mathcal{A}$ that $K(x)$ is an orthogonal tensor, so that $K(x)k$ also is a unit vector. We propose the definition $n(x) := K(x)k$ for the director at x in the given structured deformation, and we may use the Approximation Theorem to justify this definition. In fact, by the Approximation Lemma, we may chose a sequence $m \mapsto (\kappa_m, f_m)$ of piecewise affine simple deformations that converge to $(\emptyset, i, K)$. Thus, for each $x \in \mathcal{A} \backslash \kappa_m$ and $m \in \mathbb{N}$, $\nabla f_m(x)$ approximately is an orthogonal tensor, so that $\nabla f_m(x)k$ approximately is a unit vector. Moreover, because f_m is piecewise affine, $\{\nabla f_m(x)k \mid x \in \mathcal{A} \backslash \kappa_m\}$ is a finite set of vectors, each with magnitude approximately one. We interpret each of the the approximately rigid deformations $(f_m)_j := f_m \mid_{\mathcal{A}_j}$, $j \in \{1, \cdots, J_m\}$ (with the sets $\mathcal{A}_j$ fit regions on each of which ∇f_m is constant) as taking a molecule with orientation k into the same molecule with new orientation $\nabla(f_m)_j k$. Because $m \mapsto \nabla f_m$ converges to K, $\nabla f_m k$ converges to Kk. More precisely, for each $x \in \mathcal{A}$ there is a subsequence $m' \mapsto (\kappa_{m'}, f_{m'})$ such that

$$\lim_{m' \to \infty} \nabla f_{m'}(x)k = K(x)k.$$

The next result, whose proof can be found in ([11, Part One]), gives a precise sense in which the director field $n := Kk$ represents a limit of the average orientations of molecules.

Proposition 5.1 *:Let a unit vector $k \in \mathcal{V}$ and $(\emptyset, i, K) \in Std(\mathcal{A})$ be given with K orthogonal valued. For each $x \in \mathcal{A}$ and $m \mapsto (\kappa_m, f_m)$ converging to $(\emptyset, i, K)$*

$$n(x) = \lim_{j \to \infty} \frac{\int_{\mathcal{B}(x, \frac{1}{j+1}) \cap \mathcal{A}} \nabla f_j(y)k \, dV_y}{vol(\mathcal{B}(x, \frac{1}{j+1}) \cap \mathcal{A})}. \tag{5.6}$$

In descriptions of nematic liquid crystals one finds a measure of deviation of molecular orientations from the director $n(x)$ that corresponds here to the quantity

$$S(x) := \lim_{m \to \infty} \frac{3}{2} \left[\frac{\int_{\mathcal{B}(x, \frac{1}{j+1}) \cap \mathcal{A}} (n(x) \cdot \nabla f_j(y)k)^2 \, dV_y}{vol(\mathcal{B}(x, \frac{1}{j+1}) \cap \mathcal{A})} - \frac{1}{3} \right].$$

The inner product $n(x) \cdot \nabla f_j(y)k$ measures the angular deviation from $n(x)$ of a molecule containing the point y. It is easy to prove from the convergence of ∇f_m to K that $S(x) = 1$ for all $x \in \mathcal{A}$, a relation that describes the so-called "completely oriented" nematic phase. Thus, the strong convergence of ∇f_m to K limits the deviation of $\nabla f_m(y)k$ from $n(x)$ for points y near x. To obtain values of S different from 1 one would have to weaken the type of convergence as, for example, was done by Choksi & Fonseca [?] (not in the context of liquid crystals).

5.3 Mixtures

We begin with a useful example described in non-mathematical terms. Take a deck with $2n$ cards, cut it at the n^{th} card from the bottom, including that card with the bottom half, and then shuffle the deck by alternating cards from the top and bottom half. If we count the $2n-1$ interfaces as the set κ_{2n}, then we obtain a simple deformation $(\kappa_{2n},\ f_{2n})$. The cards in the top and bottom halves intermingle but do not interpenetrate as a result of the shuffling deformation $(\kappa_{2n},\ f_{2n})$. It is also useful to consider the effect of $f_{2n}\mid_{\mathcal{T}\backslash\kappa_{2n}}$ and $f_{2n}\mid_{\mathcal{B}\backslash\kappa_{2n}}$, where $\mathcal{T}$ and $\mathcal{B}$ denote the top and the bottom (open) halves, respectively, of the deck before shuffling. The first mapping $f_{2n}\mid_{\mathcal{T}\backslash\kappa_{2n}}$takes the cards in the top half and separates each adjacent pair by enough space to insert a card from the bottom half between them, while the second mapping $f_{2n}\mid_{\mathcal{B}\backslash\kappa_{2n}}$does the same for the bottom half. We note that the surface $\mathcal{C}$ at which the deck is cut in two is the same for every n, and the following observations are easy to verify:

1. $(\kappa_{2n}\cap\mathcal{T}\ ,\ f_{2n}\mid_{\mathcal{T}\backslash\kappa_{2n}})\in Sid(\mathcal{T})$ for every n and the sequence $n\mapsto(\kappa_{2n}\cap\mathcal{T}\ ,\ f_{2n}\mid_{\mathcal{T}\backslash\kappa_{2n}})$ converges to the structured deformation $(\emptyset,g_{\mathcal{T}},I)\in Std(\mathcal{T})$, where $g_{\mathcal{T}}$ is a homogeneous deformation that maps the top half $\mathcal{T}$ onto the entire deck $int(clo(\mathcal{B}\cup\mathcal{T}))$.

2. $(\kappa_{2n}\cap\mathcal{B}\ ,\ f_{2n}\mid_{\mathcal{B}\backslash\kappa_{2n}})\in Sid(\mathcal{B})$ for every n and the sequence $n\mapsto(\kappa_{2n}\cap\mathcal{B}\ ,\ f_{2n}\mid_{\mathcal{B}\backslash\kappa_{2n}})$ converges to the structured deformation $(\emptyset,g_{\mathcal{B}},I)\in Std(\mathcal{B})$, where $g_{\mathcal{B}}$ is a homogeneous deformation that maps the bottom half $\mathcal{B}$ onto the entire deck $int(clo(\mathcal{B}\cup\mathcal{T}))$.

3. The volume fraction $y\mapsto\varphi(y):=\det G(g^{-1}(y))/\det\nabla g(g^{-1}(y))$ for a general, structured deformation (κ,g,G) reduces to the constant function $x\mapsto\frac{1}{2}$ for both $(\emptyset,g_{\mathcal{T}},I)$ and $(\emptyset,g_{\mathcal{B}},I)$.

4. The sequence of simple deformations $n\mapsto(\kappa_{2n},\ f_{2n})\in Sid(int(clo(\mathcal{B}\cup\mathcal{T})))$ converges to the limit of simple deformations $(C,g,I)\in LimSid(int(clo(\mathcal{B}\cup\mathcal{T})))$, where $g:\mathcal{B}\cup\mathcal{T}\to\mathcal{E}$ is defined by the relations $g\mid_{\mathcal{T}}:=g_{\mathcal{T}}$ and $g\mid_{\mathcal{B}}:=g_{\mathcal{B}}$.

5. $(C,g,I)\in LimSid\backslash\ Std$.

In item 5, $(C, g, I) \notin Std$ because g is not injective. In fact, g maps each half of the deck onto the entire deck: $g(\mathcal{T}) = g(\mathcal{B}) = int(clo(\mathcal{B} \cup \mathcal{T}))$. The non-injectivity of g tells us that the two regions $\mathcal{T}$ and $\mathcal{B}$ interpenetrate under the action of the transplacement g . However, each approximating simple deformation $(\kappa_{2n},\ f_{2n})$ is such that f_{2n} is injective, so that the top and bottom halves of the deck do not interpenetrate, but rather intermingle under the action of f_{2n}. Motivated by this example, we make the following definition:

Definition 5.1 *Let a piecewise fit region $\mathcal{A}$ and $(\kappa, g, G) \in \mathrm{LimSid}(\mathcal{A})$ be given. The triple (κ, g, G) is called a mixing deformation from $\mathcal{A}$, and we write $(\kappa, g, G) \in Mix(\mathcal{A})$, if there exists a finite collection $\{\mathcal{C}_j \mid j \in \{1, \cdots, n\}\}$ of pairwise disjoint, piecewise fit regions such that*

1. $\mathcal{A} \backslash \kappa = \bigcup_{j=1}^{n} \mathcal{C}_j$;
2. *for each* $j \in \{1, \cdots, n\}$, $(\emptyset, g\mid_{\mathcal{C}_j}, G\mid_{\mathcal{C}_j}) \in Std(\mathcal{C}_j)$.

If we put $g_j := g\mid_{\mathcal{C}_j}$ and $G_j := G\mid_{\mathcal{C}_j}$, then we call $(\emptyset, g_j, G_j)$ the *deformation of the j^{th} constituent of the mixture*, and, because $(\emptyset, g_j, G_j)$ is a structured deformation from $\mathcal{C}_j$, we may speak of its *volume fraction* $\varphi_j : g(\mathcal{A}\backslash\kappa) \to \mathbb{R}$ defined by

$$\varphi_j(y) := \begin{cases} 0 & if \quad y \notin g(\mathcal{C}_j) \\ \frac{\det G_j\,(g_j^{-1}(y))}{\det \nabla g_j\,(g_j^{-1}(y))} & if \quad y \in g(\mathcal{C}_j) \end{cases} \tag{5.7}$$

We may also treat each piecewise fit region $\mathcal{C}_j$ as the virgin configuration, identify a Piola-Kirchhoff stress field $S_j : \mathcal{C}_j \to Lin\mathcal{V}$, a body force field $b_j : \mathcal{C}_j \to \mathcal{V}$, and, following the analysis in Section 1, write down the *balance of forces and moments for the j^{th} constituent in its virgin configuration*:

$$\begin{aligned} div(S_j K_j^*) - S_j div K_j^* + \nabla S_j\,[\varphi_j \circ g_j I - K_j^*] + \rho_j b_j &= 0 & (5.8)\\ Sk(S_j K_j^* \nabla g_j^T) + Sk(S_j(\varphi_j \circ g_j I - K_j^*)\nabla g_j^T) &= 0. & (5.9)\end{aligned}$$

We call the term $div(S_j K_j^*)$ the *volume density in the j^{th} constituent of the contact forces without dispersion,* because the internal surfaces in the jth constituent, across which voids are formed in placing that constituent in the mixture, do not contribute to $div(S_j K_j^*)$ (see the interpetation of the identification relations in Section 1.2). Similarly, we may call the terms $-S_j div K_j^* + \nabla S_j\,[\varphi_j \circ g_j I - K_j^*]$ the *volume density in the* j^{th} *constituent of the contact forces due to dispersion.* These terms reflect the separation of pieces of the jth constituent and the accompanying formation of voids that occur in the purely microscopic deformation $(\emptyset, i, K_j)$, with $K_j := (\nabla g_j)^{-1} G_j$.

6 Structured Motions

The preceding sections focused on the goal of prescribing and analyzing a geometrical setting broad enough to describe deformations at more than one length scale. In this section we broaden that goal to include prescribing motions that occur at more than one length scale. Thus, we wish to be able to study kinematics at multiple length scales and, for example, to assign meanings to such terms as "velocity due to slip", "velocity without slip", "velocity due to dispersion", and "velocity without dispersion". Generally speaking, we wish to be able to distinguish between non–smooth kinematical changes at smaller lengths scales and smooth kinematical changes at smaller length scales.

6.1 Four-dimensional, "space-time" structured deformations

Let $\mathcal{E}$ and $\mathcal{V}$ denote a three-dimensional Euclidean point space and its translation space, respectively, and put $\mathcal{E}^{(4)} := \mathcal{E} \times \mathbb{R}$ and $\mathcal{V}^{(4)} := \mathcal{V} \times \mathbb{R}$. The objects $\mathcal{E}^{(4)}$ and $\mathcal{V}^{(4)}$ then define a four-dimensional Euclidean point space that we view as describing non-relativistic, "space-time". Because our study of structured deformations is applicable in any finite-dimensional Euclidean point space, we may consider for each piecewise fit region $\mathcal{A} \subset \mathcal{E}$ and each $T > 0$ the piecewise fit region $\mathcal{A} \times (0,T) \subset \mathcal{E}^{(4)}$ and let $(\kappa^{(4)}, g^{(4)}, G^{(4)}) \in Std(\mathcal{A} \times (0,T))$ be given. We call $(\kappa^{(4)}, g^{(4)}, G^{(4)})$ a space-time structured deformation, and we note that the pair $(\kappa^{(4)}, g^{(4)}) \in Sid(\mathcal{A} \times (0,T))$ is a simple deformation. Moreover, $G^{(4)} : \mathcal{A} \times (0,T) \backslash \kappa^{(4)} \to Lin\mathcal{V}^{(4)}$ is a tensor field, so that each of its values

$G^{(4)}(x,t)$ for $(x,t) \in \mathcal{A} \times (0,T)$ has the block form

$$G^{(4)}(x,t) = \left[\begin{array}{cc} G^{11}(x,t) & G^{12}(x,t) \\ G^{21}(x,t) & G^{22}(x,t) \end{array} \right] \in Lin\mathcal{V}^{(4)} \tag{6.1}$$

with

$$\begin{array}{rcl} G^{11}(x,t) & \in & Lin\mathcal{V}, \quad G^{12}(x,t) \in Lin(\mathbb{R},\mathcal{V}) \approx \mathcal{V} \\ G^{21}(x,t) & \in & Lin(\mathcal{V},\mathbb{R}) \approx \mathcal{V}, \quad G^{22}(x,t) \in Lin(\mathbb{R},\mathbb{R}) \approx \mathbb{R}. \end{array} \tag{6.2}$$

Similarly, $\nabla^{(4)}g^{(4)}$, the gradient of the transplacement $g^{(4)} = (g,\tau) : \mathcal{A} \times (0,T) \rightarrow \mathcal{E}^{(4)}$, gives rise to the block form

$$\nabla^{(4)}g^{(4)}(x,t) = \left[\begin{array}{cc} \nabla g(x,t) & \dot{g}(x,t) \\ \nabla \tau(x,t) & \dot{\tau}(x,t) \end{array} \right] \in Lin\mathcal{V}^{(4)} \tag{6.3}$$

with

$$\begin{array}{rcl} \nabla g(x,t) & \in & Lin\mathcal{V}, \quad \dot{g}(x,t) \in Lin(\mathbb{R},\mathcal{V}) \approx \mathcal{V} \\ \nabla \tau(x,t) & \in & Lin(\mathcal{V},\mathbb{R}) \approx \mathcal{V}, \quad \dot{\tau}(x,t) \in Lin(\mathbb{R},\mathbb{R}) \approx \mathbb{R}. \end{array} \tag{6.4}$$

Of course, the Approximation Theorem can be applied to obtain a sequence of "space-time" simple deformations that converges to the space-time structured deformation $(\kappa^{(4)}, g^{(4)}, G^{(4)})$. Henceforth, the symbol "∇" denotes differentiation with respect to the spatial variable "x", and the superimposed "$\cdot$" denotes differentiation with respect to the time variable "t".

We do not pursue the details of the theory of "space-time" structured deformations, because of one shortcoming of this setting: in general, the time-coordinate $\tau(x,t)$ of the transplacement value $g^{(4)}(x,t)$ does not equal t. In other words, "time-travel" can occur through a space-time structured deformation. This is a shortcoming, because it makes it possible for a body occupying the reference configuration $\mathcal{A}$ to disappear during an interval of time and then reappear. Therefore, we shall develop our kinematical ideas by assuming the relation

$$\tau(x,t) = t \quad \text{for all } (x,t) \in \mathcal{A} \times (0,T). \tag{6.5}$$

This assumption leads us to notions of "classical motion", "simple motion", and "structured motion" as described in the next subsections.

6.2 Classical motions

We call a mapping $\chi : \mathcal{A}\times(0,T) \to \mathcal{E}$ a *classical motion* of the fit region $\mathcal{A}$ during the time interval $(0,T)$, and write $\chi \in Clm(\mathcal{A}\times(0,T))$, if the mapping

$$(x,t) \mapsto \mathsf{t}_\chi(x,t) := (\chi(x,t),t) \tag{6.6}$$

defines a "space-time" classical deformation, i.e., if $\mathsf{t}_\chi \in Cld(\mathcal{A}\times(0,T))$. We call t_χ the *trajectory mapping* for the classical motion χ. For example, if $e \in \mathcal{V}$ is a given vector, we put

$$\chi_e(x,t) := x + te \tag{6.7}$$

and obtain the *uniform translation* χ_e as an instance of a classical motion. Here, the corresponding trajectory mapping t_{χ_e} is given by $\mathsf{t}_{\chi_e}(x,t) = (x,0) + t(e,1) = (x+te,t)$.

The following properties of classical motions follow easily from this definition and from the block forms in (**??**) and (**??**):

- Clm1: For all $\chi \in Clm(\mathcal{A}\times(0,T))$ and $t \in (0,T)$, $\chi(\cdot,t)$ is injective.
- Clm2: For all $\chi \in Clm(\mathcal{A}\times(0,T))$ and $(x,t) \in \mathcal{A}\times(0,T)$,

$$\begin{aligned}\nabla^{(4)}\mathsf{t}_\chi(x,t) &= \begin{bmatrix} \nabla\chi(x,t) & \dot\chi(x,t) \\ 0 & 1 \end{bmatrix} \\ \nabla^{(4)}\mathsf{t}_\chi^{-1}(\chi(x,t),t) &= \nabla^{(4)}\mathsf{t}_\chi(x,t)^{-1} = \begin{bmatrix} \nabla\chi(x,t)^{-1} & -\nabla\chi(x,t)^{-1}\dot\chi(x,t) \\ 0 & 1 \end{bmatrix}.\end{aligned}$$

- Clm3: For all $\chi \in Clm(\mathcal{A}\times(0,T))$, $\det\nabla\chi = \det^{(4)}(\nabla^{(4)}\mathsf{t}_\chi)$.

6.3 Simple motions

Let a subset $\kappa^{(4)}$of $\mathcal{A}\times(0,T)$ and $\chi : (\mathcal{A}\times(0,T))\backslash\kappa^{(4)} \to \mathcal{E}$ be given. We call the pair $(\kappa^{(4)},\chi)$ a *simple motion* of the piecewise fit region $\mathcal{A}$ during the time interval $(0,T)$ if the pair $(\kappa^{(4)},\mathsf{t}_\chi)$, with t_χ the trajectory mapping defined in (**??**), is a "space-time " simple deformation, i.e., if $(\kappa^{(4)},\mathsf{t}_\chi) \in Sid(\mathcal{A}\times(0,T))$.

Example ("blinking motion"): Let $m \in \{1,2,3,\cdots\}$, $e \in \mathcal{V}$, $t \in (0,1)$, and let $\lfloor(mt)$ denote the greatest integer less than or equal to mt. We define

$$\begin{aligned} \chi_m(x,t) &: = x + \frac{\lfloor(mt)}{m} e \text{ for } (x,t) \in (\mathcal{A} \times (0,1)) \backslash \kappa_m^{(4)} \\ \kappa_m^{(4)} &: = \left\{ (x, \frac{k}{m}) \mid x \in \mathcal{A},\ k \in \{1,2,\cdots,m-1\} \right\}. \end{aligned} \tag{6.8}$$

In this simple motion, the points of the region $\mathcal{A}$ do not move during the time interval $(0, \frac{1}{m})$, but they suddenly all move at time $\frac{1}{m}$ to gain a displacement $\frac{1}{m}e$. The points again remain static during the interval $(\frac{1}{m}, \frac{2}{m})$ and suddenly displace at time $\frac{2}{m}$, again by amount $\frac{1}{m}e$, and so on. Thus, if one happened to blink at each of the times $\frac{1}{m}, \frac{2}{m}, \cdots, \frac{m-1}{m}$, one would not observe any motion. Nevertheless, at the end of the time interval $(0,1)$, the region would have displaced by an amount $\frac{m-1}{m}e$. Note that we have

$$\nabla^{(4)} \mathsf{t}_{\chi_m}(x,t) = \left[\begin{array}{cc} I & 0 \\ 0 & 1 \end{array} \right] =: I^{(4)}$$

for all $(x,t) \in (\mathcal{A} \times (0,1)) \backslash \kappa_m^{(4)}$; this relation reflects the fact that in this example movement only occurs at a finite set of times and distances between points in the body never change.

We write $Sim(\mathcal{A} \times (0,T))$ for the collection of simple motions $(\kappa^{(4)}, \chi)$ of $\mathcal{A}$ during $(0,T)$.

6.4 Structured motions

Let a simple motion $(\kappa^{(4)}, \chi) \in$S$im(\mathcal{A} \times (0,T))$ be given, and let $G : \mathcal{A} \times (0,T) \to Lin\mathcal{V}$ and $w : \mathcal{A} \times (0,T) \to \mathcal{V}$ be given tensor-valued and vector-valued functions of position and time. We say that the array $(\kappa^{(4)}, \chi, G, w)$ is a *structured motion*, and we write $(\kappa^{(4)}, \chi, G, w) \in Stm(\mathcal{A} \times (0,T))$, if
$(\kappa^{(4)}, \mathsf{t}_\chi, \left[\begin{array}{cc} G & w \\ 0 & 1 \end{array} \right]) \in Std(\mathcal{A} \times (0,T))$, i.e., if the triple $(\kappa^{(4)}, \mathsf{t}_\chi, \left[\begin{array}{cc} G & w \\ 0 & 1 \end{array} \right])$ is a "space-time" structured deformation. This last condition implies that
$\det \nabla^{(4)} \mathsf{t}_{\chi_m}(x,t) \geq \det \left[\begin{array}{cc} G & w \\ 0 & 1 \end{array} \right]$,and, by a formula in Clm2, this condition is

equivalent to the inequality $\det \nabla\chi \geq \det G$, corresponding to the inequality $\det \nabla g \geq \det G$ in the definition of structured deformations.

We note that the mapping $\chi \mapsto (\emptyset, \chi)$ imbeds $Clm(\mathcal{A} \times (0,T))$ into $Sim(\mathcal{A} \times (0,T))$, while the mapping $(\kappa^{(4)}, \chi) \mapsto (\kappa^{(4)}, \chi, \nabla\chi, \dot{\chi})$ imbeds $Sim(\mathcal{A}\times(0,T))$ into $Stm(\mathcal{A}\times(0,T))$. Thus, both classical motions and simple motions may be regarded as structured motions. For example, for each $e \in \mathcal{V}$, the uniform translation χ_e is a classical motion, so that

$$(\emptyset, \chi_e, \nabla\chi_e, \dot{\chi}_e) = (\emptyset, \chi_e, I, e) \in \; Stm(\mathcal{A} \times (0,T)).$$

We note also that for each non-zero vector e there holds $(\emptyset, \chi_e, I, 0) \in Stm(\mathcal{A}\times(0,T)) \setminus Clm(\mathcal{A}\times(0,T))$, i.e., by replacing the non-zero vector e in the last component of $(\emptyset, \chi_e, I, e)$ by the zero vector we obtain a non-classical structured motion.

In the next two sections we develop a version of the Approximation Theorem that permits us to give a useful interpretation to both G and w for a general structured motion $(\kappa^{(4)}, \chi, G, w)$.

6.5 Factorizations and the Approximation Theorem

One can factor structured motions $(\kappa^{(4)}, \chi, G, w)$ first by factoring the associated "space-time" structured deformation

$$\begin{aligned}
(\kappa^{(4)}, \mathsf{t}_\chi, \begin{bmatrix} G & w \\ 0 & 1 \end{bmatrix}) &= (\emptyset, \mathsf{t}_\chi, \begin{bmatrix} \nabla\chi & \dot{\chi} \\ 0 & 1 \end{bmatrix}) \circ (\kappa^{(4)}, i^{(4)}, \begin{bmatrix} \nabla\chi & \dot{\chi} \\ 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} G & w \\ 0 & 1 \end{bmatrix}) \\
&= (\emptyset, \mathsf{t}_\chi, \begin{bmatrix} \nabla\chi & \dot{\chi} \\ 0 & 1 \end{bmatrix}) \circ (\kappa^{(4)}, i^{(4)}, \begin{bmatrix} \nabla\chi^{-1} & -\nabla\chi^{-1}\dot{\chi} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} G & w \\ 0 & 1 \end{bmatrix})
\end{aligned}$$

$$= (\emptyset, \mathsf{t}_\chi, \begin{bmatrix} \nabla\chi & \dot{\chi} \\ 0 & 1 \end{bmatrix}) \circ (\kappa^{(4)}, i^{(4)}, \begin{bmatrix} \nabla\chi^{-1}G & \nabla\chi^{-1}(w - \dot{\chi}) \\ 0 & 1 \end{bmatrix}), \tag{6.9}$$

where in the last member the symbol $i^{(4)}$ denotes the identity map on $\mathcal{A} \times (0,T)$, and then by translating the resulting "space-time" factors into structured motions:

$$(\kappa^{(4)}, \chi, G, w) = \left(\kappa^{(4)}, \chi, \nabla\chi, \dot{\chi}\right) \circ \left(\emptyset, \pi, \nabla\chi^{-1}G, \nabla\chi^{-1}(w - \dot{\chi})\right). \tag{6.10}$$

Here, π denotes the projection $(x,t) \mapsto x$. A similar argument yields the alternative factorization

$$(\kappa^{(4)},\chi,G,w) = \left(\emptyset,\pi,(G\nabla\chi^{-1})\circ \mathsf{t}_\chi^{-1},(w-G\nabla\chi^{-1}\dot{\chi})\circ \mathsf{t}_\chi^{-1}\right)\circ\left(\kappa^{(4)},\chi,\nabla\chi,\dot{\chi}\right). \tag{6.11}$$

Each factor containing the projection depicts a structured motion that is static at the macroscopic level but that involves disarrangements at the microlevel. The remaining factors are simple motions and involve only disarrangements at the macrolevel.

We recall now that the Approximation Theorem (Part One, Section 4) permits us to write every structured deformation and, therefore, every "space-time" structured deformation of the form $(\kappa^{(4)},\mathsf{t}_\chi,\begin{bmatrix} G & w \\ 0 & 1\end{bmatrix})$, as a limit of simple deformations. However, the Approximation Theorem by itself does not guarantee that the approximating simple deformations $(\kappa_m^{(4)},\ f_m^{(4)}) \in Sid(\mathcal{A}\times(0,T))$ correspond to simple *motions*. Thus, terms in the determining sequence provided by the Approximation Theorem might cause time travel. Consequently, we need to reexamine the proof of the Approximation Theorem and, in particular, the proof of the Approximation Lemma (Part One, Section 4) to determine whether the approximations can be chosen so that they correspond to simple motions. Indeed, we have the following

Lemma 6.1 *(Approximation Lemma for Purely Microscopic Structured Motions): For each $(\emptyset,\pi,K,u) \in Stm(\mathcal{A}\times(0,T))$, there exists a sequence $m \mapsto (\kappa_m^{(4)},\chi_m)$ of simple motions such that*

$$\lim_{m\to\infty}\chi_m = \pi, \quad \lim_{m\to\infty}\nabla\chi_m = K, \quad \lim_{m\to\infty}\dot{\chi} = u \tag{6.12}$$

in the sense of L^∞-convergence, and such that $\liminf_{m\to\infty}\kappa_m^{(4)} = \emptyset$.

Examination of the proof of the Approximation Lemma (Lemma 5.7, reference [11, Part One]) reveals that relations (5.36) and (5.57), in which piecewise affine approximating simple deformations are chosen, guarantee that the approximating piecewise affine "space-time" simple deformations for the present case correspond to simple motions. Moreover, the piecewise rigid "space-time" simple deformations, corresponding to those chosen just above (5.49) and below (5.57) in [11, Part One], can be chosen here as those associated with piecewise rigid motions, because the inequality

$$\det{}^{(4)} \begin{bmatrix} K & u \\ 0 & 1 \end{bmatrix} \leq \det \nabla^{(4)} \mathrm{t}_{\chi} \tag{6.13}$$

is equivalent to the inequality $\det K \leq \det \nabla\pi = 1$. The present Approximation Lemma for purely microscopic structured motions implies the main result on structured motions.

Theorem 6.1 *(Approximation Theorem for Structured Motions): Every structured motion* $(\kappa^{(4)}, \chi, G, w) \in Stm(\mathcal{A} \times (0,T))$ *is a limit of simple motions, i.e., there exists* $m \mapsto (\kappa_m^{(4)}, \chi_m) \in Sim(\mathcal{A} \times (0,T))$ *such that*

$$\lim_{m\to\infty} \chi_m = \chi, \quad \lim_{m\to\infty} \nabla\chi_m = G, \quad \lim_{m\to\infty} \dot{\chi}_m = w \tag{6.14}$$

in the sense of L^∞*-convergence, and such that* $\liminf_{m\to\infty} \kappa_m^{(4)} = \kappa^{(4)}$.

6.6 Velocity and deformation with and without disarrangements

The integral-gradient formula (7.7), Part One applied to "space-time" structured deformations yields the following *identification relations* for $\nabla\chi - G$ and for $\dot{\chi} - w$ in a given structured motion $(\kappa^{(4)}, \chi, G, w)$: for every $(x,t) \in (\mathcal{A} \times (0,T)) \backslash \kappa^{(4)}$

$$\nabla\chi(x,t) - G(x,t) =$$

$$\lim_{r\to 0} \lim_{m\to\infty} vol\mathcal{B}(x,t;r)^{-1} \int_{\Gamma(\chi_m)\cap\mathcal{B}(x,t;r)} \left((\chi_m)_\nu - (\chi_m)_{-\nu}\right)(\zeta) \otimes \nu^{(3)}(\zeta) dA_\zeta \tag{6.15}$$

$$\dot{\chi}(x,t) - w(x,t) =$$

$$lim_{r\to 0} \lim_{m\to\infty} vol\mathcal{B}(x,t;r)^{-1} \int_{\Gamma(\chi_m)\cap\mathcal{B}(x,t;r)} \nu^{(1)}(\zeta) \left((\chi_m)_\nu - (\chi_m)_{-\nu}\right)(\zeta) dA_\zeta . \tag{6.16}$$

Here, for each $r > 0$, $\mathcal{B}(x,t;r) \subset \mathcal{E} \times \mathbb{R}$ is the ball centered at (x,t) of radius r, $\Gamma(\chi_m) \subset \mathcal{E} \times \mathbb{R}$ is the jump set for χ_m, and $(\nu^{(3)}(\zeta), \nu^{(1)}(\zeta)) \subset \mathcal{V} \times \mathbb{R}$ is the "space-time" unit normal to $\Gamma(\chi_m)$ at ζ. In addition, ${}^{(4)}_{m}, \chi_m)$ is a sequence of simple motions chosen as in the Approximation Theorem.

The identification relations (**??**) and (**??**) justify our calling $\nabla\chi - G$ the *deformation due to disarrangements* and $\dot{\chi} - w$ the *velocity due to disarrangements* , respectively. Moreover, the formulas $(\mathbf{??})_2$ and $(\mathbf{??})_3$ justify our calling G and w the *deformation without disarrangements* and the *velocity without disarrangements*, respectively. These quantities show that specification of a structured motion permits one to describe with precision the amount of deformation and of velocity associated with smooth geometrical changes on a smaller length scale, as well as the amount of deformation and of velocity associated with non-smooth changes at a smaller length scale. According to (**??**) and (**??**), whether a jump $((\chi_m)_\nu - (\chi_m)_{-\nu})(\zeta)$ in position across a given surface contributes to $\nabla\chi - G$ alone, to $\dot{\chi} - w$ alone, or to both depends upon whether the normal $(\nu^{(3)}(\zeta), \nu^{(1)}(\zeta))$ has only the space-like component $\nu^{(3)}(\zeta)$ non-zero, only the time-like component $\nu^{(1)}(\zeta)$ non-zero, or both non-zero. In addition, we may conclude from the identification relations the following transformation rules for the deformation due to disarrangements and the velocity due to disarrangements:

$$
\begin{array}{cc}
\textbf{Change of observer} & \textbf{Change of virgin configuration} \\[1em]
\nabla\chi - G \to Q(\nabla\chi - G) & \nabla\chi - G \to (\nabla\chi - G)H \\
\dot{\chi} - w \to Q(\dot{\chi} - w) & \dot{\chi} - w \to \dot{\chi} - w
\end{array}
\tag{6.17}
$$

It is worth noting that the velocity due to disarrangements $\dot{\chi} - w$ transforms objectively under a change in observer, in spite of the fact that neither $\dot{\chi}$ nor w transforms objectively.

Let us return to the two examples of structured motions in Subsection 6.4: $(\emptyset, \chi_e, I, e)$ and $(\emptyset, \chi_e, I, 0)$, where χ_e is the uniform translation defined in (**??**). For both of these motions, the deformation due to disarrangements $\nabla\chi - G$ vanishes. For the classical motion $(\emptyset, \chi_e, I, e)$, the velocity due to disarrangements $\dot{\chi} - w = e - e$ also vanishes, while for the non-classical structured motion $(\emptyset, \chi_e, I, 0)$ the velocity due to disarrangements is given by $\dot{\chi} - w = \dot{\chi} - 0 = e = \dot{\chi}$. Thus, in the non-classical motion $(\emptyset, \chi_e, I, 0)$, the macroscopic velocity $\dot{\chi}$ equals the velocity due to disarrangements $\dot{\chi} - w$, and we may say that the macroscopically uniform translation associated with $(\emptyset, \chi_e, I, 0)$ is due entirely to disarrangements.

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