The discrete origin of configurational forces

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In Memory of Morton E. Gurtin

Abstract

We develop a discrete formulation of configurational forces for open subsystems of a finite particle system. Membership in an open subsystem may change by particle admission or deletion. We first use zero-one membership functions to formulate standard balances for mass, standard momentum, angular momentum, and kinetic energy: continuous terms are evaluated on fixed-membership subintervals, but admission and deletion enter through jump-transfer sums. We then introduce a configurational momentum balance for open subsystems and configurational contact-force resultants associated with the ordered separation between a subsystem and its complement. To describe membership changes geometrically, we introduce an auxiliary smooth description based on a scalar membership field on the Euclidean space of particle placements. For each particle, the level set through the current particle position is used as a local membership cut, and the gradient at that position defines a normal to the cut. We assign an observed velocity to these level sets; its tangential component can be changed without altering the smooth membership value or its rate. We require the working associated with membership transfer to be invariant under such tangential changes, and we refer to this invariance as intrinsicity. If this invariance is imposed on a working involving only standard contact-force assignments and standard momentum transfer, then an artificial normality condition is imposed on the standard contact-force assignment. We therefore add configurational contact-force assignments. For a particle with assigned mass, standard momentum, standard velocity, and specific configurational momentum, we impose the intrinsicity requirement and obtain that the specific configurational momentum is the negative of the standard velocity. For nondissipative membership transfer, we use a mechanical energy imbalance to identify the particlewise membership tension: the combined standard-plus-configurational cut-force assignment equals the difference between the membership interaction-energy increment and the kinetic energy, multiplied by the cut normal. After imposing localization hypotheses for contact-force assignments, current representative volumes, and energy increments, we obtain the continuum relation $\boldsymbol{u} = -\boldsymbol{v}$ for the specific configurational momentum and the spatial inertial Eshelby relation $\boldsymbol{C} = \rho(\psi - \frac{1}{2}|\boldsymbol{v}|^2)\boldsymbol{1} - \boldsymbol{T}$, where $\boldsymbol{C}$ is the spatial configurational stress, $\boldsymbol{T}$ is the Cauchy stress, ρ is the mass density, ψ is the specific free energy, $\boldsymbol{v}$ is the standard velocity, and $\boldsymbol{1}$ is the identity tensor.

1 Introduction

Configurational forces enter continuum mechanics when changes of material structure must be described independently of the standard motion. The classical source of this viewpoint is Eshelby's [1–4] work on elastic singularities, lattice defects, and the energy-momentum tensor. Gurtin [5, 6] treated configurational forces as primitive objects by assigning working to migrating control volumes, rather than by treating configurational forces only as quantities obtained from variational arguments.

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For a finite particle system, the discrete counterpart of transfer across a nonmaterial migrating control-volume boundary is time-dependent membership in an open subsystem. We obtain such a subsystem by changing which particles of the system are included; admission and deletion change the subsystem, not the particle system itself. We therefore pursue the following particle-level program: formulate balances for open subsystems, introduce configurational working, and impose intrinsicity with respect to nonintrinsic descriptions of membership change.

We use two descriptions of membership. The first is a zero-one description: at each time, the open subsystem is the collection of particles currently included in it, and changes of membership occur by admission or deletion jumps. The second is a smooth membership-field description: for an auxiliary smooth scalar field $\chi : \mathcal{E} \times I \to [0, 1]$, the value $\theta_i(t) = \chi(x_i(t), t)$ is attached to particle p_i at its current place. This scalar is a smooth bookkeeping variable for regularized admission or deletion, and we use its time derivative as the associated membership-transfer rate. We use the level surfaces of χ as local membership cuts, their gradients as normals to those cuts, and an observed velocity assigned to the level surfaces has a tangential part that does not affect θ_i or $\dot{\theta}_i$. Intrinsicity means that the cut working must be insensitive to this nonintrinsic tangential part. The auxiliary field is used only for this geometric and kinematic description; zero-one membership remains the description of actual admission and deletion.

Because the places of particles are points of the current Euclidean space, we formulate the theory spatially from the outset. By working in the spatial configuration, we remain consistent with the migrating-spatial-control-volume theory of Anderson et al. [7], where configurational momentum and the inertial Eshelby relation are obtained without recourse to a reference configuration. We also remain consistent with Ericksen's [8] observation, in the setting of line defects, that the choice between referential and spatial independent variables can affect the interpretation of mechanical and configurational forces.

Methodologically, we follow Gurtin's [5, 6] continuum treatment. For migrating control volumes, Gurtin imposed invariance with respect to changes in the velocity field used to describe the migrating boundary before introducing constitutive restrictions. We regard this order of development as one of the principal strengths of his framework. He then used a mechanical version of the second law to identify the bulk tension. The boundary of Gurtin's [5, 6] migrating control volume is not material; material is transferred across it, and its tangential velocity is nonintrinsic. We retain this separation of steps in a finite-particle setting. We use time-dependent membership in the role played, in the continuum theory, by transfer across the migrating boundary. In place of the complete thermomechanical treatment of Anderson et al. [7], we use a purely mechanical energy imbalance for smooth membership-field descriptions.

The particle-level formulation is intended as a complement to, rather than a replacement for, Gurtin's [5, 6] continuum formulation. Our aim is to show that the same order of development can be carried out using changes of membership in a fixed finite particle system. In place of a migrating control-volume boundary, we use admission and deletion of particles. We then write the bookkeeping directly in terms of particle labels, positions, velocities, momenta, pair forces, and interaction-energy increments before introducing continuum stress, density, or free-energy fields. Using this bookkeeping, we distinguish explicitly between continuous evolution on fixed-membership intervals and transfer by admission or deletion, and we identify the particlewise origins of the configurational momentum and cut-force relations. This change of level also has costs: the zero-one membership description does not supply local normals or tangential descriptors, so the intrinsicity argument uses an auxiliary smooth membership-field description; moreover, comparison with continuum stresses and energy densities requires the localization hypotheses introduced later.

With this comparison in mind, we organize our developments around two particle-level relations and their continuum counterparts. We first formulate open-subsystem balances for mass, standard momentum, angular momentum, and kinetic energy using zero-one membership functions and explicit jump transfers. We then introduce a configurational momentum balance for open subsystems. After adding a smooth membership-field description, we use intrinsicity to obtain the particlewise configurational momentum relation. For a particle p_i with mass m_i, standard momentum $\boldsymbol{p}_i$, and specific configurational momentum $\boldsymbol{u}_i$, this relation is

$$m_i \boldsymbol{u}_i = -\boldsymbol{p}_i. \tag{1.1}$$

We next use intrinsicity to obtain a discrete pre-Eshelby cut relation. We then combine the mechanical energy imbalance for smooth membership-field descriptions with the specialization to nondissipative membership transfer. Writing $\boldsymbol{f}_i^\chi$ and $\boldsymbol{c}_i^\chi$ for the standard and configurational cut-force assignments associated with p_i, ψ_i^θ for the interaction-energy increment conjugate to the smooth membership value θ_i, k_i for the kinetic energy of p_i, and $\boldsymbol{h}_i$ for the cut normal obtained from χ, we obtain the energetically identified cut relation

$$\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi = (\psi_i^\theta - k_i)\boldsymbol{h}_i. \tag{1.2}$$

The relations (1.1) and (1.2) are relations among particle quantities, cut normals, and cut-force assignments. They do not require continuum stress, density, or free-energy fields.

To compare the particlewise relations with continuum theory, we impose the localization hypotheses described in Section 7. Under the sampling assumption for specific quantities, we pass from (1.1) to the continuum relation between the specific configurational momentum $\boldsymbol{u}$ and the standard velocity $\boldsymbol{v}$:

$$\boldsymbol{u} = -\boldsymbol{v}. \tag{1.3}$$

Under the traction representations for the particlewise cut-force assignments and the energy-density representation for the extensive scalar $\psi_i^\theta - k_i$, we pass from (1.2) to the spatial inertial Eshelby relation

$$\boldsymbol{C} = \rho\Big(\psi - \frac{1}{2}|\boldsymbol{v}|^2\Big)\boldsymbol{1} - \boldsymbol{T}. \tag{1.4}$$

Here $\boldsymbol{C}$ is the spatial configurational stress, $\boldsymbol{T}$ is the Cauchy stress, ρ is the mass density, ψ is the specific free energy, and $\boldsymbol{1}$ is the identity tensor. The continuum relations (1.3) and (1.4) are formal consequences of the localization hypotheses; they are not imposed at the particle level.

We proceed as follows. In Section 2, we describe open subsystems of a particle system, zero-one membership functions, and the jump-transport identity for quantities carried by particles. In Section 3, we combine that transport identity with balances for closed subsystems to obtain the standard balances for open subsystems. In Section 4, we introduce configurational momentum and formulate its open-subsystem balance. In Section 5, we pass from zero-one membership to a smooth membership-field description, examine the inadequacy of standard-only working, introduce configurational cut forces, and use intrinsicity to derive the configurational momentum relation and the reduced discrete cut relation. In Section 6, we use a mechanical energy imbalance for smooth membership-field descriptions to identify the membership tension. In Section 7, we impose localization hypotheses and derive the continuum counterparts of the particlewise configurational momentum and cut-force relations. We close in Section 8 with a discussion of configurational cut forces, dissipative membership transfer, the status of the localization step, and possible extensions.

2 Open subsystems of a given particle system

Let $\mathcal{E}$ be three-dimensional Euclidean point space, and let $\mathcal{V}$ be its associated translation space. We consider the finite particle system

$$\mathcal{B} = \{p_1, \dots, p_N\} \tag{2.1}$$

of $N \geq 1$ particles. A motion of $\mathcal{B}$ on a time interval I is a list of functions $x_i : I \to \mathcal{E}$, $i = 1, \dots, N$, such that

$$x_i(t) \in \mathcal{E}, \qquad t \in I, \qquad i = 1, \dots, N. \tag{2.2}$$

At each time $t \in I$, we assume that the placement of $\mathcal{B}$ in $\mathcal{E}$ is one-to-one; hence $x_i(t) \neq x_j(t)$ whenever $i \neq j$. The velocity $\boldsymbol{v}_i$ and acceleration $\boldsymbol{a}_i$ of p_i are the vectors

$$\boldsymbol{v}_i = \dot{x}_i \qquad \text{and} \qquad \boldsymbol{a}_i = \dot{\boldsymbol{v}}_i. \tag{2.3}$$

The standard momentum, angular momentum about a chosen origin $o \in \mathcal{E}$, and kinetic energy of p_i are denoted by

$$\boldsymbol{p}_i = m_i \boldsymbol{v}_i, \qquad \boldsymbol{l}_i = (x_i - o) \times \boldsymbol{p}_i, \qquad \text{and} \qquad k_i = \frac{1}{2} m_i |\boldsymbol{v}_i|^2. \tag{2.4}$$

Here, $x_i - o$ is the vector in $\mathcal{V}$ directed from o to x_i.

Throughout what follows, subscripts such as i and j label particles, not vector or tensor components. Repetition of particle labels is not meant to imply summation; whenever a sum over particles or ordered particle pairs is intended, we display the summation sign explicitly. We do not use component notation for vector or tensor components.

2.1 Particle subsystems and elementary membership changes

At a given time, we call a nonempty subset P of $\mathcal{B}$ a particle subsystem. Thus, for each particle p_i in the ambient system $\mathcal{B}$, exactly one of the alternatives $p_i \in P$ and $p_i \notin P$ holds. We therefore consider subsystems P with

$$P \subset B \quad \text{and} \quad P \neq \varnothing. \tag{2.5}$$

For a subsystem P, we write α_i for the characteristic membership value of p_i:

$$\alpha_i = \begin{cases} 1, & p_i \in P, \\ 0, & p_i \notin P. \end{cases} \tag{2.6}$$

Thus, in this set-valued description, the membership values are zero-one valued.

A subsystem whose membership is independent of time will be called closed. Thus a closed subsystem is a nonempty subset P of $\mathcal{B}$; the particles in P may move, but no particles are admitted to, or deleted from, P. We use the adjective open for a subsystem with time-varying membership. An open subsystem is therefore a map from the time interval I into the nonempty subsets of $\mathcal{B}$:

$$P : I \to \mathcal{P}(\mathcal{B}) \setminus \{\varnothing\}, \qquad t \mapsto P(t). \tag{2.7}$$

For each time $t \in I$, the collection of particles $P(t)$ is a subsystem of $\mathcal{B}$. Changes of $P(t)$ represent changes of membership within $\mathcal{B}$. If p_i is admitted to $P(t)$, then p_i passes from the complement $P'(t) = \mathcal{B} \setminus P(t)$ of $P(t)$ into $P(t)$. If p_i is deleted from $P(t)$, then p_i passes from $P(t)$ into $P'(t)$. Neither operation changes $\mathcal{B}$.

Elementary changes of a subsystem are oriented edges of the Boolean lattice of subsets of $\mathcal{B}$, with the empty vertex removed when nonemptiness is imposed throughout. If $p_i \notin P$, an elementary admission is represented by

$$P \xrightarrow{\alpha_i : 0 \mapsto 1} P \cup \{p_i\}. \tag{2.8}$$

If, alternatively, $p_i \in P$ and $P \setminus \{p_i\} \neq \varnothing$, an elementary deletion is represented by

$$P \xrightarrow{\alpha_i : 1 \mapsto 0} P \setminus \{p_i\}. \tag{2.9}$$

The labels above the arrows record the change of the membership value associated with p_i. The orientation is the direction of traversal in the Boolean lattice.

For a subsystem P, we define the *ordered cut* of P by

$$\partial P = \{(i, j) : p_i \in P,\ p_j \in P'\}. \tag{2.10}$$

At this stage, the word “cut” has only a combinatorial meaning: ∂P is the set of ordered index pairs whose first index labels a particle in P and whose second index labels a particle in P'. After pair quantities have been introduced, expressions indexed by $(i, j) \in \partial P$ are therefore evaluated with the first slot associated with a particle in P and the second slot associated with a particle in P'. If $(i, j) \in \partial P$, then $(j, i) \in \partial P'$.

2.2 Zero-one membership functions

We represent an open subsystem $P : I \to \mathcal{P}(\mathcal{B}) \setminus \{\varnothing\}$ by its characteristic membership functions. For each particle p_i, the function $\alpha_i : I \to \{0,1\}$ is given for each $t \in I$ by

$$\alpha_i(t) = \begin{cases} 1, & p_i \in P(t), \\ 0, & p_i \notin P(t). \end{cases} \tag{2.11}$$

Conversely, given a list

$$\alpha = (\alpha_1, \ldots, \alpha_N), \qquad \alpha_i : I \to \{0,1\}, \tag{2.12}$$

of membership functions taking only the values zero and unity, we associate with α, at each time $t \in I$, the subset

$$P_\alpha(t) = \{p_i \in \mathcal{B} : \alpha_i(t) = 1\}. \tag{2.13}$$

The requirement $(2.5)_2$, applied to $P_\alpha(t)$, is equivalent to

$$\sum_{i=1}^{N} \alpha_i(t) \geq 1 \qquad \text{for each } t \in I. \tag{2.14}$$

When (2.14) holds, P_α is an open subsystem. Consistent with the notation P' for the complement of P, we denote the complementary membership of p_i by α_i' and define it by

$$\alpha_i'(t) = 1 - \alpha_i(t) \qquad \text{for each } t \in I. \tag{2.15}$$

Because each α_i depends on time, its differentiability on I must be addressed. A nonconstant function from an interval into the two-point set $\{0,1\}$ cannot be classically differentiable on that interval. Indeed, if the function is differentiable on the interval then it must be continuous. However, the continuous image of an interval is connected, and the only connected subsets of $\{0,1\}$ are singletons. A differentiable zero-one membership function $\alpha_i : I \to \{0,1\}$ is therefore constant on every connected interval of I. Thus, a change of zero-one membership at an instant of admission or deletion cannot be described by a classical time derivative.

For the foregoing reason, we describe changes of zero-one membership by jumps. We assume that each α_i is right-continuous, piecewise constant, and has only finitely many jumps on each compact subinterval of I. At a time τ at which at least one membership function jumps, we denote the left limit of α_i by $\alpha_i(\tau-)$ and define the jump of α_i by

$$\Delta\alpha_i(\tau) = \alpha_i(\tau) - \alpha_i(\tau-). \tag{2.16}$$

For a fixed i, the value $\Delta\alpha_i(\tau)$ may vanish. Since α_i is equal to either zero or unity, the only possible nonzero alternatives are

$$\Delta\alpha_i(\tau) = +1 \qquad \text{or} \qquad \Delta\alpha_i(\tau) = -1. \tag{2.17}$$

We interpret the first alternative in (2.17) as the admission of p_i to the open subsystem and the second as the deletion of p_i from the open subsystem. In Figure 1, we provide a schematic representation of the two elementary zero-one membership jumps: admission of a particle to P_α and deletion of a particle from P_α. When exactly one membership function has a nonzero jump at τ, the transition from $P_\alpha(\tau-)$ to $P_\alpha(\tau)$ is an elementary edge of the form (2.8) or (2.9). When several membership functions have nonzero jumps at the same time, we specify only the transition from $P_\alpha(\tau-)$ to $P_\alpha(\tau)$. An ordering into elementary admissions and deletions is additional data. In the framework developed in this section, only zero-one memberships and explicit jumps are used. Additional structure is needed for regularized or spatially generated memberships; such descriptions will be introduced subsequently.

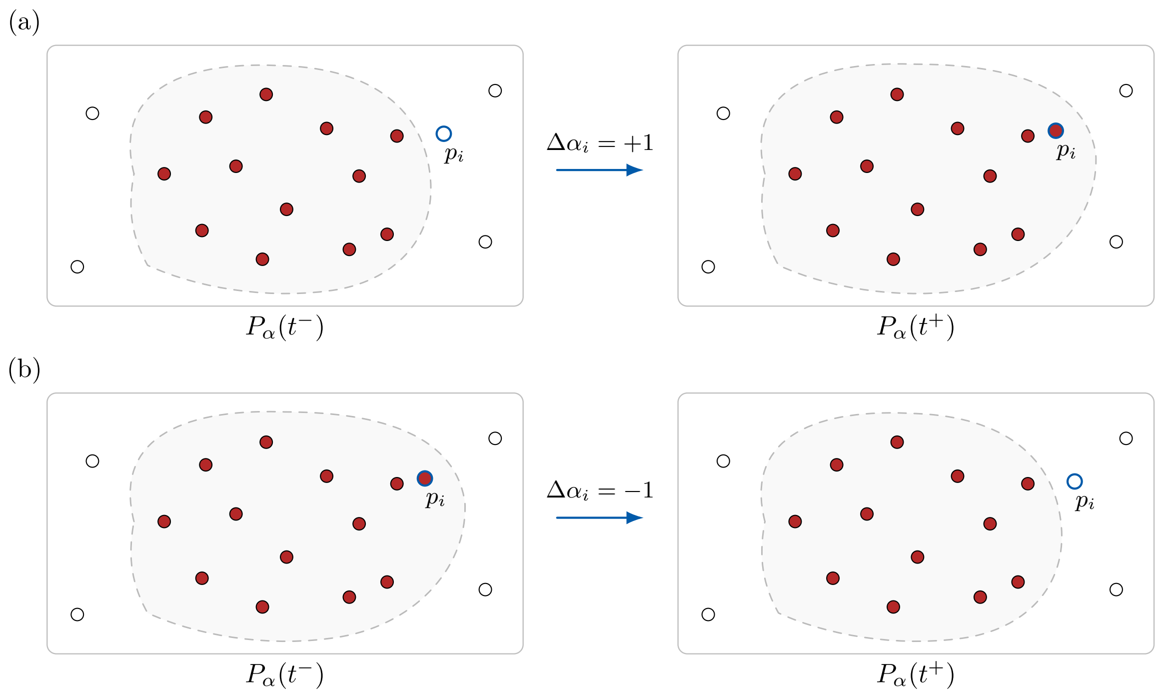

Figure 1: Open subsystems and membership jumps. Each boxed snapshot represents a particle system together with a schematic dashed contour grouping the particles that belong to the open subsystem P_α; the dashed contour does not represent a material boundary. Red filled particles have membership $\alpha_i = 1$, while open particles have membership $\alpha_i = 0$. In (a), particle p_i is outside $P_\alpha(t^-)$ and inside $P_\alpha(t^+)$, so that $\Delta\alpha_i = +1$. In (b), particle p_i is inside $P_\alpha(t^-)$ and outside $P_\alpha(t^+)$, so that $\Delta\alpha_i = -1$.

2.3 Particle-carried content and the jump-transport identity

For each $i = 1, \ldots, N$, let a_i be a time-dependent quantity carried by p_i. We assume that the quantities a_i are either all scalar-valued, all vector-valued, or all tensor-valued, so that sums over particles are meaningful, and we write

$$a = (a_1, \ldots, a_N) \tag{2.18}$$

for the corresponding list of carried quantities. At time t, we define the content $\langle a \rangle_\alpha(t)$ of a in the open subsystem $P_\alpha(t)$ by the sum

$$\langle a \rangle_\alpha(t) = \sum_{i=1}^{N} \alpha_i(t) a_i(t). \tag{2.19}$$

We next separate two mechanisms that contribute to changes of content: continuous evolution on intervals on which membership is fixed, and instantaneous transfer at membership jumps. To this end, we assume that each a_i is continuous on I and continuously differentiable except possibly at finitely many times on each compact subinterval of I. Under this assumption, and using the piecewise constancy of the membership functions, the time integrands used below are piecewise continuous. Throughout this subsection, time integrals are understood in the usual one-dimensional sense for such integrands; values assigned at finitely many exceptional times do not affect their values.

On an open interval on which no membership jump occurs, the membership list α is constant. At any time in such an interval at which each carried quantity a_i is differentiable, we differentiate only the carried quantities and obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle a \rangle_\alpha = \sum_{i=1}^{N} \alpha_i \dot{a}_i. \tag{2.20}$$

At a time τ at which one or more membership values change, we record the change for each particle by

$\Delta\alpha_i(\tau) = \alpha_i(\tau) - \alpha_i(\tau-)$. This value is positive for admission, negative for deletion, and zero for particles whose membership does not change at τ. Since the carried quantities are continuous at τ, the jump in content is

$$\langle a\rangle_\alpha(\tau) - \langle a\rangle_\alpha(\tau-) = \sum_{i=1}^{N} a_i(\tau)\Delta\alpha_i(\tau). \tag{2.21}$$

For zero-one memberships, the values $\Delta\alpha_i(\tau)$ record admission and deletion at jump times; we do not use time derivatives of the membership functions α_i for this purpose.

For $s < t$, let $J_\alpha(s,t)$ denote the finite set of times in $(s,t]$ at which at least one membership function has a nonzero jump. The set $J_\alpha(s,t)$ is finite by the assumed finiteness of membership jumps on compact subintervals of I. We use the half-open interval $(s,t]$ in accord with the right-continuous convention: a jump at t is included in the transfer from s to t, whereas a jump at s is excluded because the value $\langle a\rangle_\alpha(s)$ already uses the post-jump membership at s. For compactness in subsequent balances, we write the cumulative membership transfer of a over $(s,t]$ as

$$\mathcal{A}_\alpha(a; s,t) = \sum_{\tau\in J_\alpha(s,t)} \sum_{i=1}^{N} a_i(\tau)\Delta\alpha_i(\tau). \tag{2.22}$$

We use the same jump set to identify the subintervals on which the membership list is fixed. Let m be the number of elements of $J_\alpha(s,t)\cap(s,t)$. If $m > 0$, write these elements as $\tau_1 < \cdots < \tau_m$; if $m = 0$, there are no interior jump times. In either case, set $\tau_0 = s$ and $\tau_{m+1} = t$. On each open interval (τ_q, τ_{q+1}), no membership jump occurs, and the right-continuous value $\alpha_i(\tau_q)$ equals the value of α_i immediately after τ_q. Hence $\alpha_i(r) = \alpha_i(\tau_q)$ for $r \in (\tau_q, \tau_{q+1})$. By the convention on time integrals stated above, the values assigned at the finitely many endpoints do not affect the integral. Leveraging additivity of the integral, we therefore find that

$$\int_s^t \sum_{i=1}^{N} \alpha_i(r)\dot{a}_i(r)\,\mathrm{d}r = \sum_{q=0}^{m} \int_{\tau_q}^{\tau_{q+1}} \sum_{i=1}^{N} \alpha_i(\tau_q)\dot{a}_i(r)\,\mathrm{d}r. \tag{2.23}$$

If a membership jump occurs at t, that jump is not part of the last fixed-membership subinterval; it contributes only to the transfer sum in (2.22).

Adding the fixed-membership contributions in (2.23) and the jump contributions in (2.22), we obtain the transport identity

$$\begin{aligned}\langle a\rangle_\alpha(t) - \langle a\rangle_\alpha(s) &= \int_s^t \sum_{i=1}^{N} \alpha_i(r)\dot{a}_i(r)\,\mathrm{d}r + \sum_{\tau\in J_\alpha(s,t)} \sum_{i=1}^{N} a_i(\tau)\Delta\alpha_i(\tau) \\ &= \int_s^t \sum_{i=1}^{N} \alpha_i(r)\dot{a}_i(r)\,\mathrm{d}r + \mathcal{A}_\alpha(a; s,t). \end{aligned} \tag{2.24}$$

In (2.24), we use the integral to collect only continuous changes of the carried quantities on fixed-membership subintervals between membership jumps. The transfer term is the explicit sum over membership jump times in $(s,t]$. In Figure 2, we provide a visual representation of the bookkeeping underlying (2.24).

For subsequent use, we specialize the content notation to the standard particle quantities introduced in (2.4). Specifically, choosing a_i in (2.19) successively as m_i, $\boldsymbol{p}_i$, $\boldsymbol{l}_i$, and k_i, we define M_α, $\boldsymbol{\varpi}_\alpha$, $\boldsymbol{\ell}_\alpha$, and K_α by

$$M_\alpha = \langle m\rangle_\alpha, \qquad \boldsymbol{\varpi}_\alpha = \langle \boldsymbol{p}\rangle_\alpha, \qquad \boldsymbol{\ell}_\alpha = \langle \boldsymbol{l}\rangle_\alpha, \qquad \text{and} \qquad K_\alpha = \langle k\rangle_\alpha. \tag{2.25}$$

For these same choices of a_i, we denote the corresponding cumulative transfers over $(s,t]$ by

$$\mathcal{A}_\alpha(m; s,t), \qquad \mathcal{A}_\alpha(\boldsymbol{p}; s,t), \qquad \mathcal{A}_\alpha(\boldsymbol{l}; s,t), \qquad \text{and} \qquad \mathcal{A}_\alpha(k; s,t). \tag{2.26}$$

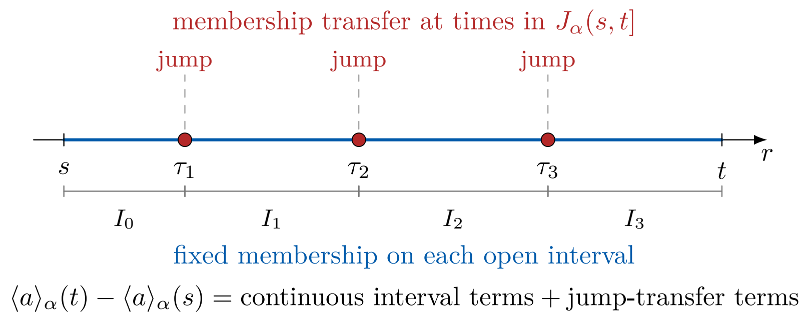

Figure 2: Transport-by-jumps structure for an open subsystem. The membership list is fixed on each open interval $I_0, \ldots, I_3$ between successive jump times. At each jump time $\tau_k \in J_\alpha(s,t]$, admission or deletion of particles enters the transport identity through a separate transfer term. Thus, the change $\langle a\rangle_\alpha(t) - \langle a\rangle_\alpha(s)$ in the content $\langle a\rangle_\alpha$ of a generic quantity a over the half-open time interval $(s,t]$ is decomposed into continuous contributions over fixed-membership intervals and jump-transfer contributions at the jump times.

2.4 Pair weights and cuts

For subsequent sums over ordered particle pairs, only the membership values at the time under consideration are needed. Throughout this subsection, we therefore suppress the common time argument, writing α_i, α'_i, P_α, P'_α, and ∂P_α for $\alpha_i(t)$, $\alpha'_i(t)$, $P_\alpha(t)$, $P'_\alpha(t)$, and $\partial P_\alpha(t)$, respectively. The same convention applies to the weights introduced below. With this convention, we use the membership values introduced in Subsection 2.2 to define the weights that retain, respectively, pairs for which both particles belong to P_α and pairs for which both particles belong to $P'_\alpha = \mathcal{B} \setminus P_\alpha$:

$$\iota^\alpha_{ij} = \alpha_i\alpha_j \qquad \text{and} \qquad \iota^{\alpha'}_{ij} = \alpha'_i\alpha'_j = (1-\alpha_i)(1-\alpha_j). \tag{2.27}$$

For pairs whose particles have different memberships, we use two related weights. To retain the ordering in which the first index labels a particle in P_α and the second index labels a particle in P'_α, we introduce the oriented cut weight

$$\beta^\alpha_{ij} = \alpha_i\alpha'_j = \alpha_i(1-\alpha_j). \tag{2.28}$$

For zero-one membership, β^α_{ij} is equal to unity precisely when $(i,j) \in \partial P_\alpha$ and vanishes otherwise. To compare this ordering with its reverse, we introduce the signed cut weight δ^α_{ij}, defined by

$$\delta^\alpha_{ij} = \alpha_i - \alpha_j. \tag{2.29}$$

Combining (2.11), (2.13), and (2.29) with the definition (2.10) of the ordered cut of a subsystem, we find that, for zero-one membership, δ^α_{ij} is positive on the ordered cut, negative on the reverse orientation of the cut, and zero for pairs whose particles have the same membership:

$$\delta^\alpha_{ij} = \begin{cases} 1, & (i,j) \in \partial P_\alpha, \\ -1, & (j,i) \in \partial P_\alpha, \\ 0, & \alpha_i = \alpha_j. \end{cases} \tag{2.30}$$

The zero-one membership characterization in (2.30) is a pointwise interpretation of δ^α_{ij}. The relation needed below is algebraic and does not rely on zero-one membership. Subtracting the version of (2.28) with i and j interchanged from (2.28), and using (2.29), we obtain the identity

$$\beta^\alpha_{ij} - \beta^\alpha_{ji} = \alpha_i(1-\alpha_j) - \alpha_j(1-\alpha_i) = \alpha_i - \alpha_j = \delta^\alpha_{ij}. \tag{2.31}$$

2.5 Forces and moments

We next introduce standard force and moment resultants. The adjective standard is used to distinguish these quantities from configurational forces, which will be introduced later.

We first consider arbitrary disjoint subsets P and Q of $\mathcal{B}$. This choice separates the definition of the force resultants from a particular membership process $t \mapsto P_\alpha(t)$. For each $t \in I$, let $\boldsymbol{f}_{ij}(t)$ be the force exerted on p_i by p_j, $j \neq i$, and let $\boldsymbol{f}_i^{\text{env}}(t)$ be the force exerted on p_i by agencies external to $\mathcal{B}$. The force on P due to Q and the environmental force on P are the resultants $\boldsymbol{f}(P, Q; t)$ and $\boldsymbol{f}^{\text{env}}(P; t)$ defined by

$$\boldsymbol{f}(P, Q; t) = \sum_{p_i \in P} \sum_{p_j \in Q} \boldsymbol{f}_{ij}(t) \qquad \text{and} \qquad \boldsymbol{f}^{\text{env}}(P; t) = \sum_{p_i \in P} \boldsymbol{f}_i^{\text{env}}(t). \tag{2.32}$$

To include empty subsets without further qualification, we use the normalizations

$$\boldsymbol{f}(P, \varnothing; t) = \boldsymbol{f}(\varnothing, Q; t) = \boldsymbol{0}, \qquad \boldsymbol{f}^{\text{env}}(\varnothing; t) = \boldsymbol{0}. \tag{2.33}$$

In particular, $\boldsymbol{f}(P, P'; t)$ is the standard cut force on P.

To prepare for angular-momentum balances, we also use moments about the chosen point $o \in \mathcal{E}$. Corresponding to the force resultants in (2.32), we write

$$\boldsymbol{m}(P, Q; o, t) = \sum_{p_i \in P} \sum_{p_j \in Q} (x_i(t) - o) \times \boldsymbol{f}_{ij}(t) \qquad \text{and} \qquad \boldsymbol{m}^{\text{env}}(P; o, t) = \sum_{p_i \in P} (x_i(t) - o) \times \boldsymbol{f}_i^{\text{env}}(t). \tag{2.34}$$

The moment resultants are normalized consistently with (2.33):

$$\boldsymbol{m}(P, \varnothing; o, t) = \boldsymbol{m}(\varnothing, Q; o, t) = \boldsymbol{0}, \qquad \boldsymbol{m}^{\text{env}}(\varnothing; o, t) = \boldsymbol{0}. \tag{2.35}$$

We now specialize the force and moment resultants defined in (2.32) and (2.34) to the open subsystem associated with the membership list α. At time t, we choose $P = P_\alpha(t)$ and $Q = P'_\alpha(t)$ in $(2.32)_1$ and $(2.34)_1$. The relevant pair forces are those exerted on particles in $P_\alpha(t)$ by particles in $P'_\alpha(t)$. We use the oriented cut weight (2.28) to select those ordered pairs and express the cut force resultant $\boldsymbol{f}_\alpha^{\text{cut}}(t)$ as

$$\boldsymbol{f}_\alpha^{\text{cut}}(t) = \sum_{i=1}^{N} \sum_{j \neq i} \beta_{ij}^{\alpha}(t) \boldsymbol{f}_{ij}(t) = \boldsymbol{f}(P_\alpha(t), P'_\alpha(t); t) \tag{2.36}$$

and the cut moment resultant $\boldsymbol{m}_\alpha^{\text{cut}}(o, t)$ about o as

$$\boldsymbol{m}_\alpha^{\text{cut}}(o, t) = \sum_{i=1}^{N} \sum_{j \neq i} \beta_{ij}^{\alpha}(t)(x_i(t) - o) \times \boldsymbol{f}_{ij}(t) = \boldsymbol{m}(P_\alpha(t), P'_\alpha(t); o, t). \tag{2.37}$$

For environmental actions, only the subsystem on which the external agencies act must be specified. Thus, at time t, we choose $P = P_\alpha(t)$ in $(2.32)_2$ and $(2.34)_2$. Using the membership values to select the particles in $P_\alpha(t)$, we express the environmental force resultant $\boldsymbol{f}_\alpha^{\text{env}}(t)$ as

$$\boldsymbol{f}_\alpha^{\text{env}}(t) = \sum_{i=1}^{N} \alpha_i(t) \boldsymbol{f}_i^{\text{env}}(t) = \boldsymbol{f}^{\text{env}}(P_\alpha(t); t) \tag{2.38}$$

and the environmental moment resultant $\boldsymbol{m}_\alpha^{\text{env}}(o, t)$ about o as

$$\boldsymbol{m}_\alpha^{\text{env}}(o, t) = \sum_{i=1}^{N} \alpha_i(t)(x_i(t) - o) \times \boldsymbol{f}_i^{\text{env}}(t) = \boldsymbol{m}^{\text{env}}(P_\alpha(t); o, t). \tag{2.39}$$

2.6 Internal and external powers

We next associate power expenditures with the standard forces introduced in Subsection 2.5. For each $t \in I$, a particle-particle force $\boldsymbol{f}_{ij}(t)$ and an environmental force $\boldsymbol{f}_i^{\text{env}}(t)$ are paired with the velocity $\boldsymbol{v}_i(t)$ of the particle on which they act.

For a closed subsystem P of $\mathcal{B}$, the internal power at time t is the power expended on particles in P by pair forces from other particles in P:

$$w^{\text{int}}(P;t) = \sum_{p_i \in P} \sum_{p_j \in P \setminus \{p_i\}} \boldsymbol{f}_{ij}(t) \cdot \boldsymbol{v}_i(t). \tag{2.40}$$

The power expended on particles in P by forces external to P has a cut contribution, due to pair forces from particles in P', and an environmental contribution, due to agencies external to $\mathcal{B}$:

$$w^{\text{cut}}(P;t) = \sum_{p_i \in P} \sum_{p_j \in P'} \boldsymbol{f}_{ij}(t) \cdot \boldsymbol{v}_i(t) \qquad \text{and} \qquad w^{\text{env}}(P;t) = \sum_{p_i \in P} \boldsymbol{f}_i^{\text{env}}(t) \cdot \boldsymbol{v}_i(t). \tag{2.41}$$

The external power on P is the sum of these two contributions:

$$w^{\text{ext}}(P;t) = w^{\text{cut}}(P;t) + w^{\text{env}}(P;t). \tag{2.42}$$

We now specialize the power expenditures defined for an arbitrary closed subsystem P to the time-dependent subsystem associated with a membership list α. This specialization is made only at times at which no membership jump occurs. At any such time $t \in I$, the membership list is locally constant, and the closed subsystem definitions may be applied with $P = P_\alpha(t)$ and $P' = P'_\alpha(t)$. Using the zero-one membership representation (2.11)–(2.13), the complement relation (2.15), and the pair weights $(2.27)_1$ and (2.28), we write the instantaneous powers as sums over all particle labels. The internal power of the open subsystem is

$$w_\alpha^{\text{int}}(t) = \sum_{i=1}^{N} \sum_{j \neq i} \iota_{ij}^{\alpha}(t) \boldsymbol{f}_{ij}(t) \cdot \boldsymbol{v}_i(t) = w^{\text{int}}(P_\alpha(t);t). \tag{2.43}$$

The cut and environmental contributions to the external power are

$$w_\alpha^{\text{cut}}(t) = \sum_{i=1}^{N} \sum_{j \neq i} \beta_{ij}^{\alpha}(t) \boldsymbol{f}_{ij}(t) \cdot \boldsymbol{v}_i(t) = w^{\text{cut}}(P_\alpha(t);t) \tag{2.44}$$

and

$$w_\alpha^{\text{env}}(t) = \sum_{i=1}^{N} \alpha_i(t) \boldsymbol{f}_i^{\text{env}}(t) \cdot \boldsymbol{v}_i(t) = w^{\text{env}}(P_\alpha(t);t). \tag{2.45}$$

Consequently, the instantaneous external power of the open subsystem is

$$w_\alpha^{\text{ext}}(t) = w_\alpha^{\text{cut}}(t) + w_\alpha^{\text{env}}(t) = w^{\text{ext}}(P_\alpha(t);t). \tag{2.46}$$

At membership jump times, we use the jump relation (2.21) to account for changes of content; we do not assign an instantaneous power expenditure to the jump itself.

2.7 Consequences of power invariance

We next record the consequences of requiring that the power expenditures (2.40) and (2.42) for a closed subsystem be frame-indifferent for every closed subsystem P of $\mathcal{B}$. Our arguments are pointwise in time. In algebraic particle-level calculations, we suppress the common time argument on positions, velocities, forces, and membership weights. We retain explicit time arguments in subsystem resultants, powers, and balances when needed to ensure clarity.

2.7.1 Internal-power invariance

We first consider the consequence of frame indifference for the internal power (2.40). For the present power expression, the relevant requirement is invariance under the addition of an arbitrary rigid velocity field $\boldsymbol{c} + \boldsymbol{\omega} \times (x - o)$, where $\boldsymbol{c}$ and $\boldsymbol{\omega}$ are arbitrary vectors. We apply this requirement to doubleton subsystems. For $P = \{p_i, p_j\}$, the change in internal power caused by adding this rigid velocity field is

$$(\boldsymbol{f}_{ij} + \boldsymbol{f}_{ji}) \cdot \boldsymbol{c} + \big((x_i - o) \times \boldsymbol{f}_{ij} + (x_j - o) \times \boldsymbol{f}_{ji}\big) \cdot \boldsymbol{\omega}. \tag{2.47}$$

We require the expression in (2.47) to vanish for all choices of $\boldsymbol{c}$ and $\boldsymbol{\omega}$. The coefficient of $\boldsymbol{c}$ then gives $\boldsymbol{f}_{ij} = -\boldsymbol{f}_{ji}$. With this relation imposed, the coefficient of $\boldsymbol{\omega}$ reduces to $(x_i - x_j) \times \boldsymbol{f}_{ij}$. Hence, for $i \neq j$, we obtain the mutual-action and collinearity relations

$$\boldsymbol{f}_{ij} = -\boldsymbol{f}_{ji} \qquad \text{and} \qquad (x_i - x_j) \times \boldsymbol{f}_{ij} = \boldsymbol{0}. \tag{2.48}$$

We next use the mutual-action relation $(2.48)_1$ to obtain a useful representation of the cut force on an open subsystem. Starting from (2.36), we use the mutual-action relation $(2.48)_1$ to average the ordered-pair sum with its label-interchanged counterpart and invoke the connection (2.31) between $\beta^{\alpha}_{ij} - \beta^{\alpha}_{ji}$ and δ^{α}_{ij} to find that

$$\begin{aligned}
\boldsymbol{f}^{\text{cut}}_{\alpha}(t) &= \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}(\beta^{\alpha}_{ij}\boldsymbol{f}_{ij} + \beta^{\alpha}_{ji}\boldsymbol{f}_{ji}) \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}(\beta^{\alpha}_{ij} - \beta^{\alpha}_{ji})\boldsymbol{f}_{ij} \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}\delta^{\alpha}_{ij}\boldsymbol{f}_{ij}.
\end{aligned} \tag{2.49}$$

We next use the collinearity relation $(2.48)_2$. For the fixed ordered pair (i, j) with $i \neq j$, we write the relative-position vector, its length, and the associated unit orientation as

$$\boldsymbol{r}_{ij} = x_i - x_j, \qquad r_{ij} = |\boldsymbol{r}_{ij}|, \qquad \text{and} \qquad \boldsymbol{n}_{ij} = \frac{\boldsymbol{r}_{ij}}{r_{ij}}, \tag{2.50}$$

respectively. Since the placement is one-to-one, $r_{ij} > 0$ and $\boldsymbol{n}_{ij}$ is well-defined. By $(2.48)_2$, there is a scalar φ_{ij} such that

$$\boldsymbol{f}_{ij} = \varphi_{ij}\boldsymbol{n}_{ij}. \tag{2.51}$$

The mutual-action relation $(2.48)_1$ and the identity $\boldsymbol{n}_{ji} = -\boldsymbol{n}_{ij}$ imply $\varphi_{ji} = \varphi_{ij}$. We also write the relative velocity of p_i with respect to p_j and the rate of change of the distance between these particles as

$$\boldsymbol{v}_{ij} = \boldsymbol{v}_i - \boldsymbol{v}_j \qquad \text{and} \qquad s_{ij} = \dot{r}_{ij} = \boldsymbol{n}_{ij} \cdot \boldsymbol{v}_{ij}. \tag{2.52}$$

For an unordered pair $\{p_i, p_j\}$ contained in a closed subsystem P, the two ordered terms in (2.40) associated with that pair reduce, by $(2.48)_1$, (2.51), and (2.52), to

$$\boldsymbol{f}_{ij} \cdot \boldsymbol{v}_i + \boldsymbol{f}_{ji} \cdot \boldsymbol{v}_j = \varphi_{ij}s_{ij}. \tag{2.53}$$

Summing (2.53) over all unordered pairs in P, or equivalently taking one half of the corresponding ordered-pair sum, we obtain the frame-indifferent representation

$$w^{\text{int}}(P; t) = \frac{1}{2}\sum_{p_i \in P}\sum_{p_j \in P\setminus\{p_i\}}\varphi_{ij}(t)s_{ij}(t). \tag{2.54}$$

2.7.2 External-power invariance

We next impose frame-indifference on the external power in (2.42), again for every closed subsystem P of $\mathcal{B}$. Let $\boldsymbol{c}$ and $\boldsymbol{\omega}$ be arbitrary translational and angular velocities associated with a superposed rigid change of frame at time t. Under this change, the velocity of p_i differs from $\boldsymbol{v}_i(t)$ by $\boldsymbol{c} + \boldsymbol{\omega} \times (x_i(t) - o)$. Inserting this additional velocity in (2.42) and subtracting the original value, we express frame-indifference as

$$(\boldsymbol{f}(P, P'; t) + \boldsymbol{f}^{\mathrm{env}}(P; t)) \cdot \boldsymbol{c} + (\boldsymbol{m}(P, P'; o, t) + \boldsymbol{m}^{\mathrm{env}}(P; o, t)) \cdot \boldsymbol{\omega} = 0 \tag{2.55}$$

for every choice of $\boldsymbol{c}$ and $\boldsymbol{\omega}$. Since we may prescribe $\boldsymbol{c}$ and $\boldsymbol{\omega}$ independently, we obtain the balance of standard forces on P,

$$\boldsymbol{f}(P, P'; t) + \boldsymbol{f}^{\mathrm{env}}(P; t) = \mathbf{0}, \tag{2.56}$$

and the balance of standard moments about o,

$$\boldsymbol{m}(P, P'; o, t) + \boldsymbol{m}^{\mathrm{env}}(P; o, t) = \mathbf{0}. \tag{2.57}$$

The power balance for a closed subsystem follows from the force balance. To derive the power balance, we first choose $P = \{p_i\}$ in (2.56), giving

$$\sum_{p_j \in \mathcal{B} \setminus \{p_i\}} \boldsymbol{f}_{ij} + \boldsymbol{f}_i^{\mathrm{env}} = \mathbf{0}. \tag{2.58}$$

Taking the inner product of (2.58) with $\boldsymbol{v}_i$, summing over all $p_i \in P$, and using (2.40) and (2.42), we obtain

$$w^{\mathrm{int}}(P; t) + w^{\mathrm{ext}}(P; t) = 0. \tag{2.59}$$

We use (2.56), (2.57), and (2.59) for every closed subsystem P of $\mathcal{B}$, including $P = \mathcal{B}$.

2.8 Standard balances for closed subsystems

We have so far included inertia in the environmental force. To obtain the balances for a closed subsystem used below, we separate $\boldsymbol{f}_i^{\mathrm{env}}$ into noninertial and inertial parts:

$$\boldsymbol{f}_i^{\mathrm{env}} = \boldsymbol{f}_i^{\mathrm{ni}} + \boldsymbol{f}_i^{\mathrm{in}}. \tag{2.60}$$

In an inertial frame, we represent the inertial part by

$$\boldsymbol{f}_i^{\mathrm{in}} = -m_i \boldsymbol{a}_i = -\dot{\boldsymbol{p}}_i. \tag{2.61}$$

For a closed subsystem P, we denote the corresponding noninertial environmental force and moment resultants by

$$\boldsymbol{f}^{\mathrm{ni}}(P; t) = \sum_{p_i \in P} \boldsymbol{f}_i^{\mathrm{ni}}(t) \qquad \text{and} \qquad \boldsymbol{m}^{\mathrm{ni}}(P; o, t) = \sum_{p_i \in P} (x_i(t) - o) \times \boldsymbol{f}_i^{\mathrm{ni}}(t). \tag{2.62}$$

We also define the noninertial environmental power by

$$w^{\mathrm{ni}}(P; t) = \sum_{p_i \in P} \boldsymbol{f}_i^{\mathrm{ni}}(t) \cdot \boldsymbol{v}_i(t). \tag{2.63}$$

We now insert (2.60) and (2.61) into the force balance (2.56) and use $(2.62)_1$. This yields the balance of standard momentum for a closed subsystem:

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{p_i \in P} \boldsymbol{p}_i(t) = \boldsymbol{f}(P, P'; t) + \boldsymbol{f}^{\mathrm{ni}}(P; t). \tag{2.64}$$

For angular momentum, we differentiate $\boldsymbol{l}_i(t) = (x_i(t) - o) \times \boldsymbol{p}_i(t)$. Since $(2.4)_1$ gives $\boldsymbol{p}_i(t) = m_i \boldsymbol{v}_i(t)$, the term $\boldsymbol{v}_i(t) \times \boldsymbol{p}_i(t)$ vanishes, and $\dot{\boldsymbol{l}}_i(t) = (x_i(t) - o) \times \dot{\boldsymbol{p}}_i(t)$. We then use this identity, (2.60), (2.61), and $(2.62)_2$ in the moment balance (2.57) to obtain the balance of standard angular momentum for a closed subsystem:

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{p_i \in P} \boldsymbol{l}_i(t) = \boldsymbol{m}(P, P'; o, t) + \boldsymbol{m}^{\mathrm{ni}}(P; o, t). \tag{2.65}$$

For kinetic energy, we use $(2.4)_1$ and $(2.4)_3$ to write $\dot{k}_i = \dot{\boldsymbol{p}}_i \cdot \boldsymbol{v}_i$. We then use this identity, the definitions (2.41) and (2.63), and the relations (2.60) and (2.61) in the power balance (2.59) to obtain the balance of kinetic energy for a closed subsystem:

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{p_i \in P} k_i(t) = w^{\mathrm{int}}(P; t) + w^{\mathrm{cut}}(P; t) + w^{\mathrm{ni}}(P; t). \tag{2.66}$$

Since each particle mass is constant, the total mass of a closed subsystem is conserved:

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{p_i \in P} m_i = 0. \tag{2.67}$$

In Section 3, we pass from these balances for closed subsystems to standard balances for open subsystems. For a zero-one membership list α and times $s, t \in I$ with $s < t$, we use the interior jump times in $J_\alpha(s, t)$ to identify the fixed-membership subintervals between s and t. On those subintervals, we take $P = P_\alpha(r)$ in the closed-subsystem balances. At membership jump times in $(s, t]$, we use the transfer sums in (2.24) to include the mass, standard momentum, angular momentum, and kinetic energy carried by admitted or deleted particles.

3 Standard balances for open subsystems

We now combine the balances for closed subsystems from Subsection 2.8 with the jump-transport relation (2.24). For a zero-one membership list α and times $s, t \in I$ with $s < t$, we use the interior jump times in $J_\alpha(s, t)$ to decompose the time interval into fixed-membership subintervals, as in (2.23). On those subintervals, we use the corresponding closed-subsystem balance with $P = P_\alpha(r)$. At membership jump times, we use the transfer term in (2.24); a jump at t is included because the transfer interval is $(s, t]$, whereas a jump at s is already reflected in the initial content at time s. At a membership jump time, we account only for the quantity carried by the admitted or deleted particles; we do not add a separate jump contribution involving the force, moment, or power resultants. Throughout this section, M_α, $\boldsymbol{\varpi}_\alpha$, $\boldsymbol{\ell}_\alpha$, and K_α denote the content specializations introduced in (2.25), and $\mathcal{A}_\alpha(m; s, t)$, $\mathcal{A}_\alpha(\boldsymbol{p}; s, t)$, $\mathcal{A}_\alpha(\boldsymbol{l}; s, t)$, and $\mathcal{A}_\alpha(k; s, t)$ denote the corresponding cumulative transfer terms introduced in (2.26). Each of these transfer terms is obtained from (2.22) by replacing the generic content a_i with the indicated standard particle quantity.

3.1 Mass balance

For the mass balance, we choose $a_i = m_i$ in (2.24). Since each m_i is constant, $\dot{m}_i = 0$, in agreement with the closed-subsystem mass balance (2.67). The change in mass of the open subsystem over $(s, t]$ is therefore due entirely to cumulative admission and deletion:

$$M_\alpha(t) - M_\alpha(s) = \mathcal{A}_\alpha(m; s, t). \tag{3.1}$$

By (2.22) and (2.26), the term $\mathcal{A}_\alpha(m; s, t)$ in (3.1) is the cumulative transfer of particle masses over the jump times in $(s, t]$. We interpret positive contributions to $\mathcal{A}_\alpha(m; s, t)$ as admitted mass and negative contributions as deleted mass.

3.2 Linear momentum balance

Using (2.13) and $(2.62)_1$, we define the noninertial environmental force on the current value of the open subsystem by

$$\boldsymbol{f}_\alpha^{\mathrm{ni}}(t) = \sum_{i=1}^{N} \alpha_i(t)\boldsymbol{f}_i^{\mathrm{ni}}(t) = \boldsymbol{f}^{\mathrm{ni}}(P_\alpha(t); t). \tag{3.2}$$

We choose $a_i = \boldsymbol{p}_i$ in (2.24). For $r \in (s,t) \setminus J_\alpha(s,t)$, the membership list is fixed on a neighborhood of r, so we may use the closed-subsystem momentum balance (2.64) with $P = P_\alpha(r)$. In terms of (2.36) and (3.2), the continuous integrand in the transport relation is

$$\sum_{i=1}^{N} \alpha_i(r)\dot{\boldsymbol{p}}_i(r) = \boldsymbol{f}_\alpha^{\mathrm{cut}}(r) + \boldsymbol{f}_\alpha^{\mathrm{ni}}(r). \tag{3.3}$$

Using (3.3) in (2.24), we obtain a balance in which the change in standard momentum equals the accumulated cut and noninertial environmental forces plus the momentum transferred by membership jumps:

$$\boldsymbol{\varpi}_\alpha(t) - \boldsymbol{\varpi}_\alpha(s) = \int_s^t (\boldsymbol{f}_\alpha^{\mathrm{cut}}(r) + \boldsymbol{f}_\alpha^{\mathrm{ni}}(r))\,\mathrm{d}r + \mathcal{A}_\alpha(\boldsymbol{p}; s, t). \tag{3.4}$$

On any open interval disjoint from the membership jump set, the transfer sum is empty. Differentiating $\boldsymbol{\varpi}_\alpha$ on such an interval and using (3.3), we obtain the differential form

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\varpi}_\alpha(t) = \boldsymbol{f}_\alpha^{\mathrm{cut}}(t) + \boldsymbol{f}_\alpha^{\mathrm{ni}}(t). \tag{3.5}$$

At a membership jump time τ, the jump in $\boldsymbol{\varpi}_\alpha = \langle \boldsymbol{p} \rangle_\alpha$ comes from the change in the membership multipliers. Using the continuity of the particle momenta at τ in the jump-transport calculation, we choose $a_i = \boldsymbol{p}_i$ in (2.21) and obtain

$$\begin{aligned} \boldsymbol{\varpi}_\alpha(\tau) - \boldsymbol{\varpi}_\alpha(\tau-) &= \sum_{i=1}^{N} \alpha_i(\tau)\boldsymbol{p}_i(\tau) - \sum_{i=1}^{N} \alpha_i(\tau-)\boldsymbol{p}_i(\tau) \\ &= \sum_{i=1}^{N} \boldsymbol{p}_i(\tau)\Delta\alpha_i(\tau). \end{aligned} \tag{3.6}$$

For an elementary admission of p_i at time τ, the sum in (3.6) is $\boldsymbol{p}_i(\tau)$; for an elementary deletion of p_i, it is $-\boldsymbol{p}_i(\tau)$.

3.3 Angular momentum balance

Using (2.13) and $(2.62)_2$, we define the noninertial environmental moment on the current value of the open subsystem, about the point o, by

$$\boldsymbol{m}_\alpha^{\mathrm{ni}}(o,t) = \sum_{i=1}^{N} \alpha_i(t)(x_i(t) - o) \times \boldsymbol{f}_i^{\mathrm{ni}}(t) = \boldsymbol{m}^{\mathrm{ni}}(P_\alpha(t); o, t). \tag{3.7}$$

We choose $a_i = \boldsymbol{l}_i$ in (2.24). For $r \in (s,t) \setminus J_\alpha(s,t)$, the membership list is fixed on a neighborhood of r, so we may use the closed-subsystem angular-momentum balance (2.65) with $P = P_\alpha(r)$. In terms of (2.37) and (3.7), the continuous integrand in the transport relation is

$$\sum_{i=1}^{N} \alpha_i(r)\dot{\boldsymbol{l}}_i(r) = \boldsymbol{m}_\alpha^{\mathrm{cut}}(o,r) + \boldsymbol{m}_\alpha^{\mathrm{ni}}(o,r). \tag{3.8}$$

Using (3.8) in (2.24), we obtain a balance in which the change in standard angular momentum equals the accumulated cut and noninertial environmental moments plus the angular momentum transferred by membership jumps:

$$\boldsymbol{\ell}_\alpha(t) - \boldsymbol{\ell}_\alpha(s) = \int_s^t (\boldsymbol{m}_\alpha^{\mathrm{cut}}(o,r) + \boldsymbol{m}_\alpha^{\mathrm{ni}}(o,r))\,\mathrm{d}r + \mathcal{A}_\alpha(\boldsymbol{l}; s,t). \tag{3.9}$$

On any open interval disjoint from the membership jump set, the transfer sum is empty. Differentiating $\boldsymbol{\ell}_\alpha$ on such an interval and using (3.8), we obtain the differential form

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\ell}_\alpha(t) = \boldsymbol{m}_\alpha^{\mathrm{cut}}(o,t) + \boldsymbol{m}_\alpha^{\mathrm{ni}}(o,t). \tag{3.10}$$

At a membership jump time τ, the jump in $\boldsymbol{\ell}_\alpha = \langle \boldsymbol{l} \rangle_\alpha$ comes from the change in the membership multipliers. Using the continuity of the particle momenta at τ in the jump-transport calculation, we choose $a_i = \boldsymbol{l}_i$ in (2.21) and obtain

$$\begin{aligned} \boldsymbol{\ell}_\alpha(\tau) - \boldsymbol{\ell}_\alpha(\tau-) &= \sum_{i=1}^N \alpha_i(\tau)\boldsymbol{l}_i(\tau) - \sum_{i=1}^N \alpha_i(\tau-)\boldsymbol{l}_i(\tau) \\ &= \sum_{i=1}^N \boldsymbol{l}_i(\tau)\Delta\alpha_i(\tau). \end{aligned} \tag{3.11}$$

For an elementary admission of p_i at time τ, the sum in (3.11) is $\boldsymbol{l}_i(\tau)$; for an elementary deletion of p_i, it is $-\boldsymbol{l}_i(\tau)$.

3.4 Kinetic-energy balance

For the kinetic-energy balance, the relevant closed-subsystem balance involves the internal, cut, and noninertial environmental powers. Using (2.13) and (2.63), we define the noninertial environmental power on the current value of the open subsystem by

$$w_\alpha^{\mathrm{ni}}(t) = \sum_{i=1}^N \alpha_i(t)\boldsymbol{f}_i^{\mathrm{ni}}(t)\cdot\boldsymbol{v}_i(t) = w^{\mathrm{ni}}(P_\alpha(t);t). \tag{3.12}$$

We choose $a_i = k_i$ in (2.24). For $r \in (s,t) \setminus J_\alpha(s,t)$, the membership list is fixed on a neighborhood of r, so we may use the closed-subsystem kinetic-energy balance (2.66) with $P = P_\alpha(r)$. In terms of (2.43), (2.44), and (3.12), the continuous integrand in the transport relation is

$$\sum_{i=1}^N \alpha_i(r)\dot{k}_i(r) = w_\alpha^{\mathrm{int}}(r) + w_\alpha^{\mathrm{cut}}(r) + w_\alpha^{\mathrm{ni}}(r). \tag{3.13}$$

Using (3.13) in (2.24), we obtain a balance in which the change in kinetic energy equals the accumulated internal, cut, and noninertial environmental powers plus the kinetic energy transferred by membership jumps:

$$K_\alpha(t) - K_\alpha(s) = \int_s^t (w_\alpha^{\mathrm{int}}(r) + w_\alpha^{\mathrm{cut}}(r) + w_\alpha^{\mathrm{ni}}(r))\,\mathrm{d}r + \mathcal{A}_\alpha(k;s,t). \tag{3.14}$$

On any open interval disjoint from the membership jump set, the transfer sum is empty. Differentiating K_α on such an interval and using (3.13), we obtain the differential form

$$\frac{\mathrm{d}}{\mathrm{d}t}K_\alpha(t) = w_\alpha^{\mathrm{int}}(t) + w_\alpha^{\mathrm{cut}}(t) + w_\alpha^{\mathrm{ni}}(t). \tag{3.15}$$

By (2.22) and (2.26), the term $\mathcal{A}_\alpha(k; s, t)$ in (3.14) is the cumulative transfer of kinetic energy carried by particles admitted to or deleted from the open subsystem during $(s, t]$.

At a membership jump time τ, the jump in $K_\alpha = \langle k \rangle_\alpha$ comes from the change in the membership multipliers. Using the continuity of the particle momenta at τ in the jump-transport calculation, we choose $a_i = k_i$ in (2.21) and obtain

$$\begin{aligned} K_\alpha(\tau) - K_\alpha(\tau-) &= \sum_{i=1}^{N} \alpha_i(\tau) k_i(\tau) - \sum_{i=1}^{N} \alpha_i(\tau-) k_i(\tau) \\ &= \sum_{i=1}^{N} k_i(\tau) \Delta\alpha_i(\tau). \end{aligned} \tag{3.16}$$

For an elementary admission of p_i at time τ, the sum in (3.16) is $k_i(\tau)$; for an elementary deletion of p_i, it is $-k_i(\tau)$.

In the balances formulated above, we use the two mechanisms described in Subsection 2.3. On each fixed-membership subinterval, where r denotes the running time, we use the corresponding closed-subsystem balance with $P = P_\alpha(r)$. Over the full interval $(s, t]$, the cumulative transfer terms listed in (2.26) collect the mass, standard momentum, angular momentum, and kinetic energy carried by particles whose memberships jump. At a single jump time $\tau \in J_\alpha(s, t)$, (2.21) gives the corresponding instantaneous change in content, with signs determined by the values $\Delta\alpha_i(\tau)$. We do not supplement these jump contributions with additional terms involving force, moment, or power resultants.

4 Configurational momentum balance for open subsystems

We now introduce a configurational counterpart of the standard momentum balance developed in Section 3. Our purpose in this section is limited: we introduce configurational momentum, configurational force resultants, and the corresponding balance for open subsystems. In this balance, we account for configurational contact and body force resultants associated with changes of subsystem membership. It is not a replacement for, or a modification of, the standard momentum balance; instead, it is a separate balance for the membership degree of freedom. At this stage, the specific configurational momentum is primitive, just as configurational stress is primitive in Gurtin's [5, 6] continuum theory. When we impose the working and intrinsicity requirements below, we obtain its value as the negative of the standard velocity; no independent particle velocity is therefore retained.

For each particle p_i, let $\boldsymbol{u}_i(t) \in \mathcal{V}$ denote the specific configurational momentum assigned to p_i at time $t \in I$.The configurational momentum content of the open subsystem associated with the membership list α is equal to

$$\boldsymbol{\mu}_\alpha(t) = \sum_{i=1}^{N} \alpha_i(t) m_i \boldsymbol{u}_i(t). \tag{4.1}$$

Equivalently, $\boldsymbol{\mu}_\alpha = \langle m\boldsymbol{u} \rangle_\alpha$, where $m\boldsymbol{u}$ denotes the list $(m_1\boldsymbol{u}_1, \dots, m_N\boldsymbol{u}_N)$.

We next introduce the configurational force resultants used in the configurational momentum balance. For arbitrary disjoint subsets P and Q of $\mathcal{B}$, we write $\boldsymbol{c}(P, Q; t)$ for the configurational contact-force resultant associated with the ordered cut from P to Q. For a subsystem P, we write $\boldsymbol{g}(P; t)$ and $\boldsymbol{e}(P; t)$ for the internal and external configurational force resultants on P. To include empty cuts without further qualification, we use the normalizations

$$\boldsymbol{c}(P, \varnothing; t) = \boldsymbol{c}(\varnothing, Q; t) = \mathbf{0}, \qquad \boldsymbol{g}(\varnothing; t) = \boldsymbol{e}(\varnothing; t) = \mathbf{0}. \tag{4.2}$$

For the open subsystem associated with the membership list α, these resultants specialize to

$$\boldsymbol{c}_\alpha^{\mathrm{cut}}(t) = \boldsymbol{c}(P_\alpha(t), P'_\alpha(t); t), \qquad \boldsymbol{g}_\alpha(t) = \boldsymbol{g}(P_\alpha(t); t), \qquad \boldsymbol{e}_\alpha(t) = \boldsymbol{e}(P_\alpha(t); t). \tag{4.3}$$

For a closed subsystem P of $\mathcal{B}$, we take the configurational momentum balance to be

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{p_i\in P} m_i\boldsymbol{u}_i(t) = \boldsymbol{c}(P,P';t) + \boldsymbol{g}(P;t) + \boldsymbol{e}(P;t). \tag{4.4}$$

The balance (4.4) is the discrete counterpart of Gurtin's [6, eqn. (5–8)] configurational force balance. In Gurtin's framework, a configurational stress represents the contact traction across the boundary of a migrating control volume, and configurational body forces act within that volume. In the present discrete setting, the contact resultant $\boldsymbol{c}(P,P';t)$ is the resultant configurational contact action across the ordered cut, while $\boldsymbol{g}(P;t)$ and $\boldsymbol{e}(P;t)$ are the resultants of the internal and external configurational body-forces.

We now pass from the closed-subsystem balance (4.4) to the open subsystem associated with α. For a zero-one membership list α and times $s,t\in I$ with $s<t$, we choose $a_i = m_i\boldsymbol{u}_i$ in the jump-transport relation (2.24). For $r\in(s,t)\setminus J_\alpha(s,t)$, the membership list is fixed on a neighborhood of r, so we may use (4.4) with $P=P_\alpha(r)$. In terms of the resultants in (4.3), the continuous integrand in the transport relation is

$$\sum_{i=1}^{N}\alpha_i(r)m_i\dot{\boldsymbol{u}}_i(r) = \boldsymbol{c}_\alpha^{\mathrm{cut}}(r) + \boldsymbol{g}_\alpha(r) + \boldsymbol{e}_\alpha(r). \tag{4.5}$$

Using (4.5) in (2.24), we obtain a balance in which the change in configurational momentum equals the accumulated configurational contact, internal, and external forces plus the configurational momentum transferred by membership jumps:

$$\boldsymbol{\mu}_\alpha(t) - \boldsymbol{\mu}_\alpha(s) = \int_s^t \left(\boldsymbol{c}_\alpha^{\mathrm{cut}}(r) + \boldsymbol{g}_\alpha(r) + \boldsymbol{e}_\alpha(r)\right)\mathrm{d}r + \mathcal{A}_\alpha(m\boldsymbol{u};s,t). \tag{4.6}$$

The cumulative transfer term in (4.6) is the configurational momentum carried by particles admitted to or deleted from the open subsystem during $(s,t]$:

$$\mathcal{A}_\alpha(m\boldsymbol{u};s,t) = \sum_{\tau\in J_\alpha(s,t)}\sum_{i=1}^{N} m_i\boldsymbol{u}_i(\tau)\Delta\alpha_i(\tau). \tag{4.7}$$

On any open interval disjoint from the membership jump set, the transfer sum is empty. Differentiating $\boldsymbol{\mu}_\alpha$ on such an interval and using (4.5), we obtain the differential form

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\mu}_\alpha(t) = \boldsymbol{c}_\alpha^{\mathrm{cut}}(t) + \boldsymbol{g}_\alpha(t) + \boldsymbol{e}_\alpha(t). \tag{4.8}$$

At a membership jump time τ, we use (2.21) with $a_i = m_i\boldsymbol{u}_i$ and write the corresponding jump in configurational momentum content as

$$\boldsymbol{\mu}_\alpha(\tau) - \boldsymbol{\mu}_\alpha(\tau-) = \sum_{i=1}^{N} m_i\boldsymbol{u}_i(\tau)\Delta\alpha_i(\tau). \tag{4.9}$$

For an elementary admission of p_i at time τ, the sum in (4.9) is $m_i\boldsymbol{u}_i(\tau)$; for an elementary deletion of p_i, it is $-m_i\boldsymbol{u}_i(\tau)$. Thus, in the open configurational momentum balance, the time integral represents continuous evolution on fixed-membership subintervals, while the transfer term represents configurational momentum carried by admitted or deleted particles at membership jump times. We have so far introduced only the configurational momentum balance. In the next section, we introduce the working of the configurational forces and use intrinsicity to determine the relation between $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$ and to obtain a preliminary representation of the configurational contact-force resultant.

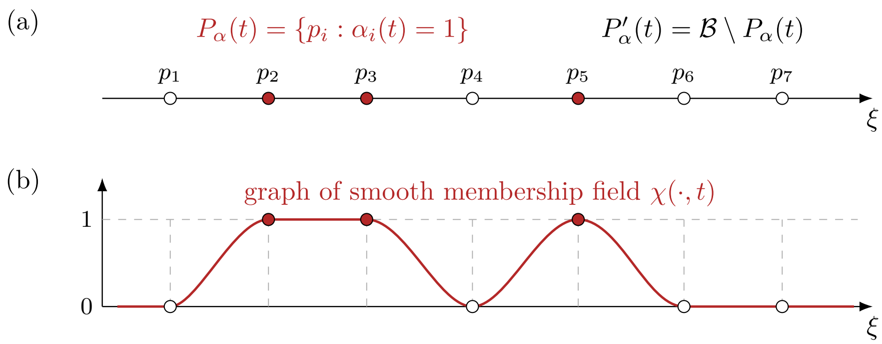

Figure 3: One-dimensional schematic of zero-one and smooth membership descriptions at a fixed time t. (a) The open subsystem $P_\alpha(t) = \{p_i : \alpha_i(t) = 1\}$ consists of the displayed particles with $\alpha_i(t) = 1$, while the complementary subsystem is $P'_\alpha(t) = \mathcal{B} \setminus P_\alpha(t)$. The horizontal coordinate ξ is used only to order the displayed particle positions. (b) Along the same schematic coordinate ξ, we draw a smooth membership profile whose values at the displayed particle positions agree with the zero-one values in (a). The graph in (b) is used only for visualization; the smooth membership field in the theory is $\chi : \mathcal{E} \times I \to [0, 1]$, and its smooth values $\theta_i(t) = \chi(x_i(t), t)$ need not be zero or unity unless a zero-one specialization is imposed.

5 Smooth membership fields, working, and intrinsicity

In Sections 3 and 4, we used zero-one membership lists and explicit jump transfers. Those balances separate continuous evolution on fixed-membership subintervals from admission and deletion at membership jump times.To formulate the intrinsicity requirement developed below, we require a local normal direction associated with membership change. Since such a direction cannot be defined from a zero-one membership list alone, we introduce a smooth membership field $\chi : \mathcal{E} \times I \to [0, 1]$ and an observed velocity field for its level sets. Throughout Sections 5 and 6, the symbol α_i remains reserved for the zero-one membership values of Sections 2–4. For the smooth membership value of p_i, we write $\theta_i(t) = \chi(x_i(t), t)$. The scalar θ_i is a smooth bookkeeping variable attached to p_i by the auxiliary field. We use θ_i to regularize admission or deletion and $\dot{\theta}_i$ as the associated membership-transfer rate. In zero-one specializations and zero-one jump limits, θ_i is required only to match or approach α_i at the relevant particle positions. For a particle p_i, the level set of $\chi(\cdot, t)$ through $x_i(t)$ plays the role of a local membership cut, the vector $\boldsymbol{h}_i(t) = -(\operatorname{grad}\chi)(x_i(t), t)$ is normal to that cut, and we use the observed level-set velocity to introduce the tangential freedom needed for the intrinsicity argument. For a fixed time t, we use the one-dimensional schematic in Figure 3 to compare zero-one membership data $\{\alpha_i(t)\}_{i=1}^N$ with a smooth membership profile drawn as a function of a schematic spatial coordinate ξ. The lower panel is only a visualization of a zero-one specialization: in the theory, $\chi : \mathcal{E} \times I \to [0, 1]$, and the values $\theta_i(t) = \chi(x_i(t), t)$ need not be zero or unity unless a zero-one specialization or a zero-one jump limit is explicitly invoked.

When a zero-one specialization is imposed at a fixed time t, the smooth field is chosen so that $\theta_i(t) = \alpha_i(t)$ at the relevant particle positions. A regularized admission or deletion is represented by a smooth change of θ_i whose integral rate tends to the corresponding jump $\Delta\alpha_i$ in the zero-one limit.

5.1 Smooth membership fields and tangential freedom

Let $\chi : \mathcal{E} \times I \to [0, 1]$ be a smooth membership field on $\mathcal{E}$. We use an observed level-set velocity field $\boldsymbol{w}$ to describe the motion of the level sets of χ by requiring that

$$\frac{\partial \chi}{\partial t}(x, t) + (\operatorname{grad}\chi)(x, t) \cdot \boldsymbol{w}(x, t) = 0 \tag{5.1}$$

for each $x \in \mathcal{E}$ and each $t \in I$. The field $\boldsymbol{w}$ is not a material velocity. Rather, it is an observed velocity field for the level sets of χ: along any curve $r \mapsto z(r)$ satisfying $\dot{z}(r) = \boldsymbol{w}(z(r), r)$, the value $\chi(z(r), r)$ is constant. In this respect, $\boldsymbol{w}$ is the spatial-membership analogue of the velocity field assigned to the boundary of a migrating control volume in Gurtin's [5, 6] formulation.

At the position $x_i(t)$ of p_i at time t, we write

$$\theta_i(t) = \chi(x_i(t), t), \qquad \boldsymbol{h}_i(t) = -(\operatorname{grad}\chi)(x_i(t), t), \qquad \text{and} \qquad \boldsymbol{w}_i(t) = \boldsymbol{w}(x_i(t), t). \tag{5.2}$$

If $\boldsymbol{h}_i(t) \neq \boldsymbol{0}$, then $\boldsymbol{h}_i(t)$ is normal to the level set of $\chi(\cdot, t)$ through $x_i(t)$ and points in the direction of decreasing membership. Thus, when χ approximates the characteristic membership of a subsystem, with values near unity in the high-membership region and values near zero in the low-membership region, $\boldsymbol{h}_i(t)$ points from the former toward the latter.

We do not assume that χ is normalized. In particular, χ is not a signed-distance function. For $\boldsymbol{h}_i(t) \neq \boldsymbol{0}$, the corresponding unit normal is $\boldsymbol{h}_i(t)/|\boldsymbol{h}_i(t)|$, and the scalar normal velocity of the level set, at $x_i(t)$, in that direction is

$$V_i(t) = \frac{1}{|\boldsymbol{h}_i(t)|}\frac{\partial \chi}{\partial t}(x, t)\Big|_{x=x_i(t)}. \tag{5.3}$$

To quantify the rate at which the membership of p_i changes, we differentiate $(5.2)_1$ along the trajectory of p_i:

$$\dot\theta_i(t) = \frac{\mathrm{d}}{\mathrm{d}t}\chi(x_i(t), t) = \Big(\frac{\partial \chi}{\partial t}(x, t) + (\operatorname{grad}\chi)(x, t)\cdot \dot x_i(t)\Big)\Big|_{x=x_i(t)}. \tag{5.4}$$

The following particle-level calculations are pointwise in time. We therefore suppress the common time argument on θ_i, $\boldsymbol{h}_i$, $\boldsymbol{w}_i$, $\boldsymbol{v}_i$, and related particle-level quantities. Using $(2.3)_1$, the transport relation (5.1) evaluated at the particle place, and the definitions $(5.2)_2$ and $(5.2)_3$ of $\boldsymbol{h}_i$ and $\boldsymbol{w}_i$, we rewrite (5.4) as

$$\dot\theta_i = \boldsymbol{h}_i \cdot (\boldsymbol{w}_i - \boldsymbol{v}_i). \tag{5.5}$$

For a prescribed smooth membership field χ and a prescribed particle trajectory, the right-hand side of (5.5) involves $\boldsymbol{w}_i$ only through its component in the direction of $\boldsymbol{h}_i$.

To express the relative motion of the level set and the particle with the sign convention used for migrating control volumes, we define

$$\boldsymbol{q}_i = \boldsymbol{w}_i - \boldsymbol{v}_i. \tag{5.6}$$

Using (5.6) in (5.5), we express the membership rate as

$$\dot\theta_i = \boldsymbol{h}_i \cdot \boldsymbol{q}_i. \tag{5.7}$$

We use (5.7) to identify the nonintrinsic part of the observed velocity. Suppose that $\boldsymbol{h}_i \neq \boldsymbol{0}$. At the time under consideration, let $\boldsymbol{\tau}_i$ be an arbitrary vector and replace $\boldsymbol{w}_i$ by $\boldsymbol{w}_i + \boldsymbol{\tau}_i$. The values of θ_i and $\dot\theta_i$ are unchanged by this replacement whenever

$$\boldsymbol{\tau}_i \cdot \boldsymbol{h}_i = 0. \tag{5.8}$$

Thus, for fixed χ and fixed particle trajectory, the component of $\boldsymbol{w}_i$ tangent to the level set of χ through x_i may be changed without changing either the membership value θ_i or its rate $\dot\theta_i$. The corresponding normal representative of the observed velocity at a point with $\boldsymbol{h}_i \neq \boldsymbol{0}$ is $\boldsymbol{w}_i^{\perp} = V_i\boldsymbol{h}_i/|\boldsymbol{h}_i|$. We do not choose this representative at the outset. The tangential part of $\boldsymbol{w}_i$ is nonintrinsic, and invariance of the working with respect to changes of that tangential part is the condition from which the configurational cut relation follows. After intrinsicity has been imposed, the normal representative may be used in computations without changing the intrinsic relations. This tangential freedom is the particle-level analogue of the freedom in the tangential part of the velocity field assigned to the boundary of a migrating control volume in Gurtin's [5, 6] formulation. We illustrate this pointwise freedom in Figure 4: at a particle with $\boldsymbol{h}_i \neq \boldsymbol{0}$, replacing $\boldsymbol{q}_i = \boldsymbol{w}_i - \boldsymbol{v}_i$ by $\boldsymbol{q}_i + \boldsymbol{\tau}_i$, with $\boldsymbol{h}_i \cdot \boldsymbol{\tau}_i = 0$, changes only the tangential part of the observed relative velocity and leaves $\dot\theta_i = \boldsymbol{h}_i \cdot \boldsymbol{q}_i$ unchanged.

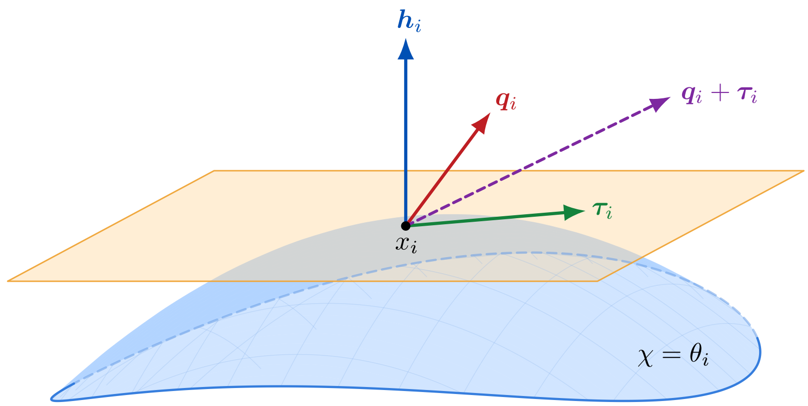

Figure 4: Tangential freedom in the smooth membership-field description. The translucent blue surface is the level set $\chi = \theta_i$ passing through the point x_i occupied by particle p_i, and the translucent orange plane is tangent to that level set at x_i. The vector $\boldsymbol{h}_i = -(\operatorname{grad}\chi)(x_i, \cdot)$ (blue arrow) is normal to the level set and points in the direction of decreasing membership. The vector $\boldsymbol{\tau}_i$ (green arrow) lies in the tangent plane, so that $\boldsymbol{h}_i \cdot \boldsymbol{\tau}_i = 0$. Hence, replacing the relative velocity $\boldsymbol{q}_i = \boldsymbol{w}_i - \boldsymbol{v}_i$ (red arrow) by $\boldsymbol{q}_i + \boldsymbol{\tau}_i$ (dashed purple arrow) does not change the membership rate, since $\dot{\theta}_i = \boldsymbol{h}_i \cdot \boldsymbol{q}_i = \boldsymbol{h}_i \cdot (\boldsymbol{q}_i + \boldsymbol{\tau}_i)$.

5.2 Smooth cut weights and standard cut-force assignments

Although the membership values defined from χ need not be zero or unity, we retain the algebraic form of the oriented cut weight (2.28) and define the smooth cut weight

$$\beta_{ij}^{\theta} = \theta_i(1 - \theta_j). \tag{5.9}$$

If the smooth membership values are specialized to the zero-one list α, then β_{ij}^{θ} reduces to β_{ij}^{α} and is equal to unity precisely when $(i, j) \in \partial P_\alpha$. For the smooth membership-field description, we use β_{ij}^{θ} as a weighted cut selector.

Guided by the cut-force representation (2.36), we define the standard cut-force assignment to p_i by

$$\boldsymbol{f}_i^{\chi} = \sum_{j \neq i} \beta_{ij}^{\theta} \boldsymbol{f}_{ij}. \tag{5.10}$$

By summing the particlewise assignments in (5.10), we obtain the corresponding weighted standard cut-force resultant:

$$\sum_{i=1}^{N} \boldsymbol{f}_i^{\chi} = \boldsymbol{f}_{\theta}^{\mathrm{cut}}. \tag{5.11}$$

Thus $\boldsymbol{f}_i^{\chi}$ is the contributionassociated with the weighted cut pair forces acting on p_i. The resultant $\boldsymbol{f}_{\theta}^{\mathrm{cut}}$ is a smooth-membership analogue of the zero-one cut force $\boldsymbol{f}_{\alpha}^{\mathrm{cut}}$.

5.3 Inadequacy of standard-only working

We next examine what would follow from applying intrinsicity to a working involving only standard cut forces. Suppose, for this purpose, that the cut working associated with the observed velocity field $\boldsymbol{w}$ is

$$\mathcal{W}_{\chi}^{\mathrm{std}} = \sum_{i=1}^{N} (\boldsymbol{f}_i^{\chi} + \dot{\theta}_i \boldsymbol{p}_i) \cdot \boldsymbol{w}_i. \tag{5.12}$$

The term $\dot{\theta}_i \boldsymbol{p}_i$ accounts for standard momentum carried by membership transfer.

We now replace $\boldsymbol{w}_i$ by $\boldsymbol{w}_i + \boldsymbol{\tau}_i$, with $\boldsymbol{\tau}_i$ satisfying (5.8). By the discussion in Subsection 5.1, this replacement

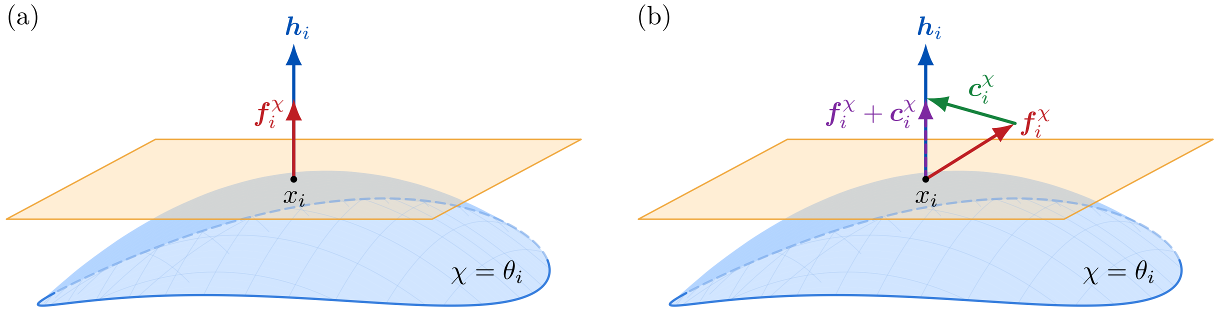

Figure 5: Standard-only obstruction and configurational resolution. In both panels, the translucent blue surface is the level surface $\chi = \theta_i$ passing through the point x_i occupied by particle p_i, and the translucent orange plane is tangent to that level surface at x_i. The vector $\boldsymbol{h}_i$ (blue arrow) is normal to the level surface. (a) For a working involving only the standard cut force $\boldsymbol{f}_i^\chi$ (red arrow), tangential invariance leads to $\boldsymbol{f}_i^\chi \parallel \boldsymbol{h}_i$, so that $\boldsymbol{f}_i^\chi$ must be normal to the level surface. (b) With the configurational cut force $\boldsymbol{c}_i^\chi$ (green arrow) included, tangential invariance leads to $\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi \parallel \boldsymbol{h}_i$, so that the combined cut force $\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi$ (dashed purple arrow) is normal to the level surface while $\boldsymbol{f}_i^\chi$ (red arrow) may have a tangential component.

changes neither θ_i nor $\dot{\theta}_i$. Intrinsicity of the standard-only working (5.12) would require

$$\sum_{i=1}^{N} (\boldsymbol{f}_i^\chi + \dot{\theta}_i \boldsymbol{p}_i) \cdot \boldsymbol{\tau}_i = 0 \tag{5.13}$$

for every family of tangential vectors satisfying (5.8). Since those vectors may be prescribed independently, (5.13) implies that, for each particle with $\boldsymbol{h}_i \neq \boldsymbol{0}$, there is a scalar λ_i^χ such that

$$\boldsymbol{f}_i^\chi + \dot{\theta}_i \boldsymbol{p}_i = \lambda_i^\chi \boldsymbol{h}_i. \tag{5.14}$$

We cannot accept (5.14) as a restriction on standard cut forces. In particular, for $\dot{\theta}_i = 0$, it follows from (5.14) that $\boldsymbol{f}_i^\chi$ must be normal to the level set of χ through x_i. That level set is part of the chosen smooth membership-field description; it is not a physical constraint on standard pair forces. Thus, an artificial normality condition would be the consequence of stipulating that the standard-only working be instrinsic.

This obstruction is the particle-level counterpart of the continuum difficulty identified by Podio-Guidugli [9]: a theory using only standard forces cannot, in general, account for the response associated with evolving material structures. We therefore introduce a configurational cut-force assignment. For each i, let $\boldsymbol{c}_i^\chi$ denote the configurational cut force assigned to p_i. We choose these particlewise contributions so that their sum equals the configurational contact-force resultant associated with the smooth membership cut:

$$\sum_{i=1}^{N} \boldsymbol{c}_i^\chi = \boldsymbol{c}_\theta^{\text{cut}}. \tag{5.15}$$

We use (5.15) as the spatial-membership counterpart of $(4.3)_1$. We interpret $\boldsymbol{c}_i^\chi$ as a particlewise share of the configurational contact resultant associated with the chosen smooth membership cut, not as a constitutive prescription. At the finite-particle level, the construction consists of labels and finite sums rather than tractions per unit area. We introduce a traction representation only in Section 7, as a localization hypothesis, where $\boldsymbol{c}_i^\chi$ is represented to leading order by the traction $\boldsymbol{C}\boldsymbol{a}_i^\chi$. With the configurational cut-force assignment now in place, we use Figure 5 to compare the artificial normality condition obtained from the standard-only working with the corresponding normality condition imposed on the combined standard-plus-configurational cut force.

5.4 Cut working

Having introduced the configurational cut-force assignment, we formulate the part of the open-system working that involves the observed velocity field $\boldsymbol{w}$. Following the structure used by Gurtin [5, 6] for migrating control volumes and by Anderson et al. [7] for migrating spatial control volumes, we include both contact forces and momentum transferred by membership change. The use of $\boldsymbol{w}_i$ in the standard part of the cut working does not replace the usual standard power $\boldsymbol{f}_i^\chi \cdot \boldsymbol{v}_i$ on a fixed-membership subsystem. Since $\boldsymbol{w}_i = \boldsymbol{v}_i + \boldsymbol{q}_i$, the product $\boldsymbol{f}_i^\chi \cdot \boldsymbol{w}_i$ contains the usual cut-power term $\boldsymbol{f}_i^\chi \cdot \boldsymbol{v}_i$ and the transfer contribution $\boldsymbol{f}_i^\chi \cdot \boldsymbol{q}_i$. This is the particle-level analogue of the standard traction working with the velocity following a migrating boundary in Gurtin's theory. If the standard cut force were paired only with $\boldsymbol{v}_i$, the standard stress contribution would be absent from the localized Eshelby relation.

In the standard force system, we pair the effective cut force $\boldsymbol{f}_i^\chi + \dot{\theta}_i \boldsymbol{p}_i$ with the observed velocity $\boldsymbol{w}_i$. In the configurational force system, we pair the effective cut force $\boldsymbol{c}_i^\chi + \dot{\theta}_i m_i \boldsymbol{u}_i$ with the relative velocity $\boldsymbol{q}_i$. We therefore define the cut working by

$$\mathcal{W}_\chi^{\mathrm{cut}} = \sum_{i=1}^{N} (\boldsymbol{f}_i^\chi + \dot{\theta}_i \boldsymbol{p}_i) \cdot \boldsymbol{w}_i + \sum_{i=1}^{N} (\boldsymbol{c}_i^\chi + \dot{\theta}_i m_i \boldsymbol{u}_i) \cdot \boldsymbol{q}_i. \tag{5.16}$$

The terms involving $\dot{\theta}_i \boldsymbol{p}_i$ and $\dot{\theta}_i m_i \boldsymbol{u}_i$ account for standard and configurational momentum carried by membership transfer.

5.5 Intrinsicity and the preliminary cut relation

We now impose intrinsicity on the cut working (5.16). Under tangential changes of the observed velocity satisfying (5.8), neither the membership value nor the membership rate changes. We therefore require $\mathcal{W}_\chi^{\mathrm{cut}}$ to be unchanged under all such tangential changes. This requirement is the discrete analogue of Gurtin's [5, 6] invariance with respect to changes in the tangential part of the velocity field assigned to the boundary of a migrating control volume. It is also the particle-level counterpart of the intrinsicity requirement used by Anderson et al. [7] for migrating spatial control volumes in the theory of sharp fluid-fluid phase interfaces.

We carry out the intrinsicity argument pointwise in time, holding the particle state, the smooth membership field χ, and the cut-force assignments fixed. For each particle with $\boldsymbol{h}_i \neq \boldsymbol{0}$, let $\boldsymbol{\tau}_i$ satisfy (5.8); for particles with $\boldsymbol{h}_i = \boldsymbol{0}$, set $\boldsymbol{\tau}_i = \boldsymbol{0}$. Replacing $\boldsymbol{w}_i$ by $\boldsymbol{w}_i + \boldsymbol{\tau}_i$ also replaces $\boldsymbol{q}_i$ by $\boldsymbol{q}_i + \boldsymbol{\tau}_i$. For particles with $\boldsymbol{h}_i \neq \boldsymbol{0}$, (5.7) and (5.8) show that $\dot{\theta}_i$ is unchanged; for particles with $\boldsymbol{h}_i = \boldsymbol{0}$, no perturbation is made. The difference between the modified and original values of the cut working must therefore vanish by intrinsicity:

$$\sum_{i=1}^{N} (\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi + \dot{\theta}_i (\boldsymbol{p}_i + m_i \boldsymbol{u}_i)) \cdot \boldsymbol{\tau}_i = 0 \tag{5.17}$$

for every such family of vectors $\boldsymbol{\tau}_i$. Since the vectors assigned to particles with $\boldsymbol{h}_i \neq \boldsymbol{0}$ may be prescribed independently subject only to (5.8), the vector $\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi + \dot{\theta}_i (\boldsymbol{p}_i + m_i \boldsymbol{u}_i)$ must be orthogonal to every tangent vector to the level set of χ at x_i. Consequently, for each particle with $\boldsymbol{h}_i \neq \boldsymbol{0}$, there is a scalar π_i^χ such that

$$\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi + \dot{\theta}_i (\boldsymbol{p}_i + m_i \boldsymbol{u}_i) = \pi_i^\chi \boldsymbol{h}_i. \tag{5.18}$$

The pointwise relations obtained from tangential freedom are imposed only at particles for which $\boldsymbol{h}_i \neq \boldsymbol{0}$. These particles constitute the active part of the smooth membership cut. When $\boldsymbol{h}_i = \boldsymbol{0}$, no local level-set normal is available and no tangential-invariance condition is imposed at that particle. Unless explicitly stated otherwise, the pointwise cut relations below are understood on the active part of the smooth membership cut. We refer to (5.18) as a preliminary Eshelby-type cut relation. In this relation, the effective standard-plus-configurational cut force assigned to p_i is normal to the local level set of χ.

5.6 Configurational momentum and the reduced cut relation

To extract the configurational momentum relation from (5.18), we use a local admissibility property of the smooth membership-field description. At a particle with $\boldsymbol{h}_i \neq \mathbf{0}$, we allow the normal component of $\boldsymbol{q}_i$ to be varied while the particle state, the membership value, the cut normal, and the force assignments are held fixed. Granted that $\boldsymbol{h}_i \neq \mathbf{0}$, we also allow its direction to be prescribed locally by changing the membership field χ while holding the corresponding membership value θ_i fixed.

The only term in (5.18) that remains to be reduced is the term multiplied by the membership rate $\dot{\theta}_i$. We now use the freedom in the normal component of the observed velocity. For a particle with $\boldsymbol{h}_i \neq \mathbf{0}$, we compare two choices of the normal component of $\boldsymbol{q}_i$ that leave the particle state, the membership value, the cut normal, and the force assignments unchanged. By (5.7), these choices give distinct values of $\dot{\theta}_i$. Writing (5.18) for the two choices and subtracting the resulting relations, we find that $\boldsymbol{p}_i + m_i\boldsymbol{u}_i$ must be parallel to $\boldsymbol{h}_i$.

The direction of a nonzero $\boldsymbol{h}_i$ can be prescribed locally by the choice of the smooth membership field while leaving the membership value at the position x_i of particle p_i fixed. Thus $\boldsymbol{p}_i + m_i\boldsymbol{u}_i$ must be parallel to every possible direction of $\boldsymbol{h}_i$, and therefore must be consistent with

$$\boldsymbol{p}_i + m_i\boldsymbol{u}_i = \mathbf{0}. \tag{5.19}$$

We read (5.19) as a particlewise configurational momentum relation: the configurational momentum carried by p_i is the negative of its standard momentum. Using $(2.4)_1$, we write this relation equivalently as

$$\boldsymbol{u}_i = -\boldsymbol{v}_i. \tag{5.20}$$

Thus $\boldsymbol{u}_i$ is the discrete particlewise counterpart of the continuum specific configurational momentum obtained by Anderson et al. [7].

Substituting (5.19) in (5.18), we obtain the reduced cut relation

$$\boldsymbol{f}_i^{\chi} + \boldsymbol{c}_i^{\chi} = \pi_i^{\chi}\boldsymbol{h}_i. \tag{5.21}$$

Equivalently, the configurational cut-force assignment has the representation

$$\boldsymbol{c}_i^{\chi} = \pi_i^{\chi}\boldsymbol{h}_i - \boldsymbol{f}_i^{\chi}. \tag{5.22}$$

We call the scalar π_i^{χ} the particlewise membership tension associated with p_i. Intrinsicity does not determine π_i^{χ}. This quantity is the particle-level analogue of the bulk tension in Gurtin's [5, 6] pre-Eshelby relation. In Section 6, we identify π_i^{χ} by combining the interaction-energy imbalance with the configurational mechanical-energy imbalance for smooth membership-field descriptions and then specializing to nondissipative membership transfer.

6 Energetic identification of the particlewise membership tension

At the end of Section 5, we used intrinsicity to obtain the configurational momentum relation (5.20) and the reduced cut relation (5.21). The particlewise membership tension π_i^{χ} remains undetermined. We now identify this scalar from a mechanical energy imbalance for smooth membership-field descriptions. Since the membership values in this section are defined from a smooth field, we use a rate form of the imbalance. The corresponding zero-one jump statement is obtained by integrating the rate form across a regularized admission or deletion and passing to the jump limit.

In this section, $\theta_i(t) = \chi(x_i(t), t)$ denotes the membership value defined from χ at the position $x_i(t)$ of p_i at time t. The rate calculations are pointwise in time. After this convention is stated, we suppress the common time argument on particle quantities, membership values, pair energies, powers, and cut-force assignments, except when values at jump times or continuum localizations are being discussed. We use w_{θ}^{int},

w_θ^{cut}, and w_θ^{ni} for the algebraic expressions in (2.43), (2.44), and (3.12), respectively, with the zero-one values α_i replaced by the smooth values θ_i; in a zero-one specialization, these powers reduce to their α-counterparts.

6.1 Interaction energy and membership increments

For each pair of particle labels, let ψ_{ij} denote an interaction energy, with self-interaction excluded and pair interaction symmetric:

$$\psi_{ij} = \psi_{ji} \qquad \text{and} \qquad \psi_{ii} = 0. \tag{6.1}$$

We do not use ψ_{ij} to prescribe the force $\boldsymbol{f}_{ij}$. Thus no force law is introduced. For the smooth membership list $\theta = (\theta_1, \ldots, \theta_N)$, we define the weighted interaction-energy content by

$$\Psi_\theta = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}\theta_i\theta_j\psi_{ij}. \tag{6.2}$$

The coefficient of a change in the membership value θ_i in (6.2) is the membership interaction-energy increment

$$\psi_i^\theta = \sum_{j\neq i}\theta_j\psi_{ij}. \tag{6.3}$$

For zero-one membership, we write $\Psi(P)$ for (6.2) evaluated with θ_j equal to the characteristic membership of the subsystem P. If $p_i \notin P$, then admission of p_i changes the interaction energy by

$$\psi_i^\alpha = \Psi(P \cup \{p_i\}) - \Psi(P). \tag{6.4}$$

If $p_i \in P$, deletion of p_i changes the interaction energy by $-\psi_i^\alpha$, where ψ_i^α denotes the zero-one specialization of (6.3).

Assume that the quantities ψ_{ij} are differentiable in time. Differentiating (6.2) and using the symmetry condition $(6.1)_1$, we write the interaction-energy rate as the sum of a fixed-membership part and a membership-transfer part:

$$\dot{\Psi}_\theta = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}\theta_i\theta_j\dot{\psi}_{ij} + \sum_{i=1}^{N}\dot{\theta}_i\psi_i^\theta. \tag{6.5}$$

We interpret the first term on the right-hand side of (6.5) as the rate associated with changes of the pair interaction energies at fixed membership, and the second as the rate associated with membership transfer. We use this decomposition to define the residual dissipation associated with fixed-membership changes of interaction energy and internal power:

$$\mathscr{D}_\theta^{\mathrm{int}} = -\Big(\frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}\theta_i\theta_j\dot{\psi}_{ij} + w_\theta^{\mathrm{int}}\Big). \tag{6.6}$$

Using (6.5), we also write

$$\mathscr{D}_\theta^{\mathrm{int}} = -\Big(\dot{\Psi}_\theta + w_\theta^{\mathrm{int}} - \sum_{i=1}^{N}\dot{\theta}_i\psi_i^\theta\Big). \tag{6.7}$$

For constant membership values, $\mathscr{D}_\theta^{\mathrm{int}}$ is the residual dissipation associated with interaction-energy change and internal power. For varying membership values, $\mathscr{D}_\theta^{\mathrm{int}}$ is the fixed-membership contribution to the total residual dissipation introduced below.

6.2 Mechanical energy imbalance for smooth membership-field descriptions

The weighted kinetic-energy content associated with the smooth membership values is

$$K_\theta = \sum_{i=1}^{N} \theta_i k_i. \tag{6.8}$$

To compute the rate of K_θ, we use the differentiable transport identity. We multiply the closed-subsystem kinetic-energy balance (2.66) with $P = \{p_i\}$ by θ_i, sum over i, and split each pair contribution with $\theta_i = \theta_i\theta_j + \theta_i(1-\theta_j)$. This gives

$$\dot{K}_\theta = w_\theta^{\mathrm{int}} + w_\theta^{\mathrm{cut}} + w_\theta^{\mathrm{ni}} + \sum_{i=1}^{N} \dot{\theta}_i k_i. \tag{6.9}$$

We take the mechanical energy imbalance for smooth membership-field descriptions to be of the form

$$\mathscr{D}_\theta = \mathcal{W}_\chi^{\mathrm{cut}} + w_\theta^{\mathrm{ni}} - \dot{K}_\theta - \dot{\Psi}_\theta \geq 0. \tag{6.10}$$

Here, $\mathscr{D}_\theta$ is the total residual dissipation for the weighted subsystem defined by the smooth membership values. The cut working $\mathcal{W}_\chi^{\mathrm{cut}}$ is the configurational form of the power supplied across the membership cut; no second, independent energy imbalance is imposed.

We next reduce the cut working in (5.16). The relation $\boldsymbol{q}_i = \boldsymbol{w}_i - \boldsymbol{v}_i$ gives $\boldsymbol{w}_i = \boldsymbol{v}_i + \boldsymbol{q}_i$, while (5.19) gives $m_i\boldsymbol{u}_i = -\boldsymbol{p}_i$. Using these identities together with the definition (5.10) of $\boldsymbol{f}_i^\chi$, we write

$$\begin{aligned} \mathcal{W}_\chi^{\mathrm{cut}} &= \sum_{i=1}^{N} (\boldsymbol{f}_i^\chi + \dot{\theta}_i \boldsymbol{p}_i) \cdot (\boldsymbol{v}_i + \boldsymbol{q}_i) + \sum_{i=1}^{N} (\boldsymbol{c}_i^\chi - \dot{\theta}_i \boldsymbol{p}_i) \cdot \boldsymbol{q}_i \\ &= w_\theta^{\mathrm{cut}} + \sum_{i=1}^{N} (\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi) \cdot \boldsymbol{q}_i + \sum_{i=1}^{N} \dot{\theta}_i\, \boldsymbol{p}_i \cdot \boldsymbol{v}_i. \end{aligned} \tag{6.11}$$

The kinetic identity $\boldsymbol{p}_i \cdot \boldsymbol{v}_i = 2k_i$, the membership-rate relation (5.7), and the reduced cut relation (5.21) allow us to reduce (6.11) to

$$\mathcal{W}_\chi^{\mathrm{cut}} = w_\theta^{\mathrm{cut}} + \sum_{i=1}^{N} \dot{\theta}_i (2k_i + \pi_i^\chi). \tag{6.12}$$

The term $2k_i$ in (6.12) comes from the identity $\boldsymbol{p}_i \cdot \boldsymbol{v}_i = m_i|\boldsymbol{v}_i|^2 = 2k_i$.

We now substitute (6.9), (6.5), and (6.12) into the mechanical energy imbalance (6.10). Using the definition (6.6) of $\mathscr{D}_\theta^{\mathrm{int}}$, we obtain the relation

$$\mathscr{D}_\theta = \mathscr{D}_\theta^{\mathrm{int}} + \sum_{i=1}^{N} (k_i + \pi_i^\chi - \psi_i^\theta)\dot{\theta}_i. \tag{6.13}$$

Thus, requiring (6.10) is equivalent to requiring nonnegative values of the right-hand side of (6.13). We interpret the first term in (6.13) as the residual dissipation associated with fixed-membership changes of particle-particle interaction energy and internal power. We interpret the remaining sum as the residual contribution associated with membership transfer.

The rate form (6.13) has a corresponding interpretation in the zero-one membership setting. Suppose that smooth membership values regularize an admission or deletion over a small time interval containing a jump time τ. If k_i, π_i^χ, and ψ_i^θ converge uniformly to their limiting values over that interval, and if the limiting zero-one interaction-energy increment is written as $\psi_i^\alpha(\tau)$, then integration of the membership-transfer contribution in (6.13) gives, in the zero-one jump limit,

$$\sum_{i=1}^{N}(k_i(\tau) + \pi_i^\chi(\tau) - \psi_i^\alpha(\tau))\Delta\alpha_i(\tau). \tag{6.14}$$

For an elementary admission of p_i, the factor multiplying the jump is $k_i + \pi_i^\chi - \psi_i^\alpha$ in the zero-one notation; for an elementary deletion, the sign of this factor is reversed. The nondissipative identification below is therefore the same whether membership transfer is represented by a smooth membership rate or by a zero-one jump limit.

6.3 Nondissipative membership transfer

To identify the particlewise membership tension π_i^χ without introducing a kinetic law for membership transfer, we now restrict attention to nondissipative membership transfer. We use this term for a state at which admissible regularized membership variations include both signs of $\dot{\theta}_i$ while the remaining state variables are held fixed, and for which the membership-transfer contribution to the residual dissipation vanishes for those variations. For each such particle, the coefficient of $\dot{\theta}_i$ in (6.13), equivalently the factor multiplying $\Delta\alpha_i$ in (6.14), must vanish:

$$k_i + \pi_i^\chi - \psi_i^\theta = 0. \tag{6.15}$$

The scalar multiplying $\boldsymbol{h}_i$ in the reduced cut relation is therefore

$$\pi_i^\chi = \psi_i^\theta - k_i. \tag{6.16}$$

For zero-one membership, if $p_i \notin P$, (6.4) gives the corresponding admission value

$$\pi_i^\chi = \Psi(P \cup \{p_i\}) - \Psi(P) - k_i. \tag{6.17}$$

Thus, we may interpret the particlewise membership tension π_i^χ as the interaction-energy increment associated with admitting p_i, corrected by the kinetic energy carried by that particle.

Using (6.16) in (5.21), we obtain the energetically identified cut relation

$$\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi = (\psi_i^\theta - k_i)\boldsymbol{h}_i. \tag{6.18}$$

Equivalently, the configurational cut-force assignment has the representation

$$\boldsymbol{c}_i^\chi = (\psi_i^\theta - k_i)\boldsymbol{h}_i - \boldsymbol{f}_i^\chi. \tag{6.19}$$

If membership transfer is dissipative, we retain (6.13) as an admissibility condition. Additional constitutive information would then be needed to determine departures of π_i^χ from the nondissipative value (6.16).

7 Continuum representations of particlewise configurational relations

The configurational momentum relation (5.20) and the energetically identified cut relation (6.18) belong to the finite-system theory developed above. They involve quantities carried by the labeled elements of $\mathcal{B}$, the smooth membership values θ_i, the cut normals $\boldsymbol{h}_i$ defined from χ, and the force assignments associated with the membership cut. We have so far used χ only to assign those local cuts, normals, and level-set velocities; we have not yet introduced continuum bulk fields such as the standard velocity field $\boldsymbol{v}$, the specific configurational momentum field $\boldsymbol{u}$, the mass density ρ, the specific free energy ψ, or the standard and configurational stresses $\boldsymbol{T}$ and $\boldsymbol{C}$. To obtain continuum counterparts, we must add a localizing family and leading-order continuum representations for the extensive quantities already present in the finite-system relations.

In the localizing family, p_i represents a small current spatial volume $\Delta V_i(t)$ centered at its current place $x_i(t)$. Since (5.20) is a specific relation, we need only compare $\boldsymbol{v}_i$ and $\boldsymbol{u}_i$ with the corresponding smooth fields at $x_i(t)$. For the cut relation (6.18), the terms to be localized are extensive. We represent the assigned cut forces by tractions acting over the area vector associated with the membership cut, and we represent the energetic scalar $\psi_i^\theta - k_i$ by a continuum energy density multiplied by $\Delta V_i(t)$.

In introducing this localizing family, we make no constitutive specification of the particle-particle interactions. Specifically, we neither prescribe ψ_{ij} nor $\boldsymbol{f}_{ij}$ through the localization, and we do not derive $\boldsymbol{T}$ by averaging a specified pair-force law. Constitutive choices for the interactions are a separate matter: once a law for the interaction energies is supplied, thermodynamic compatibility constrains the associated pair forces, so laws for ψ_{ij} and $\boldsymbol{f}_{ij}$ cannot be prescribed independently. In the localization step below, we assume only the leading-order continuum representations for the quantities that already enter the particlewise relations. With these representations in hand, we translate the particlewise configurational momentum and cut-force relations into continuum field relations and identify the continuum counterpart of $(\psi_i^\theta - k_i)/\Delta V_i(t)$.

7.1 Localization of configurational momentum

The relation (5.20) is specific, or per unit mass. For a member of the localizing family, we represent the particle velocity and the specific configurational momentum by values of smooth continuum fields at the current place of the particle:

$$\boldsymbol{v}_i(t) = \boldsymbol{v}(x_i(t), t) \qquad \text{and} \qquad \boldsymbol{u}_i(t) = \boldsymbol{u}(x_i(t), t). \tag{7.1}$$

Combining (7.1) with (5.20), we obtain, at the sampled places,

$$\boldsymbol{u}(x_i(t), t) = -\boldsymbol{v}(x_i(t), t). \tag{7.2}$$

For any continuum point x and time t, we may choose a localizing sequence for which the current particle places $x_i(t)$ approach x. Passing from the sampled relation (7.2) to the corresponding field relation, we recover the spatial continuum relation obtained by Anderson et al. [7]: the specific configurational momentum is the negative of the standard velocity,

$$\boldsymbol{u} = -\boldsymbol{v}. \tag{7.3}$$

7.2 Localization of the cut relation

We recall the energetically identified cut relation (6.18) and write it pointwise in time, while keeping explicit time arguments in the continuum representations. The particlewise relation to be localized is

$$\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi = (\psi_i^\theta - k_i)\boldsymbol{h}_i. \tag{7.4}$$

To localize the factors in (7.4), we first specify the local geometry. At the time t under consideration, suppose that, in a member of the localizing family, p_i represents a small current spatial volume $\Delta V_i(t) > 0$ centered at $x_i(t)$. Since χ is dimensionless, $\boldsymbol{h}_i(t)\Delta V_i(t)$ has the dimension of area. In the localization ansatz, we use

$$\boldsymbol{a}_i^\chi(t) = \boldsymbol{h}_i(t)\Delta V_i(t) \tag{7.5}$$

as the area vector associated with the membership cut near p_i. If χ approximates the characteristic membership of a region, with values near unity inside the region and near zero outside it, then $\boldsymbol{a}_i^\chi(t)$ approximates the outward area vector associated with the smooth membership cut.

We next introduce smooth tensor fields $\boldsymbol{T}$ and $\boldsymbol{C}$, interpreted respectively as the standard Cauchy stress and the spatial configurational stress. We use these fields only to represent, to leading order, the assigned cut forces as tractions over the membership-cut area vector $\boldsymbol{a}_i^\chi(t)$; in particular, we do not prescribe a microscopic interaction law or derive $\boldsymbol{T}$ by averaging a specified pair-force law. Thus,

$$\boldsymbol{f}_i^{\chi}(t) \sim \boldsymbol{T}(x_i(t),t)\boldsymbol{a}_i^{\chi}(t) \qquad \text{and} \qquad \boldsymbol{c}_i^{\chi}(t) \sim \boldsymbol{C}(x_i(t),t)\boldsymbol{a}_i^{\chi}(t). \tag{7.6}$$

At the same current volume scale, we relate the particle mass to the continuum mass density by

$$m_i \sim \rho(x_i(t),t)\Delta V_i(t). \tag{7.7}$$

With ψ denoting the continuum-level specific free energy, we then represent the membership interaction-energy increment and the kinetic energy of p_i, to leading order, by

$$\psi_i^{\theta}(t) \sim \rho(x_i(t),t)\psi(x_i(t),t)\Delta V_i(t) \qquad \text{and} \qquad k_i(t) \sim \frac{1}{2}\rho(x_i(t),t)|\boldsymbol{v}(x_i(t),t)|^2\Delta V_i(t). \tag{7.8}$$

Consequently, the extensive scalar $\psi_i^{\theta}(t) - k_i(t)$ has the local representation

$$\psi_i^{\theta}(t) - k_i(t) \sim \rho(x_i(t),t)\Big(\psi(x_i(t),t) - \frac{1}{2}|\boldsymbol{v}(x_i(t),t)|^2\Big)\Delta V_i(t). \tag{7.9}$$

We now insert the traction representations (7.6) and the energetic representation (7.9) into (7.4), with all particle-level factors evaluated at the same time. Since $\Delta V_i(t) > 0$, cancellation of the common factor gives the localized traction relation

$$(\boldsymbol{T}(x_i(t),t) + \boldsymbol{C}(x_i(t),t))\boldsymbol{h}_i(t) = \rho(x_i(t),t)\Big(\psi(x_i(t),t) - \frac{1}{2}|\boldsymbol{v}(x_i(t),t)|^2\Big)\boldsymbol{h}_i(t). \tag{7.10}$$

The relation (7.10) is a traction relation in the direction of the cut normal. To pass from this traction relation to a tensor relation, we require the same local representations for smooth membership fields whose nonzero gradients at $x_i(t)$ have arbitrary directions, while the continuum fields at $(x_i(t),t)$ are held fixed. Since we may prescribe the direction of $\boldsymbol{h}_i(t)$ arbitrarily under that requirement, we find from (7.10) that

$$\boldsymbol{T}(x_i(t),t) + \boldsymbol{C}(x_i(t),t) = \rho(x_i(t),t)\Big(\psi(x_i(t),t) - \frac{1}{2}|\boldsymbol{v}(x_i(t),t)|^2\Big)\boldsymbol{1}. \tag{7.11}$$

From (7.9), the quotient $(\psi_i^{\theta} - k_i)/\Delta V_i(t)$, or equivalently $\pi_i^{\chi}/\Delta V_i(t)$ in the nondissipative case, has the continuum counterpart $\rho(\psi - \frac{1}{2}|\boldsymbol{v}|^2)$. Thus, solving (7.11) for the configurational stress and replacing the sampled place by a generic continuum point, we recover the pointwise spatial inertial Eshelby relation obtained by Anderson et al. [7]:

$$\boldsymbol{C} = \rho\Big(\psi - \frac{1}{2}|\boldsymbol{v}|^2\Big)\boldsymbol{1} - \boldsymbol{T}. \tag{7.12}$$

8 Discussion

We have developed a particle-level route to configurational forces by translating Gurtin's [5, 6] continuum description of transfer across a nonmaterial migrating control-volume boundary into a discrete description based on time-dependent membership. In the zero-one membership setting, we evaluate continuous terms on fixed-membership subintervals and account for admission and deletion through transfer sums over membership jump times. In the smooth membership-field setting, we introduce the geometric and kinematic data used in the intrinsicity argument: the level sets of χ, normals to the local cuts, observed level-set velocities, and the associated tangential freedom. With these two descriptions, we obtain two particle-level configurational relations before introducing continuum bulk fields. The first is the configurational momentum relation $m_i\boldsymbol{u}_i = -\boldsymbol{p}_i$, or equivalently $\boldsymbol{u}_i = -\boldsymbol{v}_i$. The second is the energetically identified cut relation $\boldsymbol{f}_i^{\chi} + \boldsymbol{c}_i^{\chi} = (\psi_i^{\theta} - k_i)\boldsymbol{h}_i$, or equivalently $\boldsymbol{c}_i^{\chi} = (\psi_i^{\theta} - k_i)\boldsymbol{h}_i - \boldsymbol{f}_i^{\chi}$.

The particle-level route serves a different purpose from Gurtin's [5, 6] continuum formulation. In Gurtin's theory, material transfer is described through a nonmaterial migrating control-volume boundary and through the velocity assigned to that boundary. We do not view this construction as deficient. Instead, we ask what discrete structure can play the corresponding role in a finite particle system. We represent transfer by admission and deletion of particles and write the balances in terms of particle-carried quantities and the signs of membership jumps. With this representation, we separate continuous evolution on fixed-membership intervals from transfer by admission or deletion, and we derive the relations $m_i \boldsymbol{u}_i = -\boldsymbol{p}_i$ and $\boldsymbol{f}_i^\chi + \boldsymbol{c}_i^\chi = (\psi_i^\theta - k_i)\boldsymbol{h}_i$ before introducing continuum bulk fields. Thus, the particle-level formulation is useful not because it replaces the migrating-control-volume construction, but because it identifies a possible discrete origin of the configurational momentum and cut-force relations.

The same change of description also entails restrictions on the particle-level route. With a zero-one membership list, we specify which particles are admitted or deleted, but we do not obtain a local normal or a tangential descriptor for the intrinsicity argument. We therefore introduce the auxiliary smooth membership field χ and use it only to define level sets, normals to local cuts, observed level-set velocities, and tangential freedom. In addition, the particle-level relations do not contain continuum stresses, mass density, or free-energy density. To compare the particlewise relations with continuum field relations, we impose the localization hypotheses of Section 7. For continuum problems in which migrating control volumes and continuum fields are already natural primitives, Gurtin's [5, 6] formulation is more direct. The present formulation is complementary: we use it to identify possible particle-level origins of configurational momentum and pre-Eshelby cut relations, and we recover continuum relations only after introducing the auxiliary membership-field description and imposing formal localization hypotheses.

The need for the configurational cut-force assignment appears when we impose intrinsicity on a cut working that contains only the standard cut-force assignment and the standard momentum carried by membership transfer. In that case, we obtain the normality condition (5.14). For $\dot{\theta}_i = 0$, acceptance of that condition would require the standard cut-force assignment to be normal to the level set of the chosen smooth membership field. Since that level set belongs to the description of membership and not to the standard force system, we cannot accept this as a restriction on standard pair forces. We therefore introduce the configurational cut-force assignment $\boldsymbol{c}_i^\chi$ before seeking a representation for it. With this configurational cut-force assignment included in the cut working, intrinsicity requires normality of the combined effective standard-plus-configurational cut force, rather than of the standard cut-force assignment alone. This is the particle-level counterpart of Podio-Guidugli's [9] conclusion that standard forces alone are insufficient to account for evolving material structures.

The identification of the membership tension was made under the nondissipative specialization of membership transfer. Outside that specialization, we retain (6.13) as an admissibility condition. The scalar $k_i + \pi_i^\chi - \psi_i^\theta$ is the membership-transfer affinity conjugate to the rate $\dot{\theta}_i$, and admissibility requires nonnegative residual dissipation for the allowed affinity-rate pairs. This admissibility condition can serve as a starting point for kinetic modeling: in the nondissipative specialization, the affinity vanishes; in a dissipative theory, additional constitutive information would be needed to relate the affinity, the rate $\dot{\theta}_i$, and the departure of π_i^χ from the nondissipative value (6.16). In continuum theories of vacancies, substitutional and interstitial impurities, dislocations, cracks, grain boundaries, twin boundaries, and phase interfaces, such constitutive information is often supplied by a relation between the configurational driving force on the evolving material structure and the conjugate velocity with which that structure migrates. There are important antecedents in finite elasticity. Knowles [10] considered equilibrium states in which the deformation is continuous while the deformation gradient has bounded jumps across smooth surfaces satisfying the Hadamard compatibility condition, and he associated a dissipation condition with quasi-static families of such stationary gradient discontinuities. Abeyaratne [11] later introduced an admissibility condition in the same setting. Abeyaratne and Knowles [12, 13] subsequently formulated the driving traction and treated the relation between driving traction and interface velocity as a constitutive kinetic relation. In his configurational-force formulation, Gurtin [5, 6] obtained analogous evolution equations by supplementing configurational balances with thermodynamically consistent constitutive assumptions.

To compare the particle-level relations with continuum field relations, we impose the localization hypotheses introduced in Section 7; our use of those hypotheses is formal. For the configurational momentum relation, we impose only a sampling assumption for specific quantities and obtain the continuum relation $\boldsymbol{u} = -\boldsymbol{v}$. For the cut relation, we assume leading-order traction representations for the assigned cut forces and a density representation for the extensive scalar $\psi_i^\theta - k_i$. With these assumptions, and with arbitrary directions of the membership-cut area vector, we obtain the spatial inertial Eshelby relation $\boldsymbol{C} = \rho(\psi - \frac{1}{2}|\boldsymbol{v}|^2)\boldsymbol{1} - \boldsymbol{T}$. We do not prescribe pair potentials or pair-force laws from which $\boldsymbol{T}$, $\boldsymbol{C}$, or ψ would be computed by an averaging theorem; rather, we assume leading-order local representations for the quantities already present in the particlewise configurational relations. We view this localization argument as part of the broader point-particle-to-continuum tradition initiated by Irving and Kirkwood [14], clarified by Noll [15], extended by Hardy [16] and by Murdoch and Bedeaux [17], and examined more recently by DiCarlo and Podio-Guidugli [18]. Thus, localization is used here only after the needed continuum representations have been stated explicitly.

Several extensions remain open. Pair interaction energies were used only to identify the membership tension; if many-particle interaction energies are included, we would replace ψ_i^θ by the appropriate insertion or deletion increment in the zero-one membership setting, or by the coefficient conjugate to $\dot{\theta}_i$ in a smooth membership description. If interfacial energy is included, we would add lower-dimensional energetic increments and corresponding configurational working. For lower-dimensional defect structures, we would attach membership variables to carriers other than individual particles, such as bonds, faces, or defect cores. Stochastic forcing would require a nondeterministic or an averaged counterpart of the pathwise balance structure. If particle-particle interactions are dissipative, we would include their contribution in the internal residual dissipation. In each case, the details of the particle-level accounting would change, but we would retain the same central steps: use changes of membership as the discrete kinematical degree of freedom, impose intrinsicity to obtain configurational momentum and pre-Eshelby cut relations, and rely on a mechanical energy imbalance to identify the membership tension when membership transfer is nondissipative.

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References

[1] J. D. Eshelby. The force on an elastic singularity, *Philosophical Transactions of the Royal Society of London. Series A* **244** (1951), 87–112.

[2] J. D. Eshelby. The continuum theory of lattice defects, in *Solid State Physics*, Vol. 3, edited by F. Seitz and D. Turnbull, Academic Press, New York, 1956, pp. 79–144.

[3] J. D. Eshelby. Energy relations and the energy-momentum tensor in continuum mechanics, in *Inelastic Behavior of Solids*, edited by M. F. Kanninen, W. F. Adler, A. R. Rosenfield, and R. I. Jaffee, McGraw–Hill, New York, 1970, pp. 77–115.

[4] J. D. Eshelby, The elastic energy-momentum tensor, *Journal of Elasticity* **5** (1975), 321–335.

[5] M. E. Gurtin. The nature of configurational forces, *Archive for Rational Mechanics and Analysis* **131** (1995), 67–100.

[6] M. E. Gurtin. *Configurational Forces as Basic Concepts of Continuum Physics.* Applied Mathematical Sciences, Vol. 137. Springer, New York, 2000.

[7] D. M. Anderson, P. Cermelli, E. Fried, M. E. Gurtin, and G. B. McFadden. General dynamical sharp-interface conditions for phase transformations in viscous heat-conducting fluids, *Journal of Fluid Mechanics* **581** (2007), 323–370.

[8] J. L. Ericksen. Remarks concerning forces on line defects. *Zeitschrift für angewandte Mathematik und Physik* **46** (1995), S247–S271.

[9] P. Podio-Guidugli. Configurational forces: are they needed? *Mechanics Research Communications* **29** (2002), 513–519.

[10] J. K. Knowles. On the dissipation associated with equilibrium shocks in finite elasticity. *Journal of Elasticity* **9** (1979), 131–158.

[11] R. Abeyaratne. An admissibility condition for equilibrium shocks in finite elasticity. *Journal of Elasticity* **13** (1983), 175–184.

[12] R. Abeyaratne and J. K. Knowles. On the driving traction acting on a surface of strain discontinuity in a continuum. *Journal of the Mechanics and Physics of Solids* **38** (1990), 345–360.

[13] R. Abeyaratne and J. K. Knowles. Kinetic relations and the propagation of phase boundaries in solids. *Archive for Rational Mechanics and Analysis* **114** (1991), 119–154.

[14] J. H. Irving and J. G. Kirkwood. The statistical mechanical theory of transport processes. IV. The equations of hydrodynamics. *Journal of Chemical Physics* **18** (1950), 817–829.

[15] W. Noll. Die Herleitung der Grundgleichungen der Thermomechanik der Kontinua aus der statistischen Mechanik. *Journal of Rational Mechanics and Analysis* **4** (1955), 627–646.

[16] R. J. Hardy. Formulas for determining local properties in molecular-dynamics simulations: Shock waves. *Journal of Chemical Physics* **76** (1982), 622–628.

[17] A. I. Murdoch and D. Bedeaux. Continuum equations of balance via weighted averages of microscopic quantities. *Proceedings of the Royal Society of London Series A, Mathematical, Physical and Engineering Sciences* **445** (1994), 157–179.

[18] A. DiCarlo and P. Podio-Guidugli. From point particles to body points. *Mathematics in Engineering* **4** (2022), 1–29.