A general formalism for the mechanics of discrete systems and continuous media, with a view to concurrent molecular-continuum simulations

Lecture Notes for the Spring Course
Hierarchical multiscale methods using the Andersen-Parrinello-Rahman formulation of molecular dynamics
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1 The impulse functional and its balance

Force and impulse Impulse is force integrated over time. However, since integral quantities antecede their densities, it is force that should be defined as the time density of the impulse (whenever it is well defined). Force is dual to velocity. More precisely, it is a linear functional on the vector space of the velocity fields instantaneously defined over the body manifold. Its value is the power expended, i.e., another density: work per unit time. Again, it is better to consider the impulse as a linear functional on the vector space of the velocity fields defined over the body-time manifold, i.e., over the product of the body manifold times a time interval. Its value is the work done over that lapse of time.

Work and balance The basic dynamical infrastructure of this general formalism is encapsulated in the abstract formula

$$\mathcal{W} = \langle\, \mathbf{i} \,|\, \mathfrak{w} \,\rangle\,, \tag{1.0.1}$$

where $\mathbf{i}$ is the impulse functional, $\mathfrak{w}$ the velocity field on which $\mathbf{i}$ is evaluated, and the value of the duality bracket $\langle\, \cdot \,|\, \cdot \,\rangle$ is the work $\mathcal{W}$. To stress the crucial fact that the impulse has to be tested for balance on *all* the kinematically admissible velocity fields, the field $\mathfrak{w}$ entering (1.0.1) is labelled as *test* velocity. Correspondingly, $\mathcal{W}$ is often called *virtual*, to emphasize that it is *not* the work done on the velocity actually realized along the motion under consideration. Balance is enforced by requiring that the (virtual) work $\mathcal{W}$ be null for all test velocity $\mathfrak{w}$.

In each of the following subsections, (1.0.1) will be instantiated in a concrete, physically motivated representation. All of these representations—very different in detail from one another—share the following structural features:

i) the work has physical dimension *energy*:

$$[\mathcal{W}] = \mathtt{E}\,, \tag{1.0.2}$$

so that the physical dimensions of $\mathbf{i}$ and $\mathfrak{w}$ have to compensate each other;

ii) the impulse functional $\mathbf{i}$ admits of an integral representation in terms of densities on the relevant body-time manifold;

iii) the above representation is comprised of an integral over the body-time manifold and an integral over its boundary.[†]

[†]The boundary of a product manifold has a Leibniz-like property: $\partial(\mathscr{B}\times\mathscr{T}) = \partial\mathscr{B}\times\mathscr{T}\cup\mathscr{B}\times\partial\mathscr{T}$.

Time-scale gap Thinking in terms of time-integrated quantities is essential when trying to transfer physical information between theories modelling the same phenomenon on vastly different time scales. The (nominally) instantaneous value of a macroscopic quantity observed on a coarse time scale appears as a time average, when the corresponding microscopic quantity is observed on a much finer scale.

1.1 Impulse balance for a bunch of particles in 3D

Discrete system Independently of the number of particles—supposedly finite, or at most countably infinite—, a particle system is a 0D body embedded in a 3D Euclidean space. The relevant body-time manifold is the product $\mathsf{P}\times[\tau_-,\tau_+]$ of the set $\mathsf{P}=\{1,\dots,N\}$ endowed with the discrete topology (identified with the 0D body) times the time interval $[\tau_-,\tau_+]$. Its boundary is comprised of two 0D time cuts $\mathsf{P}\times\{\tau_\mp\}$ (since $\partial\mathsf{P}=\emptyset$). A superposed dot denotes differentiation with respect to time. All densities on the 1D body-time manifold are taken with respect to the time duration measure $d\tau$.

Impulse functional In this case, the space of test velocities is comprised of the collection of all smoothly differentiable particle velocities:

$$[\tau_-,\tau_+]\ni\tau\mapsto\big(\mathbf{w}_1(\tau),\dots,\mathbf{w}_N(\tau)\big)\,, \tag{1.1.1}$$

and the work done on the test velocity $\big(\mathbf{w}_i|\,i\in\mathsf{P}\big)$ is assumed to be

$$\mathcal{W}=\int_{\tau_-}^{\tau_+}d\tau\sum_{i\in\mathsf{P}}\big(\mathbf{f}_i\cdot\mathbf{w}_i+\mathbf{p}_i\cdot\dot{\mathbf{w}}_i\big)-\Big[\sum_{i\in\mathsf{P}}\boldsymbol{\varpi}_i\cdot\mathbf{w}_i\Big]_{\tau_-}^{\tau_+}\,. \tag{1.1.2}$$

Here and in what follows a superposed dot denotes time differentiation. In (1.1.2), the impulse is parameterized by $2N$ vector-valued functions of time, $\big(\mathbf{f}_i|\,i\in\mathsf{P}\big)$ and $\big(\mathbf{p}_i|\,i\in\mathsf{P}\big)$, and $2N$ vectors, $\big(\boldsymbol{\varpi}_i(\tau_-)|\,i\in\mathsf{P}\big)$ and $\big(\boldsymbol{\varpi}_i(\tau_+)|\,i\in\mathsf{P}\big)$. Since $\mathbf{w}_i$ has physical dimension *length/time* ($[\mathbf{w}_i]=\mathtt{L/T}$), the *force applied* to the i-th particle has dimension $\mathtt{E/L}$. The *momentum* $\mathbf{p}_i$ and the two *boundary momenta* of the i-th particle, $\boldsymbol{\varpi}_i(\tau_-)$ and $\boldsymbol{\varpi}_i(\tau_+)$, share the same physical dimension: $[\mathbf{p}_i]=[\boldsymbol{\varpi}_i(\tau_\pm)]=\mathtt{ET/L}$ (i.e., impulse).

Balance laws After an integration by parts, the balance principle yields the following equations:

$$\mathbf{f}_i(\tau)-\dot{\mathbf{p}}_i(\tau)=\mathbf{0}\qquad\text{for all }(i,\tau)\in\mathsf{P}\times]\,\tau_-,\tau_+[\,, \tag{1.1.3a}$$

$$\boldsymbol{\varpi}_i(\tau_\pm)=\pm\,\mathbf{p}_i(\tau_\pm)\qquad\text{for all }i\in\mathsf{P}\,. \tag{1.1.3b}$$

Motion, velocity, and test velocities The evolution equations governing the *motion*

$$[\tau_-, \tau_+] \ni \tau \mapsto \big(\boldsymbol{q}_1(\tau), \dots, \boldsymbol{q}_N(\tau)\big) \tag{1.1.4}$$

will be produced by (1.1.3), once augmented with constitutive information relating the force applied to each particle and its momentum to the motion itself $\big(\boldsymbol{q}_i |\, i \in \mathsf{P}\big)$. The (unique) velocity realized along the motion $\big(\boldsymbol{q}_i |\, i \in \mathsf{P}\big)$ is its time derivative:

$$[\tau_-, \tau_+] \ni \tau \mapsto \big(\dot{\boldsymbol{q}}_1(\tau), \dots, \dot{\boldsymbol{q}}_N(\tau)\big)\,. \tag{1.1.5}$$

Test velocities are best conceived of by embedding the motion in a one-parameter family of putative motions, smoothly parameterized by a pseudo-time ϵ, such that the motion of interest is recovered for $\epsilon = 0$:

$$\boldsymbol{q}_i^\epsilon(\tau) := \boldsymbol{q}_i(\tau) + \epsilon\, \mathbf{w}_i(\tau) + o(\epsilon)\,.$$

1.2 Impulse balance for a 1D continuum in 1D

The simplest continuum The medium, regarded here as a 1D continuum embedded in a 1D Euclidean space, is comprised of uncountably many body points—*not* to be conceived of as particles—one for each real number in the interval $[x_-, x_+]$. Body points should neither be mistaken for elements (places) of the 1D ambient space in which they move. They are best thought of as the tiniest macroscopic markers that can conceivably be produced and somehow followed during the time lapse $[\tau_-, \tau_+]$. Each of them may be identified with its *reference* position $x \in [x_-, x_+]$, given once for all. The relevant body-time manifold is the product of the interval $[x_-, x_+]$ of the real line, identified with the 1D body, times the time interval $[\tau_-, \tau_+]$. Its boundary is comprised of two body cuts $\{x_\mp\} \times [\tau_-, \tau_+]$ and two time cuts $[x_-, x_+] \times \{\tau_\mp\}$. A superposed dot denotes differentiation with respect to time, as before, while a prime denotes differentiation with respect to the body coordinate. All densities on the body-time manifold are taken with respect to the product measure $d\tau \wedge dx$, with $d\tau$ the time duration measure (the same as before) and dx the length (1D volume). Space-like tensor fields of all orders will be identified with their single component in a Cartesian coordinate system. In order to avoid mathematical technicalities, the necessary smoothness is taken for granted and left unspecified.

Impulse functional The space of test velocities is comprised of the collection of all sufficiently smooth $\mathbb{R}$-valued fields:

$$[x_-, x_+] \times [\tau_-, \tau_+] \ni (x, \tau) \mapsto w(x, \tau)\,. \tag{1.2.1}$$

To see the analogy with (1.1.1), consider that (1.1.1) could have been written in a perfectly legitimate—though less usual—way as

$$\mathsf{P}\times[\tau_-,\tau_+]\ni(i,\tau)\mapsto\mathbf{w}(i,\tau)\,. \tag{1.1.1$_{\text{rep}}$}$$

The work done on the test velocity w is assumed to be

$$\begin{aligned}\mathcal{W}=&\int_{\tau_-}^{\tau_+}d\tau\int_{x_-}^{x_+}\big(b\,w+m\,\dot{w}-t\,w'\big)\,dx\\&+\int_{\tau_-}^{\tau_+}d\tau\,\Big[t^{\,\mathsf{cut}}\,w\Big]_{x_-}^{x_+}-\left[\int_{x_-}^{x_+}m^{\mathsf{cut}}\,w\,dx\right]_{\tau_-}^{\tau_+}\end{aligned} \tag{1.2.2}$$

In (1.2.2), the impulse is parameterized by three sufficiently smooth $\mathbb{R}$-valued bulk fields:

$$]x_-,x_+[\times]\tau_-,\tau_+[\ni(x,\tau)\mapsto\big(b(x,\tau),m(x,\tau),t(x,\tau)\big)\,, \tag{1.2.3}$$

and two $\mathbb{R}$-valued boundary field, one defined on the union of the body cuts at x_- and x_+:

$$\{x_\mp\}\times]\tau_-,\tau_+[\ni(x,\tau)\mapsto t^{\,\mathsf{cut}}(x,\tau)\,, \tag{1.2.4a}$$

and the other defined on the union of the body cuts at τ_- and τ_+:

$$]x_-,x_+[\times\{\tau_\mp\}\ni(x,\tau)\mapsto m^{\mathsf{cut}}(x,\tau)\,. \tag{1.2.4b}$$

Since w has physical dimension $\mathtt{L/T}$, the *specific bulk force* b has physical dimension $\mathtt{E/L}^2$ (i.e., force per unit reference length), while the *traction* t and the *boundary traction* $t^{\,\mathsf{cut}}$ share the physical dimension $\mathtt{E/L}$ (i.e., force). The *specific bulk momentum* m and the *specific boundary momentum* m^{cut} share the same physical dimension $\mathtt{ET/L}^2$ (i.e., impulse per unit reference length).

Balance laws After an integration by parts, the balance principle yields the following equations:

$$b(x,\tau)-\dot{m}(x,\tau)+t'(x,\tau)=0\qquad\text{for all }(x,\tau)\in]x_-,x_+[\times]\tau_-,\tau_+[\,, \tag{1.2.5a}$$

$$t^{\,\mathsf{cut}}(x_\pm,\tau)=\pm\,t(x_\pm,\tau)\qquad\text{for all }\tau\in]\tau_-,\tau_+[\,, \tag{1.2.5b}$$

$$m^{\mathsf{cut}}(\tau_\pm)=\pm\,m(\tau_\pm)\qquad\text{for all }x\in]x_-,x_+[\,. \tag{1.2.5c}$$

Motion, velocity, and test velocities The evolution equations governing the *motion*

$$[x_-,x_+]\times[\tau_-,\tau_+]\ni(x,\tau)\mapsto y(x,\tau)\,, \tag{1.2.6}$$

will be produced by (1.2.5), once augmented with constitutive information relating the traction t and the boundary traction t^{cut}, the specific bulk force b, and the specific momenta m and m^{cut}, to the motion itself y. The section $y(\,\cdot\,,\tau)$, i.e., the *configuration* assumed at time τ along the motion y, is assumed to be invertible at all time τ. In other words, two or more body points can never sit in the same place simultaneously. This requires that

$$y'(x,\tau) \neq 0 \qquad \text{for all } (x,\tau) \in]x_-, x_+[\times]\tau_-, \tau_+[\,, \tag{1.2.7a}$$

which, because of continuity, implies that $y(\,\cdot\,,\tau)$ is either strictly monotonically increasing or strictly monotonically decreasing. Since the choice of the reference configuration is conventional, we may always assume that

$$y'(x,\tau) > 0\,, \tag{1.2.7b}$$

by flipping the reference configuration about 0, if necessary: $x \mapsto -x$. The (unique) velocity realized along the motion y is its time derivative:

$$[x_-, x_+] \times [\tau_-, \tau_+] \ni (x,\tau) \mapsto \dot{y}(x,\tau)\,. \tag{1.2.8}$$

Also in a continuum field theory, test velocities are best conceived of by embedding the motion in a one-parameter family of putative motions, smoothly parameterized by a pseudo-time ϵ, such that the motion of interest is recovered for $\epsilon = 0$:

$$y^\epsilon(x,\tau) := y(x,\tau) + \epsilon\, w(x,\tau) + o(\epsilon)\,. \tag{1.2.9}$$

Spatial description The *referential* velocity field (1.2.8), while mathematically convenient and well defined, is *not* directly observable. What is observable is the *spatial* velocity field

$$v(\,\cdot\,,\tau) := \dot{y}(\,\cdot\,,\tau) \circ y(\,\cdot\,,\tau)^{-1}, \tag{1.2.10}$$

whose domain is the current shape $y\big([x_-, x_+], \tau\big)$. If the reference configuration is the one actually taken by the body at a given time t, then the motion y may be reconstructed from the observed spatial field v by integrating (in parallel) the x-parameterized family of ordinary differential equations (ODEs)

$$\dot{y}(x,\tau) = v\big(y(x,\tau),\tau\big) \tag{1.2.11}$$

with initial conditions $y(x,t) = x$. Let

$$\xi := y(x,\tau) \tag{1.2.12}$$

be the current position of the body point whose reference body coordinate is x. Since

$$x = y^{-1}(\xi,\tau) := \big(y(\,\cdot\,,\tau)^{-1}\big)(\xi)\,, \tag{1.2.13}$$

each referential field considered so far has a spatial counterpart, analogous to (1.2.10). In particular, the referential test field w has a spatial counterpart $w_>$ such that[†]

$$w(x,\tau) = w_>\big(y(x,\tau),\tau\big)\,. \tag{1.2.14}$$

Its time and space derivatives appearing in (1.2.2) transform accordingly:

$$\dot w = w_>' v + \dot w_>\,, \tag{1.2.15a}$$

$$w' = w_>' y'\,, \tag{1.2.15b}$$

it being intended that a prime applied to spatial fields denotes differentiation with respect to the current body coordinate. In (1.2.15), as in all other equations to follow where referential and spatial fields coexist, it is intended that the spatial fields are evaluated at the current coordinate ξ corresponding to the referential coordinate x where the referential fields are evaluated. The traction transforms like the velocity:

$$t_> = t \quad\Rightarrow\quad t' = t_>' y'\,, \qquad\qquad t_>^{\mathsf{cut}} = t^{\mathsf{cut}}\,. \tag{1.2.16}$$

Differentiating (1.2.12) yields

$$d\xi = y'\,dx\,. \tag{1.2.17}$$

Densities transform contravariantly, so that the work (1.2.2) is parameterization-invariant:

$$y' b_> = b\,, \qquad y' m_> = m\,, \qquad y' m_>^{\mathsf{cut}} = m^{\mathsf{cut}}\,. \tag{1.2.18}$$

In conclusion, the spatial representations of the impulse functional (1.2.2) and of the balance laws (1.2.5) read

$$\begin{aligned}\mathcal{W} =& \int_{\tau_-}^{\tau_+} d\tau \int_{\xi_-}^{\xi_+} \big(b_> w_> + m_> \dot w_> + (v m_> - t_>)\, w_>'\big)\, d\xi \\ &+ \int_{\tau_-}^{\tau_+} d\tau \Big[t_>^{\mathsf{cut}} w_>\Big]_{\xi_-}^{\xi_+} - \bigg[\int_{\xi_-}^{\xi_+} m_>^{\mathsf{cut}} w_>\, d\xi\bigg]_{\tau_-}^{\tau_+};\end{aligned} \tag{1.2.19}$$

[†]To avoid a proliferation of symbols, most spatial fields will be denoted by attaching the subscript '$>$' to the same symbol used for the corresponding referential field (one notable exception being the velocity field: spatial v vs. referential $\dot y$). Eschewing the bad habit of denoting different fields that represent the same physical quantity with the same symbol frees us from the necessity of introducing a zoo of derivatives. In particular, the same dot derivative of a referential or of a spatial field holds constant the homonymous body coordinate, x or ξ, respectively.

$$b_>(\xi,\tau) - \dot{m}_>(\xi,\tau) - \big(v m_> - t_>\big)'(\xi,\tau) = 0\,, \tag{1.2.20a}$$

$$t_>^{\mathsf{cut}}(\xi_\pm,\tau) = \pm\, t_>(\xi_\pm,\tau)\,, \tag{1.2.20b}$$

$$m_>^{\mathsf{cut}}(\tau_\pm) = \pm\, m_>(\tau_\pm)\,. \tag{1.2.20c}$$

A quick comparison of (1.2.19) and (1.2.20) with the corresponding referential representations (1.2.2) and (1.2.5) makes it apparent why referential fields are a convenient mathematical contrivance, in spite of the fact that spatial fields are the natural physical observables. This issue is peculiar to continuum mechanics, where by construction the body manifold is modeled after a region of the ambient space and places in that region are used to label body points.

1.3 Impulse balance for a 3D continuum in 3D

The standard 3D continuum *Mutatit mutandis*, this section follows the same lines of Section 1.2. Once the leap from discrete (0D) systems to 1D continua is made, augmenting the dimension of space does not demand the introduction of radically new concepts—such as the notion of traction in (1.2.2)—at least when the body and the space manifold keep the same dimension, as we admit here. However, the mathematical apparatus required for administering the same basic concepts is a multidimensional space is definitely more sophisticated (cf. the next two paragraphs). The medium is regarded here as a 3D manifold $\mathscr{B}$ embeddable in a 3D Euclidean space $\mathscr{E}$. Body points should not be mistaken for particles nor for elements (places) of the 3D ambient space in which they move. Each of them may be conveniently—but conventionally—identified with its *reference* position $\boldsymbol{x} \in \mathscr{E}$, given once for all. The relevant body-time manifold is the 4D product $\mathscr{B}\times[\tau_-,\tau_+]$. Its boundary is comprised of a body cut $\partial\mathscr{B}\times[\tau_-,\tau_+]$ (possibly disconnected) and two time cuts $\mathscr{B}\times\{\tau_\mp\}$. All densities on the body-time manifold are taken with respect to the product measure $d\tau\wedge\omega$, with $d\tau$ the time duration measure (the same as before) and ω the volume form. Densities defined on the time-wise component of its boundary, i.e., the body cut $\partial\mathscr{B}\times[\tau_-,\tau_+]$, are taken with respect to the product measure $d\tau\wedge\alpha$, with α the area form. Densities defined on the body-wise component of its boundary, i.e., the time cuts $\mathscr{B}\times\{\tau_\mp\}$, are taken with respect to the volume form ω.

A bit of multilinear algebra in Euclidean spaces Let $\mathbf{a},\mathbf{b}$ be space vectors. Then, their tensor product $\mathbf{a}\otimes\mathbf{b}$ is the dyad such that, for all vector $\mathbf{u}$, $(\mathbf{a}\otimes\mathbf{b})\mathbf{u} = (\mathbf{a}\cdot\mathbf{u})\mathbf{v}$. Not all double tensors are dyads, but all of them are linear combinations of dyads. The transpose of a double tensor $\mathbf{L}$ is the (unique) double tensor $\mathbf{L}^\top$ such

that $(\mathbf{L}\mathbf{u})\cdot\mathbf{v} = \mathbf{u}\cdot(\mathbf{L}^\top\mathbf{v})$ for all vectors $\mathbf{u},\mathbf{v}$. It is easily seen that $(\mathbf{a}\otimes\mathbf{b})^\top = (\mathbf{b}\otimes\mathbf{a})$. The trace tr is the (unique) linear $\mathbb{R}$-valued functional on double tensors such that $\mathrm{tr}(\mathbf{a}\otimes\mathbf{b}) = \mathbf{a}\cdot\mathbf{b}$. The Euclidean inner product is extended to double tensors $\mathbf{L},\mathbf{M}$ by defining $\mathbf{L}\cdot\mathbf{M} := \mathrm{tr}\,(\mathbf{L}^\top\mathbf{M})$ or, equivalently, $(\mathbf{a}\otimes\mathbf{b})\cdot(\mathbf{u}\otimes\mathbf{v}) := (\mathbf{a}\cdot\mathbf{u})(\mathbf{b}\cdot\mathbf{v})$. It is easy to prove that $\mathbf{L}\cdot(\mathbf{a}\otimes\mathbf{b}) = (\mathbf{L}\mathbf{a})\cdot\mathbf{b}$, while $\mathbf{L}(\mathbf{a}\otimes\mathbf{b}) = \mathbf{a}\otimes(\mathbf{L}\mathbf{b})$, and $(\mathbf{a}\otimes\mathbf{b})\mathbf{L} = (\mathbf{L}^\top\mathbf{a})\otimes\mathbf{b}$.

A bit of multivariate calculus in Euclidean spaces The Euclidean derivative will be denoted ∇. The derivative along a space vector field $\mathbf{u}$ of a tensor field of any order $\mathfrak{L}$ is the tensor field of the same order denoted $\nabla_{\mathbf{u}}\mathfrak{L}$. If f is a scalar field, $\nabla_{\mathbf{u}}f = (\nabla f)\cdot\mathbf{u}$, where the gradient ∇f of f is a vector field. If $\mathbf{v}$ is a vector field, $\nabla_{\mathbf{u}}\mathbf{v} = (\nabla\mathbf{v})\mathbf{u}$, where the gradient $\nabla\mathbf{v}$ of $\mathbf{v}$ is a (double) tensor field. The divergence of a vector field $\mathbf{v}$ equals the trace of its gradient: $\mathrm{div}\mathbf{v} = \mathrm{tr}\nabla\mathbf{v}$. The divergence of a tensor field $\mathbf{L}$ is a vector field characterized by the defining property: $\mathrm{div}\,(\mathbf{L}^\top\mathbf{u}) = (\mathrm{div}\,\mathbf{L})\cdot\mathbf{u} + \mathbf{L}\cdot(\nabla\mathbf{u})$ for all vector field $\mathbf{u}$. It is not difficult to prove the identities:

$$\begin{aligned}\nabla(\mathbf{u}\cdot\mathbf{v}) &= (\nabla\mathbf{u})^\top\mathbf{v} + (\nabla\mathbf{v})^\top\mathbf{u},\\ \mathrm{div}(f\,\mathbf{v}) &= f\,\mathrm{div}\,\mathbf{v} + (\nabla f)\cdot\mathbf{v},\\ \mathrm{div}(\mathbf{u}\otimes\mathbf{v}) &= (\mathrm{div}\,\mathbf{u})\mathbf{v} + (\nabla\mathbf{v})\cdot\mathbf{u}.\end{aligned}$$

Impulse functional The space of test velocities is comprised of the collection of all sufficiently smooth vector-valued fields

$$\mathscr{B}\times[\tau_-,\tau_+] \ni (\boldsymbol{x},\tau) \mapsto \mathbf{w}(x,\tau) \tag{1.3.1}$$

having physical dimension $\mathtt{L}/\mathtt{T}$. The work done on $\mathbf{w}$ is assumed to be

$$\begin{aligned}\mathcal{W} = &\int_{\tau_-}^{\tau_+} d\tau \int_{\mathscr{B}} \big(\mathbf{b}\cdot\mathbf{w} + \mathbf{m}\cdot\dot{\mathbf{w}} - \mathbf{S}\cdot(\nabla\mathbf{w})\big)\,\omega\\ &+ \int_{\tau_-}^{\tau_+} d\tau \int_{\partial\mathscr{B}} \mathbf{s}^{\mathsf{cut}}\cdot\mathbf{w}\,\alpha - \Big[\int_{\mathscr{B}} \mathbf{m}^{\mathsf{cut}}\cdot\mathbf{w}\,\omega\Big]_{\tau_-}^{\tau_+}\end{aligned} \tag{1.3.2}$$

In (1.3.2), the impulse is parameterized by three sufficiently smooth bulk fields: the vector-valued *specific bulk force* $\mathbf{b}$ having physical dimension $\mathtt{E}/\mathtt{L}^4$ (i.e., force per unit reference volume), the vector-valued *specific bulk momentum* $\mathbf{m}$ having physical dimension $\mathtt{E}/\mathtt{L}^4$ (i.e., impulse per unit reference volume), the *Piola stress* $\mathbf{S}$ having physical dimension $\mathtt{E}/\mathtt{L}^3$ (i.e., energy per unit reference volume), and two vector-valued boundary fields: the *boundary traction* $\mathbf{s}^{\mathsf{cut}}$ sharing the same physical dimension of $\mathbf{S}$ (to be intended here as force per unit reference area), the *specific boundary momentum* $\mathbf{m}^{\mathsf{cut}}$ sharing the same physical dimension of $\mathbf{m}$.

Balance laws After an integration by parts, the balance principle yields the following equations:

$$\mathbf{b}(\boldsymbol{x},\tau) - \dot{\mathbf{m}}(\boldsymbol{x},\tau) + \operatorname{div}\mathbf{S}|_{(\boldsymbol{x},\tau)} = \mathbf{0} \qquad \text{for all } (\boldsymbol{x},\tau) \in \overset{\circ}{\mathscr{B}} \times]\tau_-,\tau_+[\,, \tag{1.3.3a}$$

$$\mathbf{s}^{\mathsf{cut}}(\boldsymbol{x},\tau) = \mathbf{S}(\boldsymbol{x},\tau)\,\mathbf{n}^{\mathsf{cut}}(\boldsymbol{x}) \qquad \text{for all } (\boldsymbol{x},\tau) \in \partial\mathscr{B} \times]\tau_-,\tau_+[\,, \tag{1.3.3b}$$

$$\mathbf{m}^{\mathsf{cut}}(\boldsymbol{x},\tau_\pm) = \pm\,\mathbf{m}(\boldsymbol{x},\tau_\pm) \qquad \text{for all } \boldsymbol{x} \in \overset{\circ}{\mathscr{B}}\,, \tag{1.3.3c}$$

where a superposed $\circ$ denotes the interior. In (1.3.3b) $\mathbf{n}^{\mathsf{cut}}(\boldsymbol{x})$ is the unit outer normal to $\partial\mathscr{B}$ at $\boldsymbol{x}$ in the reference configuration. In hindsight, comparing (1.2.2) with (1.3.2), it is easy to recognize that the prime in (1.2.2) is the 1D gradient, while the prime in (1.2.5a) is the 1D divergence (cf. (1.3.3a)). Also the factor ± 1 in (1.2.5b) represents the unit outer normal to the body cuts in 1D.

Motion, velocity, and test velocities The evolution equations governing the *motion*

$$\mathscr{B} \times [\tau_-,\tau_+] \ni (\boldsymbol{x},\tau) \mapsto \boldsymbol{y}(\boldsymbol{x},\tau)\,, \tag{1.3.4}$$

will be produced by (1.3.3), once augmented with constitutive information relating the Piola stress $\mathbf{S}$ and the boundary traction $\mathbf{s}^{\mathsf{cut}}$, the specific bulk force $\mathbf{b}$, and the specific momenta $\mathbf{m}$ and $\mathbf{m}^{\mathsf{cut}}$, to the motion itself $\boldsymbol{y}$. The section $\boldsymbol{y}(\,\cdot\,,\tau)$, i.e., the *configuration* assumed at time τ along the motion $\boldsymbol{y}$, is assumed to be invertible at all time τ. This requires the *Jacobian determinant*

$$J(\boldsymbol{x},\tau) := \det\big(\nabla\boldsymbol{y}|_{(\boldsymbol{x},\tau)}\big) \tag{1.3.5a}$$

to stay away from zero. Because of continuity, this implies that $J(\boldsymbol{x},\tau)$ takes either positive or negative values everywhere. Since the choice of the reference configuration is conventional, we may always assume that

$$J(\boldsymbol{x},\tau) > 0 \quad \text{for all } (\boldsymbol{x},\tau) \in \overset{\circ}{\mathscr{B}} \times]\tau_-,\tau_+[\,, \tag{1.3.5b}$$

by replacing the reference configuration with any of its mirror images, if necessary. The (unique) velocity realized along the motion $\boldsymbol{y}$ is its time derivative:

$$\mathscr{B} \times [\tau_-,\tau_+] \ni (\boldsymbol{x},\tau) \mapsto \dot{\boldsymbol{y}}(\boldsymbol{x},\tau)\,. \tag{1.3.6}$$

Test velocities are best conceived of by embedding the motion in a one-parameter family of putative motions, smoothly parameterized by a pseudo-time ϵ, such that the motion of interest is recovered for $\epsilon = 0$:

$$\boldsymbol{y}^\epsilon(\boldsymbol{x},\tau) := \boldsymbol{y}(\boldsymbol{x},\tau) + \epsilon\,\mathbf{w}(\boldsymbol{x},\tau) + o(\epsilon)\,. \tag{1.3.7}$$

Spatial description The *referential* velocity field (1.3.6), while mathematically convenient and well defined, is *not* directly observable. What is observable is the *spatial* velocity field

$$\mathbf{v}(\,\cdot\,,\tau) := \dot{\boldsymbol{y}}(\,\cdot\,,\tau) \circ \boldsymbol{y}(\,\cdot\,,\tau)^{-1}, \tag{1.3.8}$$

whose domain is the current shape $\boldsymbol{y}\big(\mathscr{B},\tau\big)$. If the reference configuration is the one actually taken by the body at a given time t, then the motion $\boldsymbol{y}$ may be reconstructed from the observed spatial field $\mathbf{v}$ by integrating (in parallel) the $\boldsymbol{x}$-parameterized family of ODEs

$$\dot{\boldsymbol{y}}(\boldsymbol{x},\tau) = \mathbf{v}\big(\boldsymbol{y}(\boldsymbol{x},\tau),\tau\big) \tag{1.3.9}$$

with initial conditions $\boldsymbol{y}(\boldsymbol{x},t) = \boldsymbol{x}$. Let

$$\boldsymbol{\xi} = \boldsymbol{y}(\boldsymbol{x},\tau) \tag{1.3.10}$$

be the current position of the body point whose reference position is $\boldsymbol{x}$. Since

$$\boldsymbol{x} = \boldsymbol{y}^{-1}(\boldsymbol{\xi},\tau) := \big(\boldsymbol{y}(\,\cdot\,,\tau)^{-1}\big)(\boldsymbol{\xi}), \tag{1.3.11}$$

each referential field considered so far has a spatial counterpart, analogous to (1.3.8). In particular, the referential test field $\mathbf{w}$ has a spatial counterpart $\mathbf{w}_{>}$ such that[†]

$$\mathbf{w}(\boldsymbol{x},\tau) = \mathbf{w}_{>}\big(\boldsymbol{y}(\boldsymbol{x},\tau),\tau\big). \tag{1.3.12}$$

Its time and space derivatives appearing in (1.3.2) transform accordingly:

$$\dot{\mathbf{w}} = (\nabla \mathbf{w}_{>})\,\mathbf{v} + \dot{\mathbf{w}}_{>}\,, \tag{1.3.13a}$$

$$\nabla \mathbf{w} = (\nabla \mathbf{w}_{>})\nabla \boldsymbol{y}, \tag{1.3.13b}$$

The referential volume form ω transforms into the current volume form $\omega_{>}$ in such a way that

$$\omega_{>} = J\,\omega, \tag{1.3.14}$$

(cf. (1.3.5a)), while the current area $\alpha_{>}(\boldsymbol{\xi},\tau)$ and the unit normal vector $\mathbf{n}_{>}(\boldsymbol{\xi},\tau)$ to a facet currently at $\boldsymbol{\xi}$ depend also on its reference unit normal vector $\mathbf{n}(\boldsymbol{x})$ at $\boldsymbol{x}$:

$$\mathbf{n}_{>}\alpha_{>} = (\nabla \boldsymbol{y})^{\star}\,\mathbf{n}\,\alpha\,, \tag{1.3.15}$$

where

$$(\nabla \boldsymbol{y})^{\star} = J\,(\nabla \boldsymbol{y})^{-\top} \tag{1.3.16}$$

[†]See footnote on page 8 and the explanations following (1.2.15).

is the *adjugate* of $\nabla \boldsymbol{y}$. Bulk and surface densities transform contravariantly, so that the work (1.3.2) is parameterization-invariant. In particular,

$$J\,\mathbf{b}_{>} = \mathbf{b}\,, \qquad J\,\mathbf{m}_{>} = \mathbf{m}\,, \qquad J\,\mathbf{m}^{\mathsf{cut}}_{>} = \mathbf{m}^{\mathsf{cut}}, \tag{1.3.17a}$$

$$\mathbf{S}\cdot(\nabla \mathbf{w})\,\omega = \mathbf{T}\cdot(\nabla \mathbf{w}_{>})\,\omega_{>}\,, \tag{1.3.17b}$$

$$\mathbf{s}^{\mathsf{cut}}\,\alpha = \mathbf{S}\,\mathbf{n}\,\alpha = \mathbf{T}\,\mathbf{n}_{>}\,\alpha_{>} = \mathbf{t}^{\mathsf{cut}}\,\alpha_{>}\,, \tag{1.3.17c}$$

where

$$\mathbf{T} = J^{-1}\mathbf{S}\,(\nabla \boldsymbol{y})^{\top} \tag{1.3.18a}$$

is the *Cauchy stress* (energy per unit current volume), and

$$\mathbf{t}^{\mathsf{cut}} = \mathbf{T}\,\mathbf{n}_{>} \tag{1.3.18b}$$

is the spatial boundary traction (force per unit current area). Moreover,

$$(\mathrm{div}\mathbf{S})\,\omega = (\mathrm{div}\mathbf{T})\,\omega_{>}\,. \tag{1.3.18c}$$

In conclusion, the spatial representations of the impulse functional (1.3.2) and of the balance laws (1.3.3) read[†]

$$\begin{aligned}\mathcal{W} =& \int_{\tau_-}^{\tau_+} d\tau \int_{\mathscr{B}_{>}} \big(\mathbf{b}_{>}\cdot \mathbf{w}_{>} + \mathbf{m}_{>}\cdot \dot{\mathbf{w}}_{>} + (\mathbf{v}\otimes \mathbf{m}_{>} - \mathbf{T})\cdot(\nabla \mathbf{w}_{>})\big)\,\omega_{>} \\ &+ \int_{\tau_-}^{\tau_+} d\tau \int_{\partial\mathscr{B}_{>}} \mathbf{s}^{\mathsf{cut}}_{>}\cdot \mathbf{w}_{>}\,\alpha - \left[\int_{\mathscr{B}_{>}} \mathbf{m}^{\mathsf{cut}}_{>}\cdot \mathbf{w}_{>}\,\omega_{>}\right]_{\tau_-}^{\tau_+};\end{aligned} \tag{1.3.19}$$

$$\mathbf{b}_{>}(\boldsymbol{\xi},\tau) - \dot{\mathbf{m}}_{>}(\boldsymbol{\xi},\tau) - \mathrm{div}\big(\mathbf{v}\otimes \mathbf{m}_{>} - \mathbf{T}\big)(\boldsymbol{\xi},\tau) = \mathbf{0}\,, \tag{1.3.20a}$$

$$\mathbf{t}^{\mathsf{cut}}_{>} = \mathbf{T}\,\mathbf{n}_{>}\,, \tag{1.3.20b}$$

$$\mathbf{m}^{\mathsf{cut}}_{>}(\tau_{\pm}) = \pm\,\mathbf{m}_{>}(\tau_{\pm})\,, \tag{1.3.20c}$$

where $\mathscr{B}_{>} := \boldsymbol{y}(\mathscr{B},\tau)$.

[†]The closing remark of Section 1.2 applies *a fortiori* to the comparison of (1.3.19) and (1.3.20) with the corresponding referential representations (1.3.2) and (1.3.3).

3D stress vs. 1D traction The close affinity between the 1D concept of traction (1.2.2), (1.2.16) and the 3D notions of Piola (1.3.2) and Cauchy (1.3.18a) stress is better perceived by representing the stress tensors as linear combinations of dyads. Let us introduce a field of bases (not necessarily orthonormal) $(\mathbf{e}_i|\, i=1,2,3)$ and of their reciprocals $(\mathbf{e}^j|\, j=1,2,3)$, such that $\mathbf{e}_i\cdot\mathbf{e}^j=\delta_i^j$. Then,

$$\mathbf{S}=\mathbf{e}_k\otimes\mathbf{s}^k \text{ (sum over } k) \qquad \text{with} \qquad \mathbf{s}^k:=\mathbf{S}\,\mathbf{e}^k. \tag{1.3.21a}$$

Moreover,

$$\operatorname{div}\mathbf{S}=(\operatorname{div}\mathbf{e}_k)\mathbf{s}^k+\big(\nabla\mathbf{s}^k\big)\mathbf{e}_k\,. \tag{1.3.21b}$$

In Section 1.2, when identifying any tensor with its unique component, we assumed a constant field of basis $\mathbf{e}_1=\mathbf{e}$, trivially orthonormal, hence coincident with its reciprocal $\mathbf{e}^1=\mathbf{e}$. Therefore, in 1D (1.3.21a) boils down to $\mathbf{S}=\mathbf{e}\otimes(t\,\mathbf{e})$, and (1.3.21b) to $\operatorname{div}\mathbf{S}=t'\mathbf{e}$. Substituting each field $\mathbf{e}_i$ with $\mathbf{e}_i^{>}:=(\nabla\boldsymbol{y})\mathbf{e}_i$ and the corresponding reciprocal $\mathbf{e}^i$ with $\mathbf{e}^i_{>}:=(\nabla\boldsymbol{y})^{-\top}\mathbf{e}^i$ in (1.3.21a) yields the dyadic representation of the Cauchy stress:

$$\mathbf{T}=\mathbf{e}_k^{>}\otimes\mathbf{t}^k \text{ (sum over } k) \qquad \text{with} \qquad \mathbf{t}^k=\mathbf{T}\,\mathbf{e}^k_{>}. \tag{1.3.22}$$

In 1D, $\mathbf{e}_1^{>}:=y'\mathbf{e}$ and $\mathbf{e}^1_{>}:=(1/y')\mathbf{e}$, so that $\mathbf{T}=\mathbf{e}_1^{>}\otimes(t_{>}\mathbf{e}^1_{>})=\mathbf{e}\otimes(t_{>}\mathbf{e})$, and $\operatorname{div}\mathbf{T}=t'_{>}\mathbf{e}$ (cf. (1.3.18c), (1.3.14) and (1.2.16)).

2 Modeling interactions

To close the system of equations—ODEs for discrete systems, such as (1.1.3), or PDEs, such as (1.2.5) or (1.3.3)—enforcing impulse balance, it is necessary to augment them with constitutive information relating impulse to motion, i.e., to the evolution of the degrees of freedom (DOFs) *explicitly* described by the theory. This is the reason why the coarser the theory—i.e., the greater the number of relevant DOFs it leaves implicit—the more complex (and more doubtful) the constitutive recipes it requires to work properly—i.e., to *predict* quantitatively realistic results. Reducing the complexity of constitutive prescriptions without having recourse to a significantly finer theory—i.e., without a substantial increase of the number of DOFs explicitly described by the theory—inevitably narrows down its scope, to the limit of making it either too special or unmanageable. Trying to evade such a frustrating dilemma is the main motivation for our multiscale endeavor.

This section is devoted to the thorniest constitutive issue, namely, the modeling of dynamical interactions. In all its subsections, a central role is played by the concept of change in observer—a global gauge transformation. It will therefore be introduced here in a 3D setting—its restriction to 1D being obvious.

Change in observer Explicitly or implicitly, motions are defined from the point of view of an observer. The evolution that the hitherto implied observer describes as the motion (1.1.4) or (1.3.4)

$$(i,\tau)\mapsto \boldsymbol{q}_i(\tau)\,,\qquad\qquad (\boldsymbol{x},\tau)\mapsto \boldsymbol{y}(\boldsymbol{x},\tau) \tag{2.0.1}$$

is perceived by another, equally legitimate, "starred" observer as the $\star$-corresponding motion

$$(i,\tau)\mapsto \boldsymbol{q}^\star_i(\tau)\,,\qquad\qquad (\boldsymbol{x},\tau)\mapsto \boldsymbol{y}^\star(\boldsymbol{x},\tau) \tag{2.0.2}$$

where

$$\begin{aligned}\boldsymbol{q}^\star_i(\tau)&=\boldsymbol{q}^\star_0(\tau)+\mathbf{Q}(\tau)\big(\boldsymbol{q}_i(\tau)-\boldsymbol{q}_0(\tau)\big)\,,\\ \boldsymbol{y}^\star(\boldsymbol{x},\tau)&=\boldsymbol{q}^\star_0(\tau)+\mathbf{Q}(\tau)\big(\boldsymbol{y}(\boldsymbol{x},\tau)-\boldsymbol{q}_0(\tau)\big)\,,\end{aligned} \tag{2.0.3}$$

with $\boldsymbol{q}_0$, $\boldsymbol{q}^\star_0$ two arbitrary place-valued and $\mathbf{Q}$ an arbitrary orthogonal-tensor-valued (smooth) functions of time, parameterizing the change in observer.[†] Differentiation with respect to time yields the $*$-corresponding velocity:

$$\begin{aligned}\dot{\boldsymbol{q}}^\star_i(\tau)&=\mathbf{Q}(\tau)\,\dot{\boldsymbol{q}}_i(\tau)+\mathbf{v}_0(\tau)+\mathbf{W}_0(\tau)\big(\boldsymbol{q}^\star_i(\tau)-\boldsymbol{q}^\star_0(\tau)\big)\,,\\ \dot{\boldsymbol{y}}^\star(\boldsymbol{x},\tau)&=\mathbf{Q}(\tau)\,\dot{\boldsymbol{y}}(\boldsymbol{x},\tau)+\mathbf{v}_0(\tau)+\mathbf{W}_0(\tau)\big(\boldsymbol{y}^\star(\boldsymbol{x},\tau)-\boldsymbol{q}^\star_0(\tau)\big)\,,\end{aligned} \tag{2.0.4}$$

where $\mathbf{v}_0(\tau):=\dot{\boldsymbol{q}}^\star_0(\tau)-\mathbf{Q}(\tau)\,\dot{\boldsymbol{q}}_0(\tau)$, and $\mathbf{W}_0(\tau):=\dot{\mathbf{Q}}(\tau)\mathbf{Q}(\tau)^\top$ is skew. Test velocities transform accordingly:

$$\begin{aligned}\mathbf{w}^\star_i(\tau)&=\mathbf{Q}(\tau)\,\mathbf{w}_i(\tau)+\mathbf{v}_0(\tau)+\mathbf{W}_0(\tau)\big(\boldsymbol{q}^\star_i(\tau)-\boldsymbol{q}^\star_0(\tau)\big)\,,\\ \mathbf{w}^\star(\boldsymbol{x},\tau)&=\mathbf{Q}(\tau)\,\mathbf{w}(\boldsymbol{x},\tau)+\mathbf{v}_0(\tau)+\mathbf{W}_0(\tau)\big(\boldsymbol{y}^\star(\boldsymbol{x},\tau)-\boldsymbol{q}^\star_0(\tau)\big)\,.\end{aligned} \tag{2.0.5}$$

2.1 Interactions between particles in 3D

Internal and external force The force $\mathbf{f}_i(\tau)$ applied to the general i-th particle at the current time τ splits into the sum of an *internal* and an *external* contribution:

$$\mathbf{f}^{\mathtt{I}}_i(\tau)=\hat{\mathbf{f}}^{\mathtt{I}}_i\big(\boldsymbol{q}_j(\tau)\big|\,j\in\mathsf{P}\big)\,, \tag{2.1.1a}$$

$$\mathbf{f}^{\mathtt{E}}_i(\tau)=\hat{\mathbf{f}}^{\mathtt{E}}_i\big(\boldsymbol{q}_i(\tau),\tau\big)\,, \tag{2.1.1b}$$

the distinguishing features being: (i) $\mathbf{f}^{\mathtt{I}}_i(\tau)$ depends—in principle—on the position of *all* of the N particles in the system, while $\mathbf{f}^{\mathtt{E}}_i(\tau)$ depends on the position of the i-th

[†]In order to be as unbiased as possible towards the two observers, this parameterization is somewhat more redundant than necessary: either $\boldsymbol{q}_0$ or $\boldsymbol{q}^\star_0$ may be chosen at will by one observer, and the other has to follow suit.

particle only, and (ii) $\mathbf{f}_i^{\mathtt{E}}(\tau)$ may depend *also* directly on time τ, such a dependence representing an external control; $\mathbf{f}_i^{\mathtt{I}}(\tau)$, on the contrary, is assumed to be *positional*, i.e., it is allowed to depend on time only through the particle positions. Both the internal and the external force are typically assumed to be *conservative*, i.e.,

$$\mathbf{f}_i^{\mathtt{I}}(\tau) = -\mathsf{D}_i \mathscr{V}^{\mathtt{I}}\big|_{(\boldsymbol{q}_j(\tau)|\, j=1,\dots,N)} \tag{2.1.2a}$$

where

$$(\boldsymbol{x}_1,\dots,\boldsymbol{x}_N) \mapsto \mathscr{V}^{\mathtt{I}}(\boldsymbol{x}_1,\dots,\boldsymbol{x}_N) \tag{2.1.2b}$$

is a real-valued *interaction* potential, and D_i denotes the derivative with respect to the i-th position. The external potential is unary, and possibly time dependent:

$$\mathbf{f}_i^{\mathtt{E}}(\tau) = -\mathsf{D}\mathscr{V}_i^{\mathtt{E}}|_{(\boldsymbol{q}_i(\tau),\tau)} \tag{2.1.3a}$$

with

$$(\boldsymbol{x},\tau) \mapsto \mathscr{V}^{\mathtt{E}}(\boldsymbol{x},\tau)\,. \tag{2.1.3b}$$

Invariance under change in observer The basic invariance requirement is twofold: (i) the *internal* response function $\hat{\mathbf{f}}_i^{\mathtt{I}}$, and (ii) the *internal* work done on any test velocity, should both be invariant under all change in observer:

$$\big(\hat{\mathbf{f}}_i^{\mathtt{I}}\big)^\star = \hat{\mathbf{f}}_i^{\mathtt{I}} \qquad \& \qquad \int_{\tau_-}^{\tau_+} d\tau \sum_{i\in\mathsf{P}} \mathbf{f}_i^\star \cdot \mathbf{w}_i^\star = \int_{\tau_-}^{\tau_+} d\tau \sum_{i\in\mathsf{P}} \mathbf{f}_i \cdot \mathbf{w}_i\,. \tag{2.1.4}$$

Covariance of the internal force A necessary and sufficient condition for (i) and (ii) to be satisfied is that there exists a *reduced* potential function

$$\begin{aligned} \big(\mathbb{R}^+\big)^{N(N-1)/2} &\to \mathbb{R} \\ \big(\rho_{jk}\big|\, j,k=1,\dots,N, j<k\big) &\mapsto \check{\mathscr{V}}^{\mathtt{I}}\big(\rho_{jk}\big|\, j,k=1,\dots,N, j<k\big) \end{aligned} \tag{2.1.5}$$

such that the interaction potential depends only on the mutual distances between all particle pairs:

$$\mathscr{V}^{\mathtt{I}}(\boldsymbol{q}_j(\tau)|\, j=1,\dots,N) = \check{\mathscr{V}}^{\mathtt{I}}\big(d_{jk}(\tau)\big|\, j,k=1,\dots,N, j<k\big) \tag{2.1.6a}$$

where

$$d_{jk}(\tau) := |\boldsymbol{q}_j(\tau) - \boldsymbol{q}_k(\tau)|\,. \tag{2.1.6b}$$

This entails a *compatibility* issue, since in general $(N-1)N/2$ positive real numbers $\big\{\rho_{jk}>0\,\big|\, j,k=1,\dots,N, j<k\big\}$ cannot be given at will if they have to be the distances between pairs of N distinct places in $\mathscr{E}$ (think of the triangle inequality).

Moreover, if such an N-tuple exists, it is essentially non unique: if $|\boldsymbol{x}_j - \boldsymbol{x}_k| = \rho_{jk}\,(j,k=1,\dots,N, j<k)$, then, for all $\widetilde{\boldsymbol{x}}_1 \in \mathscr{E}$ and all orthogonal tensor $\mathbf{Q}$, the $N-1$ places $\{\widetilde{\boldsymbol{x}}_j \,|\, j=2,\dots,N\}$ such that

$$\widetilde{\boldsymbol{x}}_i - \widetilde{\boldsymbol{x}}_1 = \mathbf{Q}\,(\boldsymbol{x}_i - \boldsymbol{x}_1) \qquad (i=2,\dots,N) \tag{2.1.7}$$

satisfy the condition $|\widetilde{\boldsymbol{x}}_j - \widetilde{\boldsymbol{x}}_k| = |\boldsymbol{x}_j - \boldsymbol{x}_k| = \rho_{jk}\,(j,k=1,\dots,N, j<k)$. The internal force is accordingly *covariant*: let $\mathbf{f}_i^{\mathtt{I}}$ be the internal force acting on the general i-th particle when the general j-th particle is located in $\boldsymbol{x}_j$ $(i,j=1,\dots,N)$; then, if the general j-th particle is displaced to $\boldsymbol{x}_j^\star$ $(j=1,\dots,N)$, the internal force acting on the general i-th particle (now located in $\boldsymbol{x}_i^\star$) is

$$\mathbf{f}_i^{\mathtt{I}\star} = \mathbf{Q}\,\mathbf{f}_i^{\mathtt{I}} \qquad (i=1,\dots,N)\,, \tag{2.1.8}$$

i.e., internal forces co-rotate with place differences (cf. (2.1.7)). It should be stressed that this property is more general than (2.1.6), since it is a *necessary* condition for (2.1.4) to hold even if the internal force were not conservative.

Law of action-reaction Plugging (2.1.8) into $(2.0.5)_1$, it is found that the *resultant internal force* and the *resultant internal torque* should be null at all time:

$$\sum_{i\in\mathsf{P}} \mathbf{f}_i = \mathbf{0}\,, \tag{2.1.9a}$$

$$\sum_{i\in\mathsf{P}} \big(\boldsymbol{q}_i - \boldsymbol{q}_0\big) \otimes \mathbf{f}_i = \mathbf{0}\,. \tag{2.1.9b}$$

Equations (2.1.9) and (2.1.8), taken together, constitute a necessary and sufficient condition for requirement (2.1.4) to be satisfied, independently of whether the internal force is conservative or not. If it is conservative, and its potential satisfies (2.1.6), then (2.1.9) ensues.