Granular Matter (2010) 12:239–252
DOI 10.1007/s10035-010-0181-z

Stress, stress asymmetry and couple stress: from discrete particles to continuous fields

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Received: 5 October 2009 / Published online: 26 March 2010

Abstract Explicit and closed expressions for the stress and couple-stress fields for discrete (classical) mechanical systems in terms of the constituents' degrees of freedom and interactions are derived and compared to previous results. This is done by using an exact and general coarse graining formulation, which allows one to predetermine the resolution of the continuum fields. Since the full dynamics of the pertinent fields is considered, the results are not restricted to static states or quasi-static deformations; the latter comprise mere limiting cases, which are discussed as well. The fields automatically satisfy the equations of continuum mechanics. An explicit expression for the antisymmetric part of the stress field is presented; the question whether the latter vanishes, much like its nature when it does not, have been debated in the literature. Physical explanations of some of the obtained results are offered; in particular, an interpretation of the expression for the stress field provides an argument in favor of its uniqueness, yet another topic of debate in the literature. The formulation and results are valid for single realizations, and can of course be used in conjunction with ensemble averaging. Part of the paper is devoted to a biased discussion of the notion of coarse graining in general, in order to set the presented results in a certain perspective. Although the results can be applied to molecular (nanoscale included) and granular systems alike, the presentation and some simplifying assumptions (which can be easily relaxed) target granular systems. The results should be useful for the analysis of experimental and numerical findings as well as the development of constitutive relations.

Keywords Coarse graining · Averaging · Homogenization · Stress · Stress asymmetry · Couple Stress · Cosserat · Continuum mechanics · Discrete mechanical systems · Granular systems · Nanoscale systems

The author gratefully acknowledges partial support from the Israel Science Foundation, grant No. 412/08 and the US-Israel Binational Science Foundation, grant No. 2004391.

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1 Introduction

Efforts to connect molecular scale dynamics with macroscopic continuum dynamics date back to classical studies by Boltzmann (for gases), Kirkwood [1], Born and Huang [2], and others [3]. Coarse graining approaches to granular matter appeared much later, perhaps starting with Weber's work [4], but are mostly based on similar principles, cf. a selection of some relatively recent (1995 and later) studies and reviews [5–18] and references therein; also see [19] for a review that includes historic references, and [20] concerning the coarse graining of granular gases. Although the present paper does not focus on granular gases, the presented results are valid for them as well, but, in models where the collisions are taken to be instantaneous temporal as well as spatial coarse graining need to be invoked [21] (a minor modification of the presented formulation).

The classical expression for the stress tensor in terms of the constituents' degrees of freedom and their interactions, often referred to as the Born-Huang [2] or Love [22] or Voigt [23] formula, was originally derived for molecular systems and is based on the "limit" of large REV's or coarse graining scales. This is justified for typical molecular systems since the latter possess strong scale separation between the molecular and macroscopic scales. For instance, in gases the scales that correspond to typical gradients of the continuum fields are much

larger than the corresponding mean free paths (else one deals with the Knudsen regime); this fact is among other things the basis for the fundamental and useful notion of local equilibrium. Similar statements can be made concerning molecular solids. When the gradients (or strain) are sufficiently "small" one can employ very large REV's, i.e., much larger than the microscopic scales, e.g., the lattice constant in ordered solids, yet much smaller than the typical scales on which the physical entities of interest undergo significant changes.

The above mentioned classical expressions for stress and other fields have often been adopted in the realm of granular matter and for relatively small (e.g., nanoscale) systems and very fine resolutions, where scale separation is weak and at times nonexistent. This is particularly true for some experiments which involve relatively small (granular) systems. It is not a-priori obvious that results obtained for systems that possess strong scale separation can be carried over to the realm of granular media or small systems; as a matter of fact, it is often untrue. When care is taken to coarse grain in such a way that the issue of scales is properly handled, one can indeed apply the same methods to granular and molecular systems, in particular one can study nanoscale systems [24]. This topic will be further discussed below.

The formulation presented below is exact and fully compatible with continuum mechanics. The resolution of the continuum fields can be chosen at will, although certain choices are advantageous over others. Some of the results presented below are known, cf. e.g., [8,21,24–29] and references therein, and repeated here using a somewhat simpler presentation and for sake of completeness. New results presented below include an exact and explicit formula for the stress asymmetry, which has been a subject of debate in the literature, see Bardet and Vardoulakis [12], references therein and citations thereof, an explicit expression for the couple stress field, and a novel derivation and interpretation of the formula for the stress field which offers a possible answer to the question whether this field is unique or not [25,26,30,31].

As mentioned, the results are of rather general validity, but some simplifying assumptions are made for sake of convenience of presentation. In particular, it is assumed that the particle interactions are binary and additive (these need to be relaxed, e.g., for molecular solids). It is also assumed that interacting pairs of particles possess (effective) discrete contact points (easy to generalize to contact areas) and that the force distribution at a contact area can be replaced by a contact force acting at the corresponding contact point and a couple or torque; physically this amounts to assuming that the particles are quite stiff. The couples that arise from the distribution of forces at the contact areas are referred to as torques due to rolling friction. Each pair of particles is assumed to possess at most one contact point, i.e., the particles are taken to be convex; this assumption can be easily relaxed. In addition, effects such as attrition and breakup are ignored, hence the particle masses are taken to be constant. It is *not assumed* that the particles are rigid or spherical or the system is monodisperse, but, as mentioned, it is convenient to envisage that the particles are not "too soft".

The structure of this article is as follows. Section 2 provides a brief and biased introduction to coarse graining. Section 3 sets the notation, and provides additional general comments. Section 4 starts with a demonstration of the method through a derivation of the equation of continuity, and provides closed expressions for the stress field and its antisymmetric part. A derivation of the continuum mechanical equation for the angular momentum density is presented in Sect. 5, in which a closed expression for the couple-stress is obtained. Finally, Sect. 6 provides concluding remarks.

2 On coarse graining

The goal of coarse graining is to produce continuum equations of motion out of microscopic dynamics. The first step involved in the process of coarse graining is to choose and define a set of continuum fields for which equations of motion are desired. The choice is usually dictated by symmetries, conservation laws, measurability and other considerations, not the least of which is the wish to obtain closed sets of equations of motion, i.e., the time derivatives of the fields should depend on the chosen set of fields alone. The fields should be defined everywhere in the space occupied by the considered system, not only, e.g., at the centers of mass of the discrete particles or in the interior of the particles. For instance, the strain and stress fields of a solid have to be continuous function of space, not restricted in their definitions to the positions of the atoms. Coarse graining involves a spatial coarse graining scale (when temporal coarse graining is invoked as well one also needs a temporal coarse graining scale, see [21]). This scale, or resolution, is important both for obtaining smooth fields and constitutive relations. As explained, e.g., in Batchelor [32], the density field is strongly fluctuating as a function of the coarse graining scale (or resolution) for very fine resolutions (e.g., when one uses a REV whose linear dimension is smaller than the corresponding mean free path in a gas), yet its value plateaus to a space-dependent number as a function of resolution. The latter *is* what one refers to as the macroscopic density. For very coarse resolutions the density becomes space dependent again due to macroscopic variations. The same holds for practically any other macroscopic field, see e.g., [33,34] for the case of the stress field. When the macroscopic gradients of a field are "large" the corresponding plateaus may be narrow but still identifiable [33,34]. In some cases, such as fluid turbulence, there is no separation between the smallest and largest relevant scales of certain fields and fluxes, and then these fields, as well as the corresponding constitutive relations, are reso-

lution or scale dependent (e.g., the "eddy viscosity" depends on scale). This may also happen in granular systems [35].

Coarse graining is a projection process through which information is lost. Subresolution scale information is not included in the fields. Therefore attempts to, e.g., define displacement fields that coincide with the particle displacements at their respective centers of mass clash with the notion of coarse graining both in terms of physics and underlying philosophy, even if such interpolations are mathematically feasible. Not only is information not lost this way but the fields one produces may possess large gradients (whose scale, except for the case of ordered systems under small strains, is typically an inverse particle diameter); practically all gradient expansions may fail for such fields. Such interpolation would be tantamount to requiring that the values of the momentum field of a gas at the positions of the centers of mass of the molecules equals the corresponding momenta of the molecules. As is well known the molecules of a gas (macroscopically) at rest have speeds of the order of the speed of sound in the gas, yet the macroscopic momentum and velocity fields vanish. Of course this description requires the use of spatial (and often temporal) coarse graining of finite resolution.

In statistical mechanical theories of fluids it is common to define fields by first using discrete Fourier transforms of the microscopic entities (such as momentum) and then invoking a cutoff in the wave-vector space upon back-transforming. The inverse cutoff is the resolution of the coarse grained fields. In Boltzmann's kinetic theory the spatial resolution is the mean free path.

As mentioned, in early studies of elasticity (see e.g., [2]) the coarse graining scale was taken to be very large compared to the molecular scale (e.g., the lattice constant), yet still small with respect to the macroscopic scales. This is possible when the system of interest is sufficiently large compared to its microscopic scale and the gradients are "small", i.e., the properties of the system are nearly constant on the coarse graining scale. Clearly, such a choice is not possible for nanoscale systems or granular materials due to the lack of good scale separation. As stressed in the Introduction, this in turn requires one to revisit the ways to coarse grain these classes of systems, paying due attention to the resolutions involved. When a system is coarse grained with a spatial resolution, w, no gradient involves a scale that is smaller than w, and therefore one expects to obtain smooth fields whose spatial variation is characterized by scales that exceed the resolution or coarse graining scale. When only a particle and its nearest neighbors are involved in the definition of coarse grained fields, the resolution is very fine and one may not obtain proper continuum descriptions. Ensemble averaging (when relevant) may enable one to use finer resolution but then some features of interest may be smeared out, cf. [33,34]. It is though particularly useful for stationary states (also for cases with good scale separation).

3 Definitions and notation

Consider a finite or infinite number of particles, identified by lower case Latin indices, e.g., the mass of particle i is denoted by m_i. Vectorial and tensorial components are denoted by Greek letters. The positions of the centers of mass of the particles are denoted by $\mathbf{r}_i(t)$, where t denotes time, and the α component of this vector is $r_{i\alpha}(t)$. The corresponding center of mass velocity is $\mathbf{v}_i(t) \equiv \dot{\mathbf{r}}_i(t)$. In addition, $\mathbf{r}_{ij}(t) \equiv \mathbf{r}_i(t) - \mathbf{r}_j(t)$, denotes the relative positions of the centers of mass of two particles, and $\mathbf{v}_{ij}$, the corresponding relative center of mass velocities. The resultant force on particle i is denoted by $\mathbf{f}_i(t)$, and it equals $m_i\dot{\mathbf{v}}_i(t)$ by Newton's second law. Similarly, the angular momentum of particle i is denoted by $\mathbf{S}_i(t)$, and it satisfies $\dot{\mathbf{S}}_i(t) = \mathbf{M}_i(t)$ where $\mathbf{M}_i(t)$ is the resultant torque on particle i (this does not require the particle to be rigid). The force exerted by particle j on particle i is denoted by $\mathbf{f}_{ij}(t)$, and thus $\mathbf{f}_i(t) = \sum_j \mathbf{f}_{ij}(t)$, i.e., we assume binary and additive interactions (as mentioned, it is not difficult to relax this assumption but we don't do it here for sake of simplicity). Bulk forces are easy to include in the formulation but they are not. By Newton's third law: $\mathbf{f}_{ij}(t) = -\mathbf{f}_{ji}(t)$; this is used below quite frequently. Nearly all factors of $\frac{1}{2}$ that appear below stem from the following trivial identity: when expression, A, equals another expression, B, they both also equal $\frac{1}{2}(A + B)$.

A point in space, $\mathbf{r}$, is a point where we choose to measure a physical entity (e.g., the value of the stress tensor field) and it is not "time dependent". The fields depend on $\mathbf{r}$ and t, their time dependence being dictated by that of the particles' positions, $\mathbf{r}_i(t)$, velocities $\mathbf{v}_i(t)$, orientations and angular velocities. The time dependence of the particles' degrees of freedom is often not explicitly spelled out below, nor is that of the fields, for notational simplicity. The Einstein summation convention is used below only for Greek letters (i.e., vector/tensor components) but not Latin indices (that represent the particles' identities); the latter are explicitly summed over. Note that for numerical simulations one needs to restrict the definitions to a set of discrete (e.g., on a grid) points. This causes no problem. The formulation here is Eulerian and can be changed to Lagrangian by standard means, cf. e.g., [24,27].

4 Equation of continuity, stress and stress asymmetry

First we derive the equation of continuity as a trivial example of how the formulation presented here can be used. Then we proceed to the equation of motion for the momentum density and derive an explicit formula for the stress tensor field. The latter expression is used to obtain the antisymmetric part of the stress tensor.

4.1 The equation of continuity

The most trivial and well known equation of motion for any system in which mass is conserved is the equation of continuity for the mass density, a similar statement holding for the number density (or densities in polydisperse systems). The derivation presented below helps further set the notation and demonstrates part of the method used throughout this paper.

The microscopic mass density at a point $\mathbf{r}$ at time t, $\rho^{\rm mic}(\mathbf{r}, \mathbf{t})$, is defined in statistical mechanics by:

$$\rho^{\rm mic}(\mathbf{r}, t) \equiv \sum_i m_i \delta(\mathbf{r} - \mathbf{r}_i(t)), \tag{1}$$

where $\delta(\mathbf{r})$ is the Dirac delta function. This definition complies with the basic requirement that the integral of the mass density over a volume in space equals the mass contained in this volume. It is however a singular entity. A nonsingular mass density can be defined by

$$\rho(\mathbf{r}, t) = \sum_i m_i \phi(\mathbf{r} - \mathbf{r}_i(t)), \tag{2}$$

i.e., by replacing the delta-function by a (real) "coarse graining" function of space, ϕ, which possesses a predetermined "width", w (the coarse graining scale or resolution) and which is required to be positive semi-definite and normalizable (its integral over space is unity). A simple example is $\phi(\mathbf{r}) \equiv \frac{1}{\Omega_d(w)} H(w - \| \mathbf{r} \|)$, where H represents the Heaviside function and $\Omega_d(w)$ is the volume of a sphere of radius w in d-dimensions. Often it is more useful to take ϕ to be a Gaussian of width w since then the resulting field is smoother. In the limit $w \longrightarrow 0$, Eq. 2 becomes identical to Eq. 1. The above coarse graining procedure can also be viewed as being defined by a convolution of the microscopic density with the coarse graining function, i.e.,

$$\rho(\mathbf{r}, t) = \int d\mathbf{r}' \phi(\mathbf{r} - \mathbf{r}') \rho^{\rm mic}(\mathbf{r}', t). \tag{3}$$

In most cases known to the author the values of the fields depend mostly on w and not the precise choice of the coarse graining function as long as the latter is not chosen to be singular or highly anisotropic. Similar definitions will be used for the other coarse grained fields below. Note that (chain rule):

$$\frac{\partial}{\partial t} \phi(\mathbf{r} - \mathbf{r}_i) = -\dot{r}_{i\beta} \frac{\partial}{\partial r_\beta} \phi(\mathbf{r} - \mathbf{r}_i) = -v_{i\beta} \frac{\partial}{\partial r_\beta} \phi(\mathbf{r} - \mathbf{r}_i).$$

Also note that $\frac{\partial}{\partial r_\beta}$ (a component of the gradient) commutes with all variables that describe the particles' degrees of freedom (i.e., it can be moved to front of sums) since the latter are just time dependent entities.

The mass conservation (continuity) equation can be derived by taking the time derivative of the coarse grained mass density:

$$\frac{\partial \rho(\mathbf{r}, t)}{\partial t} = \frac{\partial}{\partial t} \sum_i m_i \phi(\mathbf{r} - \mathbf{r}_i) = -\frac{\partial}{\partial r_\beta} \sum_i m_i v_{i\beta} \phi(\mathbf{r} - \mathbf{r}_i) = -\frac{\partial p_\beta(\mathbf{r}, t)}{\partial r_\beta}, \tag{4}$$

where the coarse grained momentum density is defined by

$$\mathbf{p}(\mathbf{r}, t) \equiv \sum_i m_i \mathbf{v}_i \phi(\mathbf{r} - \mathbf{r}_i), \tag{5}$$

corresponding to the following microscopic momentum density field: $\mathbf{p}^{\rm mic}(\mathbf{r}, t) \equiv \sum_i m_i \mathbf{v}_i(t) \delta(\mathbf{r} - \mathbf{r}_i(t))$ (here the time dependence is explicitly presented). Note that the above result holds even for a single particle and therefore one does not need to resort to arguments involving swarms of particles or ensembles, as in some derivations in the literature. In the limit $w \to 0$ one obtains the same result for microscopic resolution. These observations hold for all fields discussed below and will not be repeated. The coarse grained velocity field *is defined* by

$$\mathbf{V}(\mathbf{r}, t) \equiv \mathbf{p}(\mathbf{r}, t) / \rho(\mathbf{r}, t). \tag{6}$$

Notice that the velocity field is meaningful only as a coarse grained field, unlike the mass and momentum density fields, which are densities of well defined physical entities (from a thermodynamic point of view the velocity field is the vector chemical potential conjugate to the momentum density field). Substituting Eq. 6 in Eq. 4, one obtains the standard form for the equation of continuity: $\dot{\rho} = -\frac{\partial}{\partial r_\beta}(\rho V_\beta)$.

4.2 Equation for the momentum density

The momentum equation can be derived in a similar way. Taking the time derivative of Eq. 5 one obtains:

$$\begin{aligned} \frac{\partial p_\alpha(\mathbf{r}, t)}{\partial t} &= \frac{\partial}{\partial t} \sum_i m_i v_{i\alpha} \phi(\mathbf{r} - \mathbf{r}_i) \\ &= \sum_i m_i \dot{v}_{i\alpha} \phi(\mathbf{r} - \mathbf{r}_i) + \sum_i m_i v_{i\alpha} \frac{\partial \phi(\mathbf{r} - \mathbf{r}_i)}{\partial t} \\ &= \underbrace{\sum_i m_i \dot{v}_{i\alpha} \phi(\mathbf{r} - \mathbf{r}_i)}_{A_\alpha} \underbrace{- \frac{\partial}{\partial r_\beta} \sum_i m_i v_{i\alpha} v_{i\beta} \phi(\mathbf{r} - \mathbf{r}_i)}_{B_\alpha}. \end{aligned} \tag{7}$$

Here the time dependence of the particles' positions and velocities is no longer spelled out. Next, each part of Eq. 7 is treated separately. The first part is:

$$\begin{aligned} A_\alpha &\equiv \sum_i m_i \dot{v}_{i\alpha} \phi(\mathbf{r} - \mathbf{r}_i) = \sum_i f_{i\alpha} \phi(\mathbf{r} - \mathbf{r}_i) \\ &= \sum_{ij} f_{ij\alpha} \phi(\mathbf{r} - \mathbf{r}_i), \end{aligned} \tag{8}$$

where Newton's second law was used and the assumption of additive binary interactions invoked. Upon exchanging the names of the dummy summation variables, i and j, one obtains:

$$A_\alpha = \sum_{ij} f_{ji\alpha}\phi(\mathbf{r}-\mathbf{r}_j).$$

Using Newton's third law one further obtains:

$$A_\alpha = -\sum_{ij} f_{ij\alpha}\phi(\mathbf{r}-\mathbf{r}_j). \tag{9}$$

Upon summing expressions Eq. 8 and Eq. 9 for A_α, and dividing the sum by 2 one obtains:

$$A_\alpha = \frac{1}{2}\sum_{ij} f_{ij\alpha}\left[\phi(\mathbf{r}-\mathbf{r}_i)-\phi(\mathbf{r}-\mathbf{r}_j)\right]. \tag{10}$$

The following identity, which holds for any smooth function, ϕ, will be useful in the sequel:

$$\begin{aligned}\phi(\mathbf{r}-\mathbf{r}_j)-\phi(\mathbf{r}-\mathbf{r}_i) &= \int_0^1 ds\ \frac{\partial}{\partial s}\,\phi(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij})\\ &= \int_0^1 ds\, r_{ij\beta}\frac{\partial}{\partial r_\beta}\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right)\\ &= r_{ij\beta}\frac{\partial}{\partial r_\beta}\int_0^1 ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right),\end{aligned} \tag{11}$$

where integration by parts has been invoked to go from the first to the second line in the above. Substituting the identity, Eq. 11, in Eq. 10 one obtains:

$$A_\alpha = -\frac{1}{2}\frac{\partial}{\partial r_\beta}\sum_{ij} f_{ij\alpha}r_{ij\beta}\int_0^1 ds\,\phi(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}), \tag{12}$$

where again, the commutation of the gradient operator, $\frac{\partial}{\partial r_\beta}$, with the (time dependent) particle position vectors and forces has been invoked. Note that Eq. 11 corresponds to a specific choice of an integration path from $\mathbf{r}_i$ to $\mathbf{r}_j$ (a straight line) and is therefore not the most general possibility for representing the difference in Eq. 10. This issue will be further discussed below.

In rewriting the expression for B_α, defined in Eq. 7, it is convenient to define the *fluctuating velocity* of particle i at time t:

$$\mathbf{v}_i'(\mathbf{r},t) \equiv \mathbf{v}_i(t) - \mathbf{V}(\mathbf{r},t). \tag{13}$$

Note that the reference coarse grained velocity is at the "coarse graining-center", $\mathbf{r}$, and not at the particle's position [21]. This also corresponds to the numerical method of defining fluctuations: one divides the system into boxes and computes the center of mass velocity of the particles in each box. The fluctuating velocity of a particle in a given box is then measured with respect to the center of mass velocity of the particles in the corresponding box and not the velocity field at the particle's position. There are other ways to define fluctuations but they do not always yield results that are consistent with the equations of continuum mechanics. In the realm of kinetic theory (which is a coarse grained theory, as mentioned above) one does define fluctuations with respect to the local value of the pertinent field in the framework of an ensemble average but a discussion of this issue is beyond the goals of this paper. Below we write $\mathbf{v}_i'$ for $\mathbf{v}_i'(\mathbf{r},t)$ for sake of notational brevity.

The following identity follows from the definition, Eq. 13, and the definition of the coarse grained velocity, Eq. 6:

$$\begin{aligned}\sum_i m_i\mathbf{v}_i'\phi(\mathbf{r}-\mathbf{r}_i) &\equiv \sum_i m_i\left[\mathbf{v}_i-\mathbf{V}\right]\phi(\mathbf{r}-\mathbf{r}_i)\\ &= \sum_i m_i\mathbf{v}_i\phi(\mathbf{r}-\mathbf{r}_i) - \mathbf{V}\sum_i m_i\phi(\mathbf{r}-\mathbf{r}_i)\\ &= \mathbf{p}-\rho\mathbf{V} = 0,\end{aligned} \tag{14}$$

i.e., the coarse-grained velocity fluctuation field vanishes by construction, as it should.

Using this result (which implies: $\sum_i V_\alpha v_{i\beta}\phi(\mathbf{r}-\mathbf{r}_i) = V_\alpha\sum_i v_{i\beta}\phi(\mathbf{r}-\mathbf{r}_i) = 0$) and Eq. 7 one obtains:

$$\begin{aligned}B_\alpha &= -\frac{\partial}{\partial r_\beta}\sum_i m_i v_{i\alpha}v_{i\beta}\phi(\mathbf{r}-\mathbf{r}_i)\\ &= -\frac{\partial}{\partial r_\beta}\sum_i m_i(V_\alpha+v_{i\alpha}')(V_\beta+v_{i\beta}')\phi(\mathbf{r}-\mathbf{r}_i)\\ &= -\frac{\partial}{\partial r_\beta}\left[\sum_i m_i V_\alpha V_\beta\phi(\mathbf{r}-\mathbf{r}_i)+\sum_i m_i v_{i\alpha}'v_{i\beta}'\phi(\mathbf{r}-\mathbf{r}_i)\right]\\ &= -\frac{\partial}{\partial r_\beta}\left[\rho V_\alpha V_\beta+\sum_i m_i v_{i\alpha}'v_{i\beta}'\phi(\mathbf{r}-\mathbf{r}_i)\right].\end{aligned} \tag{15}$$

Combining Eqs. 12, 15, yields the momentum conservation equation:

$$\frac{\partial p_\alpha}{\partial t} = -\frac{\partial}{\partial r_\beta}\left[\rho V_\alpha V_\beta - \sigma_{\alpha\beta}\right], \tag{16}$$

where (on the basis of continuum mechanics) we *identify* the following expression for the stress tensor, σ, in terms of microscopic entities:

$$\begin{aligned}\sigma_{\alpha\beta} = &-\frac{1}{2}\sum_{i,j} f_{ij\alpha}r_{ij\beta}\int_0^1 ds\,\phi(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij})\\ &-\sum_i m_i v_{i\alpha}'v_{i\beta}'\phi(\mathbf{r}-\mathbf{r}_i),\end{aligned} \tag{17}$$

The first term on the right hand side of Eq. 17 is the "contact" or "collisional" stress, $\boldsymbol{\sigma}^c$, while the second term is the "kinetic" or "streaming" stress, $\boldsymbol{\sigma}^k$ (with $\boldsymbol{\sigma} = \boldsymbol{\sigma}^c + \boldsymbol{\sigma}^k$) and it is negligible for quasi-static deformations. Note that in static states (all velocities vanish), Eq. 16 identically reduces to $\mathrm{div}\boldsymbol{\sigma}^c = 0$, as expected.

When the coarse graining scale, w, is far larger than the typical distance between interacting particles one can neglect $s\mathbf{r}_{ij}$ in the integral in Eq. 17, since for most particle pairs that contribute to the sum in this equation $\| \mathbf{r} - \mathbf{r}_i \| >> \| \mathbf{r}_{ij} \|$. In this case: $\sigma^c_{\alpha\beta} \approx -\frac{1}{2}\sum_{i,j} f_{ij\alpha} r_{ij\beta} \phi(\mathbf{r} - \mathbf{r}_i)$, where $\boldsymbol{\sigma}^c$ stands for "the contact stress contribution". Furthermore, when $\phi(\mathbf{r} - \mathbf{r}_i)$ is chosen to equal $\frac{1}{\Omega_d(w)} H(w - \| \mathbf{r} - \mathbf{r}_i \|)$, i.e., one averages over a sphere around $\mathbf{r}$, the formula reduces to the well known (and frequently used) Born-Huang expression: $\sigma^c_{\alpha\beta} \approx -\frac{1}{2}\frac{1}{\Omega_d(w)}\sum_{i,j;\|(\mathbf{r}-\mathbf{r}_i)\|<w} f_{ij\alpha} r_{ij\beta}$. In other words, the standardly employed formula is only justified in the limit of large coarse graining scales and spherical coarse graining volumes, and needs to be replaced by the exact expression presented above when one is concerned with mesoscopic scales, else the error can be large [24,33,34]. As mentioned, the original, e.g., in Born and Huang [2], derivation of this formula pertains to molecular systems that possess strong scale separation and therefore the use of the limit of "coarse" resolution compared to molecular dimensions is practically always justified. Also note that the coarse graining center in many applications of the Born–Huang formula is taken to be the center of mass of "particle i". A one dimensional demonstration of this formulation can be found in Goldenberg and Goldhirsch [24].

One may criticize [25,26,30,31] the above derivation of the expression for the stress since it is not unique, in the sense that any tensor whose divergence vanishes can be added to the expression without changing the equation of motion. Furthermore, the choice in Eq. 11 of a straight line interpolation may seem arbitrary (other choices amount to adding a divergence free tensor to the obtained expression). However, in addition to the fact that the above choice of the integration path is simple to implement (when Maxwellian or Heaviside coarse-graining functions are used one can perform the integration analytically and obtain an explicit expression, hence the numerical application of this formula is not more expensive than that of other expressions) it can be shown [31] that additional symmetry requirements (e.g., that the stress tensor is invariant to permutations of the particles' identities, symmetric for particles interacting by binary central forces, reduces to the well known formula for equilibrium pressure and more) render this a unique choice. A stronger argument in favor of the above expression for the contact part of the stress tensor is provided in Sect. 4.3. Note that the integral of the above expression for the normal stress over a closed surface yields the total force acting on the material enclosed by the surface. The expression does not a-priori guarantee the same for an open surface. As shown in Sect. 4.3 the force exerted across any smooth (even open) geometric surface is given by an integral of the normal stress over this surface, in accordance with Cauchy's definition of stress.

4.3 A direct derivation and physical interpretation of Eq. 17

It is sufficient to derive the contact part of the stress tensor since the expression for the kinetic contribution is not disputed. To this end recall that the classical (Cauchy) definition of stress is related to the force per unit area applied through a small area that is normal to direction, $\hat{\mathbf{n}}$, by the material on the side to which $\hat{\mathbf{n}}$ points on the material on the other side, in the limit of "vanishing" area. In a system comprising discrete particles one needs to identify the forces transmitted through this small area. To this end consider for simplicity (and without loss of generality) a square of side ϵ whose normal points in the positive y direction and whose center is at the "origin" $\mathbf{r}^0 \equiv (x^0, y^0, z^0)$, as depicted in Fig. (1). It is reasonable to define a force as penetrating the square (or acting through it) if a particle to the right of the square, whose center of mass is at $\mathbf{r}_j$, i.e., $y_j > y^0$, exerts a force on a particle whose center of mass is at $\mathbf{r}_i$ to the left of the square, i.e., $y_i < y^0$. This condition is not sufficiently restrictive since by it alone any particle whose center of mass resides to the right of the $x - z$ plane and which interacts with a particle whose center of mass is located to the left of the $x - z$ plane will contribute to the stress. A further restriction is obtained when one requires the line connecting the centers of mass of the interacting particles to intersect the above mentioned square. Note that the actual point of contact can be either on the right or left of the $x - z$ plane (or on it), depending on the particles' shapes, orientations and positions. Now, the contact stress component contributed by particles i and j, $\sigma^{c;i,j}_{\alpha 2}$, at $\mathbf{r}^0$ can be written as follows (the subscript 2 stands for the y direction):

$$\sigma^{c;i,j}_{\alpha 2} = \lim_{\epsilon \to 0} \frac{1}{\epsilon^2} f_{ij\alpha} \times (\text{expression for the constraints})$$

The first constraint on the locations of the centers of mass of particles i and j can be expressed as follows: $H(y_j - y^0)H(y^0 - y_i) \neq 0$, where H denotes the Heaviside function. Next, in order for the line connecting the centers of mass to cut through the $x - z$ plane there must be a number $0 \leq s^* \leq 1$ such that $y_i + s^*(y_j - y_i) = y^0$. Denoting $y_{ij} \equiv y_i - y_j$ this condition amounts to $y^0 - y_i + s^* y_{ij} = 0$. It can be enforced as a constraint by noting that

$$|y_{ij}| \int_0^1 \delta(y^0 - y_i + s y_{ij}) ds = \begin{cases} 1 & \text{when a value, } s^*, \\ & \text{with } 0 \leq s^* \leq 1 \\ & \text{satisfies the} \\ & \text{above constraint} \\ 0 & \text{otherwise} \end{cases}$$

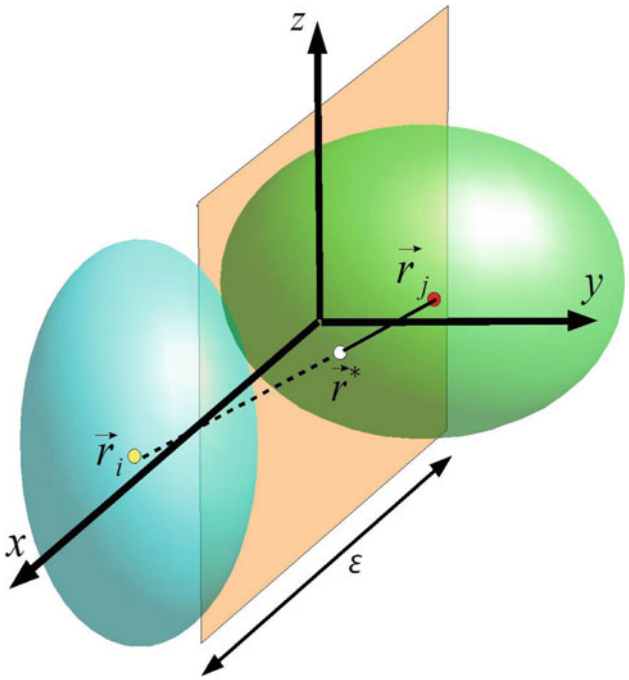

Fig. 1 Demonstration of the procedure for finding the contact stress: note the *square* of side ϵ in the (x, z) plane around the origin at (x^0, y^0, z^0). The center of mass of particle j, denoted by $\mathbf{r}_j$ is to the right of the plane, i.e., $y_j > y^0$, and the center of mass of particle i is to the left of the plane, i.e., $y_i < y^0$. A *straight line* connects these two centers of mass and pierces through the *square*, else these particles would not have been considered to contribute to the force exerted "through the square" by particle j on particle i. The intersection point of this line with the *square* is denoted by $\mathbf{r}^*$

hence the constraint is $|y_{ij}| \int_0^1 \delta(y^0 - y_i + s y_{ij}) ds \neq 0$. For the same value of $s = s^*$ one would like the line that connects the centers of mass to actually intersect the square (not only the $x - z$ plane). This means that one needs the x and z components of the point of intersection, $\mathbf{r}^*$, not to be farther away than a distance $\frac{\epsilon}{2}$ from the origin, i.e., the following needs to be satisfied: $H(\frac{\epsilon}{2} - |x^0 - x_i + s^* x_{ij}|)\, H(\frac{\epsilon}{2} - |z^0 - z_i + s^* z_{ij}|) \neq 0$. All of these conditions can be combined into:

$$H(y_j - y^0)\, H(y^0 - y_i)|y_{ij}| \int_0^1 ds \, \Big(\delta(y^0 - y_i + s y_{ij}) \times H\left(\frac{\epsilon}{2} - |x^0 - x_i + s x_{ij}|\right) H\left(\frac{\epsilon}{2} - |z^0 - z_i + s z_{ij}|\right)\Big) \neq 0$$

This condition can be further simplified by noting that the delta function implies that the y-component of the point of intersection, i.e., y^0 (which also equals y^*, since both are in the same $x - z$ plane), is between y_i and y_j; therefore one can replace $H(y_j - y^0) H(y^0 - y_i)$ in the last expression by $H(y_{ji})$. In addition, given the last condition one can also replace $|y_{ij}|$ in the prefactor of the delta function by $-y_{ij}$. With these, the expression for the contact stress can be written as:

$$\sigma^c_{\alpha 2} = \lim_{\epsilon \to 0} \frac{1}{\epsilon^2} \sum_{ij} f_{ij\alpha}(-y_{ij}) H(y_{ji}) \times \int_0^1 ds \, \Big(\delta(y^0 - y_i + s y_{ij}) \times H\left(\frac{\epsilon}{2} - |x^0 - x_i + s x_{ij}|\right) H\left(\frac{\epsilon}{2} - |z^0 - z_i + s z_{ij}|\right)\Big)$$

where a summation over all particle pairs has been invoked. Next, note that $\lim_{\epsilon \to 0} \frac{1}{\epsilon} H(\frac{\epsilon}{2} - |G|) = \delta(G)$ for any real variable or function, G (the Heaviside function defines a rectangle of width ϵ and its prefactor defines a height of $\frac{1}{\epsilon}$). Therefore the limit $\epsilon \to 0$ in the last equation can be executed, the result being:

$$\sigma^c_{\alpha 2} = -\sum_{ij} f_{ij\alpha} y_{ij}\, H(y_{ji}) \int_0^1 ds \, \Big(\delta(y^0 - y_i + s y_{ij}) \times \delta(x^0 - x_i + s x_{ij}) \delta(z^0 - z_i + s z_{ij})\Big) \tag{18}$$

or

$$\sigma^c_{\alpha 2} = -\sum_{ij} f_{ij\alpha} y_{ij}\, H(y_{ji}) \times \int_0^1 ds \, \delta(\mathbf{r}^0 - \mathbf{r}_i + s \mathbf{r}_{ij})$$

Next, it is convenient to replace the general point $\mathbf{r}^0$ by just $\mathbf{r}$ and it is clearly allowed to replace the index '2' in the above equation by a general index, β. The result is:

$$\sigma^c_{\alpha\beta} = -\sum_{ij} f_{ij\alpha} r_{ij\beta} H(r_{ji\beta}) \int_0^1 ds \, \delta(\mathbf{r} - \mathbf{r}_i + s \mathbf{r}_{ij}) \tag{19}$$

Note that (by a simple change of variables, $s \longrightarrow 1 - s$):

$$\chi_{ji} \equiv \int_0^1 ds \, \phi(\mathbf{r} - \mathbf{r}_j + s \mathbf{r}_{ji}) = \int_0^1 ds \, \phi(\mathbf{r} - \mathbf{r}_i + s \mathbf{r}_{ij}) = \chi_{ij} \tag{20}$$

i.e., the integral χ_{ij} is symmetric under the exchange of i and j. This also clearly holds when ϕ is replaced by a delta function (the limit $w \to 0$). Also note that the product $f_{ij\alpha} r_{ij\beta}$ is symmetric under the same exchange of indices. Therefore, this exchange of dummy indices yields from Eq. 19:

$$\sigma^c_{\alpha\beta} = -\sum_{ij} f_{ij\alpha} r_{ij\beta} H(r_{ij\beta}) \int_0^1 ds \, \delta(\mathbf{r} - \mathbf{r}_i + s \mathbf{r}_{ij}). \tag{21}$$

Since Eqs. 19, 21 represent the same entity one can add up the corresponding expressions and divide by 2. Also, since the only difference between these expressions is the sign inside the Heaviside function one obtains:

$$\sigma^c_{\alpha\beta} = -\frac{1}{2}\sum_{ij} f_{ij\alpha} r_{ij\beta} \int_0^1 \delta(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}) ds. \tag{22}$$

Equation 22 provides an exact expression for the contact stress with microscopic resolution (corresponding to $w = 0$). We shall rename the result $\boldsymbol{\sigma}^{c,\mathrm{mic}}$ to denote this fact. The coarse grained contact stress can now be obtained by convoluting the latter expression with the coarse graining function, i.e., computing

$$\sigma^c_{\alpha\beta}(\mathbf{r}) = \int d\mathbf{r}' \phi(\mathbf{r} - \mathbf{r}')\, \sigma^{c,\mathrm{mic}}_{\alpha\beta}(\mathbf{r}').$$

Alternatively and equivalently one may replace the delta function in Eq. 22 by the coarse graining function.

This derivation shows that indeed the identification of the stress tensor field in Eq. 17 is justified in the sense that the same expression complies with Cauchy's definition of stress and clearly the integration of the normal stress over an open surface yields the force transmitted "through" this surface. This should answer at least part of the above mentioned criticism [25,26,30,31] raised against the validity of the expression for the contact stress in Eq. 17.

4.4 The antisymmetric part of the stress tensor field

The kinetic stress is manifestly symmetric and therefore it does not contribute to the antisymmetric part of the stress tensor, i.e., $\sigma_{\alpha\beta} - \sigma_{\beta\alpha} = \sigma^c_{\alpha\beta} - \sigma^c_{\beta\alpha}$, where we recall that:

$$\sigma^c_{\alpha\beta} = -\frac{1}{2}\sum_{i,j} f_{ij\alpha} r_{ij\beta} \int_0^1 ds\, \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}). \tag{23}$$

It follows that:

$$\sigma_{\alpha\beta} - \sigma_{\beta\alpha} = -\frac{1}{2}\sum_{i,j} \left(f_{ij\alpha} r_{ij\beta} - f_{ij\beta} r_{ij\alpha}\right) \times \int_0^1 ds\, \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}), \tag{24}$$

hence

$$\sigma_{\alpha\beta} - \sigma_{\beta\alpha} = -\frac{1}{2}\sum_{i,j} \epsilon_{\alpha\beta\gamma} \left[\mathbf{r}_{ij} \times \mathbf{f}_{ij}\right]_\gamma \times \int_0^1 ds\, \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}) \tag{25}$$

where $\epsilon_{\alpha\beta\gamma}$ is the antisymmetric isotropic tensor. It follows immediately that when only normal contact forces are present and the particles are (internally) homogeneous spheres (or inhomogeneous in such a way that their centers of mass coincide with their respective geometric centers) the stress tensor is symmetric, else the vector product in the last equation need not vanish and a stress asymmetry arises even for spheres. For central interactions (i.e., $\mathbf{f}_{ij} \parallel \mathbf{r}_{ij}$) the stress is always symmetric. Other possibilities are discussed below.

Denote by $\mathbf{M}^f_{ij}$ the torque applied on particle i by the *force* exerted by particle j on particle i. This torque can be due to frictional forces as well as normal forces, e.g., when the particles are not spherical. Clearly: $\mathbf{M}^f_{ij} = (\mathbf{r}^c_{ij} - \mathbf{r}_i) \times \mathbf{f}_{ij}$, where $\mathbf{r}^c_{ij}$ denotes the point of contact of particles i and j; when the contact is not approximated by a point one can still define an effective point of contact but this is not important here. Also, the theory can easily be extended to the case when several points of contact between a pair of particles (e.g., for concave particles) exist. Clearly $\mathbf{r}^c_{ij} = \mathbf{r}^c_{ji}$. Similarly, the torque exerted by particle i on particle j is given by $\mathbf{M}^f_{ji} = (\mathbf{r}^c_{ij} - \mathbf{r}_j) \times \mathbf{f}_{ji} = -(\mathbf{r}^c_{ij} - \mathbf{r}_j) \times \mathbf{f}_{ij}$. Notice that $\mathbf{r}_{ij} = -(\mathbf{r}^c_{ij} - \mathbf{r}_i) + (\mathbf{r}^c_{ij} - \mathbf{r}_j)$. It follows that: $\mathbf{r}_{ij} \times \mathbf{f}_{ij} = -\mathbf{M}^f_{ij} - \mathbf{M}^f_{ji}$. Substitution of the latter result into Eq. 25 yields:

$$\begin{aligned}\sigma_{\alpha\beta} - \sigma_{\beta\alpha} &= \frac{1}{2}\sum_{i,j} \epsilon_{\alpha\beta\gamma}\left(M^f_{ij\gamma} + M^f_{ji\gamma}\right) \int_0^1 ds \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}) \\ &= \frac{1}{2}\sum_{i,j} \epsilon_{\alpha\beta\gamma} M^f_{ij\gamma} \int_0^1 ds\, \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}) \\ &\quad + \frac{1}{2}\sum_{i,j} \epsilon_{\alpha\beta\gamma} M^f_{ji\gamma} \int_0^1 ds\, \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}).\end{aligned} \tag{26}$$

Upon exchanging i and j in the last line of Eq. 26 and using the symmetry, Eq. 20, one obtains:

$$\sigma_{\alpha\beta} - \sigma_{\beta\alpha} = \sum_{i,j} \epsilon_{\alpha\beta\gamma} M^f_{ij\gamma} \int_0^1 ds\, \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}). \tag{27}$$

This is one way to express the antisymmetric part of the stress tensor field. One can obtain further insights by rewriting this exact result in a different way. Details can be found in Appendix A-1. The result is:

$$\begin{aligned}\sigma_{\alpha\beta} - \sigma_{\beta\alpha} &= \epsilon_{\alpha\beta\gamma} \sum_i \dot{S}_{i\gamma} \phi(\mathbf{r} - \mathbf{r}_i) \\ &\quad + \epsilon_{\alpha\beta\gamma} \frac{\partial}{\partial r_\delta} \sum_{i,j} \left(\frac{1}{2} M^{rf}_{ij\gamma} r_{ij\delta} \int_0^1 ds \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}) \right. \\ &\quad \left. + M^f_{ij\gamma} r_{ij\delta} \int_0^1 ds(1-s) \phi(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij}) \right).\end{aligned} \tag{28}$$

The three terms in the above equation represent the contributions of the rotations (dynamics), rolling friction and "reg-

ular" friction (and normal forces for non-spherical particles that give rise to torques) to the stress asymmetry (which, in general, stems from localized sources of torques, or angular momentum).

Note that even in the quasistatic limit (i.e., for $\dot{\mathbf{S}}_i = 0$), there are contributions to the stress asymmetry that are not nominally vanishing. However, these contributions take on the form of a divergence. One can try to naively estimate the values of these contributions as follows (for different approaches to estimate length scales associated with Cosserat formulations, cf. e.g., [36] and references therein). The largest value of a derivative, given the resolution, is of the order of $\frac{1}{w}$. The typical value of the rolling friction term, up to a constant, is the product df, where f represents the norm of a typical force, and d stands for a typical particle diameter (the same holding for the force contribution to the torque). Also, the norm of $\mathbf{r}_{ij}$ can be represented by d. Therefore the overall contribution of this term can be roughly estimated by $\frac{1}{w\Omega_d(w)} f d^2 N_c q_1$, where $\Omega_d(w)$ is the coarse graining volume (the normalization of ϕ when it is taken to be a Heaviside function), N_c is the number of contacts in the volume and q_1 is a "reduction factor" due to cancellations stemming from possible different signs of the summands. To within an O(1) factor, $\Omega_3(w) \approx w^3$ in three dimensions. Therefore one can estimate the antisymmetric part of the stress tensor in three dimensions by $f\frac{d^2}{w^4} N_c q_1$. Compare this to a similar rough estimate of the stress: $\frac{f d N_c q_2}{w^3}$, where q_2 plays a similar role to q_1. The ratio of the former to the latter is $\frac{d}{w}$ when $q_1 \approx q_2$ (unjustified), and it is rather small for large coarse graining scales, irrespective of the neglected numerical factors. However, it can be rather significant for small coarse graining scales. Note that even in the absence of rolling friction there is a contribution to the stress asymmetry which is approximately of the same order as the above estimate. When the dynamics is not "slow" the antisymmetric part of the stress has a contribution from the time dependence of the particles' angular momenta. For frictionless spherical homogeneous particles the stress tensor is symmetric as already mentioned above. Finally, note that the above result is similar but not identical to that obtained in Bardet and Vardoulakis [12] since they do not use controlled resolution fields and their results are basically valid in the limit of low resolution (or large w in the language of this paper); the similarity can be easily appreciated by comparing Eq. 27 with (47–48) in Bardet and Vardoulakis [12].

5 Equation for the angular momentum density field, and the couple-stress tensor

In order to define the angular momentum of a system or parts of it one needs a fixed reference point (in an inertial frame) with respect to which angular momentum is measured (the center of mass of the system can also be used, even when it accelerates, but this is not convenient here). We denote this point by $\mathbf{r}_o$. The reference point does not have to be "inside" the system or otherwise related to it. Since angular momentum is conserved in the absence of external torques, its density should satisfy a conservation equation similar to that that is satisfied by the momentum density. In the case of momentum density the flux accounts both for the flow of momentum due to the mere motion of the particles and the transfer of momentum by forces that are exerted on a subsystem (e.g., within the coarse graining volume) by the complementary subsystem (its exterior). In the case of angular momentum the flux accounts for the transfer of angular momentum by the mere motion of the particles and by torques on a given subsystem exerted by the complementary subsystem. It does not matter whether the torques are the results of forces or couples, such as those involved in rolling friction.

The angular momentum of particle i with respect to $\mathbf{r}_0$ is given by: $(\mathbf{r}_i - \mathbf{r}_o) \times m_i \mathbf{v}_i + \mathbf{S}_i$. Recall that $\mathbf{S}_i$ denotes the angular momentum of particle i around its center of mass. On the basis of this we define the angular momentum density as follows:

$$\mathbf{L} \equiv \sum_i [(\mathbf{r}_i - \mathbf{r}_o) \times m_i \mathbf{v}_i + \mathbf{S}_i]\, \phi(\mathbf{r} - \mathbf{r}_i). \tag{29}$$

Clearly a microscopic angular momentum density field can be defined by replacing ϕ by a delta function. It follows from the definition of $\mathbf{L}$ that:

$$\begin{aligned}\mathbf{L} &= \sum_i [(\mathbf{r}_i - \mathbf{r} + \mathbf{r} - \mathbf{r}_o) \times m_i \mathbf{v}_i + \mathbf{S}_i]\, \phi(\mathbf{r} - \mathbf{r}_i) \\ &= (\mathbf{r} - \mathbf{r}_o) \times \mathbf{p} + \sum_i [m_i\, (\mathbf{r}_i - \mathbf{r}) \times \mathbf{v}_i \\ &\quad + \mathbf{S}_i]\, \phi(\mathbf{r} - \mathbf{r}_i) = (\mathbf{r} - \mathbf{r}_o) \times \mathbf{p} + \mathbf{J},\end{aligned} \tag{30}$$

where the local angular momentum (LAM) density, $\mathbf{J}$ (with respect to the coarse graining center, $\mathbf{r}$), is defined as:

$$\mathbf{J} \equiv \sum_i [m_i\, (\mathbf{r}_i - \mathbf{r}) \times \mathbf{v}_i + \mathbf{S}_i]\, \phi(\mathbf{r} - \mathbf{r}_i). \tag{31}$$

Note that this entity does not depend on the reference point, $\mathbf{r}_o$. The physical interpretation of the above is obvious: the angular momentum corresponding to a coarse graining volume in the system is the sum of its internal angular momentum (measured with respect to the center of coarse graining, $\mathbf{r}$), $\mathbf{J}$, and the angular momentum due to the resultant momentum in this volume with respect to the reference point, $\mathbf{r}_o$. A derivation of the continuum mechanical equation for the LAM density, $\mathbf{J}$, is presented in Appendix A-2. The result is:

$$\frac{\partial J_\alpha}{\partial t} = -\frac{\partial}{\partial r_\delta} [V_\delta J_\alpha - C_{\alpha\delta}] - \varepsilon_{\alpha\beta\gamma}\sigma_{\beta\gamma}, \tag{32}$$

where the *couple stress* tensor is given by:

$$C_{\alpha\delta} = -\frac{1}{2}\sum_{ij}\left[\left(\left(\mathbf{r}_{ij}^{c}-\mathbf{r}\right)\times\mathbf{f}_{ij}\right)_{\alpha}+M_{ij\alpha}^{rf}\right]\mathbf{r}_{ij\delta} \times\int_{0}^{1}ds\,\phi\left(\mathbf{r}-\mathbf{r}_{i}+s\mathbf{r}_{ij}\right)-\sum_{i}\left[\varepsilon_{\alpha\beta\gamma}\left(r_{i\beta}-r_{\beta}\right) \times m_{i}v_{i\gamma}+S_{i\alpha}\right]v_{i\delta}'\phi(\mathbf{r}-\mathbf{r}_{i}). \quad (33)$$

In the quasi-static limit Eq. 33 simplifies to:

$$C_{\alpha\delta} = -\frac{1}{2}\sum_{ij}\left[\left(\left(\mathbf{r}_{ij}^{c}-\mathbf{r}\right)\times\mathbf{f}_{ij}\right)_{\alpha}+M_{ij\alpha}^{rf}\right]\mathbf{r}_{ij\delta} \times\int_{0}^{1}ds\,\phi\left(\mathbf{r}-\mathbf{r}_{i}+s\mathbf{r}_{ij}\right). \quad (34)$$

Like in Eq. 28 note that the couple stress has terms due to friction and rolling friction. When the dynamic part is not neglected there is also a contribution to the particles' rotation and angular momentum with respect to the coarse-graining center, $\mathbf{r}$.

A further simplification is obtained when rolling friction is neglected:

$$C_{\alpha\delta} = -\frac{1}{2}\sum_{ij}\left(\left(\mathbf{r}_{ij}^{c}-\mathbf{r}\right)\times\mathbf{f}_{ij}\right)_{\alpha}\mathbf{r}_{ij\delta} \times\int_{0}^{1}ds\,\phi\left(\mathbf{r}-\mathbf{r}_{i}+s\mathbf{r}_{ij}\right). \quad (35)$$

In the limit of large coarse graining scales and a spherical coarse graining volume one obtains:

$$C_{\alpha\delta} = -\frac{1}{2\Omega_{d}(w)}\sum_{ij;\|\mathbf{r}-\mathbf{r}_{i}\|<w}\left(\left(\mathbf{r}_{ij}^{c}-\mathbf{r}\right)\times\mathbf{f}_{ij}\right)_{\alpha}\mathbf{r}_{ij\delta}. \quad (36)$$

This formula is very similar to, e.g., the expression used by Lätzel et al. [11] and others for the same entity (rewritten in the language of this article): $\frac{1}{\Omega_d(w)}\sum_{j\text{contacts of }i}((\mathbf{r}_{ij}^{c}-\mathbf{r}_i)\times\mathbf{f}_{ij})_{\alpha}r_{ij\delta}$, where $\mathbf{r}$ in Eq. 36 is replaced by $\mathbf{r}_i$, the latter serving as the "coarse graining center" in the phenomenological approaches. However, the effective value of w in the latter approaches is basically a diameter and therefore the limit of large w does not apply there.

Note that Eq. 32 is not a strict conservation equation for the LAM density, $\mathbf{J}$, since the latter does not represent the density of a conserved quantity by itself. Therefore its time derivative includes a source term, $-\varepsilon_{\alpha\beta\gamma}\sigma_{\beta\gamma}$, which is proportional to the antisymmetric part of the stress tensor. The full momentum density, $\mathbf{L}(\mathbf{r},t)$, is conserved, as can be verified by adding the contribution of the time derivative of $(\mathbf{r}-\mathbf{r}_0)\times\mathbf{p}$ to that of $\mathbf{J}$:

$$\frac{\partial L_{\alpha}}{\partial t} = \frac{\partial}{\partial t}\left[\varepsilon_{\alpha\beta\gamma}\left(r_{\beta}-r_{0\beta}\right)p_{\gamma}+J_{\alpha}\right] = -\frac{\partial}{\partial r_{\delta}}\left\{V_{\delta}L_{\alpha}-\varepsilon_{\alpha\beta\gamma}\left(r_{\beta}-r_{0\beta}\right)\sigma_{\gamma\delta}-C_{\alpha\beta}\right\}. \quad (37)$$

Note that three terms contribute to the angular momentum flux. The first is a convective term, the second is a torque due to the stress and the third is the couple stress, in agreement with continuum mechanics [37].

6 Concluding remarks

One of the main objectives of coarse graining is to produce constitutive relations for the continuum equations as well as appropriate boundary conditions. This has been achieved for gases and granular gases using the Boltzmann equation and its extensions, and for molecular liquids by employing the powerful methods of response and projection operator theory. When it comes to disordered solids and dense granular systems in static or "liquid" states or under quasi-static deformations, there is still much to be done, see however the derivation of elasticity in Goldhirsch and Goldenberg [27].

When attempting to coarse grain from the level of the constituents to that of continuum theory one needs to bear in mind that the fields thus obtained and their corresponding fluxes, sources and sinks should actually be smooth (with possible exceptions, e.g., when shocks are concerned), preferably have a well defined resolution (as is the case in non-equilibrium statistical mechanical derivations) and obey the equations of continuum mechanics. These "rules" are not always "obeyed" in phenomenological studies, in particular one often considers "fields" that are only defined on the discrete set of particle centers of mass, one uses expressions that are justified for large coarse graining scales when only a particle and the particles with which it is in contact (typically, its nearest neighbors) are accounted for, and one does not pay attention to the boundaries. Furthermore, it is not clear whether some of the definitions employed for these "fields" actually satisfy the equations of continuum mechanics. Concerning boundaries, it is known from, e.g., fluid dynamics that near boundaries there is a thin (Knudsen) layer where the constitutive relations (which are usually based on gradient expansions) do not hold since *there* the gradients are "large". A proper way to incorporate the effects of boundaries in kinetic theories has been developed and it involves the matching of the kinetics near the boundaries to the continuum descriptions away (i.e., a few mean free paths) from them, cf. [38] for a general description and [39] for an application to granular gases. A similar procedure has not yet been developed for dense granular systems. However, one may note the following. The stress field defined above, and even those defined phenomenologically, does not vanish at

the surface of a "sand pile". At first this looks surprising but then consider the above definition of the stress *field* at points which are a few w's from the surface: there the stress automatically vanishes and this is fully compatible with the understanding that the description has a finite resolution.

Even before one uses coarse graining to obtain constitutive relations one can employ the above (and other) expressions for the study of results of computations or experiments and their characterization in terms of stress, strain (not discussed in this paper), couple-stress and other fields; for application of the above formulation (including the strain field), see [24,27,28,40,41].

It is important to reiterate the issue of plateaus. Experimental results concerning purely sheared two dimensional slabs [41], as well as numerical findings [24,33,34] show that even when the gradients of various fields are relatively large one can observe plateaus, e.g., in the stress as a function of resolution, or w. This allows one to define "objective" continuum fields.

In summary, this paper describes a coarse graining approach, stresses the meaning of coarse graining and presents novel results concerning the couple stress and stress asymmetry, and the question of uniqueness of the stress field. These and other results should be relevant for other systems such as disordered solids, and since one can control the resolution and define it to be quite fine, one may apply them to nanoscale materials [24]. The above results can easily be extended to include temporal coarse graining, when needed, see [21].

Acknowledgments Section 4 is based on published work with Ben Glasser and Chay Goldenberg. Part of Sect. 5 is based on preliminary work with Chay Goldenberg. Discussions with Jens Boberski, Chay Goldenberg, Joe Goddard, Hans Herrmann, Niels Kruyt, Stefan Luding, Thorsten Pöschel, Ioannis Vardoulakis, and Dietrich Wolf are gratefully acknowledged. The results presented in Sect. 4.3 were obtained by IG in the summer of 2009, in Kyoto, Japan, during the workshop "Frontiers in Nonequilibrium Physics". The author is grateful to Hisao Hayakawa and the Yukawa Institute for their kind hospitality.

Appendix A: Details of some derivations

This appendix presents technical details of the derivations of some expressions in the main text.

A-1: the stress asymmetry

Following Eq. 27:

$$\begin{aligned}\sigma_{\alpha\beta}-\sigma_{\beta\alpha}&=\sum_{i,j}\epsilon_{\alpha\beta\gamma}M^f_{ij\gamma}\int_0^1 ds\left(\phi(\mathbf{r}-\mathbf{r}_i)\right.\\&\left.+\int_0^s\frac{\partial}{\partial s'}\phi(\mathbf{r}-\mathbf{r}_i+s'\mathbf{r}_{ij})ds'\right)\\&=\sum_i\epsilon_{\alpha\beta\gamma}M^f_{i\gamma}\phi(\mathbf{r}-\mathbf{r}_i)\\&+\epsilon_{\alpha\beta\gamma}\frac{\partial}{\partial r_\delta}\sum_{i,j}M^f_{ij\gamma}r_{ij\delta}\int_0^1 ds\\&\times\int_0^s\phi(\mathbf{r}-\mathbf{r}_i+s'\mathbf{r}_{ij})ds'\end{aligned}\tag{38}$$

where $\mathbf{M}^f_i\equiv\sum_j\mathbf{M}_{ij}$ is the resultant torque on particle i *due to forces*; note that integration by parts has been invoked in the above chain of equations. A simple transformation of the above double integral yields:

$$\begin{aligned}\sigma_{\alpha\beta}-\sigma_{\beta\alpha}&=\epsilon_{\alpha\beta\gamma}\sum_i M^f_{i\gamma}\phi(\mathbf{r}-\mathbf{r}_i)\\&+\epsilon_{\alpha\beta\gamma}\frac{\partial}{\partial r_\delta}\sum_{i,j}M^f_{ij\gamma}r_{ij\delta}\int_0^1 ds(1-s)\phi(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}).\end{aligned}\tag{39}$$

Recalling that $\dot{\mathbf{S}}_i=\mathbf{M}_i$, the resultant torque on particle i, and noting that: $\mathbf{M}_i=\mathbf{M}^f_i+\mathbf{M}^{rf}_i$, where $\mathbf{M}^{rf}$ denotes the contribution of rolling friction (or couples in general), one can replace $\mathbf{M}^f_i$ in Eq. 39 by $\dot{\mathbf{S}}_i-\mathbf{M}^{rf}_i$. The result is:

$$\begin{aligned}\sigma_{\alpha\beta}-\sigma_{\beta\alpha}&=\epsilon_{\alpha\beta\gamma}\sum_i(\dot{S}_{i\gamma}-M^{rf}_{i\gamma})\phi(\mathbf{r}-\mathbf{r}_i)\\&+\epsilon_{\alpha\beta\gamma}\frac{\partial}{\partial r_\delta}\sum_{i,j}\mathbf{M}^f_{ij\gamma}r_{ij\delta}\int_0^1 ds(1-s)\phi(\mathbf{r}-\mathbf{r}_i+\mathbf{r}_{ij})\end{aligned}\tag{40}$$

Denote by M^{rf}_{ij} the couple exerted by particle j on particles i. Clearly,

$$\begin{aligned}\sum_i M^{rf}_{i\gamma}\phi(\mathbf{r}-\mathbf{r}_i)&=\sum_{ij}M^{rf}_{ij\gamma}\phi(\mathbf{r}-\mathbf{r}_i)\\&=\sum_{ij}M^{rf}_{ji\gamma}\phi(\mathbf{r}-\mathbf{r}_j)\\&=-\sum_{ij}M^{rf}_{ij\gamma}\phi(\mathbf{r}-\mathbf{r}_j),\end{aligned}$$

where use has been made of $\mathbf{M}^{rf}_{ij}=-\mathbf{M}^{rf}_{ji}$. Therefore:

$$\sum_i M^{rf}_{i\gamma}\phi(\mathbf{r}-\mathbf{r}_i)=-\frac{1}{2}\sum_{ij}M^{rf}_{\gamma ij}\left(\phi(\mathbf{r}-\mathbf{r}_j)-\phi(\mathbf{r}-\mathbf{r}_i)\right)$$

$$= -\frac{\partial}{\partial r_\delta}\frac{1}{2}\sum_{ij} M^{rf}_{ij\gamma} r_{ij\delta}\int_0^1 ds\phi(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}). \tag{41}$$

Upon substituting this result in Eq. 40 one obtains another expression for the stress difference, Eq. 28.

A-2: the equation of motion for the LAM

Consider the time derivative of the α component of the LAM density, Eq. 31:

$$\begin{aligned}
\frac{\partial J_\alpha}{\partial t} &= \frac{\partial}{\partial t}\sum_i \left[\varepsilon_{\alpha\beta\gamma} m_i \left(r_{i\beta}-r_\beta\right) v_{i\gamma}+S_{i\alpha}\right]\phi(\mathbf{r}-\mathbf{r}_i) \\
&= \underbrace{\varepsilon_{\alpha\beta\gamma}\sum_i m_i v_{i\beta} v_{i\gamma}\phi(\mathbf{r}-\mathbf{r}_i)}_{C_\alpha} \\
&\quad + \underbrace{\varepsilon_{\alpha\beta\gamma}\sum_i m_i \left(r_{i\beta}-r_\beta\right)\dot{v}_{i\gamma}\phi(\mathbf{r}-\mathbf{r}_i)}_{D_\alpha} \\
&\quad + \underbrace{\sum_i \dot{S}_{i\alpha}\phi(\mathbf{r}-\mathbf{r}_i)}_{E_\alpha} \\
&\quad + \underbrace{\varepsilon_{\alpha\beta\gamma}\sum_i m_i \left(r_{i\beta}-r_\beta\right) v_{i\gamma}\frac{\partial\phi(\mathbf{r}-\mathbf{r}_i)}{\partial t}}_{F_\alpha} \\
&\quad + \underbrace{\sum_i S_{i\alpha}\frac{\partial\phi(\mathbf{r}-\mathbf{r}_i)}{\partial t}}_{G_\alpha}
\end{aligned} \tag{42}$$

Each part of Eq. 42 is treated separately below. First note that $C_\alpha = 0$ since the tensor $\sum_i m_i v_{i\beta} v_{i\gamma}\phi(\mathbf{r}-\mathbf{r}_i)$ is symmetric. Next, using the antisymmetry of $\epsilon_{\alpha\beta\gamma}$, changes of dummy summation variables and Newton's second and third laws, one can obtain expressions for the other terms in Eq. 42. We start with D_α.

$$\begin{aligned}
D_\alpha &= \varepsilon_{\alpha\beta\gamma}\sum_{ij}\left(r_{i\beta}-r_\beta\right) f_{ij\gamma}\phi(\mathbf{r}-\mathbf{r}_i) \\
&= \varepsilon_{\alpha\beta\gamma}\sum_{ij}\left(r_{j\beta}-r_\beta\right) f_{ji\gamma}\phi(\mathbf{r}-\mathbf{r}_j) \\
&= -\varepsilon_{\alpha\beta\gamma}\sum_{ij}\left(r_{j\beta}-r_\beta\right) f_{ij\gamma}\phi(\mathbf{r}-\mathbf{r}_j)
\end{aligned} \tag{43}$$

Summing up the first and last lines on the rhs of Eq. 43, and dividing by 2 one obtains:

$$\begin{aligned}
D_\alpha &= \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\sum_{ij} f_{ij\gamma}\left[\left(r_{i\beta}-r_\beta\right)\phi(\mathbf{r}-\mathbf{r}_i)\right. \\
&\quad \left.-\left(r_{j\beta}-r_\beta\right)\phi(\mathbf{r}-\mathbf{r}_j)\right] \\
&= \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\left\{\sum_{ij} f_{ij\gamma} r_{ij\beta}\phi(\mathbf{r}-\mathbf{r}_i)\right. \\
&\quad \left.+\sum_{ij} f_{ij\gamma}\left(r_{j\beta}-r_\beta\right)\left[\phi(\mathbf{r}-\mathbf{r}_i)-\phi(\mathbf{r}-\mathbf{r}_j)\right]\right\} \\
&= \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\left\{\sum_{ij} f_{ij\gamma} r_{ij\beta}\phi(\mathbf{r}-\mathbf{r}_i)\right. \\
&\quad \left.-\sum_{ij} f_{ij\gamma}\left(r_{j\beta}-r_\beta\right)\frac{\partial}{\partial r_\delta}\int_0^1 r_{ij\delta} ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right)\right\} \\
&= \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\sum_{ij} f_{ij\gamma} r_{ij\beta}\phi(\mathbf{r}-\mathbf{r}_i) \\
&\quad -\frac{1}{2}\varepsilon_{\alpha\beta\gamma}\frac{\partial}{\partial r_\delta}\sum_{ij}\left(r_{j\beta}-r_\beta\right) f_{ij\gamma} r_{ij\delta} \\
&\quad \times\int_0^1 ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right) \\
&\quad -\frac{1}{2}\varepsilon_{\alpha\beta\gamma}\sum_{ij} f_{ij\gamma} r_{ij\beta}\int_0^1 ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right).
\end{aligned} \tag{44}$$

Since the product $f_{ij\gamma} r_{ij\delta}$ is symmetric to the exchange of i and j and so is the integral over ϕ (see Eq. 20), one can invoke a exchange of indices in the second term on the right hand side of Eq. 44 to obtain:

$$\begin{aligned}
D_\alpha &= \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\sum_{ij} f_{ij\gamma} r_{ij\beta}\phi(\mathbf{r}-\mathbf{r}_i) \\
&\quad -\frac{1}{2}\varepsilon_{\alpha\beta\gamma}\frac{\partial}{\partial r_\delta}\sum_{ij}\left(r_{i\beta}-r_\beta\right) f_{ij\gamma} r_{ij\delta} \\
&\quad \times\int_0^1 ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right) \\
&\quad -\frac{1}{2}\varepsilon_{\alpha\beta\gamma}\sum_{ij} f_{ij\gamma} r_{ij\beta}\int_0^1 ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right).
\end{aligned} \tag{45}$$

Next (recalling that $\mathbf{M}_i$ denotes the resultant torque on particle i):

$$\begin{aligned}
E_\alpha &= \sum_i \dot{S}_{i\alpha}\phi(\mathbf{r}-\mathbf{r}_i) \\
&= \sum_i M_{i\alpha}\phi(\mathbf{r}-\mathbf{r}_i) = \sum_{ij} M_{ij\alpha}\phi(\mathbf{r}-\mathbf{r}_i) \\
&= \sum_{ij} M_{ji\alpha}\phi(\mathbf{r}-\mathbf{r}_j)
\end{aligned}$$

$$= \frac{1}{2}\sum_{ij}\left(M_{ij\alpha}\phi(\mathbf{r}-\mathbf{r}_i) + M_{ji\alpha}\phi(\mathbf{r}-\mathbf{r}_j)\right)$$
$$= \frac{1}{2}\sum_{ij}\left(M_{ij\alpha} + M_{ji\alpha}\right)\phi(\mathbf{r}-\mathbf{r}_i)$$
$$+\frac{1}{2}\sum_{ij} M_{ji\alpha}\left(\phi(\mathbf{r}-\mathbf{r}_j) - \phi(\mathbf{r}-\mathbf{r}_i)\right). \quad (46)$$

At this stage recall that $\mathbf{M}_{ij} = \mathbf{M}^f_{ij} + \mathbf{M}^{rf}_{ij}$, where $\mathbf{M}^f_{ij} = (\mathbf{r}^c_{ij} - \mathbf{r}_i)\times\mathbf{f}_{ij}$. Also note that $\mathbf{M}^{rf}_{ij} = -\mathbf{M}^{rf}_{ji}$. We have seen before that $\mathbf{M}_{ij} + \mathbf{M}_{ji} = -\mathbf{r}_{ij}\times\mathbf{f}_{ij}$. Substituting these facts in Eq. 46 one obtains:

$$E_\alpha = \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\sum_{ij} f_{ij\beta}r_{ij\gamma}\phi(\mathbf{r}-\mathbf{r}_i)$$
$$+\frac{1}{2}\sum_{ij} M_{ji\alpha}\left[\phi(\mathbf{r}-\mathbf{r}_j)-\phi(\mathbf{r}-\mathbf{r}_i)\right]$$
$$= \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\sum_{ij} f_{ij\beta}r_{ij\gamma}\phi(\mathbf{r}-\mathbf{r}_i)$$
$$-\frac{1}{2}\sum_{ij} M_{ij\alpha}\left[\phi(\mathbf{r}-\mathbf{r}_j)-\phi(\mathbf{r}-\mathbf{r}_i)\right]$$
$$= \frac{1}{2}\varepsilon_{\alpha\beta\gamma}\sum_{ij} f_{ij\beta}r_{ij\gamma}\phi(\mathbf{r}-\mathbf{r}_i)$$
$$-\frac{1}{2}\frac{\partial}{\partial r_\beta}\sum_{ij} M_{ij\alpha}r_{ij\beta}\int_0^1 ds\,\phi(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}). \quad (47)$$

Next, rewrite F_α as follows:

$$F_\alpha = -\varepsilon_{\alpha\beta\gamma}\sum_i m_i(r_{i\beta}-r_\beta)v_{i\gamma}v_{i\delta}\frac{\partial}{\partial r_\delta}\phi(\mathbf{r}-\mathbf{r}_i)$$
$$= -\varepsilon_{\alpha\beta\gamma}\frac{\partial}{\partial r_\delta}\sum_i m_i(r_{i\beta}-r_\beta)v_{i\gamma}v_{i\delta}\phi(\mathbf{r}-\mathbf{r}_i)$$
$$-\varepsilon_{\alpha\beta\gamma}\sum_i m_i v_{i\gamma}v_{i\beta}\phi(\mathbf{r}-\mathbf{r}_i)$$
$$= -\varepsilon_{\alpha\beta\gamma}\frac{\partial}{\partial r_\delta}\sum_i m_i(r_{i\beta}-r_\beta)v_{i\gamma}v_{i\delta}\phi(\mathbf{r}-\mathbf{r}_i)$$
$$= -\varepsilon_{\alpha\beta\gamma}\frac{\partial}{\partial r_\delta}\left[V_\delta\sum_i m_i\left(r_{i\beta}-r_\beta\right)v_{i\gamma}\phi(\mathbf{r}-\mathbf{r}_i)\right.$$
$$\left.+\sum_i m_i\left(r_{i\beta}-r_\beta\right)v_{i\gamma}v'_{i\delta}\phi(\mathbf{r}-\mathbf{r}_i)\right], \quad (48)$$

where use has been made of $\epsilon_{\alpha\beta\gamma}\sum_i m_i v_{i\gamma}v_{i\beta}\phi(\mathbf{r}-\mathbf{r}_i) = 0$, by symmetry considerations. Finally,

$$G_\alpha \equiv \sum_i S_{i\alpha}\frac{\partial\phi(\mathbf{r}-\mathbf{r}_i)}{\partial t} = -\frac{\partial}{\partial r_\delta}\sum_i S_{i\alpha}v_{i\delta}\phi(\mathbf{r}-\mathbf{r}_i)$$
$$= -\frac{\partial}{\partial r_\delta}\left[V_\delta\sum_i S_{i\alpha}\phi(\mathbf{r}-\mathbf{r}_i) + \sum_i S_{i\alpha}v'_{i\delta}\phi(\mathbf{r}-\mathbf{r}_i)\right]. \quad (49)$$

Adding up all contributions on the right hand side of Eq. 42, as calculated in Eq. 45, 47, 48, 49, and employing the antisymmetry of $\varepsilon_{\alpha\beta\gamma}$, one obtains:

$$\frac{\partial J_\alpha}{\partial t} = -\frac{\partial}{\partial r_\delta}\left[V_\delta J_\alpha - C_{\alpha\delta}\right] - \varepsilon_{\alpha\beta\gamma}\sigma_{\beta\gamma}, \quad (50)$$

where the *couple stress tensor* is identified as:

$$C_{\alpha\delta} \equiv -\frac{1}{2}\sum_{ij}\left[\varepsilon_{\alpha\beta\gamma}\left(r_{i\beta}-r_\beta\right)f_{ij\gamma}r_{ij\delta}\right.$$
$$\left.+M_{ij\alpha}r_{ij\delta}\right]\int_0^1 ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right)$$
$$-\sum_i\left[\varepsilon_{\alpha\beta\gamma}\left(r_{i\beta}-r_\beta\right)m_i v_{i\gamma}+S_{i\alpha}\right]v'_{i\delta}\phi(\mathbf{r}-\mathbf{r}_i).$$
$$= -\frac{1}{2}\sum_{ij}\left[\left((\mathbf{r}_i-\mathbf{r})\times\mathbf{f}_{ij}\right)_\alpha + M_{ij\alpha}\right]\mathbf{r}_{ij\delta}$$
$$\times\int_0^1 ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right)$$
$$-\sum_i\left[\varepsilon_{\alpha\beta\gamma}\left(r_{i\beta}-r_\beta\right)m_i v_{i\gamma}+S_{i\alpha}\right]v'_{i\delta}\phi(\mathbf{r}-\mathbf{r}_i). \quad (51)$$

Using $M_{ij\alpha} = M^f_{ij\alpha} + M^{rf}_{ij\alpha} = (\mathbf{r}^c_{ij}\times\mathbf{f}_{ij})_\alpha + M^{rf}_{ij\alpha}$, the couple stress tensor can be further rewritten as follows:

$$C_{\alpha\delta} = -\frac{1}{2}\sum_{ij}\left[\left((\mathbf{r}_i-\mathbf{r})\times\mathbf{f}_{ij}\right)_\alpha + \left(\left(\mathbf{r}^c_{ij}-\mathbf{r}_i\right)\times\mathbf{f}_{ij}\right)_\alpha\right.$$
$$\left.+M^{rf}_{ij\alpha}\right]\mathbf{r}_{ij\delta}\int_0^1 ds\,\phi\left(\mathbf{r}-\mathbf{r}_i+s\mathbf{r}_{ij}\right)$$
$$-\sum_i\left[\varepsilon_{\alpha\beta\gamma}\left(r_{i\beta}-r_\beta\right)m_i v_{i\gamma}+S_{i\alpha}\right]v'_{i\delta}\phi(\mathbf{r}-\mathbf{r}_i)$$

The above is presented in a somewhat more compact form in the main text, Eq. 33.

References

1. Irving, J.H., Kirkwood, J.G.: The statistical mechanical theory of transport properties IV. The equations of hydrodynamics. J. Chem. Phys. **18**, 817–829 (1950)
2. Born, M., Huang, K.: Dynamical Theory of Crystal Lattices. Oxford (1954, reissue 2000)

3. Reichl, L.E.: A Modern Course in Statistical Physics. Wiley and numerous references therein (1998)
4. Weber, J.: Recherches concernantes les contraintes intergranulaires dans les milieux pulvérantes. Bull. de Liais P. C. **20**, 1–31 (1966)
5. Cambou, B., Dubujet, P., Emeriault, F., Sidoroff, F.: Homogenization for granular media. Eur. J. Mech. A Solids **14**, 255–276 (1995)
6. Chang, C.S., Gao, J.: Kinematic and static hypotheses for constitutive modeling of granulates considering particle rotation. Acta Mech. **115**, 213–229 (1996)
7. Bagi, K.: Stress and strain in granular assemblies. Mech. Mat. **22**(3), 165–177 (1996)
8. Babic, M.: Average balance equations for granular materials. Int. J. Eng. Sci. **35**, 523–548 (1997)
9. Goddard, J.D.: Continuum modeling of granular assemblies: quasistatic dilatancy and yield. In: Herrmann, H.J., Hovi, J.-P., Luding, S. (eds.) Physics of Dry Granular Media, pp. 1–24. Kluwer, Dordrecht (1998)
10. Nemat-Nasser, S.: A micromechanically-based constitutive model for frictional deformation of granular materials. J. Mech. Phys. Solids **48**, 1541–1563 (2000)
11. Lätzel, M., Luding, S., Herrmann, H.J. : From discontinuous models towards a continuum description. In: Vermeer, P.A., Diebels, S., Ehlers, W., Herrmann, H.J., Luding, S., Ramm, E. (eds.) Continuous and Discontinuous Models of Cohesive-Frictional Materials, Lecture Notes in Physics 568, pp. 215–230. Springer, Berlin (2001)
12. Bardet, J.P., Vardoulakis, I.: The asymmetry of stress in granular media. Int. J. Solids Struct. **38**, 353–367 (2001)
13. Zhu, H.P., Yu, A.B.: Averaging method for granular materials. Phys. Rev. **E 66**, 021302 (2002)
14. Ball, R.C., Blumenfeld, R.: Stress field in granular systems, loop forces and potential formulation. Phys. Rev. Lett. **88**, 115505 (2002)
15. Ehlers, W., Ramm, E., Diebels, S., D'Addetta, G.A.: From particle ensembles to Cosserat continua: homogenization of contact forces towards stresses and couple stresses. Int. J. Solids Struct. **40**, 6681–6702 (2003)
16. Kruyt, N.P., Rothenburg, L.: Kinematic and static assumptions for homogenization in micromechanics of granular media. Mech. Mater. **36**(22), 1157–1173 (2004)
17. Froiio, F., Tomassetti, G., Vardoulakis, I.: Mechanics of granular materials: the discrete and continuum descriptions juxtaposed. Int. J. Solids Struct. **43**, 7684–7720 (2006)
18. Goddard, J.D. : From granular matter to generalized continuum. In: Capriz, G., Giovine, P., Mariano, P.M. (eds.) Mathematical Models of Granular Matter, Lecture Notes in Applied Mathematics, vol. 1937, Ch. 1, pp. 1–20. Springer, Berlin (2008)
19. Goddard, J.D: Microstructural origins of continuum stress fields—a brief history and some unresolved issues. In: DeKee, D., Kaloni, P.N. (eds.) Recent Developments in Structured Continua, Pitman Research Notes in Mathematics, No. 143, pp. 179–208. Longman/Wiley, New York (1986)
20. Goldhirsch, I.: Rapid granular flows. Ann. Rev. Fluid Mech. **35**, 267–293 (2003)
21. Glasser, B.J., Goldhirsch, I.: Scale dependence, correlations and fluctuations of stresses in rapid granular flows. Phys. Fluids **13**, 407–420 (2001)
22. Love, A.E.H.: Treatise of Mathematical Theory of Elasticity. Cambridge, UP, London (1927)
23. Voigt, W.: Theoretische Studien über die Elasticitätverhhältnisse der Krystalle. Abhandt. Ges. Wiss. Gött. **34**, 3–52 (1887)
24. Goldenberg, C., Goldhirsch, I. : Continuum mechanics for small systems and fine resolutions. In: Rieth, M., Schommers, W. (eds.) Handbook of Theoretical and Computational Nanotechnology, pp. 330–386. American Scientific, New York (2006)
25. Murdoch, A.I.: On the microscopic interpretation of stress and couple stress. J. Elast. **71**(1–3), 105–131 (2003)
26. Murdoch, A.I.: A critique of atomistic definitions of the stress tensor. J. Elast. **88**(2), 113–140 (2007)
27. Goldhirsch, I., Goldenberg, C.: On the microscopic foundations of elasticity. Eur. Phys. J. **E 9**(3), 245–251 (2002)
28. Goldenberg, C., Goldhirsch, I.: Small and large scale granular statics. Granul. Matter **6**(2–3), 87–96 (2004)
29. Goldhirsch, I., Goldenberg, C. : Stress in dense granular materials. In: Wolf, D.E., Hinrichsen, H. (eds.) The Physics of Granular Media, pp. 3–22. Wiley, Weinheim (2004)
30. Schofield, P., Henderson, J.R.: Statistical mechanics of inhomogeneous fluids. Prof. R. Soc. Lond. Ser. A **379**(1776), 231–246 (1982)
31. Wajnryb, E., Altenberger, A.R., Dahler, J.S.: Uniqueness of the microscopic stress tensor. J. Chem. Phys. **103**, 9782–9787 (1995)
32. Batchelor, G.K.: An Introduction to Fluid Dynamics. Cambridge, UP, Cambridge (1967)
33. Goldenberg, C., Atman, A.P.F., Claudin, P., Combe, G., Goldhirsch, I.: Scale separation in granular packings: stress plateaus and fluctuations. Phys. Rev. Lett. **96**(16), 168001 (2006)
34. Goldenberg, C., Goldhirsch, I.: Effects of friction and disorder on the quasistatic response of granular solids to a localized force. Phys. Rev. **E 77**(4), 041303 (2008)
35. Tan, M.-L., Goldhirsch, I.: Rapid granular flows as mesoscopic systems. Phys. Rev. Lett. **81**(14), 3022–3025 (1998)
36. Arslan, H., Sture, S.: Evaluation of a physical length scale for granular materials. Comput. Mater. Sci. **42**, 525–530 (2008)
37. Eringen, A.C.: Theory of micropolar elasticity. In: Leibowitz, H. (ed.) Fracture: An Advanced Treatise, vol. I, Mathematical Fundamentals, pp. 621–729. Academic Press, New York (1968)
38. Cercignani, C.: The Boltzmann Equation and Its Applications, Ser. "Applied Mathematical Sciences", No. 67. Springer, Berlin (1988)
39. Goldhirsch, I.: Scales and kinetics of granular flows. CHAOS **9**(3), 659–672 (1999)
40. Goldenberg, C., Goldhirsch, I.: Friction enhances elasticity in granular solids. Nature **435**(7039), 188–191 (2005)
41. Zhang, J., Behringer, R.P., Goldhirsch, I.: Coarse graining of a physical granular system. Prog. Theor. Phys. Suppl. (2010, in press)