Virial Theorems and Virial Stresses of Micropolar Media

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Abstract

A generalization of virial theorems and virial stresses to micropolar continuum mechanics is explored. The linear momentum balance in dyadic product with translation leads to (i) the first virial theorem of micropolar continuum mechanics involving the infinite-time limit of the kinetic translational energy and (ii) a classical formula for computing the virial force-stress known in molecular dynamics. The angular momentum balance in dyadic product with rotation leads to (i) the second virial theorem of micropolar continuum mechanics involving the infinite-time limit of the kinetic rotational energy and (ii) a virial couple-stress along with a formula for its computation. The latter stress is also uncovered in the dyadic product of linear momentum balance with rotation. The virial force-stress and virial couple-stress contain, respectively, the Reynolds force-stress and turbulent couple-stress.

1 Introduction

This communication reports a generalization of the virial theorem and virial stress from classical to micropolar continuum mechanics. The study is set in the spatial (Eulerian) description [Eringen, 2001; Lukaszewicz, 1999] in $\mathbb{E}^d$, $d = 2$ or 3. For reference, the kinematics of such a continuum is described through a field with two degrees of freedom ($u_i, \varphi_i$) and their rates:

\[
\dot{u}_i; \quad \dot{\varphi}_i.
\]

(1)

The overdot stands for the material time derivative. Standard index as well as symbolic tensor notations are used.

The local form of linear momentum balance reads

\[
\rho \ddot{v}_i = \rho \ddot{f}_i + \tau_{ki,k},
\]

(2)
where $\rho$ is the mass density, $f_i$ is the body force per unit mass, and $\tau_{ji}$ is the (generally non-symmetric) Cauchy force-stress. The latter is related to the force- traction on any surface element specified by the outer normal $n_k$ through $t_{i}^{(n)} = \tau_{ji}n_j$.

The local form of angular momentum balance, after accounting for (2), reads

$$\rho J \frac{D\dot{\phi}_i}{Dt} = \rho g_i + \mu_{ki} + T_i \quad \text{where} \quad T_i = \epsilon_{ijk}\tau_{jk},$$

where $J$ is the (micro)inertia tensor of a particle, $g_i$ is the body torque per unit mass, and $\mu_{ki}$ is the couple-stress, which is related to the surface moment- traction $m_{i}^{(n)}$ through $m_{i}^{(n)} = \mu_{ki}n_k$. If $T_i = 0$, $\tau_{jk}$ becomes symmetric, in which case we write $\sigma_{jk}$ instead. In (2) and henceforth, we work with a microisotropic medium, i.e. where $J_{ij} = J\delta_{ij}$.

In general, we consider the material properties to be constant, while the displacement, rotation, force-stress, and couple stress, as well as their derivatives, to be tensor-valued random fields [Malyarenko and Ostoja-Starzewski, 2019]. Denoting by $F(x,t,\omega)$ a realization of any such random field, it is clearly seen to be parametrized by the (spatial) position $x$ and time $t$, where $\omega$ is a realization drawn from a probability space $(\Omega,\mathcal{F},P)$. Thus, there are three basic types of averaging:

(i) Space (volume) averaging of volume integrals:

$$\mathcal{F}_V(x,t,\omega) := \frac{1}{V} \int_B F(x',t,\omega) dV,$$

where $V = |B|$ is the volume of domain $B$ having a bounding surface $\partial B$. In the language of stochastic processes, this is local averaging transforming the original random field $F$ into a new, smoother random field $\mathcal{F}_V$. In general, $\mathcal{F}_V$ is a function of $x$ but, if spatial ergodicity (i.e., equivalence of spatial averaging with time averaging and/or ensemble averaging) is assumed, this dependence vanishes. This situation corresponds to passing from a statistical to a representative volume element (RVE), with the RVE size heavily dependent on the random microstructural properties involved [Ostoja-Starzewski et al., 2016]. In the following, to simplify the notation, we will simply write $\mathcal{F}$.

(ii) Time averaging, wherein fluctuations observed on a fine time scale get smoothed (smeared) on a coarse time scale;

$$F_T(x,t,\omega) := \frac{1}{T} \int_0^T F(x,t',\omega) dt'.$$

In the language of stochastic processes, this is local averaging in the time domain, transforming the original random field $F$ into a new, smoother-in-time random field $F_T$. In general, $F_T$ is still a random function of $t$ but, if temporal ergodicity (i.e., equivalence with space and/or ensemble averaging) is assumed, this dependence vanishes. The latter situation typically implies taking the $T \to \infty$ limit.


(iii) **Ensemble (statistical) averaging.**

While in either case, one obtains a coarser description than the original one, in the present study only space averaging over arbitrary volumes and time averaging over infinitely long times is considered. The latter operation, called *infinite-time averaging*, is indicated by

\[ \{ F(\mathbf{x}, t, \omega) \}_\infty = \lim_{T \to \infty} \{ F(\mathbf{x}, t, \omega) \}_T. \]  

(6)

The reason for considering such a limit as well as the spatial averaging resides in our focus on the exploration of the virial theorem(s) and virial stress(es) in micropolar media. The ensuing study aims to generalize the deterministic exposition of those topics in the setting of classical media [Podio-Guidugli, 2019], whereby we follow a similar line of reasoning. The statistical exposition in the vein of that paper is not discussed here.

## 2 Consequences of linear momentum balance

First, we take a dyadic product of a test function \( \phi_j \) with (2) and integrate over an arbitrary (and simply-connected) domain \( \mathcal{B} \) to get

\[ \int_\mathcal{B} (\phi_j \rho f_i + \phi_j \tau_{ki,k}) \, dV = \int_\mathcal{B} \phi_j \rho \dot{v}_i \, dV. \]  

(7)

We now consider two choices for the test function.

### 2.1 Translation as test function

Taking translation as the test function \( \phi_j = x_j \) in (7), we perform these steps

\[
\begin{align*}
\int_\mathcal{B} x_j \rho f_i \, dV + \int_{\partial \mathcal{B}} x_j \tau_{ki} \, dS - \int_\mathcal{B} \tau_{ji} \, dV &= \frac{d}{dt} \left( \int_\mathcal{B} x_j \rho v_i \, dV \right) - \int_\mathcal{B} \rho v_j v_i \, dV
\end{align*}
\]

(8)

Hence, we can write

\[ \int_\mathcal{B} \rho x_j f_i \, dV + \int_{\partial \mathcal{B}} x_j t_i^{(m)} \, dS - V \tau_{ji}^* = \frac{d}{dt} \left( \int_\mathcal{B} \rho x_j v_i \, dV \right), \]  

(9)

where

\[ \tau_{ji}^* := \tau_{ji} - \rho v_j v_i \]  

(10)

is the *virial stress*. The term \( \rho v_j v_i \) contains \( \rho v'_j v'_i \), as can be seen from the Reynolds decomposition \( (v_j = \overline{v}_j + v'_j) \) with \( \overline{v}'_j = 0 \). Depending on a convention, \( \rho v_j v_i \) or \( \rho v'_j v'_i \) (with a plus or minus sign) is called the Reynolds stress. From the standpoint of turbulent flows, \( \tau_{ji}^* \) is the *modified stress* in the sense that the
linear momentum, angular momentum, and energy balances are unchanged in form upon volume averaging [Ostoja-Starzewski, 2021].

Going from continuum to discrete systems such as molecular dynamics, (10) is consistent with the very well-known prescription for computation of the instantaneous volume-averaged virial (generally non-symmetric) force-stress

$$\tau_{ji}^*: = \frac{1}{V} \sum_{k \in B} \left[ \frac{1}{2} \sum_{l \in B} \left( x_i^{(l)} - x_i^{(k)} \right) f_j^{(kl)} - m^{(k)} \left( v_j^{(k)} - \bar{v}_j \right) \left( v_i^{(k)} - \bar{v}_i \right) \right], \quad (11)$$

where
- \( k \) and \( l \) are particles in the domain \( B \),
- \( m^{(k)} \) is the mass of particle \( k \),
- \( v_j^{(k)} \) is the \( j \)-th component of the velocity of particle \( k \),
- \( \bar{v}_j \) is the \( j \)-th component of the average velocity of particles in the volume,
- \( x_i^{(k)} \) is the \( i \)-th component of the position of particle \( k \), and
- \( f_j^{(kl)} \) is the \( j \)-th component of the force applied on particle \( k \) by particle \( l \).

No symmetry of the Cauchy stress is required in the above derivation. Also, (10) does not imply the symmetry of \( \tau_{ji}^* \) unless all the body torques and couple-stresses are zero: this is seen by applying (3) on the lengthscale \( L = \sqrt[3]{V} \) (\( d = 2 \) or 3) on which the space averaging is carried out. This would imply writing \( \rho J_{ij} \frac{\partial}{\partial t} \dot{\phi}_j = \rho g_i + \mu_{ki,k}^* + \epsilon_{ijk} \tau_{jk}^* \), where \( \mu_{ki}^* \) is given by (26) below. In essence, the formula (2.5) alone is not sufficient to judge whether this force-stress will be symmetric or not.

Taking the trace of (9) we get:

$$\int_B \rho x_i f_i dV + \int_{\partial B} x_i \dot{v}_i^{(n)} dS - \int_B \tau_{ii} dV = \dot{W}_u (B) - 2K_u (B), \quad (12)$$

where

$$W_u (B) := V \rho x_i \dot{v}_i, \quad K_u (B) := \frac{V}{2} \rho x_i \dot{v}_i,$$

with the latter being the kinetic translational energy.

Performing the infinite-time averaging (6), with the argument given in [Podio-Guidugli, 2019], the above becomes

$$\left\{ \int_B \rho x_i f_i dV + \int_{\partial B} x_i \dot{v}_i^{(n)} dS - \int_B \tau_{ii} dV \right\}_\infty = -2 \{ K_u (B) \}_\infty, \quad (14)$$

which, in view of Section 3 below, is called the first virial theorem of micropolar continuum mechanics. The arguments accompanying this infinite time limit include the assumption of kinematic uniform or periodic boundary conditions (Costanzo et al., 2005).

Taking the dual vector of (9) we find two relations to be satisfied by the skew-symmetric part of the Cauchy stress tensor and, essentially, linking all the
quantities appearing in (2) and (3):

\[ \int_B (\rho J \dddot{\phi}_k - \rho g_k - \mu_{ik,n}) \, dV = \int_B T_k dV \]
\[ = \int_B \rho e_{kji} x_j f_i dV + \int_{\partial B} e_{kji} x_j t_i^{(n)} dS - \int_B \rho e_{kji} x_j \dot{v}_i dV. \]  

(15)

In the special case of micropolar effects in (2)–(3) being absent, \( W_{\phi}(B) = 0 \) and \( K_{\phi}(B) = 0 \) in (22), so that (14) simplifies to the virial theorem of classical continuum mechanics

\[ \left\{ \int_B \rho x_i f_i dV + \int_{\partial B} x_i t_i^{(n)} dS - \int_B \sigma_{ii} dV \right\}_\infty = -2 \{ K(B) \}_\infty. \]  

(16)

Note: there are various ways for couple-stress effects to arise, typically involving some internal material structure, and these include:
- presence of moment interactions in granular media or suspensions, e.g. [Cowin, 1974; Eringen, 2001; Vardoulakis, 2019];
- presence of defects, phase boundaries, e.g. [Chen et al., 2006; Rigelesaiyin et al. 2018];
- homogenization of random media, e.g. [Trovalusci et al., 2015];
- fractal media in which the fractal structure (homogenized in the vein of dimensional regularization) is anisotropic [Li & Ostoja-Starzewski, 2011].

The symmetric part of (9) was discussed in [Podio-Guidugli, 2019].

2.2 Rotation as test function

Taking rotation as the test function \((\phi_j = x_j)\) in (7), we obtain

\[ \int_B \phi_j \rho f_i dV + \int_{\partial B} \phi_j t_i^{(n)} dS - \int_B \phi_j \tau_{ki} dV + \int_B \rho \phi_j \dot{v}_i dV = \frac{d}{dt} \left( \int_B \rho \phi_j \dot{v}_i dV \right) \]  

(17)

Multiplying this equation by \(J\) yields

\[ \int_B \rho J \phi_j f_i dV + \int_{\partial B} J \phi_j t_i^{(n)} dS - \int_B J \phi_j \tau_{ki} dV - \int_B J \phi_j \dot{v}_i dV = \frac{d}{dt} \left( \int_B \rho J \phi_j \dot{v}_i dV \right). \]  

(18)

The new term in parenthesis on the left-hand side, \(-V \rho J \phi_j \dot{v}_i\), will independently arise in Section 3.2.

3 Consequences of angular momentum balance

Consider a dyadic product of test function \(\phi_j\) with the vector (3) and integrate over \(B\) to get

\[ \int_B \phi_j (\rho g_i + \mu_{ki,n} + \epsilon_{ink} \tau_{nk}) \, dV = \int_B \phi_j \rho J \phi_j \dot{v}_i dV. \]  

(19)

Again, there are two basic options for choosing the test function.
3.1 Rotation as test function

On account of the Green-Gauss Theorem and taking rotation as the test function \( \phi_j = \varphi_j \), we find

\[
\int_B \varphi_j \rho g_i dV + \int_{\partial B} \varphi_j m_i^{(n)} dS - \int_B \varphi_j \mu_{ki} dV + \int_B \varphi_j \epsilon_{ink} \tau_{nk} dV = \frac{d}{dt} \left( \int_B \rho J \varphi_j \varphi_i dV \right) - \int_B \rho J \varphi_j \dot{\varphi}_i dV. \tag{20}
\]

Taking the trace of (20) we obtain (with \( T_i \) defined in (3)\textsuperscript{2})

\[
\int_B \varphi_i \rho g_i dV + \int_{\partial B} \varphi_i m_i^{(n)} dS - \int_B \varphi_{i,k} \mu_{ki} dV + \int_B \varphi_i T_i dV = W_\varphi (B) - 2K_\varphi (B), \tag{21}
\]

where

\[
W_\varphi (B) := V \rho J \varphi_j \varphi_i, \quad K_\varphi (B) := \frac{1}{2} \rho J \varphi_j \varphi_i, \tag{22}
\]

with the latter being the kinetic rotational energy; compare with (13).

Under the infinite-time averaging (6), we find

\[
\left\{ \int_B \rho \varphi_j g_i dV + \int_{\partial B} \varphi_i m_i^{(n)} dS - \int_B \varphi_{i,k} \mu_{ki} dV + \int_B \varphi_i T_i dV \right\} \rightarrow -2 \left\{ K_\varphi (B) \right\}_\infty, \tag{23}
\]

which we call the second virial theorem of micropolar continuum mechanics.

3.2 Translation as test function

Considering \( \phi_j = x_j \) in (19) we get:

\[
\int_B x_j \rho g_i dV + \int_{\partial B} x_j m_i^{(n)} dS - \int_B \mu_{ji} dV + \int_B x_j \epsilon_{ink} \tau_{nk} dV = \frac{d}{dt} \left( \int_B \rho J x_j \varphi_i dV \right) - \int_B \rho J x_j \dot{\varphi}_i dV, \tag{24}
\]

which can be written as

\[
\int_B x_j \rho g_i dV + \int_{\partial B} x_j m_i^{(n)} dS - V \mu_{ji} + \int_B x_j T_i dV = \frac{d}{dt} \left( \int_B \rho J x_j \varphi_i dV \right), \tag{25}
\]

where

\[
\mu_{ji} := \mu_{ji} - \rho J \varphi_j v_i \tag{26}
\]

is the virial couple-stress. As can be seen from the Reynolds decomposition of \( \varphi_j \) and \( v_i \), the term \( -\rho J \varphi_j v_i \) contains

\[
S_{ji} := -\rho J \varphi_j' v_i', \tag{27}
\]

which was called the turbulent couple-stress in [Ostoja-Starzewski, 2021]. No microisotropy restriction was assumed there, so the formula for \( S_{ji} \) was a bit more general. This couple-stress may be thought of as an analogue of the Reynolds stress \( -\rho v_j' v_i' \) brought up in Section 2.1.
Interestingly, $-\rho J_i \dot{\varphi}_i$ appeared via a completely different route in \[18\]. As discussed in [Ostoja-Starzewski, 2021], from the standpoint of turbulent flows, $\mu^*_ij$ is the modified stress in the sense that, if it replaces $\mu_{ij}$ along with the heat flux and internal energy density being also replaced by modified expressions, then the angular momentum and energy balance equations are unchanged in form upon volume averaging.

Again, going from continuum to discrete systems such as the molecular/particle dynamics, \[26\] gives a prescription for computation of the instantaneous volume-averaged virial couple-stress

$$
\mu^*_ji := \frac{1}{V} \sum_{k \in B} \left[ \frac{1}{2} \sum_{l \in B} \left( x^{(l)}_i - x^{(k)}_i \right) m^{(kl)}_j - J^{(k)} \left( \bar{\varphi}^{(k)}_j - \bar{\varphi}^i_j \right) \left( v^{(k)}_i - \bar{v}_i \right) \right], \tag{28}
$$

where

- $k$ and $l$ are particles in the domain $B$,
- $J^{(k)}$ is the mass moment of inertia of particle $k$,
- $v^{(k)}_j$ is the $j$-th component of the velocity of particle $k$,
- $\bar{v}_j$ is the $j$-th component of the average velocity of particles in the volume,
- $\dot{\varphi}^{(k)}_i$ is the $i$-th component of the velocity of particle $k$,
- $\bar{\varphi}^i_j$ is the $j$-th component of the average velocity of particles in the volume,
- $x^{(k)}_i$ is the $i$-th component of the position of particle $k$, and
- $m^{(kl)}_j$ is the $j$-th component of the moment applied on particle $k$ by particle $l$.

Note the analogy between the formulas \[28\] and \[11\].

4 Conclusions

This communication generalizes the virial theorem and virial stress to micropolar continuum mechanics. The study hinges on exploring the dyadic products of linear and angular momentum balances with translational and rotational test functions. In generic terms, the results are summarized as follows.

- The linear momentum balance with translation leads to:
  
  (i) A virial theorem known in classical continuum theories involving the infinite-time limit of the kinetic translational energy. It is called the first virial theorem of micropolar continuum mechanics.
  
  (ii) A classical formula for computing the virial force-stress known in molecular dynamics.

- The angular momentum balance with rotation leads to a new virial theorem involving the infinite-time limit of the kinetic rotational energy. It is called the second virial theorem of micropolar continuum mechanics.
• The angular momentum balance with translation leads to a virial couple-stress along with a formula for its computation. The same stress arises independently in the linear momentum balance with rotation.

• The virial couple-stress contains the turbulent couple-stress, just like the virial force-stress contains the Reynolds stress.

• The virial force-stress and couple-stress formulas do not require ‘infinitely’ large volumes (on the RVE level) and can be used to assess tensor-valued random fields on mesoscale levels as in [Ostoja-Starzewski and Laudani [2020].

These results have applicability in computational studies as well as a stepping-stone to micropolar extensions of various complex phenomena such as presented in, say, [Ganghoffer, 2015; Chen and Diaz, 2016, 2018].

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