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DISCUSSION OF STRESS TENSOR NONUNIQUENESS WITH APPLICATION TO NONUNIFORM, PARTICULATE SYSTEMS

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The indeterminacy of the mechanical stress tensor has been noted in several developments of expressions for stress in a system of particles. It is generally agreed that physical quantities related to the stress tensor must be insensitive to this nonuniqueness, but there is no definitive prescription for insuring it. Kröner's tensor decomposition theorem is applied to the mechanical stress tensor σ_{ij} to show that its complete determination requires specification of its "incompatibility," $\epsilon_{ijk} \epsilon_{lmn} \partial_j \partial_m \sigma_{kn}$, in addition to its divergence, which is obtained from the momentum conservation relation. For a particulate system, stress tensor incompatibility is shown to vanish to recover the correct expression for macroscopically observable traction. This result removes concern about nonuniqueness without requiring equilibrium or arbitrarily defined force lines.

INTRODUCTION

Expressions for the configurational (interaction) contribution to the stress density tensor, σ , for particulate systems can be derived from the momentum conservation relation.¹⁻³ This part of the stress density tensor, exclusive of kinetic contributions, will be referred to here as the mechanical stress tensor. This quantity is of interest for molecular dynamics simulations, where the continuum stress can be obtained from it as an appropriate space and time average.^{1,4} Because momentum conservation involves only the divergence of the stress density, mechanical stress expressions developed from it are indeterminate up to the addition of a divergence-free tensor, as has been commented on by several authors.^{1-3,5} It is generally agreed that physical quantities related to the stress tensor must be insensitive to this nonuniqueness. Nielsen and Martin claim that the divergence-free part of the stress density σ (incorrectly identified as the curl of an arbitrary tensor) does not contribute to volume integrals of σ over all space for finite systems, over a periodic cell for periodic systems, or to surface integrals of σ over infinite planes.³

At least for classical systems, these claims are unsubstantiated and the divergence-free part of σ must either be constrained, or physical quantities must be invariant to it. Here the physical content of the stress tensor is discussed and it is argued that its divergence-free part must vanish to yield the correct expression for traction, which is a physical observable.

THEORY

Kroner's decomposition theorem⁶ provides the framework for evaluating stress tensor nonuniqueness. Like the Helmholtz decomposition theorem for vectors, Kroner's decomposition theorem for second rank tensors establishes that the information required to uniquely determine a tensor (to within a constant) is its divergence and incompatibility. The incompatibility operator, Inc , is defined as

$$\text{Inc } A = \nabla \times [\nabla \times A]^T \quad (1a)$$

$$\text{or } [\text{Inc } A]_{ij} = \epsilon_{ijk} \epsilon_{lmn} \partial_m \partial_k A_{ln} \quad (1b)$$

Defining the deformation operator, Def , as

$$\text{Def } \underline{a} \equiv \frac{1}{2} [\underline{\nabla a} + (\underline{\nabla a})^T] \quad (2a)$$

$$\text{or } [\text{Def } \underline{a}]_{ij} \equiv \frac{1}{2} (\partial_i a_j + \partial_j a_i), \quad (2b)$$

the stress tensor can be decomposed as⁶

$$\sigma = \text{Def } \underline{a} + \text{Inc } \underline{C}^S + \sigma^\Lambda + \underline{K} \quad (3)$$

where $\underline{K}$ is a constant tensor. Superscript S (Λ) denotes the (anti)symmetric part of the tensor and superscript T denotes a transpose. The vector $\underline{q}^\Lambda$, which generates the antisymmetric part of the stress tensor according to

$$\sigma^\Lambda_{ij} \equiv \epsilon_{ijk} \sigma^\Lambda_k, \quad (4)$$

is subject to the Helmholtz decomposition,

$$\underline{q}^\Lambda = \underline{\nabla} \phi + \underline{\nabla} \times \underline{G}, \quad (5)$$

Substituting from Eqs. (4) and (5), the indicial form of the tensor decomposition, Eq. (3), becomes

$$\sigma_{ij} = \frac{1}{2} (\partial_i a_j + \partial_j a_i) + \epsilon_{ikl} \epsilon_{jmn} \partial_k \partial_m C_{ln}^S + \epsilon_{ijk} \partial_k \phi + \partial_i G_j - \partial_j G_i + K_{ij} \quad (6)$$

Kröner⁶ demonstrated that the decomposition quantities $\underline{a}$ and C^S are determined by $\text{Div } \sigma^S$ and $\text{Inc } \sigma^S$, respectively, while $\underline{G}$ and $\nabla \phi$ are determined from $\text{Div } \sigma^\Lambda$ and $\text{Inc } \sigma^\Lambda$, as follows:

$$\underline{G} = -\frac{1}{4\pi} \int_V \frac{\text{Div } \sigma^\Lambda(r_2)}{r_{12}} d^3r_2, \quad (7)$$

where, without loss of generality, $\text{Div } \underline{G}$ is taken to vanish,

$$(\nabla \cdot \underline{G})_i = \frac{1}{2} \epsilon_{ijk} (\nabla \cdot \underline{\nabla} \times \underline{G})_k, \quad (8a)$$

where

$$\underline{\nabla} \times \underline{G} = -\frac{1}{4\pi} \int_V \frac{\text{Inc } \sigma^\Lambda(r_2)}{r} d^3r \quad (8b)$$

and $\underline{I}$ is the identity tensor. Hence, a general second rank tensor is completely determined by its divergence and incompatibility. Like Helmholtz' theorem,⁷ Kröner's decomposition theorem applies to a continuous (tensor) field having continuous first derivatives and occupying either a finite or infinite region. It is not restricted only to fields with infinite extent, as Kröner indicated. If the integration volume V is taken to be finite, $\underline{K}$ may be nonzero. If V is all of space, then $r^2|\phi|$ must be bounded for large r .

DISCUSSION

To evaluate the physical content of σ , recall that it is introduced in the development of the continuum momentum conservation relation so that a local differential relation can be obtained. Using the purely mathematical procedure of representing the traction vector as the contraction of a tensor with the system surface normal,⁸ the surface integral of the traction is converted into a volume integral of the stress tensor divergence by application of the divergence theorem. This mathematical representation of traction constrains only the stress tensor divergence,

$$\nabla_i \cdot \sigma = \nabla \cdot [\text{Def } \underline{a} + \nabla \cdot \underline{G} + (\nabla \cdot \underline{G})^T] = \nabla \cdot \underline{F}, \quad (9)$$

which suffices for determining $\underline{a}$ and $\underline{G}$ only. Having no knowledge of $\text{Inc } \sigma$ leaves the stress tensor indeterminate by $\underline{A} \equiv \sigma - \underline{F}$:

$$\Lambda_{ij} \equiv \epsilon_{ikl} \epsilon_{jmn} \partial_k \partial_m C_{ln}^S + \epsilon_{ijk} \partial_k \phi. \quad (10)$$

The following relations hold:

$$\sigma = \underline{F} + \underline{A}; \quad \text{Div } \sigma = \text{Div } \underline{F}; \quad \text{Inc } \sigma = \text{Inc } \underline{A};$$

$$\text{but } \text{Curl } \underline{a} = \text{Curl } (\underline{F} + \underline{A}), \quad (11a-d)$$

This kind of indeterminacy is typical in continuum field equations.³ It occurs as the additive constant for scalar potentials, the gauge for the vector potential, and the divergence-free tensor for stress-energy tensors.^{9,10} If no dynamical principle constrains $\text{Inc } \sigma$, it does not contribute to any observable quantity and is, thus, unphysical and completely arbitrary.^{3,10,11} Hence, though the stress tensor σ has some physical content, if it is nonunique it is not itself a physical quantity. Traction is physical quantities. In discrete systems where the fundamental mechanics assumption of material continuity does not hold, a traction, t , is the areal average force applied to a finite area S .

$$t = \int_S dS \cdot \sigma / \int_S dS \quad (12)$$

$\underline{Y} \cdot \sigma$ is also a physical quantity. It is the force produced indirectly at a location in the interior of the system by application of tractions at its surface.

Though the divergence free part of the stress-energy tensor may be completely arbitrary for some fields,^{9,10} a generalization of Irving and Kirkwood's argument¹ demonstrates that the divergence free part of the mechanical stress tensor considered here is constrained by its relation to traction: When $\nabla \cdot \sigma = 0$, as for a stress-free state, the traction also vanishes, leaving and Eq. (12) reduces to

$$0 = \underline{Y} + \underline{A}, \quad (13)$$

because S is arbitrary. Because $\underline{Y}$ has no constant part, Eqs. (11b) and (13) provide that $\underline{Y}$ and $\underline{A}$ are each zero. Hence, the correct expression for the force or traction on a finite surface is obtained only for the choice of a null $\text{Inc } \sigma$ tensor. This result holds for a general internal potential and does not require specification of paths along which forces act. In contrast, Irving and Kirkwood's argument depends on the choice for the arbitrarily defined force lines. For a general potential, as well as from the more fundamental quantum mechanical viewpoint, paths of interactions between particles cannot be identified, only the total force on a particle.

The indeterminacy of the divergence-free part of σ occurs as an integration-contour dependence in Schofield and Henderson's expression.² Consistent with Irving and Kirkwood's arbitrary definition of interactions as being along the line of centers between particles,¹ they regard the integration contour as the path along which forces act.^{2,12} From this they conclude that the nonuniqueness of the stress density expression is equivalent to uncertainty as to exactly where the forces between particles are acting. However, their expression holds for a general internal potential, in which case a contour integral multiplies the total internal force on each particle. Hence, the integral and the cited nonuniqueness are not simply related to interactions between particles.

Baus and Lovett^{5,13} recently presented independent arguments that lead them to conclude that, for a symmetric stress tensor, constraining $\text{Inc } \sigma S$ to vanish makes earlier stress tensor expressions unique.^{1,2} Though the present discussion leads to a similar conclusion, their arguments based on equilibrium continuum relations are not applicable to the dynamic systems treated in those earlier developments. In their analysis they define stress as the strain derivative of free energy and invoke strain compatibility.⁵ The equivalence of the purported nonuniqueness in strain derivatives of free energy and the nonuniqueness of the mechanical stress tensor defined in the continuum momentum conservation relation remains to be established. Additionally, when stress is defined as the strain derivative of free energy, it lacks the clear applicability to discrete, dynamic systems possessed by the earlier stress density tensors to which it is supposed to be equivalent. Two factors contribute to this deficiency. First, this stress definition is specifically suited to conditions at or near equilibrium. Second, strain cannot be defined as a point quantity in a discrete system, but only as an average quantity in some region, as done, for example, in [14]. In contrast, the present argument for vanishing of $\text{Inc } \sigma$ is independent of strain-related concepts and applies in general to dynamic systems with arbitrary constitutive behavior, which includes those with nonsymmetric stress tensors.

CONCLUSION

The constraint on the divergence-free part of the stress tensor discussed here removes several difficulties encountered in attempts to derive expressions for physical observables that are invariant to the choice of Λ .^{2,5,15} No such invariance is required² because Λ is physically limited to being the null tensor.

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