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Objective decomposition of the stress tensor in granular flows

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A model for the stress tensor in granular flows [Volfson, Tsimring, and Aranson, Phys. Rev. Lett. **90**, 254301 (2003)] is correctly generalized to an objective form that is independent of the coordinate system. The objective representation correctly models the isotropic and anisotropic parts of the stress tensor, whereas the original model for stress tensor components is dependent on the coordinate system. This general objective form of the model also relaxes the assumption in the original model that the principal axes of the granular stress tensor be coaxial with that of the "fluid" stress tensor. This generalization expands the applicability of the model to a wider class of granular flows. The objective representation is also useful in analyzing other models based on additive decomposition of the stress tensor in granular flows.

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I. INTRODUCTION

Granular flows can exhibit different types of material characteristics and constitutive behavior, depending on the volume fraction and the magnitude of applied shear rate (relative to relevant particle time scales). Many recent attempts [1–3] to characterize the stress in granular flows involve an additive decomposition of the granular stress. In a recent continuum theory proposed by Aranson and Tsimring (AT) [1], the stress tensor σ_{ij} in a granular flow is decomposed into σ_{ij}^{f}, a "fluid" part, and σ_{ij}^{s} a "solid" part. Models are then proposed for the "fluid" and "solid" parts. Similar decompositions into impulsive and enduring parts [2], or kinetic and frictional parts [3], are common in the granular flow literature.

It is important to note that although the term "fluid" or "fluidlike" is used in the granular flow literature, this is potentially misleading since it may imply that the systems under consideration are granular mixtures (solid particles with interstitial fluid). The focus of this work (and those cited in Refs. [1,2]) is on the decomposition of the *particulate solid stress* into "solidlike" and "fluidlike" parts. If the ambient fluid is present, as in the case of granular mixtures, then an additional stress associated with the fluid will appear in the models (see Ref. [3] for example). With this clarification the quotation marks on fluid and solid are dropped.

In the AT model [4,5], the fluid and solid parts of the stress tensor are modeled in terms of the granular stress tensor σ_{ij}. It is then assumed that the principal axes of all the stress tensors are coaxial. The coefficients in the AT model (which are ratios of stress components) are then determined by matching individual components of the fluid stress tensor to data obtained from molecular dynamics (MD) simulations of zero-gravity Couette flow [4,5].

Models for the fluid (or solid) stress tensor which require specification of coefficients that depend on ratios of individual stress components are obviously coordinate-system dependent, and do not guarantee the important requirement that the stress tensor be objective [6]. In Euclidean space the objectivity requirement is that the tensor components in different coordinate systems satisfy a transformation rule (see for example Malvern [15]). Therefore models such as the AT model are not general, but are restricted to the coordinate system and flow configurations in which they are specified. Specifically, it is unclear how to generalize the AT model, which is formulated for two-dimensional (2D) Couette flow,[1] to a coordinate-system-independent form so that it may be applied to granular flows in more complex 3D geometries. Here we show how the AT model may be generalized to 3D, while satisfying the objectivity requirement.

If the fluid and solid parts of the stress tensor are modeled in terms of the granular stress tensor σ_{ij}, the general objective form of the decomposition can obtained by using representation theorems [7,8]. The assumption of coaxial principal axes for all the stress tensors is shown to be unnecessary, and an objective model which does not require this assumption is derived. The special case of coaxial principal axes is subsumed in the general objective form. This objective model is

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[1]More precisely this is a 2C flow, where by 2C we mean that the *componentiality* [13] of the stress tensor is 2, i.e., the stress tensor has only two nonzero singular values and the component index range is $i,j=1,2$. A 2D simulation can at best yield a 2C stress tensor, whereas in 3D the stress tensor can be either 3C or 2C. For simplicity of exposition we assume the stress tensor is nonsingular in the rest of this paper, in which case componentiality and dimensionality are the same.

easily extended to 3D. While the AT model in 2D specifies three model coefficients, it is shown that proper application of the requirement of objectivity results in fewer coefficients: only two coefficients can be independently specified for this tensor decomposition. The objective model also shows that the stress components can only be matched in a least-squares sense [9–11], regardless of the assumption of coaxial principal axes for all stress tensors. The objective form of the granular stress tensor decomposition is essential to compute granular flows using constitutive relations in continuum two-fluid formulations such as MFIX [12]. The physical significance of using the objective form (which allows for noncoaxial stress tensors) is that it extends the applicability of the model to granular flows with nonspherical grains, or other sources of noncoaxiality.

II. DECOMPOSITION OF GRANULAR STRESS

The basic idea in AT's additive stress decomposition is to express the stress tensor in a granular flow as the sum of a fluid stress tensor and a solid stress tensor:

$$\sigma_{ij} = \sigma^f_{ij} + \sigma^s_{ij}. \tag{1}$$

The goal is to propose models for each of the solid and fluid parts in terms of an order parameter ρ and the granular stress tensor σ_{ij}, and thereby come up with a model for stress in the granular flow. The order parameter ρ is defined by Volfson *et al.* [4] as a mesoscopic space-time average fraction of solidlike contacts between the particles in the granular system. (A contact is considered "solidlike" if it is in a stuck state and its duration is longer than a typical collision time. Additional details of the calculation of the order parameter from MD are given in [4].) Aranson and Tsimring [1] express the fluid stress in terms of the granular stress, the general form of such a model being

$$\boldsymbol{\sigma}^f = \mathbf{M}(\boldsymbol{\sigma}), \tag{2}$$

where $\mathbf{M}$ is an isotropic tensor function in the sense of Smith and Smith [7]. [Isotropic tensor functions satisfy the invariance property of Eq. (3) when subjected to unitary transformations.] The remaining stress that is obtained by subtracting the fluid stress from total stress is denoted the solid stress.

III. OBJECTIVE FORM

The objectivity requirement is that if $\boldsymbol{\sigma}^f$ is an isotropic tensor function $\mathbf{M}$ of the tensor $\boldsymbol{\sigma}$ as in Eq. (2), and $\mathbf{Q}$ is an arbitrary unitary transformation of the coordinate axes, such that

$$\boldsymbol{\sigma}^{f*} = \mathbf{Q}\boldsymbol{\sigma}^f\mathbf{Q}^{\mathrm{T}}$$

is the "fluid" stress tensor in the transformed coordinate system, then

$$\mathbf{Q}\mathbf{M}(\boldsymbol{\sigma})\mathbf{Q}^{\mathrm{T}} = \mathbf{M}(\mathbf{Q}\boldsymbol{\sigma}\mathbf{Q}^{\mathrm{T}}). \tag{3}$$

It is convenient to express the granular stress σ_{ij}, a second-order tensor that is assumed to be symmetric, [2] in isotropic and deviatoric parts:

$$\sigma_{ij} = \frac{1}{3}\sigma_{ii}\delta_{ij} + \tau_{ij} = \sigma_0\{\delta_{ij} + b_{ij}\}, \tag{4}$$

where τ_{ij} is the symmetric deviatoric stress defined as

$$\tau_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{ii}\delta_{ij}, \tag{5}$$

and b_{ij} is the normalized, symmetric, traceless, anisotropy tensor defined as

$$b_{ij} = \frac{1}{\sigma_0}\tau_{ij} = \frac{1}{\sigma_0}\sigma_{ij} - \delta_{ij}. \tag{6}$$

Here $\sigma_0 = \sigma_{ii}/3$ is the scale of the stress.[3] (Einstein notation is used so summation is implied over repeated indices.)

An objective form[4] in which the fluid (or solid) stress tensor may by expressed as a function of the granular stress tensor is

$$\sigma^f_{ij} = \sigma_0\left\{\alpha\delta_{ij} + \beta b_{ij} + \gamma\left[(\mathbf{b}^2)_{ij} - \frac{1}{3}(\mathbf{b}^2)_{ll}\delta_{ij}\right]\right\} \tag{7}$$

where α, β, γ are undetermined scalar coefficients that are functions of the invariants of b_{ij} and the order parameter ρ. (Note that b_{ij} has zero trace by definition, so only its second and third invariants may be nonzero.) The components of the second-order tensor $\mathbf{b}^2$ are defined as

$$(\mathbf{b}^2)_{ij} = b_{ik}b_{kj}, \tag{8}$$

and $(\mathbf{b}^2)_{ll}$ is a scalar that is defined as

$$(\mathbf{b}^2)_{ll} = b_{lk}b_{kl}. \tag{9}$$

If the solid stress tensor is also represented in a similar form, then the requirement that the fluid and solid stresses sum to the granular stress requires that the solid stress model expression be

[2]The stress tensor in granular flows is assumed to be symmetric [14]. However, in particle dynamics simulations which incorporate angular momentum transfer between particles, this assumption needs to be verified. Malvern [15] states that a symmetric stress tensor is implied by the moment of momentum principle for a collection of particles interacting through equal, opposite, and collinear forces, but the symmetry property is lost when even equal and opposite couples are included. Nevertheless, the objectivity requirements that we impose here can be extended to the general nonsymmetric stress tensor by decomposing it into symmetric and skew-symmetric parts.

[3]In 2D the scale of the stress is defined as $\sigma_0 = \sigma_{ii}/2$, and appropriate modifications are needed for the definition of the deviatoric and anisotropy tensors.

[4]This simpler version of the more general form proposed by Pope [16] follows from Eq. (2).

$$\sigma_{ij}^s = \sigma_0 \left\{ (1-\alpha)\delta_{ij} + (1-\beta)b_{ij} - \gamma\left[(\mathbf{b}^2)_{ij} - \frac{1}{3}(\mathbf{b}^2)_{ll}\delta_{ij} \right] \right\}. \tag{10}$$

Clearly one can exactly match three components of the fluid stress tensor model (or the solid stress model, but not both) to data from MD simulations by specifying the three model coefficients α, β, γ. In a 3D granular flow there are six independent nonzero components of the fluid stress tensor. Therefore one can specify the three model coefficients α, β, γ to match the six components from simulation data only in a least-squares sense [9–11].

In the 2D case one can show that the characteristic equation for the stress tensor is a quadratic (instead of a cubic for the 3D case), and there are only two invariants (instead of three for the 3D case): the sum and product of the two principal values of the stress tensor. The Cayley-Hamilton theorem in the 2D case shows that $\mathbf{b}^2$ (instead of $\mathbf{b}^3$ in the 3D case) itself can be expressed as a linear combination of $\mathbf{b}$, and therefore the term in γ is redundant and can be dropped. Then there are only two coefficients α and β. Noting that in 2D there are three independent nonzero components of the fluid stress tensor, again the two coefficients must be determined by matching the three stress components in a least-squares sense.

The accuracy of the "fluid" stress model for a given set of data is defined in terms of the p-norm [11] of the error matrix, which is defined as the difference between the modeled "fluid" stress tensor and the data. Here we use $p=1$ and define the matrix error measure as χ:

$$\chi = \|\boldsymbol{\sigma}^f_{\text{model}} - \boldsymbol{\sigma}^f_{\text{data}}\|_1 / \|\boldsymbol{\sigma}^f_{\text{data}}\|_1. \tag{11}$$

This measure of modeling error is useful because it applies to all the models considered in this study.

Another way to measure the errors is specific to the objective model and results in the norm of an error vector. For the 2D case the objective form of stress tensor representation in Eq. (7) has three equations and two unknowns, which requires solving

$$\begin{bmatrix} \sigma_0 & \sigma_{11} - \sigma_0 \\ 0 & \sigma_{12} \\ \sigma_0 & \sigma_{22} - \sigma_0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \sigma_{11}^f \\ \sigma_{12}^f \\ \sigma_{22}^f \end{bmatrix}. \tag{12}$$

In matrix notation this least-squares problem is

$$\mathbf{Kx} = \mathbf{y}$$

with $\mathbf{K}$ the coefficient matrix, and $\mathbf{x}$ the unknown vector of model coefficients. The error in the objective model can also be quantified by calculating the vector norm of the relative error in the least-squares solution:

$$\varepsilon = \|\mathbf{Kx} - \mathbf{y}\|_2 / \|\mathbf{y}\|_2. \tag{13}$$

Using the data ($\boldsymbol{\sigma}$, $\boldsymbol{\sigma}^f$, and ρ from Figs. 6, 7, and 8) reported in Volfson *et al.* [4] we obtain the coefficients for the objective model. The values of the coefficients α and β in the objective model are shown as functions of the order parameter ρ in Fig. 1. As expected the coefficients approach 1 as the order parameter ρ approaches zero, corresponding to

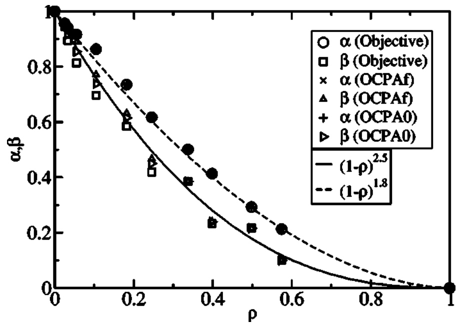

FIG. 1. Model coefficients as functions of order parameter ρ: α and β for the general objective form, and α_{CPA} and β_{CPA} (for models OCPA0 and OCPAf) for the equivalent objective form assuming coaxial principal axes.

the granular flow reaching the fully fluidized state. It is also to be expected that the coefficients will approach zero as the order parameter ρ approaches 1. In this case it would be preferable to solve for the model coefficients of the "solid" stress tensor, $(1-\alpha)$ and $(1-\beta)$. The errors incurred in terms of the matrix norm χ and the vector norm ε are depicted in Fig. 2. Over the entire range of the order parameter $(0.1 < \rho < 1.0)$ it is gratifying to note that the errors of the objective model are less than 10%. As ρ approaches zero the granular flow becomes more fluidized, and the error drops rapidly (i.e., the "solid" stress is negligible). Therefore, for the granular Couette flow the objective form [Eqs. (7) and (10)] accurately decomposes the stress into "fluid" and "solid" parts with the following expressions that fit the variation of model coefficients with order parameter:

$$\alpha = (1-\rho)^{1.8}, \tag{14}$$

$$\beta = (1-\rho)^{2.5}. \tag{15}$$

These expressions ensure the correct limiting behavior of the model at $\rho=0$ and 1.

IV. COAXIAL PRINCIPAL AXES CASE

In the AT model it is assumed that the principal axes of all three stress tensors $\boldsymbol{\sigma}$, $\boldsymbol{\sigma}^f$, and $\boldsymbol{\sigma}^s$ are coaxial. The coefficients in the AT model are then determined by matching

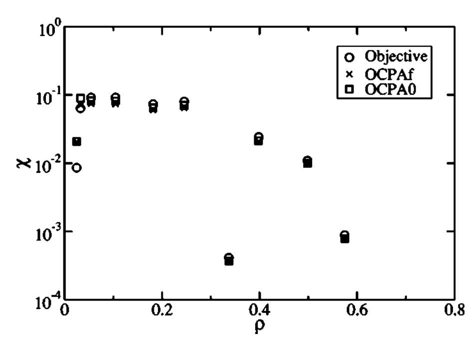

FIG. 2. Error in modeled "fluid" stress characterized by matrix one-norm χ for all models: general objective and equivalent objective under coaxial principal axes assumption (OCPA0 and OCPAf).

individual components σ_{xx}, σ_{xy}, σ_{yy} of the fluid stress tensor to data obtained from molecular dynamics simulations of a canonical granular flow [1,4].

The objective model can be investigated under the assumption of coaxial principal axes. If the objective model is written in principal axes coordinates, then the deviatoric tensor is diagonal and given by

$$\tau_{ij} = \sigma_{(i)}\delta_{ij} - \sigma_0\delta_{ij}. \tag{16}$$

The normalized symmetric traceless anisotropy tensor b_{ij} is also diagonal and is given by

$$b_{ij} = \left[\frac{\sigma_{(i)}}{\sigma_0} - 1\right]\delta_{ij}. \tag{17}$$

In the 2D case there are only two coefficients α and β. Note that in principal coordinates we have

$$\sigma_1^f = \alpha\sigma_0 + \beta(\sigma_1 - \sigma_0),$$

$$\sigma_2^f = \alpha\sigma_0 + \beta(\sigma_2 - \sigma_0).$$

By eliminating α and β from the above equations we obtain the equivalent *objective* specification of the coaxial principal axes (CPA) model to be

$$\alpha_{\mathrm{CPA}} = \frac{\sigma_1^f}{\sigma_0} - \left(\frac{\sigma_1^f - \sigma_2^f}{\sigma_1 - \sigma_2}\right)(\sigma_1 - \sigma_0), \tag{18}$$

$$\beta_{\mathrm{CPA}} = \frac{\sigma_1^f - \sigma_2^f}{\sigma_1 - \sigma_2}. \tag{19}$$

A technical detail arising from nonzero angle between the principal axes of the fluid and total granular stress data results in two slightly different ways in which the CPA model coefficients can be calculated. In both approaches σ_1 and σ_2 in Eqs. (18) and (19) are the singular values of the total granular stress matrix. In the first approach (OCPAf) we use the singular values of the "fluid" stress matrix for (σ_1^f, σ_2^f), even though the principal directions of the fluid and total stress tensors are not identical. In the second approach (OCPA0), the "fluid" stress tensor is transformed into the principal coordinates of the total stress tensor, and the diagonal components of the transformed matrix are taken to be (σ_1^f, σ_2^f). The values of α_{CPA} and β_{CPA} as a function of the order parameter ρ are shown in Fig. 1.

It is found that α_{CPA} is practically identical to α for the objective model without the coaxial principal axes assumption. There are some differences between β_{CPA} and β for the objective model without the coaxial principal axes assumption. The modeling error measure χ is shown for both models in Fig. 2, and it is found that the error incurred in the various models is comparable.

V. VALIDITY OF COAXIAL PRINCIPAL AXES ASSUMPTION

Denoting the principal axes of $\boldsymbol{\sigma}$ as $\{\mathbf{u}_1, \mathbf{u}_2\}$, and similarly the principal axes of $\boldsymbol{\sigma}^f$ as $\{\mathbf{u}_1^f, \mathbf{u}_2^f\}$ [11], one can calculate the angle θ between the principal axes of $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}^f$ as

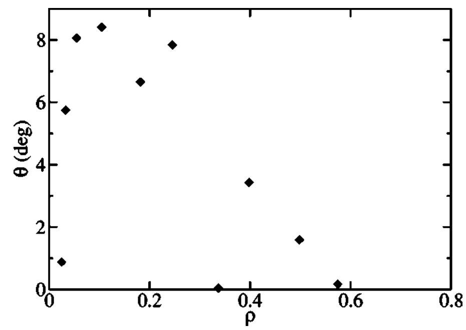

FIG. 3. Angle between principal axes of the total granular stress $\boldsymbol{\sigma}$ and the "fluid" stress $\boldsymbol{\sigma}^f$.

$$\theta = \arccos(|\mathbf{u}_1 \cdot \mathbf{u}_1^f|) = \arccos(|\mathbf{u}_2 \cdot \mathbf{u}_2^f|). \tag{20}$$

The angles for the data obtained from Volfson *et al.* [4] are shown in Fig. 3. It is found that the maximum angle between the two principal axis systems is about 8°, so the principal axes of the stress tensors are almost collinear. As ρ decreases, the angle increases to the maximum, and then drops rapidly when ρ approaches zero. Whether this near-collinearity of the stress tensors is a universal characteristic of granular flow in this regime is questionable. Certainly coaxial principal axes are not expected if the grains are anisotropic (e.g., ellipsoids).

The small angle between the principal axes explains why the orthotropic model incurs errors that are of the same magnitude as the objective model for this flow. We also see from Figs. 2 and 3 that the modeling errors follow the same trend as the angle between the principal axes. The small angle between the principal axes also explains why the model coefficients with the coaxial principal axes assumption $(\alpha_{\mathrm{CPA}}, \beta_{\mathrm{CPA}})$ are very close to the general objective model. One may expect larger differences in other granular flows, although these comparisons are difficult to make because only the objective model is truly generalizable and independent of the coordinate system.

VI. OBJECTIVE MODEL PERFORMANCE IN THICK GRANULAR LAYER

Volfson *et al.* [4] also report MD simulations for a thick granular layer under nonzero gravity driven by a moving upper plate, a granular system that is different from the zero-gravity Couette flow with which the model coefficients were calibrated. The objective model is tested in this thick granular system, and these results of the model predictions for the granular layer driven by a moving upper plate under nonzero gravity [4] (case P10V5) are shown in Fig 4. The agreement of the objective model's predicted stresses to the simulation data is remarkably good.

VII. CONCLUSIONS

An objective generalization of the stress model based on the order parameter [4,5] has been developed [see Eqs. (7),

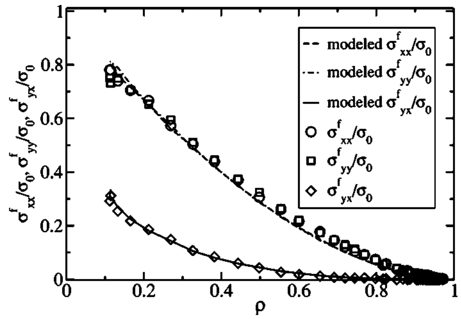

FIG. 4. Comparison of objective model predictions of "fluid" stress components with MD data for a thick granular system driven by a moving upper plate under nonzero gravity.

(14), and (15)]. The objective model does not assume that the principal axes of the "fluid" and total granular stress are coaxial. The objective model has fewer model coefficients than the original model and therefore the "fluid" stress is matched only in a least-squares sense. Model coefficients and error measures are compared for both the general objective model and the equivalent objective model under coaxial principal axes assumption. It is found that the error is comparable for both models and is below 10% for all values of the order parameter in the Couette flow configuration for which data from MD are available.

The angle between principal axes of $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}^f$ is computed and it was found to increase sharply at very small ρ ($\rho<0.1$, fluidlike regime), reach a maximum of about 10° for the granular Couette flow, and then decrease again at larger ρ (solidlike regime). The modeling errors follow the same trend. This nonlinear variation with order parameter ρ tells us that the stress in granular matter does not become fluidlike in direct proportion to the order parameter ρ. Further study is needed to understand if the discontinuity in the angle that is observed around $\rho=0.05$ is indicative of a sort of phase transition, or not. The objective model is used to predict the stresses in a *different* granular system from the one using which the model coefficients were calibrated (thin Couette flow with zero gravity). In this thick granular flow driven by a moving upper plate under nonzero gravity, the objective model predictions are in excellent agreement with the simulation data, even though the objective model has fewer coefficients than the previous model. However, a more rigorous test of the objective model would require data from MD of a fully 3D granular flow for a range of order parameter and stress tensor anisotropy values.

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