Evolution of spatially structured elastic materials using a harmonic density function

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A study is presented of the evolution of a heterogeneous material that is subjected to an increment-by-increment persistent, deviatoric strain path. The internal evolution of the stiffness components may be effected in various ways; some simple ones are studied here and the resulting structure formation is detected via the spatial Fourier transform of the stiffness fluctuations. [S1063-651X(97)06010-8]

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I. INTRODUCTION

The mechanical response of materials as they progress through an imposed stress or strain path generally depends on the evolution of the internal state of the medium. The complete description of materials should therefore include information about the internal state. This is especially necessary for granular and other geological or biological materials, which are often heterogeneous in nature and exhibit measurable changes in the ''microstructure.'' Oda [1,2], for example, has measured the angular variation of the contact distribution of a noncohesive sand under deviatory loading and has found strong effects of both contacts being made and contacts being broken, in contact directions that coincide with the major and minor principal stress axes, respectively. Experiments on photoelastic assemblies in both two [3–5] and three [6,7] dimensions on systems of disks or spheres give information on the development of contact forces during a load path. More recently, relatively reliable computer simulations have been developed in which small assemblies are subjected to various loading conditions [8–10], with results that can be verified against photoelastic experiments. The advantage of simulated tests is obviously that data gathering is far easier than for the physical experiments. Also, changes in microscopic properties can be effected with little effort, which may facilitate the study of conceptual mechanisms, insofar as they operate on a particle scale. All these are relevant to noncohesive granular materials.

While it is completely clear that changes in microstructure do take place, there is a lack of theoretical support that needs urgent remedy. A number of papers deal with the behavior of small assemblies. These consist either of one particle surrounded by (stochastically described) neighboring presences [11–13] or of two neighboring particles embedded in a mean field [14,15]. The behavior of the medium as a whole is carried out either by a traditional homogenization technique [12] or via a least-squares procedure in which mean-field properties are assigned to variables that appear in the single-particle equilibrium equations [15,16]. All these techniques give reasonable answers at low stress ratios for noncohesive materials [16,17] and up to quite high stress ratios for cemented materials [18]. As such these methods have contributed to reduce the traditionally high number of describing parameters required for the material description.

Nearly all geological materials exhibit rupture phenomena at some critical stress ratio. These are extremely important for the predictions of catastrophic events. Landslides [19] and planetoid breakup in the gravity field of a large planetary body [20,21] are two well-known examples. Questions associated with these events pertain mostly to the variety of rupture phenomena as well to with the theoretical framework that is required to make adequate predictions. The challenge is to link the micromechanical models that work over length scales of a couple of particles to large-scale phenomena working over a length scale that encompasses the whole assembly.

Both experimental and theoretical studies of rupture layers have been published. The experimental technique relies on either x-ray or surface displacement imaging of a sample. The x-ray studies [22] show very clearly that various types of ''shearbands'' become evident under deviatoric loading. Once the rupture takes place the material loses the ability to support further increased deviatoric stress and therefore the onset of rupture is associated with peak stress ratio. In addition to shearbands at different distinct angles, a ''diffuse'' mode of failure is sometimes observed; in this mode there is no localized shearband, but the stress ratio attains a maximum value [22,23].

Theoretical studies on shearband formation have been published and rely on a continuum description of the material (often in the framework of a plasticity theory) [24,25]. The drawback is that a certain constitutive behavior has to be assumed that has all the various rupture modes already built in. These methods do not explain what it is that physically changes inside the material that causes rupture; it merely sets out what constitutive assumptions are needed to cause rupture under the criterion imposed for failure to take place. Some understanding, however, can be derived from models in which a microstructure near the peak stress ratio is assumed. A well-developed example of this is the double shearing model, which assumes built-in directions along which the incremental velocity must take place. Anand [26] has shown that the most commonly observed shearband directions follow from this model. It is intriguing that the directions of the model (the maximum obliquity directions, that is, the directions along which the the macroscopic stress ratio is maximal) are only one of the three sets of directions of shearband formation. Koenders [27] has demonstrated that when a similar model is extended to include higher-order gradients the thickness of the bands can also be obtained.

While these descriptions are useful in understanding the onset of rupture they do not explain what evolution the ma-

terial has experienced to get into a state where instability may occur. It is also noteworthy that materials with an entirely different microstructure from noncohesive granular materials exhibit similar qualitative stress-strain behavior and rupture layer formation (for jointed rock [28] and for clays [29]), suggesting that the development of these properties depends more on the type of internal evolution as the material is subjected to a deviatoric stress path than on the precise microscopic interactive properties between the fundamental elements that constitute the medium.

In the analysis below an analytical exploration of evolution of internal heterogeneity is carried out. To keep the model analytical, simplifying assumptions obviously have to be made. While these assumptions limit the model to the most primitive of materials, the analysis demonstrates very clearly that structure formation takes place when the material is subjected to a persistent deviatoric strain path. The term ''structure'' is here meant as a directional dependence of the two-point correlation function of the components of the position-dependent stiffness. Not only does structure arise quite naturally, the theory reveals very clearly how localized phenomena may arise. By particularly studying two types of evolution rules, those that depend on either the local volume strain or the local deviator invariant, it is demonstrated that the manner in which structure is created depends directly on the sort of rule that is deployed.

It turns out that a transparent picture of the two-point correlation function of the stiffness is achieved by using its Fourier transform, the harmonic density. At the same time the wave vector that is involved in this representation gives a measure of when the internal state of the material is such that the finite dimension of the constituents becomes relevant. In line with other theories the constituents themselves are believed to be much stiffer than the assembly of which they are elements, the main cause of deformation being the relative motion between the particles due either to sliding or to spinning.

II. THEORETICAL PRINCIPLES

A medium is characterized by its position-dependent stiffness $\mathbf{A}(\mathbf{x})$, connecting a stress increment $\mathbf{s}(\mathbf{x})$ to a strain increment $\mathbf{e}(\mathbf{x})$ in geometrical linearization, implying that the displacement increment $\mathbf{u}$ is much smaller than the length scale of a mesodomain [30] D:

$$s_{ij}(\mathbf{x})=A_{ijkl}(\mathbf{x})e_{kl}(\mathbf{x})=\frac{1}{2}A_{ijkl}(\mathbf{x})\left(\frac{\partial u_k}{\partial x_l}+\frac{\partial u_l}{\partial x_k}\right). \quad (1)$$

The stiffness is defined over the length scale D, the typical dimension of a small assembly, in such a way that it portrays the average motion between the grains that constitute the material. The representation of the medium is here as ''point functions''; the alternative representation as ''set functions'' is developed by Axelrad [30], Sec. 3.5. In this reference also relevant probability space measures are discussed. On the scale of the mesodomain the stress cannot be expected to represent the force between the grains in its entirety. There is a correction, not necessarily small, that describes the erratic part of the force that is left after the local homogenization that yields the small-scale stress measure; this part of the force is represented by its volume density and is called $\mathbf{f}_D(\mathbf{x})$. The variation in the stiffness is crucial and needs to be characterized in some way. This is done here by specifying the harmonic density. It will be demonstrated that this is a very natural measure that fits in directly with the methodology for the quasistatic equilibrium equations. These are

$$\frac{\partial s_{ij}}{\partial x_j}+(f_D)_i=0,$$

$$\frac{\partial}{\partial x_j}\left[A_{ijkl}(x)\left(\frac{\partial u_k}{\partial x_l}+\frac{\partial u_l}{\partial x_k}\right)\right]=-2(f_D)_i. \quad (2)$$

The moduli change as the motion goes on, but the motion is assumed to be so slow that at any point quasistatic equilibrium may be used. For a first-order solution Kröner [31] is followed, where the solution is expressed as a sum of n-point correlation functions. In lowest order the two-point correlation function is sufficient, which is obtained by neglecting the possible correlation between first-order fluctuations. The latter are defined as the deviation from the volume averages of the various significant variables

$$\overline{A_{ijkl}}=\frac{1}{V}\int_V dV\, A_{ijkl}(\mathbf{x}), \quad B_{ijkl}(\mathbf{x})=A_{ijkl}(\mathbf{x})-\overline{A_{ijkl}}; \quad (3)$$

$$\alpha_{kl}=\frac{1}{V}\int_V dV\frac{\partial u_k}{\partial x_l}(\mathbf{x}), \quad \frac{\partial v_k}{\partial x_l}(\mathbf{x})=\frac{\partial u_k}{\partial x_l}(\mathbf{x})-\alpha_{kl}. \quad (4)$$

When this decomposition of the stiffness tensor and the deformation is substituted into the equilibrium equations an ordering on the basis of products of fluctuating terms is found:

$$\frac{\partial B_{ijkl}(x)}{\partial x_j}(\alpha_{kl}+\alpha_{lk})+\overline{A_{ijkl}}\left(\frac{\partial^2 v_k}{\partial x_l\partial x_j}+\frac{\partial^2 v_l}{\partial x_k\partial x_j}\right)+\frac{\partial}{\partial x_j}\left[B_{ijkl}(x)\left(\frac{\partial v_k}{\partial x_l}+\frac{\partial v_l}{\partial x_k}\right)\right]=-2(f_D)_i. \quad (5)$$

A solution hierachy was put forward by Kröner [31]: Neglect first the last term and solve the ensuing linear equation; then substitute back and solve for the first-order fluctuations and so on. Here the first-order fluctuations are retained only and the solution is expressed as a Fourier transform in n dimensions $(n=2,3)$

$$B_{ijkl}(\mathbf{x})=\frac{1}{(2\pi)^n}\int d_n k\ \hat{B}_{ijkl}(\mathbf{k})e^{ik_m x_m},$$

$$v_k(\mathbf{x})=\frac{1}{(2\pi)^n}\int d_n k\ \hat{v}_k(\mathbf{k})e^{ik_m x_m}. \quad (6)$$

Thus

$$ik_j\hat{B}_{ijkl}(\alpha_{kl}+\alpha_{lk})+2(\hat{f}_D)_i-\overline{A_{ijkl}}(k_j k_l\hat{v}_k+k_j k_k\hat{v}_l)\approx 0. \quad (7)$$

This equation is valid for each value of $\mathbf{k}$; the analysis below is particularly aimed at investigating the range of small k,

whereas the harmonic content of $\hat{\mathbf{f}}_D$ is nonzero in the range $|\mathbf{k}|D>1$. For the moment this term is then neglected, but the issue will be taken up again in Sec. IV.

The symmetry in the indices of both $\overline{\mathbf{A}}$ and $\hat{\mathbf{B}}$ ($A_{ijkl}=A_{jikl}=A_{ijlk}$, and similarly for $\hat{\mathbf{B}}$) ensures that one may write

$$ik_j\hat{B}_{ijkl}\alpha_{kl}-\overline{A}_{ijkl}k_jk_l\hat{v}_k=0. \tag{8}$$

The acoustic tensor is defined as

$$\hat{P}_{ik}=\overline{A}_{ijkl}k_jk_l \tag{9}$$

and therefore

$$\hat{v}_a=i\hat{P}^{-1}_{ab}k_j\hat{B}_{bjkl}\alpha_{kl}. \tag{10}$$

From this first-order approximation the following relevant parameters can be derived. The Fourier transform of the fluctuation of the distortion is

$$ik_c\hat{v}_a=-\hat{P}^{-1}_{ab}k_jk_c\hat{B}_{bjkl}\alpha_{kl}=-\hat{H}_{acbj}\hat{B}_{bjkl}\alpha_{kl}. \tag{11}$$

The homogenized stress increment is

$$\overline{s_{pq}}=\overline{A}_{pqkl}\alpha_{kl}+\frac{1}{2V}\int_V dV\ B_{pqkl}(\mathbf{x})\left(\frac{\partial v_k}{\partial x_l}(\mathbf{x})+\frac{\partial v_l}{\partial x_k}(\mathbf{x})\right). \tag{12}$$

The second term is conveniently reevaluated by making use of the development

$$\begin{aligned}\frac{1}{V}\int_V dV\ B_{pqkl}(\mathbf{x})\frac{\partial v_k}{\partial x_l}(\mathbf{x})&=\frac{i}{V(2\pi)^{2n}}\int_V dV\int d_nk\int d_n\eta\ \hat{B}_{pqkl}(\mathbf{k})\\&\quad\times e^{ik_mx_m+i\eta_mx_m}\eta_l\hat{v}_k(\boldsymbol{\eta})\\&=\frac{1}{V(2\pi)^n}\int d_nk\ \hat{B}_{pqkl}(\mathbf{k})\int d_n\eta\ i\eta_l\hat{v}_k(\boldsymbol{\eta})\delta_n(\boldsymbol{\eta}+\mathbf{k})\\&=-\frac{1}{V(2\pi)^n}\int d_nk\ \hat{B}_{pqac}(-\mathbf{k})\hat{H}_{acbj}(\mathbf{k})\hat{B}_{bjkl}(\mathbf{k})\alpha_{kl}.\end{aligned} \tag{13}$$

This expression is now interpreted with the aid of a harmonic density rather than (as does Kröner [31]) express it as a correlation function. The following definitions of correlation function and harmonic density are used. The autocorrelation function $\Phi_y(\tau)$ of a function $y(t)$ is

$$\Phi_y(\tau)=\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\ y(t)y(t+\tau). \tag{14}$$

It follows that $\Phi(-\tau)=\Phi(\tau)$. A truncated Fourier transform is defined as $F_T=\int_0^T dt\ y(t)e^{-ikt}$; using this the harmonic density of $y(t)$ is now defined as

$$S_y(k)=\frac{2}{T}F_T(k)F^*_T(k). \tag{15}$$

The connection with the correlation function is given by the familiar Wiener-Khinchin theorem

$$\int_0^T d\tau\ \Phi(\tau)e^{-ik\tau}=\frac{1}{T}F_T(-k)F_T(k)=\frac{1}{T}F^*_T(k)F_T(k). \tag{16}$$

Cross correlations may be defined analogously. The cross correlation function is

$$\Phi_{xy}(\tau)=\lim_{T\to\infty}\int_0^T dt\ x(t)y(t+\tau) \tag{17}$$

and the cross harmonic density is

$$S_{xy}(k)=2\int_{-\infty}^{\infty}d\tau\ \Phi_{xy}(\tau)e^{ik\tau}=\frac{2}{T}(F_T)_x(k)(F_T)^*_y(k). \tag{18}$$

This has the property $S_{xy}(k)=S^*_{yx}(k)=S_{yx}(-k)$.

Using these formulas, extended to n dimensions, to evaluate formula (13), it is seen that the first-order correction on the stress is a filtered cross harmonic density

$$\begin{aligned}&\frac{-\alpha_{kl}}{2V(2\pi)^n}\int d_nk\ \hat{B}_{pqac}(-\mathbf{k})[\hat{H}_{acbj}(\mathbf{k})+\hat{H}_{cabj}(\mathbf{k})]\hat{B}_{bjkl}(\mathbf{k})\\&\quad=-\frac{\alpha_{kl}}{4(2\pi)^n}\int d_nk\ S_{B_{bjkl},B_{pqac}}(\mathbf{k})\\&\qquad\times[\hat{H}_{acbj}(\mathbf{k})+\hat{H}_{cabj}(\mathbf{k})].\end{aligned} \tag{19}$$

Kröner [31] does the same calculation but expresses the correction in terms of the cross correlation function. He also discusses higher-order terms and applies these to a perfectly random material. In this way he achieves an estimate for the effective stiffness of the medium, an estimate somewhere between the Reuss and Voight estimates. While the estimate of the overall stiffness is not irrelevant for the purposes of this paper, the central question here is the evolution of the internal structure of the medium. It is therefore required that evolution rules are phrased. The criterion for these is that they must be sufficiently simple for the theory to retain its analytical form. The effect of the evolution rules is studied under persistent strain paths.

The study is most straightforwardly carried out if the medium is composed of a material with few parameters. The simplest, nontrivial material is an isotropic medium that has two parameters, for which $\mathbf{A}(\mathbf{x})$ has the form

$$A_{ijkl}(\mathbf{x})=\lambda(\mathbf{x})\delta_{ij}\delta_{kl}+\mu(\mathbf{x})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{kj}). \tag{20}$$

The spatial distributions of $\lambda(\mathbf{x})$ and $\mu(\mathbf{x})$ then completely define the first-order stiffness correction given by formula (13). The material may consist of isotropic mesodomains and the overall moduli may exhibit anisotropy due to an anisotropic distribution of $\lambda(\mathbf{x})$ and $\mu(\mathbf{x})$.

For an average isotropic medium the stiffnesses $\overline{\mathbf{A}}$ take the form

$$\overline{A}_{ijkl}=\overline{\lambda}\delta_{ij}\delta_{kl}+\overline{\mu}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{kj}). \tag{21}$$

It is easily verified that the following relations hold:

$$\hat{P}_{ik}=(\overline{\lambda}+\overline{\mu})k_i k_k+\overline{\mu}k^2\delta_{ik}, \tag{22}$$

$$\hat{H}_{acbj}=\left(\frac{-(\overline{\lambda}+\overline{\mu})k_a k_b}{\overline{\mu}(\overline{\lambda}+2\overline{\mu})k^4}+\frac{\delta_{ab}}{\overline{\mu}k^2}\right)k_j k_c. \tag{23}$$

Let the fluctuations be generated by another isotropic tensor

$$B_{ijkl}(\mathbf{x})=\nu(\mathbf{x})\,\delta_{ij}\delta_{kl}+\rho(\mathbf{x})(\,\delta_{ik}\delta_{jl}+\delta_{il}\delta_{kj}) \tag{24}$$

and so

$$i\hat{v}_a k_c=-\hat{\nu}\alpha_{kk}\frac{k_a k_c}{(\overline{\lambda}+2\overline{\mu})k^2} -2\hat{\rho}\alpha_{kl}k_c k_1\frac{-(\overline{\lambda}+\overline{\mu})k_a k_k+\delta_{ak}k^2(\overline{\lambda}+2\overline{\mu})}{\overline{\mu}(\overline{\lambda}+2\overline{\mu})k^4}. \tag{25}$$

The evolution in the internal parameters is phrased as a microstrain-dependent ''law''. The strain increment at location $\mathbf{x}$, $\mathbf{e}(\mathbf{x})$, is the average strain $\boldsymbol{\alpha}$ plus a fluctuation $\boldsymbol{\beta}(\mathbf{x})$; the Fourier transform of the latter is $\hat{\beta}_{ab}=(i/2)\,(\hat{v}_a k_b+\hat{v}_b k_a)$. As isotropy has been imposed, the coefficients that appear in the evolution rule can only depend on the local invariants. These are the isotropic strain increment $e_{aa}(\mathbf{x})=\alpha_{aa}+\beta_{aa}(\mathbf{x})$ and the first nonzero invariant of the deviatoric strain increment $(1/2)e'_{ab}(\mathbf{x})e'_{ba}(\mathbf{x})$, where the deviatoric strain increment is defined as $e'_{ab}(\mathbf{x})=e_{ab}(\mathbf{x})-(1/n)\,e_{kk}(\mathbf{x})\delta_{ab}$. The third invariant exists only in the three-dimensional case and may be introduced if required.

Changes associated with isotropic and deviatoric strain increments are of key relevance to the geological materials mentioned in the Introduction. The change due to the isotropic strain increment can be related to the mechanism of local contact deletion or contact making. The physical interaction takes place at contacts; the mechanical contact law may naturally depend on local conditions, but the number of interactive points in a small volume is certainly important. Experimental findings as well as modeling have been reported to bear out these facts. Yanagisawa [32] draws together results from the theoretical study of various regular and random packings and experiments on glass beads and sand, demonstrating a systematic connection between the shear modulus, the coordination number, and the voids ratio. Brotzmeyer and Abouaf [33] similarly show the relation between the applied pressure, the voids ratio, and the coordination number for a numerical simulation of a ceramic powder compaction (acknowledging the heterogeneous character of the problem). The effects of the deviatoric strain are reported by Cundall *et al.* [34], who with a numerical simulation of a densely packed assembly of disks with elastofrictional interactive properties show that the local deletion of contacts is accompanied by a local slip and thus a concomitant reduction in the stiffness parameters. Both the isotropic and deviatoric strain increments influence the stress ratio in a mesodomain and where the contact law has a frictional character the stiffness coefficients of the mesodomain will be influenced by these two invariants.

With these considerations in mind, the following evolution rules are put forward:

$$\mathring{\lambda}(\mathbf{x})\,\delta t=c_I^{(\lambda)}e_{aa}(\mathbf{x})+c_D^{(\lambda)}\sqrt{\frac{1}{2}e'_{ab}(\mathbf{x})e'_{ba}(\mathbf{x})}, \tag{26}$$

$$\mathring{\mu}(\mathbf{x})\,\delta t=c_I^{(\mu)}e_{aa}(\mathbf{x})+c_D^{(\mu)}\sqrt{\frac{1}{2}e'_{ab}(\mathbf{x})e'_{ba}(\mathbf{x})}. \tag{27}$$

The coefficients $c_{I,D}^{(\lambda,\mu)}$ can be functions of local state variables: components of the local stress, invariants of the local stress, the mass density, or even independent variables that change with the local strain (local contact point distribution, for example). None of these are considered here; the material-dependent coefficients $c_{I,D}^{(\lambda,\mu)}$ will be assumed to be constants throughout the persistent strain path. The effect of evolution for the material properties as a whole and pattern of microstructure that evolves are studied as the material is subjected to a succession of strain increments.

III. EXAMPLES OF DIFFERENT CASES OF EVOLUTION RULE

Two examples of evolution rule are studied in some detail. The two cases are extremes, but demonstrate that the medium under persistent straining can become highly structured and that the type of structure that materializes depends crucially on the type of evolution rule that is deployed.

A. Isotropic rule

For this case $c_D^{(\lambda,\mu)}=0$. The evolution rule takes the form

$$\delta\lambda(\mathbf{x})=c_I^{(\lambda)}e_{aa}(\mathbf{x})=c_I^{(\lambda)}[\,\alpha_{aa}+\beta_{aa}(\mathbf{x})], \tag{28}$$

$$\delta\mu(\mathbf{x})=c_I^{(\mu)}e_{aa}(\mathbf{x})=c_I^{(\mu)}[\,\alpha_{aa}+\beta_{aa}(\mathbf{x})]. \tag{29}$$

Distinguishing averages and fluctuations gives

$$\delta\overline{\lambda}=c_I^{(\lambda)}\alpha_{aa}, \quad \delta\nu(\mathbf{x})=c_I^{(\lambda)}\beta_{aa}(\mathbf{x}); \tag{30}$$

$$\delta\overline{\mu}=c_I^{(\mu)}\alpha_{aa}, \quad \delta\rho(\mathbf{x})=c_I^{(\mu)}\beta_{aa}(\mathbf{x}). \tag{31}$$

Time is mesaured as a fraction of α_{11}: $\alpha_{11}=\alpha_0\delta t$. Let the intial state be isotropic. A persistent strain path is defined as $\alpha_{22}=m_2\alpha_0\delta t$, $\alpha_{33}=m_3\alpha_0\delta t$ with constant coefficients m. Thus $\alpha_{aa}=\alpha_0(1+m_2+m_3)\,\delta t=\mathring{\alpha}_{aa}\delta t$. The four differential equations (30) and (31) have a solution in the Fourier domain. The averages satisfy

$$\overline{\lambda}(t)=\overline{\lambda}(0)+c_I^{(\lambda)}\alpha_0(1+m_2+m_3)t, \tag{32}$$

$$\overline{\mu}(t)=\overline{\mu}(0)+c_I^{(\mu)}\alpha_0(1+m_2+m_3)t. \tag{33}$$

For the solution of the fluctuating parts of the stiffness field the quantity $\hat{\beta}_{aa}(\mathbf{k})$ is obtained from Eq. (25): $\hat{\beta}_{aa}(k)=-[\,\hat{\nu}(\mathbf{k})\alpha_{kk}-2\hat{\rho}(\mathbf{k})\alpha_{kl}k_k k_l]/[(\overline{\lambda}+2\overline{\mu})(t)]$. The equations for the fluctuating parts of the stiffnesses are seen to represent a linear system of two differential equations. The solution has the form

$$\hat{\nu}(t)=\hat{\nu}(0)+M(e^{\eta(w)\tau(t)}-1),$$

$$\hat{\rho}(t)=\hat{\rho}(0)+\frac{c_I^{(\mu)}}{c_I^{(\lambda)}}M(e^{\eta(w)\tau(t)}-1), \tag{34}$$

where

$$\eta(w)=-c_I^{(\lambda)}\mathring{\alpha}_{aa}-2c_I^{(\mu)}\frac{k_1^2+m_2k_2^2+m_3k_3^2}{k^2}\alpha_0,$$

$$\tau(t)=\frac{\ln\left(\dfrac{(\overline{\lambda+2\mu})(t)}{(\overline{\lambda+2\mu})(0)}\right)}{(c_I^{(\lambda)}+2c_I^{(\mu)})\mathring{\alpha}_{aa}},$$

$$M=\frac{c_I^{(\lambda)}\hat{\nu}(0)\mathring{\alpha}_{aa}+2c_I^{(\lambda)}\hat{\rho}(0)(k_1^2+m_2k_2^2+m_3k_3^2)\alpha_0/k^2}{c_I^{(\lambda)}\mathring{\alpha}_{aa}+2c_I^{(\mu)}(k_1^2+m_2k_2^2+m_3k_3^2)\alpha_0/k^2}. \tag{35}$$

For the interpretation below on structure formation it is convenient to write the exponential part of the solution in the form

$$e^{\eta(\mathbf{k})\tau(t)}=\left\{\frac{(\overline{\lambda+2\mu})(t)}{(\overline{\lambda+2\mu})(0)}\right\}^{-p}=\left\{\frac{(c_I^{(\lambda)}+2c_I^{(\mu)})\mathring{\alpha}_{aa}t}{(\overline{\lambda+2\mu})(0)}+1\right\}^{-p}$$

with

$$p=\frac{c_I^{(\lambda)}+\dfrac{2c_I^{(\mu)}(k_1^2+m_2k_2^2+m_3k_3^2)}{k^2(1+m_2+m_3)}}{c_I^{(\lambda)}+2c_I^{(\mu)}}. \tag{36}$$

The isotropic distribution of the fluctuations of the stiffness parameters retains its shape in space (and only changes in magnitude) when the deformation is isotropic ($m_2=1$ and $m_3=1$). But the shape becomes distorted if a deviatoric component is present in the average strain. The latter case is most easily studied in two dimensions, so set $m_3=0$.

The salient features are captured by the parameters $f=c_I^{(\mu)}/c_I^{(\lambda)}$ and m_2. The dependence on $\mathbf{k}$ of Eq. (36) is as a function of the angle in the k-plane only. Therefore, for strain paths in which $(c_I^{(\lambda)}+2c_I^{(\mu)})(1+m_2)\alpha_0 t$ is positive, that is, when $(m_2+1)(2f+1)>0$, the harmonic density of $\hat{\nu}$ will inflate in the direction for which the exponent of Eq. (36) is positive. When the value of $(\overline{\lambda+2\mu})(t)$ decreases with time, or $(m_2+1)(2f+1)<0$, the same will happen for directions for which the exponent is negative. Expressed in f and m_2, the exponent has the form $-[(m_2+1+2f)k_1^2+(m_2+1+2fm_2)k_2^2]/(m_2+1)(2f+1)k^2$. If this theory is pushed to the point where $(\overline{\lambda+2\mu})(t)$ vanishes there will be problems with diverging integrals when doing the perturbation calculus. Much more subtle evolution rules are then required. However, the tendency for the harmonic density to concentrate in certain directions will occur.

As the exponent depends homogeneously on k_1^2 and k_2^2 the directions in which an extreme concentration of harmonic density may occur after persistent straining is either the major or the minor principal strain direction. Reckoning compressive strain positive, as is usual in soil mechanics, the ranges of f and m_2 for which the polar angle in the k plane is the extreme concentration direction are as follows [$\phi=\arctan(k_2/k_1)$] $\phi=0$ and $\phi=\pi$ are obtained when either

$$(m_2+1)(2f+1)>0, \quad f<fm_2$$

or

$$(m_2+1)(2f+1)<0, \quad f>fm_2; \tag{37a}$$

$\phi=\pi/2$ and $\phi=3\pi/2$ are obtained when either

$$(m_2+1)(2f+1)>0, \quad f>fm_2$$

or

$$(m_2+1)(2f+1)<0, \quad f>fm_2. \tag{37b}$$

B. Deviatoric rule

For this case $c_I^{(\lambda,\mu)}=0$. The evolution rule is nonlinear; Eqs. (26) and (27) take the form

$$\delta\lambda(\mathbf{x})=c_D^{(\lambda)}\sqrt{\frac{1}{2}e'_{ab}(\mathbf{x})e'_{ba}(\mathbf{x})}, \tag{38}$$

$$\delta\mu(\mathbf{x})=c_D^{(\mu)}\sqrt{\frac{1}{2}e'_{ab}(\mathbf{x})e'_{ba}(\mathbf{x})}. \tag{39}$$

The perturbation theory produces results with an accuracy of the order $(\hat{\nu}/\hat{\mu},\hat{\rho}/\hat{\mu})$, or equivalently $|\beta|/|\alpha|$. The nonlinear terms of Eqs. (38) and (39) are therefore inaccurate and a linear approximation is appropriate. As before, a coordinate system is chosen in which α takes the diagonal form. Depending on the dimension of the problem, the following is obtained:

$$\sqrt{\frac{1}{2}e'_{ab}(\mathbf{x})e'_{ba}(\mathbf{x})}\approx\frac{1}{2}[|\alpha_{11}-\alpha_{22}|+(\beta_{11}-\beta_{22})\mathrm{sgn}(\alpha_{11}-\alpha_{22})], \quad n=2. \tag{40a}$$

For $n=3$ define

$$\gamma=\sqrt{\alpha_{11}^2+\alpha_{22}^2+\alpha_{33}^2-\alpha_{22}\alpha_{33}-\alpha_{11}\alpha_{22}-\alpha_{11}\alpha_{33}};$$

then

$$\sqrt{\frac{1}{2}e'_{ab}(\mathbf{x})e'_{ba}(\mathbf{x})}\approx\frac{\gamma}{\sqrt{3}}+\frac{1}{2\sqrt{3}}\frac{\beta_{11}(2\alpha_{11}-\alpha_{22}-\alpha_{33})}{\gamma}+\frac{1}{2\sqrt{3}}\frac{\beta_{22}(-\alpha_{11}+2\alpha_{22}-\alpha_{33})+\beta_{33}(-\alpha_{11}-\alpha_{22}+2\alpha_{33})}{\gamma}. \quad (40b)$$

These formulas are obviously ill defined for isotropic loading. Averages and fluctuations can be distinguished, leading to differential equations similar to the case of the isotropic evolution rule. A two-dimensional specialization is pursued here to acquire insight into the physical properties of the solutions for persistent loading. The following four equations are obtained:

$$\delta\overline{\lambda}=\frac{1}{2}c_D^{(\lambda)}|\alpha_{11}-\alpha_{22}|,$$

$$\delta\overline{\mu}=\frac{1}{2}c_D^{(\mu)}|\alpha_{11}-\alpha_{22}|, \quad (41)$$

$$\delta\nu(\mathbf{x})=\frac{1}{2}c_D^{(\lambda)}[\beta_{11}(\mathbf{x})-\beta_{22}(\mathbf{x})]\mathrm{sgn}(\alpha_{11}-\alpha_{22}),$$

$$\delta\rho(\mathbf{x})=\frac{1}{2}c_D^{(\mu)}[\beta_{11}(\mathbf{x})-\beta_{22}(\mathbf{x})]\mathrm{sgn}(\alpha_{11}-\alpha_{22}), \quad (42)$$

where

$$\hat{\beta}_{11}-\hat{\beta}_{22}=(\alpha_{11}+\alpha_{22})\frac{(\hat{\rho}-\hat{\nu})(k_2^4-k_1^4)}{(\overline{\lambda}+2\overline{\mu})k^4}-(\alpha_{11}-\alpha_{22})\times\frac{\hat{\rho}[4\overline{\lambda}k_1^2k_2^2+\overline{\mu}(k_1^4+6k_1^2k_2^2+k_2^4)]}{\overline{\mu}(\overline{\lambda}+2\overline{\mu})k^4}. \quad (43)$$

Using once more the shorthand $\alpha_{11}=\alpha_0\delta t$, $\alpha_{22}=m\alpha_0\delta t$ and assuming that the intial state is isotropic, Eqs. (41) and (42) have solutions. These are rather more complicated in form than the equivalent solution for the isotropic evolution rule. The averages are straightforward:

$$\overline{\lambda}(t)=\overline{\lambda}(0)+\frac{1}{2}c_D^{(\lambda)}\alpha_0|1-m|t, \quad (44)$$

$$\overline{\mu}(t)=\overline{\mu}(0)+\frac{1}{2}c_D^{(\mu)}\alpha_0|1-m|t. \quad (45)$$

The solution for the fluctuations is found in the following manner. The evolution equations in the Fourier domain take the form

$$\frac{\delta\hat{\nu}(\mathbf{k})}{\delta t}=\frac{1}{2}c_D^{(\lambda)}[A_\nu(\mathbf{k},t)\hat{\nu}(\mathbf{k})+A_\rho(\mathbf{k},t)\hat{\rho}(\mathbf{k})]\alpha_0 s, \quad (46)$$

$$\frac{\delta\hat{\rho}(\mathbf{k})}{\delta t}=\frac{1}{2}c_D^{(\mu)}[A_\nu(\mathbf{k},t)\hat{\nu}(\mathbf{k})+A_\rho(\mathbf{k},t)\hat{\rho}(\mathbf{k})]\alpha_0 s, \quad (47)$$

where $s=\mathrm{sgn}(m-1)$. The solution has the form

$$\hat{\nu}(t)=\hat{\nu}(0)+e^{\eta(t,\mathbf{k})}\int_0^t G(\tau,\mathbf{k})e^{-\eta(\tau,\mathbf{k})}d\tau, \quad (48)$$

$$\hat{\rho}(t)=\hat{\rho}(0)+\frac{c_D^{(\mu)}}{c_D^{(\lambda)}}e^{\eta(t,\mathbf{k})}\int_0^t G(\tau,w)e^{-\eta(\tau,\mathbf{k})}d\tau, \quad (49)$$

with

$$G(\tau,\mathbf{k})=\frac{1}{2}c_D^{(\lambda)}\alpha_0 s[A_\nu(\tau,\mathbf{k})\hat{\nu}(0)+A_\rho(\tau,\mathbf{k})\hat{\rho}(0)], \quad (50)$$

$$\frac{\delta\eta(\tau,\mathbf{k})}{\delta\tau}=\frac{1}{2}c_D^{(\lambda)}\alpha_0 s\left(A_\nu(\tau,\mathbf{k})+\frac{c_D^{(\mu)}}{c_D^{(\lambda)}}A_\rho(\tau,\mathbf{k})\right). \quad (51)$$

While the solution for the Fourier transform of the fluctuations is given implicitly, the structure formation is dictated by the asymptotic behavior $t\to\infty$. The leading term is obviously the term $e^{\eta(t,\mathbf{k})}$ in Eqs. (48) and (49) and therefore Eq. (51) is investigated in the limit of large t. The behavior of $\eta(t,k)$ in this limit is read from the structure of $A_\nu(\tau,k)$ and $A_\rho(\tau,k)$: Eq. (48). Introducing the ratio $g=c_D^{(\mu)}/c_D^{(\lambda)}$, it is found that

$$\frac{\delta\eta(\tau,\mathbf{k})}{\delta\tau}\sim\frac{1}{\tau}\theta(\mathbf{k}), \quad (52)$$

with

$$\theta(\mathbf{k})=-\frac{\alpha_0k_1^4(2g-m-1)}{k^4(2g+1)(m-1)}+\frac{2\alpha_0k_1^2k_2^2(3g+2)}{k^4(2g+1)}+\frac{\alpha_0k_2^4(2gm-m-1)}{k^4(2g+1)(m-1)}. \quad (53)$$

Angles corresponding to maxima for positive $\theta(\mathbf{k})$ represent a concentration of the harmonic density, as well as angles corresponding to minima for negative $\theta(\mathbf{k})$. While for the case of the isotropic rule the angle of concentration always coincided with the coordinate axes, for the case considered here other angles are also possible, depending on the combination of g and m. These angles satisfy

$$\cos\phi=\pm\frac{\sqrt{g(m-3)+3m-1}}{2\sqrt{g+1}\sqrt{m-1}}. \quad (54)$$

These angles are possible when

$$\left|\frac{(g-1)(m+1)}{(m-1)(2g+1)}\right|\leqslant 1, \quad (54a)$$

while the sign of

$$S=g^2(9m^2-14m+9)+4g(m^2-4m+1)+2(m^2+1) \quad (54b)$$

determines whether $\theta(\mathbf{k})$ is positive or negative and the sign of the second derivative

$$S_2=[g(m-3)+2m][2-g(3m-1)] \tag{54c}$$

indicates a maximum when $S_2<0$ or a minimum if $S_2>0$.

When for any given m and g these angles become the directions of concentration of harmonic density, the medium is dominated by an intrinsic microstructure with preferential directions according to Eq. (54). This is a typical result of an evolution rule that depends on the local deviatoric strain. Other concentration directions may appear simultaneously and coincide with one of the coordinate axes. This completes the study of the two extreme cases of evolution rule.

IV. EFFECTS DUE TO THE FINITE CONSTITUENT SIZE

The analysis in Sec. II relies on the fact that a local stiffness can be defined. For a material consisting of finite constituents the local stiffness is derived by characterizing a small assembly of particles. Thus the stiffness is defined over a length scale of the order of the small assembly size D. Wave vectors with a magnitude greater than D^{-1} have no meaning for the problem. But there is an effect due to the residue force $\mathbf{f}_D$, which adds a contribution to the overall stiffness. This contribution is obtained in a way similar to the manner in which Eq. (13) was found and is equal to

$$-\frac{1}{4(2\pi)^n}\int d_n k\ \hat{P}_{kb}(\mathbf{k}) \times[S_{\partial B_{pqkl}/\partial x_l,(f_D)_b}(\mathbf{k})+S_{\partial B_{pqlk}/\partial x_l,(f_D)_b}(\mathbf{k})].$$

The correlation between the gradient in $\mathbf{B}$ and $\mathbf{f}_D$ manifests itself on the scale of D^{-1} in the wave-vector space. The presence of $\hat{\mathbf{P}}$, however, damps the influence of the correlation as this quantity declines rapidly with increasing $|\mathbf{k}|$.

As the harmonic density changes due to persistent (mostly deviatoric) loading, the typical dominant wave number also changes. The order of magnitude of the maximum wave number corresponds to a sphere in k space with radius D^{-1}. The whole problem must be constrained to remain within this sphere and when the dominant wave number approaches the permissible outer region certain measures must be taken.

A suitable measure for the magnitude of a component of the dominant wave number is derived from interpreting the harmonic density as a probability density function

$$\langle k_1^2\rangle=\frac{\int d_2k\ k_1^2\hat{\nu}(\mathbf{k})\hat{\nu}^*(\mathbf{k})}{\int d_2k\ \hat{\nu}(\mathbf{k})\hat{\nu}^*(\mathbf{k})}. \tag{55}$$

The value changes with time as persistent deviatoric loading takes place.

By way of example, the case of the isotropic evolution rule is considered. To ensure an analytical result, which is desirable for transparency, a special assumption is made to make the parameter M in Eq. (34) independent of the wave number. This assumption is that $c_I^{(\mu)}\hat{\nu}(0)=c_I^{(\lambda)}\hat{\rho}(0)$; then the harmonic density has the form

$$[\hat{\nu}(\mathbf{k})\hat{\nu}^*(\mathbf{k})](t)=[\hat{\nu}(\mathbf{k})\hat{\nu}^*(\mathbf{k})](0)q(t)^{a+b\ \cos^2(\phi)+c\ \sin^2(\phi)}, \tag{56}$$

where $q(0)=1$. Assuming an initial isotropic harmonic density, expression (55) is expressed in the modified Bessel functions I_0 and I_1 [35]:

$$\langle k_1^2\rangle(t)=\frac{\int dk\ k^3[\hat{\nu}(\mathbf{k})\hat{\nu}^*(\mathbf{k})](0)}{\int dk\ k[\hat{\nu}(\mathbf{k})\hat{\nu}^*(\mathbf{k})](0)} \times\left(\frac{I_1\left(\frac{1}{2}(b-c)\ln[q(t)]\right)}{2I_0\left(\frac{1}{2}(b-c)\ln[q(t)]\right)}\right)\left(\frac{1}{2}\ln[q(t)]+1\right). \tag{57}$$

It follows from the properties of the modified Bessel functions that if the 1 direction is the direction in which the harmonic density concentrates, $\langle k_1^2\rangle$ always increases with time. Therefore, there must come a point when contributions close to the sphere in k space with radius D^{-1} become important. More generally, when structure formation takes place an interaction between effects on the macroscale and those on a microscale is inevitable. Naturally, if the assumption $c_I^{(\mu)}\hat{\nu}(0)=c_I^{(\lambda)}\hat{\rho}(0)$ is not made the result will be similar, but it is not so easily expressed in analytical form.

The above is a powerful argument in favor of the study of small assemblies under intense straining conditions as well as an initial and tentative guide to the possible form any correction might have. The fact that the problem has a spherical character implies that any correction terms in the constitutive relations must be of an even power in $\mathbf{k}$, the simplest one being quadratic. This points to a second-order gradient correction term in the stress-strain relationship. A stress increment s calculated by conventional means, Eq. (1), needs to be corrected by a term proportional to $\partial^2 s_{mn}/\partial x_p\partial x_q D^2$. In k space this type of term will not be noticed, while $k^2D^2\ll 1$, in which case the theory reverts to the classical form. The correction term detects when the magnitude of the wave number approaches D^{-1}.

It is reasonable to assume that the correction term is sensitive to the directions in which the harmonic density concentrates. Calling the unit vectors of these directions $\mathbf{N}$, with a superscript to distinguish between them if there is more than one, and employing a set of geometrical tensors $\mathbf{Q}^{(i)}$, a plausible corrective term may have the form

$$s'_{ij}=\frac{\partial^2 s_{mn}}{\partial x_r\partial x_s}D^2\sum_{(p)}Q^{(p)}_{ijmn}N^{(p)}_r N^{(p)}_s. \tag{58}$$

This needs to be expressed in the displacement field. To avoid problems with objectivity (see [36]) primary variables are used, that is, the distortion and the spin tensor

$$s_{mn}=X_{mnkl}\left(\frac{\partial u_k}{\partial x_l}-k_{kl}\right), \tag{59}$$

$$X_{mnkl}+X_{mnlk}=2A_{mnkl}. \tag{60}$$

The total stress increment is

$$s_{ij}+s'_{ij}=X_{ijkl}\left(\frac{\partial u_k}{\partial x_l}-k_{kl}\right)+\frac{\partial^2 s_{mn}}{\partial x_r \partial x_s}D^2\sum_{(p)} Q^{(p)}_{ijmn}N^{(p)}_r N^{(p)}_s$$
$$=X_{ijkl}\left(\frac{\partial u_k}{\partial x_l}-k_{kl}\right)+D^2\sum_{(p)} Q^{(p)}_{ijmn}N^{(p)}_r N^{(p)}_s$$
$$\times\frac{\partial^2}{\partial x_r \partial x_s}\left[X_{mnkl}\left(\frac{\partial u_k}{\partial x_l}-k_{kl}\right)\right]. \quad (61)$$

X is defined to work on a scale greater than D and therefore the corrective term contains contributions of higher-order displacement and spin gradients only. The spin is solved from the requirement that the total stress increment is symmetric.

The form for the correction suggested here may not be the most general or even the most appropriate one, but on the basis of more specific studies [27] there is little doubt that it should contain higher-order gradients and gradients of spin tensors. Alternatively, the corrective term may be viewed as a more precise description of the forces between the particles than is achieved by an ''ordinary'' stress. The term then approximates the short-range force residue $\mathbf{f}_D$, giving a more precise description of interconstituent forces.

V. INDUCED ANISOTROPY

Persistent deviatoric loading of an initially isotropic sample will lead to overall anistropic properties, even though the constituents themselves are isotropic. The anisotropy is induced by the deviatoric character of the succession of strain increments as the fluctuation intensity of the parameters that make up the stiffness are ordered in a specific direction in k space. The most accessible parameter, illustrative of the anisotropy induction, is the difference in the 1111 and 2222 components of the overall stiffness. Equation (19) is evaluated for this purpose:

$$-\frac{1}{4}\frac{1}{(2\pi)^n}\int d_n k[S_{B_{bj11},B_{11ac}}(\mathbf{k})-S_{B_{bj22},B_{22ac}}(\mathbf{k})]$$
$$\times[\hat{H}_{acbj}(\mathbf{k})+\hat{H}_{cabj}(\mathbf{k})]$$
$$=-\frac{1}{\overline{(\lambda+2\mu)}t}\frac{1}{(2\pi)^2}\int_0^\infty dk\int_0^{2\pi} d\phi k\,\cos(2\phi)$$
$$\times[\hat{\nu}(-\mathbf{k})\hat{\rho}(\mathbf{k})+\hat{\nu}(\mathbf{k})\hat{\rho}(-\mathbf{k})+2\hat{\rho}(\mathbf{k})\hat{\rho}(-\mathbf{k})](t). \quad (62)$$

Clearly, while the distribution of the fluctuations is isotropic, Eq. (62) vanishes, but as the distribution builds up in certain directions, as explained in Sec. III, the angular integral of Eq. (62) becomes nonvanishing and anisotropy is induced.

The anisotropy so obtained is entirely due to the spatial ordering of the material under the influence of the evolution rules. Another type of anisotropy may also occur, but it has been neglected here. This type is inherent anisotropy, which may become manifest as the constituents themselves aquire anistropy due to changing local state variables. For example, if the material consists of an assembly of grains with an elastofrictional interaction contacts are lost and broken while the material is strained through a deviatoric path. The constituents of the material are small subassemblies, each consisting of a handful of grains; these subassemblies themselves become anisotropic when contacts concentrate in a particular direction. The calculus presented here can be amended to allow for such effects, but it is unlikely that this can be done under a purely analytical scheme; numerical approaches will have to be devised to estimate these phenomena.

VI. DISCUSSSION AND CONCLUSIONS

The approximation that has been made throughout is that on the basis of the first-order approximation of the strain field, sufficient information is available to estimate the extent of the local evolution of the material properties. This can obviously be refined. For persistent strain paths and constant evolution rules it is then found that structure formation and induced anisotropy become manifest, even though the constituents themselves are perfectly isotropic; the structure formation appears as a result of spatial distrubution of stiffness and not necessarily due to intrinsic anisotropy on a microlevel.

For extreme structure formation it is clear that an extension of the stress strain theory is required to stop the deformation taking place on the scale of the (rigid) constituents of the medium. In principle, the inhibition can also be phrased in terms of the evolution rules themselves, but whichever way is chosen a clear need has been identified for the investigation of small assemblies of grains in severe straining.

To compare the results reported here with other works two papers are mentioned: those of Williams and Rege [37] and Cundall [38]. These are both numerical papers, thus the methodology for solving the properties of the heterogeneous medium is entirely different from the one described above. Both papers describe the fate of a heterogeneous medium under persistent straining, with evolution rules that are similar (if not identical) to the deviatoric rule deployed here. Both papers find that coherent structures appear at high deviatoric strain, similar to the ones that are predicted by more theoretical means in the present paper, that is, structures at certain preferred angles. While a direct comparison with the present theory is difficult to carry out, the effect of spatial distribution in structures is clearly, though qualitatively, validated.

A more quantitave validation could be carried out if a numerical simulation of an assembly of particles is run and a Fourier transform of a local stiffness measure is carried out. If the interparticle force displacement is given by the tensor **K** and the center-to-center vector between neighboring grains is called **c**, then a simple measure for the stiffness A_{pqrs} representing one particle with N contacts is proportional to a symmetrized form of $\Sigma_{n=1}^{N} K^{(n)}_{pr} c^{(n)}_q c^{(n)}_s$.

The cross harmonic density of this quantity can be determined. Suppose that structure formation takes place on a linear scale of some ten particles. To evaluate the harmonic content with an accuracy of, say, 10%, 100 adjacent spatial frequency points need to be averaged (assuming that the harmonic content does not change markedly in the vicinity of the point; see [39]), requiring a linear dimension of some 1000 particles. For a three-dimensional simulation some 10^9 particles are needed and for a two-dimensional one some-

thing on the order of 10^6 particles are needed. These numbers are in line with experiments on laboratory-prepared samples of soil; Arthur [40] has shown in an experiment using an x-ray grain displacement measurement technique [41] that reproducibility in the standard deviation of the displacement is achieved for samples consisting of some 10^8 particles. This number is stress-ratio dependent though; the number quoted pertains to a value of two-thirds of the stress ratio at failure (dense sample of Leighton-Buzzard sand). For lower stress ratios it is smaller: greater than 10^4 for the stress ratio at roughly half the failure value.

The numerical tests in two dimensions by Williams and Rege [37] contain maximally 2000 particles in two dimensions and while a structure formation of some sort is observed, it is difficult to make conclusive statistical statements about it. The two-dimensional sample size that is needed is just within the reach of current simulation practice.

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