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Fluctuations and the effective moduli of an isotropic, random aggregate of identical, frictionless spheres

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Abstract

We consider a random aggregate of identical frictionless elastic spheres that has first been subjected to an isotropic compression and then sheared. We assume that the average strain provides a good description of how stress is built up in the initial isotropic compression. However, when calculating the increment in the displacement between a typical pair of contaction particles due to the shearing, we employ force equilibrium for the particles of the pair, assuming that the average strain provides a good approximation for their interactions with their neighbors. The incorporation of these additional degrees of freedom in the displacement of a typical pair relaxes the system, leading to a decrease in the effective moduli of the aggregate. The introduction of simple models for the statistics of the ordinary and conditional averages contributes an additional decrease in moduli. The resulting value of the shear modulus is in far better agreement with that measured in numerical simulations.
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1. Introduction

Digby (1981) and Walton (1987) considered a random aggregate of frictional spheres in which the distribution of contacts was isotropic. They considered a random aggregate

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of identical spheres that was first compressed by an average pressure p. They assumed that the relative displacement of the centers of two contacting particles was given by the average strain, and they obtained expressions for the effective shear modulus μ^{E} and Lamé coefficient λ^{E}. Their expressions for these moduli are

$$\mu^{\mathrm{E}} = \frac{kv}{5\pi}\,\frac{\mu}{(1-v)}\left[\frac{3\pi}{2}\,\frac{(1-v)}{vk}\,\frac{p}{\mu}\right]^{1/3}\frac{[2-v+3\alpha(1-v)]}{(2-v)} \tag{1}$$

and

$$\lambda^{\mathrm{E}} = \frac{kv}{5\pi}\,\frac{\mu}{(1-v)}\left[\frac{3\pi}{2}\,\frac{(1-v)}{vk}\,\frac{p}{\mu}\right]^{1/3}\frac{[2-v-2\alpha(1-v)]}{(2-v)}, \tag{2}$$

where k is the average number of contacts per particle (the coordination number) and v is the solid volume fraction. The parameter α describes the strength of the transverse stiffness of the grain-to-grain contact; $\alpha = 0$ is appropriate to frictionless interactions (perfect slip), whereas $\alpha = 1$ describes the fully frictional interactions (perfect stick). The effective bulk modulus, κ^{E}, and the effective Poisson ratio, v^{E}, are given in terms of these by

$$\kappa^{\mathrm{E}} \equiv \lambda^{\mathrm{E}} + \frac{2}{3}\,\mu^{\mathrm{E}} = \frac{kv}{3\pi}\,\frac{\mu}{(1-v)}\left[\frac{3\pi}{2}\,\frac{(1-v)}{vk}\,\frac{p}{\mu}\right]^{1/3} \tag{3}$$

and

$$v^{\mathrm{E}} = \frac{\lambda^{\mathrm{E}}}{2(\lambda^{\mathrm{E}} + \mu^{\mathrm{E}})}, \tag{4}$$

respectively. Note that the bulk modulus, κ^{E}, does not depend upon α because the transverse forces do not enter at all into this average strain approximation.

The effective moduli of the corresponding aggregate of frictionless spheres can be obtained simply from Eqs. (1) and (2) by setting $\alpha = 0$:

$$\mu^{\mathrm{E}} = \lambda^{\mathrm{E}} = \frac{3}{5}\,\kappa^{\mathrm{E}} = \frac{kv}{5\pi}\,\frac{\mu}{(1-v)}\left[\frac{3\pi}{2}\,\frac{(1-v)}{vk}\,\frac{p}{\mu}\right]^{1/3}. \tag{5}$$

The equality of the coefficients is consistent with Cauchy's use of the average strain assumption to obtain a single independent modulus for random arrays of grains that interact through central forces (e.g., Love, 1927, Note B).

Jenkins et al. (1989) compared the predicted values of the effective shear and bulk moduli of frictional spheres with the results of computer simulations and physical experiments on a binary mixture of glass spheres with rather large differences in diameters that were isotropically compressed to an average pressure of 138 kPa. They found that the effective shear and bulk modulus predicted by Digby (1981) and Walton (1987) were, respectively, three times and one and one-half times greater than the values measured in the experiments and the simulations. Makse et al. (1999) also compared values of the effective moduli with the results of computer simulations. For a binary mixture of frictional spheres that differed little in diameter, they found the effective shear modulus to be about two-thirds of the value predicted using the average strain assumption. They explained this difference as being due to the relaxation of the particles associated with their achieving equilibrium in the numerical simulation. More surprisingly, they found that the effective shear modulus for frictionless spheres in the simulation was less than ten per cent of the predicted effective medium value, Eq. (5). It is the central goal of the present article to understand why this is so. (By contrast the bulk modulus agreed reasonably well with Eq. (3) regardless whether there was perfect slip or perfect stick.)

Because the difficulty with the shear modulus was shown to be due to the relaxation of the particles from the average strain, we first perform the simplest investigation that allows for some relaxation. From the simulations, we know the rest positions of each of the particles, as well as the vectors between the centers. Consider a specific particle. We make the approximation that when a macroscopic strain increment is applied, the particles in contact with it move according to the average strain. Because the specific particle is not, in general, in a symmetric environment, it experiences an unbalanced force. Consequently, it will, in general, move to a position different than that expected from the average strain, in order to reduce the net force to zero. So, for the specific particle, we calculate its new position. We next calculate the energy stored within each of the contact "springs" for each of the particles in the simulation and calculate the total stored energy due to the applied strain. We set this equal to the usual expression for strain energy and deduce new estimates for the bulk and shear moduli of the aggregate. This procedure is detailed in Appendix A.

It is obvious that such a procedure can only reduce the moduli relative to those of the average strain prediction. Note that if we were to neglect the relaxation of each particle and assume each that particle sees the same coordination number, k, distributed uniformly around it, we would reproduce the average strain predictions, Eqs. (1) and (3), as detailed in Norris and Johnson (1997). We find that for a static confining pressure of 100 kPa, there is a small reduction of the bulk modulus from 223 MPa predicted by the average strain analysis to 206 MPa. There is a much larger reduction of the shear modulus from 134 to 100 MPa; however, the results of the simulations for the shear modulus give the much, much smaller value $\mu^{\mathrm{E}} = 8 \pm 3$ MPa. We see that relaxation effects at the single particle level, while significant, are by no means sufficient to explain the effect.

We are thus led to consider a more sophisticated theory in which we explicitly account for fluctuations in pairs of contacting particles. Here, we specialize specifically to the frictionless case, where the reduction in shear modulus is most dramatic and for which we can derive an analytic result using some fairly weak assumptions. We employ the relatively simple model of a static aggregate introduced by Jenkins (1997) in which the assumption that the increment in the contact displacement is given by the increment of the average strain is relaxed. Instead, the centers of a typical pair of contacting particles are assumed to be able to translate in order to equilibrate force, while their surrounding neighbors are constrained to move with the increment in the average strain. Incremental strains are employed because the contact forces are nonlinear functions of the displacement. When the equilibrium equations are phrased in terms of increments in displacements, they provide linear equations for their determination in terms of the increment in average strain. We obtain an approximate analytical solution to the equilibrium equations that determine the increments in displacements of the pair in terms of the increment of average strain. This solution contains quantities that involve the geometry and interactions of a particle with its neighbors; we provide relatively simple statistical models for the averages of these and their correlations. This permits the calculation of the increment of contact force between the pair. Summation of the increments of contact force over all pair orientations provides the relationship between the increment of stress and the increment in strain and, hence, the effective moduli. In this way, we calculate a decrease of the effective shear modulus of about seventy per cent from the value predicted by the more elementary theory.

2. Theory

We focus our attention on a pair of contacting spheres, label them A and B, and denote the vector from the center of A to the center of B by $\mathbf{d}^{(BA)}$. We write the increment $\dot{\mathbf{F}}^{(BA)}$ in the contact force exerted by particle B on particle A in terms of the increment $\dot{\mathbf{u}}^{(BA)}$ in the relative displacement of the points of contact:

$$\dot{F}_i^{(BA)} = K_{ij}^{(BA)} \dot{u}_j^{(BA)}, \tag{6}$$

where $\mathbf{K}^{(BA)}$ is the contact stiffness.

Here, we assume that the contact stiffness is given in terms of the unit vector $\hat{\mathbf{d}}^{(BA)}$ in the direction of $\mathbf{d}^{(BA)}$ by

$$K_{ij}^{(BA)} = K_N^{(BA)} \hat{d}_i^{(BA)} \hat{d}_j^{(BA)}, \tag{7}$$

where $K_N^{(BA)}$ is the normal contact stiffness, given in terms of the contact displacement $\mathbf{u}^{(BA)}$ by

$$K_N^{(BA)} = \frac{\mu d^{1/2}}{(1-\nu)} [\delta^{(BA)}]^{1/2}, \tag{8}$$

with

$$\delta^{(BA)} \equiv -\hat{d}_i^{(BA)} u_i^{(BA)}.$$

Using the Hertz contact law, the normal displacement can be related to average pressure p through the average strain assumption (Jenkins et al., 1989) by

$$\delta^{(BA)} = d \left[\frac{3\pi}{2} \frac{(1-\nu)}{\nu k} \frac{p}{\mu} \right]^{2/3}, \tag{9}$$

where d is the sphere diameter. Because computer simulations (Jenkins et al., 1989) indicate that the bulk modulus is rather well predicted by the average strain theory, we believe it appropriate to use this expression to relate the modulus K_N to the pressure p in the initial isotropic state.

The increment $\dot{\mathbf{u}}^{(BA)}$ in contact displacement may be written in terms of the increments $\dot{\mathbf{c}}^{(B)}$ and $\dot{\mathbf{c}}^{(A)}$ in the translations of the centers of the two spheres by

$$\dot{u}_i^{(BA)} = \dot{c}_i^{(B)} - \dot{c}_i^{(A)}.$$

Alternatively, the relative displacement of the two contacting points may be written in terms of the increments in the averages of quantities and their fluctuations as

$$\dot{u}_i^{(BA)} = \dot{E}_{ij} d_j^{(BA)} + \delta \dot{c}_i^{(B)} - \delta \dot{c}_i^{(A)}, \tag{10}$$

where $\dot{\mathbf{E}}$ is the increment in the average strain of the aggregate and, for example, $\delta\dot{\mathbf{c}}^{(B)}$ is the departure of the displacement of sphere B from the average strain assumption. The relative displacement can be written more compactly by introducing $\dot{\mathbf{\Delta}}^{(BA)} \equiv \delta\dot{\mathbf{c}}^{(B)} - \delta\dot{\mathbf{c}}^{(A)}$, the increment in the difference of the fluctuations in displacement.

Given $\dot{\mathbf{F}}$, the increment $\dot{\mathbf{T}}$ in the stress may be written as the average over all N particles in a region of relatively homogeneous strain as

$$\dot{T}_{ij} = \left\langle \frac{1}{V^{(A)}} \sum_{n=1}^{N^{(A)}} \dot{F}_i^{(nA)} d_j^{(nA)} \right\rangle \equiv \frac{1}{2N} \sum_{A=1}^{N} \frac{1}{V^{(A)}} \sum_{n=1}^{N^{(A)}} \dot{F}_i^{(nA)} d_j^{(nA)}, \qquad (11)$$

where $N^{(A)}$ is the number of particles in contact with particle A and $V^{(A)}$ is the volume of the Voroni polyhedron associated with particle A. A continuous form of this may be written in terms of a distribution function $f(\hat{\mathbf{d}})$, defined so that $f(\hat{\mathbf{d}})\,\mathrm{d}\Omega$ is the number of contacts in an element $\mathrm{d}\Omega$ of solid angle centered at $\hat{\mathbf{d}}$:

$$\dot{T}_{ij} = \frac{1}{2} \frac{6v}{\pi d^2} \int\!\!\int_{\Omega} f(\hat{\mathbf{d}}) \dot{F}_i(\hat{\mathbf{d}}) \hat{d}_j \, \mathrm{d}\Omega,$$

where the factor multiplying the integral is the half the number of particles per unit volume, expressed in terms of the solid volume fraction v. For an isotropic distribution of contacts, the distribution can be expressed in terms of the coordination number

$$f(\hat{\mathbf{d}}) = \frac{k}{4\pi}.$$

Given the increments $\dot{\mathbf{E}}$ in average strain, the calculation of the increment in stress requires the increment in contact force,

$$\dot{F}_i^{(BA)} = K_N^{(BA)} \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} (\dot{E}_{jm} d_m^{(BA)} + \dot{\Delta}_j^{(BA)}),$$

determined in terms of the fluctuations $\dot{\mathbf{\Delta}}$ for all pairs of particles in the region. These fluctuations can be obtained as solutions of the equations of balance of force for each of the N particles.

3. Pair fluctuations

Here, we analyze a far simpler situation in which two contacting particles, A and B, have sufficient translational freedom to satisfy force equilibrium. In order that the equilibrium equations for the two particles determine these translations, we assume that the other particles in contact with the pair translate with the average deformation.

We denote the increment in the translation of center of the nth neighbor of particle A by $\dot{\mathbf{c}}^{(n)}$. Then, as before,

$$\dot{u}_i^{(nA)} = \dot{c}_i^{(n)} - \dot{c}_i^{(A)}.$$

For $n \neq B$, only the fluctuations in the translation of particle A occur; so, for these pairs, we may write

$$\dot{c}_i^{(n)} - \dot{c}_i^{(A)} = \dot{E}_{ij} d_j^{(nA)} - \delta\dot{c}_i^{(A)} = \dot{E}_{ij} d_j^{(nA)} + \tfrac{1}{2}\dot{\Delta}_i^{(BA)} - \tfrac{1}{2}\dot{\Sigma}_j^{(BA)},$$

where $\dot{\mathbf{\Sigma}}^{(BA)} \equiv \delta\dot{\mathbf{c}}^{(B)} + \delta\dot{\mathbf{c}}^{(A)}$ is the increment in the sum of the fluctuations in displacement.

The equations of force equilibrium for particle A are, then,

$$0 = K_N^{(BA)} \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} (\dot{E}_{jk} d_k^{(BA)} + \dot{\Delta}_j^{(BA)}) + \sum_{n \neq B}^{N^{(A)}} K_N^{(nA)} \hat{d}_i^{(nA)} \hat{d}_j^{(nA)} (\dot{E}_{jk} d_k^{(nA)} + \tfrac{1}{2} \dot{\Delta}_j^{(BA)} - \tfrac{1}{2} \dot{\Sigma}_j^{(BA)}). \tag{12}$$

The corresponding equilibrium equations for particle B are obtained by interchanging A and B, keeping in mind that $\mathbf{d}^{(AB)} = -\mathbf{d}^{(BA)}$.

The equilibrium equations for the particles A and B lead to a system of equations that we use to evaluate the unknown incremental fluctuations $\dot{\Delta}^{(BA)}$ and $\dot{\Sigma}^{(BA)}$ for the pair BA. In order to phrase the equilibrium equations in terms of the neighbors of the individual particles of the pair, we write, for example,

$$\sum_{n \neq B}^{N^{(A)}} K_N^{(nA)} \hat{d}_i^{(nA)} \hat{d}_j^{(nA)} d_l^{(nA)} = \sum_{n=1}^{N^{(A)}} K_N^{(nA)} \hat{d}_i^{(nA)} \hat{d}_j^{(nA)} d_l^{(nA)} - K_N^{(BA)} \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} d_l^{(BA)}.$$

We then characterize the neighborhoods of particles A and B through the tensors

$$A_{ij}^{(BA)} \equiv \sum_{n=1}^{N^{(A)}} K_N^{(nA)} \hat{d}_i^{(nA)} \hat{d}_j^{(nA)} \quad \text{and} \quad A_{ij}^{(AB)} \equiv \sum_{n=1}^{N^{(B)}} K_N^{(nB)} \hat{d}_i^{(nB)} \hat{d}_j^{(nB)}$$

and

$$J_{ijk}^{(BA)} \equiv \sum_{n=1}^{N^{(A)}} K_N^{(nA)} \hat{d}_i^{(nA)} \hat{d}_j^{(nA)} \hat{d}_k^{(nA)} \quad \text{and} \quad J_{ijk}^{(AB)} \equiv \sum_{n=1}^{N^{(B)}} K_N^{(nB)} \hat{d}_i^{(nB)} \hat{d}_j^{(nB)} \hat{d}_k^{(nB)}.$$

The definitions of $\mathbf{A}^{(BA)}, \mathbf{A}^{(AB)}, \mathbf{J}^{(BA)}$ and $\mathbf{J}^{(AB)}$ are based on the existence of the contact between A and B and it is this that gives them their directionality.

Eq. (12) can be written in terms of these tensors as

$$dJ_{ijk}^{(BA)} \dot{E}_{jk} + \tfrac{1}{2} A_{ij}^{(BA)} (\dot{\Delta}_j^{(BA)} - \dot{\Sigma}_j^{(BA)}) + \tfrac{1}{2} K_N^{(BA)} \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} (\dot{\Delta}_j^{(BA)} + \dot{\Sigma}_j^{(BA)}) = 0.$$

Upon interchanging A and B, an equivalent expression is obtained for the force equilibrium for particle B:

$$dJ_{ijk}^{(AB)} \dot{E}_{jk} - \tfrac{1}{2} A_{ij}^{(AB)} (\dot{\Delta}_j^{(BA)} + \dot{\Sigma}_j^{(BA)}) - \tfrac{1}{2} K_N^{(BA)} \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} (\dot{\Delta}_j^{(BA)} - \dot{\Sigma}_j^{(BA)}) = 0.$$

The summations for $\mathbf{A}^{(BA)}$ and $\mathbf{A}^{(AB)}$ involve a number of contacts equal, on average, to the coordination number; so, up to an error of $1/k$, the last term in these equations may be neglected. In this case, their solution is

$$\dot{\Sigma}_i^{(BA)} = d[(A_{ij}^{(BA)})^{-1} J_{jkm}^{(BA)} + (A_{ij}^{(AB)})^{-1} J_{jkm}^{(AB)}] \dot{E}_{km} \tag{13}$$

and

$$\dot{\Delta}_i^{(BA)} = -d[(A_{ij}^{(BA)})^{-1} J_{jkm}^{(BA)} - (A_{ij}^{(AB)})^{-1} J_{jkm}^{(AB)}] \dot{E}_{km}. \tag{14}$$

Given the tensors $\mathbf{A}^{(BA)}, \mathbf{J}^{(BA)}, \mathbf{A}^{(AB)}$ and $\mathbf{J}^{(AB)}$, Eqs. (13) and (14) provide the increments in the sum and difference of the fluctuations of the pair BA in terms of the increment in average strain.

Eqs. (13) and (14) apply to each pair of contacting particles in the assembly with orientation near $\hat{\mathbf{d}}^{(BA)}$. However, detailed information regarding the tensors $\mathbf{A}^{-1}\mathbf{J}$ for each such pair is available only from the numerical simulations. Consequently, we introduce an average of such tensors. The average is taken over all pairs of particles with their orientation in an increment of solid angle centered on the unit vector that points in the direction indicated by the superscripts. For example, with $\Delta\Omega^{(BA)}$ the increment of solid angle centered on the unit vector $\hat{\mathbf{d}}^{(BA)}$:

$$\overline{(A_{ji}^{(BA)})^{-1}J_{imn}^{(BA)}} \equiv \frac{1}{M}\sum_{\mathbf{d}^{(CD)}\subset\Delta\Omega^{(BA)}} (A_{ji}^{(CD)})^{-1}\,J_{imn}^{(CD)}$$

where M is the number of pairs in the increment of solid angle.

Then, the existence of the contact between particle A and B provides a symmetry about the plane perpendicular to $\hat{\mathbf{d}}^{(BA)}$:

$$\overline{(A_{ji}^{(AB)})^{-1}J_{imn}^{(AB)}} = -\overline{(A_{ji}^{(BA)})^{-1}J_{imn}^{(BA)}}.$$

With this, the average value of the sum and difference of the fluctuations over all pairs with orientation near $\hat{\mathbf{d}}^{(BA)}$ are

$$\overline{\dot{\Sigma}_j^{(BA)}} = 0$$

and

$$\overline{\dot{\Delta}_j^{(BA)}} = -\,2d\overline{(A_{ji}^{(BA)})^{-1}J_{imn}^{(BA)}}\,\dot{E}_{mn}. \tag{15}$$

In what follows, we also employ the corresponding averages for the individual tensors

$$\overline{A_{ij}^{(BA)}} \equiv \frac{1}{M}\sum_{\mathbf{d}^{(CD)}\subset\Delta\Omega^{(BA)}} A_{ij}^{(CD)}$$

and

$$\overline{J_{ijk}^{(BA)}} \equiv \frac{1}{M}\sum_{\mathbf{d}^{(CD)}\subset\Delta\Omega^{(BA)}} J_{ijk}^{(CD)}.$$

Because of the role played by $\hat{\mathbf{d}}^{(BA)}$ in the definition of the average, $\overline{\mathbf{A}^{(AB)}} = \overline{\mathbf{A}^{(BA)}}$ and $\overline{\mathbf{J}^{(AB)}} = -\overline{\mathbf{J}^{(BA)}}$; while the average of $\mathbf{J}^{(BA)}$ over all orientations of the pair is zero.

In order to evaluate the average on the right-hand side of (15), we first express the tensors involved as the sum of an average and a fluctuation. For example,

$$A_{ij}^{(BA)} = \overline{A_{ij}^{(BA)}} + A_{ij}^{(BA)\prime}.$$

Then, in Eq. (15), we express the inverse of $\mathbf{A}^{(BA)}$ in terms of the inverse of $\overline{\mathbf{A}^{(BA)}}$ and the fluctuation $\mathbf{A}^{(BA)\prime}$ by

$$(A_{ij}^{(BA)})^{-1} = [\delta_{il} + (\overline{A_{ik}^{(BA)}})^{-1}A_{kl}^{(BA)\prime}]^{-1}(\overline{A_{lj}^{(BA)}})^{-1},$$

or, up to an error proportional to the cube of the fluctuations

$$(A_{ij}^{(BA)})^{-1} \doteq [\delta_{il} - (\overline{A_{ik}^{(BA)}})^{-1} A_{kl}^{(BA)\prime} + (\overline{A_{ik}^{(BA)}})^{-1} A_{km}^{(BA)\prime} (\overline{A_{mp}^{(BA)}})^{-1} A_{pl}^{(BA)\prime}](\overline{A_{lj}^{(BA)}})^{-1}.$$

With this,

$$\overline{A_{ji}^{(BA)-1} J_{imn}^{(BA)}} = (\overline{A_{ji}^{(BA)}})^{-1} \overline{J_{imn}^{(BA)}} - \overline{(A_{jk}^{(BA)})}^{-1} \overline{(A_{li}^{(BA)}})^{-1} \overline{A_{kl}^{(BA)\prime} J_{imn}^{(BA)\prime}} + (\overline{A_{jk}^{(BA)}})^{-1} (\overline{A_{sp}^{(BA)}})^{-1} (\overline{A_{li}^{(BA)}})^{-1} \overline{A_{ks}^{(BA)\prime} A_{pl}^{(BA)\prime}}\, \overline{J_{imn}^{(BA)}}. \tag{16}$$

We next introduce simple assumptions regarding the distribution of contacts and calculate these averages.

4. Averages

We introduce an orthogonal Cartesian system with its center coincident with the center of the sphere A and characterize a typical contact vector α through its equatorial and polar angles ϕ and θ: $\alpha = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$.

In calculating the tensors $\overline{\mathbf{A}^{(BA)}}$ and $\overline{\mathbf{J}^{(BA)}}$, we replace the summation over the discrete contacts of a particle by integration over a contact distribution function $g^{(BA)}(\alpha)$, defined so that $g^{(BA)}(\alpha)\,\mathrm{d}\Omega$ is the number of contacts in an element of solid angle $\mathrm{d}\Omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$ centered at α, given that there is a contact at $\hat{\mathbf{d}}^{(BA)}$ along the polar axis. Then, for example,

$$\overline{A_{ij}^{(BA)}} = K_N \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} + K_N \int_{\Omega_\alpha} g(\alpha)\, \alpha_i \alpha_j \,\mathrm{d}\Omega_\alpha,$$

where the integration is over all solid angle Ω_α consistent with the presence of particle B. The first term is associated with the presence of this contact. We assume that the distribution is uniform in the upper and lower hemispheres. That is, in the upper hemisphere, there are, on average, $k/2 - 1$ contacting particles uniformly distributed over the orientations not excluded by the solid angle of π associated with particle B at the pole; while there are, on average, $k/2$ contacting particles uniformly distributed over the lower hemisphere. Then

$$g(\alpha) = \begin{cases} 0, & 0 \leqslant \theta_\alpha \leqslant \dfrac{\pi}{3}, \\ \dfrac{(k-2)}{2\pi}, & \dfrac{\pi}{3} \leqslant \theta_\alpha \leqslant \dfrac{\pi}{2}, \\ \dfrac{k}{4\pi}, & \dfrac{\pi}{2} \leqslant \theta_\alpha \leqslant \pi \end{cases}$$

and

$$\overline{A_{ij}^{(BA)}} = K_N \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} + K_N \left[\int_0^{2\pi} \int_{\frac{\pi}{3}}^{\frac{\pi}{2}} \frac{k-2}{2\pi} \alpha_i \alpha_j \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi + \int_0^{2\pi} \int_{\frac{\pi}{2}}^{\pi} \frac{k}{4\pi} \alpha_i \alpha_j \sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi \right].$$

It is a straightforward calculation to determine that

$$\overline{A_{ij}^{(BA)}} \equiv K_N(\alpha_1 \delta_{ij} + \alpha_2 \hat{d}_i^{(BA)} \hat{d}_j^{(BA)}), \tag{17}$$

where $\alpha_1 = (19k - 22)/48$ and $\alpha_2 = (22 - 3k)/16$.

In a similar way, we determine that

$$\overline{J_{ijk}^{(BA)}} \equiv K_N[\omega_1 \hat{d}_i^{(BA)} \hat{d}_j^{(BA)} \hat{d}_k^{(BA)} + \omega_2(\delta_{ik} \hat{d}_j^{(BA)} + \delta_{ij} \hat{d}_k^{(BA)} + \delta_{kj} \hat{d}_i^{(BA)})], \tag{18}$$

where $\omega_1 = (166 - 11k)/128$ and $\omega_2 = -(k + 14)/128$.

For simplicity, we approximate the tensor $\overline{\mathbf{A}^{(BA)}}$ by its isotropic part

$$\overline{A_{ij}^{(BA)}} = \psi K_N \delta_{ij},$$

where $\psi = k/3$. Then its inverse is simply

$$\overline{A_{ij}^{(BA)}}^{-1} = (\psi K_N)^{-1} \delta_{ij}. \tag{19}$$

With this, the terms in Eq. (16) that remain to be evaluated are $\overline{\mathbf{A}^{(BA)\prime}\mathbf{J}^{(BA)\prime}}$ and $\overline{\mathbf{A}^{(BA)\prime}\mathbf{A}^{(BA)\prime}}$

Now, by definition,

$$\overline{A_{ji}^{(BA)\prime} J_{imn}^{(BA)\prime}} = \overline{A_{ji}^{(BA)} J_{imn}^{(BA)}} - \overline{A_{ji}^{(BA)}}\, \overline{J_{imn}^{(BA)}}.$$

In order to calculate $\overline{\mathbf{A}^{(BA)}\mathbf{J}^{(BA)}}$ we introduce the joint probability density function $F(\alpha, \beta)$, defined so that $F(\alpha, \beta)\mathrm{d}\Omega_\alpha \, \mathrm{d}\Omega_\beta$ is the fraction of contacts with α in $\mathrm{d}\Omega_\alpha$ and β in $\mathrm{d}\Omega_\beta$, given that there is the contact at $\hat{\mathbf{d}}^{(BA)}$, including the possibility that the two directions can coincide. Then

$$\overline{A_{ji}^{(BA)} J_{imn}^{(BA)}} = K_N^2 \hat{d}_j^{(BA)} \hat{d}_m^{(BA)} \hat{d}_n^{(BA)} + K_N^2 \hat{d}_i^{(BA)} \hat{d}_m^{(BA)} \hat{d}_n^{(BA)} \int_{\Omega_\beta} g(\beta) \, \beta_j \beta_i \, \mathrm{d}\Omega_\beta + K_N^2 \hat{d}_j^{(BA)} \hat{d}_i^{(BA)} \int_{\Omega_\alpha} g(\alpha) \, \alpha_i \alpha_m \alpha_n \, \mathrm{d}\Omega_\alpha + K_N^2 \int_{\Omega_\beta} \int_{\Omega_\alpha} F(\alpha, \beta) \beta_j \beta_i \alpha_i \alpha_m \alpha_n \, \mathrm{d}\Omega_\alpha \, \mathrm{d}\Omega_\beta,$$

where the integrals are taken over all solid angles consistent with the presence of particle B. Then

$$\overline{A_{ji}^{(BA)\prime} J_{imn}^{(BA)\prime}} = K_N^2 \int_{\Omega_\beta} \int_{\Omega_\alpha} F(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n \,\mathrm{d}\Omega_\alpha \,\mathrm{d}\Omega_\beta - K_N^2 \int_{\Omega_\beta} g(\beta)\,\beta_j\beta_i \,\mathrm{d}\Omega \int_{\Omega_\alpha} g(\alpha)\,\alpha_i\alpha_m\alpha_n \,\mathrm{d}\Omega, \tag{20}$$

in which the contributions associated with the presence of the contact at $\hat{\mathbf{d}}^{(BA)}$ have canceled.

The unconditional averages are

$$\int_{\Omega_\beta} g(\beta)\,\beta_j\beta_i \,\mathrm{d}\Omega = \alpha_1\delta_{ji} + \widetilde{\alpha}_2 \hat{d}_j^{(BA)}\hat{d}_i^{(BA)},$$

where α_1 has been defined in Eq. (17) and $\widetilde{\alpha}_2 = (18-9k)/48$, and

$$\int_{\Omega_\beta} g(\alpha)\,\alpha_i\alpha_m\alpha_n \,\mathrm{d}\Omega_\beta = \widetilde{\omega}_1 \hat{d}_i^{(BA)}\hat{d}_m^{(BA)}\hat{d}_n^{(BA)} - \omega_2(\delta_{im}\hat{d}_n^{(BA)} + \delta_{mn}\hat{d}_i^{(BA)} + \delta_{ni}\hat{d}_m^{(BA)}), \tag{21}$$

where $\widetilde{\omega}_1 = (38-11k)/128$ and ω_2 is defined in Eq. (18).

The joint probability density can be expressed as the product of the simple probability $g(\beta)$ and the conditional joint probability $h_{\alpha\,|\,\beta}(\alpha,\beta)$, defined so that $h_{\alpha\,|\,\beta}(\alpha,\beta)\,\mathrm{d}\Omega_\alpha$ is the fraction of contacts with α in $\mathrm{d}\Omega_\alpha$, given that β is in $\mathrm{d}\Omega_\beta$:

$$F(\alpha,\beta) = g(\beta)\,h_{\alpha\,|\,\beta}(\alpha,\beta).$$

Here $h_{\alpha\,|\,\beta}(\alpha,\beta)$ includes the possibility that α equals β. We take this possibility into account explicitly and introduce the conditional probability $z_{\alpha\,|\,\beta}(\alpha,\beta)\,\mathrm{d}\Omega_\alpha$ that expresses the fraction of contacts at α in $\mathrm{d}\Omega_\alpha$, given that β is in $\mathrm{d}\Omega_\beta$ with $\alpha \neq \beta$. Then

$$\int_{\Omega_\beta}\int_{\Omega_\alpha} F(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n \,\mathrm{d}\Omega_\alpha \,\mathrm{d}\Omega_\beta = \int_{\Omega_\beta} g(\beta)\,\beta_j\beta_m\beta_n \,\mathrm{d}\Omega_\beta + \int_{\Omega_\beta}\int_{\Omega_\alpha} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n \,\mathrm{d}\Omega_\alpha \,\mathrm{d}\Omega_\beta. \tag{22}$$

The conditional probability $z_{\alpha\,|\,\beta}(\alpha,\beta)$ is not uniform; it depends on the locations of spheres at β and $\hat{\mathbf{d}}^{(BA)}$.

From the above results, we have

$$\overline{A_{js}^{(BA)\prime} A_{sl}^{(BA)\prime}} = K_N^2 \int_{\Omega_\beta}\int_{\Omega_\alpha} F(\alpha,\beta)\beta_j\beta_s\alpha_s\alpha_l \,\mathrm{d}\Omega_\beta \,\mathrm{d}\Omega_\alpha - K_N^2 \int_{\Omega_\beta} g(\beta)\,\beta_j\beta_s \,\mathrm{d}\Omega \int_{\Omega_\alpha} g(\alpha)\,\alpha_s\alpha_l \,\mathrm{d}\Omega, \tag{23}$$

with

$$\int_{\Omega_\beta}\int_{\Omega_\alpha} F(\alpha,\beta)\beta_j\beta_s\alpha_s\alpha_l\,\mathrm{d}\Omega\,\mathrm{d}\Omega$$
$$=\int_{\Omega_\beta} g(\beta)\,\beta_j\beta_l\,\mathrm{d}\Omega+\int_{\Omega_\beta}\int_{\Omega_\alpha} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_s\alpha_s\alpha_l\,\mathrm{d}\Omega_\beta\,\mathrm{d}\Omega_\alpha. \tag{24}$$

The integrals in Eqs. (22) and (24) that involve the conditional probability are complicated because the limits of integration for θ_α and ϕ_α can depend upon θ_β and ϕ_β. We illustrate this in the calculation of $\overline{\mathbf{A}^{(BA)\prime}\mathbf{J}^{(BA)\prime}}$ with the order of integration taken to be $\mathrm{d}\phi_\alpha, \mathrm{d}\phi_\beta, \mathrm{d}\theta_\alpha, \mathrm{d}\theta_\beta$. Then

$$\int_{\Omega_\beta}\int_{\Omega_\alpha} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta$$
$$=\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\theta_\beta+\frac{\pi}{3}}\int_0^{2\pi}\int_{\Phi+\phi_\beta}^{2\pi-\Phi+\phi_\beta} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta$$
$$+\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}\int_0^{2\pi}\int_0^{2\pi} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta$$
$$+\int_{\frac{2\pi}{3}}^{\pi}\int_{\frac{\pi}{3}}^{\theta_\beta-\frac{\pi}{3}}\int_0^{2\pi}\int_0^{2\pi} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta$$
$$+\int_{\frac{2\pi}{3}}^{\pi}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{5\pi}{3}-\theta_\beta}\int_0^{2\pi}\int_{\Phi+\phi_\beta}^{2\pi-\Phi+\phi_\beta} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta. \tag{25}$$

The angle $\Phi(\theta_\alpha,\theta_\beta)$ follows from the fact that the arc on the unit sphere that links the centers of the spheres at α and β has length $d(\alpha,\beta)=\cos^{-1}(\alpha\cdot\beta)$. When α is taken to be in the x–z plane, $\phi_\alpha=0$ and $\phi_\beta=\Phi$; then, because the spheres are in contact, $d=\pi/3$ and

$$\Phi=\arccos\left(\frac{1-2\cos\theta_\alpha\cos\theta_\beta}{2\sin\theta_\alpha\sin\theta_\beta}\right).$$

The distribution function $z_{\alpha\,|\,\beta}(\alpha,\beta)$ is determined over the range of polar angles in each of these integrals in Appendix B. Then, in Appendix C, it is used to complete the calculation of $\overline{\mathbf{A}^{(BA)\prime}\mathbf{J}^{(BA)\prime}}$ and $\overline{\mathbf{A}^{(BA)\prime}\mathbf{A}^{(BA)\prime}}$.

The final results, obtained in Appendix C, are

$$\overline{A_{ji}^{(BA)\prime}J_{imn}^{(BA)\prime}}=K_N^2[S_{jmn}^{(BA)}-\omega_2\alpha_1(\delta_{jm}\hat{d}_n^{(BA)}+\delta_{nj}\hat{d}_m^{(BA)})-(\omega_2\widetilde{\alpha}_2+\omega_2\alpha_1)\,\delta_{nm}\hat{d}_j^{(BA)}$$
$$-(\alpha_1\widetilde{\omega}_1+\widetilde{\omega}_1\widetilde{\alpha}_2+2\omega_2\widetilde{\alpha}_2)\,\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}] \tag{26}$$

and

$$\overline{A_{js}^{(BA)\prime}A_{sl}^{(BA)\prime}}=K_N^2[H_{jl}^{(BA)}-\alpha_1^2\delta_{jl}-(2\alpha_1\widetilde{\alpha}_2+\widetilde{\alpha}_2^2)\,\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}], \tag{27}$$

where $\mathbf{S}^{(BA)}$ and $\mathbf{H}^{(BA)}$ are given as functions of k and $\mathbf{d}^{(BA)}$ in Eqs. (C.5) and (C.6), respectively, of Appendix C.

Eqs. (26) and (27) may be written more compactly as

$$\overline{A_{ji}^{(BA)\prime}J_{imn}^{(BA)\prime}} = K_N^2[\kappa_1\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)} + \kappa_2(\delta_{jm}\hat{d}_n^{(BA)} + \delta_{nj}\hat{d}_m^{(BA)}) + \kappa_3\delta_{nm}\hat{d}_j^{(BA)}] \tag{28}$$

and

$$\overline{A_{js}^{(BA)\prime}A_{sl}^{(BA)\prime}} = K_N^2(\eta_1\delta_{jl} + \eta_2\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}), \tag{29}$$

where, with the information provided, the coefficients κ and η may be expressed as functions of k; they are evaluated for a specific value of k in Appendix C. Then, the last term of Eq. (16) is

$$(\overline{A_{jk}^{(BA)}})^{-1}(\overline{A_{sp}^{(BA)}})^{-1}(\overline{A_{li}^{(BA)}})^{-1}\overline{A_{ks}^{(BA)\prime}A_{pl}^{(BA)\prime}}\,\overline{J_{imn}^{(BA)}} = \psi^{-3}[\xi_1\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}\hat{d}_m^{(BA)} + \xi_2(\delta_{jm}\hat{d}_n^{(BA)} + \delta_{jn}\hat{d}_m^{(BA)}) + \xi_3\delta_{nm}\hat{d}_j^{(BA)}], \tag{30}$$

where $\xi_1 \equiv (\eta_1\omega_1 + \eta_2\omega_1 + 2\eta_2\omega_2)$, $\xi_2 \equiv \eta_1\omega_2$, and $\xi_3 \equiv (\eta_2\omega_2 + \eta_1\omega_2)$, with the coefficients η and ω defined in Eqs. (29) and (18), respectively.

5. Effective moduli

We use Eqs. (6), (7), and (10) to write the increment in contact force as

$$\overline{\dot{F}_i^{(BA)}} = K_N^{(BA)}\hat{d}_i^{(BA)}\hat{d}_j^{(BA)}(\dot{E}_{jm}d_m^{(BA)} + \overline{\dot{\Delta}_j^{(BA)}}),$$

where K_N is given by Eqs. (8) and (9) and

$$\begin{aligned}\overline{\dot{\Delta}_j^{(BA)}} &= -2\,\overline{A_{ji}^{(BA)-1}J_{imn}^{(BA)}}\,\dot{E}_{mn}\\ &= -2\{\psi^{-1}[\omega_1\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}\hat{d}_m^{(BA)} + \omega_2(\delta_{jm}\hat{d}_n^{(BA)} + \delta_{jn}\hat{d}_m^{(BA)}) + \omega_2\delta_{nm}\hat{d}_j^{(BA)}]\\ &\quad - \psi^{-2}[\kappa_1\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}\hat{d}_m^{(BA)} + \kappa_2(\delta_{jm}\hat{d}_n^{(BA)} + \delta_{jn}\hat{d}_m^{(BA)}) + \kappa_3\delta_{nm}\hat{d}_j^{(BA)}]\\ &\quad + \psi^{-3}[\xi_1\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}\hat{d}_m^{(BA)} + \xi_2(\delta_{jm}\hat{d}_n^{(BA)} + \delta_{jn}\hat{d}_m^{(BA)}) + \xi_3\delta_{nm}\hat{d}_j^{(BA)}]\}\dot{E}_{mn}.\end{aligned}$$

With the increment contact force known, the increment in stress,

$$\dot{T}_{ij} = \frac{3v}{\pi d^2}\frac{k}{4\pi}\int_\Omega \overline{\dot{F}_i^{(BA)}}\,\hat{d}_j^{(BA)}\,\mathrm{d}\Omega,$$

may be calculated, making use of the identities

$$\int_\Omega \hat{d}_i^{(BA)}\hat{d}_j^{(BA)}\,\mathrm{d}\Omega = \frac{4\pi}{3}\delta_{ij}$$

and

$$\int_{\Omega_i} \hat{d}_i^{(BA)}\hat{d}_j^{(BA)}\hat{d}_k^{(BA)}\hat{d}_l^{(BA)}\,\mathrm{d}\Omega = \frac{4\pi}{15}(\delta_{ij}\delta_{kl} + \delta_{jl}\delta_{ik} + \delta_{il}\delta_{jk}).$$

Therefore, the incremental response of an isotropic, random aggregate of identical frictionless spheres is given by

$$\begin{aligned}\dot{T}_{ij} = \frac{vkK_N}{5\pi d}\{&2[1 - 2\psi^{-1}(\omega_1 + 2\omega_2) + 2\psi^{-2}(\kappa_1 + 2\kappa_2) - 2\psi^{-3}(\xi_1 + 2\xi_2)]\dot{E}_{ij}\\ &+[1 - 2\psi^{-1}(\omega_1 + 2\omega_2) - 10\psi^{-1}\omega_2 + 2\psi^{-2}(\kappa_1 + 2\kappa_2) + 10\psi^{-2}\kappa_3\\ &-2\psi^{-3}(\xi_1 + 2\xi_2) - 10\psi^{-3}\xi_3]\dot{E}_{kk}\delta_{ij}\}.\end{aligned}$$

From this, the effective moduli are

$$\mu^{\mathrm{E}} = \frac{kv}{5\pi d}K_N\{1 - 2[\psi^{-1}(\omega_1 + 2\omega_2) - \psi^{-2}(\kappa_1 + 2\kappa_2) + \psi^{-3}(\xi_1 + 2\xi_2)]\} \tag{31}$$

and

$$\begin{aligned}\lambda^{\mathrm{E}} = \frac{kv}{5\pi d}K_N[&1 - 2\psi^{-1}(\omega_1 + 7\omega_2) + 2\psi^{-2}(\kappa_1 + 2\kappa_2 + 5\kappa_3)\\ &- 2\psi^{-3}(\xi_1 + 2\xi_2 + 5\xi_3)],\end{aligned} \tag{32}$$

where, we recall that $\psi = k/3$ and the coefficients κ, ω, and ξ are defined in Eqs. (28), (18), and (30), respectively. The dependence of the effective moduli on the pressure occurs only through K_N and k, the other coefficients are functions only of the geometry. A dependence on $p^{1/3}$ enters through K_N.

6. Comparisons

We compare the results of computer simulations with the predictions of the model. The numerical simulations were carried out using the code TRUBAL developed by Cundall (1988). Each simulation employed spheres of two different radii: $R_1 = 0.105 \times 10^{-3}$ m and $R_2 = 0.095 \times 10^{-3}$ m in equal numbers. The shear modulus of the material of the spheres was $\mu = 2.9 \times 10^{10}$ Pa and the Poisson ratio was $v = 0.2$. This simulation employed a system of 10,000 spheres. The initial state was obtained in the manner described by Makse et al. (1999). An initial random aggregate of frictionless spheres without contacts was homogeneously and isotropically contracted, bringing the spheres into contact, until a pressure p of 100×10^3 Pa was reached. In this state, $k = 6.067$ and $v = 0.637$.

The numerical results for the shear and bulk moduli were

$$\mu^{\mathrm{E}} = 8 \text{ MPa and } \kappa^{\mathrm{E}} = 200 \text{ MPa}.$$

The predictions are based on identical spheres made of the same material with the average diameter $d = 0.1995 \times 10^{-3}$ m in an initial state with the same coordination number, volume fraction, and confining pressure. Then, from Eqs. (8) and (9), we first calculate the average normal stiffness:

$$K_N = 1.08 \times 10^5 \text{ Pa m}.$$

In this case, the effective moduli calculated from the average strain assumption are

$$\mu^{\mathrm{E}} = \lambda^{\mathrm{E}} = 134 \text{ MPa}$$

and

$$\kappa^{\mathrm{E}} = \lambda^{\mathrm{E}} + \frac{2}{3}\mu^{\mathrm{E}} = \frac{5}{3}\mu^{\mathrm{E}} = 223 \text{ MPa}.$$

On the other hand, the effective moduli determined from Eqs. (31) and (32) are

$$\mu^{\mathrm{E}} = \frac{kv}{5\pi d} K_N(1 - 0.69) = 41 \text{ MPa}$$

and

$$\lambda^{\mathrm{E}} = \frac{kv}{5\pi d} K_N(1 + 0.57) = 208 \text{ MPa};$$

so, the bulk modulus is

$$\kappa^{\mathrm{E}} = 235 \text{ MPa}.$$

The predicted value of the effective shear modulus is about 70% less than that resulting from the average strain assumption. This is encouraging. The increase in the bulk modulus over that based on the average strain assumption can be reversed by incorporating the anisotropic part of $\overline{(\mathbf{A}^{(BA)})^{-1}}$ into the calculation.

7. Conclusion

We have considered a random aggregate of identical, frictionless, elastic spheres subjected to an initial confining pressure followed by a general increment in strain. We have incorporated the deviation from the average of the difference in the displacement of a typical pair of particles into the contact force. We then determined the approximate value of this fluctuation in terms of statistical measures of the geometry of the packing and the contact stiffnesses using force equilibrium in a way suggested by Jenkins (1997). We then made simple but plausible assumptions regarding the form of the simple and conditional probabilities that determined the geometry of the packing and used these to carry out the averages. Of particular interest was the quantity $\overline{(\mathbf{A}^{(BA)})^{-1}\mathbf{J}^{(BA)}}$. This involved the product of averages and the average of the product of fluctuations. We found that the product of the averages provides 46% of the reduction of the shear modulus and the average of the product provides the remaining 24%. Other sources of a reduction in moduli were not considered.

For example, Trentadue (2001), apparently following Jenkins (1997), carries out a similar calculation of the bulk and shear moduli for elastic, frictional spheres and includes a reduction in moduli due to fluctuations during the initial isotropic compression and a reduction due to the retention of the anisotropic part of $\overline{(\mathbf{A}^{(BA)})^{-1}}$. On the other hand, he does not include a contribution from the product of the averages. Our experience with the computer simulations indicates that the reduction of the shear modulus associated with the former two contributions are relatively small, but that associated with the latter is significant.

Independently, Paine (1997) introduced fluctuations in displacement and used the equilibrium equations to determine them in terms of the packing and stiffness. She then employed computer simulations, measured the statistical distributions, and calculated the reduction of the bulk modulus.

We believe that the correct modeling of the statistical distributions is crucial to the prediction of the mechanical behavior of granular materials. In our modeling, we have assumed them to be the most homogeneous possible. This assumption is plausible and seems to be effective. We have focused on frictionless particles in an isotropic compressed state, because, for frictionless particles, the difference in the values of the shear modulus based on the average strain assumption and those measured in the numerical simulation is very large. Consequently, this material provides a good test of any improved theory. We believe that we have incorporated the essential features of the correct distributions into such a theory and have established an appropriate basis for the extension of the theory to frictional particles and more complicated states of stress.

Finally, it is natural to question why the average strain assumption provides a relative good approximation to the bulk modulus and a relatively poor approximation to the shear modulus. An indication of why this is so can be obtained by considering a behavior of a simple model neighborhood of the sphere A in which sphere B is on the polar axis in the upper hemisphere and three other spheres in the lower hemisphere are distributed symmetrically about the polar axis at an angle $\phi = \cos^{-1}(1/3)$ below the equator. Then, when this neighborhood is subjected to a isotropic compression, the relative displacement of the particles A and B is given by the average strain and there is no fluctuation. However, when the neighborhood is subjected to a deviatoric strain, there must be a deviation from the displacements associated with the average strain, whose direction and magnitude varies with the orientation of the neighborhood with respect to the principal axes of the strain, in order for the pair to be in equilibrium. That is, a typical neighborhood is closer to being equilibrated by a average isotropic strain than by an average deviatoric strain.

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Appendix A. Single particle relaxation

Consider a specific particle, labelled A, which we take to be centered at the origin. It has contacts with particles centered at $\mathbf{d}^{(nA)}$, $n = 1, 2, \ldots, N^{(A)}$. Assuming that one of the particle centers is displaced by an increment $\dot{\mathbf{u}}^{(nA)}$ the form of Eq. (6) is

$$\dot{F}_i^{(nA)} = K_N(\hat{d}_k^{(nA)} \dot{u}_k^{(nA)})\, \hat{d}_i^{(nA)}, \tag{A.1}$$

where K_N is given by

$$K_N = \frac{\mu d^{1/2}}{1-\nu}\,\delta^{1/2}$$

with δ given by Eq. (9).

As written, the total force on the specific particle, due to the sum of all the incremental contact forces is not zero:

$$\dot{F}_i^{(A)} \equiv \sum_{n=1}^{N^{(A)}} \dot{F}_i^{(nA)} \neq 0.$$

Accordingly, that particle will move to a new incremental position, $\dot{\mathbf{X}}^{(A)}$. The generalization of Eq. (A.1) that takes into account the new position and orientation is

$$\dot{F}_i^{(nA)} = K_N[\hat{d}_k^{(nA)}(\dot{u}_k^{(nA)} - \dot{X}_k^{(A)})]\hat{d}_i^{(nA)}.$$

Now, the requirement that the particle is in equilibrium with its contact forces gives three linear equations in the three unknowns $\dot{\mathbf{X}}^{(A)}$. It is straightforward to solve these equations numerically.

Having determined the new equilibrium position and orientation, one can show that the total increment in work done by the increment in contact forces on particle A is simply

$$\dot{W}^{(A)} = \frac{1}{2}\left[K_N \sum_{n=1}^{N^{(A)}} (\hat{d}_i^{(nA)}\dot{u}_i^{(nA)})^2 - \dot{F}_i^{(A)}\dot{X}_i^{(A)}\right], \tag{A.2}$$

where $\mathbf{X}^{(A)}$ is determined as described above. In order to calculate $\dot{W}^{(A)}$ we make the average strain assumption that the displacement at the contact point is simply related to the macroscopic strain

$$\dot{u}_i^{(nA)} = \dot{E}_{ij} d_j^{(nA)}. \tag{A.3}$$

Because we know the exact positions of each center, $\mathbf{d}^{(nA)}$, from the simulations, we are able to evaluate Eq. (A.2) for each particle in the ensemble.

We now evaluate the elastic moduli by setting the total deformation in the contacts equal to the macroscopic strain energy

$$\frac{1}{V}\sum_{A=1}^{N} \dot{W}^{(A)} = \frac{1}{2}\left[\left(\bar{\kappa} - \frac{2}{3}\,\bar{\mu}\right)(\dot{E}_{ll})^2 + 2\bar{\mu}\dot{E}_{ij}\dot{E}_{ij}\right], \tag{A.4}$$

where the sum is taken over all particles in the computational unit cell of volume V. The left-hand side of Eq. (A.4) can be evaluated once for a pure compression and once for a simple shear in order to deduce the values of $\bar{\kappa}$ and $\bar{\mu}$. The point of the exercise is to investigate the extent to which relaxation, at the single particle level, can explain the large reduction of the shear modulus relative to the prediction of the average strain approximation.

If, in Eqs. (A.2) and (A.3), we assume there is no relaxation ($\dot{\mathbf{X}}^{(A)} = \mathbf{0}$), and if we replace the sum over contacts by an integral over a presumed uniform distribution of contact directions, we reproduce the average strain theory, Eqs. (1) and (2), as detailed in Norris and Johnson (1997).

Appendix B. $z_{\alpha\,|\,\beta}(\alpha, \beta)$

Here, we determine the appropriate form of the distribution function $z_{\alpha\,|\,\beta}(\alpha,\beta)$ for the intervals of polar angles θ_α and θ_β indicated in Eq. (25), given that particle B is on the pole. We assume that the distribution $z_{\alpha\,|\,\beta}(\alpha,\beta)$ is independent of the circumferential angle ϕ_α and that there are the same number of α contacts in each infinitesimal circumferential strip about the pole whether or not the particle β intrudes on the strip. This is the simplest kind of homogeneity that applies in this case.

We first consider the range of polar angles in the first integral:

$$\pi/3 \leqslant \theta_\beta \leqslant 2\pi/3 \quad \text{and} \quad \pi/3 \leqslant \theta_\alpha \leqslant \theta_\beta + \pi/3.$$

In the subinterval $\pi/3 \leqslant \theta_\beta \leqslant \pi/2$, $g(\beta)=[(k/2)-1]/\pi=(k-2)/2\pi$. For $\pi/3 \leqslant \theta_\alpha \leqslant \pi/2$, the expected average number of α particles in the upper hemisphere, given the presence of β there, is $(k/2)-2$, so

$$\frac{k-4}{2} = \int_{\frac{\pi}{3}}^{\frac{\pi}{2}} \int_{\Phi(\theta_\alpha)}^{2\pi-\Phi(\theta_\alpha)} z_{\alpha\,|\,\beta}(\alpha,\beta)\sin\theta_\alpha\,\mathrm{d}\phi_\alpha\,\mathrm{d}\theta_\alpha$$

$$= 2\int_{\frac{\pi}{3}}^{\frac{\pi}{2}} z_{\alpha\,|\,\beta}(\theta_\alpha)\,[\pi-\Phi(\theta_\alpha)]\sin\theta_\alpha\,\mathrm{d}\theta_\alpha.$$

If $z_{\alpha\,|\,\beta}(\theta_\alpha)[\pi-\Phi(\theta_\alpha)]$ is to be constant, then

$$z_{\alpha\,|\,\beta}(\alpha,\beta) = \frac{k-4}{2(\pi-\Phi)}.$$

When $\pi/2 \leqslant \theta_\alpha \leqslant \theta_\beta + \pi/3$, the average number k_1 of α particles in this strip, given the presence of β in the upper hemisphere, is obtained from the proportion

$$k/2 : 2\pi = k_1 : \int_0^{2\pi} \int_{\frac{\pi}{2}}^{\theta_\beta+\frac{\pi}{3}} \sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\phi_\alpha$$

as

$$k_1 = -\frac{k}{2}\cos\left(\theta_\beta + \frac{\pi}{3}\right).$$

Then

$$-\frac{k}{2}\cos\left(\theta_\beta+\frac{\pi}{3}\right) = \int_{\frac{\pi}{2}}^{\theta_\beta+\frac{\pi}{3}} \int_{\Phi(\theta_\alpha)}^{2\pi-\Phi(\theta_\alpha)} z_{\alpha\,|\,\beta}(\alpha,\beta)\sin\theta_\alpha\,\mathrm{d}\phi_\alpha\,\mathrm{d}\theta_\alpha$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta) = \frac{k}{4(\pi-\Phi)}.$$

In the subinterval $\pi/2 \leqslant \theta_\beta \leqslant 2\pi/3$, $g(\beta) = (k/2)/2\pi = k/4\pi$. For $\pi/3 \leqslant \theta_\alpha \leqslant \pi/2$, the average number of α particles in the upper hemisphere, given the presence β in the lower hemisphere, is $(k/2)-1$, so

$$\frac{k-2}{2}=\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}\int_{\Phi(\theta_\alpha)}^{2\pi-\Phi(\theta_\alpha)} z_{\alpha\,|\,\beta}(\alpha,\beta)\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\phi_\alpha$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta)=\frac{k-2}{2(\pi-\Phi)}.$$

For $\pi/2\leqslant\theta_\alpha\leqslant 2\pi/3$, the average number of α particles in this strip is $(k/4)-1$, so

$$\frac{k-4}{4}=\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\Phi(\theta_\alpha)}^{2\pi-\Phi(\theta_\alpha)} z_{\alpha\,|\,\beta}(\alpha,\beta)\sin\theta_\alpha\,\mathrm{d}\phi_\alpha\,\mathrm{d}\theta_\alpha$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta)=\frac{k-4}{2(\pi-\Phi)}.$$

Finally, for $2\pi/3\leqslant\theta_\alpha\leqslant\theta_\beta+\pi/3$,

$$k/2:2\pi=k_2:\int_0^{2\pi}\int_{\frac{2\pi}{3}}^{\theta_\beta+\frac{\pi}{3}}\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\phi_\alpha,$$

so

$$k_2=-\frac{k}{2}\left[\cos\left(\theta_\beta+\frac{\pi}{3}\right)+\frac{1}{2}\right],$$

$$-\frac{k}{2}\left[\cos\left(\theta_\beta+\frac{\pi}{3}\right)+\frac{1}{2}\right]=\int_{\frac{2\pi}{3}}^{\theta_\beta+\frac{\pi}{3}}\int_{\Phi(\theta_\alpha)}^{2\pi-\Phi(\theta_\alpha)} z_{\alpha\,|\,\beta}(\alpha,\beta)\sin\theta_\alpha\,\mathrm{d}\phi_\alpha\,\mathrm{d}\theta_\alpha$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta)=\frac{k}{4(\pi-\Phi)}.$$

The range of polar angles in second integral is

$$\pi/3\leqslant\theta_\beta\leqslant 2\pi/3\quad\text{and}\quad\theta_\beta+\pi/3\leqslant\theta_\alpha\leqslant\pi.$$

In the subinterval $\pi/3\leqslant\theta_\beta\leqslant\pi/2$, $g(\beta)=(k-2)/2\pi$; and in the subinterval $\pi/2\leqslant\theta_\beta\leqslant 2\pi/3$, $g(\beta)=k/4\pi$. For $\theta_\beta+\pi/3\leqslant\theta_\alpha\leqslant\pi$, given β in the first subinterval, the average number k_3 of α particles in the strip is determined by

$$k/2:2\pi=k_3:\int_0^{2\pi}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\phi_\alpha$$

as

$$k_3=\frac{k}{2}\left[1+\cos\left(\theta_\beta+\frac{\pi}{3}\right)\right].$$

Then

$$\frac{k}{2}\left[1+\cos\left(\theta_\beta+\frac{\pi}{3}\right)\right]=\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}\int_0^{2\pi} z_{\alpha\,|\,\beta}(\alpha,\beta)\sin\theta_\alpha\,\mathrm{d}\phi_\alpha\,\mathrm{d}\theta_\alpha$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta) = \frac{k}{4\pi}.$$

Then for $\theta_\beta + \pi/3 \leqslant \theta_\alpha \leqslant \pi$ and β in the second subinterval, the distribution function is the same.

The range of polar angles in third integral is

$$2\pi/3 \leqslant \theta_\beta \leqslant \pi \quad \text{and} \quad \pi/3 \leqslant \theta_\alpha \leqslant \theta_\beta - \pi/3.$$

In the subinterval $2\pi/3 \leqslant \theta_\beta \leqslant 5\pi/6$, $g(\beta) = k/4\pi$ and the average number k_4 of α particles in the strip $\pi/3 \leqslant \theta_\alpha \leqslant \theta_\beta - \pi/3$ is determined by

$$(k-2)/2 : \pi = k_4 : \int_0^{2\pi} \int_{\frac{\pi}{3}}^{\theta_\beta - \frac{\pi}{3}} \sin\theta_\alpha \, \mathrm{d}\theta_\alpha \, \mathrm{d}\phi_\alpha$$

as

$$k_4 = (k-2)\left[\frac{1}{2} - \cos\left(\theta_\beta - \frac{\pi}{3}\right)\right].$$

Then

$$(k-2)\left[\frac{1}{2} - \cos\left(\theta_\beta - \frac{\pi}{3}\right)\right] = \int_{\frac{\pi}{3}}^{\theta_\beta - \frac{\pi}{3}} \int_0^{2\pi} z_{\alpha\,|\,\beta}(\alpha,\beta) \sin\theta_\alpha \, \mathrm{d}\phi_\alpha \, \mathrm{d}\theta_\alpha,$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta) = \frac{(k-2)}{2\pi}.$$

In the subinterval $5\pi/6 \leqslant \theta_\beta \leqslant \pi$, $g(\beta){=}k/4\pi$. For $\pi/3 \leqslant \theta_\alpha \leqslant \pi/2$, the average number of α particles in the upper hemisphere, given the presence of β in the lower hemisphere, is $(k/2) - 1$, so

$$z_{\alpha\,|\,\beta}(\alpha,\beta) = \frac{(k-2)}{2\pi}.$$

For $\pi/2 \leqslant \theta_\alpha \leqslant \theta_\beta - \pi/3$, the average number k_5 of α particles in the strip is determined by

$$k/2 : 2\pi = k_5 : \int_0^{2\pi} \int_{\frac{\pi}{2}}^{\theta_\beta - \frac{\pi}{3}} \sin\theta_\alpha \, \mathrm{d}\theta_\alpha \, \mathrm{d}\phi_\alpha$$

as

$$k_5 = -\frac{k}{2}\cos\left(\theta_\beta - \frac{\pi}{3}\right).$$

Then

$$-\frac{k}{2}\cos\left(\theta_\beta - \frac{\pi}{3}\right) = \int_{\frac{\pi}{2}}^{\theta_\beta - \frac{\pi}{3}} \int_0^{2\pi} z_{\alpha\,|\,\beta}(\alpha,\beta) \sin\theta_\alpha \, \mathrm{d}\phi_\alpha \, \mathrm{d}\theta_\alpha$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta) = \frac{k}{4\pi}.$$

The range of polar angles in the fourth integral is

$$2\pi/3 \leqslant \theta_\beta \leqslant \pi \quad \text{and} \quad \theta_\beta - \pi/3 \leqslant \theta_\alpha \leqslant 5\pi/3 - \theta_\beta,$$

where $g(\beta) = k/4\pi$. In the subinterval $\theta_\beta - \pi/3 \leqslant \theta_\alpha \leqslant \pi/2$, with $2\pi/3 \leqslant \theta_\beta \leqslant 5\pi/6$,

$$(k-2)/2 : \pi = k_6 : \int_0^{2\pi} \int_{\theta_\beta - \frac{\pi}{3}}^{\frac{\pi}{2}} \sin\theta_\alpha \, \mathrm{d}\theta_\alpha \, \mathrm{d}\phi_\alpha,$$

$$k_6 = (k-2)\cos\left(\theta_\beta - \frac{\pi}{3}\right);$$

so

$$(k-2)\cos\left(\theta_\beta - \frac{\pi}{3}\right) = \int_{\theta_\beta - \frac{\pi}{3}}^{\frac{\pi}{2}} \int_{\Phi(\theta_\alpha)}^{2\pi - \Phi(\theta_\alpha)} z_{\alpha\,|\,\beta}(\alpha,\beta) \sin\theta_\alpha \, \mathrm{d}\phi_\alpha \, \mathrm{d}\theta_\alpha$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta) = \frac{k-2}{2(\pi - \Phi)}.$$

Similarly, from

$$k/2 : 2\pi = k_7 : \int_0^{2\pi} \int_{\frac{\pi}{2}}^{\frac{5\pi}{3} - \theta_\beta} \sin\theta_\alpha \, \mathrm{d}\theta_\alpha \, \mathrm{d}\phi_\alpha,$$

$$k_7 = -\frac{k}{2}\cos\left(\frac{5\pi}{3} - \theta_\beta\right);$$

so

$$k_7 = \int_{\frac{\pi}{2}}^{5\pi/3 - \theta_\beta} \int_{\Phi(\theta_\alpha)}^{2\pi - \Phi(\theta_\alpha)} z_{\alpha\,|\,\beta}(\alpha,\beta) \sin\theta_\alpha \, \mathrm{d}\phi_\alpha \, \mathrm{d}\theta_\alpha$$

and

$$z_{\alpha\,|\,\beta}(\alpha,\beta) = \frac{k}{4(\pi - \Phi)}.$$

Finally, for $\theta_\beta - \pi/3 \leqslant \theta_\alpha \leqslant 5\pi/3 - \theta_\beta$, with $5\pi/6 \leqslant \theta_\beta \leqslant \pi$, the distribution function is the same.

Appendix C. Details of the calculation

C.1. $\overline{\mathbf{A}^{(BA)\prime}\mathbf{J}^{(BA)\prime}}$

We consider first the integrals in Eq. (25) in which the limits of the integration over ϕ_α depend upon Φ and define

$$Q_{jmn}^{(BA)} \equiv \int_0^{2\pi} \beta_j \beta_i \, \mathrm{d}\phi_\beta \int_{\Phi + \phi_\beta}^{2\pi - \Phi + \phi_\beta} \alpha_i \alpha_m \alpha_n \, \mathrm{d}\phi_\alpha.$$

When expressed in terms of the angles, this is

$$
\begin{aligned}
Q^{(BA)}_{jmn} = {} & \pi[2(\pi-\Phi)\sin^2\theta_\alpha\cos\theta_\alpha\cos^2\theta_\beta - \sin\Phi\sin 2\theta_\beta\sin^3\theta_\alpha]\,\delta_{mn}\hat{d}^{(BA)}_j \\
& + \frac{\pi}{2}[2(\pi-\Phi)\sin^2\theta_\alpha\cos\theta_\alpha\sin^2\theta_\beta - \sin 2\Phi\sin^2\theta_\alpha\cos\theta_\alpha\sin^2\theta_\beta \\
& -2\sin\Phi\sin\theta_\alpha\cos^2\theta_\alpha\sin 2\theta_\beta](\delta_{mj}\hat{d}^{(BA)}_n + \delta_{jn}\hat{d}^{(BA)}_m) \\
& + \frac{\pi}{2}[4\sin\Phi\sin\theta_\beta\cos\theta_\beta\sin^3\theta_\alpha + 8(\pi-\Phi)\cos^3\theta_\alpha\cos^2\theta_\beta \\
& -4(\pi-\Phi)\sin^2\theta_\alpha\cos\theta_\alpha + 2\sin 2\Phi\sin^2\theta_\alpha\cos\theta_\alpha\sin^2\theta_\beta]\,\hat{d}^{(BA)}_m\hat{d}^{(BA)}_j\hat{d}^{(BA)}_n.
\end{aligned}
$$

With this, the integral

$$
R^{(BA)}_{jmn} \equiv \int_{\Omega_\beta}\int_{\Omega_\alpha} g(\beta)\, z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta
$$

in Eq. (25) can be written as

$$
\begin{aligned}
R^{(BA)}_{jmn} = {} & \int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\theta_\beta+\frac{\pi}{3}} g(\beta)\, z_{\alpha\,|\,\beta}(\alpha,\beta)\, Q^{(BA)}_{jmn}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha \\
& + \int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}\int_0^{2\pi}\int_0^{2\pi} g(\beta) z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta \\
& + \int_{\frac{2\pi}{3}}^{\pi}\int_{\frac{\pi}{3}}^{\theta_\beta-\frac{\pi}{3}}\int_0^{2\pi}\int_0^{2\pi} g(\beta)\, z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta \\
& + \int_{\frac{2\pi}{3}}^{\pi}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{5\pi}{3}-\theta_\beta} g(\beta)\, z_{\alpha\,|\,\beta}(\alpha,\beta) Q^{(BA)}_{jmn}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha,
\end{aligned}
$$

We use the appropriate distribution function for each range of variation of the polar angles and distinguish the integrals that involve $\mathbf{Q}^{(BA)}$ from those not.

Then, for example,

$$
\begin{aligned}
& \int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\theta_\beta+\frac{\pi}{3}} g(\beta)\, z_{\alpha\,|\,\beta}(\alpha,\beta)\, Q^{(BA)}_{jmn}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha, \\
& = \frac{(k-2)}{4\pi}(k-4)\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}\int_{\frac{\pi}{3}}^{\frac{\pi}{2}} \frac{Q^{(BA)}_{jmn}}{(\pi-\Phi)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha \\
& \quad + \frac{(k-2)}{8\pi}k\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}\int_{\frac{\pi}{2}}^{\theta_\beta+\frac{\pi}{3}} \frac{Q^{(BA)}_{jmn}}{(\pi-\Phi)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha
\end{aligned}
$$

$$+\frac{k}{8\pi}(k-2)\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}\frac{Q_{jmn}^{(BA)}}{(\pi-\Phi)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$+\frac{k}{16\pi}(k-4)\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\frac{Q_{jmn}^{(BA)}}{(\pi-\Phi)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$+\frac{k^2}{16\pi}\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\frac{2\pi}{3}}^{\theta_\beta+\frac{\pi}{3}}\frac{Q_{jmn}^{(BA)}}{(\pi-\Phi)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha.$$

Upon evaluation the integrals over θ_β and θ_α numerically, we obtain

$$\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\theta_\beta+\frac{\pi}{3}} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\,Q_{jmn}^{(BA)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$=\left[-\,0.13\,\frac{(k-2)}{4\pi}(k-4)+0.57\,\frac{k(k-2)}{8\pi}-0.38\,\frac{k(k-2)}{8\pi}\right.$$

$$\left.+0.13\,\frac{k}{16\pi}(k-4)+0.19\,\frac{k^2}{16\pi}\right]\hat{d}_n^{(BA)}\,\hat{d}_j^{(BA)}\,\hat{d}_m^{(BA)}$$

$$+\left[0.11\,\frac{(k-2)}{4\pi}(k-4)-0.23\,\frac{(k-2)}{8\pi}k+0.13\,\frac{k}{8\pi}(k-2)\right.$$

$$\left.-0.11\,\frac{k}{16\pi}(k-4)-\,0.11\,\frac{k^2}{16\pi}\right](\delta_{mj}\hat{d}_n^{(BA)}+\delta_{jn}\hat{d}_m^{(BA)})$$

$$+\left[-\,0.11\,\frac{(k-2)}{4\pi}(k-4)-0.16\,\frac{(k-2)}{8\pi}k+0.14\,\frac{k}{8\pi}(k-2)\right.$$

$$\left.+0.11\,\frac{k}{16\pi}(k-4)+0.01\,\frac{k^2}{16\pi}\right]\delta_{mn}\,\hat{d}_j^{(BA)}$$

In the same way,

$$\int_{\frac{2\pi}{3}}^{\pi}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{5\pi}{3}-\theta_\beta} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\,Q_{jmn}^{(BA)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\,\theta_\alpha$$

$$=\frac{k(k-2)}{8\pi}\int_{\frac{2\pi}{3}}^{\frac{5\pi}{6}}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{\pi}{2}}\frac{Q_{jmn}^{(BA)}}{(\pi-\Phi)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$+\frac{k^2}{16\pi}\int_{\frac{2\pi}{3}}^{\frac{5\pi}{6}}\int_{\frac{\pi}{2}}^{\frac{5\pi}{3}-\theta_\beta}\frac{Q_{jmn}^{(BA)}}{(\pi-\Phi)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$+\frac{k^2}{16\pi}\int_{\frac{5\pi}{6}}^{\pi}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{5\pi}{3}-\theta_\beta}\frac{Q_{jmn}^{(BA)}}{(\pi-\Phi)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$=\frac{k(k-2)}{8\pi}[-0.15\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}+0.03(\delta_{mj}\hat{d}_n^{(BA)}+\delta_{jn}\hat{d}_m^{(BA)})$$

$$+0.10\delta_{mn}\hat{d}_j^{(BA)}]+\frac{k^2}{16\pi}(-0.23\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}-0.05\delta_{mn}\hat{d}_j^{(BA)}).$$

In the integrals that are independent of Φ, we can easily carry out the integration of

$$P_{jmn}^{(BA)}\equiv\frac{1}{2\pi}\int_0^{2\pi}\beta_j\beta_i\,\mathrm{d}\phi_\beta\,\frac{1}{2\pi}\int_0^{2\pi}\alpha_i\alpha_m\alpha_n\,\mathrm{d}\phi_\alpha,$$

$$P_{jmn}^{(BA)}=\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}[\cos^2\theta_\beta(\cos^3\theta_\alpha-\tfrac{3}{2}\cos\theta_\alpha\sin^2\theta_\alpha)$$

$$-\tfrac{1}{2}\sin^2\theta_\beta\cos\theta_\alpha\sin^2\theta_\alpha+\cos^2\theta_\beta\cos\theta_\alpha\sin^2\theta_\alpha]$$

$$+\tfrac{1}{2}\cos^2\theta_\beta\cos\theta_\alpha\sin^2\theta_\alpha\,\hat{d}_j^{(BA)}\delta_{mn}$$

$$+\tfrac{1}{4}\sin^2\theta_\beta\cos\theta_\alpha\sin^2\theta_\alpha(\delta_{jm}\hat{d}_n^{(BA)}+\delta_{nj}\hat{d}_m^{(BA)}).$$

With this,

$$\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}\int_0^{2\pi}\int_0^{2\pi}g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta$$

$$=\frac{k(k-2)}{2}\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}P_{jmn}^{(BA)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\beta$$

$$+\frac{k^2}{4}\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}P_{jmn}^{(BA)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$=\frac{k(k-2)}{8\pi}[0.10\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}-0.09(\delta_{jm}\hat{d}_n^{(BA)}+\delta_{jn}\hat{d}_m^{(BA)})-0.03\hat{d}_j^{(BA)}\delta_{mn}]$$

$$+\frac{k^2}{16\pi}[0.03\hat{d}_i^{(BA)}\hat{d}_j^{(BA)}\hat{d}_p^{(BA)}-0.01(\delta_{ji}\hat{d}_p^{(BA)}+\delta_{ip}\hat{d}_j^{(BA)})]$$

and

$$\int_{\frac{2\pi}{3}}^{\pi}\int_{\frac{\pi}{3}}^{\theta_\beta-\frac{\pi}{3}}\int_0^{2\pi}\int_0^{2\pi}g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta$$

$$=\frac{k(k-2)}{2}\int_{\frac{2\pi}{3}}^{\frac{5\pi}{6}}\int_{\frac{\pi}{3}}^{\theta_\beta-\frac{\pi}{3}}P_{jmn}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$
\begin{aligned}
&+\frac{k(k-2)}{2}\int_{\frac{5\pi}{6}}^{\pi}\int_{\frac{\pi}{3}}^{\frac{\pi}{2}} P_{jmn}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha\\
&+\frac{k^2}{4}\int_{\frac{5\pi}{6}}^{\pi}\int_{\frac{\pi}{2}}^{\theta_\beta-\frac{\pi}{3}} P_{jmn}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha\\
=&\frac{k(k-2)}{8\pi}[-0.12\,\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}+0.03(\delta_{jm}\hat{d}_n^{(BA)}+\delta_{jn}\hat{d}_m^{(BA)})\\
&+0.08\,\hat{d}_j^{(BA)}\delta_{mn}]\\
&+\frac{k(k-2)}{8\pi}[-0.07\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}+0.01(\delta_{jm}\hat{d}_n^{(BA)}+\delta_{jn}\hat{d}_m^{(BA)})\\
&+0.08\hat{d}_j^{(BA)}\delta_{mn}]\\
&+\frac{k^2}{16\pi}(0.02\,\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}-0.02\,\hat{d}_j^{(BA)}\delta_{mn}).
\end{aligned}
$$

Then

$$
\begin{aligned}
16\pi R_{jmn}^{(BA)}=&-[0.52(k-2)(k-4)+0.10k(k-2)\\
&-0.13k(k-4)-0.01k^2]\hat{d}_j^{(BA)}\hat{d}_m^{(BA)}\hat{d}_n^{(BA)}\\
&+[0.44(k-2)(k-4)-0.24k(k-2)\\
&-0.11k(k-4)-0.14k^2](\delta_{jm}\hat{d}_n^{(BA)}+\delta_{nj}\hat{d}_m^{(BA)})\\
&-[0.44(k-2)(k-4)-0.42k(k-2)\\
&-0.11k(k-4)+0.04k^2]\delta_{mn}\hat{d}_j^{(BA)}.
\end{aligned}
\tag{C.1}
$$

Finally, we write the first integral in Eq. (20) as

$$
\begin{aligned}
S_{jmn}^{(BA)}\equiv&\int_{\Omega_\beta}\int_{\Omega_\alpha}F(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_m\alpha_n\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta\\
=&\,\widetilde{\omega}_1\hat{d}_j^{(BA)}\hat{d}_m^{(BA)}\hat{d}_n^{(BA)}+\omega_2(\delta_{jm}\hat{d}_n^{(BA)}+\delta_{nj}\hat{d}_m^{(BA)})+\omega_2\delta_{mn}\hat{d}_j^{(BA)}+R_{jmn}^{(BA)}.
\end{aligned}
\tag{C.2}
$$

C.2. $\overline{\mathbf{A}^{(BA)\prime}\mathbf{A}^{(BA)\prime}}$

For the calculation of $\overline{A_{js}^{(BA)\prime}A_{sl}^{(BA)\prime}}$ we introduce the integral

$$
F_{jl}\equiv\int_0^{2\pi}\beta_j\beta_s\,\mathrm{d}\phi_\beta\int_{\Phi+\phi_\beta}^{2\pi-\Phi+\phi_\beta}\alpha_s\alpha_l\,\mathrm{d}\phi_\alpha.
$$

When expressed in terms of the angles,

$$
\begin{aligned}
F_{jl} = &-\frac{\pi}{2}[\sin 2\Phi \sin^2\theta_\alpha \sin^2\theta_\beta + \sin\Phi \sin 2\theta_\alpha \sin 2\theta_\beta \\
&-2(\pi-\Phi)\sin^2\theta_\alpha \sin^2\theta_\beta]\delta_{jl} \\
&+\frac{\pi}{2}[\sin 2\Phi \sin^2\theta_\alpha \sin^2\theta_\beta - \sin\Phi \sin 2\theta_\alpha \sin 2\theta_\beta \\
&-2(\pi-\Phi)\sin^2\theta_\alpha \sin^2\theta_\beta + 8(\pi-\Phi)\cos^2\theta_\alpha \cos^2\theta_\beta]\hat{d}_j\hat{d}_l
\end{aligned}
$$

With this, the integral

$$
Y_{jl}^{(BA)} \equiv \int_{\Omega_\beta}\int_{\Omega_\alpha} F_{jl}^{(BA)} g(\beta) z_{\alpha\mid\beta}(\alpha,\beta)\beta_j\beta_s\alpha_s\alpha_m \,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta
$$

in Eq. (25) can be written as

$$
\begin{aligned}
Y_{jl}^{(BA)} = &\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\theta_\beta+\frac{\pi}{3}} F_{jl}^{(BA)} g(\beta)\, z_{\alpha\mid\beta}(\alpha,\beta)\sin\theta_\alpha \sin\theta_\beta \,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha \\
&+\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}\int_0^{2\pi}\int_0^{2\pi} g(\beta)\, z_{\alpha\mid\beta}(\alpha,\beta)\beta_j\beta_s\alpha_s\alpha_l \,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta \\
&+\int_{\frac{2\pi}{3}}^{\pi}\int_{\frac{\pi}{3}}^{\theta_\beta-\frac{\pi}{3}}\int_0^{2\pi}\int_0^{2\pi} g(\beta)\, z_{\alpha\mid\beta}(\alpha,\beta)\beta_j\beta_s\alpha_s\alpha_l \,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta \\
&+\int_{\frac{2\pi}{3}}^{\pi}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{5\pi}{3}-\theta_\beta} F_{jl}^{(BA)} g(\beta)\, z_{\alpha\mid\beta}(\alpha,\beta)\sin\theta_\alpha \sin\theta_\beta \,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha.
\end{aligned}
$$

Then, for example, the first integral is

$$
\begin{aligned}
&\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\theta_\beta+\frac{\pi}{3}} g(\beta)\, z_{\alpha\mid\beta}(\alpha,\beta) F_{jl}^{(BA)} \sin\theta_\alpha \sin\theta_\beta \,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha \\
&= \frac{(k-2)}{4\pi}(k-4)\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}\int_{\frac{\pi}{3}}^{\frac{\pi}{2}} \frac{F_{jl}^{(BA)}}{(\pi-\Phi)}\sin\theta_\beta \sin\theta_\alpha \,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha \\
&+\frac{(k-2)}{8\pi}k\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}\int_{\frac{\pi}{2}}^{\theta_\beta+\frac{\pi}{3}} \frac{F_{jl}^{(BA)}}{(\pi-\Phi)}\sin\theta_\beta \sin\theta_\alpha \,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha \\
&+\frac{k}{8\pi}(k-2)\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\frac{\pi}{2}} \frac{F_{jl}^{(BA)}}{(\pi-\Phi)}\sin\theta_\beta \sin\theta_\alpha \,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha
\end{aligned}
$$

$$+\frac{k}{16\pi}(k-4)\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\frac{F_{jl}^{(BA)}}{(\pi-\Phi)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$+\frac{k^2}{16\pi}\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\frac{2\pi}{3}}^{\theta_\beta+\frac{\pi}{3}}\frac{F_{jl}^{(BA)}}{(\pi-\Phi)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha.$$

Upon evaluating the integrals over θ_α and θ_β numerically, we obtain

$$\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\frac{\pi}{3}}^{\theta_\beta+\frac{\pi}{3}} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)F_{jl}^{(BA)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$

$$=\frac{(k-2)}{4\pi}(k-4)(0.49\delta_{jl}-0.54\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})$$

$$+\frac{(k-2)}{8\pi}k(0.71\delta_{jl}-0.59\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})$$

$$+\frac{k}{8\pi}(k-2)(0.55\delta_{jl}-0.47\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})$$

$$+\frac{k}{16\pi}(k-4)(0.49\delta_{jl}-0.54\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})$$

$$+\frac{k^2}{16\pi}(0.17\delta_{jl}-0.16\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}).$$

Similarly, for the second integral,

$$\int_{\frac{2\pi}{3}}^{\pi}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{5\pi}{3}-\theta_\beta} g(\beta)\,z_{\alpha\,|\,\beta}(\alpha,\beta)\,F_{jl}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\theta_\beta$$

$$=\frac{k(k-2)}{8\pi}\int_{\frac{2\pi}{3}}^{\frac{5\pi}{6}}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{\pi}{2}}\frac{F_{jl}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\theta_\beta}{(\pi-\Phi)}$$

$$+\frac{k^2}{16\pi}\int_{\frac{2\pi}{3}}^{\frac{5\pi}{6}}\int_{\frac{\pi}{2}}^{\frac{5\pi}{3}-\theta_\beta}\frac{F_{jl}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\theta_\beta}{(\pi-\Phi)}$$

$$+\frac{k^2}{16\pi}\int_{\frac{5\pi}{6}}^{\pi}\int_{\theta_\beta-\frac{\pi}{3}}^{\frac{5\pi}{3}-\theta_\beta}\frac{F_{jl}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\theta_\beta}{(\pi-\Phi)}$$

$$=\frac{k(k-2)}{8\pi}(0.16\,\delta_{jl}-0.12\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})$$

$$+\frac{k^2}{16\pi}(0.14\,\delta_{jl}+0.08\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})$$
$$-\frac{k^2}{16\pi}(0.01\,\delta_{jl}-0.14\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}).$$

In order to calculate the last two integrals, we first introduce

$$C_{jl}^{(BA)}\equiv\frac{1}{2\pi}\int_0^{2\pi}\beta_j\beta_s\,\mathrm{d}\phi_\beta\,\frac{1}{2\pi}\int_0^{2\pi}\alpha_s\alpha_l\,\mathrm{d}\phi_\alpha$$
$$=\frac{1}{4}\sin^2\theta_\beta\sin^2\theta_\alpha\delta_{jl}+\left(\cos^2\theta_\beta\cos^2\theta_\alpha-\frac{1}{4}\sin^2\theta_\beta\sin^2\theta_\alpha\right)\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}.$$

Then,

$$\int_{\frac{\pi}{3}}^{\frac{2\pi}{3}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}\int_0^{2\pi}\int_0^{2\pi}g(\beta)z_{\alpha\,|\,\beta}(\alpha,\beta)\beta_j\beta_s\alpha_s\alpha_l\,\mathrm{d}\Omega_\alpha\,\mathrm{d}\Omega_\beta$$
$$=\frac{k(k-2)}{2}\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}C_{jl}^{(BA)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\beta$$
$$+\frac{k^2}{4}\int_{\frac{\pi}{2}}^{\frac{2\pi}{3}}\int_{\theta_\beta+\frac{\pi}{3}}^{\pi}C_{jl}^{(BA)}\sin\theta_\alpha\sin\theta_\beta\,\mathrm{d}\theta_\beta\,\mathrm{d}\theta_\alpha$$
$$=\frac{k(k-2)}{8\pi}(0.12\,\delta_{jl}+0.01\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})+\frac{k^2}{16\pi}\,0.01\delta_{jl}.$$

and

$$\int_{\frac{2\pi}{3}}^{\pi}\int_{\frac{\pi}{3}}^{\theta_\beta-\frac{\pi}{3}}g(\beta)z_{\alpha\,|\,\beta}(\alpha,\beta)C_{jl}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\theta_\beta$$
$$=\frac{k(k-2)}{2}\int_{\frac{2\pi}{3}}^{\frac{5\pi}{6}}\int_{\frac{\pi}{3}}^{\theta_\beta-\frac{\pi}{3}}C_{jl}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\theta_\alpha$$
$$+\frac{k(k-2)}{2}\int_{\frac{5\pi}{6}}^{\pi}\int_{\frac{\pi}{3}}^{\frac{\pi}{2}}C_{jl}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\theta_\beta$$
$$+\frac{k^2}{4}\int_{\frac{5\pi}{6}}^{\pi}\int_{\frac{\pi}{2}}^{\theta_\beta-\frac{\pi}{3}}C_{jl}^{(BA)}\sin\theta_\beta\sin\theta_\alpha\,\mathrm{d}\theta_\alpha\,\mathrm{d}\theta_\beta$$
$$=\frac{k(k-2)}{8\pi}(0.09\delta_{jl}-0.02\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})$$
$$+\frac{k(k-2)}{8\pi}(0.02\delta_{jl}+0.04\hat{d}_j^{(BA)}\hat{d}_l^{(BA)})+\frac{k^2}{16\pi}\,0.01\delta_{jl}.$$

So,

$$16\pi Y_{jl}^{(BA)} = [1.96(k-2)(k-4) + 3.30k(k-2) + 0.49k(k-4) + 0.32k^2]\delta_{jl} - [2.16(k-2)(k-4) + 2.30k(k-2) + 0.54k(k-4) - 0.06k^2]\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}. \tag{C.3}$$

Finally, we write the first integral in Eq. (23) as

$$H_{jl}^{(BA)} = \int_{\Omega_\beta}\int_{\Omega_\alpha} F(\alpha,\beta)\beta_j\beta_i\alpha_i\alpha_l \,d\Omega_\alpha\, d\Omega_\beta = Y_{jl}^{(BA)} + \alpha_1\delta_{jl} + \widetilde{\alpha}_2\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}. \tag{C.4}$$

C.3. Final evaluation

In order to compare the values of the elastic moduli obtained by numerical simulation with what predicted by the theory, we have to evaluate all the previous quantities. These are functions of the coordination number, which is assumed to be $k = 6.07$. Therefore, with Eq. (C.1), we can write

$$R_{jmn}^{(BA)} = \chi_1\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)} + \chi_2(\delta_{mj}\hat{d}_n^{(BA)} + \delta_{jn}\hat{d}_m^{(BA)}) + \chi_3\delta_{mn}\hat{d}_j^{(BA)},$$

where $\chi_1 = -0.10$, $\chi_2 = -0.17$, and $\chi_3 = 0.13$ and, with, Eq. (C.3)

$$Y_{jl}^{(BA)} = \rho_1\delta_{jl} + \rho_2\hat{d}_j^{(BA)}\hat{d}_l^{(BA)},$$

where $\rho_1 = 2.31$ and $\rho_2 = -1.58$.

We can also evaluate all of the coefficients involved in the tensor formulas introduced earlier. So we have $\alpha_1 = 1.94$, $\alpha_2 = 0.24$, $\omega_1 = 0.78$, $\omega_2 = -0.16$, $\psi = 2.02$, $\widetilde{\alpha}_2 = -0.76$, and $\widetilde{\omega}_1 = -0.22$.

Using Eqs. (C.2), (C.1), and (21), we derive

$$S_{jmn}^{(BA)} = a_1\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)} + a_2(\delta_{mj}\hat{d}_n^{(BA)} + \delta_{jn}\hat{d}_m^{(BA)}) + a_3\delta_{mn}\hat{d}_j^{(BA)}, \tag{C.5}$$

where $a_1 = -0.32$, $a_2 = -0.33$, and $a_3 = -0.03$ and

$$H_{jl}^{(BA)} = b_1\delta_{jl} + b_2\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}, \tag{C.6}$$

where $b_1 = 4.25$ and $b_2 = -2.34$. Then, from Eq. (26),

$$\overline{A_{ji}^{(BA)\prime}J_{imn}^{(BA)\prime}} = K_N^2[\kappa_1\hat{d}_m^{(BA)}\hat{d}_j^{(BA)}\hat{d}_n^{(BA)} + \kappa_2(\delta_{jm}\hat{d}_n^{(BA)} + \delta_{nj}\hat{d}_m^{(BA)}) + \kappa_3\delta_{nm}\hat{d}_j^{(BA)}],$$

where $\kappa_1 = -0.31$, $\kappa_2 = -0.02$, and $\kappa_3 = 0.15$. This permits the calculation of the second term in Eq. (16). In a similar way, from Eq. (27),

$$\overline{A_{js}^{(BA)\prime}A_{sl}^{(BA)\prime}} = K_N^2(\eta_1\delta_{jl} + \eta_2\hat{d}_j^{(BA)}\hat{d}_l^{(BA)}),$$

where $\eta = 0.49$ and $\eta_2 = 0.03$. Then, with this and Eq. (18), the last term in Eq. (16) is

$$(\overline{A_{jk}^{(BA)}})^{-1}(\overline{A_{sp}^{(BA)}})^{-1}(\overline{A_{li}^{(BA)}})^{-1}\overline{A_{ks}^{(BA)\prime}A_{pl}^{(BA)\prime}}\,\overline{J_{imn}^{(BA)}} = \psi^{-3}[\xi_1\hat{d}_j^{(BA)}\hat{d}_n^{(BA)}\hat{d}_m^{(BA)} + \xi_2(\delta_{jm}\hat{d}_n^{(BA)} + \delta_{jn}\hat{d}_m^{(BA)}) + \xi_3\delta_{nm}\hat{d}_j^{(BA)}],$$

where $\xi_1 = 0.40$, $\xi_2 = -0.08$, and $\xi_3 = -0.08$. Finally, the first term in Eq. (16) is the simple average

$$\overline{(A_{ji}^{(BA)})^{-1}}\,\overline{J_{imn}^{(BA)}} = \psi^{-1}[\omega_1 \hat{d}_j^{(BA)} \hat{d}_m^{(BA)} \hat{d}_n^{(BA)} + \omega_2(\delta_{jn}\hat{d}_m^{(BA)} + \delta_{jm}\hat{d}_n^{(BA)} + \delta_{nm}\hat{d}_j^{(BA)})]$$

that follows from Eqs. (19) and (18).

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