Supplement for Quantifying Interparticle Forces and Heterogeneity in 3D Granular Materials

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OPTIMIZATION PROBLEM FOR INTERPARTICLE FORCES

In this supplement, we describe the equations used in the multi-objective optimization algorithm discussed in the *Letter*. As mentioned in the *Letter*, this information is also available in [1, 2], but is provided here for completeness.

The linear and angular momentum equations for each particle are written as

$$\sum_{i=1}^{N_c^\alpha} \boldsymbol{F}_\alpha^{(i)} = 0 \quad \text{and} \quad \sum_{i=1}^{N_c^\alpha} \boldsymbol{x}_\alpha^{(i)} \times \boldsymbol{F}_\alpha^{(i)} = 0, \tag{1}$$

and combined to form the objective function $|\boldsymbol{K}_{eq}\boldsymbol{f}|_2$, where $|...|_2$ is the 2-norm, i are contact IDs ranging from 1 to N_c^α for grain α, $\boldsymbol{x}_\alpha^{(i)}$ is the location of contact i on grain α in cartesian space and $\boldsymbol{F}_\alpha^{(i)}$ is the corresponding force vector. The matrix $\boldsymbol{K}_{eq}$ and vector $\boldsymbol{f}$ take the forms

$$\boldsymbol{K}_{eq} = \begin{array}{c} \\ \\ \alpha \\ \\ \beta \\ \\ \end{array} \begin{array}{c} \begin{array}{ccccc} & i & & j & \end{array} \\ \begin{pmatrix} \ddots & \mathbf{0} & \ldots & \mathbf{0} & \ldots \\ \mathbf{0} & \boldsymbol{k}_m^i & \mathbf{0} & \boldsymbol{k}_m^j & \mathbf{0} \\ \vdots & \mathbf{0} & \ddots & \mathbf{0} & \vdots \\ \mathbf{0} & -\boldsymbol{k}_m^i & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \vdots & \mathbf{0} & \vdots & \mathbf{0} & \ddots \end{pmatrix} \end{array} \quad \text{and} \quad \boldsymbol{f} = \begin{pmatrix} \vdots \\ \boldsymbol{F}^{(i)} \\ \vdots \\ \boldsymbol{F}^{(j)} \\ \vdots \end{pmatrix}, \tag{2}$$

where α and β are now distinct grain IDs, contact i is between grains α and β, and contact j is between grain α and a boundary. The vector $\boldsymbol{f}$ contains all unknown force vector components in the system. The matrix $\boldsymbol{k}_m^i$ and vector $\boldsymbol{F}^{(i)}$ incorporate Eq. (1), taking the forms

$$\boldsymbol{k}_m^i = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & -x_3^{(i)} & x_2^{(i)} \\ x_3^{(i)} & 0 & -x_1^{(i)} \\ -x_2^{(i)} & x_1^{(i)} & 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{F}^{(i)} = \begin{bmatrix} F_1^{(i)} \\ F_2^{(i)} \\ F_3^{(i)} \end{bmatrix}, \tag{3}$$

where subscripts indicate cartesian directions in a global coordinate frame.

Stress equations for each particle are written as

$$\sum_{i=1}^{N_c^\alpha} \boldsymbol{x}_\alpha^{(i)} \otimes \boldsymbol{F}_\alpha^{(i)} = V_\alpha \boldsymbol{\sigma}_\alpha \tag{4}$$

and combined to form a second objective function $|\boldsymbol{K}_{st}\boldsymbol{f} - \boldsymbol{b}_{st}|_2$, where $\boldsymbol{\sigma}_\alpha$ is the average stress tensor for grain α obtained from the 3D X-ray diffraction data. Matrix $\boldsymbol{K}_{st}$ and vector $\boldsymbol{b}_{st}$ incorporate Eq. (4), taking the forms

$$\boldsymbol{K}_{st} = \begin{array}{c} \\ \\ \alpha \\ \\ \beta \\ \\ \end{array} \begin{array}{c} \begin{array}{ccccc} & i & & j & \end{array} \\ \begin{pmatrix} \ddots & \mathbf{0} & \ldots & \mathbf{0} & \ldots \\ \mathbf{0} & \boldsymbol{k}_{st}^i & \mathbf{0} & \boldsymbol{k}_{st}^j & \mathbf{0} \\ \vdots & \mathbf{0} & \ddots & \mathbf{0} & \vdots \\ \mathbf{0} & -\boldsymbol{k}_{st}^i & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \vdots & \mathbf{0} & \vdots & \mathbf{0} & \ddots \end{pmatrix} \end{array} \quad \text{and} \quad \boldsymbol{b}_{st} = \begin{pmatrix} \vdots \\ \boldsymbol{b}_\alpha \\ \vdots \\ \boldsymbol{b}_\beta \\ \vdots \end{pmatrix}, \tag{5}$$

where the matrix $\boldsymbol{k}_{st}^{(i)}$ and $\boldsymbol{b}_\alpha$ are written as

$$\boldsymbol{k}_{st}^{i} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ x_2^{(i)} & x_1^{(i)} & 0 \\ x_3^{(i)} & 0 & x_1^{(i)} \\ 0 & x_3^{(i)} & x_2^{(i)} \end{bmatrix} \quad \text{and} \quad \boldsymbol{b}^{\alpha} = \begin{bmatrix} V_\alpha \sigma_{11} \\ V_\alpha \sigma_{22} \\ V_\alpha \sigma_{33} \\ 2V_\alpha \sigma_{12} \\ 2V_\alpha \sigma_{13} \\ 2V_\alpha \sigma_{23} \end{bmatrix}, \tag{6}$$

where V_α is the volume of grain α.

The non-cohesive force and Coulomb friction constraints are written as

$$\boldsymbol{e}_\alpha^{(i)} \cdot \boldsymbol{F}_\alpha^{(i)} \geq 0, \tag{7}$$

$$\mu \boldsymbol{e}_\alpha^{(i)} \cdot \boldsymbol{F}_\alpha^{(i)} - \sqrt{(\boldsymbol{t}_1^{(i)} \cdot \boldsymbol{F}_\alpha^{(i)})^2 + (\boldsymbol{t}_2^{(i)} \cdot \boldsymbol{F}_\alpha^{(i)})^2} \geq 0, \tag{8}$$

where $\boldsymbol{e}_\alpha^{(i)}$ is an inward-pointing unit normal vector at contact i of particle α, $\boldsymbol{t}_1^{(i)}$ and $\boldsymbol{t}_2^{(i)}$ form an orthogonal basis for the corresponding contact plane, and μ is the interparticle friction coefficient. The forces $\boldsymbol{f}$ were obtained by minimizing the sum of the two objective functions, $|\boldsymbol{K}_{eq}\boldsymbol{f}|_2$ and $|\boldsymbol{K}_{st}\boldsymbol{f} - \boldsymbol{b}_{st}|_2$, subject to the constraints in Eq. (7) and (8). The optimal trade-off parameter was therefore unity [2], which we found to provide good minimization of both objectives. More information on the optimization problem, including the choice of norms, can be found in [1, 2].

[1] R. Hurley, E. Marteau, G. Ravichandran, and J. E. Andrade, Journal of the Mechanics and Physics of Solids **63**, 154 (2014).

[2] R. Hurley, K. Lim, G. Ravichandran, and J. Andrade, Experimental Mechanics **56**, 217 (2016).