# A normal cohesive force implementation (USE_DEM_COHESION)

Written by Yun Zhang (12/27/16), edits by DCR (12/27/16)

Lastly update 06/11/20

In addition to the normal and tangential forces and the rotational torques, a normal cohesive force can be applied between two particles in contact when the 'USE_DEM_COHESION' macro is uncommented in PKDGRAV's Makefile.in file.

- **Cohesion mechanism in regolith on asteroids**

    The cohesive forces on asteroids mainly arise from the van der Waals forces due to molecular or atomic polarization effects between micro-sized particles (Scheeres et al., 2010). In the DEM community, there are numerous contact models developed for the van der Waals forces that are based on the microscopic contact mechanics of two micro-sized particles, e.g., Bradley model, DMT model, M-D model, and JKR model (see Marshall and Li 2014 for reviews on these models). Taking the model developed by Jiang et al. (2013) as an example, the attractive force between two micro-sized spheres of radius $r_i$ and $r_j$ is

$$f_c = \frac{A}{24D^3}(2\beta r)^2 , \qquad (1)$$

where $A$ is the Hamaker coefficient, and $D$ and $r$ are the micro-separation and the effective radius $r = r_i r_j/(r_i + r_j)$ of the two spheres, respectively. The contact area is described by a square of sides $2\beta r$, where $\beta$ is a shape parameter. Normally, the Hamaker coefficient is on the order of $10^{-20}$ J (e.g., $4.3\times10^{-20}$ J for lunar regolith after Perko et al. 2001), and the micro-separation is on the order of $10^{-6} \sim 10^{-8}$ m.

    These microscopic contact models cannot be directly used for particles larger than ~100 $\mu$m. The rationale for the cohesive force in PKDGRAV for larger particles is based on the granular bridge idea proposed by Sánchez and Scheeres (2014, 2016; their model is implemented as iCohesionModel = 1 in PKDGRAV). With the assumption that there exist substantial micro-sized grains to cover larger boulders, the model can mimic the cumulative effect of cohesive regolith between two large boulders without simulating each individual fine grain.

- **Cohesion model in PKDGRAV**

    We implemented two different cohesion models, which can be selected by setting iCohesionModel in ss.par. Model 0 was developed on our own and is well-tested in PKDGRAV (Zhang et al., 2018).

(1) iCohesionModel = 0

    This model is based on a hypothetical contact area characterized by a shape parameter, $\beta$, used in the microscopic contact model of Jiang et al. (2013, 2015). We use $\beta$ to represent a statistical measure of the area where the interstitial grains are in contact and use a rectangular area to approximate this effective contact area

$$A_{\text{eff}} = 4\left(\beta R\right)^2,\qquad(2)$$

where the effective radius $R = R_i R_j/(R_i + R_j)$, and $R_i$ and $R_j$ are the radii of the corresponding boulders.[1] The corresponding cohesive force between two boulders can be modeled as

$$\mathbf{F}_C = cA_{\text{eff}}\hat{\mathbf{n}},\qquad(3)$$

where the interparticle cohesive tensile strength $c$ is designed to reflect the physical properties of the interstitial regolith, e.g., porosity, size distribution, surface energy etc. The cohesive force will be neglected if the two particles are not in contact.

Users can determine the interparticle cohesive coefficient $c$ by using demparams, and then specify it in ss.par (i.e., dCohesiveCoeff; note that PKDGRAV units are used in ss.par). The magnitude of the resulting cohesive force of the typical particle is calculated and reported within demparams.

(2) dCohesionModel = 1

This model of cohesive force was introduced by Sánchez and Scheeres (2014, 2016). In their model, the cohesive force also results from the van der Waals forces between molecules of two perfectly smooth spheres of radius $r_i$ and $r_j$ and can be computed as (Israclachvili, 1985)

$$\mathbf{f}_C = Ar\hat{\mathbf{n}},\qquad(4)$$

where $A$ is a constant related to the micro-separation of the two spheres and the Hamaker coefficient, and the effective radius $r = r_i r_j /(r_i + r_j)$. Through adding this cohesive force to the interaction between the regolith grains in contact, Sánchez and Scheeres (2014) empirically determine the tensile strength for a randomly packed matrix based on a series of uniaxial tensile stress simulations, i.e.,

$$\sigma_{yy} = \frac{S_Y}{\bar{r}},\qquad(5)$$

and the corresponding cohesive force between two boulders of radius $R_i$ and $R_j$ can be modeled as

$$\mathbf{F}_C = \sigma_{yy}\frac{2\pi R_i^2 R_j^2}{R_i^2 + R_j^2}\hat{\mathbf{n}}.\qquad(6)$$

The cohesive strength coefficient $S_Y$ is a semi-empirically determined factor combining the effects of the particle geometry, the coordination number, the filling fraction, and the Hamaker coefficient. The effect of mean grain radius $\bar{r}$ is also reflected in this expression, in which a smaller mean grain size would result in a stronger cohesive regolith.

Here the coefficient $\sigma_{yy}$ is the cohesive coefficient, which can be set in ss.par (i.e.,

---

[1] When using the actual contact radius, $r_c$ (i.e., bUseContactRadius = 1), the contact area is given by $A_{\text{eff}} = \pi(\beta r_c)^2$. The contact radius $r_c = [(r_i^2 - r_j^2 + d^2)/(2d)]^{1/2}$, where $d$ is the distance between the sphere centers.

dCohesiveCoeff). Its value can be obtained by using demparams.

● **Cohesion model for particle-wall contacts**

For particle-wall contacts, the contact area is given by assuming that the radius of the wall is infinite. Other setup is the same as for interparticle cohesion. The cohesive strength for each wall can be given in the walls data file; otherwise, it will take the value in ss.par by default.

● **Cohesive strength estimate**

Based on the analyses of Sánchez and Scheeres (2016), for dCohesionModel = 1, the tensile strength of the aggregate ($\sigma_{yy}^a$) can be determined by the following expression,

$$\sigma_{yy}^a = \sigma_{yy} \frac{\eta \cos\left(45°\right)}{\sqrt[3]{3}}, \tag{7}$$

where $\eta$ is the packing efficiency. Similarly, for dCohesionModel = 0,

$$\sigma_{yy}^a = c \frac{\eta \cos\left(45°\right)}{\sqrt[3]{3}}, \tag{8}$$

● **Variable cohesive strength**

With an additional cohesion data file, the interparticle cohesive coefficient $c$ can be specified for different particle pairs. The file name, e.g., "cohesion.dat", should be assigned to, achCohesionFile, in ss.par.
The format of the cohesion data file is:

*nC    nStrategy*
*iColor_1  dCohesiveCoeff_1*
*iColor_2  dCohesiveCoeff_2*
*...*
*iColor_nC    dCohesiveCoeff_nC*

where *nC* is the total number of cohesive coefficient values intend to use. For each particle, the cohesive coefficient value is assigned according to its color, as specified in this file. If the two particles in contact have the same color, their interparticle cohesive coefficient is *dCohesiveCoeff_#* corresponding to *iColor_#*. Otherwise, the interparticle cohesive coefficient is derived according to the given strategy, *nStrategy*. Current version of PKDGRAV supports four strategies. *nStrategy* = 0 means no cohesion between particles with different colors, *nStrategy* = 1 means using the averaged cohesive coefficient value between particles with different colors, *nStrategy* = 2 means using the maximum cohesive coefficient value between particles with different colors, and *nStrategy* = 3 means using the minimum cohesive coefficient value between particles with different colors.

- **References**

Israclachvili J.N., 1985. Intermolecular and surface forces. Academic Press, London.

Marshall, J.S., Li, S., 2014. Adhesive particle flow. Cambridge University Press.

Jiang, M., Shen, Z., Thornton, C., 2013. Microscopic contact model of lunar regolith for high efficiency discrete element analyses. Computers and Geotechnics 54, 104–116.

Jiang, M., Shen, Z., Wang, J., 2015. A novel three-dimensional contact model for granulates incorporating rolling and twisting resistances. Computers and Geotechnics 32(5), 340–357.

Perko H.A., Nelson J.D., Sadeh W.Z., 2001. Surface cleanliness effect on lunar soil shear strength. J Geotech Geoenviron Eng, 127(4):371–83.

Sánchez, P., Scheeres, D.J., 2014. The strength of regolith and rubble pile asteroids. Meteoritics & Planetary Science, 49(5), 788–811.

Sánchez, P., Scheeres, D.J., 2016. Disruption patterns of rotating self-gravitating aggregates: A survey on angle of friction and tensile strength. Icarus 271, 453–471.

Scheeres, D.J., Hartzell, C.M., Sánchez, P., Swift, M., 2010. Scaling forces to asteroid surfaces: The role of cohesion. Icarus 210(2), 968–984.

Zhang, Y., Richardson, D.C., Barnouin O.S., et al. 2018. Rotational failure of rubble-pile bodies: influences of shear and cohesive strengths. Astrophysical Journal, 857, 15.