Implementation of a DEM scalable crushing model in PFC3d.

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A new rigorous breakage criterion for elasto-brittle spheres is formulated and implemented as a contact model in the discrete element method DEM. The practical upscaling rules proposed and validated Ciantia et al., (2015) allow for a dramatic reduction of computational costs. The efficiency and the ability to reproduce realistic behaviour of three different soils is further discussed in Ciantia et al., (2019). The computational speedup of the model led to 3D CPT and pile penetration simulations in crushable sands for the first time by Ciantia et al., (2016a; 2019a).

Model description:

The failure criterion is based on work by Russell and Muir Wood (2009); a two-parameter material strength criterion is used together with consideration of the elastic stresses induced by point loads on a sphere. A particle subject to a set of external point forces reaches failure when the maximum applied force reaches the following limit condition:

$$F \leq \sigma_{\lim} A_F \tag{1}$$

where σ_{lim} is the limit strength of the particle and A_F the contact area. To incorporate the natural material variability into the model, the particle limit strength, σ_{lim}, is assumed to be normally distributed for a given sphere size. The coefficient of variation of that distribution, *var*, is taken to be a material parameter. To incorporate particle scale effects the mean strength value for given sphere size, $\bar{\sigma}_{\lim}$ depends on the particle diameter:

$$\bar{\sigma}_{\lim} = \bar{\sigma}_{\lim 0} \left(\frac{d}{d_0} \right)^{-3/m} \tag{2}$$

where $\bar{\sigma}_{\lim 0}$ is a material constant. A_F depends on the contact force and the particle's elastic properties; applying Hertzian contact theory the following expression for the breakage criterion is obtained:

$$F \leq \left\{ \bar{\sigma}_{\lim 0} f(\text{var}) \left(\frac{d}{d_0} \right)^{-3/m} \pi \left[\frac{3}{4} \frac{\left(\frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2} \right)}{\left(\frac{1}{r_1} + \frac{1}{r_2} \right)} \right]^{2/3} \right\}^3 \tag{3}$$

where f(var) indicates the effect of variability of particle strength; r_1 and r_2 are the radii of the contacting spheres and E_i, v_i are the Young's Moduli and Poisson's ratio respectively. Note that this breakage criterion does not involve exclusively the maximum force on the particle: there is a strong inbuilt dependency on the characteristics of the contacting particles. For particle wall contacts, $r_2=\infty$ and E_2, v_2 assume the elastic properties of the wall.

Once the limit condition is reached, the spherical particle will split into smaller inscribed tangent spheres. The crushed fragments assume the velocity and material parameters of the original particle apart from the intrinsic strength (σ_{lim0}) which is randomly assigned sampling its normal distribution. Ciantia *et al.*, (2015; 2016b) concluded that a 14-ball crushed configuration can adequately represent macroscopic behaviour. The capability of this model to capture real test behaviour has been demonstrated by Ciantia et al. (2016a; 2019b).

To further limit the computational cost the crushing procedure may only applied for particles above a certain minimum particle size, d_{comm}, called the comminution limit. Calibration parameters for various sands are reported in Table 1.

Table 1 DEM crushing model paramters for three types of sand. Refer to the paper reference for full details of

SAND	d_{50} *mm*	d_0 *mm*	d_{100} *mm*	μ* -	***G*** ***GPa***	ν -	$\sigma_{lim,0}$ ***MPa***	***m*** -	d_0 *mm*	***var*** -	d_{comm}/d_{50} -
Fontainebleau sand	0.21	0.01	0.27	0.275	9	0.2	190	10	2	0.36	0.55
Pumice sand	0.88	0.3	2.36	0.4	0.33	0.3	116	5	2	0.5	0.25
Petroleum coke	7.5	5.0	10.0	0.4	0.33	0.3	200	10	2	1.0	0.25

*The interparticle friction coefficient is calibrated inhibiting particle rotation to capture shape effects.

Particle splitting and lost mass:

Once the limit condition is reached, a particle, modelled with a sphere in PFC 3D, will split into smaller inscribed tangent spheres. When interpreting the test results, this mass should be accounted for. This is particularly important when tracking the void ratio (or porosity) evolution of the particle size distribution (PSD) during the test, a result that is frequently obtained in experiments. For porosity evolution it is important to record the initial volume of solids making the sample while for the PSD evolution refer to Ciantia et al. (2015-19b) for the PSD evolution.

Particle scaling:

Scaling up the particle size while maintaining constant other geometrical dimensions of the problem reduces the number of particles in the model. An upscaling procedure is judged successful if the macroscopic quantities of interest such as compressibility, yield stress and so on, remain unchanged. For this to be possible, the formulation of the contact laws needs to be modified to consider the particle scaling factor, *N*. Also the PSD evolution computed during compression should be correct when scaled back. The crushing model is framed to be scalable. Without a scalable crushing model, because of size effects on particle strength, upscaled models would return incorrect macroscopic behaviour related to particle crushing. The scaled crushing criteria results:

$$F \le \left\{ \bar{\sigma}_{\lim 0} f\left(\text{var}\right) \left(\frac{d}{N d_0} \right)^{-3/m} \pi \left[\frac{3}{4} \frac{\left(\frac{1-\nu_1^2}{E_1} + \frac{1-\nu_2^2}{E_2} \right)}{\left(\frac{1}{r_1} + \frac{1}{r_2} \right)} \right]^{2/3} \right\}^3 \tag{4}$$

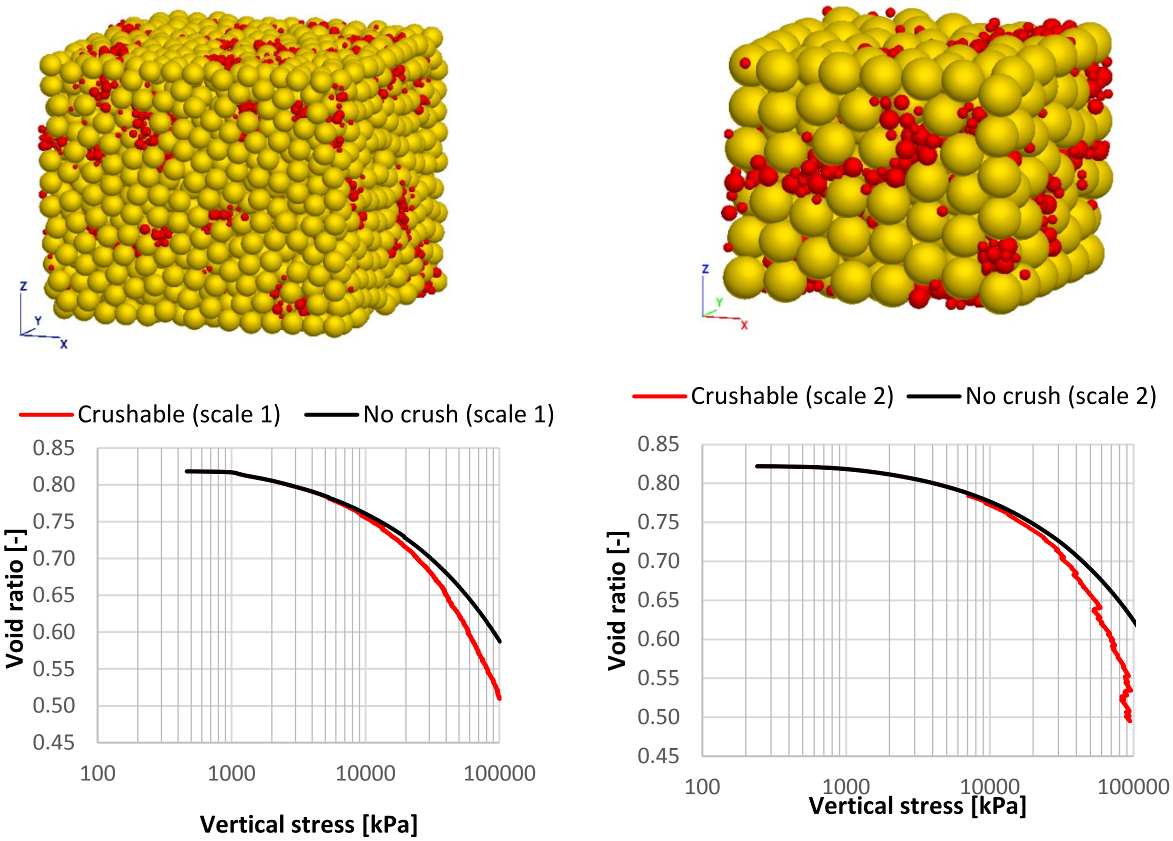
On the PFC6.proj

The example provided consists in a 1D compression problem of crushable spheres. The .dat file has plenty of comments that are intended to ease the reading of the example. After generating a monodisperse sample. The strength parameters are assigned to each particle. In theory only the *f(var)* is required as a property of the particles as all the other can be introduced directly to the cmat. However in this project for sake of clarity all crushing elastic parameters are also assigned to the particles.

There is an initial phase where friction is set to zero in order to make the particles redistribute and obtain a more homogeneous sample. This phase can be improved as initial conditions are trivial but this is not the objective of the example. Once the large contact forces disappear because of this particle rearranmgemet, friction is reactivated and the top and bottom walls are moved towards each other. This is done until a vertical stress of 100MPa. The number of cycles in the script might have to be adjusted to reach to this value.

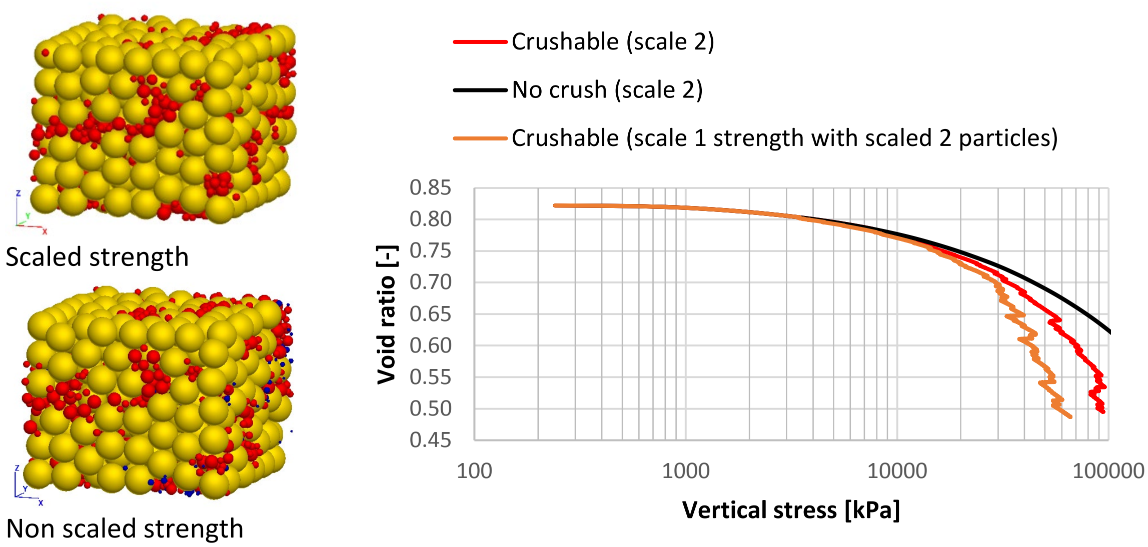
First the model is run using scale=1. Then after exporting the histories and modifying the .p3sav names the mode is re-run using scale =2. Restring the initial state and deactivating crushing (by not executing the (*fish callback add @break_balls -1* and *fish callback add @my_function event broken_ball*) the uncrushable response of the model is obtained. The result of the uncrushabke and crushable 1D compression of both scale 1 and 2 models are represented in the figure below.

Re-running the same project with scale=2 would make the initial sample of 382 particles against the 3062 obtained with scale=1. The simulation would complete in about 35 minutes for scale 1 while in just 5 minutes for scale=2. As expected, the uncrushable model is stiffer. The yielding stress for both models is about 30 MPa. To highlight the importance of using a scalable crushing model the scale 2 model is rerun setting scale=1 but using scaled particles. In this case the macroscopic response is very different as the model is considering the particles as larger particles without considering the strength of the size they are representing. In this project the 14-particle splitting configuration is used. However, this can be changed, and any sort of replacement configuration may be used.



a) Scale 1 b) Scale 2

Figure 1. Comparison of 1D compression for crushable and uncrushable response of scaled and non scaled models.



a) b)

Figure 2. Effect of not employing a non-scalable crushing strength on scaled models: a) Samples at e=0.5 and b) comparison of 1D compression between the uncrushable, the crushable using the correct strength scaling and the one without scaling the particle strength.

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