Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

High Performance Computing for Science and Engineering II

Spring semester 2016

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Project # 4

Issued: 30.05.2016

- In these scripts, we outline five computational engineering problems. Choose one and work either individually or in a group of two people. Communication is allowed to the extent that you do not copy the work of other groups.
- You are encouraged to contact one of the TAs in order to arrange a meeting to discuss your chosen project. These meetings are meant for clarifying and detailing the projects, give early feedback on your approach, *not* for correcting your code.
- In evaluating your work, we will consider your ability to analyse the problem and the hardware at your disposal, to appropriately apply the principles taught during the whole HPCSE class, and to report your reasoning and findings.
- The report (including text, code, figures) needs to be emailed to one of the TAs before the day of the exam. If working in a group of two, each student has to write an *individual* report.

Granular Flow

Discrete Element Method

The Discrete Element Method (DEM) is a widely used method to simulate granular material with a broad range of industrial applications ranging from oil and gas to pharmaceutical and metallurgy. The granular material is modeled as a set of particles of various shapes with translational and rotational degrees of freedom accompanies by models of interparticle collisions. Each particle has its own mass, velocity and friction properties. The contact force between particles consist of elastic, viscous and frictional resistance forces.

The DEM includes no long-range interaction forces, that is a pairwise force $F_{ij} \neq 0$ only if particle i touches particle j. For integration we assume the spheres are not perfectly stiff but "soft". This means that during the simulation particles may overlap one with each other, which corresponds to their physical deformation.

Method description

In this project we consider two-dimensional systems. Two disks with radii R_i, R_j are assumed to be in mechanical contact if $\xi_{ij}^n \equiv R_i + R_j - |\mathbf{r}_i - \mathbf{r}_j| > 0$. Here $\mathbf{r}_i - \mathbf{r}_j = \mathbf{r}_{ij}$ is the vector connecting the center of the particle i to the contact point with particle j and ξ_{ij} is the mutual compression between the particles. The force exerted on particle i due to contact with particle j is given as $\mathbf{F}_{ij} = \mathbf{F}_{ij}^n + \mathbf{F}_{ij}^t$ where (F^t) and (F^n) are its tangential and normal contributions. The contact force components (see fig. 1) can be written as

$$\mathbf{F_{ij}}^n = F_{ij}^n \mathbf{e_{ij}}^n, \quad \mathbf{F_{ij}}^t = F_{ij}^t \mathbf{e_{ij}}^t \tag{1}$$

with the unit vectors

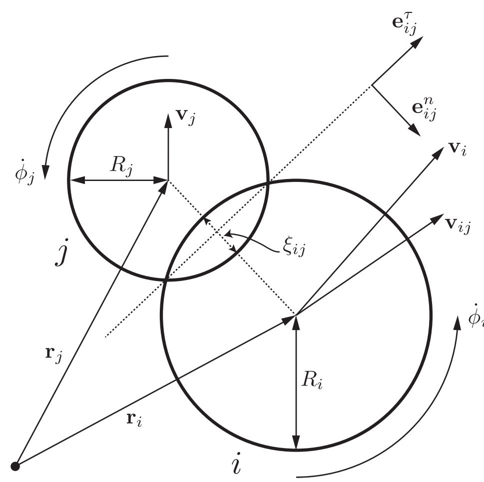

Figure 1: Sketch indicating the various F-D components for a binary collision between particle i and j.

$$\mathbf{e_{ij}}^n = \frac{\mathbf{r_j} - \mathbf{r_i}}{|\mathbf{r_j} - \mathbf{r_i}|}, \quad \mathbf{e_{ij}}^t = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \cdot \mathbf{e_{ij}}^n$$

Particles evolve according to the two-dimensional Newton's equations of motion (2):

$$m_i \ddot{\mathbf{r}}_i = m_i \mathbf{g} + \sum_j \mathbf{F}_{ij}, \qquad I_i \ddot{\phi}_i = \sum_j (\mathbf{r}_{ij} \cdot \mathbf{F}_{ij}) \tag{2}$$

where each particles $i,\ i = 1, ..., N$ has a mass (m_i) and moment of inertia (I_i), translational $(\ddot{\mathbf{r}}_i)$ and rotational $(\ddot{\phi}_i)$ acceleration and g denotes gravity. These ordinary differential equations (eq. (2)) are solved with a 3rd order Gear's Predictor-Corrector scheme (look it up in the literature).

A contact force model to be used in the current project is an extended non-linear spring-dashpot model. For the collision of two particles it reads as follows:

$$\begin{aligned}
\mathbf{F}^n &= -k^n \xi^n \mathbf{e}^n - \gamma^n \frac{d\xi^n}{dt} \mathbf{e}^n \cdot \sqrt{\xi^n}, \\
\mathbf{F}^t &= \mathbf{e}^t \cdot \min\left(\frac{2}{3} k^s \zeta^t, \mu F^n\right) \\
\zeta^t &= \int_{t_0}^{t} v^t_{rel}(\tau)\, d\tau, \\
k^n &= \frac{4}{3} E \sqrt{R\,\xi^n}, \\
k^s &= 8G\sqrt{R\,\xi^n}.
\end{aligned} \tag{3}$$

Here we assume particles of the same size $R_i = R$ and mass, E is the Young's modulus of the material, G is the shear modulus, γ is damping coefficient and v_{rel} is the relative tangential velocity of the disks at the contact point. Important to mention that quantity ζ^t depends on the previous collision history and therefore has to be tracked throughout the whole collision duration.

Problem setup

Place a number of identical disks (around $100,000$) in a square box such that half of the box is empty. Note that collisions with box walls should be treated as collisions with "ghost" particles. A ghost is a particle image mirrored with respect to the wall and having the mirrored (not necessarily opposite) velocity and no angular velocity.

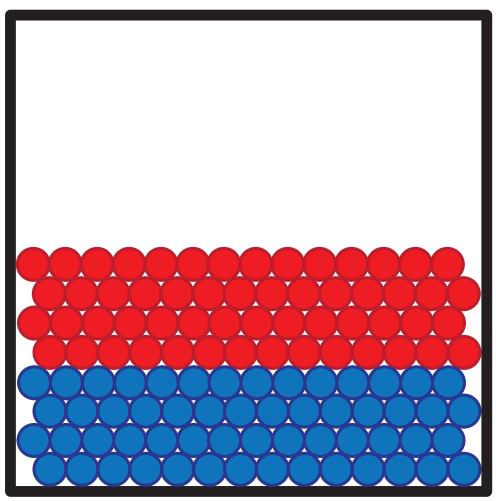

Figure 2: Sketch of the initial configuration of the simulated system

Half of the particles on top should be colored red, half on the bottom – blue (see fig. 2). At the time $t = 0$ the box start rotating with a constant angular velocity and the beads of different colors will start to mix.

Implement the DEM solver. Use stainless steel as the material and damping coefficient $\gamma = 10^{-3}$. Verify the correctness of your code by studying just one collision (particle-particle or particle-wall): look at the properties that the code should conserve (mind that energy is not conserved), direction of rotation after the impact, etc.

Optional: think of a criterion (a formula or a procedure producing a number) of the granular material to be "well-mixed". Study the evolution of this criterion over time and an impact of rotational velocity of the box on the mixing time.