

SIMULATOR

Simulator is parallelized DEM-solver, based on fast-contact detection algorithm and efficient integration scheme. Several parameters of simulator can be specified:

- *Simulation Step* – time step which is used in the integration scheme
- *Saving Step* – how often data will be saved into result file
- *End Time* – end time point when simulation should be finished (there is no possibility to continue simulation)
- *External Acceleration* – vector of external acceleration
- *Simulation Domain* – volume which is used for calculation. If some particle leaves simulation domain – it will be automatically become inactive status. All bonds connected to this particle will also become inactive status
- *Collisions Saving* – this option allows to save information about collisions during simulation. **Note:** saving of collision data can significantly slow down calculations and can lead to large amount of generated data. Tipp: save collisions for case studies where relative short time interval is modeled.

For the systems which are consisting only from primary particles recommended time step is calculated based on Rayleigh time. **Note:** that for this calculation only active particles existing on scene are considered. If new particles will be generated during simulation or solid bonds existing on the scene, then other simulation time step should be used. Rayleigh time is calculated depending on particle radius R_i , Poisson ratio ν_i , Young's modulus E_i and density ρ_i :

$$\Delta t_{sim,recom} = T_{Rayleigh} = \min \left\{ \frac{\pi \cdot R_i \sqrt{2\rho_i(1 + \nu_i)}}{\sqrt{E_i(0.163\nu_i + 0.8766)}} \right\}$$

If scene consisting of primary particles, as well as solid bonds the recommended simulation time step calculated as 10% (factor 0.1) of:

$$\Delta t_{sim,recom} = 0.1 * \min\{T_{Rayleigh}, T_{sim,bond}\}$$

where $T_{sim,bond}$ is estimated according following equation (O'Sullivan and Bray, 2003; Brown et al., 2014),

$$T_{sim,bond} = \min\left\{2 \sqrt{\frac{m_{min}}{K_{b,i,max}}}\right\}$$

where m_{min} is the minimal mass of particles connected with this bond and $K_{b,i,max}$ is the largest bond stiffness calculated for elastic solid beam theory, depending on Young's modulus E_b , Poisson ratio ν_b , initial length L_{init} , cross-cut surface A_b as:

$$K_{b,i,max} = \max\left\{\frac{E_b \cdot A_b}{L_{init}}, \frac{E_b \cdot A_b}{2 \cdot L_{init} \cdot (1 + \nu_b)}\right\}$$

When the simulation has been started there is exist a possibility to pause simulation. **However, this option is made only to check current state visually.** In order to save scene, or to analyze results the simulation should be continued and correctly stopped.

Literature

- N. Brown, J.-F. Chen, J.Y. Ooi (2014). A bond model for DEM simulation of cementitious materials and deformable structures, *Granular Materials* 16, 299-311.
- C. O'Sullivan, J.D. Bray (2003). Selecting a suitable time step for discrete element simulations that use the central difference time integration scheme, *Engineering Computations* 21, 278-303.