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DEVELOPMENT OF A SIMULATION ENVIRONMENT OF GRANNULAR MATERIALS

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Today In the chemical industry more than 60% of processes are solids processes. Typical industries using solids are:

- Mining
- Mineral processing
- Pharmaceutical
- Agriculture and food handling
- Chemical

With a purpose to optimize production process and develop more effective approaches of production processing should be done their simulation. This gives a possibility to predict behavior of materials and to avoid undesirable results and make an analysis of particle handling and manufacturing operations. Designs can be analyzed and modified on the computer before expensive and time consuming design decisions are finalized.

Any physical process that involves the disaggregation and movement of material is best modeled with DEM rather than continuum methods such as finite elements. Discrete element methods have been under development since the early 1970's. Until recently, most of the capabilities available allowed treatment of certain particle shapes such as spheres or ellipses. The examples of processes which can be simulated by DEM (discrete element methods) are precipitation, breakage, attrition, mixing and other solids processes.

Coupled processes present significant challenges to engineers today. One of those challenges is treatment of the coupling between solid particles and fluid flow. Processes of this type include sand production in oil wells and manufacturing processes where particles are carried by fluids to their final destination.

The major Molecular Dynamics simulation problems are:

- Summation of the forces and torques according
- Integration of the equation of motion
- Data extraction from the computed particle trajectories

The project will be used in educational purposes. The students will be able to study particle processes more comprehensive and see how the particles act in different situations with initial circumstances. Visual overview of these processes will help them to understand the nature of granular materials better.

The other purpose of the project is scientific. All the experiments which are connected with granular processes nature can be first simulated by the software. This can prevent of unexpected results and see how some processes occur in closed spases. Many companies and research institutes are using modelling software for various projects. The simulation environment can handle several situations which can't be tested during experiments.

Nowadays expensive commercial software packages for DEM simulation exist. A set of open source projects have been created, but they can't be effectively applied for simulation of real granular materials.

The main purpose of this project is to develop a new open-source system for DEM Simulation of granular processes which will have good agreement with an experimental data.

For the development of the project it's necessary to make an analysis of:

- Existing systems for DEM simulation

- DEM methods and the most modern scientific approaches, contact models
- Existing packages for solving systems of equations

Analysis of existing simulation environments for granular materials processes

The result of the analysis is a table of advantages and disadvantages of the environment:

Table 1

Comparison of existing systems

	EDEM	PFC	Chute Maven	ELFEN	Passage	Ascalaph	Yade	LAMMPS	Pasi-modo	Esys-P.
Commercial	+	+	+	+	+	+	-	-	-	-
Parallelization	+	+	-	+	-	+	+	+	+	+
Coupling CFD	+	-	-	-	-	-	+	+	-	-
Coupling FEM	+	-	-	+	-	-	+	+	-	-
CAD import	+	-	+	+	-	-	-	+/-	-	-
Contact model variety	+	+	-	+	+	+	-	+	+	+
Adjust particle shape	+	+	-	+	+	+	+	+	+	-
3-D	+	+	+	+	+	+	+	+	+	-
Particles information in process	+	+	+	+	+	+	+	+	+	-

The modelling environments EDEM, Itasca PFC 3D, Chute Maven, ELFEN, PASSAGE DEM and Ascalaph belong to commercial. The modelling environments Yade, LAMMPS, Pasimodo and Esys-P. belong to non-commercial.

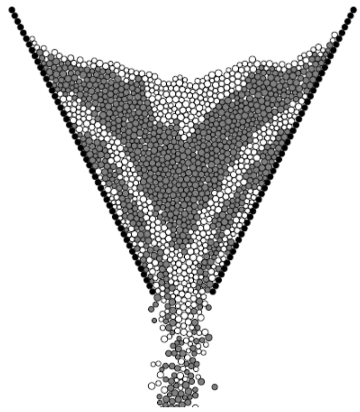
There is no sense to develop the modelling system from the beginning, when some of them are already created. The aim of the project is to modify, change and optimize an already made open-source system. As the basic the LAMMPS system was chosen.

DEM methods and the most modern scientific approaches, contact models

The dynamics of a granular material are covered by Newton's equation of motion for the center of mass coordinates and the Euler angles if its particles i (i=1 , ... , N):

$$\frac{\partial^2 \vec{r_i}}{\partial t^2} = \frac{1}{m_i} \vec{F_i}(\vec{r_j}, \vec{\upsilon_j}, \vec{\varphi_j}, \vec{\omega_j})$$

$$\frac{\partial^2 \vec{\varphi_i}}{\partial t^2} = \frac{1}{\hat{I_i}} \vec{M_i}(\vec{r_j}, \vec{\upsilon_j}, \vec{\varphi_j}, \vec{\omega_j}) \qquad (j = (1..N))$$



Picture 1 – Precipitation process

The force *Fi* and the torque *Mi*, which act on particle *i* of mass *mi* and the tensorial moment of inertia *Ji*, are functions of the particle positions rj , their angular orientations ϕj , and the corresponding velocities vj and ωj. The computation of the forces and torques is the central part of each Molecular Dynamics simulation. The contact condition:

$$\xi_{ij} = R_i + R_j - \left|\vec{r_i} - \vec{r_j}\right| > 0$$

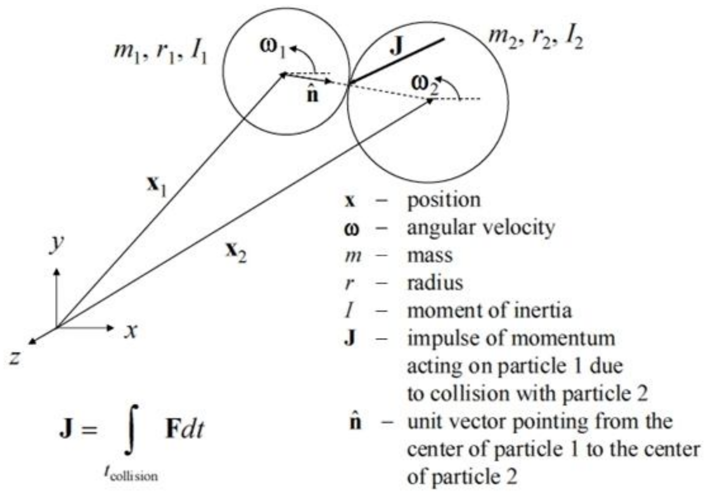
R_i and R_j are the particles radii.

If the condition of contact is true, then force exists and it's divided into normal and tangential part.

$$\vec{F}_{ij} = \begin{cases} \vec{F}_{ij}^{n} + \vec{F}_{ij}^{t} & if\ \xi_{ij} > 0 \\ 0 & otherwise \end{cases}$$

Two major types of particle interaction handling exist: soft sphere model and hard sphere model:

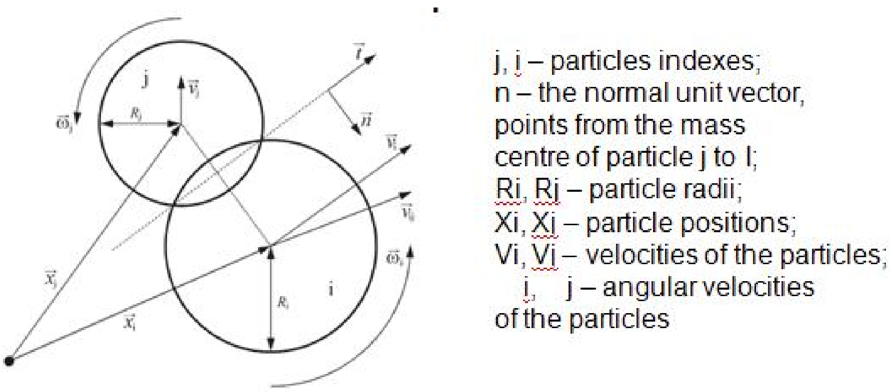
Hard sphere model collision dynamics:



Picture 2 - Hard sphere model collision dynamics

Main features of this model:
- particles do not deform during a collision
- collisions occur instantaneously
- only binary (two particle) collisions occur
- used most often for modeling dilute, energetic granular flows

Soft sphere model collision dynamics:

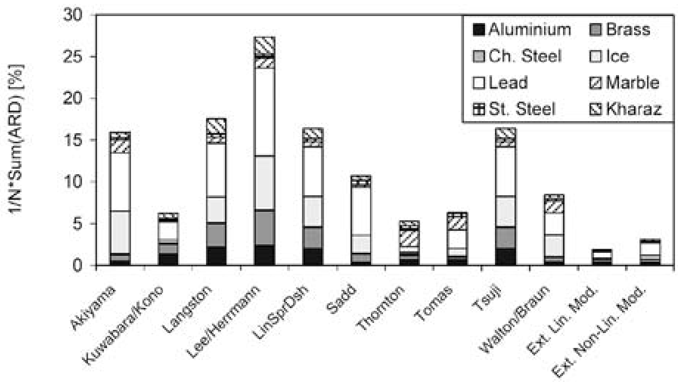


Picture 3 - Soft sphere model collision dynamics

When granular particles collide, part of the kinetic energy of their relative motion is dissipated, i.e. transformed into heat. Deformations of the particles are assumed to be small and their spherical shape is assumed to be conserved on average after many collisions. The change of the temperature of the particles is neglected.

The project will use soft sphere model for real simulations where particles deform.

The average deviation from experimental results for normal force models is presented on the plot:



Picture 4 – Average deviation of models from experimental data

The best is Extended Linear Model, because of its results that are in the best agreement with experimental data and because linear model reduces the computational costs in comparison with non-linear models. For tangential force the best linear model was presented by Di Maio and Di Renzo.

The result of analysis of the existing packages for solving systems of linear equations is: Intel MKL, LAPACK, Hips and pARMS solvers and frameworks are the best in computational costs and precision of results.

Conclusions

The aim of the project is:

- Extending of the existing system and it's optimization for DEM simulation of granular materials
- Implementation of different new contact models
- Computations and models validation by comparison of simulation and experimental results
- Implementation of more effective parallelization strategies

Literature

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