Particle Matching in Cyclic DEM Simulations based on Quantum Annealing

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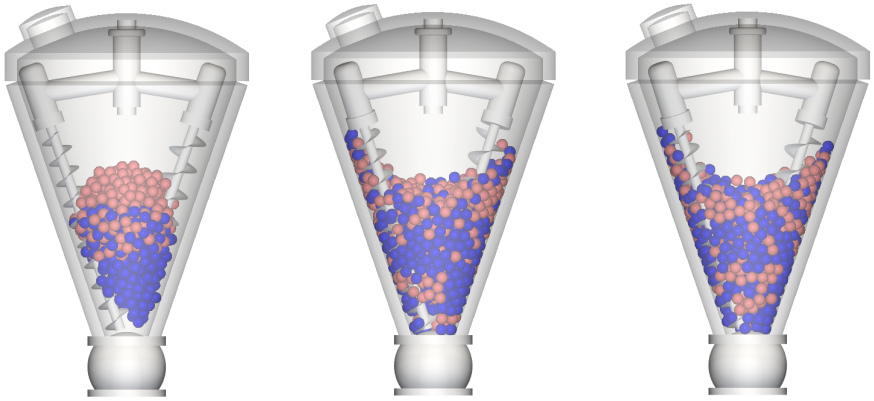
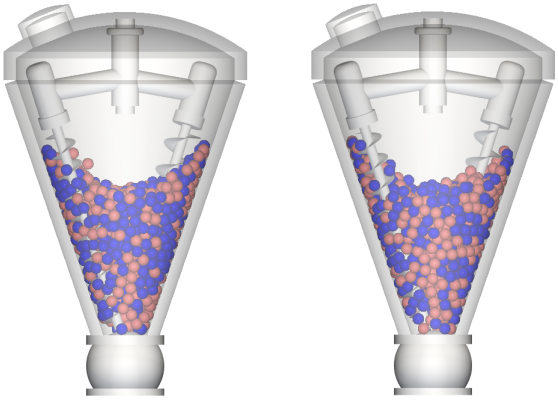
Short Description

In this project we want to speed up cyclic particle simulations of mixing processes by assuming pure permutation over a single cycle. Quantum Annealing is to be used to retrieve the permutation information from simulation data obtained by the Discrete-Element Method (DEM).



(a) Starting configuration (b) Configuration after 1 cycle (c) Configuration after 2 cycles



(d) Configuration after 3 cycles (e) Configuration after 4 cycles

Figure 1: Binary particle configurations in a mixer after filling the mixer (a) and after four subsequent mixing cycles (b) - (e).

Introduction

Application-relevant mixing processes, e.g., for the production of concrete, medication, food, etc., can be simulated via the Discrete-Element Method (DEM), also referred to as particle simulation.

Depending on the field of application the purpose of the simulation might differ. While for the mixing of cereal the ratio of oats to nuts is more of customers' personal preference, there are also applications such as tablet production, where a homogeneous mixing quality is of crucial importance, for instance when mixing medical agents. In any case it is desirable to have a mixing process that fulfills certain criteria, such as mixing time, mixing quality, abrasion, power consumption, etc. Complementary simulations allow for analyzing and optimizing mixer and process, preceding the prototype stage. Conducting DEM simulations over the whole mixing time is, however, computationally very expensive, especially as the particles get smaller and their number increases.

The basic challenge

Many mixing processes reach a somewhat periodic state. One might think about stirring a pot of sand, as shown in fig. 1. After inserting a stirrer and filling the pot with sand, the sand occupies a certain volume in the pot, with a certain shape of the surface. After one cycle, the surface of the sand has changed, and also the sand in the volume was moved. After a second cycle, the surface has changed again, but probably less than after the first cycle. Here, we assume that after a number of mixing cycles, the mixing process reaches a cyclic equilibrium, meaning that particles permute, while the bulk surface shape and volume is unchanged.
In case we knew the permutation of the particles after one cycle, e.g., by means of a permutation matrix, evaluating the mixing after more cycles would boil down to some matrix vector products, in contrast to a DEM simulation that could take hours or even days. The main difficulty now is finding the permutation information.

Mathematical background

One possible approach, to retrieve the permutation information, might be to run the DEM simulation for some n cycles, until the cyclic state of the mixer has been reached, and our assumption seems reasonable. Then run the simulation for one more cycle $n+1$. From the displacements of the particles during cycle $n+1$, we now want to extract the permutation information. As the assumption of pure permutation is usually not satisfied perfectly, the particle positions do not perfectly match after cycles n and $n+1$. Therefore, we need find a suitable assignment for every position after cycle $n+1$ to a position after cycle n. Mathematically this is a discrete optimization problem, i.e. find an assignment of particle positions after cycle $n+1$, to positions after cycle n, s.t. overall the distance between the assigned positions is minimal (in some measure). The difficulty comes from the fact that only exactly one particle position after cycle $n+1$ can be assigned exactly one particle position after cycle n. Simply assigning the positions to their closest counterpart might end up in having two or more particles at the same location, which was physically implausible. Thus the problem is a constrained discrete optimization problem.

Status Quo

Literature provides a suitable algorithm called the Hungarian Method [4]. The original algorithm inherits $\mathcal{O}(n^4)$ time complexity. Later variants, e.g. listed in [3], claim $\mathcal{O}(n^3)$ time complexity, however for large DEM simulations, containing millions of particles, such "classic" approaches are still very expensive, in terms of runtime. Luckily, Quantum Annealing is capable of solving certain optimization problems way faster. A well known formulation of problems for Quantum Annealing is given using the so called *Ising Model* [2]. However, it is not trivial to implement constraints for the Ising Model. This is where you come into play. We are looking for an approach that can be solved, using methods of Quantum Annealing, to match particles in terms of a permutation.

Software

You will be provided data of various DEM simulations, so there is no need for you to get your head around that. You can have access to a state of the art Quantum Annealer by D-Wave [1]. This uses a python interface. So basic programming skills in python are helpful. Apart from that you can use any programming language and/or software you want, we don´t have any restrictions or requirements.

References

[1] D-Wave. Homepage D-Wave Systems. `https://www.dwavesys.com/`, 2023. [Online; accessed 15-May-2023].

[2] D-Wave. What is Quantum Annealing? `https://docs.dwavesys.com/docs/latest/c_gs_2.html`, 2023. [Online; accessed 15-May-2023].

[3] Hungarian Algorithm. Hungarian algorithm. `https://en.wikipedia.org/wiki/Hungarian_algorithm#External_links`, 2023. [Online; accessed 15-May-2023].

[4] H. W. Kuhn. The hungarian method for the assignment problem. *Naval Research Logistics Quarterly*, 2:83–97, 1955.