Coupling COPSS and Evolutionary Optimization

Applications to Inverse Charge Measurement of Dielectric Particles

Xikai Jiang[1], Jiyuan Li[1], Victor Lee[2], Heinrich M. Jaeger[2], Olle G. Heinonen[3,4], and Juan J. de Pablo[1,3]

[1]Institute for Molecular Engineering, University of Chicago; [2]James Franck Institute, University of Chicago; [3]Materials Science Division, Argonne National Laboratory; [4]Northwestern-Argonne Institute for Science and Engineering

INTRODUCTION

- **Why granular particles?** Granular particles are important in a wide variety of contexts, ranging from particulate matter pollution, to industrial handling of pharmaceutical products, food grains, and toner particles.
- **Why are granular particles often charged?** Granular particles often acquire charges due to tribocharging during collisions with other granular particles or container materials.

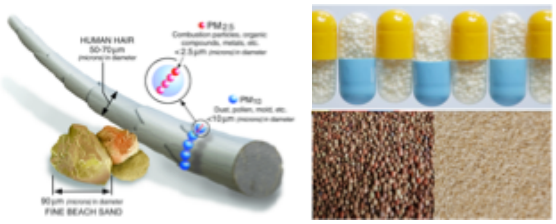

Figure 1. Granular particles and their applications in pharmaceutical and food products.[1]

- **Why do we care about the charges?** Charges on granular particles can significantly affect particles' interactions with their surrounding environment. It is important to know the amount of charges on particles to better understand their dynamics and charge transfer mechanism during contact charging.
- **Why is it difficult to measure charges on individual particles?** Charged granular particles tend to form clusters due to electrostatic, Van der Waals, and capillary forces, etc. It is difficult to separate individual particles and observe their dynamics in these small clusters, and there lack efficient methods for charge measurements.

COUPLING COPSS WITH CMA-ES

- CMA-ES (Covariance Matrix Adaption Evolutionary Strategy) is one type of evolutionary optimization algorithms that does not require derivative information of the fitness function.
- The fitness function *f* to minimize is the difference between trajectories extracted from experiment and simulated trajectories based on electrostatic polarizable force fields[2,3]. In the following formula, N_f is total number of frames excludes the initial configuration, N_p is the number of particles, $\mathbf{r}_{i,trial}(k)$ and $\mathbf{r}_{i,target}(k)$ are the positions of the *i*-th particle at *k*-th frame in the trial and target trajectories, respectively.

$$f = \frac{1}{N_f}\sum_{k=1}^{N_f}\left(\frac{1}{N_p}\sum_{i=1}^{N_p}\left|\mathbf{r}_{i,\mathrm{trial}}^{(k)} - \mathbf{r}_{i,\mathrm{target}}^{(k)}\right|\right)$$

- As validations, we use a simulated trajectory of 10 charged particles as the target trajectory and apply the coupled COPSS-CMA-ES to it to extract charges. 10 particles' charges are assigned as +/- 1, 2, 3, 4, and 5 pC, respectively. The equation of motion for particles is integrated using LAMMPS. The electrostatic polarizable forces fields is used to calculate Coulombic and polarization interactions between particles[2,3].

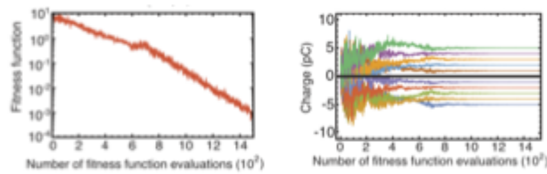

Figure 4. left) Evolution of the fitness function as a function of the number of fitness function evaluations. right) Evolution of charges on 10 individual particles as a function of the number of fitness function evaluations.[6]

EXPERIMENTS ON CHARGED DIELECTRIC PARTICLES

Using a falling high-speed camera, we observe how charged grains in their mutual electrostatic potentials can undergo attractive as well as repulsive Kepler-like trajectories. Our results demonstrate directly how electrostatic interactions provide efficient capturing and aggregation of dielectric grains via multiple collisions in vacuum.

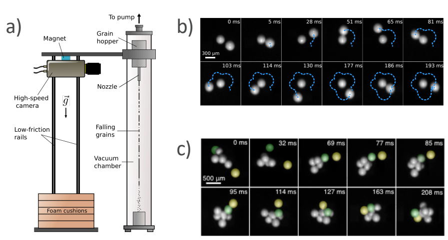

Figure 2. a) Charged ZrO_2:SiO_2 grains fall freely inside a vacuum chamber, while their motion is captured by a co-falling high-speed camera. b) Sequence of frames tracking the interaction of two oppositely charged grains. c) Particle aggregation caused by electrostatic forces.[4]

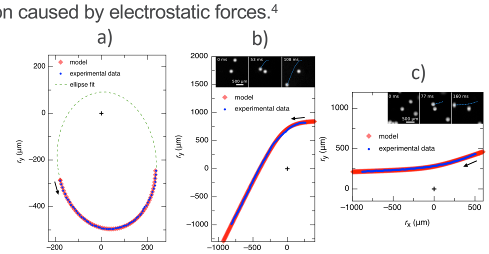

Figure 3. Kepler-like trajectories. a) Elliptical trajectory. b) Attractive hyperbolic trajectory. c) Repulsive hyperbolic trajectory.[4]

APPLYING COPSS-CMA-ES TO EXPERIMENTAL DATA

- We apply coupled COPSS-CMA-ES to experimental trajectories to extract charges on particles in vacuum.
- The inversely calculated charges are found to be within ranges reported in previous experimental measurements.

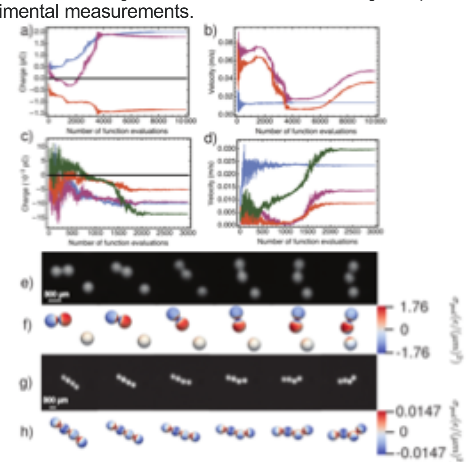

Figure 6. (a) and (b) The evolution of charges and initial velocities of three particles as a function of the number of fitness function evaluations; (c) and (d) the evolution of charges and initial velocities of four particles as a function of the number of fitness function evaluations; (e) and (f) snapshots of three particles moving in a vacuum environment from experiment (e) and simulations (f), and the time interval between two consecutive snapshots is 5 ms; (g) and (h) snapshots of four particles from experiment (g) and simulations (h), and the time interval between two consecutive snapshots is 4 ms.[6]

REFERENCES

[1] *www.epa.gov, en.wikipedia.org, www.howtoaddlikebutton.com*; [2] *J. Qin, et. al., J. Colloid Interface Sci., 469, 237 (2016)*; [3] *X. Jiang, et. al., J. Chem. Phys., 145, 064307, (2016)*; [4] *V. Lee, et. al., Nature Physics, 11, 733-737 (2015)*; [5] *en.wikipedia.org/wiki/CMA-ES*; [6] *X. Jiang, et. al., J. Chem. Phys., 148, 234302, (2018)*

U.S. DEPARTMENT OF ENERGY — Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

THE UNIVERSITY OF CHICAGO · MICCoM · Argonne NATIONAL LABORATORY