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MercuryDPM: Fast, flexible, particle simulations

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We introduce the open-source package MercuryDPM, a code for discrete particle simulations, that we are developing [1]. It simulates the motion of particles, by applying forces and torques that stem either from external body forces, (e.g. gravity, magnetic fields, etc.) or from particle interaction laws. For granular particles, these are typically contact forces (elastic, plastic, viscous, frictional).

MercuryDPM is an object-oriented C++ algorithm with an easy-to-use user interface and a flexible core, allowing developers to quickly add new features. It is parallelised using both MPI and OpenMP and released open-source under the BSD 3-clause licence. Its developers' community has developed many features, including moving (wearable) curved walls (polygons, cone sections, helices, screw threads, level-sets, nurbs, triangulated, etc.); state-of-the-art granular contact models (wet, charged, sintered, melting, cohesive, etc.); specialised classes for common geometries (inclined planes/chutes, hoppers, etc.); non-spherical particles (multisphere, superquadric, bonded particles, deformable clusters); general interfaces (particles/walls/boundaries can all be changed with the same set of commands); liquid droplet/spray models; STL readers for industrial geometries; restarting; visualisation (xBalls and Paraview); a large self-test suite; extensive Doxygen documentation; and numerous tutorials/demos.

For efficiency, it uses an advanced contact detection method, the hierarchical grid. This algorithm has a lower complexity than the traditional linked list algorithm for polydispersed flows, which allows large simulations with wide size distributions.

It also contains a coarse-graining tool: MercuryCG, which is both integrated and usable as a stand-alone tool. Coarse-graining is a novel way to extract continuum fields from discrete particle systems. It ensures by definition that the resulting continuum fields conserve mass, momentum and energy, a crucial requirement for accurate coupling with continuum models. The approach is flexible and the latest version can be applied to both bulk and mixtures; boundaries and interfaces; time-dependent, steady and static situations; and, even experimental data. It is available in MercuryDPM either as a post-processing tool, or it can be run in real-time, e.g. to define pressure-controlled walls.

Finally, MercuryDPM is coupled with the open-source FEM solver oomph-lib via the integrated coarse-graining tool. There are many uses of this coupling (in development), including interaction with elastic bodies, both fully and unresolved fluids, and heterogeneous multiscale coupling.

We will demonstrate the features of the code via several examples including: (wet) highly-polydisperse mixing in a rotating drum, wear on vibrating sieves, and sack filling.

Visit https://mercurydpm.org for more information about MercuryDPM. Training and consultancy is available via our spin-off company MercuryLab (https://mercurylab.org).

References

[1] T. Weinhart, L. Orefice, M. Post, M. P. van Schrojenstein Lantman, I. F. C. Denissen, D. R. Tunuguntla, J. M. F. Tsang, H. Cheng, M. Yousef Shaheen, H. Shi, P. Rapino, E. Grannonio, N. Losacco, J. Barbosa, L. Jing, J. E. Alvarez Naranjo, S. Roy, W. K. den Otter, A. R. Thornton. Fast, flexible particle simulations – An introduction to MercuryDPM. *Computer Physics Communications*, 249, 107129, 2020.