# Molecular dynamics algorithm for simulating a system of ellipsoids on GPU architecture

S.M. Rubio-Largo*, Pedro G. Lind†, R.C. Hidalgo
*Departamento de Física y Matemática Aplicada. Facultad de Ciencias. Universidad de Navarra. Navarra. Spain.
†Institute of Physics. Carl Von Ossiatzky. University of Oldenburg.D-26111. Oldenburg. Germany.

General-purpose computation on Graphics Processing Units (GPU) has recently become an attractive alternative to parallel computing on clusters and supercomputers[1]. We present a hybrid GPU-CPU implementation of an accurate molecular dynamics algorithm for a system of ellipsoids (see Fig. 1).

Following our procedure, the ellipsoids has three translational degrees of freedom and its rotational movement is described by a quaternion formalism[1]. The contact interaction between two generalized ellipsoids ($A$ and $B$) is described by a very accurate force law $\vec{F}_{AB} = F^N_{AB}\cdot\vec{n} + F^T_{AB}\cdot\vec{t}$, which accounts for the elastic and dissipative interactions. Following our approach, the contact plane $\vec{n}$ is analytically obtained by solving the characteristic equation $|A+\lambda B| = 0$ and deducing its corresponding eigenvectors. Based on some algebraic conditions[2–5], we have implemented an accurate algorithm to solve this problem. In our poster we will show several details about this implementation (see Fig. 2).

Finally, we show that the algorithm complies with the statistical mechanical laws by examining the homogeneous cooling of a granular gas of polydisperse generalized ellipsoids. The new algorithm dramatically reduces computational time, compared with a traditional CPU implementation.

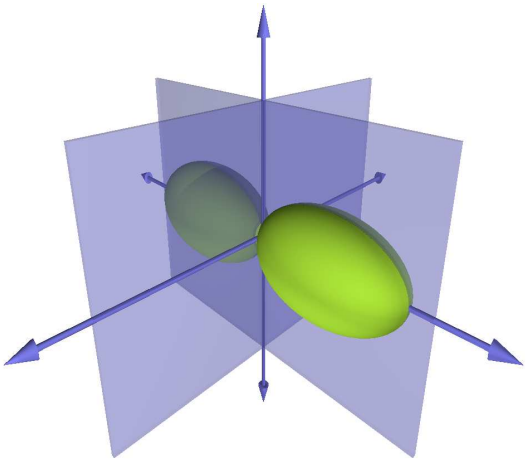

FIG. 1. Normal and tangential contact planes of two colliding ellipsoids.

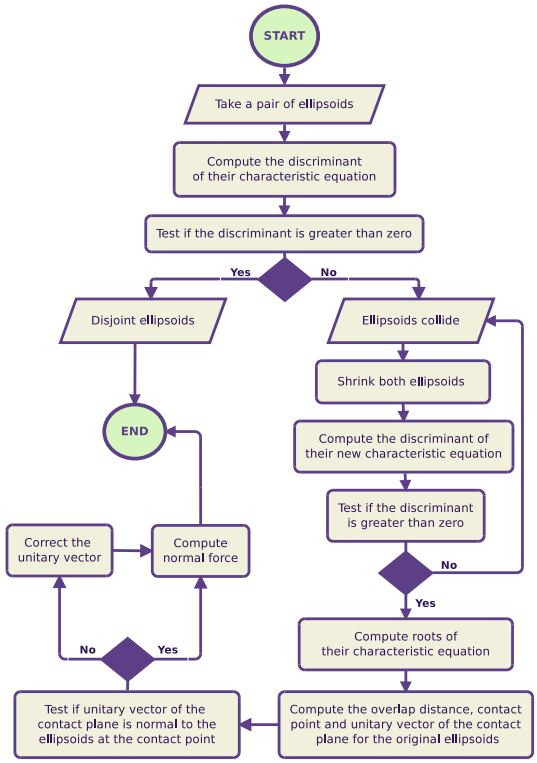


FIG. 2. Flow-chart of the algorithm for computation of normal contact force between two arbitrary ellipsoids.

* srubio.4@alumni.unav.es

[1] R. C. Hidalgo, T. Kanzaki, F. Alonso-Marroquin, and S. Luding. On the use of graphics processing units (GPUs) for molecular dynamics simulation of spherical particles. *AIP. Conference Proceedings* (2013).
[2] W. Wang, Y-K.Choi, B. Chand, Hong kong, M-S.Kim, Seoul, J.Wang, Jinan. Efficient collision detection for moving ellipsoids using seperating planes. *Computing. Springer.* (2004).
[3] Xiaohong Jia, Yi-King Choi, Bernard Mourrain, Wenping Wang. An algebraic approach to continuous collision detection for ellipsoids. *Computer Aided Geometric Design.* (2011).
[4] P. G. Lind. Sequential random packings of spheres and ellipsoids. *Powders and Grains 2009, Proc. 6. Int. Conf. on Micromechanics of Granular Media, pp. 219-222.* (2009).
[5] Reza M. Baram, and Pedro G. Lind. Deposition of general ellipsoidal particles. *Physical Review E 85 041301* (2012).