Molecular dynamics simulation of particles with complex interactions.

Oleg Vasilyev[a b]

[a] *Max-Planck-Institut für Intelligente systeme, Heisenbergstr. 3, D-70569 Stuttgart, Germany*

[b] *Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany*

Molecular dynamics is an important computational tool for studying details of liquid behavior on an atomic scale. Some applications (for example, the study of patchy colloids, virus particles, liquid crystals etc.) requires the simulation of a liquid that contains or consists of particles of complex shape with non-central interactions.

In the simplest case the complex object may be represented as a group of connected atoms. In that situation we should keep in computer memory and perform computations for coordinates and velocities of each atom that requires significant computational efforts.

The numerical algorithm is proposed for the description of the motion of the particle of non-spherical shape with non-central interaction as a single object. The orientation of such object j is described by a quaternion Λ_j. In addition to the standard pair of dynamical equations for coordinates $\vec{r}_j$ and velocity $\vec{v}_j$ we add the second pair of equations for the object orientation $\dot{\Lambda}_j$ and angular velocity $\vec{\omega}_j$. The numerical realization of these equations for a particle orientation and rotation may be realized via standard velocity Verlet scheme.

The description of the complex particle as a single object reduces the computational efforts and increases the speed of computation.