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Method for accelerating simulations of optically bound structures

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Under a coherent illumination, a collection of colloidal micro-particles tends to mutually self-arrange due to the optical forces that arise from the complex scattered field landscape ('optical binding'). With increasing number of particles, the only efficient way to determine their final arrangement is a numerical integration of the equations of motion. The particles usually relax into an equilibrium state, which may be either static, or dynamic with particles following periodic orbits.

The multiple-particle scattering problem can be efficiently solved by the T-matrix techniques, that incorporate the translation- and rotation- matrices, relating EM-field multipolar expansions centered around different particles. Construction of such matrices, at every simulation time-step and for every particle pair, is mostly the 'bottleneck' of the integrator procedure. It can be partially helped by parallelizing the task across multiple processors. For situations when this is not applicable, we propose alternative method to accelerate the calculation.

In our method, the translation matrices corresponding to an inter-particle distance d are factorized into several precalculated translation matrices. The first corresponds to one large spatial step, and is followed by a finite sequence of small discrete steps which geometrically approximate d under a specified tolerance. The final smallest step cannot be tabulated, but its calculation is rapid. The rotation matrices are treated in a similar manner.

Any acceleration resulting from such approach is not guaranteed implicitly. Rather, to ensure numerical stability and accuracy, we first need to tune the method parameters, according to the given particle and beam properties. This involves the cutoff for the maximal-multipole-order, base for the approximating steps pattern or tolerance imposed on the final step length. The main scope of this contribution is to demonstrate functionality of our method on several testing aggregates of spherical particles and, to pin down the optimal tuning.