Towards large-scale parallel simulated packings of ellipsoids with OpenMP and HyperFlow

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1. Introduction

There exist a wide spectrum of experimental and computational algorithms that can produce packings of equal spheres of different porosity and geometrical properties. However, in many applications we have to deal with granular systems of hard particles which are far from spherical. Those non-spherical particles have to be treated in quite different way due to their additional rotational degrees of freedom. In this paper we used the adaptation of the force-biased (FB) algorithm [1] to produce dense random packings of ellipsoids. The reason for this choice is that ellipsoids are excellent model for particles from spherical to very elongated or flat depending on the ratio of their axes.

The objective of this study is to verify the influence of the particle shape and rotation factor on the packing density and the orientational order of the system represented by the nematic order parameter. Moreover, a parallelization of the algorithm makes it possible to simulate bigger sets of ellipsoids (or other shapes as needed). This would be beneficial to both, computational time and statistical value of the results.

We decided to use two-level approach for parallelization: the algorithm is parallelized using OpenMP on a single node, while for the main loop of the computation, which involves multiple runs of the algorithm, we used HyperFlow as a workflow engine.

2. Parallelization with OpenMP and HyperFlow

OpenMP is a natural way to parallelize the force-biased algorithm for packing of ellipsoids. The most compute-intensive part is the calculation of the repulsive "force" defined between any two overlapping particles, which is much more complicated in the case of ellipsoids [2] than for spheres. Using OpenMP allows us to parallelize the threefold nested loops iterating over the particles and the neighboring cells.

HyperFlow [3] is a programming model and execution engine suitable for coordinating the workflow of large-scale computations. For the ellipsoid experiments the first stage of the workflow generates the parameter space, varying such parameters as shape and rotation scaling factors. In the second phase it executes the packing algorithm for each point in the parameter space as a separate task, repeating it several times with varying random seeds in order to gather better statistics of the results. The final (reduce) phase computes the averages of the runs and produces a summary file with output statistics. It is also possible to add another phase for visualization of the results using POVRay rendering program.

3. Results

Parallelization of algorihtm using OpenMP was testes on Zeus cluster, on a node with two 6-core Intel Xeon L5640 processor (12 cores total) with Intel compiler. The results in Fig. 1a shows that it is possible to achieve a speedup of over 10 on 12 cores, which we consider as a success, given the little effort of using OpenMP.

Execution of the large scale experiments with HyperFlow on Zeus cluster require setting up the workflow environment and using a pilot job mechanism to submit worker processes with HyperFlow executors, and a parallel file system for data exchange. Since the execution is pleasantly parallel, the speedup depends on the number of pilot jobs submitted and processed by the queueing system. In our early experiments we were able to run jobs with 40 nodes of 12 cores, utilizing total of 480 cores in parallel, which we consider promising.

Fig. 1b shows the dependence of the final packing density on the ellipsoid shape. It follows that the highest packing densities were obtained for $\beta = 0.5$ and α around 1.7. The practical implication is that a small deviation in shape from spherical may increase the density significantly without crystallization.

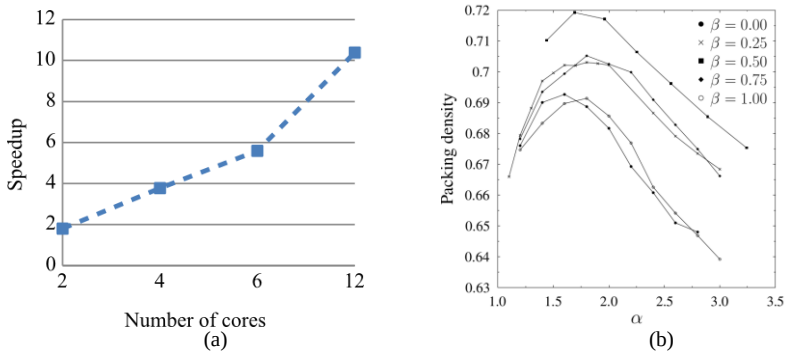

Fig. 1. (a) Parallel speedup on a single node for a system of 10000 molecules; (b) density for packings of 1000 ellipsoids with ratios between the semiaxes of $1 : \alpha^{\beta} : \alpha$ ($\alpha \geq 1$, $0 \leq \beta \leq 1$)

4. Conclusions and future work

The two-level parallelization approach of using OpenMP and HyperFlow proved to be a good match for the problem of large-scale packing of ellipsoids and can be used for other problems of similar nature. The initial results obtained give us the better understanding of the parameter space and their influence on the resulting packing density. Future work includes more large-scale studies e.g. with particle size distributions, as well as better automation of workflow execution and optimization of execution on clusters and clouds.

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References

1. Mościński, J., Bargieł, M., "C-language program for simulation of irregular close packing of hard spheres", Computer Physics Communication **64** (1991) 183-192.
2. Donev, A., Torquato, S., Stillinger, F.H., "Neighbor list collision-driven molecular dynamics simulation for nonspherical particles. II. Applications to ellipses and ellipsoids", Journal of Computational Physics **202** (2005) 765-773.
3. B. Balis, "HyperFlow: A model of computation, programming approach and enactment engine for complex distributed workflows" FGCS, Sep. 2015 (accepted)