Monte Carlo simulations of self-assembly of pentagons

Unmukt Gupta and Vikram Thapar

I. BACKGROUND AND MOTIVATION

At present, a major focus in material science is the use of Monte Carlo (MC) simulations of self-assembly of polygonal/polyhedral particles to help engineer novel materials from colloidal nanoparticles[1-5]. Recent simulations[3-5] have provided a partial roadmap of the "mesophases" (phases with partial structural order) that can be expected for different types of polyhedral/polygonal particles. Some examples include MC simulations of self-assembly of hard cubes[1] show that cubes undergo a transition from disordered phase to ordered phase (simple cubic) via a mesophase named as cubatic phase characterized by high orientational symmetry and weak translational symmetry.

The method to simulate self-assembly of hard particles ("hard" particles belongs to the class of particles which only has excluded volume interactions) of any shape involves firstly placing the N number of particles with random positions and orientations in a periodic box and then slowly compressing the box (same as increasing the pressure) while performing different types of MC moves to explore different positions and orientations of particles. For example one move that is commonly used is translational move, which is performed by choosing a particle at random and displacing it by a certain amount. The acceptance/rejection of a move is dictated by whether the displaced particle overlaps with its neighbors. The overlapping of a particle with its neighboring particles is performed through separating axis theorem, which happens to be the computational bottleneck of the MC simulation. Also, the serial implementation of MC algorithm will make the simulations computationally infeasible as the size of the system increases. These issues motivate us to firstly perform the single core optimization of overlapping algorithm and then parallelize our MC simulation by using the idea of domain decomposition (note that the similar idea is implemented before by Ref. 6).

II. OBJECTIVE

1) The serial implementation of MC code, which is currently used by our group, is written in Fortran 77. Our first objective is to transfer the code into C++.

2) We will then aim to perform the single-core optimization of the serial code, which involves optimizing the step that checks the overlapping of a particle with its neighbors using separating axes theorem.

3) We will then write a parallelized version of MC code using OpenMPI.

4) The testing of a code will be performed on understanding the self-assembly of different type of pentagons that tessellate space (shown in Fig. 1).

III. REFERENCES

[1] G. M. Whitesides and M. Boncheva, Proc. Natl. Acad. Sci. U.S.A. **99**, 4769 (2002).
[2] S. C. Glotzer and M. J. Solomon, Nature Mate. **6**, 557 (2007).
[3] U. Agarwal and F. A. Escobedo, Nature Mater. **10**, 230 (2011).
[4] P. F. Damasceno, M. Engel, and S. C. Glotzer, Science **337**, 453 (2012).
[5] A. P. Gantapara, J. de Graaf, R. van Roij, and M. Dijkstra, Phys. Rev. Lett. **111**, 015501 (2013).
[6] J. A. Anderson, E. Jankowski, T. L. Grubb, M. Engel and S. C. Glotzer, J. Comp. Phys., **254**, 27 (2013).

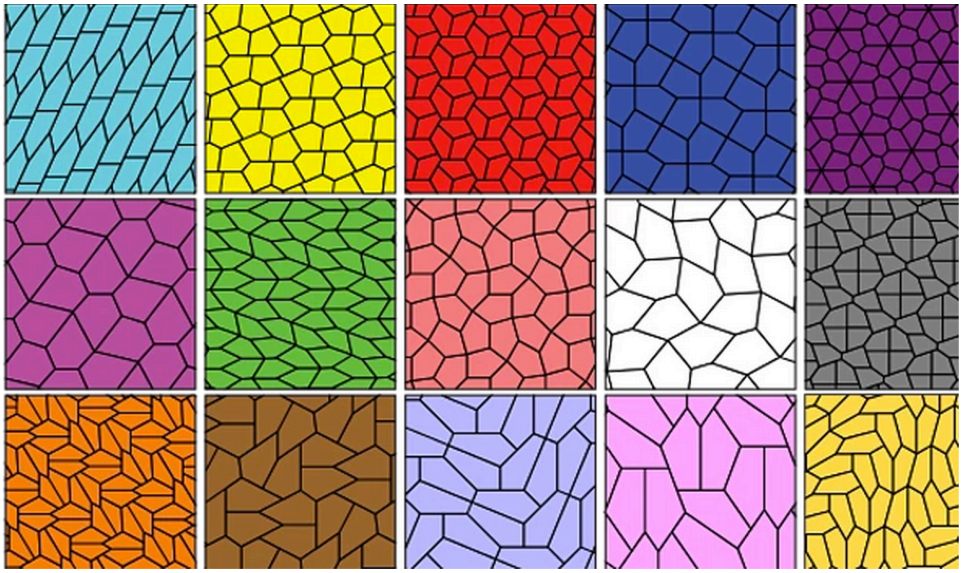

Figure 1 Different types of pentagonal tilings.