Complexity mini-project proposed by Alessandro Troisi (Chemistry)

Designing quasi crystalline molecular self-assembly using cellular automata

Molecules self-assemble in 2D forming many different patterns arising from their nearest neighbour interaction.[1] It is possible to design molecules with complementary interactions which would recognize each other like the adenine-tymine and the guanosyne-cytosine pairs in DNA. These complementary interactions are due to hydrogen bonds (HB) formed between HB donor and HB acceptor groups (the detailed chemistry will not be considered in this mini-project which does not require any chemistry background). We can indicate with "1" the HB donor and "0" the HB acceptor so that we assign a binary number to any sequence of HB donor and acceptors in a molecule. It is possible to synthesize a molecule with HB donors and acceptors and with a global shape resembling an equilateral triangle (or other regular polygons). It is chemically possible to arrange 1s and 0s (donors and acceptors) in all possible ways around the molecule. Many molecules may self-assemble in larger structures if the interaction is suitable. The example below considers many copies of the same molecule but one can consider a set of different molecules as 'tiles'.
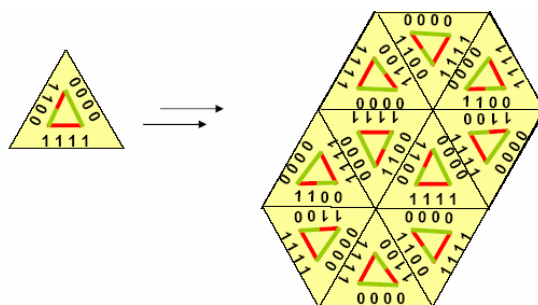
We would like to explore all the possible self-assembled structures (with fixed maximum number of HB) in a systematic way and answer the following research questions:

(i) Are there any *infinite non periodical* structures [2,3] for the model above?

(ii) What fraction of the resulting structures is zero dimensional (i.e. finite size), 1 D o 2 D?

The calculation could be implemented as a 2D *cellular automata* (for students more oriented toward computer science) using a procedure similar to the classification of cellular automata behaviour of the classical paper of Wolfram [4]. Alternatively (for more physics oriented students) a Metropolis Monte Carlo approach can be used to describe the phase diagram of these systems. The importance of this result for chemistry is related to the possibility of designing and predicting the existence of 2D quasi-crystal [2] (i.e. regular but nor periodical structure) based on simple molecules (they are not known to date). Another source of interest is the connection between this problem and the idea of *molecular computing* (i.e. using self-assembly to achieve ultra-parallel computation) [5] itself related (unsurprisingly) to the tiling problem [6].

[1] Barth, J. V. et al Nature 437, 671–679 (2005).
[2] D. Shechtman, et al. Phys. Rev. Lett. 53, 1951–1953 (1984)
[3] http://www.ics.uci.edu/~eppstein/junkyard/penrose.html
[4] S. Wolfram: Rev. Mod. Phys. 55, 601-644 (1983)
[5] Winfree, E. et al Nature 394, 539–544 (1998).
[6] Culik, K. Discrete Mathematics 160, 245–251, (1996)