Algorithmic Self Assembly and Molecular Computing: New Challenges in Performance Evaluation

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Many claim that a glimpse of the future would show a major effort in evaluating the performance of computing paradigms in which myriad particles function autonomously in a process known as algorithmic self assembly. Currently, the most successful such process, originating in the famous experiments of Adleman, is a biochemical one in that molecules fashioned from DNA are the particles of choice, since they are manipulable and abundant in nature. The material covered by this tutorial draws from biology, chemistry, computer science, and mathematics, but the presentation will be pitched at a low level, with an undergraduate degree in any of the disciplines served by the Working Group being sufficient background, The mathematics will be lightweight, with proofs rarely needed; when one does appear, it is brief and intuitive. A dominant theme of performance analysis is the formulation of fluid limits. Topics along with brief synopses are as follows:

Part I - Molecular computation by self assembly

1. Synthesis of DNA molecules that perform elementary logic, the double crossover (DX) molecule as an example, the encodings of four sticky ends (short DNA strand segments) determine the operation.
2. Modeling the DX molecule by a Wang-like tile, and hence computation as tilings of geometric figures.
3. Programs as sets of tile types. Illustration of elementary computations: the XOR molecule, parity check (mod-2 sum) of a bit string, and counting, implementing general logic circuits, Turing universality.
4. Issues of program-size and time complexity. Abstraction to tiling rectangles, extension of fixed borders to growing borders.
5. Evaluating performance in terms of computing (e.g., rectangle tiling) times, The TASEP-correspondence to tiling, fluid-limit results, explicit measures of parallelism.
6. Dealing with errors, a pulsing method applied to rectangle tiling, associating computing times with maximal-length monotone subsequences.

Part II - Self assembly and chemical kinetics

1. The linear-polymerization model of Adleman, et al.
2. Reaction rate equations (nonlinear, first-order ODEs) applied to self assembly of target polymers from an all-monomer initial state. Notions of yield and waste.
3. A discrete event simulation model and its properties.
4. Triangle self-assembly example, explicit results for self assembly times.
5. The existence of phase transitions where waste in the absorbing state vanishes, sufficient conditions.
6. Extension to reversible self assembly, controls to minimize self assembly times.