Counting with thermodynamic binding networks

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An increasing demand for chemical systems and mechanisms that implement complex computation requires that computation be efficient, not just in the time to compute a result, but also in the amount of fuel compounds used during the calculation. Many existing chemical computational systems rely on kinetic controls and driving forces; however, it is a basic result of physical chemistry that chemical systems will also be driven to a thermodynamic equilibrium. Because of this, unavoidable errors caused by thermodynamic driving forces can accumulate in the system. One way to ensure that the computation is not thermodynamically driven to error is to design a mechanism in which the states of the computation are energy neutral; that is, that they should be equivalent in energy by some measure and that the pathways between them are reversible.

Under the constraint of energy neutrality, a known result is that with space proportional to the number of steps in the computation, DSDs are Turing-universal \cite{3}. Thus, a natural question to follow is whether such computation can be conducted in a space efficient way. A result by Thachuk and Condon \cite{4} showed that space and energy efficient computation is possible in DNA strand displacement systems. They accomplish this by re-using “fuels”; the waste product of a given reaction is also a fuel for a later reaction \cite{2}. In this manner, an exponential number of states can be realized without also using a proportional amount of fuel or accumulating a proportional amount of waste. However, DSD systems rely heavily on geometry and on kinetic controls, and so a natural question is whether or not such a result relies directly on the geometry and kinetics of the system.

To address this question, we will look at a kinetic variant of the thermodynamic binding network (TBN) model \cite{1}, which considers only the energy barriers that arise from the number of bonds formed/broken and the entropic effect of colocating separate complexes at given steps in a reaction sequence. We are interested in the question if such a “recycling” method \cite{2} is applicable in the kTBN model, and will answer this in the affirmative by constructing an \( n \) bit binary (Gray code) counter, which advances as a chain through the energy wells of \( 2^n \) unique stable states, while using \( \Theta(n) \) monomers and \( \Theta(n^2) \) domains.

This result is interesting because the results do not rely upon the specific nature of the implementing substrate, and so it suggests that the same behavior could be extended to a wide variety of chemical implementations.

References

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