

Title: Thermodynamics of a multistranded scaffolded DNA computer

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Abstract:

Polynomial time dynamic programming algorithms play a crucial role in the design, analysis and engineering of nucleic acid systems including DNA computers and DNA/RNA nanostructures. However, in complex multistranded or pseudoknotted systems, computing the minimum free energy, and partition function of nucleic acid systems is NP-hard. Intuitively, the minimum free energy is the energy of the most favoured secondary structure(s) of the system, and the partition function is a Boltzmann-weighted sum of the energies of every structure--typically used as a normalisation factor to calculate the structure probabilities at equilibrium. Despite being NP-hard, multistranded and/or pseudoknotted systems represent some of the most utilised and successful systems in the field. This leaves open the tempting possibility that perhaps many of the multistranded and/or pseudoknotted systems we wish to engineer fall into restricted classes that do in fact have polynomial time algorithms, but we've just not found them yet.

Here, we give a polynomial time algorithm for minimum free energy and partition function for a restricted kind of multistranded system called the 1D scaffolded DNA computer. The scaffolded DNA computer is a thermodynamically favourable model of computation developed in our group that is computationally expressive; previously shown to simulate finite state machines in 1D and Boolean circuits in 2D, and amenable to DNA storage applications.