Solving Hard Computational Problems via *In Silico* Molecular Catalysis

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Abstract

Enormously difficult computational tasks are now hallmarks of several newly emerged disciplines such as molecular genetics (genomics), and information technology; tasks that have long been needed in the fields of robotics and operations research. NP-hard problems of combinatoric nature such as shop floor control and scheduling (i.e. job shop scheduling) distribution of goods and services (i.e. vehicle routing), aircraft landing and scheduling, product design (i.e. VLSI layout), DNA sequencing, and many others are of real world importance. The combinatoric nature of solutions varies with operand complexities and grows exponentially with the size of the problem thus making it impossible to draw solutions using deterministic algorithms within a reasonable time frame.

Solutions to combinatorial optimization have been studied extensively. Graph-based heuristics such as branch and bound, as well as distributed multi-agent based algorithms such as genetic algorithms, memetic algorithms, tabu search, simulated annealing, simulated jumping, neural networks, and swarm intelligence have been used to accurately find time-restrained optimal and near optimal solutions.

In recent years, the chemical metaphor has emerged as a computational paradigm. This is because chemical and biochemical systems of living organisms have been shown to possess inherent computational properties. In this paradigmatic framework, objects such as atoms or molecules are considered as data or solutions; while interactions (i.e. molecular collisions or reactions) among and between objects are defined by an algorithm.

In our contribution, we designed a distributed stochastic algorithm that simulates reaction systems wherein the molecular species are being represented either by a human genomic contig panel, a Hamiltonian cycle, or an aircraft landing schedule. We

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created a chemical universe governed by reactions that can alter genomic sequences, re-order Hamiltonian cycles, or reschedule an aircraft landing program. We considered molecular masses as metrics of goodness of solutions such as radiation hybrid (RH) vector similarities, costs of Hamiltonian cycles, and penalty costs for landing an aircraft before and after target landing times.

This paper is centered on the introduction of the basic ideas of simulated catalytic reactions. Tested by solving in tandem with deterministic algorithms, this novel method was demonstrated to have superior processing rate for combinatronics of finding the minima RH vector similarities of genomic data, minima costs in Hamiltonian cycles of the traveling salesman, and minima costs for landing aircraft before or after target landing times.