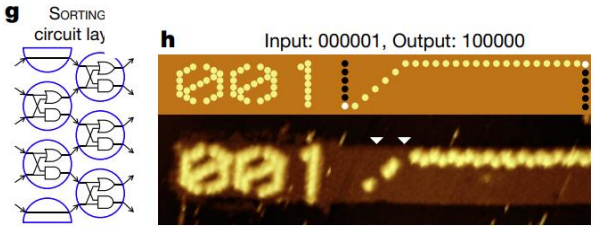
ECS 289A: Theory of Molecular Computation



Spring 2023

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The computing revolution of the 20th century focused on the systematic manipulation of information. In this century, a new revolution is underway, and its goal is the *systematic manipulation of matter* at the molecular level. DNA nanotechnology especially has established several basic low-level tools, such as tile assembly, DNA origami, and strand displacement, out of which more sophisticated molecular systems can be composed.

A traditional programming language is a simplified abstraction of the possible behaviors of the several billion low-level wires and transistors in a modern electronic computer. By analogy we introduce theoretical abstractions of molecular systems suitable for programming them with desired behavior. We emphasize formal reasoning and proofs to discover fundamental limits in the ability to engineer artificial molecular systems.

The course will cover the theory of chemical reaction networks, molecular circuits, DNA self-assembly, thermodynamics, and connections to the field of distributed computing.

Meeting time: MWF 10:00am – 10:50am

Location: Hoagland 113

Course registration number: 40818

https://web.cs.ucdavis.edu/~doty/ecs289-2023/

Prerequisites

ECS 120 or equivalent, such as Chapters 1, 3, 4, 7 of Sipser's *Introduction to the Theory of Computation*,

Or permission of instructor

Basic probability: random variables, expectation.

No chemistry/biology background needed.

Grading

Homework/Project/Participation (no exams)

Syllabus

Week 1	algorithmic self-assembly I
Week 2	algorithmic self-assembly II
Week 3	chemical reaction networks I
Week 4	chemical reaction networks II
Week 5	chemical reaction networks III
Week 6	population protocols
Week 7	DNA strand displacement/origami
Week 8	DNA sequence design
Week 9	thermodynamic binding networks
Week 10	project presentations

Textbook

No textbook. Some papers will be assigned reading.

Left image: *Crystals that count! Physical principles and experimental investigations of DNA tile self-assembly,* Constantine Evans, Ph.D. thesis, California Institute of Technology, 2014. The atomic force microscope image is of a ribbon made from DNA strands that count in binary; each bump is a streptavidin molecule, which are designed to attach to the DNA strands that represent the bit 1, to help read out the bits. **Right image:** *Diverse and robust molecular algorithms using reprogrammable DNA self-assembly*, Woods, Doty, Myhrvold, Hui, Zhou, Yin, Winfree, Nature 2019. These DNA molecules implement the even-odd transposition sort algorithm on a binary string, moving all 1's to one side.