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Programmable assembly: inverse design of materials from discrete components

Particles and discrete objects on the scale of nanometres to micrometres, such as colloids, DNA bricks, proteins, transistors, etc, are increasingly being used as building blocks for new materials, with a variety of applications such as in optics, drug delivery, energy harvesting, and nanorobotics. A goal for theory and simulation is to build algorithms and design principles to find the building blocks that assemble into a structure of interest. This is a challenge due to the high-dimensionality of the systems of interest, the presence of strong noise, and the sometimes far-from-equilibrium conditions, making standard optimization algorithms inapplicable and demanding new approaches. I will describe our group's progress on finding optimal conditions for "addressable self-assembly", a system of particles where each building block is distinct and has a specific location in the target structure, and that assembles spontaneously under thermal fluctuations. I will show how using tools derived from machine learning can generate novel solutions for small systems, and will point out challenges in extending these tools to more complex systems.