Seminar/Talk

Self-assembling kinetics: accessing a new design space with differentiable statistical-physics models

Carl Goodrich

Host:

The inverse problem of designing component interactions to target emergent structure is fundamental to numerous applications in biotechnology, materials science, and statistical physics. Equally important is the inverse problem of designing emergent kinetics, but this has received considerably less attention. Using recent advances in automatic differentiation, I will show how kinetic pathways can be precisely designed by directly differentiating through statistical-physics models, namely free energy calculations and molecular dynamics simulations. We will consider a few systems that are crucial to our understanding of structural self-assembly, including bulk crystallization and small nanoclusters, where we are able to assemble precise dynamical features using gradient information. Moreover, we use this approach to learn non-trivial features about this new, high-dimensional design space, allowing us to accurately predict when multiple kinetic features can be simultaneously and independently controlled. These results provide a concrete and generalizable foundation for studying non-structural self-assembly, including kinetic properties as well as other complex emergent properties, in a vast array of systems.

Monday, May 17, 2021 02:00pm - 03:00pm

Online Event ()

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