

"Putting the Statistics back in Statistical Mechanics"

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Statistical mechanics provides the connection between molecular scale details and macroscopic thermodynamic properties. Traditionally, analytical approaches such as mean field approximations and integral equations have been used to simplify the complicated multidimensional integrals statistical mechanics gives us. As computers have become increasingly powerful, they have allowed us over to explore the statistical mechanics of more and complicated systems by instead sampling from physical probability distributions. In this talk, I will examine ways that powerful new (and not-so-new!) techniques borrowed from statisticians can be reapplied in physical contexts to accelerate molecular simulations and more efficiently analyze the simulation data collected.