APPLIED MATHEMATICS COLLOQUIUM

A Theoretical Examination of Diffusive Molecular Dynamics

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Abstract: We give a mathematical formulation of diffusive molecular dynamics. The idea of diffusive molecular dynamics is to first minimize an approximate free energy of the system with respect to the mean atomic coordinates (averaging over many vibrational periods), and then to perform a diffusive step where atoms and vacancies (or a solute in a solvent) flow on a diffusive time scale. One of the tools we make use of in this analysis is relative entropy, or the Kullback-Leibler divergence (KL).

This is joint with Gideon Simpson and David Srolovitz.

Monday November 9, 2015
4:30 PM
Room E17-122

Applied Math Colloquium: http://www-math.mit.edu/amc/fall15/
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