Courant Institute of Mathematical Sciences

Mathematics Colloquium February 6, 2012

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Title: Nonequilibrium Thermodynamics for Mathematicians

Abstract:

Simplification should not be regarded as a necessary evil required to solve problems that are computationally too large. Simplification rather is the art of focusing on the essence of a problem and it hence leads to deeper understanding. Proper simplification should lead to physically meaningful equations with mathematically well-established solutions. It is the task of nonequilibrium thermodynamics to suggest the structures that guarantee the soundness of simplified equations. The thermodynamic structure behind sound equations is presented and illustrated by examples.

Once we know the structure of sound simplified equations, we need to fill them with life. Systematic coarse graining rules for relating models on different levels of description are offered by statistical mechanics. I suggest how efficient simulations for relating parameters should be designed, in particular, to bridge many orders of magnitude in time scales. I would further like to offer some (thought-)provoking comments on the relationship between coarse graining and mathematics.

The geometric formulation of thermodynamically sound equations is not only a tool in formulating models and performing simulations, but it moreover is the key to generalizations, for example, to accommodate boundary conditions or quantum dissipation.