Spontaneous Violations of the Clausius-Duhem Inequality

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Already in the 19th century, J.C. Maxwell recognized that "*the second law is of the nature of strong probability … not an absolute certainty*". However, it has only been in the past three decades that theoretical, simulation, and experimental results in physics in support of that old statement have been obtained. Fundamentally, there is a non-zero probability of negative entropy production rate on very small length and time scales. Thus, the Second Law needs to be replaced by the fluctuation theorem [1]. First, we discuss the consequences of these results for the axioms of continuum mechanics, arguing in favor of a framework relying on stochastic functionals of energy and dissipation [2,3] with random field coefficients of non-conservative responses which are required to satisfy the positive definiteness only on average. With the microstructure-based fluid mechanics (classical and micropolar), this framework is then employed to examine the violations of Clausius-Duhem inequality in Couette flows of molecular [4,5] and granular media [6,7]. The boundary between regimes of violations and non-violations is mapped in the parameter space. Extensive sampling of LAMMPS-generated realizations of Couette flows of granular media allows determination of the dissipation function as a wide-sense stationary random process with near-Gaussian properties and non-trivial fractal and Hurst properties.

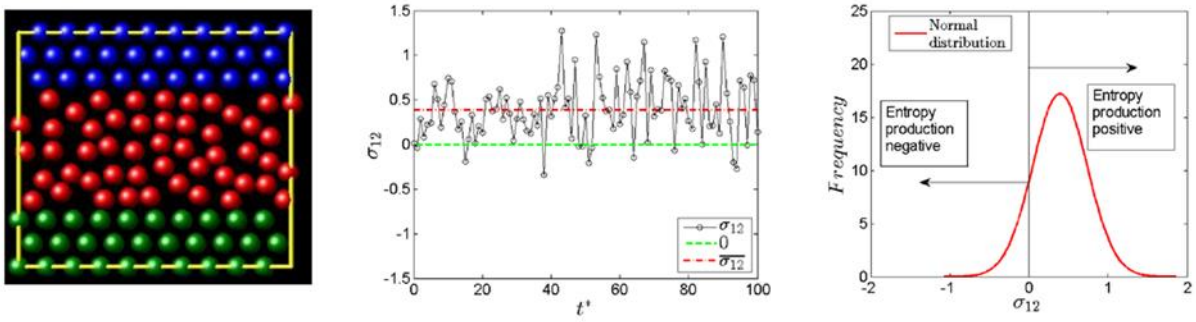

Figure: (a) Molecular dynamics simulations using LAMMPS of Couette flows in channels with (a) 50 particles. (c) Sample shear stress history with negative excursions. (e) Histogram (probability density) of shear stress. Note: with system size increasing, the scatter tends to vanish, signifying mechanics without violations of second law of thermodynamics.

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