The Fluctuation Theorem: Simulation, Theory and Experiment

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We discuss the close symbiotic relationship that algorithm development has played in the development of new fundamental science. Thermodynamics describes the framework within which all macroscopic processes operate. Until the discovery of the Fluctuation Theorem [1], there was no equivalent framework for small (nano) systems observed for short times. The Fluctuation Theorem provides a generalisation of the Second Law of thermodynamics, that applies to finite systems observed over finite times. The development of this theorem was enabled by development on nonequilibrium molecular dynamics simulation algorithms in the 1980's. These algorithms were convenient dynamical systems that were so close to experimental systems that they enabled the derivation is this generalization of the Second Law of thermodynamics. This extension was first tested with computer simulation[2] and later verified in the laboratory[3]. The Fluctuation Theorem places limits on the operation of nanomachines and biological processes taking place in small organelles. The Theorem states that as "engines" are made ever smaller, the probability that they will operate thermodynamically in reverse, increases exponentially with the size of the system and the duration of operation.

References

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