

Enhancing the understanding of entropy through computation

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(Submitted on 26 Jul 2011)

We devise a hierarchy of computational algorithms to enumerate the microstates of a system comprising N independent, distinguishable particles. An important challenge is to cope with integers that increase exponentially with system size, and which very quickly become too large to be addressed by the computer. A related problem is that the computational time for the most obvious brute-force method scales exponentially with the system size which makes it difficult to study the system in the large N limit. Our methods address these issues in a systematic and hierarchical manner. Our methods are very general and applicable to a wide class of problems such as harmonic oscillators, free particles, spin J particles, etc. and a range of other models for which there are no analytical solutions, for example, a system with single particle energy spectrum given by $\{\epsilon_{p,q}\}$ $(p,q) = \epsilon_0 (p^2 + q^4)$, where p and q are non-negative integers and so on. Working within the microcanonical ensemble, our methods enable one to directly monitor the approach to the thermodynamic limit ($N \rightarrow \infty$), and in so doing, the equivalence with the canonical ensemble is made more manifest. Various thermodynamic quantities as a function of N may be computed using our methods; in this paper, we focus on the entropy, the chemical potential and the temperature.

Comments: Trisha Salagaram and Nithaya Chetty, "Enhancing the understanding of entropy through computation" Am. J. Phys. (in press)

Subjects: **Computational Physics (physics.comp-ph)**; Popular Physics (physics.pop-ph)

Cite as: [arXiv:1107.5156](https://arxiv.org/abs/1107.5156) [physics.comp-ph]

(or [arXiv:1107.5156v1](https://arxiv.org/abs/1107.5156v1) [physics.comp-ph] for this version)

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