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Microcanonical entropy inflection points and their relationship to cooperative behavior MICHAEL BACHMANN, Center for Simulational Physics, The University of Georgia, Athens, GA 30602 — We discuss a method for the systematic classification of the analogs of phase transitions in finite systems. This completely general analysis, which is applicable to any physical system, is based on the microcanonical entropy and its energetic derivative, the inverse caloric temperature. Inflection points of this quantity signal cooperative activity and thus serve as distinct indicators of transitions. The microcanonical entropy as the logarithm of the density of states is the fundamental quantity of statistical mechanics and can directly be obtained by means of contemporary generalized-ensemble computer simulation methodologies. Nowadays, the statistics achieved by employing these methods is sufficiently high such that the accuracy of the data allows for a very precise microcanonical analysis of "phase" transitions, even in mesoscopic systems, where finite-size and surface effects are significant. This can hardly be achieved by the far more prevalent conventional canonical approach. We demonstrate the power of this method in exemplified applications to long-standing problems of polymer and protein nucleation transitions.

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