

Abstract Submitted
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Wang-Landau or Statistical Mechanics GREGORY BROWN, Oak Ridge National Laboratory / Florida State Univ, DONALD M. NICHOLSON, MARKUS EISENBACH, KH. ODBADRAKH, Oak Ridge National Laboratory — The Wang-Landau algorithm and its variations provide a method for estimating a self-consistent density of states – or equivalently the entropy – of a system with many degrees of freedom. Possible benefits from generating a self-consistent estimate of the entropy and its derivative are presented for models with both discrete and continuous values of the energy. In addition, the advantage of computing thermodynamic quantities as derivatives of the estimated entropy over summation over the density of states is shown.

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