Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Introducing the Reduced Monte Carlo Scheme (RMCS) with Application for Hard Sphere Equation of State and First Order Phase Transition UDUZEI EDGAL, Old Dominion University, DAVID HUBER, University of Wisconsin-Madison — This is the first demonstration of a novel approach, the "Reduced Monte Carlo Scheme" (RMCS), developed for the investigation of the statistical thermodynamic properties of multi-scale material systems (classical and quantum) over the entire temperature and density range, with arbitrary inter-particle interactions. RMCS employs a new ensemble, the "nearest neighbor ensemble" involving the PDF for "n" nearest neighbor configurations. RMCS results for the equation of state of the hard sphere system from low densities to densities in the neighborhood of closest packing will be discussed. The power of RMCS as a materials investigative tool will be tested within the region of first order phase transition as well as for correct asymptotic behavior of the solid phase equation of state. Early results show that RMCS provides accurate results in the fluid phase employing "small" n values, thus suggesting that RMCS may provide a highly efficient computational scheme in contrast to traditional Monte Carlo methods which normally require "large" systems for computation. Also to be discussed briefly, is the outlook for the development of the quantum version of RMCS for quantum systems.

Uduzei Edgal
Old Dominion University

Date submitted: 21 Nov 2007   Electronic form version 1.4