Employing Multiple GPU Devices over a Network to Investigate Multi-dimensional Mixtures of Hard Hyperspheres using MPI and CUDA

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A Monte Carlo code that is used to investigate the equilibrium properties of mixtures of hard hyperspheres in four dimensions has been modified to execute on multiple GPU devices. The Monte Carlo code was written in C and the GPU's were programmed using the CUDA extensions to the C language. The four dimensional domain has been subdivided into subdomains which are assigned to the host machines on the network. The majority of the random walk performed by the hyperspheres is computed on the GPU devices. When a hypersphere moves from one subdomain to another subdomain, this necessitates communication using MPI. A substantial speedup of the Monte Carlo code is observed compared with the original sequential code.