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Enhancing large-scale docking simulation on heterogeneous systems: an MPI vs rCUDA study

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Abstract

Virtual Screening (VS) methods can considerably aid clinical research by predicting how ligands interact with pharmacological targets, thus accelerating the slow and critical process of finding new drugs. VS methods screen large databases of chemical compounds to find a candidate that interacts with a given target. The computational requirements of VS models, along with the size of the databases, containing up to millions of biological macromolecular structures, means computer clusters are a must. However, programming current clusters of computers is no easy task, as they have become heterogeneous and distributed systems where various programming models need to be used together to fully leverage their resources. This paper evaluates several strategies to provide peak performance to a GPU-based molecular docking application called *METADOCK* in heterogeneous clusters of computers based on CPU and NVIDIA Graphics Processing Units (GPUs). Our developments start with an OpenMP, MPI and CUDA *METADOCK* version as a baseline case of cluster utilization. Next, we explore the virtualized GPUs provided by the *rCUDA* framework in order to facilitate the programming process. rCUDA allows us to use remote GPUs, i.e. installed in other nodes of the cluster, as if they were installed in the local node, so enabling

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