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Grid Enabled MPI (GEM) System：Toward Maximum Computational Efficiency in Molecular Docking and Virtual Screening

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Abstract

The increasing economic pressure on the pharmaceutical industry to develop new drugs in a faster and more efficient way than in the past has led to the development of a large number of new methods aimed at a more efficient and rapid lead structure discovery process. One of the key aspects of parallel computing is clusters using MPI that distributing a large computational task onto several machines. Another approach to get high computing power at low cost is grid computing. However, it would be very much attractive to integrate parallel and grid computing approaches in achieving the most effective solution.

Here, we describe Grid Enabled MPI (GEM) System that integrates individual clusters at different geographic locations as grid nodes for virtual screening. In GEM System, each node will be a single host or a cluster with its own parallel processing environment with MPI interface.

The efficiency of GEM System was evaluated by molecules docking. All 5,000 compounds were screened within UCSF DOCK. It took about 1,357,914 seconds in standalone mode and 87,626 seconds on 20 nodes GEM system, respectively.

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