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An Environment for Solving Large Scale Optimization Problems on the Grid

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The paper presents the BNB-Grid environment for solving large scale optimization problems on the grid. The environment supports Branch-and-Bound and heuristic search strategies and runs on distributed systems consisting of different nodes ranging from PCs to large publicly available supercomputers. BNB-Grid efficiently copes with difficulties arising in such systems: the software diversity, unreliability of nodes and problems with batch (queuing) systems.

Conclusions and Future Work

In the paper we described BNB-Grid –a programming environment for solving large scale optimization problems on a distributed system consisting of diverse nodes ranging from PCs to publicly available supercomputers. The efficiency of the proposed approach has been demonstrated on a hard molecular conformation problem. Our current work is focused on an interface between our system and the gLite API in order to leverage consolidated computing power by adding EGEE facilities.

Keywords

grid computing, global optimization

Impact

The distinctive feature of our approach is the use of different communication packages on different levels: on the top level we use ICE middleware and within a single cluster we use MPI. The approach imposes minimal requirements on the computing element software and efficiently utilizes the communication facilities of each cluster by using native message passing libraries. The BNB-Grid system also has an intellectual computing space manager based on a rigorous mathematical model that allocates nodes by submitting jobs to different supercomputers. This component works in cooperation with load-balancer that performs work redistribution among allocated computing nodes. BNB-Grid has been applied to molecular conformation problem that plays an important role in computational chemistry. New results were obtained demonstrating that general purposed optimization algorithm can efficiently cope with hard optimization problems providing the sufficient computational resources are employed.

URL for further information

http://dcs.isa.ru/posypkin/

Detailed analysis

Finding a solution of many practical global optimization problems requires power of hundreds and thousands of CPUs. The presented programming environment harnesses consolidated power of diverse computing resources ranging from workstations to publicly available supercomputers for solving such problems. The distributed system used for computations has a two-level hierarchical structure. The top level is formed by coarse-grain computing elements such as clusters, powerful workstations and servers connected via Internet.

Cluster nodes form the bottom level in this hierarchy. To utilize the hierarchy in a most efficient way different communication packages and load distribution schemes are used on both levels. On the top level a combination of ssh-tunneled socket connection combined with ICE (Internet Communication Engine) middleware is used. The second level nodes communicate via MPI (Message Passing Interface) –a commonly adopted library for parallel computing.

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