Structural bioinformatics

bigrHPC: creating instant computing clusters for bioinformatics and molecular dynamics

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ABSTRACT
Summary: bigrHPC, a bootable Linux Live CD has been developed to create high-performance clusters for bioinformatics and molecular dynamics studies using any Local Area Network (LAN)-networked computers. bigrHPC features automated hardware and slots detection as well as provides a simple job submission interface. The latest versions of GROMACS, NAMD, mpiBLAST and ClustalW-MPI can be run in parallel by simply booting the bigrHPC CD or flash drive from the head node, which immediately positions the rest of the PCs on the network as computing nodes. Thus, a temporary, affordable, scalable and high-performance computing environment can be built by non-computing-based researchers using low-cost commodity hardware.

Availability: The bigrHPC Live CD and relevant user guide are available for free at http://birg1.fbb.utm.my/birghpc.

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1 INTRODUCTION
The Beowulf-class computing cluster was a breakthrough in cluster computing because it enabled parallel computing to be performed utilizing low-cost commodity hardware and standard software components compared to other supercomputing solutions (Sterling et al., 1995). Typical requirements for building a Beowulf-class cluster involve setting up the number of desired personal computers (PCs) and interconnecting them on the same Local Area Network (LAN), preferably using gigabit ethernet. A similar operating system (OS) and software are then installed on each PC (node) and make install.

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2 METHODS

The scripts used to build PelicanHPC were modified to build birgHPC. It was augmented with automatic slot detection capabilities and with the ability to make modifications to the host name in order to accommodate the MPICH2 environment. We also included installations of PyMol and Grace from the Debian repository, in addition to allowing manual installations of the latest VMD, fftw libraries, GROMACS, NAMD, mpiBLAST, ClustalW-MPI, OpenMPI and MPICH2 versions from their respective web sites. Some of the original PelicanHPC scripts were incorporated unchanged into birgHPC, such as the cluster configuration script and the netboot image generation script.

3 DISCUSSION

The main feature of birgHPC is its ability to convert PCs on the same LAN into a high-performance computing cluster. PCs in computer labs are often found idle after office hours and during holidays. These untapped resources can be converted within minutes into a computing cluster by booting birgHPC and following the general cluster creation work flow (i.e. setup the head node then the computing nodes). For a PC to act as the head node, its name must be able to boot from a CD (birgHPC image) and have a monitor, a mouse and a keyboard. To act as computing nodes, the other PCs need to be bootable from the network. The birgHPC_setup script is executed upon the first cluster configuration. When additional nodes are added or removed from the existing cluster, the birg_restart_hpc script is executed. Node statuses can be monitored using the included Ganglia Monitoring System. After the final configuration, users are able to run jobs by placing their files in the /home/user directory, which is shared across the nodes using the network file system (NFS). birgHPC includes a job submission script (/usr/bin/job.sh), which provides users with an interface to run GROMACS, NAMD, mpiBLAST and ClustalW-MPI jobs.

The amount of RAM available is a concern because everything is loaded into RAM. While all the files in the /home/user/ directory should be erased from RAM when the head node is rebooted (as is common with many Live CDs), a solution has been implemented in birgHPC which automatically detects and mounts an external storage device as /home (e.g. a flash drive formatted in ext3 with a BIRG label). Testing of birgHPC has been conducted with standard benchmark processes and its performance is on par with the normal hard disk-installed parallel computing-enabled Live CD with the latest versions of GROMACS and NAMD for molecular dynamics simulations.

3 ACKNOWLEDGEMENTS

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Conflict of Interest: none declared.

4 CONCLUSION

The Linux Live CD, birgHPC, is an improvement over PelicanHPC and Debian Live because birgHPC incorporates capabilities for automatic slot detection, the use of a MPICH2 environment and a job submission interface. The ability of birgHPC to convert LAN-connected PCs into a high-performance computing cluster allows researchers to instantly utilize otherwise idle PCs in laboratories to conduct bioinformatics and molecular dynamics studies with minimal effort. birgHPC is the only freely available, parallel computing-enabled Live CD with the latest versions of GROMACS and NAMD for molecular dynamics simulations.

Table 1. A performance comparison between a permanent cluster (Ubuntu) and a birgHPC temporary cluster having identical hardware configurations based on the GROMACS with DPPC and Villin benchmarks

<table>
<thead>
<tr>
<th>Number of processes</th>
<th>DPPC (ns/day)</th>
<th>Villin (ns/day)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permanent cluster</td>
<td>2</td>
<td>6</td>
</tr>
<tr>
<td>birgHPC temporary cluster</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>Permanent cluster</td>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>birgHPC temporary cluster</td>
<td>12</td>
<td>16</td>
</tr>
</tbody>
</table>

REFERENCES