

Benchmark informed software upgrades at Quest-NUIt

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ABSTRACT

We present the work performed at Quest, a high performance computing cluster at Northwestern University regarding benchmarking of software performed to guide software upgrades. We performed extensive evaluation of all mpi libraries present on the system for functionality and performance in addition to testing a strategy to deploy architecture optimized software that can be loaded dynamically at runtime.

CCS CONCEPTS

• Software and its engineering → Software configuration management and version control systems; Software maintenance tools.

KEYWORDS

software management, software builds, software automation

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1 INTRODUCTION

Quest is a heterogenous HPC cluster[1] at Northwestern University consisting of Intel Haswell/Broadwell/Skylake nodes with varying interconnects which uses the slurm[4] as resource manager and job scheduler (should we mention fairshare?). The cluster operates with very high uptimes and only shuts down once every academic year for maintenance (for approximately two weeks). While this high uptime is great for research throughput, it compresses critical maintenance tasks into those two weeks and makes the operators prioritize in place upgrades over major redesigns. While such an operations scheme works in the short run, managing a large set of software stacks that were installed at various points in time becomes challenging. The software stack was kept stable even through maintenance cycles that involved major and minor OS upgrades.

This has led to a bloated software stack with inconsistent naming schemes for modules and executables that is challenging to continuously benchmark for functionality and performance. Thus, we are motivated to develop a strategy to maintain our software stacks that

will enable us to provide functional and performant software for our users while reducing the maintenance and support workload for the operators and software specialists. In addition to the above, we also face an immediate need to make mpi providers compatible with slurm as a slurm update is on the agenda for the next downtime.

In this article we present the results of our benchmarking studies that inform our plans for deprecating modules and preliminary tests on our beta cluster for a strategy to deploy optimized builds for each architecture that are dynamically loaded at runtime based upon the nodelist for the job.

2 MPI LIBRARIES

Over time multiple builds of libraries providing the message passing interface[2] functionality were installed. Some of these are quite old (before major OS version upgrades) and the naming scheme is inconsistent. Since none of these were installed with slurm support, we had to write a bash script to run the tests. The results are presented in the figure-abc.

In total, 42% of the available mpi libraries were faulty with 28% being nonfunctional and the rest being nonperformant.

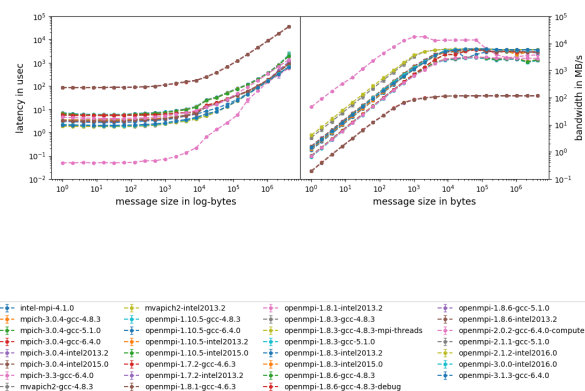


Figure 1: Benchmark of currently available mpi builds

2.1 Improvements

Spack[3] was used to build new versions of mpi libraries with slurm support. This allows us to automate a large set of parameterized builds and eases the testing. Consistent with the literature we decided to use the "UCX" transport layer for all mpi libraries and to enable the "PMIx" plugin in slurm for better performance.

What is UCX? How do we want to install it? What is PMIx? How do we want to install it?

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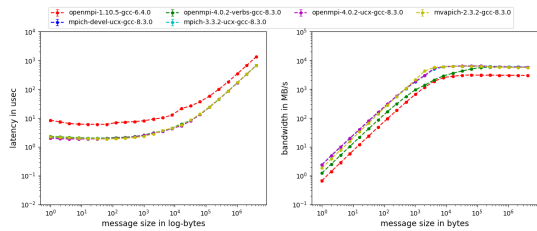


Figure 2: Benchmark of new mpi builds

Table 1: Optimized builds on Haswell nodes

Software	Current	Optimized
LAMMPS	765.8 timesteps/day	1013.4 timesteps/day
GROMACS	1.78 ns/day	2.00 ns/day

3 NODE ARCH DEPENDENT SOFTWARE

3.1 benchmarks

Table with benchmarks for LAMMPS/GROMACS.
Elaborate on the benchmark problem, add citation.

3.2 deployment strategy

On Quest, users are not required to choose a partition and the jobs are assigned to nodes dynamically based on availability. We plan to build each software package optimized for all possible architectures and configure a task prolog script that sets the modulepath based on SLURM_NODELIST as shown below.

```
short_list=${SLURM_JOB_NODELIST##worker}
if [ $short_list == "01" ]
then
echo "export MODULEPATH=/home/path1"
fi
if [ $short_list == "02" ]
then
echo "export MODULEPATH=/home/path2"
fi
```

This was tested on a virtual slurm cluster provisioned by four docker containers tied together via docker-compose. [cite].

4 CONCLUSION

Thus, an important study was conducted.

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