

Using a Hybrid Cloud approach to achieve efficiency, flexibility & high utilisation of your HPC

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Università di Pisa

What is HPC today?



HPC frequently hidden assumptions

- Linear/Polynomial complexity of algorithms
- Numerical codes
- Compute Communicate ratio
- Problem bigger than a single system
- Extreme custom code optimization



Cloud, HPC and the problem size





Flexibility IS often more important...

| Python 3 used what fraction? used how many times more? | | | | | | | | |
|--|---|---|-----|--------|-----|------|------|--|
| <u>Time-</u> <u>used</u> | - | | 25% | median | 75% | | - | |
| (Elapsed secs) | ± | ± | 6× | 43× | 62× | 106× | 106× | |

| Java used what fraction? used how many times more? | | | | | | | | |
|--|---|---|-----|--------|-----|----|----|--|
| <u>Time-</u> <u>used</u> | - | | 25% | median | 75% | | - | |
| (Elapsed secs) | ± | ± | 2× | 2× | 2× | 4× | 4× | |

Critical aspects for achieving flexible HPC



Software stack

- Library dependencies
- Package management (a nightmare): yum, apt-get, npm, nuget
- Debug/run cycle, staging
- Code and data versioning
- Open source development model is worsening this scenario
- Security hard to ensure

Code (in)-efficiency

• Experiment:

- Take a 4CPU server S with RAM
- Run CFD workload W on S with MPI multithread
- Run W on S with MPI multiprocess
- Run W on a virtual cluster on S with same resources and MPI on vSwitch

• Outcome (2010 and 2015):

Virtual execution lead to a speedup up to 30%

Algorithm complexity



Networking

- East–West traffic
- Low latency
- Topology
- IP Addressing (overlay?)
- Containers
- Data size (i.e. 300GB for a genome, remember?)





Disk size AND performance





| Avg Queue le | ngth | | |
|--------------|---------------|-------|-------|
| ratio | Virtual users | | |
| Memory | 1 | 8 | 16 |
| 4GB | 3,36 | 3,47 | 3,38 |
| 8GB | 4,71 | 4,74 | 5,08 |
| 16GB | 5,49 | 8,63 | 7,40 |
| 32GB | 10,89 | 23,70 | 10,91 |
| Unlim | 7,72 | 26,44 | 35,55 |





«Problems usually don't scale up as hardware, and so you start as enterprise to become a small business. Only then you may realize that the beautiful parallel something you devised become useless but it complicates the architecture»

A.C.

(hey, it's me :)

HPC and Cloud



Public Cloud HPC (Azure)



True HPC capabilities in the cloud, on demand

The performance and scalability of a world-class supercomputing center is now available to everyone, on demand in the cloud. Run your Windows and Linux HPC applications using high performance A8 and A9 compute instances on Azure, and take advantage of a backend network with MPI latency under 3 microseconds and non-blocking 32 Gbps throughput. This backend network includes remote direct memory access (RDMA) technology on Windows and Linux that enables parallel applications to scale to thousands of cores. Azure provides you with high memory and HPC-class CPUs to help you get results fast. Scale up and down based upon what you need and pay only for what you use to reduce costs.

Learn more about high performance A8 and A9 compute instances >

Read about the performance improvements ANEO achieved with Azure >



Public Cloud HPC (AWS)



Try out the demo framework, cfncluster, to see how to run HPC clusters in AWS

High performance computing in the cloud.

High Performance Computing (HPC) on Amazon Elastic Compute Cloud (EC2) is enabled by the Cluster Compute-optimized and GPU instance types (virtual machines). You can use them just like other EC2 instances, but they also have been specifically engineered to provide high performance networking and you can scale to tens of thousands of instances on-demand.

Get an overview of Amazon EC2 »

Announcing the Amazon EC2 C4 instance type.

You can now launch C4 instances, the latest generation of Amazon EC2 Compute-optimized instances. C4 instances are designed for computebound workloads, such as high-traffic front-end fleets, MMO gaming, media processing, transcoding, and High Performance Computing (HPC) applications.

C4 instances are available in five sizes, offering up to 36 vCPUs. C4 instances are based on Intel Xeon E5-2666 v3 (codename Haswell) processors that run at a base frequency of 2.9 GHz, and can deliver clock speeds as high as 3.5 GHz with Intel ® Turbo Boost. Each C4 instance type is EBS-optimized by default and at no additional cost. This feature provides 500 Mbps to 4,000 Mbps of dedicated throughput to EBS above and beyond the general purpose network throughput provided to the instance.



Learn more about EC2 Cluster Compute instance types

Learn more about Amazon EC2 instance types »



Private Cloud (DHCS on prem)

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OpenStack?

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| Project | | | | | |
| CURRENT PROJECT | Instances Used 1 of 10 | VCPUs Used 1 of 20 | RAM Used 512 MB of 51,200 MB | Floating IPs Used 0 of 10 | Security Groups Used 0 of 10 |
| Manage Compute | Select a period of tin | ne to query its us | age: | | |
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Containers (Docker)



Use of container for deploying different (potentially incompatible) software
Containers come with less overhead but networking can be a nightmare (latency)

It's the dawn of containers stay tuned!

Designing for specific workloads (lot of fun!)



- Design for the workload (DN, BD, traditional HPC...)
- It's not just a matter of CPU and interconnectivity
- Dimension appropriately the resource usage (bus, memory, disk, network)

New horizons



Emerging HUGE problems

- Life sciences
- Big data analytics
- Real time big data analytics
- IoT





Continuous problem solving





Democratizing HPC



- Data centers in a box
- Predefined, precooked solutions easily deployable
- Some scenarios (Fog, IoT) may benefit from a more distributed information processing



Conclusions



- HPC is redefining itself (again)
- Cloud (public or private or hybrid)
 + containers offer viable solutions for HPC-kind of problems
- Overlap with non-HPC architectures (i.e. microservices, distributed IoT)
- Flexibility will be an important pillar of the HPC in the future
- We accepted that assembly was low level, it's time to move on





OpenHPC @ University of Pisa Dell Solution Center

Antonio Cisternino Maurizio Davini IT Center University of Pisa



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OpenHPC

- Create a stable environment for testing and validation: The community will benefit from a shared, continuous integration environment, which will feature a build environment and source control; bug tracking; user and developer forums; collaboration tools; and a validation environment.
- Reduce Costs: By providing an open source framework for HPC environments, the overall expense of implementing and operating HPC installations will be reduced.
- Provide a robust and diverse open source software stack: OpenHPC members will work together on the stability of the software stack, allowing for ongoing testing and validation across a diverse range of use cases.
- Develop a flexible framework for configuration: The OpenHPC stack will provide a group of stable and compatible software components that are continually tested for optimal performance. Developers and end users will be able to use any or all of these components depending on their performance needs, and may substitute their own preferred components to fit their own use cases.



Why OpenHPC

- Many sites spend considerable effort aggregating a large suite of open-source projects to provide a capable HPC environment for their users:
 - necessary to obtain HPC focused packages that are either absent or do not keep pace from Linux distro providers
 - local packaging or customization frequently tries to give software versioning access to users (e.g. via modules or similar equivalent)
- They frequently leverage a mix of external and in-house tools for:
 - provisioning, software installations/upgrades, config management schemes, and system diagnostics mechanisms.
 - although the functionality is similar, the implementations across sites is often different which can lead to duplication of effort



OpenHPC: Early Community Members





Component Overview SW Block Diagram of Typical HPC System



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7

System Architecture

Master

Intention over time is to provide reference design(s) with use cases for big and small system designs:

- usual designation of node types by function
- current recipe example is "diskless"
- intend to include diskfull examples as well



Login

I/O Servers



Figure 1: Overview of physical cluster architecture.

OpenHPC 1.0 - Initial starting components

| Functional Areas | Components | |
|---------------------------------------|--|----|
| Base OS | CentOS 7.1 | |
| Administrative Tools | Conman, Ganglia, Intel Cluster Checker**, Lmod, LosF, Nagios, pdsh, prun, EasyBuild | No |
| Provisioning | Warewulf | • |
| Resource Mgmt. | SLURM, Munge | |
| I/O Services | Lustre client (community version) | |
| Numerical/ Scientific Libraries | Boost, GSL, FFTW, Metis, PETSc, Trilinos, Hypre, SuperLU, Mumps, Intel MKL** | • |
| I/O Libraries | HDF5 (pHDF5), NetCDF (including C++ and Fortran interfaces), Adios | |
| Compiler Families | GNU (gcc, g++, gfortran), Intel Parallel Studio XE (icc,icpc,ifort)** | · |
| MPI Families | MVAPICH2, OpenMPI, Intel MPI** | |
| Development Tools | Autotools (autoconf, automake, libtool), Valgrind,R, SciPy/NumPy, Intel Inspector ** | |
| Performance Tools | PAPI, IMB, mpiP, pdtoolkit TAU, Intel Advisor**, Trace Analyzer and Collector**, Vtune Amplifier** | |

- Additional dependencies that are not provided by the BaseOS or community repos (e.g. EPEL) are also included
- 3rd Party libraries are built for each compiler/MPI family (6 combinations typically)
- Resulting repository currently comprised of ~250 RPMs

** Bring your own license model

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8

OpenHPC++ - Potential future efforts

| Functional Areas | Components | Contributions by: |
|-------------------------------|---|------------------------------|
| Base OS | CentOS 7.1, McKernel, Kitten, mOS | RIKEN, Sandia, Intel |
| AdminTools | Conman, Ganglia, Intel Cluster Checker**, Lmod, LosF, Nagios, pdsh, prun, EasyBuild, ORCM | Intel |
| Provisioning | Warewulf, xCAT | Community |
| Resource Mgmt. | SLURM, Munge, ParaStation mgmt, PMIx, PBS Pro | ParTec, community, Altair |
| Cross Cutting | OpenStack HPC suitable components | Cray |
| Runtimes | OpenMP, OmpSs, OCR | BSC, Intel |
| I/O Services | Lustre client (community version) | |
| Numerical/ Scientific Libs | Boost, GSL, FFTW, Metis, PETSc, Trilinos, Hypre, SuperLU, Mumps, Intel MKL** | |
| I/O Libraries | HDF5 (pHDF5), NetCDF (including C++ and Fortran interfaces), Adios | |
| Compiler Families | GNU (gcc, g++, gfortran), Intel Parallel Studio XE (icc,icpc,ifort)** | |
| MPI Families | MVAPICH2, OpenMPI, Intel MPI**, MPICH, ParaStation MPI | Argonne, ParTec |
| Development Tools | Autotools (autoconf, automake, libtool), Valgrind,R, SciPy/NumPy, Intel Inspector ** | |
| Performance Tools | PAPI, Intel IMB, mpiP, pdtoolkit TAU, Intel Advisor**, Intel Trace Analyzer and Collector**, Intel Vtune Amplifier**, Paraver, Scalasca | BSC, Jülich |

** Bring your own license model

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9

Installation brief

OpenHPC 1.1 (18 April 2016)

Binary downloads are presently available in the form of RPMs. These RPMs are organized into repositories that can be accessed via standard package manager utilities (e.g. yum, zypper). OpenHPC provides builds that are compatible and tested against <u>CentOS 7.2</u> as well as <u>SUSE Linux Enterprise Server 12</u> <u>SP1</u>. A typical deployment on a new system will begin with the installation of the base operating system on a chosen *master* host identified as the system management server (SMS), followed by enabling access to a compatible OpenHPC repository.

The OpenHPC repository is created and maintained using a dedicated instance of the <u>Open Build Service</u> (OBS) that is available <u>here</u>. In addition to serving as the build server, this OBS instance also provides an RPM repository. You can scan the RPM packages that are available via this repository by browsing the x86_64/ and noarch/ subdirectories for the 1.1 release at: <u>http://build.openhpc.community/OpenHPC:/1.1</u>.

To get started, you can enable an OpenHPC repository locally through installation of an ohpc-release RPM which includes gpg keys for package signing and defines the URL locations for [base] and [update] package repositories. A copy of the ohpc-release file is available for download here:

- ohpc-release-centos7.2-1.1-1.x86_64.rpm (md5sum:f9349b2c2b117a4e3efdac8cd59cc327)
- ohpc-release-sles12sp1-1.1-1.x86_64.rpm (md5sum:a99904b08c90548faaedf7201d60e101)

Alternatively, you can use the package manager to install the RPM directly from the network as in the following examples:

yum install https://github.com/openhpc/ohpc/releases/download/v1.1.GA/ohpc-release-centos7.2-1.1-1.x86_64.rpm

or

zypper in https://github.com/openhpc/ohpc/releases/download/v1.1.GA/ohpc-release-sles12sp1-1.1-1.x86_64.rpm

Install Recipe(s)

To aid in the installation of OpenHPC packaged components, a companion installation recipe is available. This can be obtained via installation of the docsohpc RPM after the OpenHPC repository has been enabled locally. Alternatively, copies of the documentation are also provided below:

- CentOS 7.2 Install guide (PDF)
- SLE 12 SP1 Install guide (PDF)

The intent of the guide is to present a simple cluster installation procedure using components from the OpenHPC software stack. The documentation is intended to be reasonably generic, but uses the underlying motivation of a small, stateless cluster installation to define a step-by-step process. Several optional customizations are included and the intent is that these collective instructions can be modified as needed for local site use cases. Please consult the install guide for more detail and discussion regarding a companion template install script.

OpenHPC Build Service

OpenHPC Build Service

Denhpc

Welcome to the OpenHPC build service and community package repository. This community build infrastructure uses the Open Build Service to automate the build and release of a variety of RPMs under the auspices of the OpenHPC project. When combined with a matching base OS install, the collection of assembled tools and development packages can be used to deploy HPC Linux clusters. Additional information regarding the project can be found at:

- openhpc.community (General information)
- GitHub (Developer resources)
- Mailing Lists (Support)

The Open Build Service (OBS)

The Open Build Service (OBS) is an open and complete distribution development platform that provides a transparent infrastructure for development of Linux distributions, used by openSUSE, MeeGo and other distributions. It also supports Fedora, Debian, Ubuntu, RedHat and other Linux distributions.

The OBS is developed under the umbrella of the openSUSE project. Please find further informations on the openSUSE Project wiki pages.



| Latest Updates | | | |
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| 🎯 scorep | 5 days ago | | |
| 🎯 cubew | 5 days ago | | |
| 🎯 cubegui | 5 days ago | | |
| 🎯 cube | 5 days ago | | |
| 🎯 cubelib | 5 days ago | | |
| OpenHPC:Devel | 8 days ago | | |

Log In

OpenHPC on Microsoft Cloud OS



Dell HCS



Solution Brief

Dell Hybrid Cloud System for Microsoft

IT organizations have a journey to take to get to the cloud. Success with cloud requires an understanding that it is not just about the technology stack. Fundamentally, cloud is about applying technology to streamline IT operations and enable new business outcomes.

Business needs must be aligned with technology, and with cloud this relationship is more critical than ever. Dell understands these alignment challenges, having worked with our customers to build and manage some of the largest clouds on the planet.

Introducing Dell Hybrid Cloud System for Microsoft

Dell Hybrid Cloud System for Microsoft is not simply data center technology. The Dell Hybrid Cloud System for Microsoft is the industry's first integrated, cloud solution validated with Microsoft Hybrid Cloud Platform System Standard¹.

Dell Hybrid Cloud System for Microsoft is a turn-key integrated system, with powerful multi-cloud management, that uniquely adapts to and

Business needs and Cloud aligned

The Dell Hybrid Cloud System for Microsoft will make your IT services agile and more efficient. The system is designed to leverage Azure public cloud capabilities for backup and recovery to extend your data center capacity. The solution is also designed to enhance business flexibility with Dell Scale Ready Payment Solutions.

Scale Ready Payment Solutions include Cloud Flex Pay, Pay as you Grow, Provision and Pay and Scale On Demand offers, backed by Dell Financial Services. The Dell Hybrid Cloud System for Microsoft is offered with these highly flexible payment solutions so you can maximize your investments and align the acquisition of cloud technologies with your business needs.

Dell is the only tier one vendor with financing options for an end solution spanning hardware, software and services.



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One Last thing....



PBS Pro: HPC Workload Management & Job Scheduling

Faster time-to-results, better throughput and utilization

- EAL3+ security certification and SELinux support
- · Policy-driven, topology-aware scheduling
- Accelerator/Co-processor scheduling
- Green Provisioning[™] for power management
- Cgroups and fairshare available
- · Proven to run millions of jobs per day
- Backfill, sharing, and shrink-to-fit jobs maximize usage
- Extensible plugin framework
- Open architecture to implement virtually any policy



NASA's Workload Manager of Choice for All NAS HPC Resources

~200k cores scheduled by PBS Professional



PBS Pro Open Source – mid-2016

- Marry community innovations & enterprise expertise
 - Accelerate innovatic popenHPC
 for both
- Founding member c.
- Committed to openness and longevity
- Dual licensing: OSI-approved & commercial
 - No change for commercial users
- A single, common "core" for PBS Pro
- Accepted OSS practices, e.g., GitHub
- More info: pbsworks.com/opensource





PBS Pro on OpenHPC

mau — root@ohpchead:~/pbspro-14.0.1 — ssh root@131.114.137.127 — 80×24 [root@ohpchead pbspro-14.0.1]# ls aclocal.m4 config.status doc m4 README autogen.sh configure Makefile INSTALL src buildutils configure.ac libtool Makefile.am test config.log COPYRIGHT LICENSE Makefile.in [root@ohpchead pbspro-14.0.1]# qstat --version pbs_version = 14.0.1 [root@ohpchead pbspro-14.0.1]#

PBS and Docker





PBS and Docker

- PBS starts a separate Docker container to run each job; the scope of this container ends with the job.
- PBS provides the exact same environment to a job in a container that it provides to any other job when staging files in and out, managing a job's output and error files, and exporting environment variables.
- When PBS starts a Docker container, it configures the container so that the job cannot use more resources than it explicitly requested.
- For multi-vnode jobs, PBS configures any Docker containers created on sister MoMs to be network-linked to the container running on the mother superior, allowing communication between job tasks on separate execution hosts.
- When a job ends, PBS manages shutdown of the Docker containers it started for that particular job.



... to finish

- OpenHPC can be successfully used on flexible clouds platform
 A lot of scientific software will available on this platform
- We have to thanks a lot of people but a special thanks:



Bill Nitzberg CTO, PBS Works

San Francisco Bay Area Computer Software

| Current | Altair Engineering |
|-----------|----------------------|
| Previous | Veridian |
| Education | University of Oregon |

