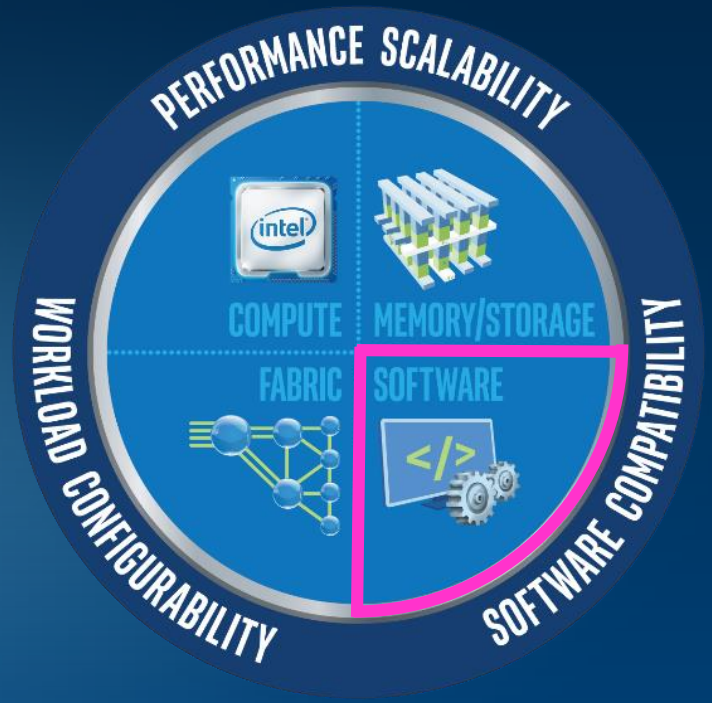
0 to 60 With Intel® HPC Orchestrator

HPC Advisory Council Stanford Conference — February 7 & 8, 2017



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Agenda

- Demo Outline
- Intel® HPC Orchestrator and OpenHPC
- Installation Walkthrough
- Intel® Parallel Studio XE
- Modules Support
- Management and Maintenance
- Workload Management
- 3rd-Party Packages
- Demo of Built Cluster
- Moving Forward

Demo Outline

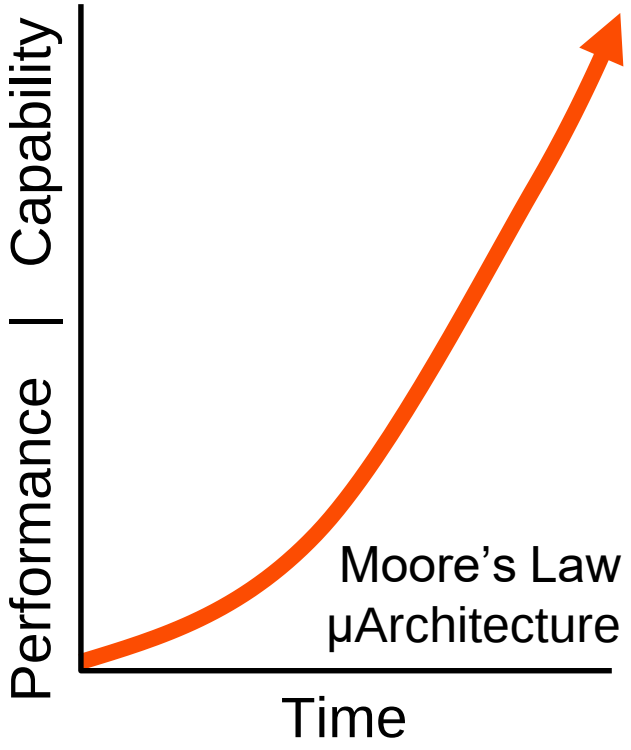
Intel® HPC Orchestrator & OpenHPC

Intel® Scalable System Framework (Intel® SSF)

A systems approach for Innovation

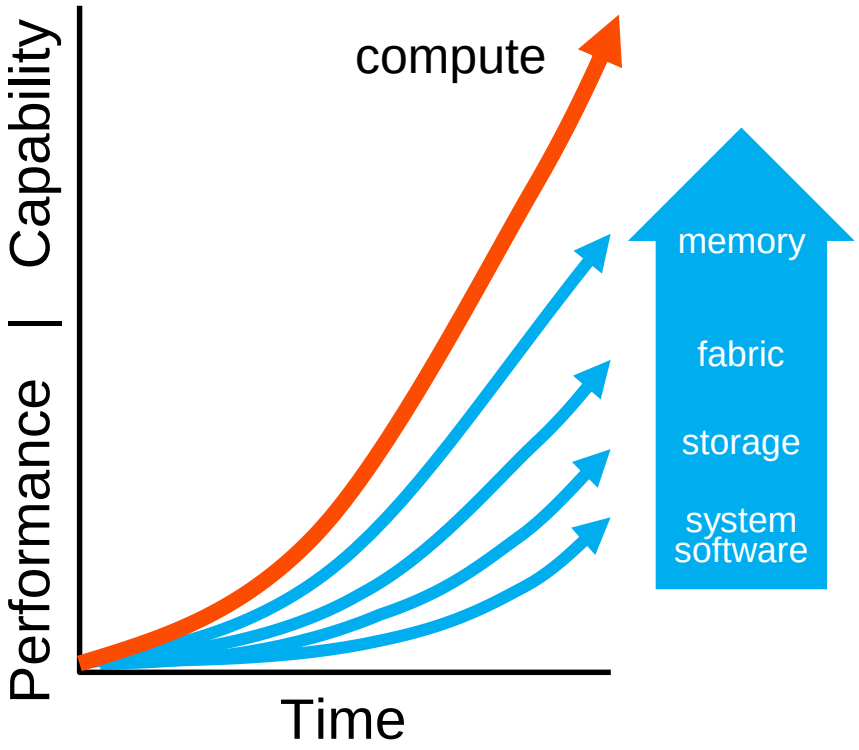
Continue the pace of

Faster Compute



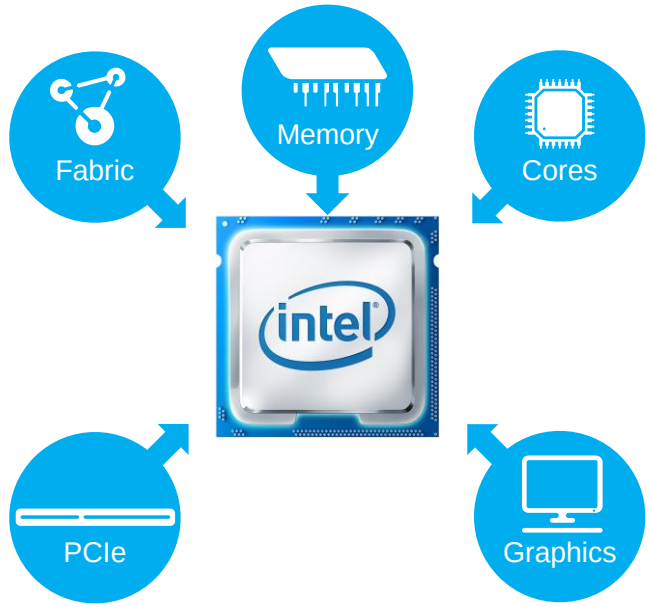
Develop new technologies to

Remove Bottlenecks



Achieve full potential via

Tighter Integration



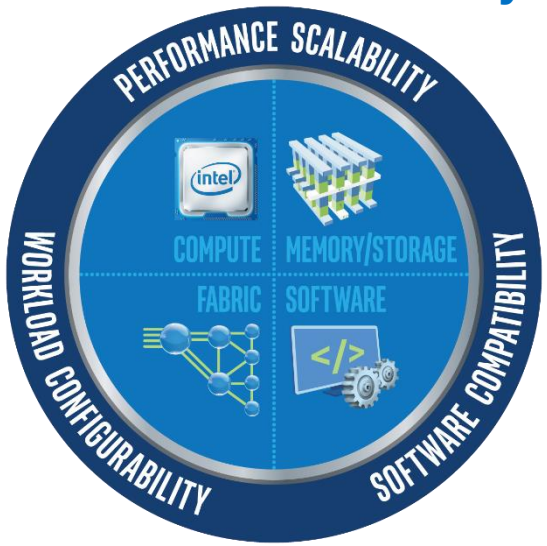
Better power, performance, density, scaling & cost

Execution of Vision

Intel® HPC Orchestrator products are the realization of the software portion of Intel® Scalable System Framework

openHPC

- Open Source Community under Linux Foundation
- Ecosystem innovation building a consistent HPC SW Platform
- Platform agnostic
- 30 global members
- Multiple distributions



Intel® Scalable System Framework (SSF)

A Holistic Design Solution for All HPC

- Small clusters through supercomputers
- Compute and data-centric computing
- Standards-based programmability
- On-Premise and cloud-based

Intel HW Validation, SW Alignment & Technical Support

Intel® HPC Orchestrator

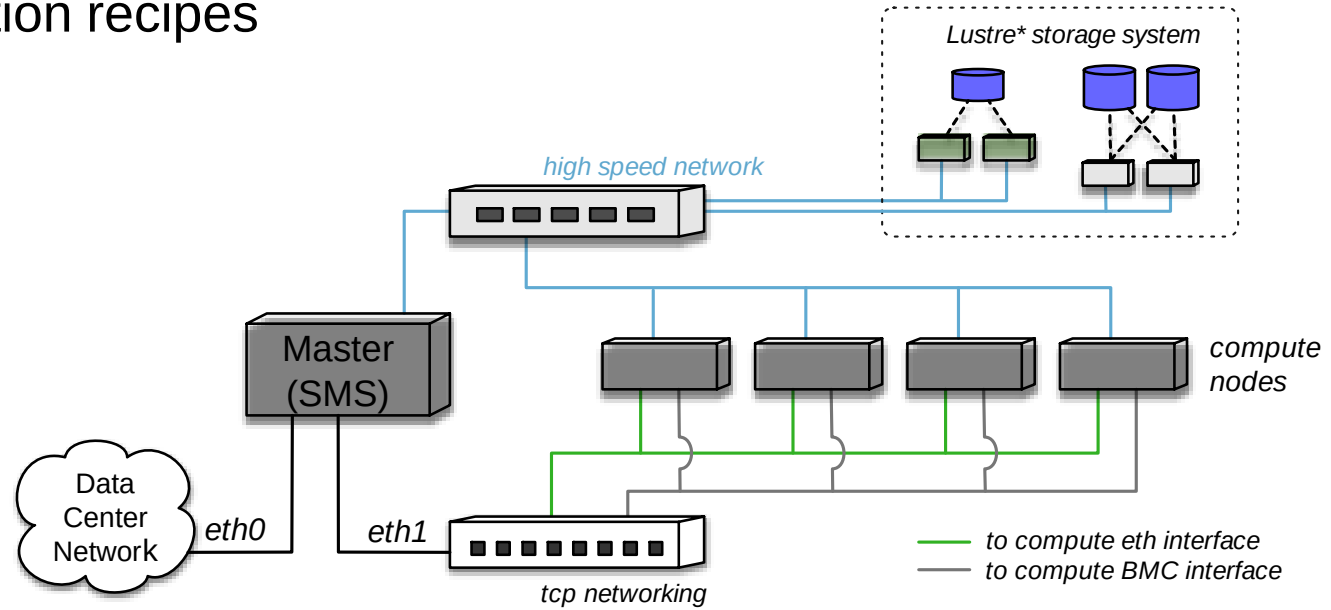
- Intel's distribution of OpenHPC
- Intel HW validation
- Expose best performance for Intel HW
- Advanced testing & premium features
- Product technical support & updates

What is OpenHPC?

OpenHPC is a community effort endeavoring to:

- provide collection(s) of pre-packaged components that can be used to help install and manage flexible HPC systems throughout their lifecycle
- leverage standard Linux delivery model to retain admin familiarity (i.e., package repos)
- allow and promote multiple system configuration recipes that leverage community reference designs and best practices
- implement integration testing to gain validation confidence
- provide additional distribution mechanism for groups releasing open-source software
- provide a stable platform for new R&D initiatives

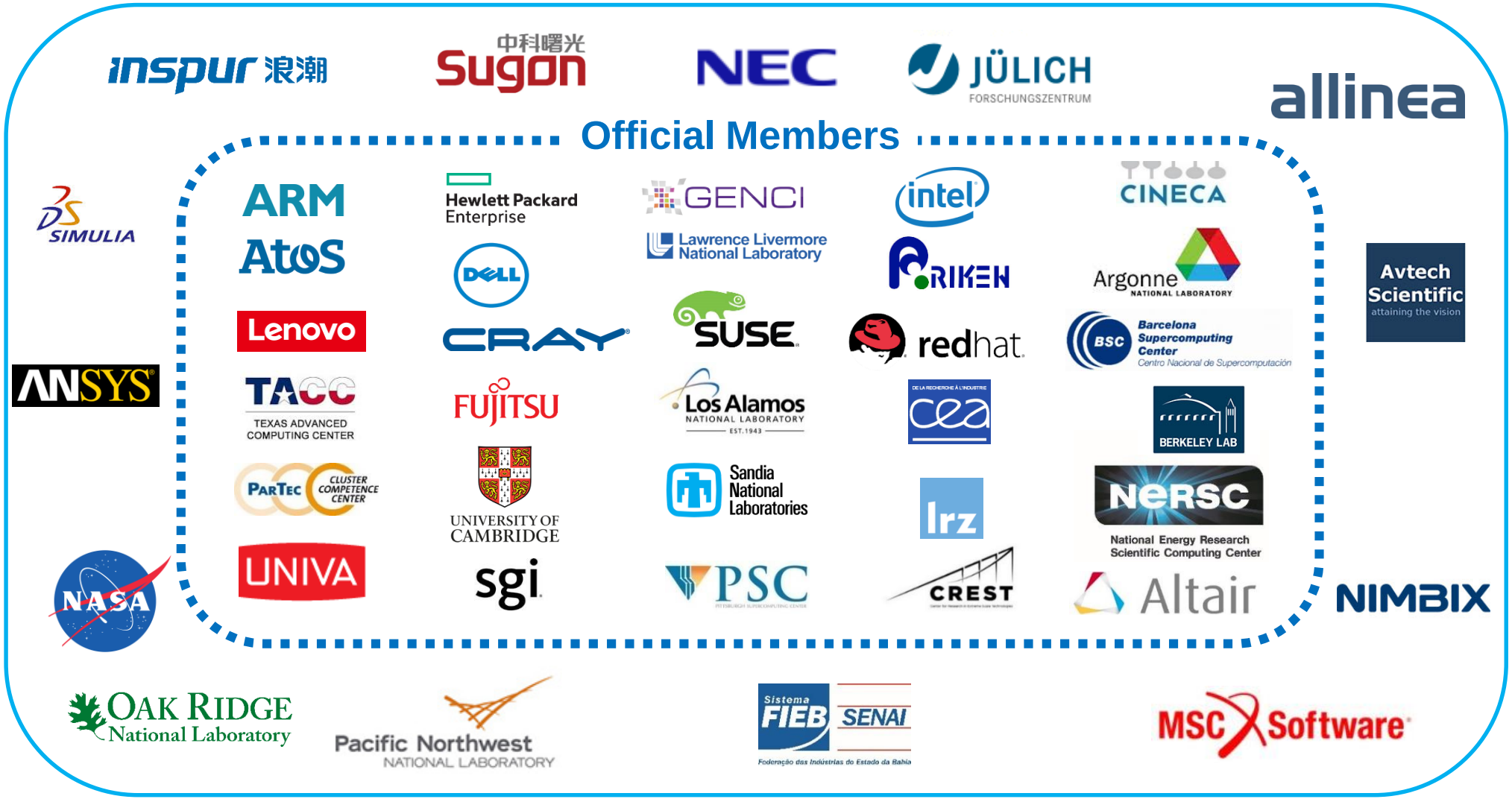
Typical cluster architecture



Courtesy of OpenHPC*

Participation as of January'17

Mixture of Academics, Labs, OEMs, and ISVs/OSVs



Courtesy of OpenHPC*

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Project member participation interest? Please contact
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Individuals

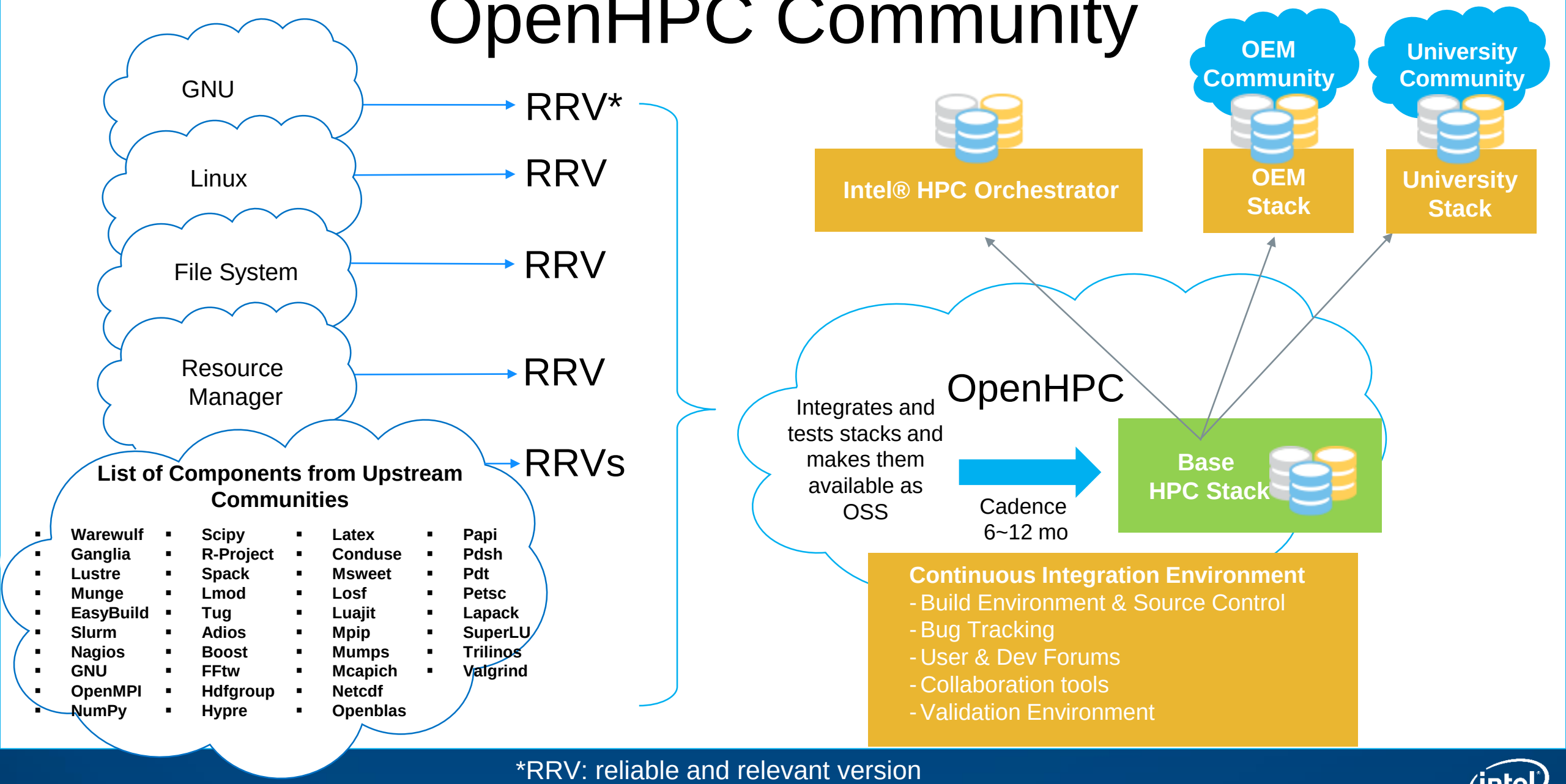
- Reese Baird, Intel (Maintainer)
- Pavan Balaji, Argonne National Laboratory (Maintainer)
- David Brayford, LRZ (Maintainer)
- Todd Gamblin, Lawrence Livermore National Labs (Maintainer)
- Craig Gardner, SUSE (Maintainer)
- Yiannis Georgiou, ATOS (Maintainer)
- Balazs Gerofi, RIKEN (Component Development Representative)
- Jennifer Green, Los Alamos National Laboratory (Maintainer)
- Eric Van Hensbergen, ARM (Maintainer, Testing Coordinator)
- Douglas Jacobsen, NERSC (End-User/Site Representative)
- Chulho Kim, Lenovo (Maintainer)
- Greg Kurtzer, Lawrence Berkeley National Labs (Component Development Representative)
- Thomas Moschny, ParTec (Maintainer)
- Karl W. Schulz, Intel (Project Lead, Testing Coordinator)
- Derek Simmel, Pittsburgh Supercomputing Center (End-User/Site Representative)
- Thomas Sterling, Indiana University (Component Development Representative)
- Craig Stewart, Indiana University (End-User/Site Representative)
- Scott Suchyta, Altair (Maintainer)
- Nirmala Sundararajan, Dell (Maintainer)

Courtesy of OpenHPC* ***https://github.com/openhpc/ohpc/wiki/Governance-Overview***

Intel® HPC Orchestrator Product Family

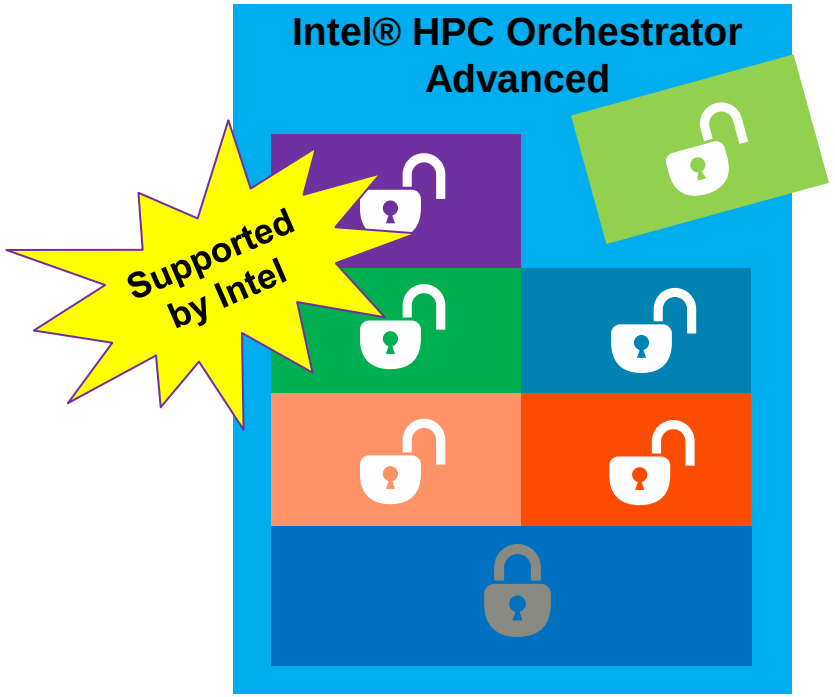
Product		Target Customer
 **CUSTOM** **Highly modular hierarchically configured stack**		**High End HPC users**
 **ADVANCED** **Modular stack with a flat configuration**	***GA today***	**Technical & commercial users with vertical HPC applications**
 **TURNKEY** **Turnkey stack with a flat configuration. A variety of stacks may be available as offerings**		**HPC ISVs, SIs and customers looking for a turnkey solution for On-Prem and CSP access methodologies, appliances**

OpenHPC Community



*RRV: reliable and relevant version

Intel® HPC Orchestrator Value Proposition



- Integrated open source and proprietary software
- Modular build; customizable; with validated updates
- Advanced integration testing, testing at scale (1,000 nodes)
- Optimization for Intel® Scalable System Framework components, such as Intel® Omni-Path Architecture and Intel® Xeon Phi™
- Level 3 technical support provided by Intel

Benefits

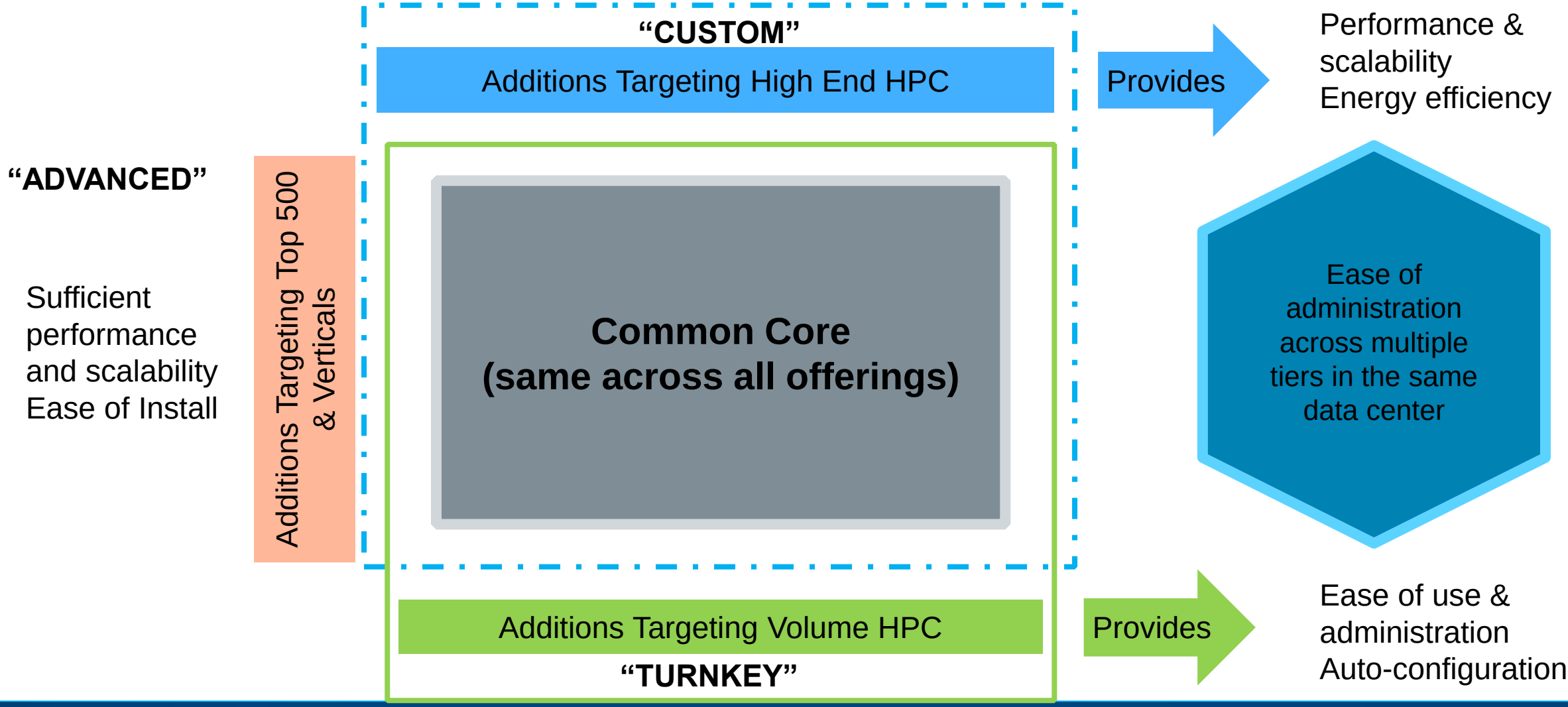
End Users - hardware innovation reflected in SW; spend time on scientific work rather than testing ; faster on path to exascale

Sys Admins - reduce R&D to build and maintain a fully integrated SW stack, easier mgmt. of clusters from multiple vendors

Developers/ISVs – reduce time and resources for constantly retesting apps as new open source components are released and updated

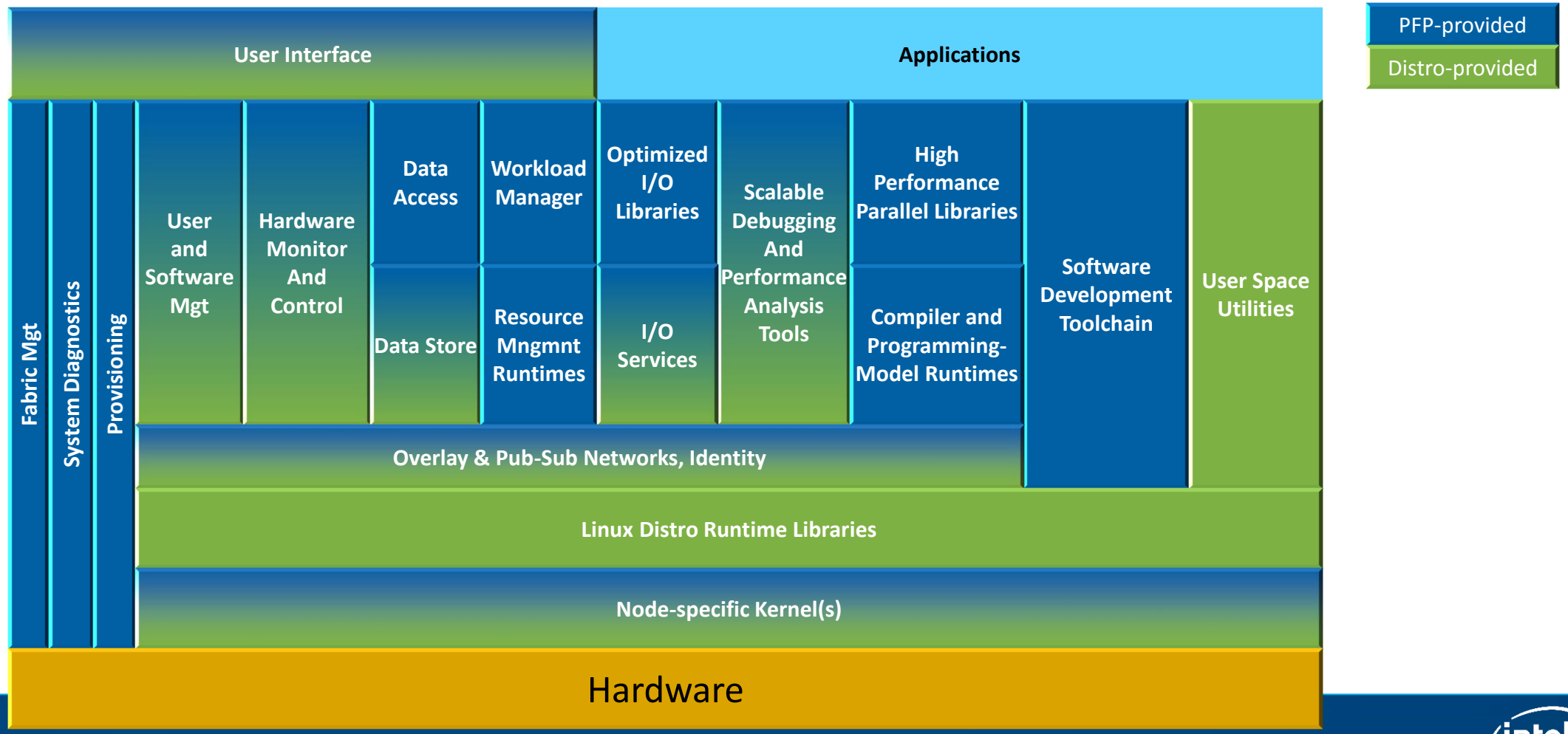
OEMs – reduce R&D to build and maintain a fully integrated SW platform, focus on providing differentiation on top of the system stack

Base Stack and Derivatives



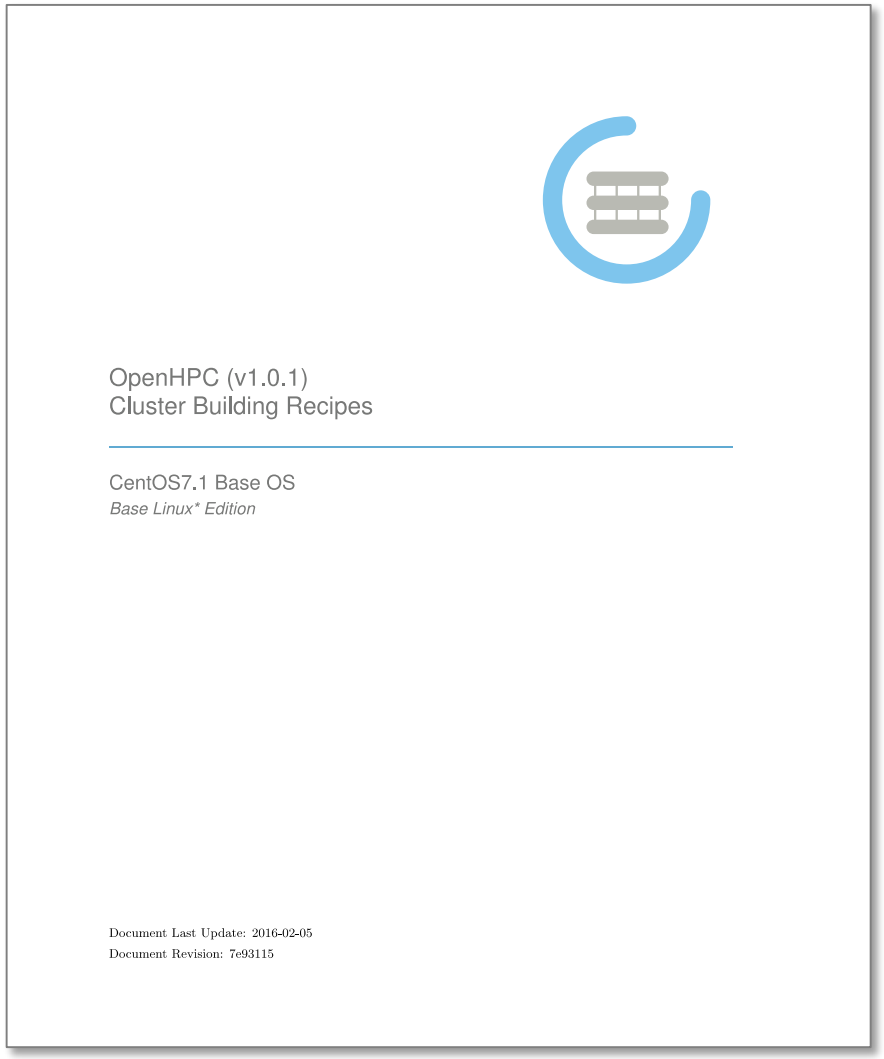
Modular Stack View

- Intra-stack APIs to allow for customization/differentiation (OEMs enabling)
- Defined external APIs for consistency across versions (ISVs)



Installation Walkthrough

Documentation Overview



OpenHPC (v1.0.1)
Cluster Building Recipes

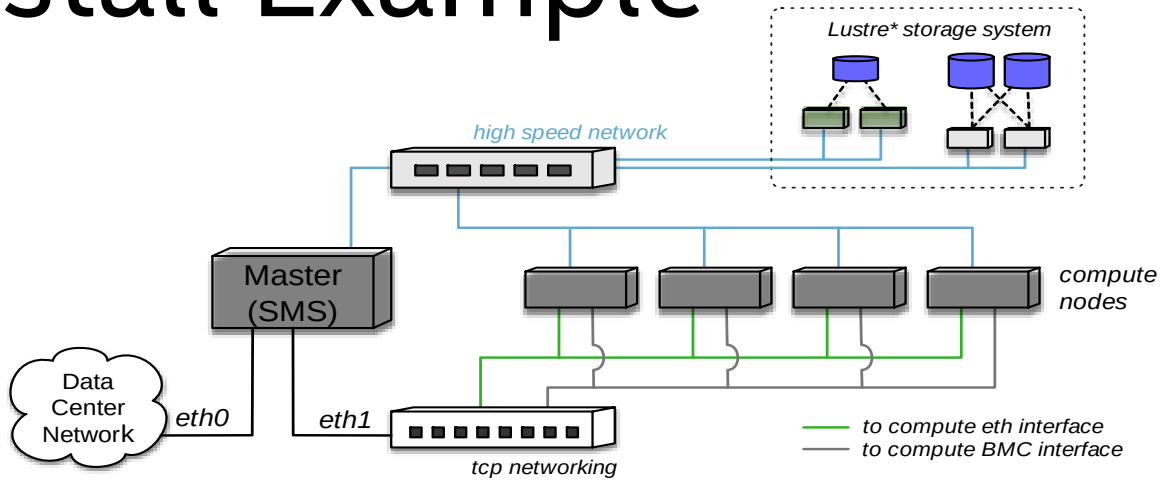
CentOS7.1 Base OS
Base Linux Edition*

Document Last Update: 2016-02-05
Document Revision: 7e93115

Contents

Basic Cluster Install Example

- Starting install guide/recipe targeted for flat hierarchy
- Image-based provisioner (Warewulf)
  - PXE boot
  - Stateless CNs
  - Optionally connect external Lustre* file system
- Hardware-specific information to support (remote) bare-metal provisioning



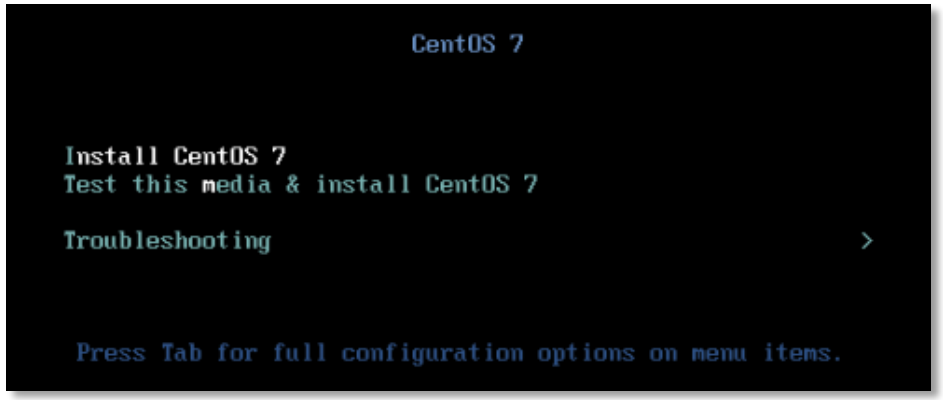
- `${sms_name}` # Hostname for SMS server
- `${sms_ip}` # Internal IP address on SMS server
- `${sms_eth_internal}` # Internal Ethernet interface on SMS
- `${eth_provision}` # Provisioning interface for computes
- `${internal_netmask}` # Subnet netmask for internal network
- `${ntp_server}` # Local ntp server for time synchronization
- `${bmc_username}` # BMC username for use by IPMI
- `${bmc_password}` # BMC password for use by IPMI
- `${c_ip[0]}, ${c_ip[1]}, ...` # Desired compute node addresses
- `${c_bmc[0]}, ${c_bmc[1]}, ...` # BMC addresses for computes
- `${c_mac[0]}, ${c_mac[1]}, ...` # MAC addresses for computes
- `${compute_regex}` # Regex for matching compute node names (e.g. c*)

Optional:

- `${mgs_fs_name}` # Lustre MGS mount name
- `${sms_ipoib}` # IPoIB address for SMS server
- `${ipoib_netmask}` # Subnet netmask for internal IPoIB
- `${c_ipoib[0]}, ${c_ipoib[1]}, ...` # IPoIB addresses for computes

Stack Overview: Bare metal install

Step1: Example OpenHPC 1.2 recipe assumes base OS is first installed on chosen master (SMS) host - e.g. install CentOS7.2 on SMS



Step2: Enable OpenHPC repo using pre-packaged ohpc-release (or mirror repo locally)

```
# export OHPC_GITHUB=https://github.com/openhpc/ohpc/releases/download
# rpm -ivh ${OHPC_GITHUB}/v1.2.1.GA/ohpc-release-1.2-1.x86_64.rpm
```

Stack Overview: Bare metal install (cont.)

– Note that ohpc-release enables two repos:

```
# yum repolist
repo id                                  repo name
OpenHPC                                  OpenHPC-1.2 - Base
OpenHPC-updates                          OpenHPC-1.2 - Updates
base                                     CentOS-7 - Base
epel                                     Extra Packages for Enterprise Linux 7 - x86_64
```

– Step3: install desired building blocks to build cluster or add development tools. **Convenience aliases** are provided to group related functionality

```
[sms]# yum -y groupinstall ohpc-base
[sms]# yum -y groupinstall ohpc-warewulf
```

Add provisioning components

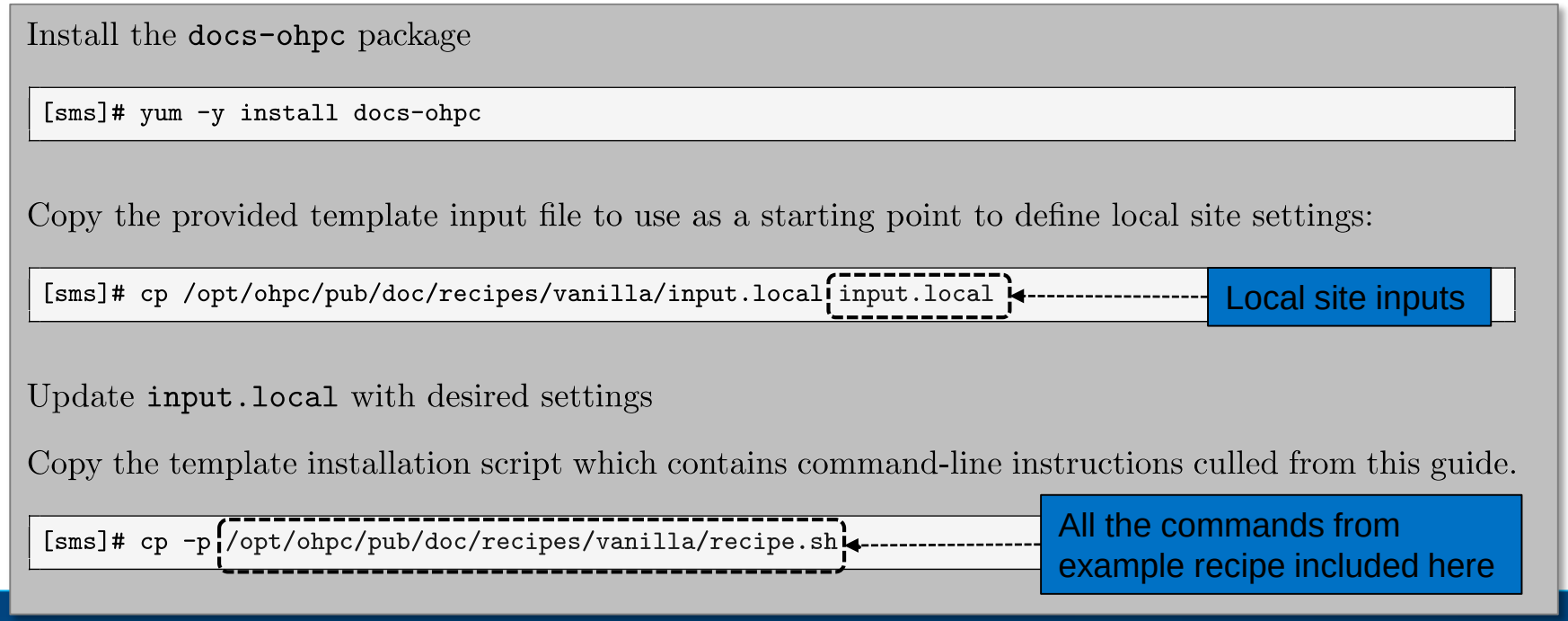
```
[sms]# yum -y install pbspro-server-ohpc
```

Add PBS Professional components

**note that community recipe is purposefully very transparent on config file edits and assumes Linux familiarity*

Stack Overview: Bare metal install (cont.)

- Recipe guides necessarily have a number of things to “cut-and-paste” if you want to reproduce them
- We have a motivating need to automate during the validation process:
  - Cull out relevant commands automatically for use during CI testing
  - A template starting script is available with the documentation RPM which can be used for local installation and customization



Intel® Parallel Studio XE

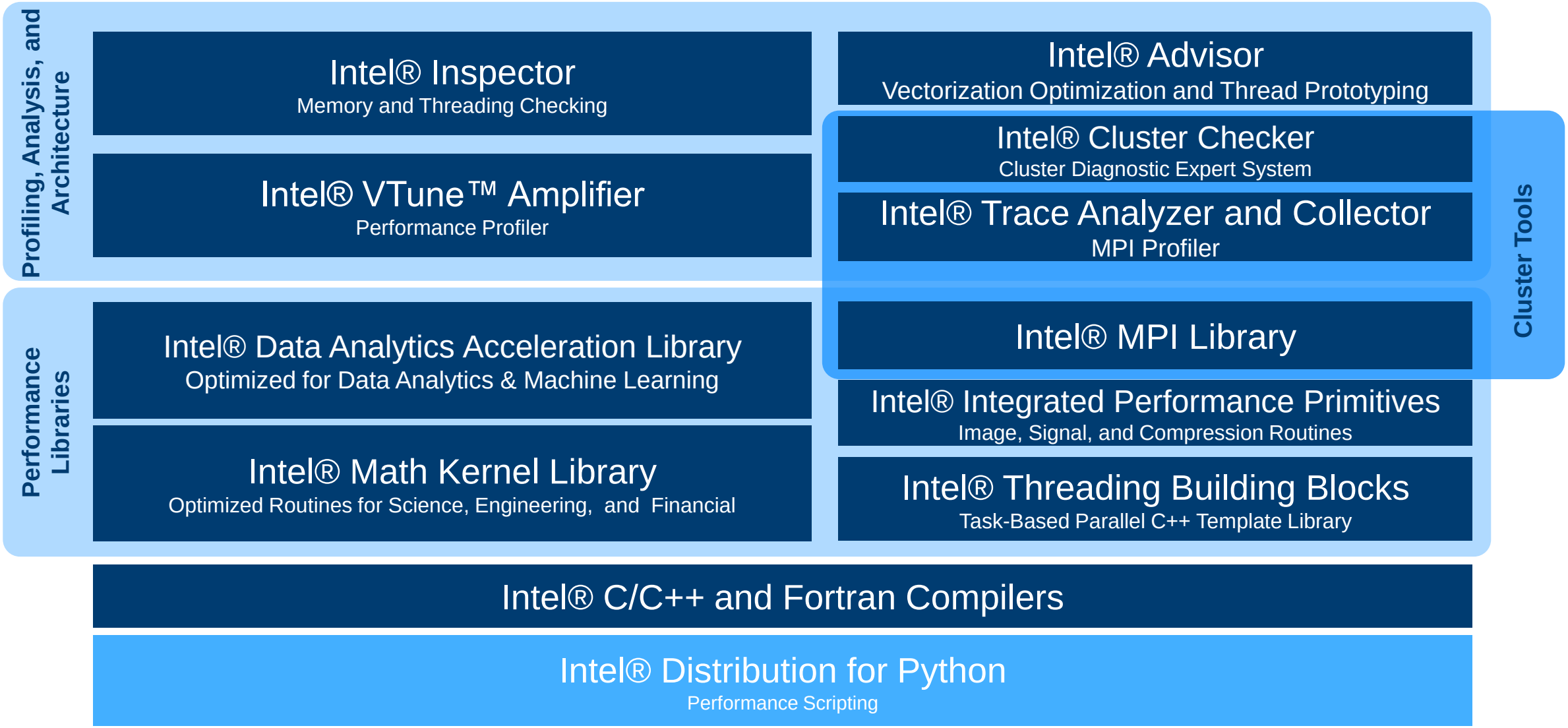
Create Faster Code…Faster

Intel® Parallel Studio XE

- High Performance Scalable Code
  - C++, C, Fortran*, Python* and Java*
  - Standards-driven parallel models: OpenMP*, MPI, and TBB
- New for 2017
  - 2nd generation Intel® Xeon Phi™ and AVX-512
    - Optimized compilers and libraries
    - Vectorization and threading optimization tools
    - High bandwidth memory optimization tools
  - Faster Python application performance
  - Faster deep learning on Intel® architecture

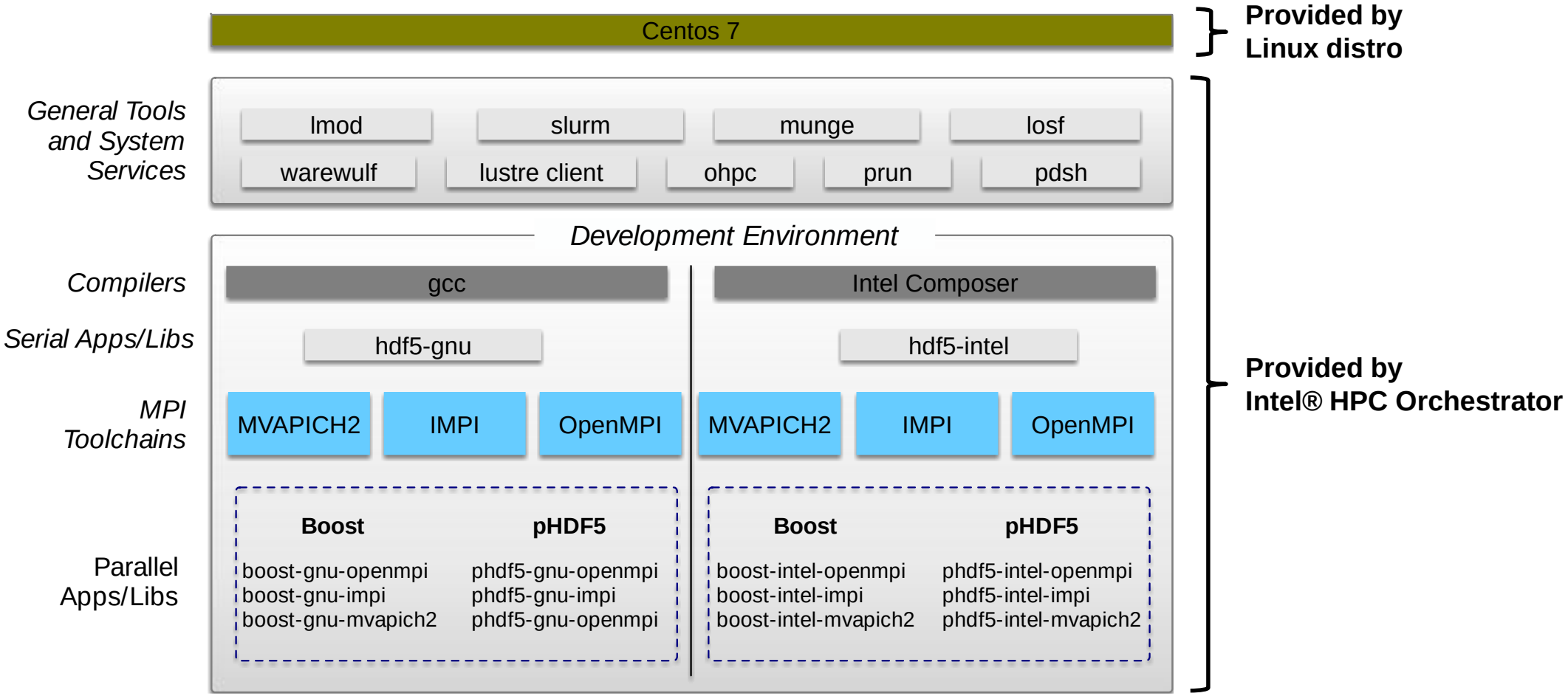
http://intel.ly/perf-tools

Intel® Parallel Studio XE



Modules Support

Hierarchical Overlay



Courtesy of OpenHPC*

Hierarchical Software - User experience

- Goal is to have a component hierarchy reflected in the user environment
- User sees compatible software based on the currently loaded environment
- Manage compiler/MPI dependencies via Lmod “families”

```
$ module list
Currently Loaded Modules:
   1) gnu/5.3.0          2) impi/5.1.3.181   3) ohpc    4) boost/1.60.0

$ module avail
------ /opt/intel/hpc-orchestrator/pub/moduledeps/gnu-impi ------
   boost/1.60.0    phdf5/1.8.16

-------- /opt/intel/hpc-orchestrator/pub/moduledeps/gnu----------
   hdf5/1.8.16    impi/5.1.3.181    mvapich2/2.1    openmpi/1.10.1

--------- /opt/intel/hpc-orchestrator/pub/modulefiles -----------
   autotools    hpc-orchestrator   gnu/5.3.0    intel/16.0.2.181

$ echo $BOOST_LIB
/opt/intel/hpc-orchestrator/pub/libs/gnu/impi/boost/1.60.0/lib

$ module swap gnu intel
Due to MODULEPATH changes the following have been reloaded:
  1) boost/1.60.0  2) impi/5.1.3.181

$ echo $BOOST_LIB
/opt/intel/hpc-orchestrator/pub/libs/intel/impi/boost/1.60.0/lib
```

Management and Maintenance

System Monitoring and Control

Control

- Intel® Cluster Checker – system health
- genders – cluster configuration DB
- mrsh – remote shell using Munge-based authentication
- pdsh – parallel distributed shell (mrsh or ssh)
- powerman – OOB power control
- prun – abstract parallel launch
- ssh – distro-provided

Monitoring

- conman – remote console access
- Ganglia – scalable node monitoring and visualization
- Nagios – servers, switches, applications, and services

Workload Management

Workload Management

- The workload managers (WLM) run user workflows on system
  - –Workflows are built around specifics of WLM
  - –WLM choice is *very important* to user community → key modularity driver!
- Two leading WLMs are supported initially
  - –SLURM (currently supported)
    - –Initially developed at LLNL; now supported by SchedMD
    - –Widely used on Top-500 systems
  - –PBS Professional (in OpenHPC; available in HPC Orchestrator presently)
    - –Initially developed for NASA; now supported by Altair
    - –Widely used in volume HPC systems

3rd-Party Packages

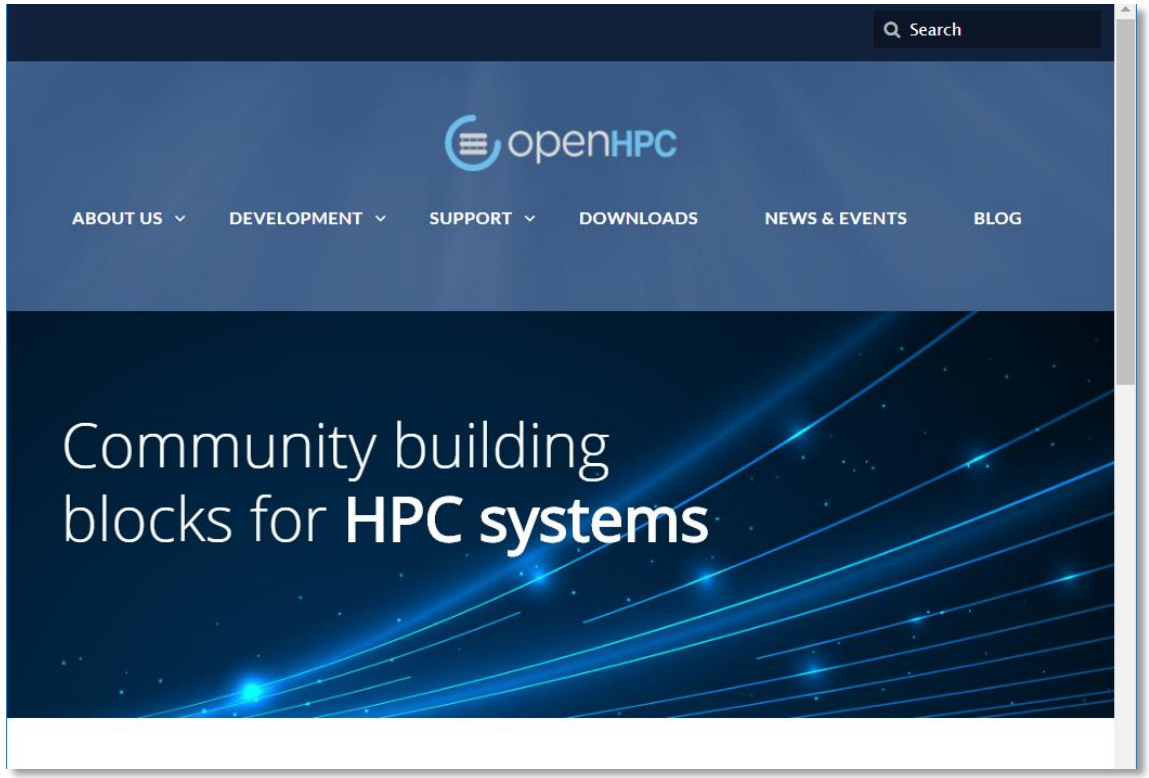
3rd-Party Packages

Functional Areas	Components
Base OS compatibility	RHEL 7.2 BU7 / SLES12 SP1 / CentOS 7.2 (coming soon)
Administrative Tools	Conman, Ganglia, Intel® Cluster Checker, Lmod, Losf, Nagios, pdsh, prun
Provisioning	Warewulf
Resource Mgmt	Slurm, Munge, (PBS Professional coming soon)
I/O Services	Lustre Client
I/O Libraries	HDF5 (pHDF5), NetCDF (including C++ & Fortran libraries), Adios
Compiler Families	GNU (gcc, g++, gfortran), Intel Parallel Studio XE** (icc, icpc, ifort)
MPI Families	OpenMPI, MVAPICH2, Intel MPI**
Development Tools	Autotools (autoconf, automake, libtool), Valgrind, R, SciPy, Numpy
Performance Tools	PAPI, Intel IMB, mpiP, pdtoolkit, TAU, Intel Advisor, Intel Trace Analyzer & Collector**, Intel VTune Amplifier**
Numerical/Scientific Libraries	Boost, GSL, FFTW, Metis, PETSc, Trilinos, Hypre, SuperLU, Mumps, Intel MKL**

Moving Forward

Further Information

openhpc.community



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Backup

OpenHPC

OpenHPC: Mission and Vision

- **Mission**: to provide a reference collection of open-source HPC software components and best practices, lowering barriers to deployment, advancement, and use of modern HPC methods and tools.

- **Vision**: OpenHPC components and best practices will enable and accelerate innovation and discoveries by broadening access to state-of-the-art, open-source HPC methods and tools in a consistent environment, supported by a collaborative, worldwide community of HPC users, developers, researchers, administrators, and vendors.

Courtesy of OpenHPC*

Information/Places to Interact

http://openhpc.community (general info)

https://github.com/openhpc/ohpc (GitHub site)

https://github.com/openhpc/submissions (new submissions)

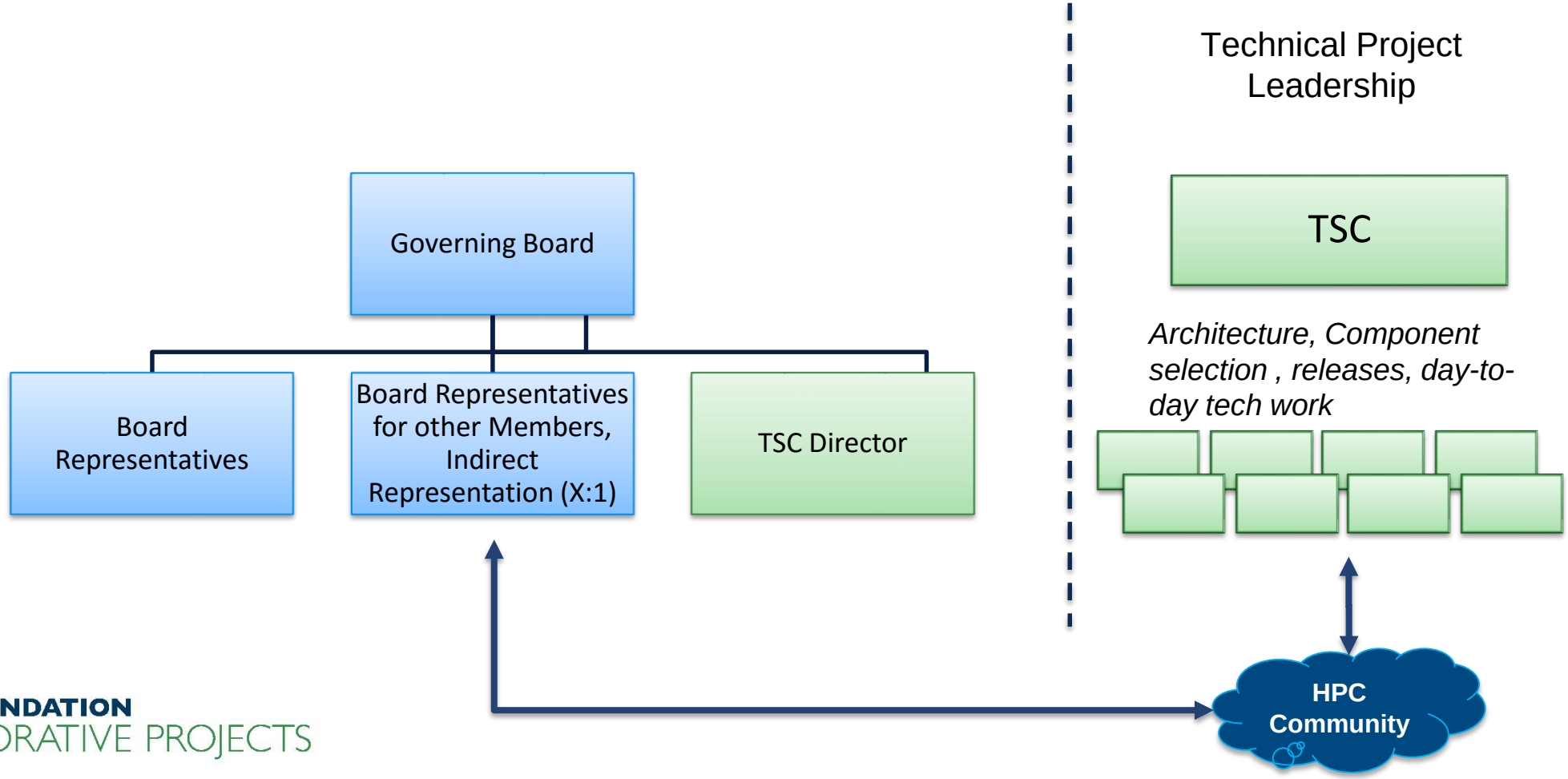
https://build.openhpc.community (build system/repos)

http://www.openhpc.community/support/mail-lists/ (email lists)

- openhpc-announce
- openhpc-users
- openhpc-devel

Community Governance Overview

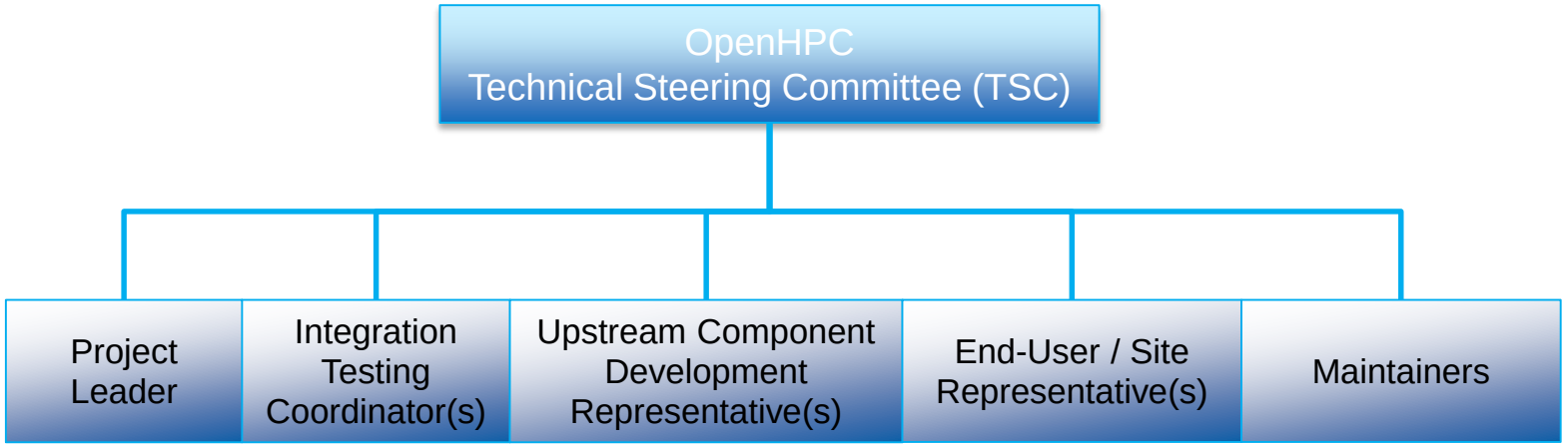
Governing Board + Technical Steering Committee



LINUX FOUNDATION
COLLABORATIVE PROJECTS

Courtesy of OpenHPC*

OpenHPC TSC - Role Overview



LINUX FOUNDATION
COLLABORATIVE PROJECTS

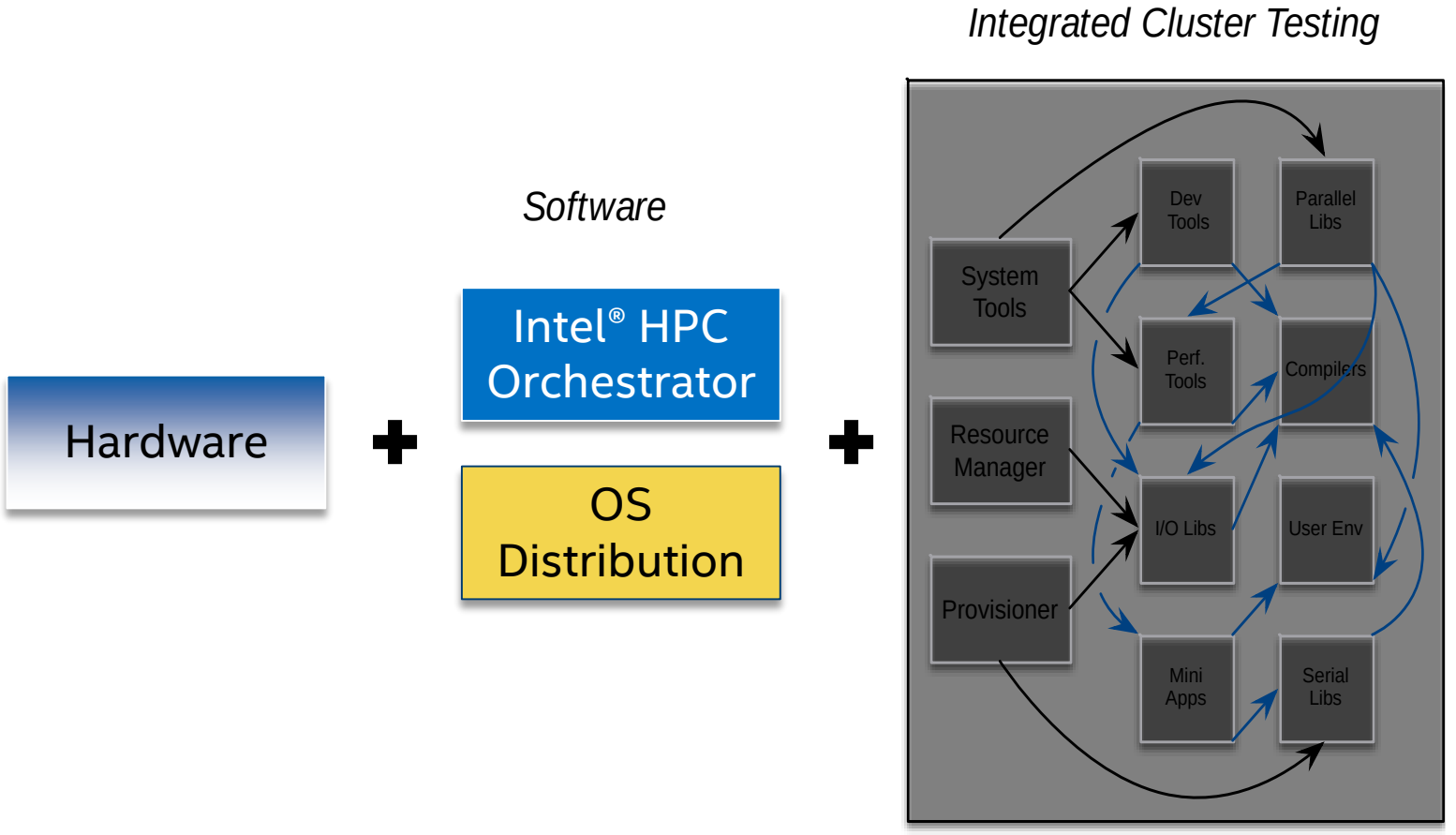
Courtesy of OpenHPC*

intel

Testing and Validation

Integration/Test/Validation

- Cross-package interaction
- Each end-user test need to touch all of the supported compiler & MPI families
- Abstracted to repeat the tests with different compiler/MPI environments:
  - gcc/Intel compiler toolchains
  - Intel MPI, OpenMPI, MVAPICH2



Post Install Integration Tests - Overview

- Major components have configuration options to enable/disable
- Suite of integration tests
  - Installed by default by the install script
  - Root-level tests
  - User-level tests: short & long versions

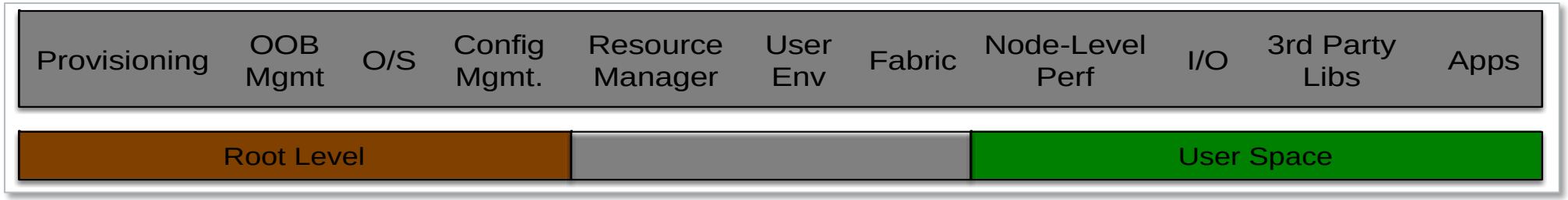
```
>>>------------Launching Integration Testsuite----------------
/home/test/jenkins

HPC Orchestrator Integration Test Configuration:

    Root Level Testing = true
    User Level Testing = true
    Enable Long Tests  = true

Running Root-Level Tests
```

Type of test	Approximate running time
Root-level	single digit number of minutes
User-level short	less than 30 minutes
User-level long	a few hours



Post Install Integration Tests – Root level

```
----------------------------------------- SUMMARY -----------------------------------------

Package version.............. : test-suite-1.0.0

Build user................... : root
Build host................... : sms002
Configure date............... : 2016-11-07 04:51
Build architecture........... : x86_64-unknown-linux-gnu
Test suite configuration..... : short

Submodule Configuration:

    Base operating system..... : enabled
    Out of band tools......... : enabled
    Hardware benchmarks....... : disabled
    Cluster checker........... : enabled
    Lustre client............. : disabled
    spack..................... : enabled
-------------------------------------------------------------
```

```
PASS: admin/run
PASS: bos/run
PASS: oob/run
PASS: clck/run
PASS: admin/spack/run
============================================================================
Testsuite summary for test-suite 1.0.0
============================================================================
# TOTAL: 5
# PASS:  5
# SKIP:  0
# XFAIL: 0
# FAIL:  0
# XPASS: 0
# ERROR: 0
============================================================================
```

Post Install Integration Tests – User level

```
Package version.............. : test-suite-1.0.0

Build user................... : orchtest
Build host................... : sms002
Configure date............... : 2016-11-07 04:56
Build architecture........... : x86_64-unknown-linux-gnu
Test suite configuration..... : long

Submodule Configuration:

User Environment:
    Packaging tests.......... :
    RMS test harness......... :
    Munge.................... :
    Compilers................ :
    MPI...................... :
    Modules.................. :
    OOM...................... :
Dev Tools:
    Autotools................ :
    EasyBuild................ :
    Valgrind................. :
    R base package........... :
    CILK..................... :
Performance Tools:
    mpiP Profiler............ :
    Papi..................... :
    TAU...................... :
```

```
Libraries:
    Adios ................... : enabled
    Boost ................... : enabled
    Boost MPI................ : enabled
    FFTW..................... : enabled
    GSL...................... : enabled
    HDF5..................... : enabled
    HYPRE.................... : enabled
    IMB...................... : enabled
    Metis.................... : enabled
    MUMPS.................... : enabled
    NetCDF................... : enabled
    Numpy.................... : enabled
    OPENBLAS................. : enabled
    PETSc.................... : enabled
    PHDF5.................... : enabled
    ScaLAPACK................ : enabled
    Scipy.................... : enabled
    Superlu.................. : enabled
    Superlu_dist............. : enabled
    Trilinos ................ : enabled
Apps:
    MiniFE................... : enabled
    MiniDFT.................. : enabled
    HPCG..................... : enabled
    PRK...................... : enabled
```

```
============================================
Testsuite summary for test-suite 1.0.0
============================================
# TOTAL: 39
# PASS:  39
# SKIP:  0
# XFAIL: 0
# FAIL:  0
# XPASS: 0
# ERROR: 0
============================================
```

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