OpenHPC Community BoF

BoF 07

Karl W. Schulz, David Brayford, Chulho Kim, Thomas Sterling
OpenHPC Technical Steering Committee (TSC) Members

ISC Conference
June 20, 2017 ◆ Frankfurt, Germany

Agenda

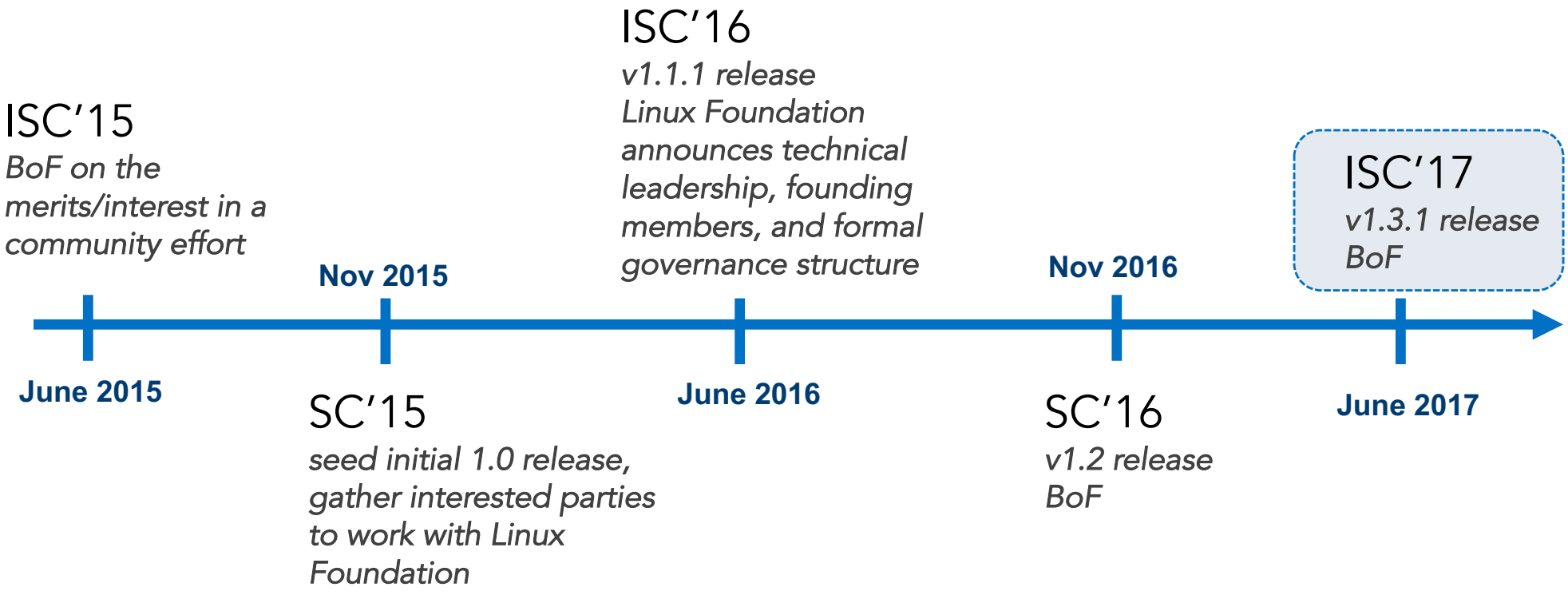
- Brief Project Overview
- Newish Items
- Latest v1.3.1 Release
- Open Forum

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.

OpenHPC: a brief History…

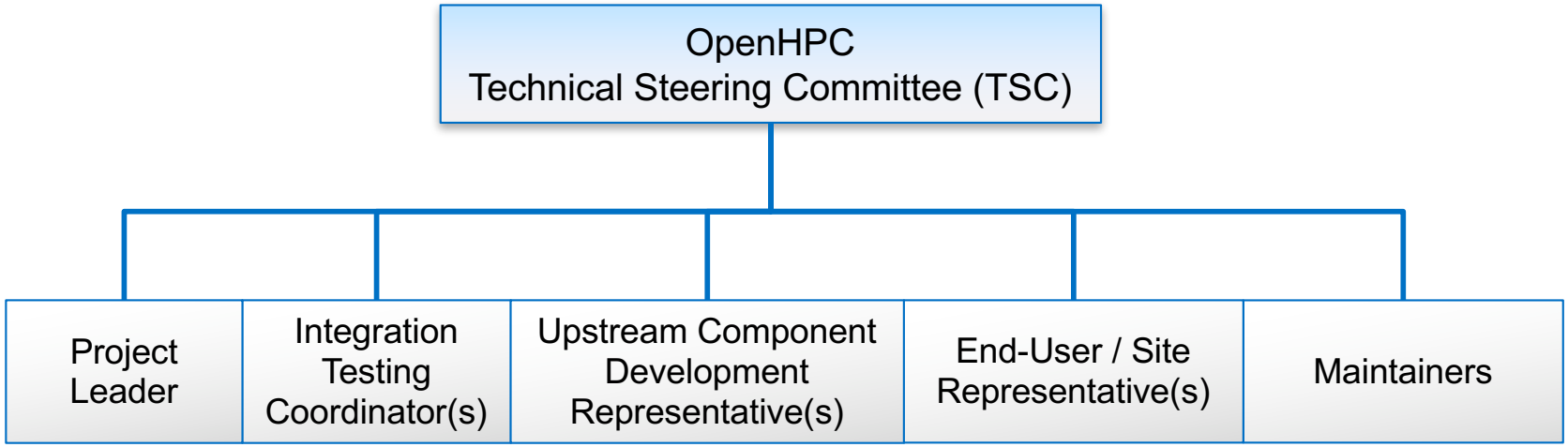


OpenHPC Project Members

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

Project member participation interest? Please contact Jeff ErnstFriedman jernstfriedman@linuxfoundation.org

OpenHPC Technical Steering Committee (TSC)
Role Overview



Note: We are currently accepting nominees for TSC volunteers for the next year:

- see recent post to openhpc-users list or email openhpc-tsc-nominations@lists.openhpc.community
- deadline is July 12

LINUX FOUNDATION
COLLABORATIVE PROJECTS

Newish Items

changes and new items since we were last together at ISC'16 BoF

Switched from ISOs -> distribution tarballs

- For those who prefer to mirror a repo locally, we have historically provided an ISO that contained all the packages/repodata
- Beginning with v1.2 release, switched to tarball based distribution
- Distribution tarballs available at:

  http://build.openhpc.community/dist
- A "make_repo.sh" script is provided that will setup a locally hosted OpenHPC repository using the contents from downloaded tarball

Index of /dist/1.2.1

Name	Last modified	Size	Description
Parent Directory		-	
OpenHPC-1.2.1.CentOS_7.2_aarch64.tar	2017-01-24 12:43	1.3G	
OpenHPC-1.2.1.CentOS_7.2_src.tar	2017-01-24 12:45	6.8G	
OpenHPC-1.2.1.CentOS_7.2_x86_64.tar	2017-01-24 12:43	2.2G	
OpenHPC-1.2.1.SLE_12_SP1_aarch64.tar	2017-01-24 12:40	1.1G	
OpenHPC-1.2.1.SLE_12_SP1_src.tar	2017-01-24 12:42	6.2G	
OpenHPC-1.2.1.SLE_12_SP1_x86_64.tar	2017-01-24 12:41	1.9G	
OpenHPC-1.2.1.md5s	2017-01-24 12:50	416	

```
# tar xf OpenHPC-1.2.1.CentOS_7.2_x86_64.tar
# ./make_repo.sh
--> Creating OpenHPC.local.repo file in /etc/yum.repos.d
--> Local repodata stored in /root/repo

# yum repolist | grep OpenHPC
OpenHPC-local           OpenHPC-1.2 - Base
OpenHPC-local-updates   OpenHPC-1.2.1 - Updates
```

More Generic Repo Paths

- Starting with the v1.3 release, we adopted more generic paths for underlying distros

```
[OpenHPC]
name=OpenHPC-1.3 - Base
baseurl=http://build.openhpc.community/OpenHPC:/1.3/CentOS_7
gpgcheck=1
gpgkey=file:///etc/pki/rpm-gpg/RPM-GPG-KEY-OpenHPC-1

[OpenHPC-updates]
name=OpenHPC-1.3 - Updates
baseurl=http://build.openhpc.community/OpenHPC:/1.3/updates/CentOS_7
gpgcheck=1
gpgkey=file:///etc/pki/rpm-gpg/RPM-GPG-KEY-OpenHPC-1
```

Similar approach for SLES12 repo config -> SLE_12

Release Roadmap Published

Release	Target Release Date	Expectations
1.3.2	August 2017	New component additions and version upgrades.
1.3.3	November 2017	New component additions and version upgrades.

Previous Releases

A history of previous OpenHPC releases is highlighted below. Clicking on the version string will take you to the `Release Notes` for more detailed information on the changes in a particular release.

Release	Date
1.3.1	June 16, 2017
1.3	March 31, 2017
1.2.1	January 24, 2017
1.2	November 12, 2016
1.1.1	June 21, 2016
1.1	April 18, 2016
1.0.1	February 05, 2016
1.0	November 12, 2015

- Have had some requests for a roadmap for future releases
- High-level roadmap now maintained on GitHub wiki:

  https://github.com/openhpc/ohpc/wiki/Release-History-and-Roadmap

Component Submission Site

- A common question posed to the project has been how to request new software components?
- We now have a simple submission site for new requests:
  - https://github.com/openhpc/submissions
  - requests reviewed on rolling basis at roughly a quarterly cadence

Next Submission Deadline: Aug 4, 2017

Subset of information requested during submission process

Software Name

Public URL

Technical Overview

Latest stable version number

Open-source license type

Relationship to component?

- ☐ contributing developer
- ☐ user
- ☐ other

If other, please describe:

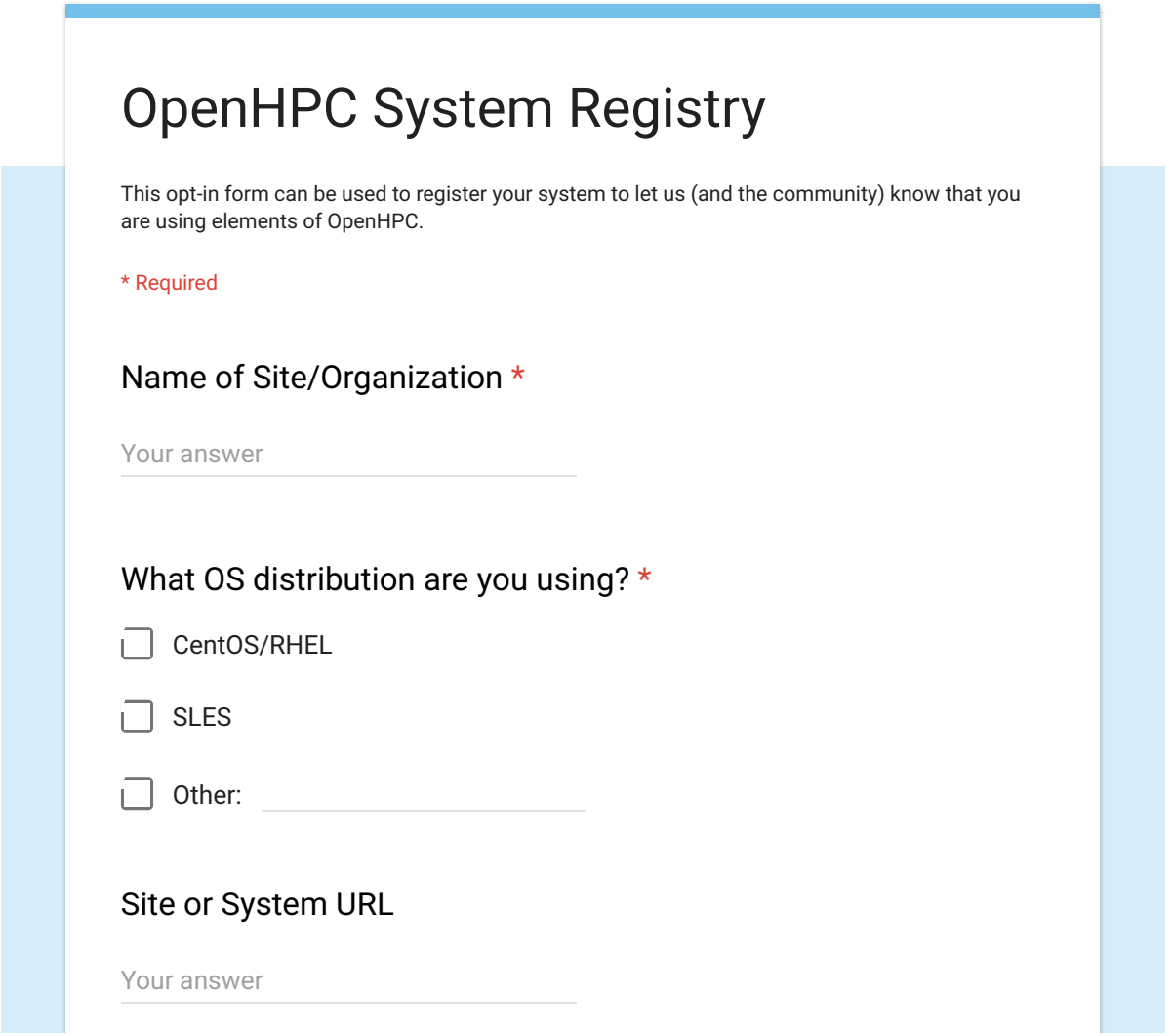
Build system

- ☐ autotools-based
- ☐ CMake
- ☐ other

Opt-in System Registry Now Available

- Interested users can now register their usage on a public system registry
- Helpful for us to have an idea as to who is potentially benefitting from this community effort
- Accessible from top-level GitHub page

System Registry



OpenHPC System Registry

This opt-in form can be used to register your system to let us (and the community) know that you are using elements of OpenHPC.

* Required

Name of Site/Organization *

Your answer

What OS distribution are you using? *

- [ ] CentOS/RHEL
- [ ] SLES
- [ ] Other:

Site or System URL

Your answer

Multiple Architecture Builds

- Starting with v1.2 release, we also include builds for **aarch64**
  - both SUSE and RHEL/CentOS now have aarch64 variants available for latest versions (SLES 12 SP2, CentOS 7.3)

- Recipes/packages being made available as a Tech Preview
  - some additional work required for provisioning
  - significant majority of development packages testing OK, but there are a few known caveats
  - please see https://github.com/openhpc/ohpc/wiki/ARM-Tech-Preview for latest info

Base OS	x86_64	aarch64	noarch
CentOS 7.3	583	361	60
SLES 12 SP2	587	363	60

v1.3.1 RPM counts

Dev Environment Consistency

x86_64

```
karl@sms001:~> module avail

---------------------------- /opt/ohpc/pub/moduledeps/gnu-mpich -----------------------------
   adios/1.10.0    mpiP/3.4.1              petsc/3.7.0        scorep/3.0
   boost/1.61.0    mumps/5.0.2             phdf5/1.8.17       sionlib/1.7.0
   fftw/3.3.4      netcdf/4.4.1            scalapack/2.0.2    superlu_dist/4.2
   hypre/2.10.1    netcdf-cxx/4.2.1        scalasca/2.3.1     tau/2.25.2
   imb/4.1         netcdf-fortran/4.4.4    scipy/0.18.0       trilinos/12.6.4

------------------------------ /opt/ohpc/pub/moduledeps/gnu -------------------------------
   R_base/3.3.1    metis/5.1.0         numpy/1.11.1       openmpi/1.10.4
   gsl/2.2.1       mpich/3.2    (L)    ocr/1.0.1          pdtoolkit/3.22
   hdf5/1.8.17     mvapich2/2.2        openblas/0.2.19    superlu/5.2.1

-------------------------------- /opt/ohpc/pub/modulefiles ---------------------------------
   EasyBuild/2.9.0        clustershell/1.7.2        ohpc       (L)    prun/1.1        (L)
   autotools       (L)    gnu/5.4.0          (L)    papi/5.4.3        valgrind/3.11.0
```

aarch64

```
karl@cavium1:~> module avail

---------------------------- /opt/ohpc/pub/moduledeps/gnu-mpich -----------------------------
   adios/1.10.0    mpiP/3.4.1              petsc/3.7.0        scorep/3.0
   boost/1.61.0    mumps/5.0.2             phdf5/1.8.17       sionlib/1.7.0
   fftw/3.3.4      netcdf/4.4.1            scalapack/2.0.2    superlu_dist/4.2
   hypre/2.10.1    netcdf-cxx/4.2.1        scalasca/2.3.1     tau/2.25.2
   imb/4.1         netcdf-fortran/4.4.4    scipy/0.18.0       trilinos/12.6.4

------------------------------ /opt/ohpc/pub/moduledeps/gnu -------------------------------
   R_base/3.3.1    metis/5.1.0         numpy/1.11.1       openmpi/1.10.4
   gsl/2.2.1       mpich/3.2    (L)    ocr/1.0.1          pdtoolkit/3.22
   hdf5/1.8.17     mvapich2/2.2        openblas/0.2.19    superlu/5.2.1

-------------------------------- /opt/ohpc/pub/modulefiles ---------------------------------
   EasyBuild/2.9.0        clustershell/1.7.2        ohpc       (L)    prun/1.1        (L)
   autotools       (L)    gnu/5.4.0          (L)    papi/5.4.3        valgrind/3.11.0
```

OpenHPC providing consistent development environment to the end user across multiple architectures

End-user software addition tools

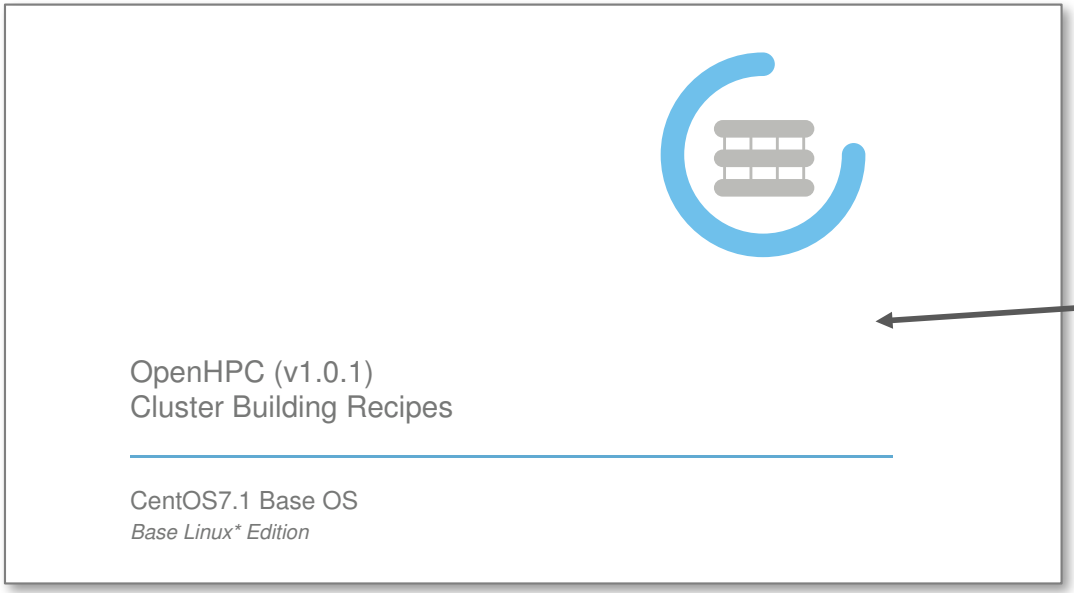
OpenHPC repositories include two additional tools that can be used to further extend a user's development environment

- EasyBuild and Spack
- leverages other community efforts for build reproducibility and best practices for configuration
- modules available for both after install

```
# module load gcc7
# module load spack
# spack compiler find
==> Added 1 new compiler to /root/.spack/linux/compilers.yaml  gcc@7.1.0
# spack install darshan-runtime
...
# . /opt/ohpc/admin/spack/0.10.0/share/spack/setup-env.sh
# module avail
----- /opt/ohpc/admin/spack/0.10.0/share/spack/modules/linux-sles12-x86_64 -----
darshan-runtime-3.1.0-gcc-7.1.0-vhd5hhg    m4-1.4.17-gcc-7.1.0-7jd575i
hwloc-1.11.4-gcc-7.1.0-u3k6dok             ncurses-6.0-gcc-7.1.0-l3mdumo
libelf-0.8.13-gcc-7.1.0-tsgwr7j            openmpi-2.0.1-gcc-7.1.0-5imqlfb
libpciaccess-0.13.4-gcc-7.1.0-33gbduz      pkg-config-0.29.1-gcc-7.1.0-dhbpa2i
libsigsegv-2.10-gcc-7.1.0-lj5rntg          util-macros-1.19.0-gcc-7.1.0-vkdpa3t
libtool-2.4.6-gcc-7.1.0-ulicbkz            zlib-1.2.10-gcc-7.1.0-gy4dtna
```

Variety of recipes now available

Choose your own adventure…



Initially, we started off with a single recipe with the intent to expand

Latest v1.3.1 release continues to expand with multiple resource managers, OSes, provisioners, and architectures:

- Install_guide-CentOS7-Warewulf-PBSPro-1.3.1-x86_64.pdf
- Install_guide-CentOS7-Warewulf-SLURM-1.3.1-aarch64.pd
- fInstall_guide-CentOS7-Warewulf-SLURM-1.3.1-x86_64.pdf
- Install_guide-CentOS7-xCAT-SLURM-1.3.1-x86_64.pdf
- Install_guide-SLE_12-Warewulf-PBSPro-1.3.1-x86_64.pdf
- Install_guide-SLE_12-Warewulf-SLURM-1.3.1-aarch64.pdf
- fInstall_guide-SLE_12-Warewulf-SLURM-1.3.1-x86_64.pdf

Additional resource manager (PBS Professional) with v1.2

Template scripts

Template recipe scripts are proved that encapsulate commands presented in the guides:

```
# yum/zypper install docs-ohpc

# ls /opt/ohpc/pub/doc/recipes/*/*/*/*/recipe.sh
/opt/ohpc/pub/doc/recipes/centos7/aarch64/warewulf/slurm/recipe.sh
/opt/ohpc/pub/doc/recipes/centos7/x86_64/warewulf/pbspro/recipe.sh
/opt/ohpc/pub/doc/recipes/centos7/x86_64/warewulf/slurm/recipe.sh
/opt/ohpc/pub/doc/recipes/centos7/x86_64/xcat/slurm/recipe.sh
/opt/ohpc/pub/doc/recipes/sles12/aarch64/warewulf/slurm/recipe.sh
/opt/ohpc/pub/doc/recipes/sles12/x86_64/warewulf/pbspro/recipe.sh
/opt/ohpc/pub/doc/recipes/sles12/x86_64/warewulf/slurm/recipe.sh

# ls /opt/ohpc/pub/doc/recipes/*/input.local
/opt/ohpc/pub/doc/recipes/centos7/input.local
/opt/ohpc/pub/doc/recipes/sles12/input.local
```

```
# compute hostnames
c_name[0]=c1
c_name[1]=c2
…
# compute node MAC addresses
c_mac[0]=00:1a:2b:3c:4f:56
c_mac[1]=00:1a:2b:3c:4f:56
…
```

input.local + recipe.sh == installed system

Test Suite

- Initiated from discussion/requests at SC'16 BoF, the OpenHPC test suite is now available as an installable RPM (introduced with v1.3 release)
- # yum/zypper install test-suite-ohpc
  - creates/relies on "ohpc-test" user to perform user testing (with accessibility to run jobs through resource manager)
  - related discussion added to recipes in Appendix C

```
[sms]# su - ohpc-test
[test@sms ~]$ cd tests
[test@sms ~]$ ./configure --disable-all --enable-fftw
checking for a BSD-compatible install... /bin/install -c
checking whether build environment is sane... yes
...
------------------------------------------- SUMMARY -------------------------------------------

Package version.............. : test-suite-1.3.0

Build user................... : ohpc-test
Build host................... : sms001
Configure date............... : 2017-03-24 15:41
Build architecture........... : x86_64
Compiler Families............ : gnu
MPI Families................. : mpich mvapich2 openmpi
```

Project CI infrastructure

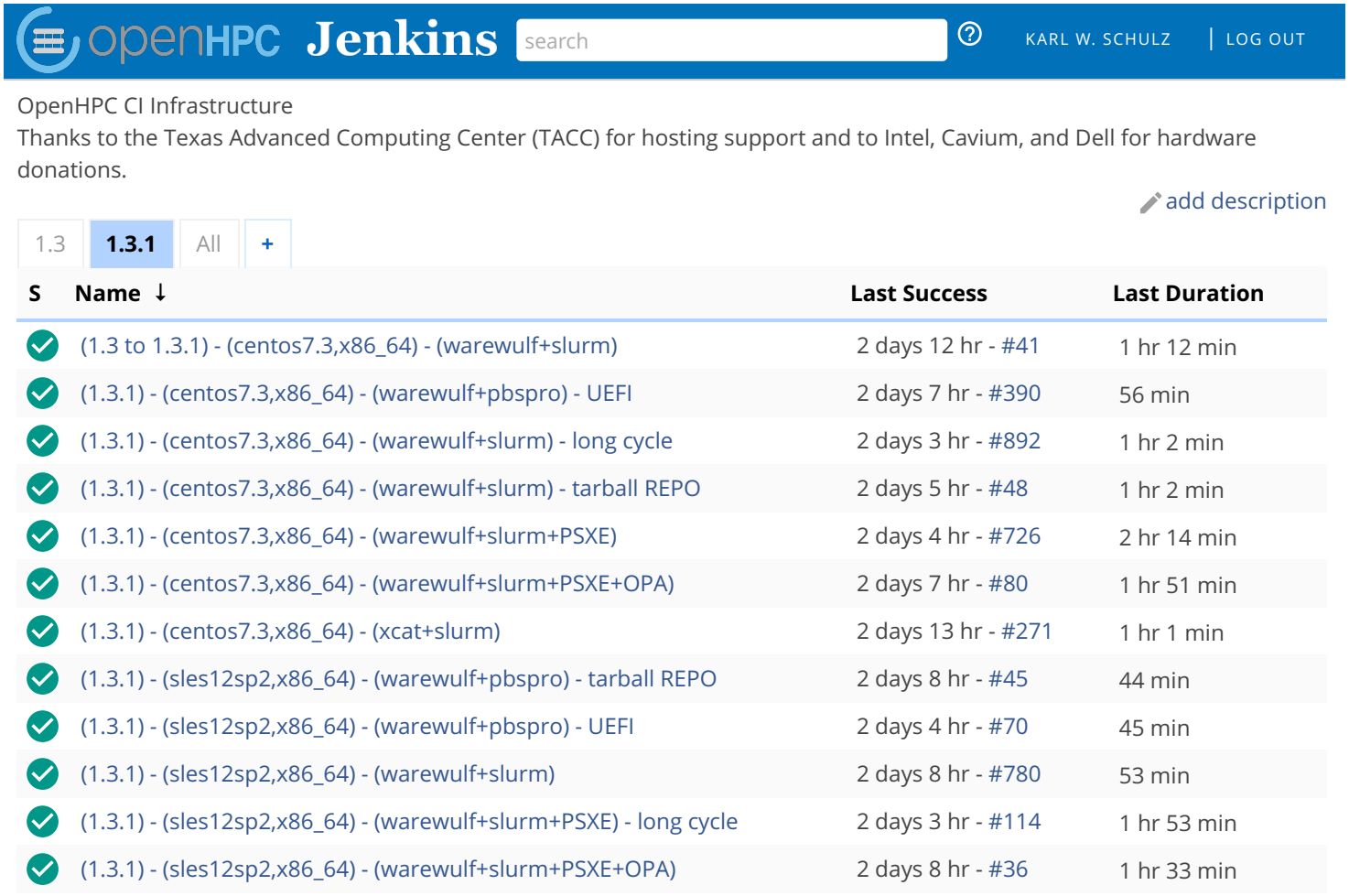
- TACC is kindly hosting some CI infrastructure for the project (Austin, TX)
- Using for build servers and continuous integration (CI) testbed.

http://test.openhpc.community:8080

Many thanks to TACC and vendors for hardware donations!!: Intel, Cavium, Dell

Community Test System for CI in use

http://test.openhpc.community:8080



All recipes exercised in CI system (start w/ bare-metal installs + integration test suite)

OpenHPC v1.3.1 Release

June 16, 2017

OpenHPC v1.3.1 - Current S/W components

components available 67 | new additions 3 | updates 44%

Functional Areas	Components
Base OS	CentOS 7.3, SLES12 SP2
Architecture	x86_64, aarch64 (Tech Preview)
Administrative Tools	Conman, Ganglia, Lmod, LosF, Nagios, pdsh, pdsh-mod-slurm, prun, EasyBuild, ClusterShell, mrsh, Genders, Shine, Spack, test-suite
Provisioning	Warewulf, xCAT
Resource Mgmt.	SLURM, Munge, PBS Professional
Runtimes	OpenMP, OCR, Singularity
I/O Services	Lustre client (community version), BeeGFS client
Numerical/Scientific Libraries	Boost, GSL, FFTW, Metis, PETSc, Trilinos, Hypre, SuperLU, SuperLU_Dist, Mumps, OpenBLAS, Scalapack
I/O Libraries	HDF5 (pHDF5), NetCDF (including C++ and Fortran interfaces), Adios
Compiler Families	GNU (gcc, g++, gfortran),
MPI Families	MVAPICH2, OpenMPI, MPICH
Development Tools	Autotools (autoconf, automake, libtool), Valgrind,R, SciPy/NumPy, hwloc
Performance Tools	PAPI, IMB, mpiP, pdtoolkit TAU, Scalasca, ScoreP, SIONLib

new with v1.3.1

Notes:

- 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
- Resulting repositories currently comprised of ~600 RPMs

Future additions approved for inclusion:

- PLASMA
- SLEPc
- pNetCDF
- Scotch
- PMIx
- Clang/LLVM

Other new items for v1.3.1 Release

Meta RPM packages introduced and adopted in recipes:

- these replace previous use of groups/patterns
- general convention remains
  - names that begin with "ohpc-*" are typically metapackges
  - intended to group related collections of RPMs by functionality
- some names have been updated for consistency during the switch over
- updated list available in Appendix E

Table 2: **Available OpenHPC Meta-packages**

Group Name	Description
ohpc-autotools	Collection of GNU autotools packages.
ohpc-base	Collection of base packages.
ohpc-base-compute	Collection of compute node base packages.
ohpc-ganglia	Collection of Ganglia monitoring and metrics packages.
ohpc-gnu7-io-libs	Collection of IO library builds for use with GNU compiler toolchain.
ohpc-gnu7-mpich-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MPICH runtime.
ohpc-gnu7-mvapich2-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the MVAPICH2 runtime.
ohpc-gnu7-openmpi-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain and the OpenMPI runtime.
ohpc-gnu7-parallel-libs	Collection of parallel library builds for use with GNU compiler toolchain.
ohpc-gnu7-perf-tools	Collection of performance tool builds for use with GNU compiler toolchain.
ohpc-gnu7-python-libs	Collection of python related library builds for use with GNU compiler toolchain.
ohpc-gnu7-runtimes	Collection of runtimes for use with GNU compiler toolchain.
ohpc-gnu7-serial-libs	Collection of serial library builds for use with GNU compiler toolchain.
ohpc-intel-impi-parallel-libs	Collection of parallel library builds for use with Intel(R) Parallel Studio XE toolchain and the Intel(R) MPI Library.
ohpc-intel-io-libs	Collection of IO library builds for use with Intel(R) Parallel Studio XE software suite.
ohpc-intel-mpich-parallel-libs	Collection of parallel library builds for use with Intel(R) Parallel Studio XE toolchain and the MPICH runtime.
ohpc-intel-mvapich2-parallel-libs	Collection of parallel library builds for use with Intel(R) Parallel Studio XE toolchain and the MVAPICH2 runtime.
ohpc-intel-openmpi-parallel-libs	Collection of parallel library builds for use with Intel(R) Parallel Studio XE toolchain and the OpenMPI runtime.
ohpc-intel-perf-tools	Collection of performance tool builds for use with Intel(R) Parallel Studio XE toolchain.
ohpc-intel-python-libs	Collection of python related library builds for use with Intel(R) Parallel Studio XE toolchain.
ohpc-intel-runtimes	Collection of runtimes for use with Intel(R) Parallel Studio XE toolchain.
ohpc-intel-serial-libs	Collection of serial library builds for use with Intel(R) Parallel Studio XE toolchain.
ohpc-nagios	Collection of Nagios monitoring and metrics packages.
ohpc-slurm-client	Collection of client packages for SLURM.
ohpc-slurm-server	Collection of server packages for SLURM.
ohpc-warewulf	Collection of base packages for Warewulf provisioning.

Other new items for v1.3.1 Release

- A new compiler variant (gnu7) was introduced
  - in the case of a fresh install, recipes default to installing the new variant along with matching runtimes and libraries
  - if upgrading a previously installed system, administrators can opt-in to enable the gnu7 variant
- The meta-packages for "gnu7" provide a convenience mechanism to add on:
  - upgrade discussion in recipes (Appendix B) amended to highlight this workflow

```
# Update default environment
[sms]# yum -y remove lmod-defaults-gnu-mvapich2-ohpc
[sms]# yum -y install lmod-defaults-gnu7-mvapich2-ohpc

# Install GCC 7.x-compiled meta-packages with dependencies
[sms]# yum -y install ohpc-gnu7-perf-tools \
                      ohpc-gnu7-serial-libs \
                      ohpc-gnu7-io-libs \
                      ohpc-gnu7-python-libs \
                      ohpc-gnu7-runtimes \
                      ohpc-gnu7-mpich-parallel-libs \
                      ohpc-gnu7-openmpi-parallel-libs \
                      ohpc-gnu7-mvapich2-parallel-libs
```

note: could skip this to leave previous gnu toolchain as default

parallel libs for gnu7/mpich

Coexistence of multiple variants

Consider an example of system originally installed from 1.3 base release and then added gnu7 variant using commands from last slide

```
$ module list

Currently Loaded Modules:
  1) autotools   2) prun/1.1   3) gnu7/7.1.0   4) mvapich2/2.2   5) ohpc

$ module avail

--------------------------- /opt/ohpc/pub/moduledeps/gnu7-mvapich2 ----------------------------
   adios/1.11.0     imb/4.1            netcdf-cxx/4.3.0        scalapack/2.0.2    sionlib/1.7.1
   boost/1.63.0     mpiP/3.4.1         netcdf-fortran/4.4.4    scalasca/2.3.1     superlu_dist/4.2
   fftw/3.3.6       mumps/5.1.1        petsc/3.7.6             scipy/0.19.0       tau/2.26.1
   hypre/2.11.1     netcdf/4.4.1.1     phdf5/1.10.0            scorep/3.0         trilinos/12.10.1

------------------------------ /opt/ohpc/pub/moduledeps/gnu7 -------------------------------
   R_base/3.3.3     metis/5.1.0          numpy/1.12.1       openmpi/1.10.7
   gsl/2.3          mpich/3.2            ocr/1.0.1          pdtoolkit/3.23
   hdf5/1.10.0      mvapich2/2.2 (L)     openblas/0.2.19    superlu/5.2.1

---------------------------------- /opt/ohpc/pub/modulefiles -----------------------------------
   EasyBuild/3.2.1            gnu/5.4.0           ohpc         (L)    singularity/2.3
   autotools           (L)    gnu7/7.1.0   (L)    papi/5.5.1          valgrind/3.12.0
   clustershell/1.7.3         hwloc/1.11.6        prun/1.1     (L)
```

everything else from 1.3.1 updates (add-on)

previously installed from 1.3 release

Other new items for v1.3.1 Release

- Two new packages introduced to add in centralization of common files for builds and file system conventions
  - introduction of "ohpc-filesystem" RPM to own top-level paths
  - introduction of "ohpc-buildroot" RPM which houses utilities used to set compiler/MPI flags for builds (formerly included in each package as OHPC_setup_compiler and OHPC_setup_mpi)
- main change is that ohpc-buildroot is now needed locally if wanting to build from .src.rpm
  - this is a published package so you can just "yum/zypper install" as usual
  - discussion in Appendix D.2 on building from source updated to reflect this addition

```
# Install rpm-build package from base OS distro
[test@sms ~]$ sudo yum -y install rpm-build

# Install OpenHPC RPM build macros
[test@sms ~]$ sudo yum -y install ohpc-buildroot

# Download SRPM from OpenHPC repository and install locally
[test@sms ~]$ rpm -i \
  http://build.openhpc.community/OpenHPC:/1.3/CentOS_7.3/src/fftw-gnu-openmpi-ohpc-3.3.6-20.3.src.rpm
```

Summary

- Technical Steering Committee has been working together for ~1 year
- Provided a highlight of changes/evolutions that have occurred since ISC'16
- Potential item of note: will have first tutorial at PEARC'17 next month
  - *Getting Started with OpenHPC*
  - *July 10, New Orleans, LA*

Community Resources

http://openhpc.community (general info)
https://github.com/openhpc/ohpc (main GitHub site)
https://github.com/openhpc/submissions (new submissions)
https://build.openhpc.community (build system/repos)
http://www.openhpc.community/support/mail-lists/ (mailing lists)

Open Forum

Now, let's open up for general discussion. Potential topics:

- what are your experiences so far?
- what's good/bad?
- suggestions for things you would like to see from OpenHPC going forward?
- general feedback, discussion…
- where can I get a lego?
- ???