



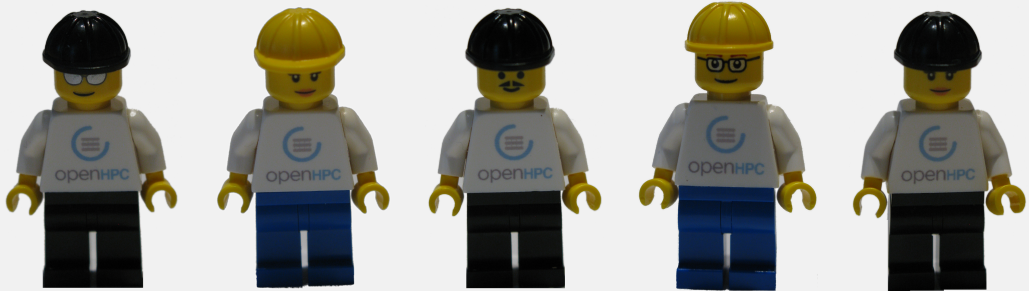
OpenHPC Introduction

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Tübix 2018
June 09, Tübingen



Building Blocks: Pick and Choose



But, Why???



Short HPC introduction

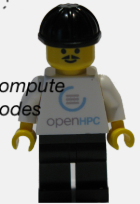
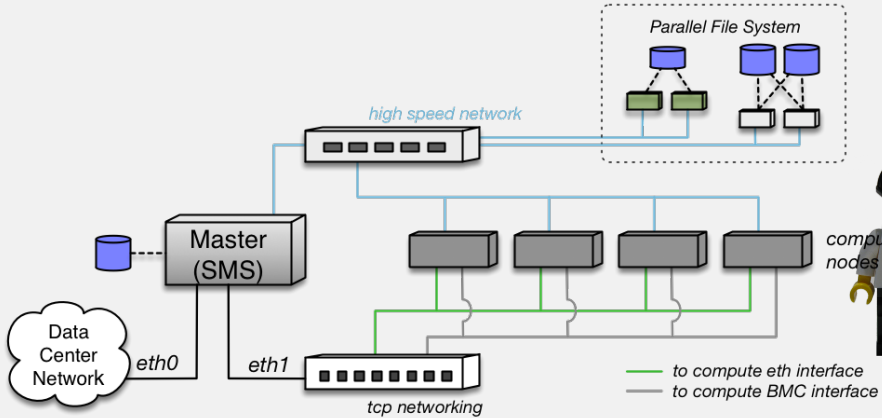


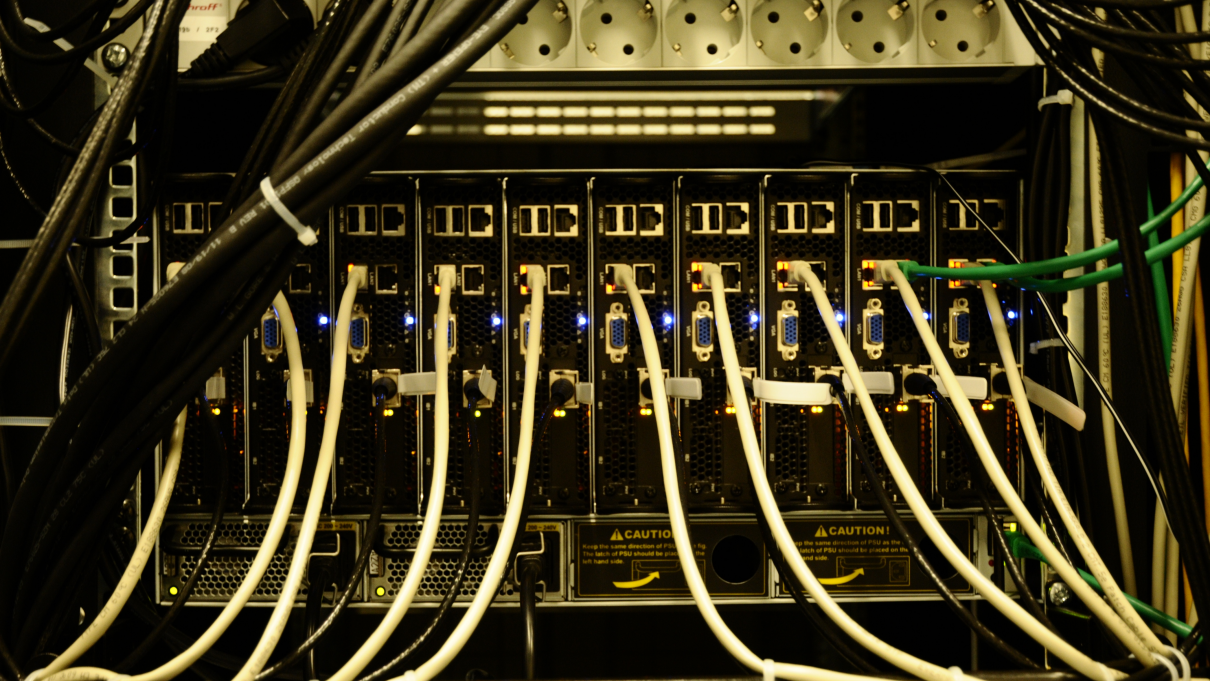
Many things can be HPC



From eight cores
to a millions of cores







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... / 292

CAUTION!
Keep the same direction of PSU airflow. The direction of PSU airflow should be preserved on the left-hand side.

CAUTION!
Keep the same direction of PSU airflow. The direction of PSU airflow should be preserved on the right-hand side.

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... / 292

Use Case Examples



Use Case Examples

Mix of free and
proprietary software



Use Case Examples

Location of wind power farms



Use Case Examples

Optimizing chemical fume hoods



Use Case Examples

Formula Student



Use Case Examples

Data Mining



Software Setup

Common for
many HPC sites



Software Setup

Each software in
multiple versions



Software Setup

Multiple Compilers



Software Setup

Multiple MPIs - Message Passing Interface



Software Setup

Open MPI
MPICH
MVAPICH2



Software Setup

Each MPI compiled
with each compiler



Software Setup

```
package-<compiler>-<mpi>
```



Software Setup

`fftw-gnu7-openmpi`

`fftw-gnu7-mvapich2`

`fftw-gnu6-mpich`



Software Setup

Three compilers
Two versions each
Already six permutations



Software Setup

Six compiler permutations

Three MPIs

Two versions each

Already 36 permutations



Software Setup

Managed using
environment modules



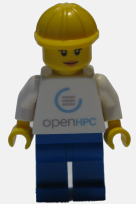
Further Common Tasks

Resource Manager



Further Common Tasks - Resource Manager

Aware of all existing resources



Further Common Tasks - Resource Manager

CPU - Memory - Network
Network Locality - Cooling
Licenses



Further Common Tasks - Resource Manager

Where to start user jobs
When to start user jobs
When to end user jobs



Further Common Tasks - Resource Manager

```
1 [ohpc@centos01 ~]$ srun hostname  
2 calvin
```



Further Common Tasks - Resource Manager

```
1 [ohpc@centos01 ~]$ srun -n 8 hostname  
2 hobbes  
3 hobbes  
4 hobbes  
5 hobbes  
6 calvin  
7 calvin  
8 calvin  
9 calvin
```



Further Common Tasks - Resource Manager

```
1 [ohpc@centos01 ~]$ cat script1.sh
2 #!/bin/sh
3 date
4 hostname
5 sleep 10
6 date
7 [ohpc@centos01 ~]$ sbatch script1.sh
8 Submitted batch job 101
```



Further Common Tasks - Resource Manager

```
1 Mon 11 Dec 16:42:31 UTC 2017
```

```
2 calvin
```

```
3 Mon 11 Dec 16:42:41 UTC 2017
```



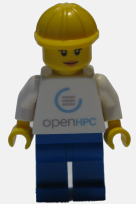
Further Common Tasks

Cluster Provisioning



OpenHPC

Reduce duplication of
all those steps



OpenHPC: Mission and Vision

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.

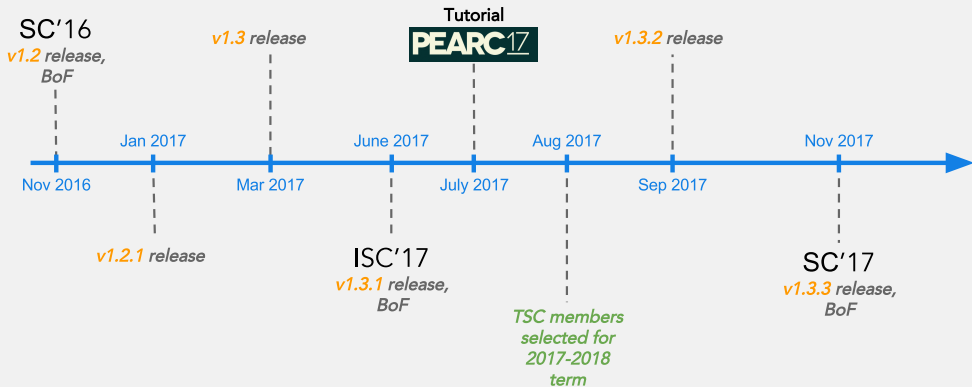
OpenHPC: Mission and Vision

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.

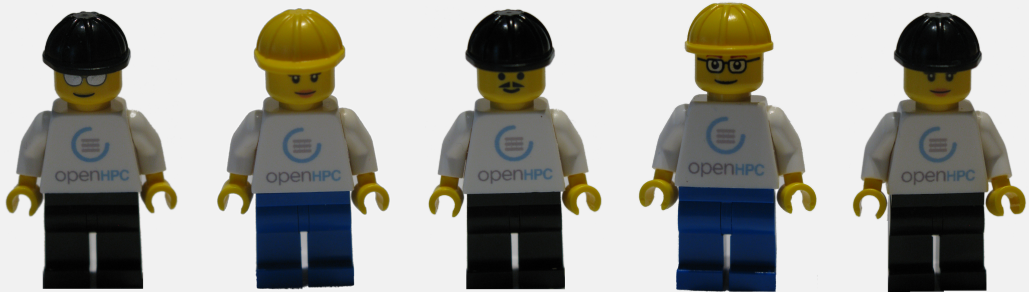
OpenHPC: Current Project Members



OpenHPC: Project History



Building Blocks: Pick and Choose



OpenHPC: Building Blocks

Important: OpenHPC provides
building blocks



OpenHPC: Building Blocks

Users can pick and choose
exactly what they need



OpenHPC: Building Blocks

x86_64 or aarch64



OpenHPC: Building Blocks

CentOS or SLES



OpenHPC: Software

Software Repository



OpenHPC: Software

Compilers



OpenHPC: Software

Message Passing Interface (MPI) libraries



OpenHPC: Software

Numerical libraries



OpenHPC: Software

I/O libraries



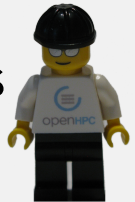
OpenHPC: Software

Performance tools



OpenHPC: Software

Software installation frameworks
Easybuild - Spack



OpenHPC: Provisioning

Warewulf



OpenHPC: Provisioning

xCAT



OpenHPC: Resource Manager

SLURM



OpenHPC: Resource Manager

PBS Professional



OpenHPC: Documentation

Very detailed documentation



OpenHPC: Documentation

For each combination of
Operating system
Provisioning System
Resource Manager



OpenHPC: Documentation

Including installation recipes
All combinations tested



OpenHPC: Same Interface Everywhere

```
[train01@sms001 ~]$ module avail
```

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

```
-----  
/opt/ohpc/pub/moduledeps/gnu7  
R/3.3.3      metis/5.1.0      numpy/1.12.1      openmpi/1.10.7  
gsl/2.3      mpich/3.2 (L)    ocr/1.0.1          pdttoolkit/3.23  
hdf5/1.10.0  mvapich
```

```
-----  
EasyBuild/3.2.1  
autotools (L)
```

x86_64

```
train01@caviu11:~> module avail
```

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

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

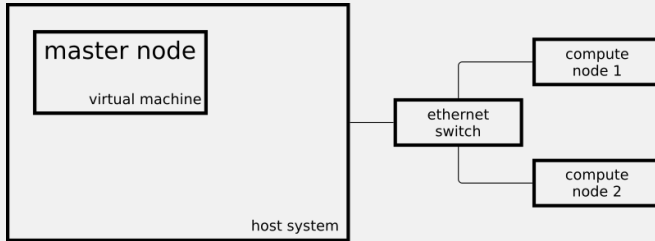
```
-----  
/opt/ohpc/pub/modulefiles  
EasyBuild/3.2.1      hwloc/1.11.6      singularity/2.3  
autotools (L)        ohpc (L)          valgrind/3.12.0
```

aarch64

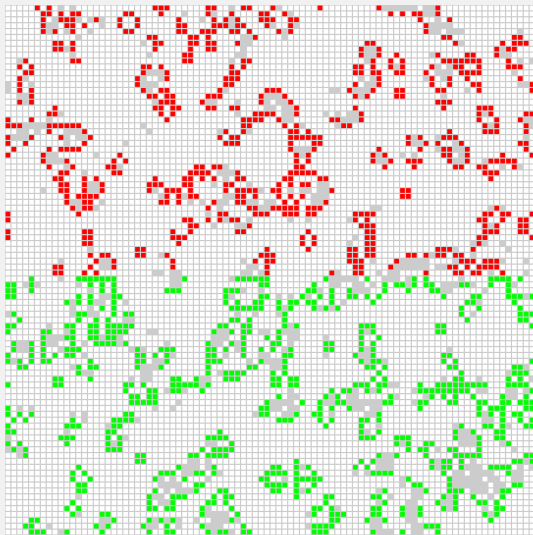


OpenHPC Demo

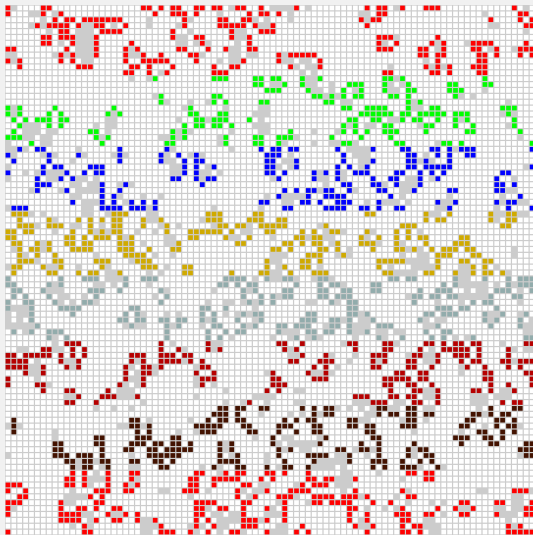
<https://opensource.com/article/18/1/how-build-hpc-system-raspberry-pi-and-openhpc>



OpenHPC Demo



OpenHPC Demo





THANK YOU

