



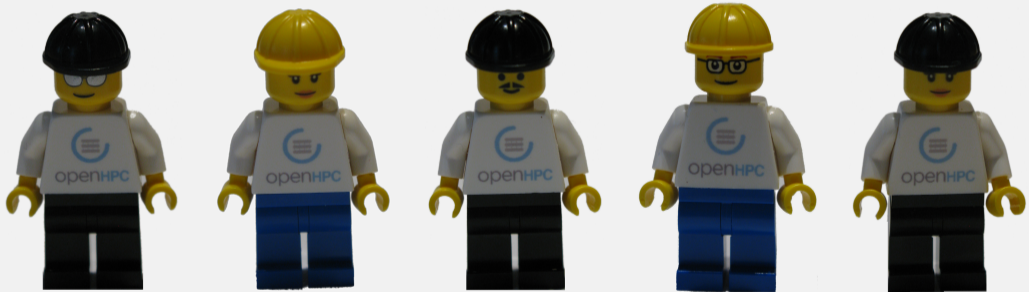
# OpenHPC and CentOS

Adrian Reber

CentOS Dojo 2018  
February 2, Brussels



# Building Blocks: Pick and Choose



# Short HPC introduction



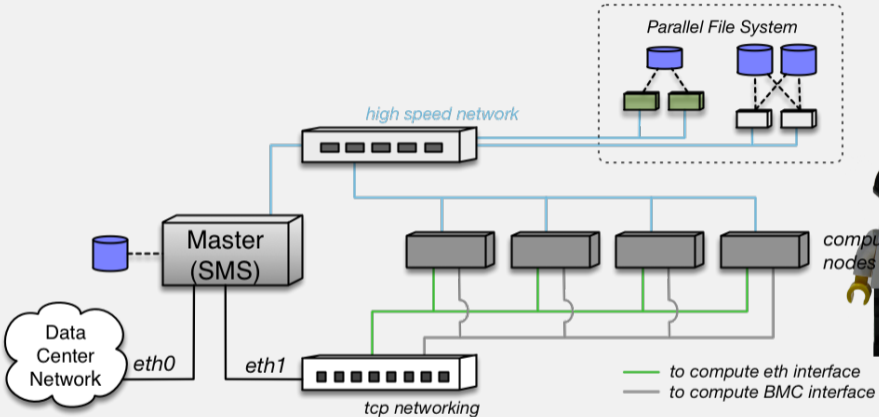


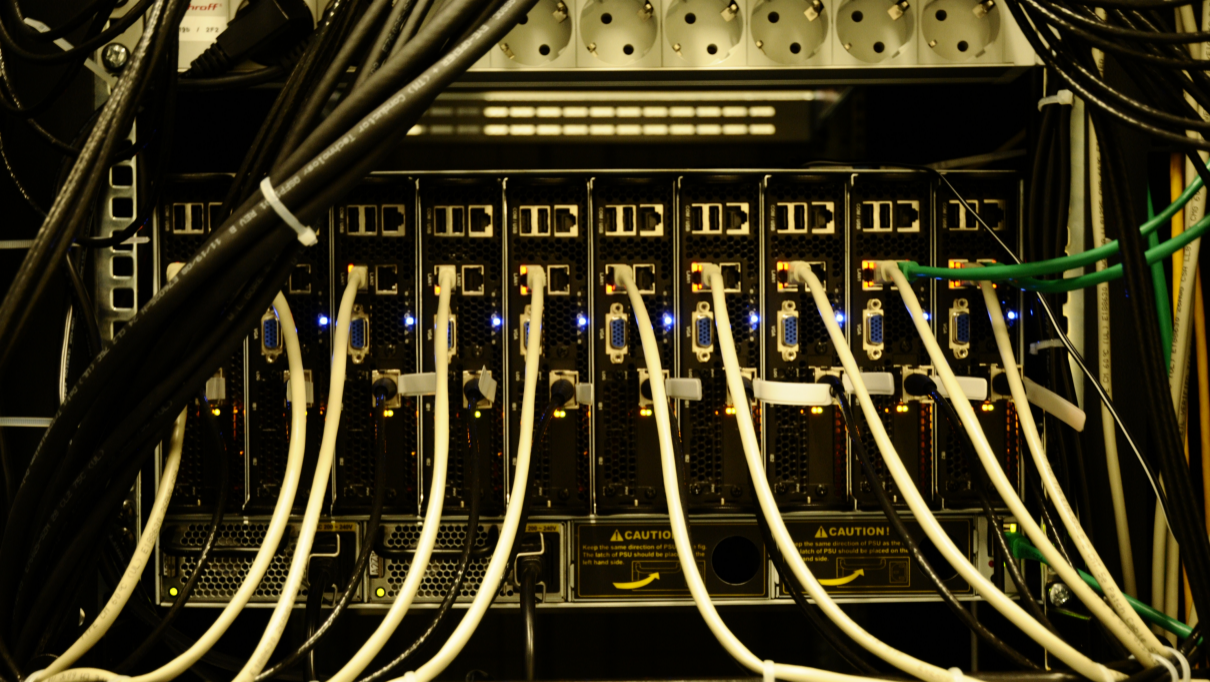
Many things can be HPC



From eight cores  
to a millions of cores







prof  
39 / 292

**CAUTION!**  
Keep the same direction of PSU airflow. The slots of PSU should be plugged on the left hand side.

**CAUTION!**  
Keep the same direction of PSU airflow. The slots of PSU should be plugged on the right hand side.

# 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.



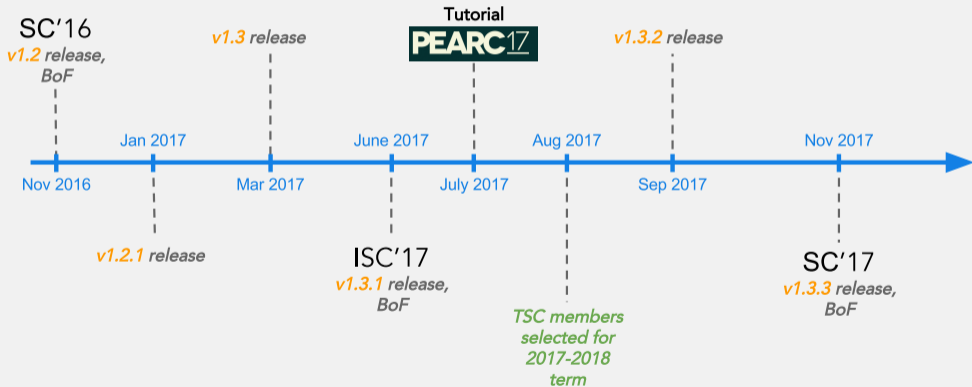
# OpenHPC: Mission and Vision

**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.

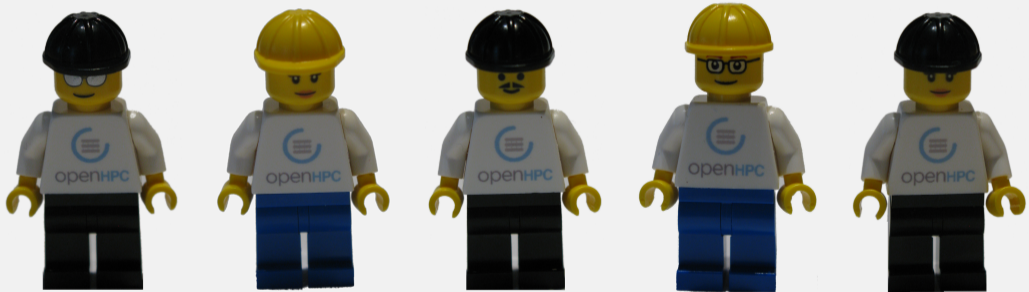
# OpenHPC: Current Project Members



# 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



# CentOS HPC SIG

Formed in April 2017





# CentOS HPC SIG

Main focus: OpenHPC



# CentOS HPC SIG

Using OpenHPC as upstream



# CentOS HPC SIG

x86\_64

aarch64

ppc64le



# CentOS HPC SIG

Better integration in CentOS  
Less package duplication



# CentOS HPC SIG

## Using devtoolset-7



ID	NVR	Tag	Built by	Finished	State
21430	pts-cotch-dts7-openmpi3-ohpc-6.0.4-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-28 08:40:09	✔
21428	trilinos-dts7-openmpi3-ohpc-12.12.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-28 03:17:57	✔
21427	netcdf-fortran-dts7-openmpi3-ohpc-4.4.4-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-28 01:19:22	✔
21426	netcdf-cxx-dts7-openmpi3-ohpc-4.3.0-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-28 01:13:09	✔
21425	slepc-dts7-openmpi3-ohpc-3.8.2-1	hpc7-openhpc-13-candidate	adrian	2018-01-28 01:06:31	✔
21424	scalasca-dts7-openmpi3-ohpc-2.3.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-30 10:45:54	✔
21423	netcdf-dts7-openmpi3-ohpc-4.5.0-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-28 00:38:07	✔
21422	scorep-dts7-openmpi3-ohpc-3.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-30 09:33:13	✔
21420	petsc-dts7-openmpi3-ohpc-3.8.3-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 23:56:02	✔
21419	plasma-dts7-ohpc-2.8.0-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-28 11:09:51	✔
21418	superlu-dist-dts7-openmpi3-ohpc-5.2.2-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-28 08:47:13	✔
21417	ftw-dts7-openmpi3-ohpc-3.3.7-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 23:03:12	✔
21416	slonlib-dts7-openmpi3-ohpc-1.7.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-30 08:53:37	✔
21415	phd5-dts7-openmpi3-ohpc-1.10.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 22:37:15	✔
21414	hd5-dts7-ohpc-1.10.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 22:26:32	✔
21413	tau-dts7-openmpi3-ohpc-2.27-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 22:16:42	✔
21412	npe-ohpc-3.2.0-2.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 22:03:45	✔
21411	mpich-dts7-ohpc-3.2.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 21:57:37	✔
21410	R-dts7-ohpc-3.4.3-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 21:44:41	✔
21409	pnetcdf-dts7-openmpi3-ohpc-1.8.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 21:28:35	✔
21408	mrsh-ohpc-2.12-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 21:21:38	✔
21407	ocr-dts7-ohpc-1.0.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 21:16:26	✔
21405	mvapich2-dts7-ohpc-2.2-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 20:53:14	✔
21404	shine-ohpc-1.5-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 20:34:14	✔
21403	pds-ohpc-2.33-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 20:29:37	✔
21402	metis-dts7-ohpc-5.1.0-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 20:24:12	✔
21401	slurm-ohpc-17.11.2-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 20:00:14	✔
21399	boost-dts7-openmpi3-ohpc-1.66.0-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 19:32:41	✔
21398	pdftoolkit-dts7-ohpc-3.25-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 19:10:33	✔
21397	mumps-dts7-openmpi3-ohpc-5.1.2-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-28 08:20:52	✔
21395	superlu-dts7-ohpc-5.2.1-0.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 18:08:58	✔
21393	imb-dts7-openmpi3-ohpc-2018.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 17:45:53	✔
21392	scalapack-dts7-openmpi3-ohpc-2.0.2-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 17:39:19	✔
21391	mpiP-dts7-openmpi3-ohpc-3.4.1-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 17:28:33	✔
21388	python-mpi4py-dts7-openmpi3-ohpc-3.0.0-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 16:47:24	✔
21387	pmix-ohpc-1.2.3-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 16:40:18	✔
21386	openblas-dts7-ohpc-0.2.20-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 16:34:32	✔
21385	openmpi3-dts7-ohpc-3.0.0-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 16:19:28	✔
21383	ohpc-filesystem-1.3-1.ohpc.1.3.4.0.2	hpc7-openhpc-13-candidate	adrian	2018-01-27 15:15:39	✔
21381	gsl-dts7-ohpc-2.4-1.ohpc.1.3.4.0	hpc7-openhpc-13-candidate	adrian	2018-01-27 15:23:34	✔

# CentOS HPC SIG

Better integration into CentOS  
Better distribution possibilities



# CentOS HPC SIG

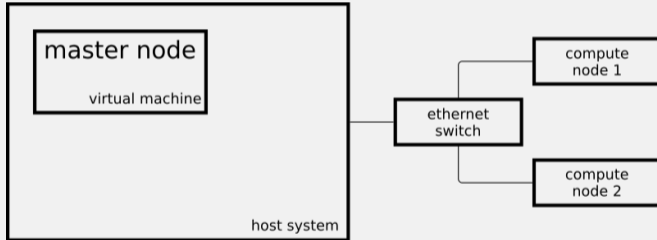
## Using the CentOS CI



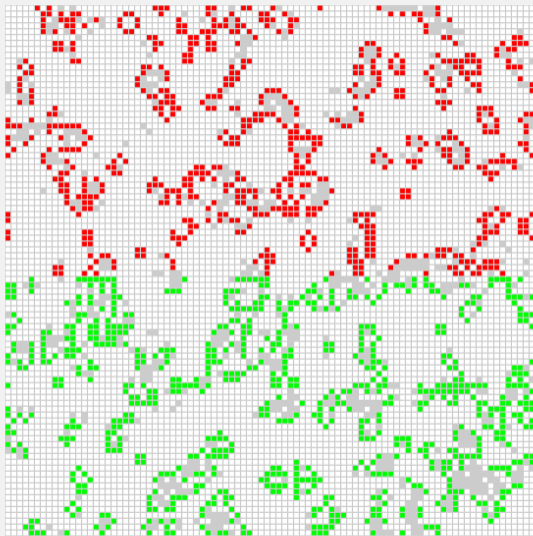


# OpenHPC Demo

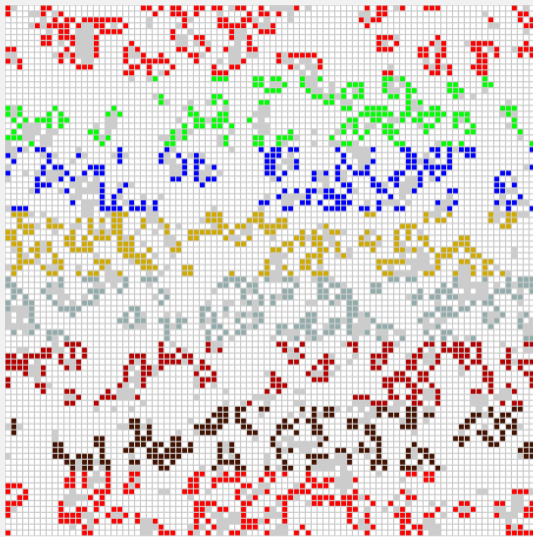
<https://opensource.com/article/18/1/how-build-hpc-system-raspberry-pi-and-openhpc>



# OpenHPC Demo



# OpenHPC Demo





**THANK YOU**

