> Content

- Options to deploy software on Maxwell

- Using Docker on Maxwell

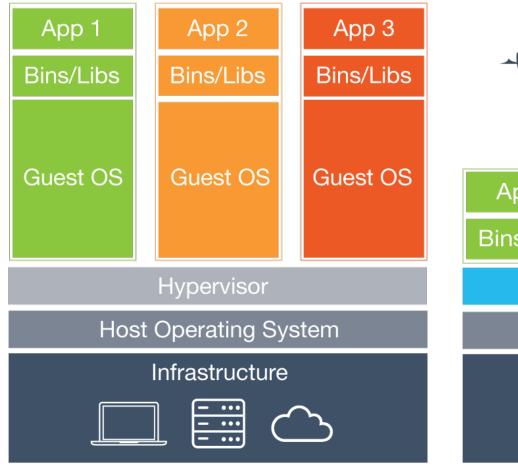- Using Singularity on Maxwell

DESY HPC User Meeting – Software deployment
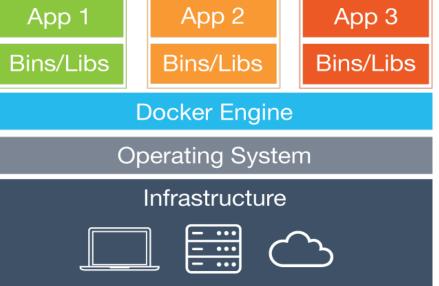
> Option One - We install the software

- System libraries

- Standard rpm packages

- Standard HPC software (compilers, …)

- Non-standard software (say thanks to Frank)

> Option Two – You install the software

- Locally – you **do not** need to be root !

- In shared group folder

- Using containers

Virtual machine

Container

> Docker is installed on Maxwell

  - You can use all Docker commands, but only when user namespaces are active (default)

> Where to store images

  - A private repository is created (max-adm01:5001)

  - Docker hub

  - Your own private repository

> Have a look at confluence pages

  https://confluence.desy.de/display/IS/Docker+containers+on+Maxwell

DESY HPC User Meeting – Docker

> ## To create an image

- Create a script with instructions – Dockerfile

```
FROM centos:7
CMD echo "Hello, World!"
```

- Build an image and push it to a repostory

```
$ docker build –t max-adm01:5001/test_image .
$ docker push max-adm01:5001/test_image
```

> ## To start a container

```
$ docker run max-adm01:5001/test_image
Hello, World!
```

DESY HPC User Meeting – Docker

> Running a non-MPI job on Maxwell

- sbatch script

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --time=00:01:00
#SBATCH --partition=all

dockerrun  max-adm01:5001/centos_mpi whoami
```

DESY HPC User Meeting – Docker

> Running an MPI job on Maxwell

- sbatch script

```
#!/bin/bash
#SBATCH --ntasks=64
#SBATCH --time=00:01:00
#SBATCH --partition=all

# start-up Docker cluster
dockercluster max-adm01:5001/centos_mpi

# run an mpi command in Docker cluster
dockerexec mpirun -np 64 hostname
```

> An alternative to Docker

- Easy to install

- No issues with user namespaces

- Can import Docker images

- Need sudo rights to build/modify images

- No out-of-the-box storage (yet)

- Parallelization outside of containers

> Gaining popularity in Grid community

> Installed on Maxwell as well

> Run a command from Singularity image

```
$ singularity exec /tmp/Centos7-ompi.img echo hello
hello
```

> Get a Docker image and run a command via Singularity

```
$ singularity exec docker.://centos:7 whoami
yakubov
```

> Running MPI job (will work only with MPI 2.x)

- sbatch script

```
#!/bin/bash
#SBATCH --ntasks=64
#SBATCH --time=00:01:00
#SBATCH --partition=all

mpirun singularity exec /tmp/Centos-7.img /usr/bin/ring
```