Singularity

enables users to have full control of their environment

Description

Singularity is a free, cross-platform and open-source computer program that performs operating-system-level virtualization also known as containerization. One of the main uses of Singularity is to bring containers and reproducibility to scientific computing and the high-performance computing (HPC) world.

The need for reproducibility requires the ability to use containers to move applications from system to system.

Using Singularity containers, developers can work in reproducible environments of their choosing and design, and these complete environments can easily be copied and executed on other platforms.

You can find the documentations on the Singularity docs page

Version	Installation Path	modulefile
3.2.1	`/opt/singularity/3.2.1`	*singularity/3.2.1*

Prerequisites

No group membership or license is needed. Singularity can be used by all HLRN users by default.

Modules

Selecting the version and loading the environment

Load the modulefile

```
$ module load singularity/3.2.1
```

This provides access to the binary singularity wich can be used to run containers.

Bash completion

By default bash completion for singularity is not loaded. To enjoy bash completion with Singularity commands and options, source the bash completion file as stated below:

```
source $SING_AUTOC
```

After loading singularity module, environment variable `SING_AUTOC` contains the necessary bash completion file.

Building images and running containers

Building images for Singularity requires root privileges. Therefore you need to prepare the image locally on your computer and then move the image into HLRN.

Or you can use Singularity or Docker hubs to run images located there. For more information please use:

```
singularity run --help
```

Example Jobscripts

Here is an example job of running the local Singularity image (.sif)

```
#!/bin/bash
#SBATCH -p medium
#SBATCH -N 1
#SBATCH -t 60:00

module load singularity

singularity run /sw/tools/singularity/lolcow.sif

Binding directories

Sometimes it is required to have some specific paths in container, which are not mounted by default. For
instance, /scratch/tmp is a default TMPDIR in the host system and is not available by default within the
container, which might cause problems with software that needs it. You can either edit the environment variable
or bind the /scratch as shown below:

singularity {run|exec|shell} --bind /scratch /path/to/singularity.sif
```