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RZ Seminar - Software

High Performance Computing with Elwetritsch

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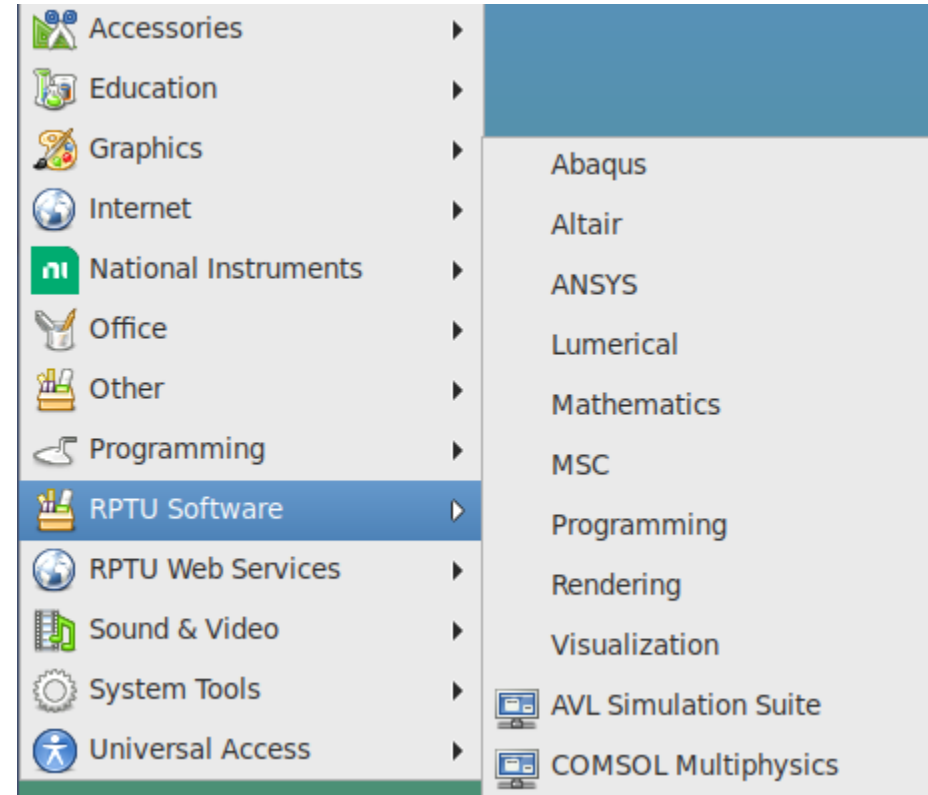
# Software

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Like most HPC systems

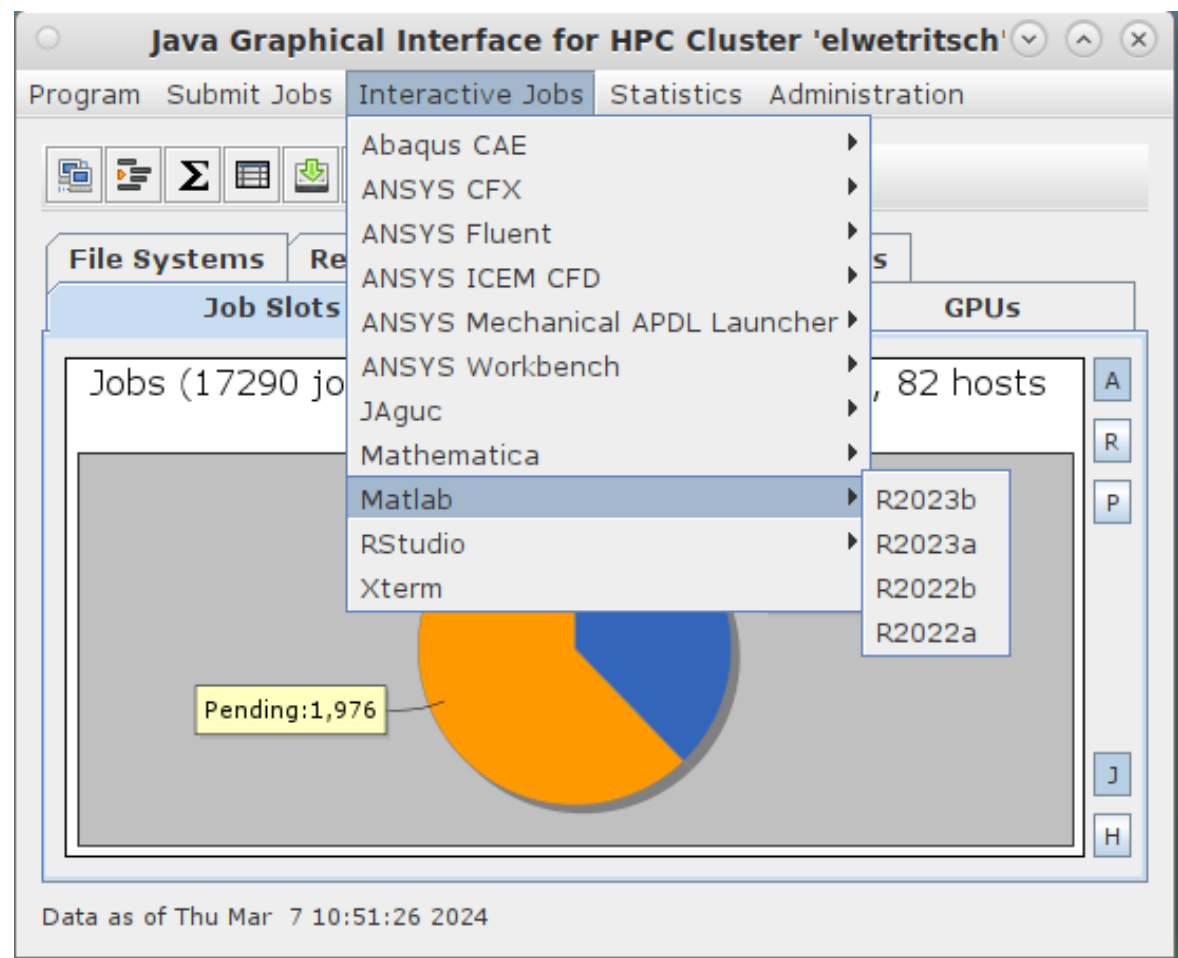
- **LINUX based**

We try to provide a Windows like facing



# Software

Or with our graphical Interface jslurm:



# Software

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Many software packages pre-installed

- some users like different versions of the software

Module package:

module is a user interface that provides for the dynamic modification of the user's environment via modulefiles.

if you need a software package

- load its module

if you need it in a different version

- remove the module
- load it in different version

if you need a second package

- add its module

**All in a single session!**

# Working with Modules

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I want to use Matlab - is it installed?

```
module avail matlab
```

```
schuele@head2 [~] module avail matlab
----- /software/modulefiles -----
matlab/latest  matlab/R2022a  matlab/R2022b  matlab/R2023a  matlab/R2023b
```

it's (at the time of this text) available in 4 versions.  
latest points to (guess it)

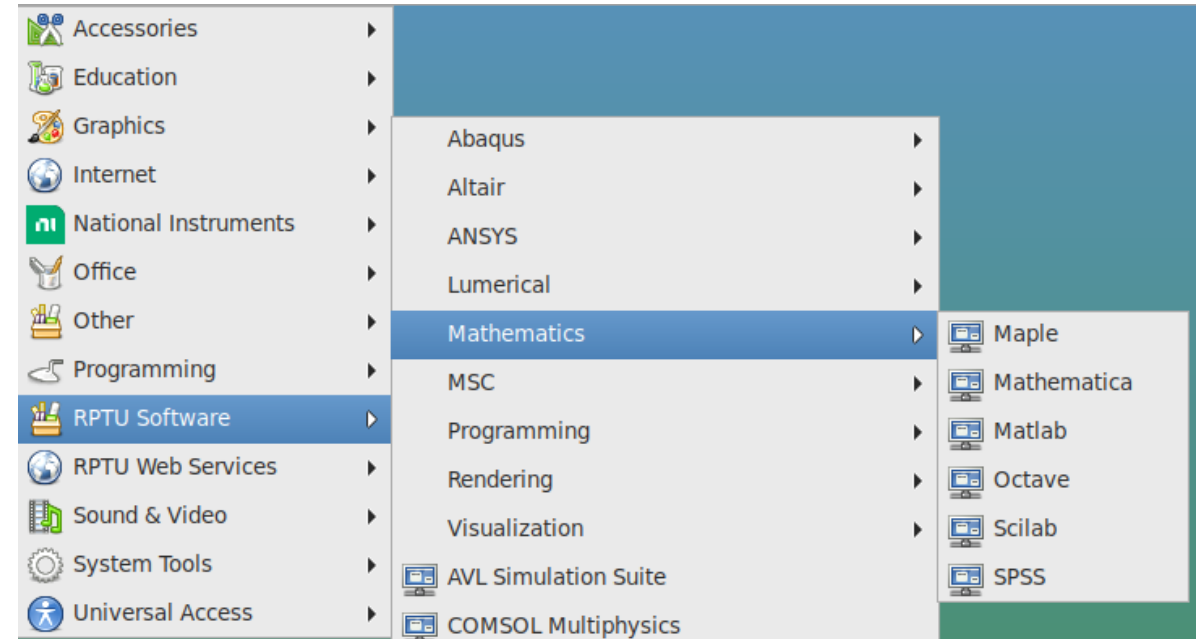
Ok. I want to use version a from of 2022:  
module load matlab/R2022a  
or - may be the last one is better  
module purge  
module load matlab/latest

# Working with Modules

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Other possibilities to start Matlab:

RDP Menue



# Working with Modules

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Some recommendations:

If you work in batch mode (SLURM):

- `add`  
`module purge`

Loaded modules are inherited to the batch environment. This will clean everything and guarantee a reproducible setup.

If you work frequently with the same module:

- don't add it into your `.bashrc`

Matters will change faster than you think and your entry in `.bashrc` will be forgotten and may cause problems

# Working with Modules

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And of course you may control your module setup:

module list

```
schuele@head2 [~] module load matlab/R2022a
schuele@head2 [~] module load matlab/latest
schuele@head2 [~] module list
Currently Loaded Modulefiles:
 1) matlab/R2022a    2) matlab/latest
schuele@head2 [~]
schuele@head2 [~] module del matlab/latest
schuele@head2 [~] module list
Currently Loaded Modulefiles:
 1) matlab/R2022a
```