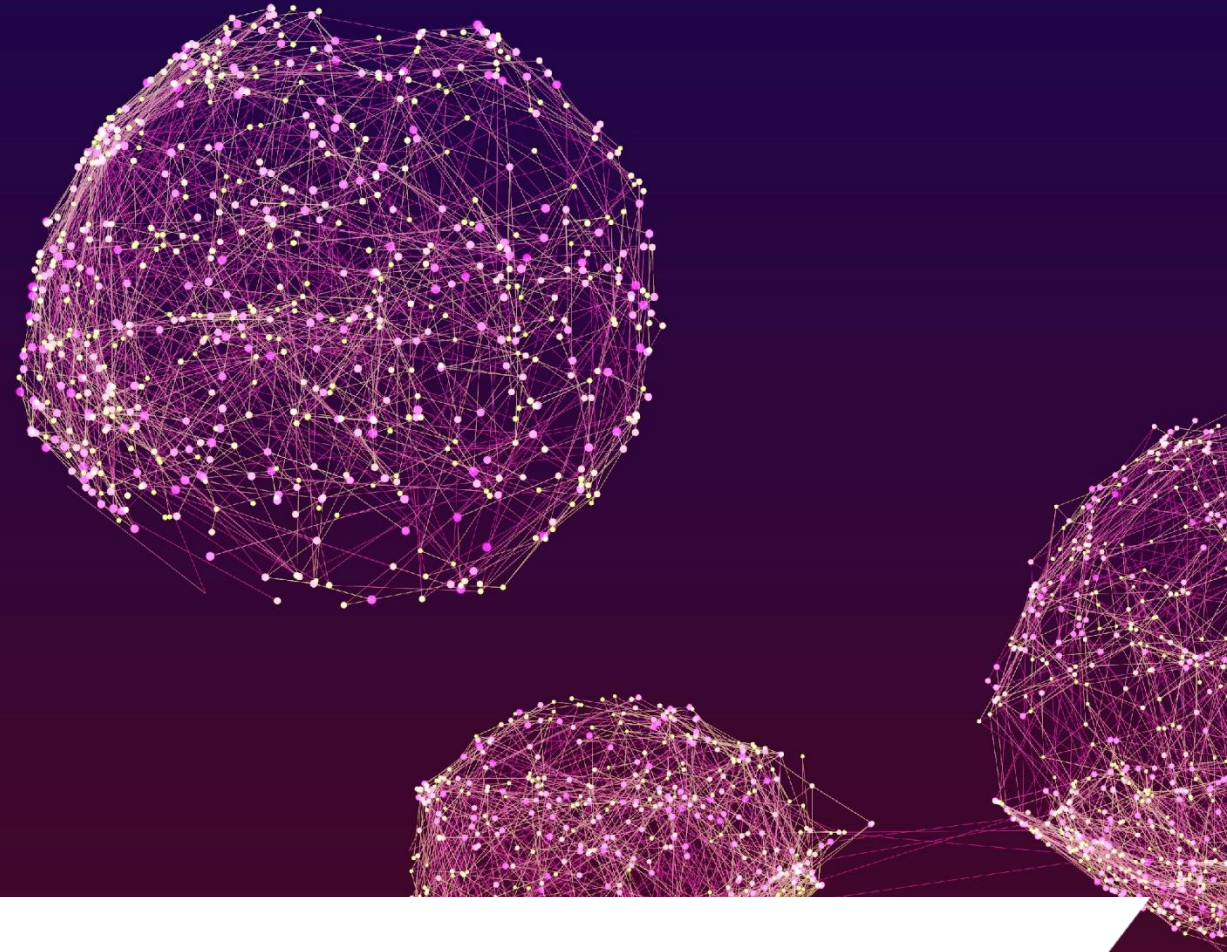


Rocky HPC Migration



Rocky HPC



<https://w>

<http>



Linux



[31999.html](https://www.ubuntu.com/31999.html)

5

Rocky HPC Migration



- CentOS will no longer be developed– Migration needed
- General Information
- New Module System
- Recompile your Software
- Revise your Batchscripts
- Where to get help?

General Information



- Rocky Linux 8.7 Green Obsidian
- only FastX 3 is supported

- Rocky batch nodes are available now
- CentOS Nodes will only be available till April 30th, 2023
- The distribution of nodes will gradually shift to Rocky
- Queue times on CentOS might increase as a result

- New Modules, we will not backport to very old software versions
(intel/2022a is new standard)

<https://help.itc.rwth-aachen.de/service/rhr4fjuttff/article/c3735af4173543b9b14a3f645a553e8a>

Rocky Front End

login18-beta.hpc.itc.rwth-aachen.de

Front Ends migrated on March 8, 2023:

login18-2.hpc.itc.rwth-aachen.de

login18-3.hpc.itc.rwth-aachen.de

login18-x-2.hpc.itc.rwth-aachen.de

login18-g-2.hpc.itc.rwth-aachen.de

copy18-2.hpc.itc.rwth-aachen.de



New Module System

LMOD und EasyBuild

- Finding Modules
- Toolchains
- Collections

Same ... but different



- PLEASE use the module system!! We provide Software for you.

- module list Lists loaded modules
- module load/unload foo Loads/Unload modules, case sensitive, Unloading has problems
- module switch foo bar Switches module foo for module bar
- module purge Purges the module system → all modules are unloaded
- module avail Lists modules available to load, different categories
C Compiler, M MPI, m mathlib, g GPU, D Default, TC Toolchain

Lots of modules



- Cfd
 - ABAQUS
 - ANSYS
 - CGNS
 - Hyperworks
 - OpenFOAM
- Chem
 - Gaussian
 - PETSc
 - QuantumESPRESSO
 - turbomole
 - VASP
- Devel
 - ARMForge
 - Boost
 - Clang
 - Cmake
 - GCC
 - GDB
- git
 - git-lfs
 - hwloc
 - iccifort
 - intel-compilers
 - Java
 - LLVM
 - MPICH
 - NCCL
 - netCDF
 - netCDF-Fortran
 - Ninja
 - NVHPC
 - OpenMPI
 - PnetCDF
 - Python
 - Qt5
 - R
 - Scons
 - Tcl
 - Tk
- Togl
 - TotalView
 - Valgrind
- Io
 - CGNS
 - HDF
 - HDF5
 - netCDF
 - netCDF-Fortran
 - PnetCDF
- Material
 - GROMACS
 - Hyperworks
 - LAMMPS
 - NWChem
 - PETSc
 - QuantumESPRESSO
 - VASP
- Math
 - arpack-ng
 - CGAL
 - Eigen
 - FFTW
 - gnuplot
 - GSL
 - Gurobi
 - Hypr
 - Maple
 - OpenBLAS
 - PETSc
 - R
 - SPRNG
- Perf
 - ARMForge
 - CubeGUI
 - CubeLib
 - CubeWriter
 - Extrae
- intel-compilers
 - likwid
 - PAPI
 - Paraver
 - Scalasca
 - Score-P
 - Vampir
 - VampirServer
- Tools
 - ARMForge
 - CubeGUI
 - CubeLib
 - CubeWriter
 - HDF
 - HDF5
 - iccifort
 - intel-compilers
 - JUBE
 - netCDF
 - netCDF-Fortran
- NVHPC
 - PnetCDF
 - Scalasca
 - Score-P
 - texlive
 - TotalView
 - Vampir
 - VampirServer



<https://help.itc.rwth-aachen.de/service/rhr4fjuttff/article/9d5dea0bfb914069a6b4bc39666206d2/>

Same ... but different



- module spider foo
- module category (foo)

Searches for modules, partial matches, case insensitive
Lists Categories for modules or modules in category foo

TC Toolchains

Grouped set of modules, (Compiler, MPI, mathlibs)
Working well together

- module save/restore <collection-name>
- module savelist
- module disable <collection-name>

Saves currently loaded modules as a collection with a name
Lists all available personal module collections
Removes a specific save module collection

<https://help.itc.rwth-aachen.de/service/rhr4fjjuttff/article/450d33cc19fd4e50b1dd07027e9b55bd/>



Same ... but different



- Live Demo
 - Login
 - module load, purge
 - How to find dependencies using spider

How to Rock(y) - Part 1



1. Change any defaults you use: (although you really should not use defaults to load modules like that)
 - `.zshrc/.bashrc`
2. Check the modules you use for name & version changes
3. Modify your SLURM jobscripts, compile- and any helper scripts with new module names (save/restore collection)

Recompile your Software

Recompile your software



- Modules/Compilers/Libraries/MPI-Runtimes change
- Make sure you are aware of changes you need to adapt to
- Recompile your own software **using current modules**
 - default toolchain (intel/2022a)
 - `$FLAGS_FAST (-xSSE4.2 -xCORE-AVX2,AVX)`
- don't forget to enable debugging and optimization (in that order): `-g -O3`
- use envvars we set for you! `$FC $CC $CXX $MPIFC $MPICC $MPIEXEC $....`
 - `$MPICC -g $FLAGS_FAST mpihelloworld.c`
 - `$MPIEXEC $FLAGS_MPI_BATCH a.out`

← try also using `-xAVX512`

How to Rock(y) - Part 2



1. Reinstall personal Software like Python packages via pip
2. Familiarize yourself with changes of newer software versions
3. Recompile your own software (use our envvars)

Revise your Batchscripts

Revise your Batchscripts



- Make sure you changed modules (see above)
- You get the same OS as your Login Node
- If you want to submit to Rocky from a CentOS7 node:
 - #SBATCH --constraint=Rocky8
- Keep it simple -> Let us/SLURM do the work and verify
- use envvars we set for you! \$MPIEXEC \$FLAG_MPI_BATCH \$....
 - \$MPICC -g \$FLAGS_FAST mpihelloworld.c
 - \$MPIEXEC \$FLAGS_MPI_BATCH a.out

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login18-g-2.hpc.itc.rwth-aachen.de

copy18-2.hpc.itc.rwth-aachen.de

How to Rock(y) - Part 3



1. Check your submit node/OS to be Rocky
2. Make sure you use the new modules and your recompiled software in your jobscript
3. Make sure you use our envvars in your jobscript

Summary

How to Rock(y)



1. Change any defaults you use: (although you really should not use defaults to load modules like that)
 - .zshrc/.bashrc
2. Check the modules you use for name & version changes
3. Modify your SLURM jobscripts, compile- and any helper scripts with new module names (save/restore collection)
4. Reinstall personal Software like Python packages via pip
5. Familiarize yourself with changes of newer software sersions
6. Recompile your own software (use our envvars)
7. Check your submit node/OS to be Rocky
8. Make sure you use the new modules and your recompiled software in your jobscript
9. Make sure you use our envvars in your jobscript

Where to get help? – HERE & NOW



Overview Rocky Changes:



<https://help.itc.rwth-aachen.de/service/rhr4fjuttff/article/c3735af4173543b9b14a3f645a553e8a/>

Overview new Module System:



<https://help.itc.rwth-aachen.de/service/rhr4fjuttff/article/450d33cc19fd4e50b1dd07027e9b55bd/>

Overview available Software:

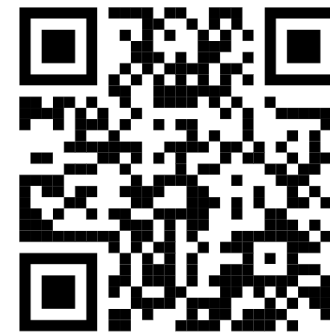


<https://help.itc.rwth-aachen.de/service/rhr4fjuttff/article/9d5dea0bf914069a6b4bc39666206d2/>



HPC
Sprechstunde

<https://blog.rwth-aachen.de/itc-events/en/hpc-consultation-hour/>



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