Environment Modules

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- Hintergrund
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- Fortgeschrittene Benutzung
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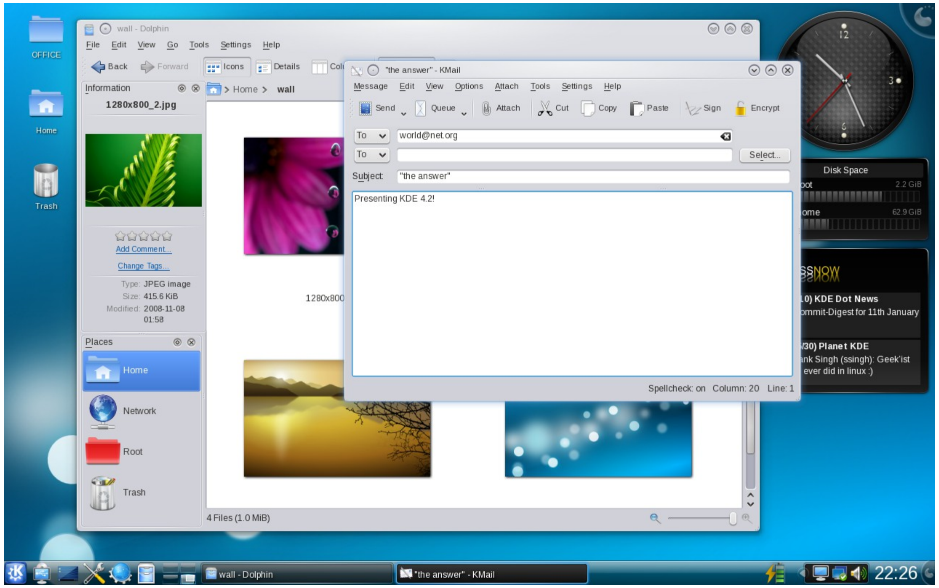
Hintergrund

Hintergrund

- Software ist im internen Netz in unterschiedlichen Versionen vorhanden
- Vor allem größere, eigenständige Anwendungen (Matlab, R, usw.) und Bibliotheken zur Kompilierung von Sourcecode (NetCDF, cernlib, usw.)
- Unix/Linux nutzt das Konzept der Umgebungsvariablen, um in Kommandoshells Programmparameter festzulegen
- Modules verändert diese, um bestimmte Versionen einer Software zur Verfügung zu stellen oder Programmen eigene Parameter mitzugeben
- Alle bekannten Kommandoshells werden unterstützt: bash, zsh, sh, csh, tcsh ...

Hintergrund

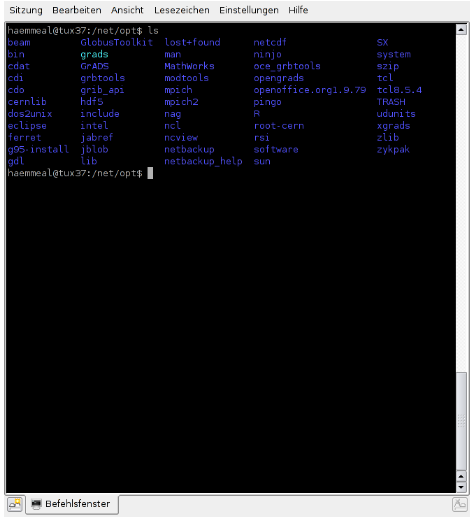
Was ist eine Kommandoshell?



To: world@net.org

Subject: "the answer"

Presenting KDE 4.2!

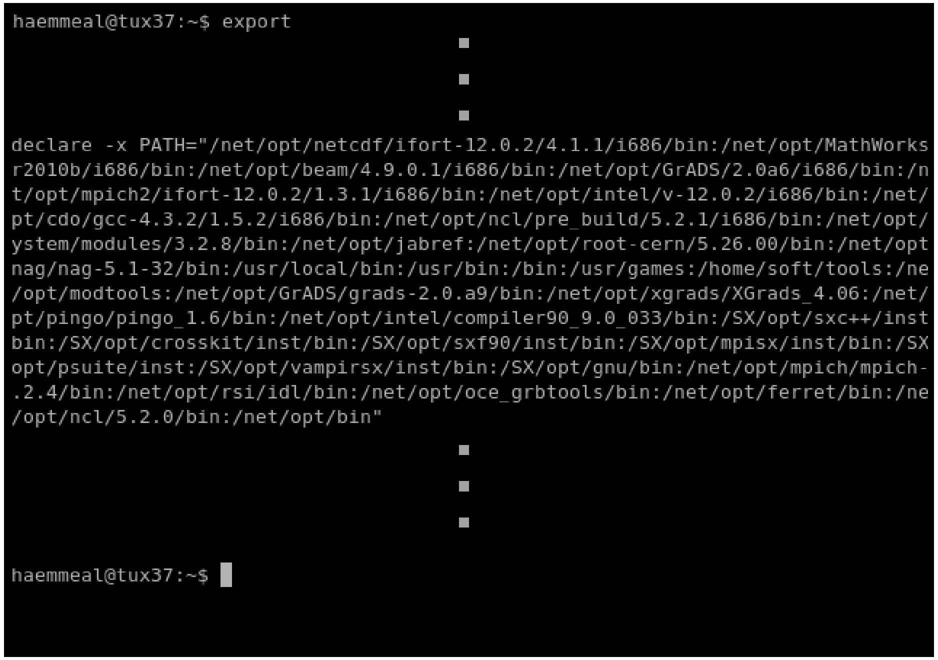


```
haemmeal@tux37:/net/opt$ ls
beam         GlobusToolkit  lost+found      netcdf                SX
bin          grads          man             ninjo                 system
cdat         GrADS          MathWorks       oce_grbtools          szip
cdi          grbtools       modtools        opengrads             tcl
cdo          grib_api       mpich           openoffice.org1.9.79  tcl8.5.4
cernlib      hdf5           mpich2          pingo                 TRASH
dos2unix     include        nag             R                     udunits
eclipse      intel          ncl             root-cern             xgrads
ferret       jabref         ncview          rsi                   zlib
g95-install  jblob          netbackup       software              zykpak
gdl          lib            netbackup_help  sun
haemmeal@tux37:/net/opt$
```

- Im Gegensatz zur grafischen Benutzeroberfläche
- Interpretiert Kommandos auf einer textbasierten Kommandozeile
- Eignet sich vor allem zur Automatisierung von Routineaufgaben

Hintergrund

Was sind Umgebungsvariablen?



```
haemmeal@tux37:~$ export
                                       ■

                                       ■

                                       ■

declare -x PATH="/net/opt/netcdf/ifort-12.0.2/4.1.1/i686/bin:/net/opt/MathWorks
r2010b/i686/bin:/net/opt/beam/4.9.0.1/i686/bin:/net/opt/GrADS/2.0a6/i686/bin:/n
t/opt/mpich2/ifort-12.0.2/1.3.1/i686/bin:/net/opt/intel/v-12.0.2/i686/bin:/net/
pt/cdo/gcc-4.3.2/1.5.2/i686/bin:/net/opt/ncl/pre_build/5.2.1/i686/bin:/net/opt/
ystem/modules/3.2.8/bin:/net/opt/jabref:/net/opt/root-cern/5.26.00/bin:/net/opt
nag/nag-5.1-32/bin:/usr/local/bin:/usr/bin:/bin:/usr/games:/home/soft/tools:/ne
/opt/modtools:/net/opt/GrADS/grads-2.0.a9/bin:/net/opt/xgrads/XGrads_4.06:/net/
pt/pingo/pingo_1.6/bin:/net/opt/intel/compiler90_9.0_033/bin:/SX/opt/sxc++/inst
bin:/SX/opt/crosskit/inst/bin:/SX/opt/sxf90/inst/bin:/SX/opt/mpisx/inst/bin:/SX
opt/psuite/inst:/SX/opt/vampirsx/inst/bin:/SX/opt/gnu/bin:/net/opt/mpich/mpich-
.2.4/bin:/net/opt/rsi/idl/bin:/net/opt/oce_grbtools/bin:/net/opt/ferret/bin:/ne
/opt/ncl/5.2.0/bin:/net/opt/bin"
                                       ■

                                       ■

                                       ■

haemmeal@tux37:~$ █
```

- Existieren innerhalb einer Kommandoshell
- Enthalten beliebige Zeichenketten
- In den meisten Fällen Pfade zu bestimmten Programmen oder Daten
- Aber auch andere Programmparameter
- Definieren eine Standardarbeitsumgebung

Die wichtigsten Befehle

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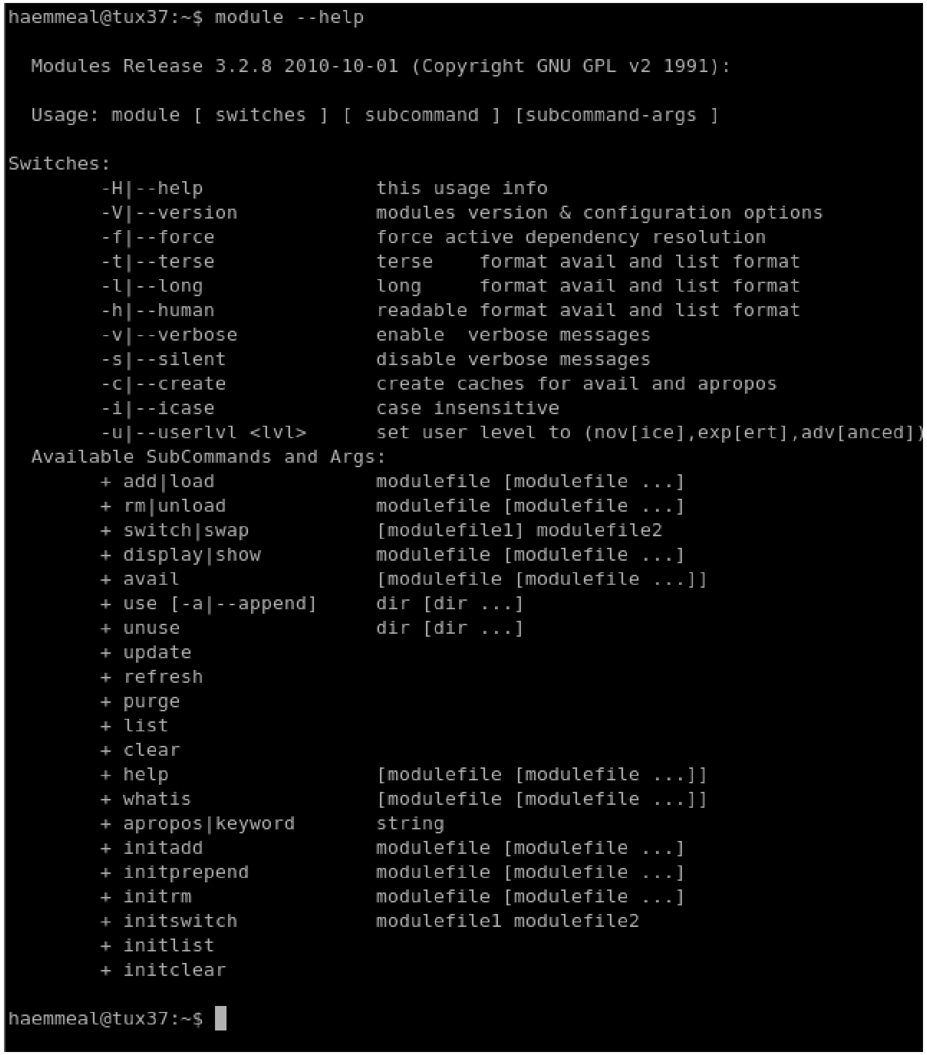
$ module --help

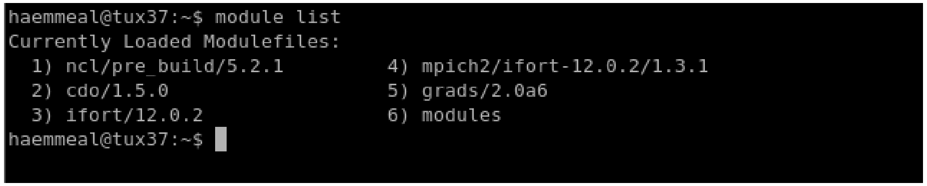


```
haemmeal@tux37:~$ module --help

  Modules Release 3.2.8 2010-10-01 (Copyright GNU GPL v2 1991):

  Usage: module [ switches ] [ subcommand ] [subcommand-args ]

Switches:
        -H|--help               this usage info
        -V|--version            modules version & configuration options
        -f|--force              force active dependency resolution
        -t|--terse              terse    format avail and list format
        -l|--long               long     format avail and list format
        -h|--human              readable format avail and list format
        -v|--verbose            enable  verbose messages
        -s|--silent             disable verbose messages
        -c|--create             create caches for avail and apropos
        -i|--icase              case insensitive
        -u|--userlvl <lvl>      set user level to (nov[ice],exp[ert],adv[anced])
  Available SubCommands and Args:
        + add|load              modulefile [modulefile ...]
        + rm|unload             modulefile [modulefile ...]
        + switch|swap           [modulefile1] modulefile2
        + display|show          modulefile [modulefile ...]
        + avail                 [modulefile [modulefile ...]]
        + use [-a|--append]     dir [dir ...]
        + unuse                 dir [dir ...]
        + update
        + refresh
        + purge
        + list
        + clear
        + help                  [modulefile [modulefile ...]]
        + whatis                [modulefile [modulefile ...]]
        + apropos|keyword       string
        + initadd               modulefile [modulefile ...]
        + initprepend           modulefile [modulefile ...]
        + initrm                modulefile [modulefile ...]
        + initswitch            modulefile1 modulefile2
        + initlist
        + initclear

haemmeal@tux37:~$ █
```

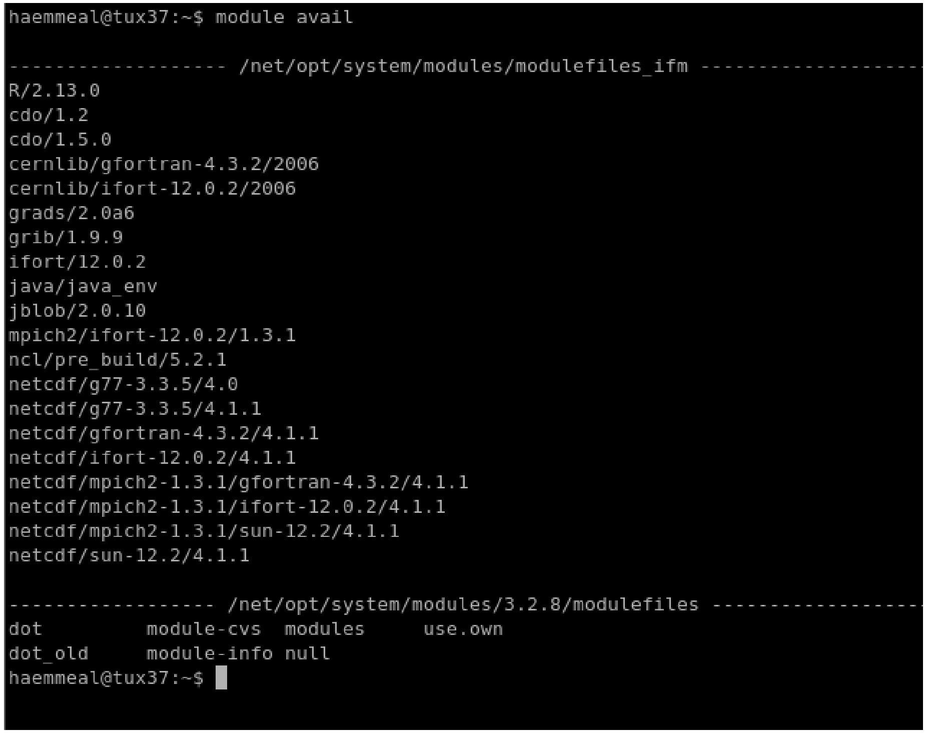
- list / available
- load / unload / switch
- help
- man module

Die wichtigsten Befehle

$ module list / avail

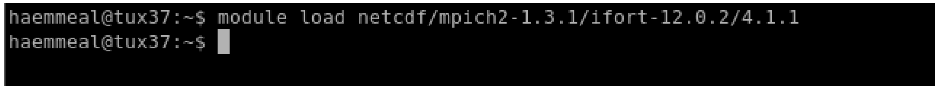


```
haemmeal@tux37:~$ module list
Currently Loaded Modulefiles:
  1) ncl/pre_build/5.2.1         4) mpich2/ifort-12.0.2/1.3.1
  2) cdo/1.5.0                   5) grads/2.0a6
  3) ifort/12.0.2                6) modules
haemmeal@tux37:~$ 
```

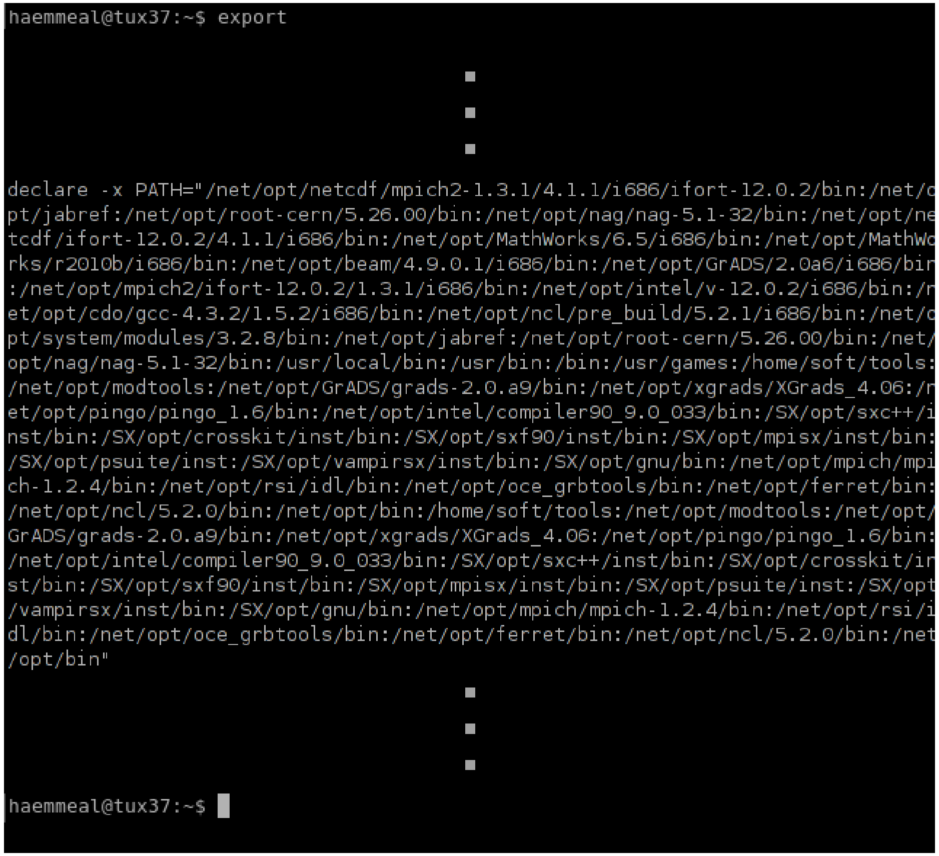


```
haemmeal@tux37:~$ module avail

------------------- /net/opt/system/modules/modulefiles_ifm -------------------
R/2.13.0
cdo/1.2
cdo/1.5.0
cernlib/gfortran-4.3.2/2006
cernlib/ifort-12.0.2/2006
grads/2.0a6
grib/1.9.9
ifort/12.0.2
java/java_env
jblob/2.0.10
mpich2/ifort-12.0.2/1.3.1
ncl/pre_build/5.2.1
netcdf/g77-3.3.5/4.0
netcdf/g77-3.3.5/4.1.1
netcdf/gfortran-4.3.2/4.1.1
netcdf/ifort-12.0.2/4.1.1
netcdf/mpich2-1.3.1/gfortran-4.3.2/4.1.1
netcdf/mpich2-1.3.1/ifort-12.0.2/4.1.1
netcdf/mpich2-1.3.1/sun-12.2/4.1.1
netcdf/sun-12.2/4.1.1

------------------ /net/opt/system/modules/3.2.8/modulefiles ------------------
dot         module-cvs  modules     use.own
dot_old     module-info null
haemmeal@tux37:~$ 
```

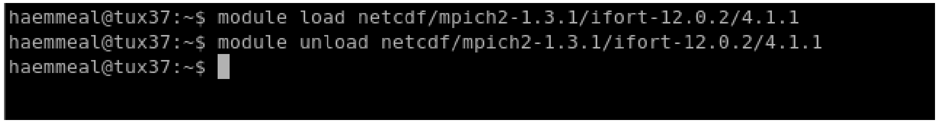
$ module load / unload <Modul>



```
haemmeal@tux37:~$ module load netcdf/mpich2-1.3.1/ifort-12.0.2/4.1.1
haemmeal@tux37:~$ 
```



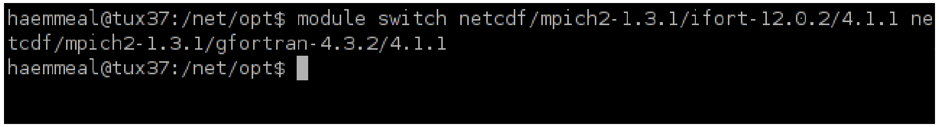
```
haemmeal@tux37:~$ export

                                        ·
                                        ·
                                        ·

declare -x PATH="/net/opt/netcdf/mpich2-1.3.1/4.1.1/i686/ifort-12.0.2/bin:/net/o
pt/jabref:/net/opt/root-cern/5.26.00/bin:/net/opt/nag/nag-5.1-32/bin:/net/opt/ne
tcdf/ifort-12.0.2/4.1.1/i686/bin:/net/opt/MathWorks/6.5/i686/bin:/net/opt/MathWo
rks/r2010b/i686/bin:/net/opt/beam/4.9.0.1/i686/bin:/net/opt/GrADS/2.0a6/i686/bin
:/net/opt/mpich2/ifort-12.0.2/1.3.1/i686/bin:/net/opt/intel/v-12.0.2/i686/bin:/n
et/opt/cdo/gcc-4.3.2/1.5.2/i686/bin:/net/opt/ncl/pre_build/5.2.1/i686/bin:/net/o
pt/system/modules/3.2.8/bin:/net/opt/jabref:/net/opt/root-cern/5.26.00/bin:/net/
opt/nag/nag-5.1-32/bin:/usr/local/bin:/usr/bin:/bin:/usr/games:/home/soft/tools:
/net/opt/modtools:/net/opt/GrADS/grads-2.0.a9/bin:/net/opt/xgrads/XGrads_4.06:/n
et/opt/pingo/pingo_1.6/bin:/net/opt/intel/compiler90_9.0_033/bin:/SX/opt/sxc++/i
nst/bin:/SX/opt/crosskit/inst/bin:/SX/opt/sxf90/inst/bin:/SX/opt/mpisx/inst/bin:
/SX/opt/psuite/inst:/SX/opt/vampirsx/inst/bin:/SX/opt/gnu/bin:/net/opt/mpich/mpi
ch-1.2.4/bin:/net/opt/rsi/idl/bin:/net/opt/oce_grbtools/bin:/net/opt/ferret/bin:
/net/opt/ncl/5.2.0/bin:/net/opt/bin:/home/soft/tools:/net/opt/modtools:/net/opt/
GrADS/grads-2.0.a9/bin:/net/opt/xgrads/XGrads_4.06:/net/opt/pingo/pingo_1.6/bin:
/net/opt/intel/compiler90_9.0_033/bin:/SX/opt/sxc++/inst/bin:/SX/opt/crosskit/in
st/bin:/SX/opt/sxf90/inst/bin:/SX/opt/mpisx/inst/bin:/SX/opt/psuite/inst:/SX/opt
/vampirsx/inst/bin:/SX/opt/gnu/bin:/net/opt/mpich/mpich-1.2.4/bin:/net/opt/rsi/i
dl/bin:/net/opt/oce_grbtools/bin:/net/opt/ferret/bin:/net/opt/ncl/5.2.0/bin:/net
/opt/bin"

                                        ·
                                        ·
                                        ·

haemmeal@tux37:~$ 
```



```
haemmeal@tux37:~$ module load netcdf/mpich2-1.3.1/ifort-12.0.2/4.1.1
haemmeal@tux37:~$ module unload netcdf/mpich2-1.3.1/ifort-12.0.2/4.1.1
haemmeal@tux37:~$ 
```

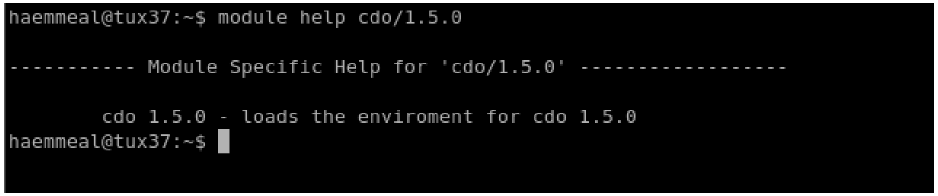
Die wichtigsten Befehle

$ module switch <alt> <neu>



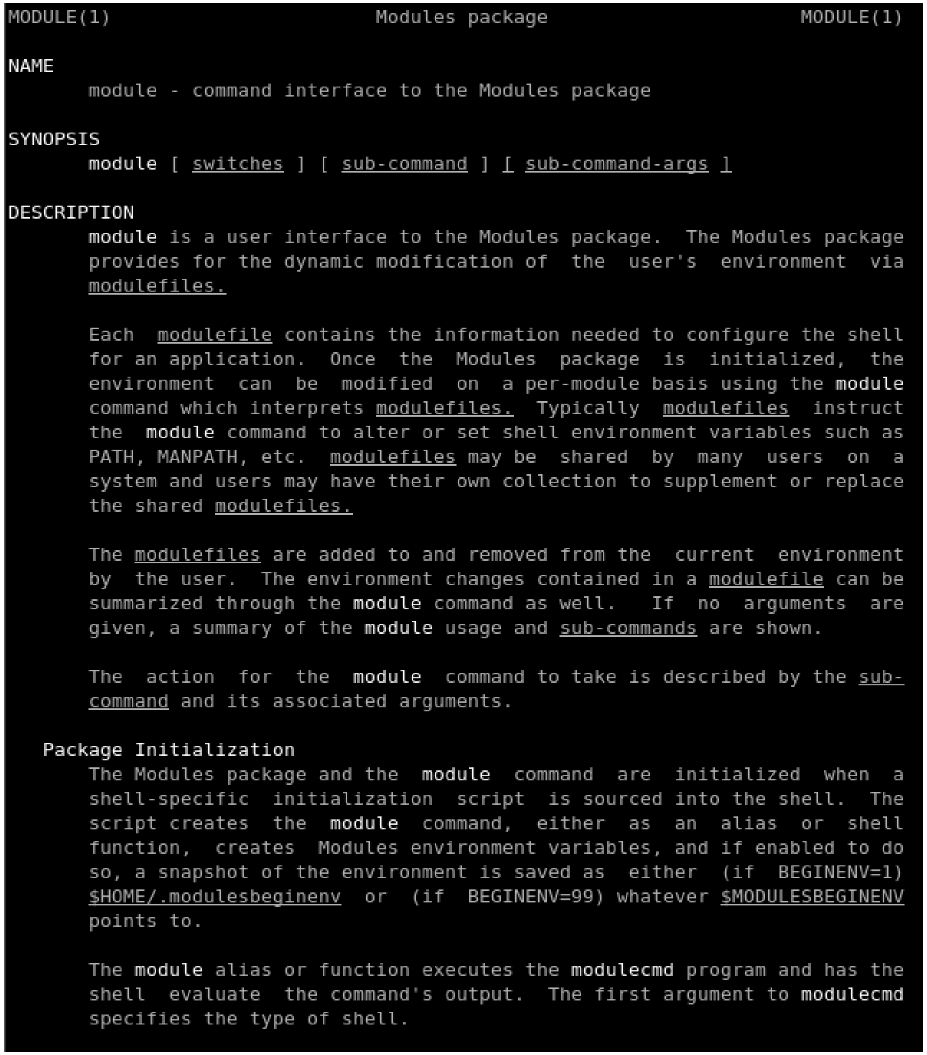
```
haemmeal@tux37:/net/opt$ module switch netcdf/mpich2-1.3.1/ifort-12.0.2/4.1.1 ne
tcdf/mpich2-1.3.1/gfortran-4.3.2/4.1.1
haemmeal@tux37:/net/opt$ 
```

$ module help <Modul>



```
haemmeal@tux37:~$ module help cdo/1.5.0

----------- Module Specific Help for 'cdo/1.5.0' ------------------

        cdo 1.5.0 - loads the enviroment for cdo 1.5.0
haemmeal@tux37:~$ 
```

$ man module



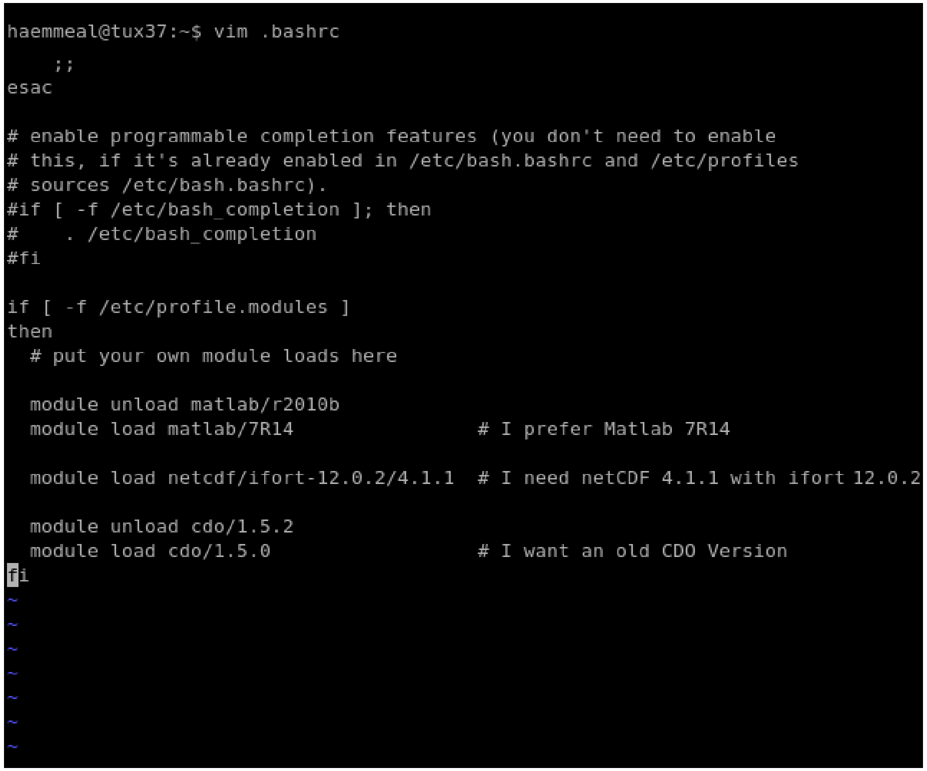
```
MODULE(1)                       Modules package                      MODULE(1)

NAME
       module - command interface to the Modules package

SYNOPSIS
       module [ switches ] [ sub-command ] [ sub-command-args ]

DESCRIPTION
       module is a user interface to the Modules package.  The Modules package
       provides for the dynamic modification of  the  user's  environment  via
       modulefiles.

       Each  modulefile contains the information needed to configure the shell
       for an application.  Once  the  Modules  package  is  initialized,  the
       environment  can  be  modified  on  a per-module basis using the module
       command which interprets modulefiles.  Typically  modulefiles  instruct
       the  module command to alter or set shell environment variables such as
       PATH, MANPATH, etc.  modulefiles may be  shared  by  many  users  on  a
       system and users may have their own collection to supplement or replace
       the shared modulefiles.

       The modulefiles are added to and removed from the  current  environment
       by  the user.  The environment changes contained in a modulefile can be
       summarized through the module command as well.   If  no  arguments  are
       given, a summary of the module usage and sub-commands are shown.

       The  action  for  the  module  command to take is described by the sub-
       command and its associated arguments.

   Package Initialization
       The Modules package and the  module  command  are  initialized  when  a
       shell-specific  initialization  script  is sourced into the shell.  The
       script creates  the  module  command,  either  as  an  alias  or  shell
       function,  creates  Modules environment variables, and if enabled to do
       so, a snapshot of the environment is saved as  either  (if  BEGINENV=1)
       $HOME/.modulesbeginenv  or  (if  BEGINENV=99) whatever $MODULESBEGINENV
       points to.

       The module alias or function executes the modulecmd program and has the
       shell  evaluate  the command's output.  The first argument to modulecmd
       specifies the type of shell.
```

Fortgeschrittene Benutzung

Fortgeschrittene Benutzung

Fortgeschrittene Benutzung

Die eigene Kommandoshell anpassen

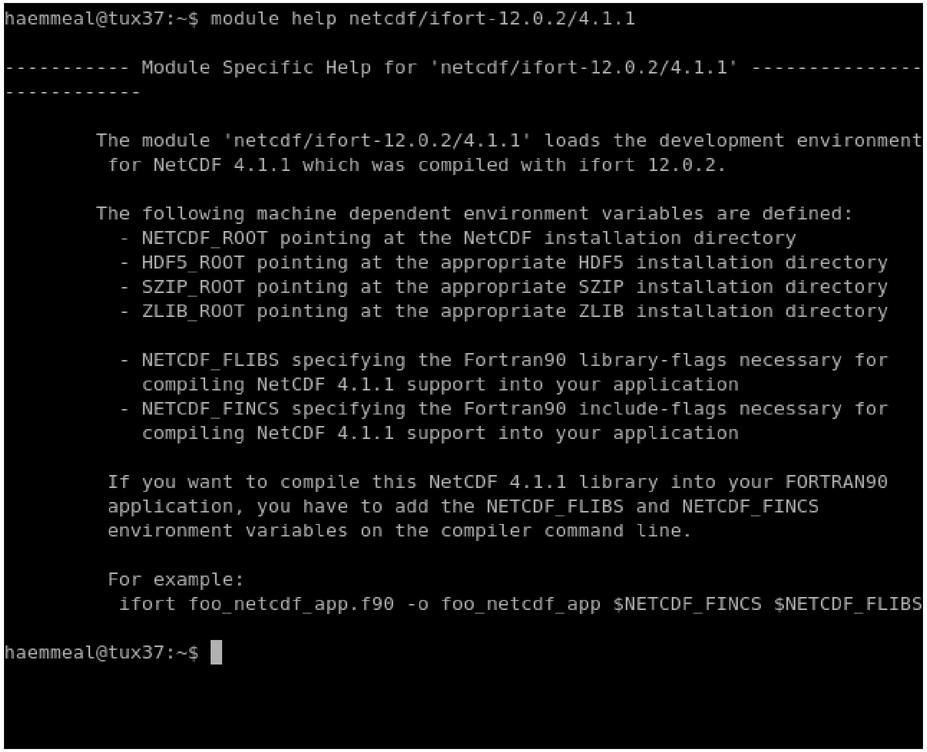


```
haemmeal@tux37:~$ vim .bashrc
    ;;
esac

# enable programmable completion features (you don't need to enable
# this, if it's already enabled in /etc/bash.bashrc and /etc/profiles
# sources /etc/bash.bashrc).
#if [ -f /etc/bash_completion ]; then
#    . /etc/bash_completion
#fi

if [ -f /etc/profile.modules ]
then
  # put your own module loads here

  module unload matlab/r2010b
  module load matlab/7R14               # I prefer Matlab 7R14

  module load netcdf/ifort-12.0.2/4.1.1  # I need netCDF 4.1.1 with ifort 12.0.2

  module unload cdo/1.5.2
  module load cdo/1.5.0                 # I want an old CDO Version
fi
~
~
~
~
~
~
~
```

- Um die standardmäßig aktivierten Module beim Login zu verändern, muss die Datei **~/.bashrc** bearbeitet werden
- Das Beispiel-Skript steht auf der internen Wiki-Seite zu Modules für Copy&Paste zur Verfügung

Fortgeschrittene Benutzung

Bibliotheken für eigene Kompilierungen nutzen

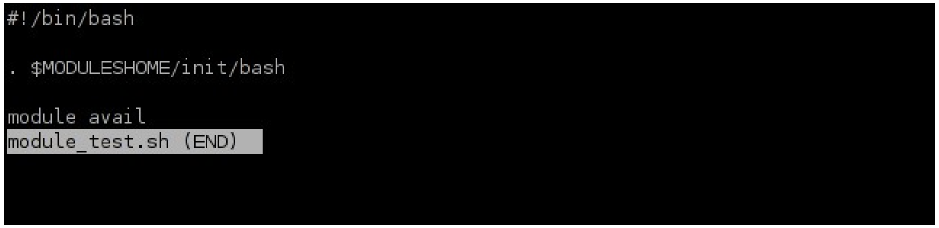


```
haemmeal@tux37:~$ module help netcdf/ifort-12.0.2/4.1.1

----------- Module Specific Help for 'netcdf/ifort-12.0.2/4.1.1' ---------------
------------

        The module 'netcdf/ifort-12.0.2/4.1.1' loads the development environment
         for NetCDF 4.1.1 which was compiled with ifort 12.0.2.

        The following machine dependent environment variables are defined:
          - NETCDF_ROOT pointing at the NetCDF installation directory
          - HDF5_ROOT pointing at the appropriate HDF5 installation directory
          - SZIP_ROOT pointing at the appropriate SZIP installation directory
          - ZLIB_ROOT pointing at the appropriate ZLIB installation directory

          - NETCDF_FLIBS specifying the Fortran90 library-flags necessary for
            compiling NetCDF 4.1.1 support into your application
          - NETCDF_FINCS specifying the Fortran90 include-flags necessary for
            compiling NetCDF 4.1.1 support into your application

         If you want to compile this NetCDF 4.1.1 library into your FORTRAN90
         application, you have to add the NETCDF_FLIBS and NETCDF_FINCS
         environment variables on the compiler command line.

         For example:
          ifort foo_netcdf_app.f90 -o foo_netcdf_app $NETCDF_FINCS $NETCDF_FLIBS

haemmeal@tux37:~$ 
```

- $ module help <Modul> liefert bei zur Kompilierung verwendbarer Software entsprechende Informationen
- Durch Modules werden Umgebungsvariablen gesetzt, die die nötigen Flags für die Kompilierung enthalten
- Macht das Auffinden der entsprechenden Dateien von Hand unnötig

Fortgeschrittene Benutzung

Modules in eigenen Skripten verfügbar machen



```
#!/bin/bash

. $MODULESHOME/init/bash

module avail
module_test.sh (END)
```

- Zu Beginn des Skripts muss die Init-Datei der entsprechenden Shell als Source eingetragen werden
- Z.B. $MODULESHOME/init/bash
- Danach lässt sich Modules innerhalb des Skripts wie auf der Kommandozeile verwenden

Linkliste

- Homepage des Projekts:

http://modules.sourceforge.net

- Wiki-Seite am Institut:

http://klimod.met.fu-berlin.de/Hilfe/index.php/Modules

- Einführung zu Umgebungsvariablen:

http://wiki.debian.org/EnvironmentVariables

Das war's ...

Danke für die Aufmerksamkeit!