Version 2.2.0

Installing from Source

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Contents

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Any use of results obtained using CONUSS-2.2.0 in related or unrelated publications have to be properly acknowledged by reference to the name of the package, to the name of the developer(s), and to the *NRIXS software* site `http://www.nrixs.com`.

2 What is CONUSS ?

The CONUSS software is a scientific application to simulate experimental data obtained using the techniques of Synchrotron Mössbauer Spectroscopy (SMS), Nuclear Forward Scattering (NFS), grazing-incidence nuclear resonant scattering (GINS), nuclear resonant Bragg/Laue diffraction (NBS), and conventional Mössbauer spectroscopy. The software calculates of time and energy spectra and supports automated parameter optimization (fitting).

The first version of the program was created from 1983 to 1986 by E. Gerdau and W. Sturhahn at the University of Hamburg shortly after the discovery of nuclear resonant scattering of synchrotron radiation using ^{57}Fe-enriched single crystals of Yttrium-iron-garnet. It was improved since then by W. Sturhahn to handle various data input formats and to provide comprehensive diagnosis tools for high-quality data evaluation. A detailed treatment of nuclear forward scattering was added in 1991, automated parameter optimization was added in 1996, and a graphical display option was provided in 2010. A new approach to parameter space exploration using randomized trials in combination with a Beam Search method was added in 2010. Nuclear resonant scattering by thin-film systems in grazing incidence geometry is supported since 2015.

CONUSS-2.2.0 supports all Mössbauer isotopes and offers great flexibility in defining sample properties, such as, arbitrary number of sites, combined hyperfine interactions, distributions of hyperfine interactions, partial alignment, and Blume-Tjon-type magnetic relaxation. The program fully implements polarization, directional, and thickness dependences for time as well as energy spectra. Further it supports sample combinations, averaging in time, energy, angle, and thickness distributions. The flexible assignment and grouping of fit parameters permits efficient evaluation of experimental data.

The CONUSS software package is mostly written in Fortran 77 and Fortran 90, and its programs have been used for data evaluation in numerous publications. CONUSS has been installed on several UNIX-like operating systems: Sun's Solaris, Apple's Mac OS X, Redhat-Enterprise Linux, and Fedora Linux. Installation on MS-Windows type operating systems requires either a Linux/Unix emulator software, e.g., cygwin, or better a virtual machine hosting a Linux-type guest-system, e.g.,VirtualBox.

3 Requirements

Before installation please verify the following list of requirements.

- Fortran90 compiler. The recommended compiler is `gfortran` version 4.8.x or higher, please visit the gcc website for more information.
- Optional: Fortran graphics tools libraries `libg2.a` and `libgd.a`. These libraries can be obtained at `http://g2.sourceforge.net/` and `http://www.libgd.org`.
- Optional: `grace` plotting tool to display data. It is available at `http://plasma-gate.weizmann.ac.il/Grace` .

On Mac OS X systems there are the following additional requirements.

- `Xcode`, Apple's developer package freely available from the Appstore. Run `Xcode` to accept the license and make sure 'linecommand tools' are installed. Install `Xcode` before you install the Fortran compiler.
- `X11` if not distributed with Mac OS X. It is available at `http://xquartz.macosforge.org` .

4 How to install

CONUSS is distributed as a compressed tar-ball named `CONUSS-2.2.0.tar.gz`. Several steps are needed to install the CONUSS software. If this is an update from an earlier version of CONUSS you may uninstall the ealier version as described in section 5. Even though this is not necessary it will avoid clutter. If you want to use both versions simultaneously you must install each version into a different location.

4.1 Extract files

Depending on the available system utilities you may have several options to extract the CONUSS files. In many cases, a double-click on `CONUSS-2.2.0.tar.gz` recovers the folder `CONUSS-2.2.0`. If this fails find out the name of the directory into which you copied `CONUSS-2.2.0.tar.gz` and open a terminal widow. Then enter the following line commands.

```
> cd <name of directory>
> gzip -dc CONUSS.2.1.1.tar.gz | tar xf -
> ls
 ...   CONUSS.2.1.1    ....
>
```

4.2 Configure

Next, run the configuration script to create the makefiles for the compilation of the source code. Several options can be specified to help a successful compilation and build of CONUSS executables. For most cases, options should not be needed. Enter the following line commands to see the options.

```
> cd CONUSS.2.2.0
> ./configure --help
Usage: configure [OPTION]...
Create Makefile(s) for CONUSS installation

      --foption=<list> colon separated list of compiler options
      --fortran=<exe>  use Fortran compiler <exe>
                       <exe> must exist in search path
      --nographics     disable graphics support
      --help           display this help and exit
      --loption=<list> colon separated list of ld options
```

```
      --lpath=<list>   prepend directories to library search path
                       <list> is a colon separated list of directories
      --prefix=<dir>   set <dir> as installation location
                       only used in 'make install'
                       preset location is <home directory>
      --spath=<list>   prepend directories to search path
                       <list> is a colon separated list of directories
      --xlarge         enforce 64bit pointers (large data section)
      --xnoquad        disable quad precision arithmetic
      --xsmall         accommodate 32bit pointers (small data section)
      --xstatic        create statically linked executables

Examples:
  configure --lpath=$HOME/lib     prepend $HOME/lib to library path
  configure --prefix=/usr/local   install into directory /usr/local
>
```

Execute the script with appropriate options and concur with the user agreement.

```
> ./configure [OPTIONS...]
  ....
  (messages)
  ....
>
```

The configuration script may be re-run with different options as needed. The last configuration command is saved in the file 'configcmd'. The script produces various messages on the progress of the configuration. The following files should have been created or overwritten: Makefile, bin/kctl, bin/kfan, bin/kfit, bin/kfmf, bin/kfor, bin/kgin, bin/kgmf, bin/kmco, bin/kmix, bin/kref, bin/krmf, bin/mca2exp, config/CONFIG, config/CONFIGgr. If graphics libraries were found also bin/kdsp should have been created or overwritten.

4.2.1 Options

Here follows a description of the functionality of each option for the configure script.

foption a list of options that will be passed to the Fortran compiler. This might be needed for some compilers. The correct syntax would be, for example, '--foption=-x1=a:-x2=b'. Everything after the first '=' character will be passed to the compiler with all ':' characters being replaced by spaces.

fortran the name of the Fortran compiler executable. By default the configuration script assigns the first compiler that is found in the search path (see description below) from this list: gfortran, g95. To use compiler 'fort' located in directory '/crazypath' the correct specification would be '--fortran=/crazypath/fort'.

nographics disable graphics support. By default the configuration script tries to find graphics libraries and compile accordingly. This option disables this behavior. The CONUSS executables still support the `xmgrace` visualization tool if found in the searchpath (see below).

loption a list of options that will be passed to the linker; see 'foption' above for syntax rules.

lpath prepend directories to the library search path. By default the path contains the following directories: /lib, /usr/lib, /usr/local/lib. Adding directories may for example be required if the graphics libraries `libg2.a` and `libgd.a` were installed at a different location, and graphics support is desired. The correct syntax would be, for example, '--lpath=/crazypath/dir1:~/dir2', where '~' symbolizes the user's home directory.

prefix set the location for installation of the CONUSS executables and their support files. By default the installation location is the installers home directory, i.e., the executables are copied into $HOME/bin and the support files are copied into $HOME/share/`CONUSS-2.2.0`. If the prefix is set to another directory it is important to have appropriate permissions as installer, e.g., '--prefix=/usr/local' requires administrator or root privileges on Mac OS X or Linux systems, respectively.

spath prepend directories to the search path for essential support programs including the compiler. By default the path contains the following directories: /bin, /usr/bin, /usr/local/bin, /opt/bin, /opt/local/bin, /opt/X11/bin, /usr/X11/bin, /usr/ccs/bin, /usr/ucb, /usr/openwin/bin. If the configuration script fails to locate support programs in this path (reported upon execution of the script) directories have to be added; see 'lpath' above for syntax rules.

xlarge override default 32bit pointer size. Some systems by default use a pointer size of 32bit instead of 64bit which would be the native size for most modern operating systems. This puts a constraint on the maximum size of data fields defined at compilation time. A typical error message contains something like '`relocation truncated to fit: R_X86_64_PC32`' and the produced executables (if any) are defective.

xnoquad disable quad precision arithmetic. Not every system permits the compiler to use quad precision expressions. However, only calculations involving nuclear Bragg/Laue reflections require quad precision and would potentially fail with this option.

xsmall reduce the size of data fields. This may restrict some calculational capabilities such as number of sites (kfor and kref) and the number of angles/thicknesses (kfor, kgin, and kref). These settings can be fine-tuned by adjusting parameters in the file 'CONUSS-2.2.0`/src/conuss.h`' followed by re-compilation.

xstatic created statically linked executables. This option is meant for developers and not recommended for normal use.

4.3 Create executables

The CONUSS executables are created using the 'make' command which by default reads the input file 'Makefile'.

```
> make
   ....
   (messages)
   ....
>
```

Inspect the output for error messages and abnormal termination. The following executables should have been created or overwritten: bin/kctl-`2.2.0`, bin/kfan-`2.2.0`, bin/kfmf-`2.2.0`, bin/kfor-`2.2.0`, bin/kgin-`2.2.0`, bin/kgmf-`2.2.0`, bin/kmco-`2.2.0`, bin/kmix-`2.2.0`, bin/kref-`2.2.0`, bin/krmf-`2.2.0`. The following libraries should have been created or overwritten: lib/libconuss-`2.2.0`.a, lib/libfit-`2.2.0`.a, lib/libforward-`2.2.0`.a, lib/libgraze-`2.2.0`.a, lib/libpolmix-`2.2.0`.a, lib/libreflex-`2.2.0`.a. If graphics libraries were found also bin/kdsp-`2.2.0` should have been created or overwritten. Errors during the 'make' execution usually indicate problems with compiler and/or linker options or their functionality.

4.4 Install files

The CONUSS program package is installed by the command

```
> make install
  ....
  (messages)
  ....
>
```

This step is optional and requires write access to the installation directory that was defined during the configuration process. If DIR is the installation directory the following files are copied into DIR/bin: kctl, kctl-2.2.0, kfan, kfan-2.2.0, kfmf, kfmf-2.2.0, kfor, kfor-2.2.0, kgin, kgin-2.2.0, kgmf, kgmf-2.2.0, kmco, kmco-2.2.0, kmix, kmix-2.2.0, kref, kref-2.2.0, krmf, krmf-2.2.0, mca2exp . and potentially kdsp, kdsp-2.2.0. Support files are copied into DIR/share/CONUSS-2.2.0. The installed executables are only accessible by line command if DIR/bin is part of the 'path' setting in the login resource file in your home directory. This can be tested by typing 'echo $PATH' or 'echo $path' at a terminal prompt. If the directory DIR/bin is not part of the listing then the login resource file, usually something like '.bash_profile', '.profile', or '.login', must be edited to include DIR/bin in the 'path' setting. After that you have to logout and login again to update the 'path' settings.

5 How to update/uninstall

5.1 Clean directories

The CONUSS directories are cleaned by using the command

```
> make clean
  ....
  (messages)
  ....
>
```

In addition to the executables bin/kctl-2.2.0, bin/kfan-2.2.0, bin/kfmf-2.2.0, bin/kfor-2.2.0, bin/kgin-2.2.0, bin/kgmf-2.2.0, bin/kmco-2.2.0, bin/kmix-2.2.0, bin/kref-2.2.0, bin/krmf-2.2.0, and the librarieslib/libconuss-2.2.0.a, lib/libfit-2.2.0.a, lib/libforward-2.2.0.a, lib/libgraze-2.2.0.a, lib/libpolmix-2.2.0.a, lib/libreflex-2.2.0.a , all compiler output will be deleted. This clean-up is highly recommended prior to re-compilation by 'make' after any of the files in directory 'include' have been edited. This step is optional after installation by 'make install'.

5.2 Uninstall files

The CONUSS program package is uninstalled by the command

```
> make uninstall
  ....
  (messages)
  ....
>
```

This step is the reverse of the above 'make install'. If a new version of CONUSS is desired to be installed this step is optional. Different versions can co-exist and the version installed last takes priority in execution. Beware that modifications and local configurations saved into <install_dir>/share/CONUSS-2.2.0 will be deleted by 'make uninstall'.

6 How to test

Examples are provided with the CONUSS package. They are located in the 'CONUSS-2.2.0/`examples`' directory and after 'make install' also in '`share`/CONUSS-2.2.0/`examples`' in the installation directory. Now change into an '`examples`' directory. If you don't have write access to the examples directory you should copy the content of an '`examples`' directory to an accessable location. For example, enter something like

```
> cd ~/CONUSS-2.2.0/examples/kctl-NFS1
> ls -px
Fe.dat Fe.mif Results/ in_kctl in_kfit in_kfor in_kmix
> kctl --help
Usage: kctl [OPTION]...
Run CONUSS executable kctl-2.2.0

      --geometry=<XxY+U+W> set the window geometry for
                           graphics display.
      --help               display this help and exit
      --infile=<file>      use <file> as input file
                           the default input file is 'in_kctl'
      --nographics         suppress visualization support
      --pipe=<fifo>        use <fifo> as pipe to output graphics data
      --quiet              suppress most print out
      --reuse              try to re-use graphics display window
      --vdelay=<val>       set visualization startup delay to <val>
      --version            display version number and exit
      --vtool=<exe>        use <exe> for data visualization

Examples:
  kctl --infile=MyFile  use 'MyFile' as input file.
  kctl --nographics     disable visualization.

> kctl

++ CONUSS-2.2.0 Copyright (C) 2017 Wolfgang Sturhahn ++

-- CONUSS module KCTL data section size: 1779.9 Mb
-- execution starting..

  ....
  (messages)
  ....

-- CPU time :  user   1.88 s  system   0.09 s
-- CONUSS module KCTL finished

> ls -px
Fe.dat        Fe.mif           Fe_exp.dat
Fe_fit.dat    Fe_fsh.dat       Fe_kctl_ptl.dat
Fe_kctl.csv   Fe_kfor_log.txt  Fe_rsd.dat
Results/      in_kctl          in_kfit
in_kfor       in_kmix          kforParms.txt
>
```

Several files were created during this fit of an forward scattering time spectrum of iron metal at ambient conditions. Compare the content with files provided in the '`Results`' directory.