



Version 2.2.0

Installing from Binary

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1 License information

CONUSS-2.2.0 is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

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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 Fortran77 and Fortran90, 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 a Linux/Unix emulator software, e.g., cygwin, or better a virtual machine hosting a Linux-type guest-system, e.g., VirtualBox.

This binary distribution does not contain source code. The complete source code is available with the regular distribution. The MacOS binaries have been compiled using `gfortran` version 6.3.0, please visit the gcc website.

3 Requirements

Before installation please verify the following list of requirements if runtime graphics are desired.

- Mac OS X: X11 if not distributed with Mac OS X. It is available at <http://xquartz.macosforge.org>.
- alternative to provided graphics: Grace plotting tool available at <http://plasma-gate.weizmann.ac.il/Grace>.

4 How to install

CONUSS is distributed as a compressed tar-ball named `CONUSS-2.2.0_<type>.tar.gz` where `<type>` describes the operating system and architecture the binaries were built for. If this is an update from an earlier binary version of CONUSS you may uninstall the earlier 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_<type>.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_<type>.tar.gz` and open a terminal window. Then enter the following line commands.

```
> cd <name of directory>
> gzip -dc CONUSS.2.2.0_<type>.tar.gz | tar xf -
> ls
... CONUSS.2.2.0 ...
>
```

4.2 Configure and Install

Next, run the installation script to install the binaries. This requires write access to the installation directory. Several options may be specified to help a successful installation and functioning of the CONUSS executables. For most cases, options should not be needed. Enter the following line commands to see the options.

```
> cd CONUSS.2.2.0
> ./install --help
Usage: install [OPTION]...
Install CONUSS

    --nographics      disable graphics support
    --help            display this help and exit
    --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

Examples:
  install --spath=$HOME/etc    prepend $HOME/etc to search path
  install --prefix=/usr/local  install into directory /usr/local
>
```

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

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

The installation script may be re-run with different options as needed. The last installation command is saved in the file 'installcmd'. The script produces various messages on the progress of the installation. If DIR is the installation directory the following files are copied into DIR/bin: kctl, kctl-2.2.0, kdsp, kdsp-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. 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.

4.2.1 Options

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

nographics disable graphics support. By default the the built-in graphics tool is activated. This option disables this behavior. The CONUSS executables still support the xmgrace visualization tool if found in the searchpath (see below).

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 installation script fails to locate support programs in this path (reported upon execution of the script) directories have to be added. The correct syntax would be, for example, '-spath=/crazypath/dir1:~/dir2', where '~' symbolizes the user's home directory.

5 How to uninstall

The CONUSS program package is uninstalled by the command

```
> cd CONUSS-2.2.0
> ./uninstall
....
(messages)
....
>
```

This step removes all files that were installed. 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 `./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 installation 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 accessible 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

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-- 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.