



Version 3.0.5

Installation Guide
Binary Distribution

June 08, 2025

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1 License information

CONUSS-3.0.5 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-3.0.5 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 <https://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 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 diagnostic 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-3.0.5 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. In 2023, various energy scan modes as well as the TDI mode have been added to support evaluation of energy-resolved Synchrotron Mössbauer Spectroscopy and time-domain-interferometry to investigate non-resonant glassy scatterers. The flexible assignment and grouping of fit parameters permits efficient evaluation of experimental data.

The software was created by W. Sturhahn to offer traceable evaluation codes for publications using coherent elastic NRS techniques. The CONUSS core programs are written in Fortran90 with wrappers using bash scripts. The CONUSS software has been used for data evaluation in numerous publications and has been extensively tested over the last three decades. Just like the other software packages of *NRIXS software*, CONUSS installs on UNIX-like operating systems: Sun's Solaris, Apple's MacOS, Ubuntu, and various other Linux versions. For installation on Microsoft's Windows operating systems, a virtual machine, e.g., VirtualBox (free) or VMware (paid), hosting a Linux-type guest-system is needed.

This binary distribution does not contain the source code. The complete source code is available with the regular distribution. The MacOS Intel/Arm binaries have been compiled using `gfortran` versions 6.3.0 and 12.2.0, respectively. The Linux binaries have been compiled using `gfortran` version 6.3.0.

3 Requirements

Before installation please verify the following list of requirements. You must install these before installation of CONUSS.

3.1 Linux and Unix

- bash shell, should be installed already.
- Optional: xmgrace plotting tool, available in native software installer.

3.2 MacOS

The order of installation is most important here.

- **Xcode**, Apple's developer package freely available from the Appstore.
Run **Xcode** to accept the license and install the 'linecommand tools': open Terminal app and type '`sudo xcode-select --install`' on the command line. You must have administrator privileges for this.
- bash shell, should be installed by Xcode.
- homebrew package installer.
- Tcl/Tk version 8.6 or higher to run the GUI, available via homebrew package installer.
- Optional: Xquartz for run-time graphics.
- Optional: macports package installer.
- Optional: xmgrace plotting tool, available via macports package installer.
- Optional: ImageMagick for image conversions, available via macports or homebrew package installers.

4 How to install

CONUSS is distributed as a compressed tar-ball named `CONUSS-3.0.5-<OS>_<arch>.tar.gz`. Here `<OS>` is the operating system the binaries were created with, and `<arch>` is the architecture the binaries were built for. If this is an update from an earlier version of CONUSS it is recommended that you uninstall the earlier version as described in section 6.

4.1 MacOS: remove restrictions

Before you extract the files, you must defeat the Gate-keeper mechanism and you need administrator privileges for this. Open Terminal app. With Dir as the folder that contains CONUSS-3.0.5-<OS>_<arch>.tar.gz enter

```
> cd Dir
> xattr CONUSS-3.0.5_<OS>_<arch>.tar.gz
> ... list of extended attributes ...
> sudo xattr -c CONUSS-3.0.5_<OS>_<arch>.tar.gz
> Password:
> xattr CONUSS-3.0.5_<OS>_<arch>.tar.gz
>
```

On more recent versions of MacOS the attribute 'com.apple.macl' cannot be removed, but this should not pose a problem.

If you are performing a local install on a non-admin account use the the following sequence

```
> cd Dir
> su <admin-account-name>
> Password:
> xattr CONUSS-3.0.5_source.tar.gz
> ... list of extended attributes ...
> sudo xattr -c CONUSS-3.0.5_source.tar.gz
> Password:
> exit
> xattr CONUSS-3.0.5_source.tar.gz
>
```

Here you have to use the password of the admin account with name <admin-account-name>.

4.2 Extract files

Depending on the available system utilities you may have several options to extract the CONUSS files. For example, the line command

```
> gzip -dc CONUSS-3.0.5_<type>.tar.gz | tar xf -
```

recovers the files on most systems. Also a double-click on CONUSS-3.0.5-<type>.tar.gz recovers the folder CONUSS-3.0.5 in many cases.

4.3 Install

Next, run the installation script to install the executables. It is generally less complicated to install locally, i.e., into a user directory. For system-wide installation, proper authorization is required. On MacOS, authorization is requested when needed during the installation. Otherwise the install script might have to be run as a 'sudo' command. The installation process can be terminated by Ctrl-c.

Several options can be specified to adjust to local circumstances. For most cases, options are probably not needed. Enter the following line commands to see the options.

```
> cd CONUSS-3.0.5
> ./install --help
Usage: install [OPTION]...
Install CONUSS-3.0.5

    --nographics      no graphics support
    --help            display this help and exit
    --prefix=<dir>    set <dir> as installation location
```

```

      default location <home directory>
--spath      show search path
--spath=<list> append or prepend directories to search path
              to prepend add leading _ to directory name
              <list> is a colon separated list of directories

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

```

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

nographics disable run-time graphics support.

prefix set the location for installation of the CONUSS executables and their support files. By default the installation location is the installer's home directory: under MacOS the CONUSS app is copied into \$HOME/Application and support files are copied into \$HOME/Library/NR-IXS/CONUSS; under other Unix systems the executables are copied into \$HOME/bin and the support files are copied into \$HOME/.NR-IXS/CONUSS. 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. Under MacOS support files are installed either into \$HOME as described above or into '/' where the CONUSS application is copied into '/Applications' and support files are copied into '/Library/NR-IXS/CONUSS'.

spath append or prepend directories to the search path for essential support programs and run-time graphics programs. By default the path contains the following directories: /bin, /usr/bin, /usr/local/bin, /opt/local/bin, /opt/X11/bin, /usr/X11/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.

Execute the script with appropriate options.

```

> ./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. After installation, you have the option to run a test of the CONUSS executables, see section 7 for more details. The test may take more than 30 minutes and can also be run at a later time.

The install requires write access to the installation directory, by default the users home directory. If DIR is the installation directory the following files are copied into DIR/bin: kcns, kctl-3.0.5, kdec-3.0.5, kfmf-3.0.5, kfor-3.0.5, kgin-3.0.5,kgmf-3.0.5, kmcc-3.0.5, kmco-3.0.5, kmix-3.0.5, kpnr-3.0.5, kref-3.0.5, krmf-3.0.5, kvzz-3.0.5, conuss_gui (Linux only), conuss_test, mca2exp. Also the following links pointing to kcns are created in DIR/bin: kctl, kdec, kfmf, kfor, kgin, kgmf, kmco, kmix, kpnr, kref, krmf, kvzz. On MacOS operating systems also the application Conuss.app should have been created or overwritten in '\$HOME/Applications' as described above or in '/Applications'.

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.

4.3.1 Search path

Pay attention to the search path.

```
> ./install --spath
/bin:/usr/bin:/usr/sbin:/usr/local/bin:/opt/local/bin:/opt/X11/bin:/usr/X11/bin
>
```

If the location of the `xmgrace` executable is not included in this search path you must add that location to the path. For example, you installed `xmgrace` into directory `'~/mybin'` (`'~'` symbolizes the user's home directory) and want the install script to use it. Then you execute the install script with option

```
> ./install --spath=~/mybin
....
(messages)
....
>
```

The directory is now appended to the original search path. Sometimes you need to overwrite an installation present in the search path. Then you must prepend the directory to the search path using a preceding underscore

```
> ./install --spath=_~/mybin
....
(messages)
....
>
```

Use the prepend option with care to avoid unwanted command overrides.

Another situation is often found on MacOS. There exists a (non-functional) system version of `Tcl/Tk` in the directory `/usr/bin` which should be avoided. You installed a working version of `Tcl/Tk` into directory `'/opt/homebrew/bin'`. Then you must prepend the directory to the search path using a preceding underscore

```
> ./install --spath=_/opt/homebrew/bin
....
(messages)
....
>
```

Again, use the prepend option with care to avoid unwanted command overrides.

5 File locations

5.1 Binaries

The executable binaries are placed into the directory `'DIR/bin'` for a install into directory `DIR`, i.e., `'./install --prefix=DIR'`. The default for `DIR` is the home directory.

5.2 GUI

For MacOS operating systems, the GUI is created as Conuss.app and placed into directories '\$HOME/Applications' or '/Applications' for a system-wide install. The app shows up automatically on Launchpad. For local installations, '\$HOME/Applications' has to be linked into '/Applications' for MacOS to see the app. Open a Terminal, then 'cd /Applications' and 'sudo ln -s \$HOME/Applications localApps'. Administrator privilege is needed for the latter command.

On Linux-type systems, the GUI is created as conuss_gui and placed into the directory 'DIR/bin' for a install into directory DIR. Depending on the particular type of window management (Gnome, KDE, etc) a launcher may be created and placed on the Desktop.

5.3 Support files

For MacOS operating systems, support files are placed into directories '\$HOME/Library/NRIXS/-CONUSS' or '/Library/NRIXS/CONUSS' for a system-wide install. On Unix-type systems, support files are placed into directories '\$HOME/.NRIXS/CONUSS' or 'DIR/share/NRIXS/CONUSS' for a system-wide install into directory DIR. If a particular directory exists the content will be saved into a same-name directory with a number appended.

6 How to uninstall

The CONUSS program package is uninstalled by the command

```
> cd CONUSS-3.0.5
> ./uninstall
....
(messages)
....
>
```

This step removes all files that were created during installation and is recommended prior to installation of a new version of CONUSS.

7 How to test

Examples are provided with the CONUSS package. They are located in the directory 'CONUSS-3.0.5/examples' and after installation also in the 'examples' directory as support files. The CONUSS self-test script is located in the directory 'CONUSS-3.0.5/bin' and can be run as follows

```
> cd CONUSS-3.0.5
> bin/conuss_test --dir=examples
....
(messages)
....
>
```

The complete test may take more than 30 minutes depending on your computing system. The test can be canceled at any time with Ctrl-c. The test of each example produces a report with extension '.log' which contains potential deviations as well as execution-time output.

```
> ls -px *.log
kctl-GINS.log kctl-MBS1.log kctl-MBS2.log kctl-NBS1.log
kctl-NBS2.log kctl-NFS1.log kctl-NFS2.log kctl-NFS3.log
kctl-NFS4.log kctl-TDI.log kdec-COMPAS.log kdec-MBS1.log
```

```
kdec-MBS2.log kfmf-MBS.log kfmf-NFS.log kfor-NFS.log
kgmf-GINS.log kgmf-GIS.log kmco-GINS.log kmco-NBS.log
kmco-NFS.log krmf-NBS1.log krmf-NBS2.log
>
```

7.1 Individual examples

Your computer system can only access the CONUSS executables if the directory that they are located in is part of the 'path' defined for your system at the time of login. You can test this, e.g., by trying something like

```
> cd ~
> which kctl
/usr/local/bin/kctl
```

If the second command doesn't succeed the location of the CONUSS executables can be made known permanently to your computer. This is done by modification of the 'path' setting in the login resource file in your home directory, usually something like '.bash_profile', '.profile', or '.login'. You have to logout and login again to update the 'path' settings.

Now change into an 'examples' directory (you need write access). If you don't have write access to the examples directory you should copy the content of an 'examples' directory to an accessible location, e.g., your home directory. For example, enter something like

```
> cd ~/CONUSS-3.0.5/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 -3.0.5

    --geometry=<XxY+U+W>  window geometry for graphics display
    --help                display this message and exit
    --infile=<file>       use <file> as input file
                          the default input file is 'in_kctl'
    --nographics          disable runtime visualization
    --quiet               suppress most print out
    --version             display version number and exit
    --vtool               list supported visualization tools
    --vtool=<tool>        use <tool> for data visualization

Examples:
  kctl --infile=MyFile  use 'MyFile' as input file
  kctl --vtool=xmgrace  use xmgrace for visualization

> kctl

++ CONUSS-3.0.5 Copyright (C) $4: Wolfgang Sturhahn ++

....
(messages)
....

-- CPU time :  user   0.29 s  system   0.01 s
-- CONUSS module KCTL finished

> ls -px
Fe.dat      Fe.mif      Fe_BestFit/
Fe_ErrEllipses/ Fe_exp.dat  Fe_exp_pwr.dat
Fe_fit.dat  Fe_fit_pwr.dat Fe_kctl.csv
Fe_kctl_ptl.txt Fe_kfor_let.dat Fe_kfor_log.txt
Fe_rsd.dat  Fe_rsd_pwr.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. The meaning of file contents is explained briefly at the end of the `Fe_kctl_ptl.txt` file and in more detail in the CONUSS Manual.

8 Get started with the graphical user interface

If Tcl/Tk 8.6 or higher was accessible during install the GUI app was created.

- MacOS

With Finder locate the Application folder into which the GUI app was installed. This is either `'$HOME/Applications'` for a local install or `'/Applications'` for a system-wide install. Start the GUI by double-click on `Conuss.app` but you might have to defeat the Gate Keeper if the app doesn't start. Defeating the Gate Keeper¹: double-click on `Conuss.app`; acknowledge that it can't be opened; select Apple -> System Preferences -> Security & Privacy -> General; at the bottom right click open `Conuss.app`. Later MacOS versions may have different mechanisms.

If the app still does not start error output is saved into file `'$HOME/Library/NRISX/-CONUSS/app.log'` or `'$HOME/CONUSSapp.log'`.

- other Unix

Use Desktop launcher or open terminal and type `'conuss_gui'` on the command line.

Select CONUSS -> Show Examples. A list of examples shows up in lower right panel; right-click on an item and select `'Open As Project'`; click on `'run'` button on top of middle panel to execute the calculation. Inspect output by left-click on thumbnail in lower left or by menu actions in upper right panel.

¹The Gatekeeper mechanism varies for different MacOS versions.