



Version 3.0.5

Installation Guide
Source Distribution

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Wolfgang Sturhahn



<https://www.nrixs.com>

support@nrixs.com

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1 License information

PHOENIX-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 PHOENIX-3.0.5 in related or unrelated publications has to be properly acknowledged by reference to the name of the package, to the name of the developer(s), to the *NRIXS software* site <https://www.nrixs.com>, and optionally to the following paper: *W. Sturhahn, Hyperfine Interact. 125 (2000) 149-172*. This paper is included but cannot be distributed under the GNU General Public License agreement.

2 What is PHOENIX ?

The PHOENIX (PHOnon Excitation by Nuclear resonant Inelastic X-ray scattering) software is a scientific application to evaluate experimental data obtained using the technique of Nuclear Resonant Inelastic X-ray Scattering (NRIXS) which is also known as Nuclear Inelastic Scattering (NIS) and Nuclear Resonant Vibrational Spectroscopy (NRVS). The first version of the program was created in 1995 by W. Sturhahn shortly after the discovery of synchrotron radiation based inelastic nuclear resonant scattering. The PHOENIX program package was improved since then to handle various data input formats and provide useful diagnosis tools for high-quality data evaluation. A detailed treatment of sound velocity extraction was added in 2007, and a graphical display option was provided in 2009. In 2019, consistency optimization in the extraction of the partial phonon density-of-states, statistical analysis of sound velocity, and a graphical user interface were introduced.

PHOENIX-3.0.5 supports all Mössbauer isotopes, the addition of raw data sets including normalization correction, the creation of an energy scale from angle and temperature data, a flexible procedure for the subtraction of the elastic peak, data normalization, detailed balance and moment calculation, a limited energy-range correction, the extraction of the partial phonon density-of-states using the Fourier-Log method, consistency checks, optional deconvolution, calculation of thermodynamic quantities, an extrapolation scheme to extract the Debye sound velocity as well as aggregate compressional and shear sound velocities.

The software was created by W. Sturhahn to offer traceable evaluation codes for publications using the NRIXS technique. The PHOENIX core programs are written in Fortran90 with wrappers using bash scripts. The GUI is implemented as Tcl/Tk script and requires Tcl version 8.6 or higher to run. The PHOENIX software has been used for data evaluation in numerous publications and has been extensively tested over the last two decades. Just like the other software packages of *NRIXS software*, PHOENIX 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.

3 Requirements

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

3.1 Linux and Unix

- bash shell, should be installed already.
- Fortran90 compiler. The recommended compiler is gfortran 4.6 or later, available in native software installer.
- Tcl/Tk version 8.6 or higher to run the GUI, available in native software installer.
- Optional: xmgrace plotting tool, available in native software installer.
- Optional: ImageMagick for image conversions, 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.
- macports or homebrew package installer.
- Fortran90 compiler. The recommended compiler is gfortran, version 4.8 or later, available via macports or homebrew package installer. Binary packages are available [here](#).
- Tcl/Tk version 8.6 or higher to run the GUI, available via homebrew package installer.
- Optional: Xquartz for run-time graphics.
- Optional: xmgrace plotting tool, available via macports or homebrew package installer.
- Optional: ImageMagick for image conversions, available via macports or homebrew package installer.

4 How to install

PHOENIX is distributed as a compressed tar-ball named `PHOENIX-3.0.5_source.tar.gz`. Several steps are needed to install the PHOENIX software. If this is an update from an earlier version of PHOENIX 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. Assume `Dir` as the location of `PHOENIX-3.0.5_source.tar.gz`. Open Terminal app and enter

```
> cd Dir
> xattr PHOENIX-3.0.5_source.tar.gz
> ... list of extended attributes ...
> sudo xattr -c PHOENIX-3.0.5_source.tar.gz
> Password:
> xattr PHOENIX-3.0.5_source.tar.gz
>
```

4.2 Extract files

Depending on the available system utilities you may have several options to extract the PHOENIX files. For example, the line command `'gzip -dc PHOENIX-3.0.5_source.tar.gz | tar xf -'` will recover the files on most systems. Also a double-click on `PHOENIX-3.0.5_source.tar.gz` recovers the folder `PHOENIX-3.0.5` in many cases.

4.3 Configure, compile, and install

Next, run the installation script to create the configuration-dependent files, to compile the source code, and 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 available options.

```
> cd PHOENIX-3.0.5
> ./install --help
Usage: install [OPTION]...
Compile and install PHOENIX-3.0.5

--foption=<list> colon separated list of compiler options
--fortran=<exe>   use Fortran compiler <exe>
                  <exe> must exist in search path
--nographics     no graphics support
--help           display this help and exit
--loption=<list> colon separated list of ld options
--prefix=<dir>   set <dir> as installation location
                  default location is <home directory>
--spath          show search path
--spath=<list>   prepend directories to search path
                  <list> is a colon separated list of directories
--static         create statically linked executables

Examples:
./install --spath=$HOME/mybin  prepend $HOME/mybin to search path
```

```
./install --prefix=/usr/local install into directory /usr/local
MacOS only: install app into /Applications
>
```

Here follows a description of the functionality of each option for the install 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 a the first compiler that is found in the search path (see description below) from this list: gfortran, g95. The correct syntax would be, for example, '-fortran=/crazypath/fort'.

nographics disable run-time graphics support.

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

prefix set the location for installation of the PHOENIX executables and their support files. By default the installation location is the installer's home directory: under MacOS the PHOENIX app is copied into \$HOME/Application and support files are copied into \$HOME/Library/NRIXS/PHOENIX; under other Unix systems the executables are copied into \$HOME/bin and the support files are copied into \$HOME/.NRIXS/PHOENIX. 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 PHOENIX application is copied into '/Applications' and support files are copied into '/Library/NRIXS/PHOENIX'.

spath append or prepend directories to the search path for essential support programs including the compiler and run-time graphics programs. By default the path contains the following directories: /bin, /usr/bin, /usr/local/bin, /opt/bin, /opt/local/bin, /opt/homebrew/bin, /opt/X11/bin, /usr/X11/bin. If the install script fails to locate essential 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.

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

Execute the install script with appropriate options.

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

The install script may be re-run with different options as needed. The last install command is saved in the file 'installcmd'. The script produces various messages on the progress of the configuration, compilation, and installation. After installation, you have the option to run a test on the PHOENIX executables, see section 7 for more details.

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': phoenix (Unix-type only), mpadd, mpbox, padd, pbox, psth, psvl, padd-3.0.5, pbox-3.0.5, psth-3.0.5, psvl-3.0.5. On MacOS

operating systems also the application Phoenix.app should have been created or overwritten in '\$HOME-/Applications' as described above or into '/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 compiler or your xmgrace executable is not included in this search path you must add those locations to the path. For example, you installed Tcl/Tk into directory '~/Tcl' ('~' symbolizes the user's home directory) and want the install script to use it then you execute the install script with option

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

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 Phoenix.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 phoenix and placed into the directory 'DIR/bin' for an 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/PHOENIX' or '/Library/NRIXS/PHOENIX' for a system-wide install. On Unix-type systems, support files are placed into directories '\$HOME/.NRIXS/PHOENIX' or 'DIR/share/NRIXS/PHOENIX' 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

6.1 Uninstall software package

The PHOENIX program package is uninstalled by the command

```
> cd PHOENIX-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 PHOENIX.

7 How to test

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

```
> cd ~/PHOENIX-3.0.5
> bin/phoenix_test --dir=examples
....
(messages)
....
>
```

For each tested example, the script produces a log file, e.g., the results of a test run in examples/bccFe are found in the file bccFe.log together with potential deviations that were detected.

The example 'mda' requires a working installation of the mdautils software maintained by the Advanced Photon Source. The test script reports a 'failed' otherwise.

7.1 Individual examples

Your computer system can only access the PHOENIX 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 padd
/usr/local/bin/padd
```

If the second command doesn't succeed the location of the PHOENIX 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 you can copy the directory to an accessible location, e.g., your home directory. For example, enter something like

```
> cd ~/PHOENIX-3.0.5/examples/bccFe
> ls -px
Results/      in_padd      in_phox      in_psvl      mono.res      scan112.raw
scan115.raw  scan118.raw  scan119.raw
> padd --help
Usage: padd [OPTION]...
Run PHOENIX executable padd-3.0.5

      --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_padd'
      --nographics        suppress visualization support
      --quiet              suppress most printout
      --version            display version number and exit
      --vtool              display list of supported visualization tools
      --vtool=<tool>      use <tool> for data visualization

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

> padd

++ PHOENIX-3.0.5 Copyright (C) 2023 Wolfgang Sturhahn
....
(messages)
....
-- CPU time :   user   0.11 s   system   0.01 s
-- PHOENIX module PADD finished

> ls -px
Fe_mon.csv  Fe_padd_ptl.txt  Fe_shf.csv
Fe_sum.csv  Results/         in_padd
in_phox     in_psvl          mono.res
scan112.raw scan115.raw      scan118.raw
scan119.raw
>
```

Several files were created during this addition of NRIXS spectra. Continue with commands `'phox'` and `'psvl'` to extract the DOS and sound velocities, respectively. Compare the content of output files with files provided in the `'Results'` directory.

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 Phoenix.app but you might have to defeat the Gate Keeper if this doesn't work. Defeating the Gate Keeper: right-click on Phoenix.app to get pull-down menu; select open; acknowledge to open. Defeating the Gate Keeper¹: double-click on Phoenix.app; acknowledge that it can't be opened; select Apple -> System Preferences -> Security & Privacy -> General; at the bottom right click open Phoenix.app. Later MacOS versions may have different mechanisms.

¹The Gatekeeper mechanism varies for different MacOS versions.

- other Linux

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

Select PHOENIX -> 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.