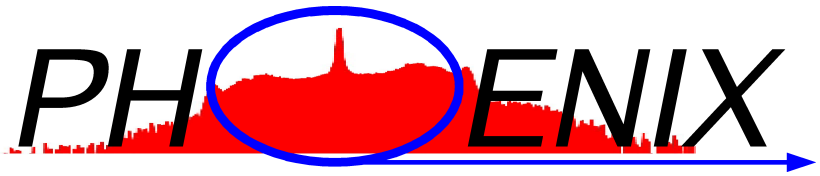

Version 2.1.4

Installing from Source

October 31, 2016

Wolfgang Sturhahn

http://www.nrixs.com support@nrixs.com Follow @NRIXS on Twitter

Contents

1 License information

PHOENIX-2.1.4 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.

PHOENIX-2.1.4 is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

A copy of the GNU General Public License is distributed with PHOENIX-2.1.4 and can also be seen at `http://www.gnu.org/licenses/`.

Any use of results obtained using PHOENIX-2.1.4 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 `http://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 is written in Fortran90. It 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.

PHOENIX-2.1.4 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 PHOENIX programs have been used for data evaluation in numerous publications. PHOENIX has been installed on several UNIX-like operating systems: Sun's Solaris, Apple's Mac OS X, Redhat-Enterprise Linux, Ubuntu, and Fedora Linux.

3 Requirements

Before installation please verify the following list of requirements.

- Fortran90 compiler. The recommended compiler is `gfortran` version 4.8 or later. Visit `http://gcc.gnu.org/fortran` 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

PHOENIX is distributed as a compressed tar-ball named `PHOENIX-2.1.4.tar.gz`. Several steps are needed to install the PHOENIX software. If this is an update from an earlier version of PHOENIX 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 PHOENIX files. In many cases, a double-click on `PHOENIX-2.1.4.tar.gz` recovers the folder `PHOENIX-2.1.4`. If this fails find out the name of the directory into which you copied `PHOENIX-2.1.4.tar.gz` and open a terminal widow. Then enter the following line commands.

```
> cd <name of directory>
> gzip -dc PHOENIX.2.1.4.tar.gz | tar xf -
> ls
 ...    PHOENIX.2.1.4    ....
>
```

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 PHOENIX executables. For most cases, options should not be needed. Enter the following line commands to see the options.

```
> cd PHOENIX-2.1.4
> ./configure --help
Usage: configure [OPTION]...
Create Makefile(s) for PHOENIX installation

      --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
      --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
```

```
      --static          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.

```
> ./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/padd, bin/phox, bin/psth, bin/psvl, bin/mpadd, config/CONFIG, config/CONFIGgr. If graphics libraries were found also bin/pdsp 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 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 graphics support. By default the configuration script tries to find graphics libraries and compile accordingly. This option disables this behavior. The PHOENIX 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 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 PHOENIX 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/`PHOENIX-2.1.4`. 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, /usr/ccs/bin, /usr/ucb, /usr/openwin/bin, /usr/X11/bin. If the configuration script fails to locate essential support programs in this path (reported upon execution of the script) directories have to be added; see 'lpath' above for syntax rules.

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

4.3 Create executables

The PHOENIX 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 files should have been created or overwritten: bin/padd-2.1.4, bin/phox-2.1.4, bin/psth-2.1.4, bin/psvl-2.1.4, lib/libphoenix-2.1.4.a. If graphics libraries were found also bin/pdsp-2.1.4 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 PHOENIX 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. By default the following files are copied into $HOME/bin: padd, padd-2.1.4, phox, phox-2.1.4, psth, psth-2.1.4, psvl, psvl-2.1.4, and potentially pdsp, pdsp-2.1.4. Support files are copied into $HOME/share/PHOENIX-2.1.4.

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 PHOENIX directories are cleaned by using the command

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

In addition to the executables bin/padd-2.1.4, bin/phox-2.1.4, bin/psth-2.1.4, bin/psvl-2.1.4, bin/pdsp-2.1.4 and the library lib/libphoenix-2.1.4.a, all compiler output will be deleted. This clean-up is highly recommended after any of the files in directory 'include' have been edited prior to re-compilation by 'make'. This step is optional after installation by 'make install'.

5.2 Uninstall files

The PHOENIX 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 PHOENIX 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/PHOENIX-2.1.4 will be deleted by 'make uninstall'.

6 How to test

Examples are provided with the PHOENIX package. They are located in the 'PHOENIX-2.1.4/examples' directory and after 'make install' also in 'share/PHOENIX-2.1.4/examples' in the installation directory. 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 accessable location. For example, enter something like

```
> cd ~/PHOENIX-2.1.4/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-2.1.4

      --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
      --vdelay=<val>       set visualization startup delay to <val>
      --version            display version number and exit
      --vtool=<exe>        use <exe> for data visualization

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

> padd
```

```
++ PHOENIX-2.1.4 Copyright (C) 2014 Wolfgang Sturhahn
++ This program comes with ABSOLUTELY NO WARRANTY.
++ This is free software.
++ You may redistribute it under certain conditions.
++ For details see <http://www.gnu.org/licenses/>.

   ....
   (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.