



Version 2.0.0

Installing from Binary

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1 License information

MINUTI-2.0.0 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 MINUTI-2.0.0 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), and to the *NRIXS software* site <http://www.nrixs.com>.

2 What is MINUTI ?

The MINUTI (MINeral physics UTILities) software is a collection of programs aimed at use by mineral physicists. At present three independent modules are provided.

- **seos**
calculation and data evaluation of compression curves including temperature dependence and spin crossover effects;
- **simx**
calculation and data evaluation of melting curves obtained by observation of time-integrated nuclear forward scattering intensity;
- **svec**
calculation of sound velocity surfaces and averages using the elastic tensor.

The software was created by W. Sturhahn to offer traceable evaluation codes for publications in mineral physics. The MINUTI core programs are written in Fortran90 with wrappers using c-shell scripts. The GUI is implemented as Tck/Tk script and requires Tcl version 8.6 or higher to run. The MINUTI software has been extensively tested over the last four years. Just like the other software packages of *NRIXS software*, MINUTI installs on UNIX-like operating systems: Sun's Solaris, Apple's MacOS, Ubuntu, and various other Linux versions. Installation on Microsoft's Windows operating systems requires a Linux/Unix emulator software, e.g., cygwin, or preferably a virtual machine hosting a Linux-type guest-system, e.g., VirtualBox.

3 Requirements

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

- alternative to built-in graphics: Grace plotting tool, on many linux-type systems available in native software installer. On MacOS it is available via the port facility;
- MacOS only: X11 is not distributed with MacOS. It is available at <http://xquartz.macosforge.org>.

4 How to install

MINUTI is distributed as a compressed tar-ball named `MINUTI-2.0.0-<type>.tar.gz` where `<type>` describes the operating system and architecture the binaries were built on. If this is an update from an earlier version of MINUTI it is recommended that you uninstall the earlier version as described in section 6.

4.1 Extract files

Depending on the available system utilities you may have several options to extract the MINUTI files. For example, the line command `'gzip -dc MINUTI-2.0.0-<type> | tar xf -'` will recover the files on most systems. Depending on your system capabilities you may be able to double-click on `MINUTI-2.0.0-<type>.tar.gz` to recover the folder `MINUTI-2.0.0`.

4.2 Configure and Install

Next, run the installation script to install the binaries. Several options can be specified to help a successful installation and functioning of the MINUTI executables. For most cases, options should not be needed. Enter the following line commands to see the options.

```
> cd MINUTI-2.0.0
> ./install --help
Usage: install [OPTION]...
Install MINUTI

    --nographics      no 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           show search path
    --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
>
```

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

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

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

spath prepend directories to the search path for essential support programs. 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 installation 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 in this example '~' symbolizes the user's home directory.

4.3 Install executables

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.

The installation 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': minuti (Linux OS only), sdsp, seos, simx, svec, sdsp-2.0.0, seos-2.0.0, simx-2.0.0, svec-2.0.0. On MacOS operating systems also the application Minuti.app was copied into '\$HOME/Applications' or into '/Applications' as described above.

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 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'.

5.2 GUI

For MacOS operating systems, the GUI is created as Minuti.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'. Admin privilege is needed for the latter command.

On Unix-type systems, the GUI is created as minuti and placed into the directory 'DIR/bin' for a install into directory DIR. Depending on the particular type of window management (Gnome, KDE, etc) you may create a launcher that points at 'DIR/bin/minuti'.

5.3 Support files

For MacOS operating systems, support files are placed into directories '\$HOME/Library/NRIXS/MINUTI' or '/Library/NRIXS/MINUTI' for a system-wide install. On Unix-type systems, support files are placed into directories '\$HOME/.NRIXS/MINUTI' or 'DIR/share/NRIXS/MINUTI' 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 MINUTI program package is uninstalled by the command

```
> cd MINUTI-2.0.0
> ./uninstall
....
(messages)
....
>
```

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

7 How to test with command line interface

Examples are provided with the MINUTI package. They are located in the 'MINUTI-2.0.0/examples' directory and after installation also in the 'examples' directory as support files. Your computer system can only access the MINUTI 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 seos
/usr/local/bin/seos
```

If the second command doesn't succeed the location of the MINUTI 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 ~/MINUTI-2.0.0/examples/seos_quartz
> ls -px
Results/      in_seos      quartz.dat
> seos --help
Usage: seos [OPTION]...
Run MINUTI executable seos -1.1.3

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

> seos

++ MINUTI-2.0.0 Copyright (C) 2017 Wolfgang Sturhahn
....
(messages)
....
-- CPU time :  user   0.02 s  system   0.00 s
-- MINUTI module SEOS finished

> ls -px
Results/
quartz_bdt.csv      in_seos              quartz_bdp.csv
quartz_csv.csv     quartz_bms.csv       quartz_ccv.csv
quartz_ffm.csv     quartz_dat.csv       quartz_dns.csv
quartz_ptl.csv     quartz_fft.csv       quartz_int.csv
quartz_thx.csv     quartz_rsd.csv       quartz_smv.csv
quartz_dsv.csv     quartz_vol.csv       quartz_vrd.csv
quartz_p02v01_eel.csv quartz_p02v01_nel.csv quartz_p02v01_nel.csv
quartz_p03v01_eel.csv quartz_p03v01_nel.csv quartz_p03v02_eel.csv
quartz_p03v02_nel.csv quartz_vkk.csv
>

```

Several files were created during this fit of p-V data of quartz. Compare the content of output files with files provided in the 'Results' directory. The meaning of file contents is explained briefly at the end of the quartz.ptl file and in more detail in the MINUTI manual.

8 How to test with 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 '~/Applications' for a local install or '/Applications' for a system-wide install. Start the GUI by double-click on Minuti.app but depending on the OS version you might have to defeat the Gate Keeper mechanism.

Defeating the Gate Keeper: right-click on Minuti.app to get pull-down menu; select open; acknowledge to open.

Defeating the Gate Keeper on MacOS 10.12 and higher: double-click on Minuti.app; acknowledge that it can't be opened; select Apple -> System Preferences -> Security & Privacy -> General; at the bottom right click open Minuti.app. The app might still be translocated by the security mechanism, so that some functionality could be lost.

Preventing the translocation: quit Minuti.app; open Terminal.app; then type 'xattr ~/Applications/Minuti.app' or 'xattr /Applications/Minuti.app'; if you see the string 'com.apple.quarantine' the app has been quarantined and only runs in translocation mode; to lift the quarantine type 'sudo xattr -dr com.apple.quarantine ~/Applications/Minuti.app' or 'sudo xattr -dr com.apple.quarantine /Applications/Minuti.app' which requires admin privileges.
- other Unix

Open terminal and type 'minuti' on the command line.

Select MINUTI -> 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 double-click on thumbnail in lower left or by actions in upper right panel.