Gwyddion user guide

Petr Klapetek, David Nečas, and Christopher Anderson

Version 2009-11-11. This guide is a work in progress.

Contents

Chapter 1

Introduction

This guide was last updated to version 2.19 of Gwyddion. The latest version this guide can be found at http://gwyddion.net/documentation/.

1.1 Motivation

Gwyddion is a modular program for SPM data analysis. Primarily it is supposed to be used for analysis of height fields obtained by means of scanning probe microscopy techniques (AFM, MFM, STM, NSOM), but generally it can be used for any other height field analysis or image analysis. Gwyddion is Free Software (and Open Source Software), covered by GNU General Public License (GNU GPL).

The main idea behind Gwyddion developement is to provide modular program for 2D data analysis that could be easily extended by modules and plug-ins with no need of core recompilation. Moreover, the status of free software enables to provide source codes to developers and users, which makes the further program improvement easier.

Gwyddion can be currently used with Linux/Unix (including Mac OS X) and Microsoft Windows operating systems. Both families of systems can be used also for developement. For graphical interface, Gtk+ widget toolkit is used, therefore it can be basically ported on any system that is supported by Gtk+.

Gwyddion core developement is currently funded by Czech Metrology Institute. The project started as a part of the Nanomet initiative (covered by Euromet) in August, 2004. It is supposed that more persons and institutions will participate on developement. Project is open for anyone. Welcome...

1.2 Licensing

Gwyddion is covered by GNU General Public License (GNU GPL). The full license text is also included as file `COPYING` in the source distribution (MS Windows installers contain it as file `COPYING.wri`). In brief, this license means that:

- You can freely use the program. You can freely make copies, modify and distribute them. You can download the program and its source code from Gwyddion web pages and modify it as you want.
- If you decide to distribute it, the modified code is still covered by the same license. In particular, you have to offer the source code too.
- The same holds for extensions, e.g. if you write an import module for a new file type or a new data analysis function it has to be licensed under GNU GPL (if you distribute it).

  However, it is also possible to execute third-party programs from Gwyddion and these do not necessarily have to be distributed under the same license – if they are not derived works of Gwyddion (which, admittely, is not always easy to determine).

The main reasons, why the program is covered by this kind of license are here: first of all, this licensing policy enables us to make modular program that can be easily developed my many persons from different institutions. Second, this license protects the rights of developers that their code, here given to public, cannot be copied and used for closed proprietary products.

Chapter 2

Installation

Gwyddion source code and binaries can be downloaded from the download web page of the project, or alternatively from raw SourceForge.net download page. The installation slightly varies depending on the operating system used. However, basically it consist of two steps:

- Installing the Gtk+ widget toolkit (if not already done).
- Installing Gwyddion

The first step is necessary at first Gwyddion installation on operating systems that do not come with Gtk+. The version of Gtk+ necessary for your system (and where to obtain it) is described in the next sections.

Generally, one needs Gtk+ libraries (run-time package) for running Gwyddion and a Gtk+ development package for Gwyddion compilation from source code and development.

Beside Gtk+, Gwyddion can optionally utilize also other software libraries and components that are described in section Build Dependencies. This is mainly important if you build Gwyddion from the source code and hence can control what features it will include.

We recommend to download sample Gwyddion files too. They are in native Gwyddion format and represent typical AFM data.

2.1 Linux/Unix Packages

Some GNU/Linux and Unix systems may provide binary packages of Gwyddion. The download page of the project also tracks known packages and packaging efforts. For instance, Debian, Ubuntu, Gentoo, openSuSE or FreeBSD offer Gwyddion packages. If your operating system provides such a package and it is recent enough, install it using the standard means of the operating system. Otherwise proceed with compilation from source code.

On Linux distributions using the RPM Package Manager, such as Fedora, openSuSE or Mandriva, you can also build a package yourself from the source code, as described below.

2.2 MS Windows Packages

If you never had any Gtk+ based application on your system (for example bitmap editor GIMP) you will need to install Gtk+ run-time environment on your computer prior to Gwyddion installation. Gtk+ is a library designed for portable creating of graphical user interface (windows, buttons, etc.) that is available on many operating systems. Therefore applications using Gtk+ can be ported to various operating systems, including Microsoft Windows.

Note that there are several Gtk+ packages for MS Windows operating systems available on the internet. Some of them include all required components (like GtkGLExt and LibXML2), some do not. We recommend GladeWin32 packages that are known to contain all required components and we build Gwyddion MS Windows executables with them.

For installation of Gwyddion follow these steps:

- Download the Gtk+ run-time environment installer from Gladewin32, version 2.8 or higher, and install it.
- Download Gwyddion installer and install Gwyddion.

The installer offers a choice of languages to use for the user interface. After installation, the lagnauge can be changed by editting registry keys in **regedit**. For user-settings, edit `HKEY_CURRENT_USER\Software\Gwyddion\1.0\gwy_locale` while `HKEY_LOCAL_MACHINE\Software\Gwyddion\1.0\gwy_locale` can be set for system-wide default. The list of available languages include:

gwy_locale	Language
cs_CZ.UTF-8	Czech (Czech Republic)
de_DE.UTF-8	German (Germany)
en_US.UTF-8	English (Unites States)
fr_FR.UTF-8	French (France)
it_IT.UTF-8	Italian (Italy)
ru_RU.UTF-8	Russian (Russia)

2.3 Build Dependencies

The following table lists packages required to build Gwyddion from source code. The table does not include common software compilation prerequisites like the C compiler or **make**. Operating system specifics are described in following sections dedicated to building on particular operating systems.

BUILD DEPENDENCIES

Gtk+ ≥ 2.8.0 *Required.*

pkg-config ≥ 0.16 *Required.*

GtkGLExt ≥ 1.0 *Optional.*

Enables OpenGL 3D data views.

The MS Windows build system is set up to require GtkGLExt and manual adjustments are necessary to disable it there.

LibXML2 ≥ 2.x *Optional.*

Enables import of SPML files.

The MS Windows build system is set up to require LibXML2 and manual adjustments are necessary to disable it there.

FFTW3 ≥ 3.0 (32bit), ≥ 3.1 (64bit), Unix only *Optional.*

Speeds up various integral transforms, power spectrum and correlation operations.

Building with FFTW3 enabled is currently unsupported on MS Windows, although it is probably possible with some effort and manual adjustments.

LibUnique ≥ 1.0 *Optional.*

Enables remote control based on D-BUS or whatever technology is currently in.

LibXmu, X11 only *Optional.*

Enables remote control on X11. This is a standard X Window System library and everyone having X probably has its runtime files. However, since the modularization of X in Xorg 7.0 it is distributed separately and therefore you might not have its development files installed.

PyGTK2, including codegen *Optional.*

Enables pygwy, the Gwyddion Python scripting interface.

Note that pygwy is not fully functional on MS Windows at this moment.

GtkSourceView *Optional.*

Enables syntax highlighting in the Python scripting console.

desktop-file-utils, Unix only *Optional.*

Enables basic desktop integration to Freedesktop-conforming environments, such as installation of Gwyddion to the menus and file associations.

GConf2, Unix only *Optional.*

Enables better GNOME and XFce integration, in particular automatic generation of SPM file thumbnails in Nautilus and Thunar.

2.4 Linux/Unix from Source Code Tarball

Gwyddion Unix build system is based on GNU autotools (autoconf, automake, libtool), like most of current Unix Free and Open Source Software. If you have ever compiled software from source code, you very likely met autotools and already know how to proceed. This section shall describe the compilation procedure in enough detail even for the uninitiated though. File INSTALL in the top-level directory of the source tarball contains generic GNU autotools installation instructions. Gwyddion specific information can be found in file INSTALL.gwyddion. Since this file comes with a particular version of Gwyddion it may contain more concrete or up-to-date information and you should follow it instead of this general guide should they disagree.

Quick Instructions

If you know the drill:

```
tar -jxvf gwyddion-2.19.tar.bz2
cd gwyddion-2.19
./configure
make install
```

Source Unpacking

Unpack the source code tarball with

```
tar -jxvf gwyddion-2.19.tar.bz2
```

replacing 2.19 with the actual version number. It will create directory `gwyddion-2.19` (again, with the actual version number in place of 2.19), **cd** to this directory. All other compilation actions will take place there.

If your operating system does not come with bzip2 you might want to download `gwyddion-2.19.tar.gz` (compressed with gzip) instead and unpack it with

```
tar -zxvf gwyddion-2.19.tar.gz
```

However, modern Unix and Unix-like systems come with both bzip2 and gzip so, the considerably smaller `gwyddion-2.19.tar.bz2` should be normally the better choice.

Configuration

Run

```
./configure
```

to configure Gwyddion.

The **configure** shell script attempts to guess correct values for various system-dependent variables used during compilation. It uses those values to create a `Makefile` in each directory of the package, a couple of header `.h` files containing system-dependent definitions and a few other system-dependent auxiliary files. Finally, it creates a shell script **config.status** that you can run in the future to recreate the current configuration, and a file `config.log`. This file contains the details of the detection process and it is helpful to include it in compilation related bug reports.

If **configure** reports missing required packages, install these packages and re-run it. The same applies to the case when **configure** passes but you find you have not installed an optional package you want to compile Gwyddion with. It is possible a package is not found or it is misdetected even if you have installed it, namely when it is installed into a non-standard directory. In this case it is necessary to adjust certain environment variables to make **configure** able to find the packages:

`PKG_CONFIG_PATH` Most packages come with so called pkg-config files (`.pc`) that describe how programs should compile and link with them. **configure** uses information from these files, therefore `PKG_CONFIG_PATH` must be set to list all non-standard directories with relevant pkg-config files. To add for instance a Gtk+ installation in `/opt/gnome` and a FFTW3 installation in `$HOME/opt/fftw3` one can do **`PKG_CONFIG_PATH=/opt/gnome/lib/pkgconfig:$HOME/opt/fftw`** **`export PKG_CONFIG_PATH`**

`PATH`, `LD_LIBRARY_PATH` It may be necessary to adjust these variables to include non-standard directories with executables and libraries of relevant packages, respectively.

CPPFLAGS, LDFLAGS It may be necessary to adjust these variables to include non-standard directories with header files and libraries of packages that do not come with pkg-config files, for example for libTIFF in `/usr/local` one can do **`CPPFLAGS=-I/usr/local/include; export CPPFLAGS`** and **`LDFLAGS=-L/usr/local/lib; export LDFLAGS`**.

The directory Gwyddion will install to and various optional features can be enabled/disabled with **configure** command line options. To obtain the complete list of these options, run

```
./configure --help
```

Option `--prefix` sets the base installation directory. Program components will be installed into its `bin`, `lib`, `share`, etc. subdirectories (they will be created if they do not exist). More detailed control is possible with options specifying particular subdirectories as `--bindir`, `--libdir`. The default prefix is `/usr/local/bin`, to install Gwyddion to your home directory you may want to use for instance

```
./configure --prefix=$HOME/opt/gwyddion
```

Configuration tweaks

Optional features can be enabled/disabled with options such as `--with-fftw3`/`--without-fftw3` (for FFTW3):

```
./configure --with-fftw3
```

By default all optional features are enabled if their prerequisites are found. A brief summary enabled and disabled optional features is printed near the end of **configure** output.

Certain auxiliary installation actions can be disabled in **configure**: Updating of Freedesktop files can be disabled with **`--disable-deskto`** Installation of GConf2 schemas can be disabled with **`--disable-schemas-install`**. However, the usual reason for disabling these actions is that Gwyddion is installed into a staging area instead of the final directory (commonly done when building Linux packages). In this case the auxiliary actions are disabled automatically by non-empty `DESTDIR` (see installation) and hence they need not be disabled in **configure**.

Compilation

Run

```
make
```

and wait until Gwyddion is compiled. If **configure** finished without errors the compilation should pass too.

If you need to do unusual things to compile the package, please try to figure out how **configure** could detect whether and what to do, and e-mail patches or instructions to the bug-report address so they can be considered for the next release.

Installation

Run

```
make install
```

to install Gwyddion to the target directory. If you install Gwyddion to a system directory you have to become root for running this command, for example using sudo:

```
sudo make install
```

Note Gwyddion has to be installed to be run, it is not possible to run it uninstalled.

To install Gwyddion to a staging area, for example for packaging, set **make** `DESTDIR` variable to a prefix that will be prepended to all target directories:

```
make install DESTDIR=/var/tmp/gwyddion-buildroot
```

Do *not* override individual directory variables as `bindir`, `libdir`.

If you do not install to a system directory, e.g. install to a subdirectory of your home directory, you may need to adjust the following variables during installation:

- `GCONF_SCHEMA_CONFIG_SOURCE` – location of GConf2 schemas
- `KDE4_MODULE_DIR` – location of KDE4 modules

Also, variable `XDG_DATA_DIRS` might need to be adjusted after installation to get full desktop integration.

Deinstallation

Run

```
make uninstall
```

in the directory you previously compiled Gwyddion to remove it. If you have lost the source directory meanwhile you can try to unpack, configure and build it exactly as before and then issue **make uninstall**, although this relies on your ability to reproduce the build process.

RPM Packages

It is possible to build RPM packages on RPM-based GNU/Linux distributions directly from source code tarballs with

```
rpmbuild -tb gwyddion-2.19.tar.bz2
```

where 2.19 is to be replaced with the actual version as above. This method was tested mainly on Fedora, openSuSE and Mandriva and the RPM spec file contains some specific provisions for these systems. Specific support for other RPM-based systems can be added on request.

2.5 Mac OS X

Much of the previous generic Unix/Linux installation section applies also to OS X. Therefore this section deals mainly with the specifics of OS X installation, some of the steps listed here are explained in more detail in the generic Unix section.

Beside building everything on your own (good luck), at this time there are two ways to install Gwyddion:

- using MacPorts (formerly Darwinports) and building from a Portfile.
- using Fink and compiling Gwyddion the common Unix way,

Preparation

To install and run Gwyddion you need the Xcode Tools and X (SDK and App) installed. They where located on your CDs/DVDs. The Xcode Tools where located on the first DVD as XcodeTools.mpkg below Xcode Tools, the X11SDK is located as X11SDK.pkg below the Packages Folder within Xcode Tools. X11 is localted as X11User.pkg below `System/Installation/Packages` even on the first DVD. If you have an CD Set the Discs may differ. The people from MacPorts recommending using the newest version of XCode. For further information look at the MacPorts Install Page. Also you should have some experience using Terminal.app. All the commands in the the rest of this section are to be entered and run in Terminal.app.

See installation dependencies section for an overview of required and optional packages to install prior to Gwyddion installation. The following table summarizes how they are called in the two software collections:

Package	Fink	MacPorts
Gtk+	gtk+2	gtk2
GtkGLExt	gtkglext1	gtkglext
FFTW3	fftw3	fftw-3
LibXML2	libxml2	libxml2

MacPorts

MacPorts is an Port based System for porting and installing Open Source/GNU software to OS X. It's based on using installation files called 'Portfiles' which where describing the steps to compile and install an application. So it's far easy to port software to OS X using MacPorts but every computer has to compile the application. Get and install MacPorts. After you installed MacPorts, run

```
sudo port selfupdate
```

to update MacPorts to the latest version.

Usually installing ports with MacPorts is easy. But since X11 is not the native Desktop for OS X, things went a litte worse. So it is recommended to install an alternative X11 before installing Gwyddion. The recommended alternatives are XQuartz on Leopard and the Port xorg-server on Tiger. After installing the suggested X11-System, Gwyddion can be then build and installed simply by

```
sudo port install gwyddion
```

To install xorg-server (Tiger) simply type

```
sudo port install xorg-server
```

this is *needed* for the 3D view on tiger. After everything is done, you will find the StartUp-Icon below `/Applications/MacPorts`.

Fink

Get and install Fink. After you installed Fink run

```
apt-get update
```

to update the database of available packages and install Gwyddion with

```
apt-get install gwyddion
```

To install Gwyddion from source code, for instance if you want to install a development version, you need to install the required packages listed in the above table and then follow the generic Unix installation section instructions.

Running

On MacPorts you simply click on the StartUp-Icon and wait until Gwyddion appears. Using Fink or an self-compiled version you should follow the steps below: Start X11.app and type in Terminal.app

```
export DISPLAY=":0"
```

Then run Gwyddion from the folder it was installed to. This is typically `/usr/local/bin` for Fink. So for example for Fink run:

```
/usr/local/bin/gwyddion
```

You can also configure X11.app to run Gwyddion via: Locate X11.app in your dock, open the menu, choose Applications, choose Customize from the next menu. Here you can choose add and enter the name (gwyddion for example) as Menu Name and the complete path to gwddion (e.g. /usr/local/bin/gwyddion) as Command. After this you can choose gwyddion from the X11 menue.

2.6 MS Windows from Source Code Tarball

Gwyddion MS Windows build system uses the Microsoft Visual C++ (MSVC) compiler (version 6 is tested and recommended, albeit it is a bit older). It primarily consists of a set of **nmake** makefiles, that is the compilation is done from the command line. This approach has several advantages with respect to reproducibility and automation of the process. Furthermore, it enables easy synchronization of Unix and MS Windows build systems. The necessity to use command line may be considered a disadvantage though you should find the compilation process quite simple even you are not used to use the command line much.

In addition to MSVC you need to install Gtk+ development environment. Again, we recommend to use the GladeWin32 package. Note it also contains the complete run-time environment, therefore you do not need to install the run-time package if you install the development one.

Unpacking

Unpack the source code tarball with your favorite (de)compression program or file manager. Tarballs compressed with bzip2 (`.bz2`) are considerably smaller than gzip compressed tarballs (`.gz`), however support for bzip2 compression used to be less widespread than gzip compression support in MS Windows programs. Most recent programs support both, for example 7zip which is also Free Software.

The unpacking will create directory `gwyddion-2.19` (with 2.19 replaced with the actual version number) where all other compilation actions will take place.

Configuration

Open file `make.msc` in a text editor. It starts approximately as follows:

```
# @(#) $Id: make.msc 8812 2008-12-02 08:49:22Z xhorak $
#
# XXX: Set following to your Gtk+-Development and MSVC paths
#
# The uncommented paths should work for default MSVC 6 installation and for
# default GladeWin32 installation.
# If you have GtkGLext separate from Gtk+, define GTKGLEXT_TOP accordingly.
# If you have LibXML2 separate from Gtk+, define LIBXML2_TOP accordingly.
GTK_TOP = C:\Gtk
GTKGLEXT_TOP = $(GTK_TOP)
LIBXML2_TOP = $(GTK_TOP)
#GTKGLEXT_TOP = C:\GtkGLExt\1.0
#LIBXML2_TOP = C:\libxml2
MSC_TOP = C:\Program Files\Microsoft Visual Studio\VC98
```

Check and correct the paths according to the instructions. Often, no modifications are necessary as the paths in the file represent the default installation directories of each program.

`GTK_TOP` It should point to the top-level directory of Gtk+ installation, that is the directory containing `bin`, `lib`, `share`, etc. subdirectories. We will refer to its value as to `$(GTK_TOP)` below.

`GTKGLEXT_TOP` It should point to the corresponding top-level directory of GtkGLExt installation. This differs from `$(GTK_TOP)` only if you do not use GladeWin32 and have installed GtkGLExt separately.

`LIBXML2_TOP` It should point to the corresponding top-level directory of LibXML2 installation. This differs from `$(GTK_TOP)` only if you do not use GladeWin32 and have installed LibXML2 separately.

`MSC_TOP` It should point to the top-level directory of MSVC installation.

Run a shell (command line, MS-DOS prompt), switch to the source directory and run **vcvars32.bat** there. This batch file is provided by MSVC and sets certain environment variables the command-line compiler and linker require, it also makes them directly executable by setting `PATH`. Note **vcvars32.bat** may not be in `PATH` itself but it should be easy to locate.

Compilation

Run

```
nmake -f makefile.msc
```

to compile Gwyddion and

```
nmake -f makefile.msc install
```

to install it into a staging area, namely subdirectory `inst` (created by this command). If something goes wrong with the second step and you wish to start it again, remove directory `inst` and file `inst.stamp` first for a clean start.

Installation

The layout of the staging area in `inst` exactly the same as of the final installation. Therefore you can also run Gwyddion directly from it (`gwyddion.exe` is found directly in `inst`). Except if you have never run Gwyddion before, it will not find the run-time Gtk+ libraries (DLLs) it needs. Run **regedit**, create in `HKEY_LOCAL_MACHINE\Software\Microsoft\Windows\Current Version\App Paths\Gwyddion.exe` a string key `Path` and put `$(GTK_TOP)\lib;$(GTK_TOP)\bin` there (here again `$(GTK_TOP)` is to be replaced with the corresponding directory set in `make.msc`, do not put '`$(GTK_TOP)`' there literally). If you have separate GtkGLExt and/or LibXML2, add also their `lib` and `bin` directories, separated by semicolons. If you cannot edit global registry under `HKEY_LOCAL_MACHINE`, set the path under `HKEY_CURRENT_USER` for the current user only.

Now you can either run Gwyddion from `inst` or copy the directory elsewhere, possibly renaming it.

Executable Installers

To create an executable installer you need Inno Setup, version 4 or newer. Open `inst/gwyddion.iss` and build the installer, it will create `Gwyddion-2.19.exe` (with 2.19 replaced with the actual version number), again in `inst`. You can repeat this procedure with `inst/gwyddion-devel.iss` to obtain `Gwyddion-Development-2.19.exe`, should you ever need it.

2.7 Subversion Checkout, Development

Gwyddion uses Subversion version control system for source code revision management. The organization of the repository is described on project web pages. For example the current head revision of the program itself can be checked out with

```
svn checkout https://gwyddion.svn.sourceforge.net/svnroot/gwyddion/trunk/gwyddion
```

The reposition does not contain any generated files, no matter how exotic tools may be necessary to generate them. Therefore additional packages are required and there are also certain platform limitations. The additional tools and packages required for development are the same as for compilation from Subversion checkout. More precisely, one needs all the tools to build from a fresh checkout, while development may require only a subset of them or even none, depending on the type and extent of the changes.

ADDITIONAL DEVELOPMENT BUILD DEPENDENCIES

- GNU autoconf ≥ 2.60
- GNU automake ≥ 1.7
- GNU libtool ≥ 1.4
- Python ≥ 2.2
- Perl5
- gtk-doc ≥ 1.8
- GNU gettext ≥ 0.12, including development stuff
- probably GNU versions of most tools: the compiler, binutils, . . .

Linux/Unix

After a fresh checkout, run **`./autogen.sh`** with any arguments you would give to **configure**. Note it automatically adds `--enable-maintainer-mode`. This option enables **make** rules for creation and updates of files that are distributed in the source code tarball (and thus they are not generated during normal compilation). Generally, you should always use this **configure** option when you intend to change the program in a non-trivial way.

autogen.sh can fail even if you have sufficient versions of autotools installed. Some operating system do not install general **autoconf** or **automake** commands, only versioned commands such as **autoconf261** or **automake19**. This makes particularly hard to find for example '**automake** 1.9 or newer' and therefore **autogen.sh** does not attempt it at all. You can either create unversioned symbolic links to the versioned commands or run **autogen.sh** as follows: **`AUTOCONF=autoconf261 AUTOHEADER=autoheader261 ./autogen.sh`** You may need to set the following variables: `ACLOCAL`, `AUTOCONF`, `AUTOHEADER`, `AUTOM4TE`, `AUTOMAKE`, `LIBTOOLIZE`. In addition, some operating systems may install **autoconf** macros in a place **aclocal** does not find them by default. This can be fixed by setting variable `ACLOCAL_FLAGS` to give **aclocal** additional search paths: **`ACLOCAL_FLAGS="-I /usr/local/share/aclocal" ./autogen.sh`**

It is often necessary to combine these adjustments. For instance on FreeBSD, where all tools are versioned, one typically invokes (broken to lines for easier reading):

```
AUTOCONF=autoconf261 \
AUTOHEADER=autoheader261 \
AUTOM4TE=autom4te261 \
AUTOMAKE=automake19 \
ACLOCAL=aclocal19 \
ACLOCAL_FLAGS="-I /usr/local/share/aclocal" \
CPPFLAGS=-I/usr/local/include \
LDFLAGS=-L/usr/local/lib \
./autogen.sh --prefix=...
```

If **autogen.sh** passes you can compile the program as usual. However, a few things remain to generate.

Developer documentation is built with **`make docs`**. This has to be done explicitly, documentation is never (re)built automatically, option `--enable-gtk-doc` of **configure** only makes the `docs` target available (this option is on by default, therefore `docs` is made available when gtk-doc is detected).

MSVC files are built with **`./utils/update-msvc.py`** which must be run from the top-level source directory (if you have Python interpreter installed elsewhere than in `/usr/bin`, run it as **`python ./utils/update-msvc.py`**). This tool takes care of keeping MSVC makefiles and other files up to date with Unix files that are taken as the primary source. More precisely **update-msvc.py** reads

- lists of source and header files, modules, libraries and data files from `Makefile.am`
- compiled libraries in `.libs` directories
- **gcc**-generated compilation dependencies in `.deps` directories
- template files to fill, these have extension `.gwt`, for example `makefile.msc.gwt` is a template for `makefile.msc`

and it writes

- filled template files (namely makefiles)
- `.def` files with lists of symbols to export from individual libraries

Evidently, it is necessary to perform a full project build first (with all optional features enabled) to generate these files properly.

One can think of **update-msvc.py** as a simple custom automake, because its basic task is to generate makefiles from `Makefile.am`.

MS Windows

As one can see from the previous section, a direct build from a Subversion checkout is not possible on MS Windows due to the inability to generate certain files there. Development is possible, although certain changes, namely additions of new files and refactorizations, require manual synchronization of files that could be updated automatically on a Unix-like system.

Fortunately plenty of free Unix-like systems is available, namely various GNU/Linux distributions. In the most desperate case one can use such a system for the checkout, build all necessary files, make a tarball and transfer it to MS Windows. This is equivalent to the use of nightly tarballs except that these tarballs can be generated any time.

However, it is also possible – and much more convenient – to build on MS Windows in the very same directory as on a GNU/Linux system. It is only necessary to share the build directory (typically in the home directory) with the Windows system using Samba. The GNU/Linux system can run either on a different physical computer or it can run on a virtual machine on the same computer as the host Windows system, for example in WMware player. (This setup can be also reversed by running MS Windows on a virtual machine but this is not the point of this section.)

When one runs builds for several operating systems from one directory, certain care has to be taken to avoid confusion due to the use of files corresponding to a different operating system. Fortunately, the only files that overlap between the Unix and MS Windows build systems are configuration headers `config.h` and `gwyconfig.h`. To update them after switch to MS Windows, just delete them, they will be re-created as a part of the build. To update them after switch to GNU/Linux, run **`./config.status`**.

Chapter 3

Getting Started

This chapter introduces various basic concepts and terms, such as masks or selections, explains the organization of data in Gwyddion and describes the user interface.

The descriptions are relatively thorough and some of the topics near the end of the chaper, such as raw file import or plug-ins, might be considered advanced and not for everyday use. So, despite the name, it is not necessary to read this entire chapter to be able to work with Gwyddion. The Gwyddion user interface is intuitive and much can be discovered by playing. The clarification of the basic ideas and components provided here will hopefully ease the discoverying.

Tip Command Meta → Tip of the Day displays data processing tips and highlights useful features that you might miss.

3.1 Main Window

The main window, also called toolbox, is one of the two Gwyddion windows that appear after program start (with no files given to open), the other is the data browser. Closing the main window causes Gwyddion to exit.

The toolbox contains the set of Gwyddion menus and from several rows of buttons connected with common functions and tools. The menus group the functions as follows:

File associates commands that are used for file loading and saving. Certain global commands (e. g. Exit) are located here too. The history of recently opened files can be browsed with File → Open Recent → Document History.

Edit provides history manipulation commands (Undo, Redo) and editors of miscellaneous global resources, such as gradients and materials for false color and 3D data representation or the default color used for data masking.

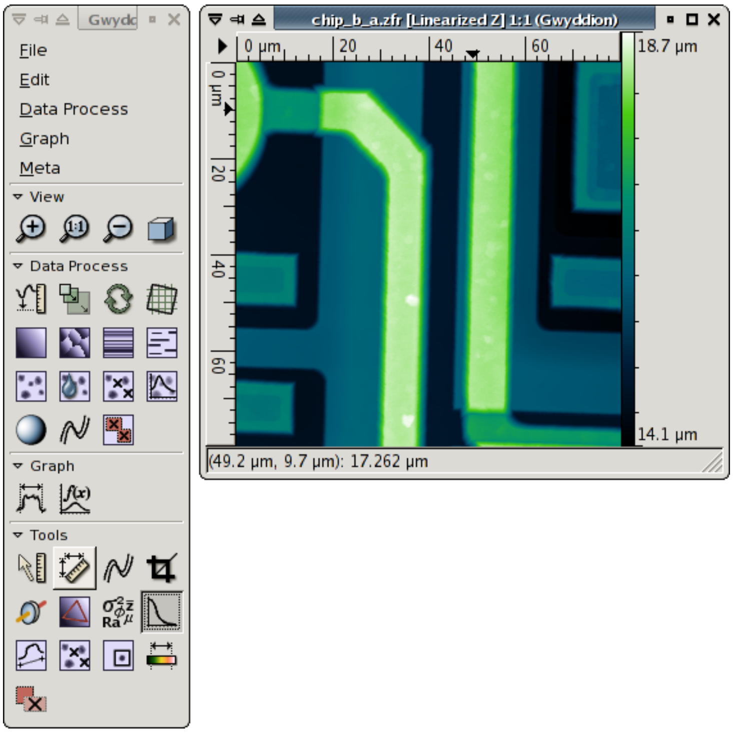
Data Process is built automatically from all data processing modules available in the Gwyddion module directory (depending on the operating system). This menu together with Tools panel of buttons contain most of the commands you will need at analyzing your SPM data. A subset of these functions is also available in Data Process button panel. These buttons serve as shortcuts to commonly used functions from Data Process menu. All functions accessible from Data Process button panel can be found in the menu too.

Graph is similar to Data Process, except it consists of graph functions. Graph processing includes function fitting, exporting graph data etc. Button panel Graph again contains a subset of the commonly used functions from Graph menu.

Meta contains commands that provide various auxiliary information. Namely height field metadata (e.g. scanning speed, tip voltage, etc.) and information about Gwyddion itself.

Finally, you can find some rows of buttons in the main window. Buttons in View panel offer zooming functions (that are often more easily invoked by keyboard shortcuts or just rezising the data window) and 3D data display. Panels Data Process and Graph contain selected functions from Data Process and Graph menus as described above.

Panel Tools contains tools, i.e. functions that directly work with selections on data windows. These functions are accessible only from this button panel.



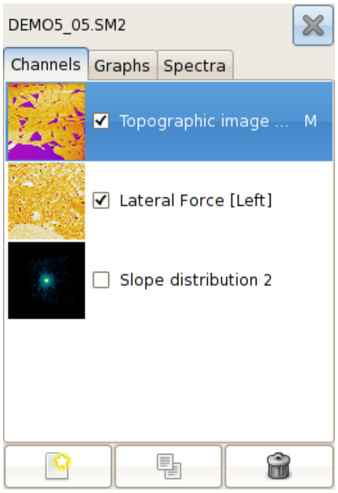
Main window and a data window showing microchip surface (Gwyddion sample file `chip.gwy`*).*

3.2 Data Browser

Data browser is a window that displays the structure of currently focused file. It shows the content as represented in Gwyddion which may differ somehwat from the organization in the original software.

Gwyddion supports an arbitrary number of two-dimensional data fields per file. Depending on the context, they are also often called channels or height fields in this guide. The dimensions of channels in one file may difffer and also the physical dimensions and values can be arbitrary physical quantities.

In addition, one-dimensional data, represented as graphs, and single-point spectra can present in the same file. The data browser is a tool for browsing and managing all the available data in the file.



☑ Topographic image ... M

☑ Lateral Force [Left]

□ Slope distribution 2

Data browser displaying several channels.

Controlling the Browser

Since the data browser always displays the structure of currently focused file, its contents change as you switch between different windows, possibly showing data from different files. There is no difference between native Gwyddion files (`.gwy`) and other files. Once a file is loaded its structure is shown as if it was a Gwyddion file.

The data browser has three tabs, one for each type of data that can be present in the file:

- Channels
- Graphs
- Spectra

Each list shows names of the data objects and some additional properties that depend on the specific data type. The names can be editted after double-clicking on them.

Individual channels, graphs or spectra can be deleted, duplicated or extracted to new Gwyddion native file using the buttons at the bottom of the browser. It is also possible to copy them to another file by dragging a data browser row to any window belonging to the target file.

The close button in the top right corner of the data browser closes the current file, discarding all unsaved changes. A file is also closed when all windows displaying data from this file are closed.

If the data browser is closed it can be recalled using the Meta → Show Data Browser command.

Channels

The channel list shows channel thumbnails, check-boxes controlling whether the channel is visible (i.e. displayed in a window) and channel names. Right to the name the presence of presentation and/or mask is indicated by the following letters:

- M – mask
- P – presentation

Graphs

The graph list shows check-boxes controlling whether the graph is visible and graph names. Right to the name the number of curves in the graph is displayed.

Spectra

The spectrum list shows the spectra name and the number of points in the set. Since single-point spectra are displayed and operated on only in connection with a two-dimensional data using the spectroscopy tool there is no check-box controlling the visibility.

3.3 Managing Files

Gwyddion uses its custom data format (`.gwy`) to store data. This format has the following important advantages:

- Capability to store the complete state of the individual data, including masks, selections and other properties.
- Arbitrary number of channels, graphs and spectrum sets, with arbitrary dimensions and units of both dimensions and values.
- Double-precision representation of all data, preventing information loss due to rounding.

Therefore, we recommned to use this format for saving of processed files.

Other data file formats are handled with appropriate file loading and saving modules. Beside a large number of file formats used in scanning probe microscopy, graphical file types (PNG, JPEG, TIFF, TARGA) and raw binary and text data can be imported too. If your SPM data format is not supported by Gwyddion yet or it is loaded incorrectly, you are encouraged to write an import module (if you can program) or contact the maintainers to help them improve the support.

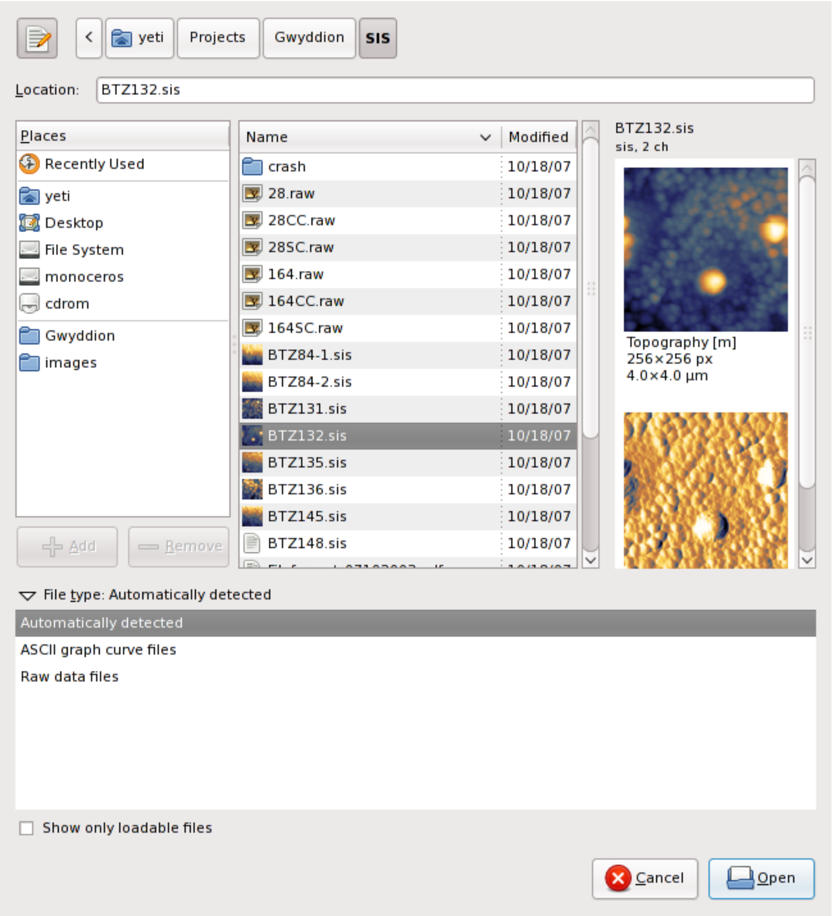
The list of all supported file formats can be found in chapter Summaries and Tables.

File Loading

Files are opened using File → Open. The file type is detected automatically, based solely on the file content. Since the same extensions such as `.img`, `.afm` or `.dat` are used by many different SPM file types this approach is superior to relying on file extensions.

The only exception is the import of various raw data, either two-dimensional or graph, that must be chosen explicitly in the file open dialog. See sections Raw Data File Import for details of import of raw data and manual extraction of data from unsupported formats and Specific Data Import for import of XYZ data, pixmap image data and graph data.

The list of files in the file open dialog can be limited to only files Gwyddion recognizes as loadable by enabling the Show only loadable files option. The file type label then indicates the filtering by appending (filtered) to the end. This can be often convenient, on the other hand it can slow down listing of directories with many files.



Location: BTZ132.sis

Name	Modified
crash	10/18/07
28.raw	10/18/07
28CC.raw	10/18/07
28SC.raw	10/18/07
164.raw	10/18/07
164CC.raw	10/18/07
164SC.raw	10/18/07
BTZ84-1.sis	10/18/07
BTZ84-2.sis	10/18/07
BTZ131.sis	10/18/07
BTZ132.sis	10/18/07
BTZ135.sis	10/18/07
BTZ136.sis	10/18/07
BTZ145.sis	10/18/07
BTZ148.sis	10/18/07

BTZ132.sis
sis, 2 ch

Topography [m]
256×256 px
4.0×4.0 µm

File type: Automatically detected

Automatically detected
ASCII graph curve files
Raw data files

□ Show only loadable files

File open dialog with expanded file type options and channel preview. The small text above the preview shows the module used to load the file (sis) and the number of channels (ch), graphs (gr) and single-point spectra (sps) in the file.

File Merging

File merging, performed by File → Open, is similar to normal file loading, except that the selected file (or files) is merged into the current open file. In other words, channels, graphs and spectra, together with all their settings and properties are added to those already present in the current file.

File Saving

Much of the previous paragraphs applies to file saving too. One of the main differences is the reliability of automatic file type determination. While loading can and does examine the file contents, saving depends on file name and extension. Combined with the large number of different file types using the same extension such as `.img`, `.afm` or `.dat` it leads to ambiguities. Select the file type explicitly before saving if you are unsure.

Since the only file type able to fully represent Gwyddion data structures is its native data format, saving to a `.gwy` file is the only proper saving. Saving to other file formats essentially consists of exporting of a limited subset of the data, typically only the active channel (without masks and presentations). Therefore it does *not* change the file name of the current file to the just saved file name.

Document History

The history of recently opened files can be accessed with File → Open Recent. The submenu contains the last 10 recently used files for quick recalling, an extensive recent file history is accessed with the last item Document History.

Document history lists the files sorted by the last access time (the most recently accessed at the top), with previews and some additional information about a selected channel. The function of the bottom row of buttons is following:

Prune Removes history entries of files that have been deleted or are no longer accessible for other reasons.

Close Closes the document history window.

Open Opens the selected file. This can be also achieved by activating the selected row, either by double-clicking or with the keyboard.

The history can be searched/filtered by file name using the filter controls above the buttons. The filter is activated by pressing **Enter** in the filter pattern entry. To display all history entries, clear the entry and activate it. The filter pattern is interpreted in two ways:

- If the pattern contains wildcards, i.e. `*` or `?`, it is interpreted as file glob. This means `?` represents a signle arbitrary character, `*` represents an arbitrary sequence of zero or more characters, and the file name has to precisely match the pattern. Note directory separators (`/` or `\`) are not treated specially, therefore in the pattern `*.sis` the initial `*` matches all leading directory components. The pattern syntax is described in GPatternSpec documentation.
- If the pattern does not contain any wildcards, it is directly searched as a part of the file name.

Search case sensitivity, controlled by option Case sensitive, is useful mainly on systems distinguishing letter case in file names, such as Unix. On systems that do not distinguish the case themselves it is recommended to keep the setting on case insensitive.

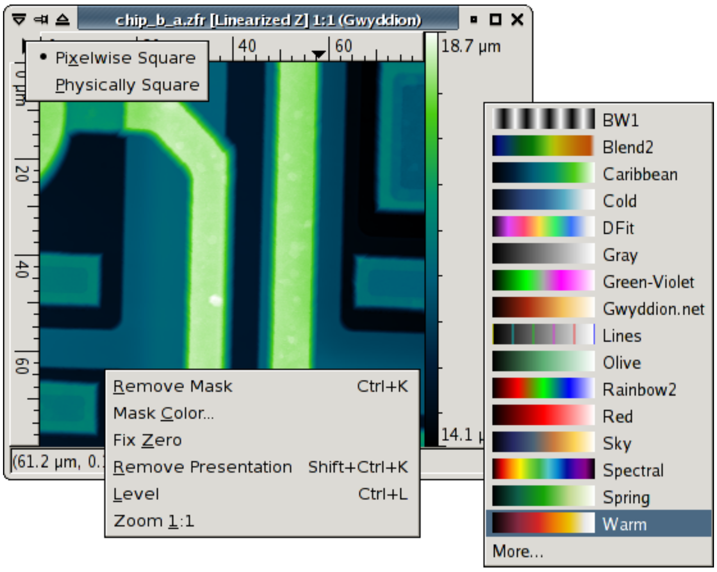
3.4 Data Window

Two-dimensional data are presented in so called data windows. It is the main widget used for working with Gwyddion. The data are presented as a field of false colors corresponding to heights. Color axis that represents mapping the colors to real height values is on the right side of the data window.

The False color palette used to represent height data can be changed by clicking on the color axis with right mouse button (i.e. invoking context menu) and selecting a palette from the list. Most frequently used palettes are available directly in the context menu; however you can reach much more of the possible palettes using the More menu entry. Moreover, you can use the color gradient editor to create your own palettes and select which palettes should be displayed in the short list.

There is a context menu available also for the data area. This menu consist of basic data and presentation operations. To reach all the possible operations use Data process... menu at the Gwyddion main window, or use some of the tools available at the Tools set of buttons at the Gwyddion main window.

The arrow in the upper left corner brings the aspect ratio switch menu. The data can be displayed either with pixels mapped with 1:1 aspect ratio to screen pixels (Pixelwise Square), or with physical dimensions mapped 1:1 onto the screen (Physically Square). For instance a sample of size 1×1 μm scanned with reduced slow axis resolution and having therefore 512×128 pixels, can be displayed either in 512×128 or 512×512 window.

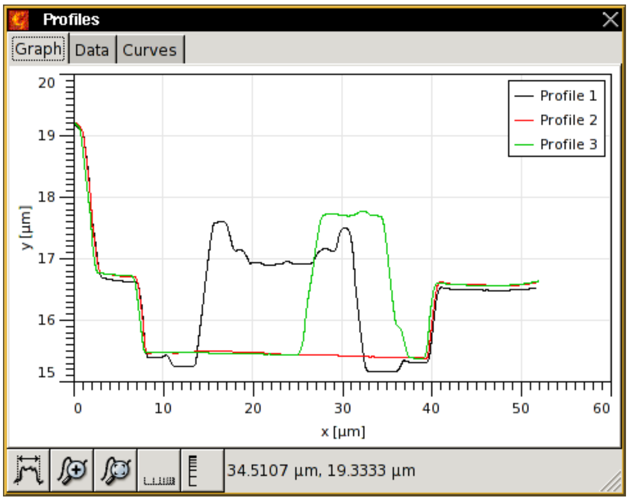


Data window with all three available context menus shown.

3.5 Graph Window

Graph window is used for 1D data processing. They are created by appropriate tools or modules that extract graphs from height field data. Currently, it is not possible to import standalone graphs into application as the main intent of Gwyddion is to provide tools for analyzing height fields, not graphs.

Graph window consist of three tabs: the first two represent graphical and tabular views of the 1D data and the third one shows a list of graph curves. Several tools connected with viewing 1D data are available directly in the graph window toolbar, namely zoom buttons and logarithmic axis buttons. To reach all the possible operations use Graph menu in the Gwyddion main window.



A graph window with three profiles.

To edit curve presentation one can either click on the curve in the graph or activate (double-click) the corresponding row in Curves. Individual curves can be deleted by selecting them in Curves and pressing **Delete**. It is also possible to copy individual curves to other graphs by dragging their curve list rows onto them (provided the graphs are unit-wise compatible).

Clicking on a graph axis brings a dialog with axis properties and graph key properties can be edited after double-clicing on it.

3.6 Tools

Functions from Data Process menu and button panel either execute immediately or after asking for parameters and settings in a dialog box. Tools, accessible from Tools button panel, work differently. Once selected, they remain active and always follow the current data window until one switches to another tool. In other words one can switch data windows freely while using a tool and it always shows information from or operates on the current data. Tools also differ by working with selections, e.g. points, lines or rectangles, on data windows. Nevertheless functionally they perform similar tasks as Data Process functions – value reading, leveling, statistics, correction, etc.

Tools can be launched only from Tools button panel located in the main window. Gwyddion includes these tools:

Read Value Reads values at the position of mouse click.

Distance Measures distances – similarly to Read value it tool enables user to measure horizontal, vertical and Euclidean distance and angle between points in the data field. In addition it displays the difference of data values between points.

Profile Extracts profiles of the data field and puts them to separate graphs. These graphs can be further processed with commands from the Graph menu.

Spectro Views and extracts single point spectroscopy data.

Statistical Quantities Computes basic statistical quantities (RMS, Ra, minimum, maximum, projected and surface area, etc.) from a selection of full data field. It can also calculate them only the masked area, or even combine these two types of selection of area of interest.

Statistical Functions Computes basic statistical functions (distribution of heights or slopes, autocorrelation function, power spectrum density function, etc.) from a selection of full data field.

Row/Column Statistics Somewhat complementary to 1D statistical functions, this tool plots characteristics such as mean, median or surface length for each row (column).

Roughness Evaluates standardized one-dimensional roughness parameters.

Three Point Level Levels data by plane obtained by clicking on three points within data window. The three values can be averaged over a small area around the selected point.

Path Level Row leveling tool equalizing the height along a set of arbitrary straight lines.

Polynomial Line Level Levels rows or columns by fitting and subtracting polynomials.

Crop Cuts part of the data.

Mask Editor Manual editing of masks: creation, exclusion, intersection, inversion, growing and shrinking, . . .

Grain Measurement Measures individual grain parameters.

Grain Remover Removes continuous parts of the mask by clicking on mask point and/or interpolates (removes) data under a continuous part of mask.

Spot Remover Manually removes spots. Select a point on a data window, mark an area to interpolate on the zoomed view and remove the defect using chosen interpolation method.

Color Range Stretches color range or changes false color mapping type. It enables the user to change the false color representation range (by default from data minimum to data maximum).

Filter Basic filters – mean, median, conservative denoise, minimum, maximum and similar simple filters to reduce noise in the data.

Selection Manager Displays selections for a channel and copies them to other channels or files.

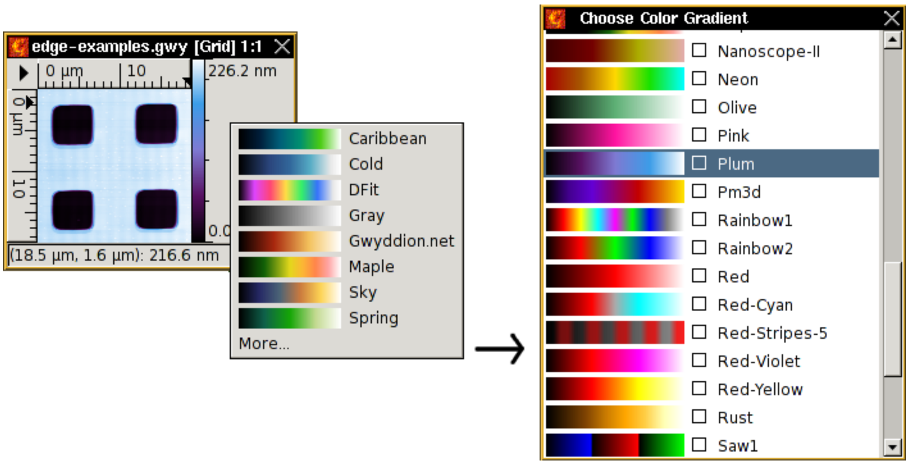
Tool dialogs can be closed (or more precisely hidden, as the current tool is still active even if its dialog is not visible), beside activating the Hide button, by pressing **Esc** or clicking the tool's button in the toolbox again.

3.7 False Color Mapping

False color mapping is the basic two-dimensional data visualization method. The color gradient (also called palette) to use can be selected after clicking on the false color map part of a data window with right mouse button.

This quick selection pop-up menu offers the list of preferred color gradients. In addition it allows to invoke the full color gradient list by selecting More. Preferred gradients can be chosen by checking the corresponding check buttons in the full list or in the gradient editor list. Selecting a row in the full list changes the gradient to the selected one, double-clicking (or pressing **Enter**) also finishes selection and closes the list window. Gradients of known names can be quickly accessed by starting to type their name. The default color gradient to use (when none is specified in the file) can be also set in the gradient editor.

More control over the way values are mapped to colors is possible with Color range tool.



A data window with the right-click color gradient pop up menu and the full color gradient list.

Color Range Tool

Color range tool is a special tool whose purpose is not to analyse or modify data, but to control the way values are mapped to colors. It offers four basic color mapping types:

Full Data values are mapped to colors linearly, the full data range corresponds to the full color range. This is the default type (unless you have changed the default).

Fixed Data values are mapped to colors linearly, a user-specified data range (which can be smaller or greater than the full range) maps onto the full color range. Values outside this range are displayed with the edge colors. The range can be set by several means:

- by entering desired values numerically in the tool window,
- by selecting a range on the height distribution graph in the tool window or
- by selecting an area on the data window, the range is then set from the minimum to maximum of the data in this area only.

If no range is manually set, fixed range type behaves identically to full range.

Note data processing operations often modify the value range – and as the fixed range remains fixed as you set it, it can result for instance in completely black data display. You may wish or have to update the range manually then, or to switch to another mapping type.

Automatic Data values are mapped to colors linearly, a heuristically determined subinterval of the full value range maps onto the full color range. Values outside this subrange are again displayed with the edge colors.

Adaptive The full data range corresponds to the full color range, however data values are mapped to colors non-linearly. The mapping function is based on inverse cumulative height distribution, therefore flat areas generally get bigger slice of the color gradient and smaller value variations can be seen on them than normally.

The false color map ruler on the right side of data windows does not display any ticks in this mode, only the minimum and maximum value.

A mapping type can be set to be default by checking the Default check button when it is active. Newly displayed data windows then use this type, unless a channel explicitly specifies other type to use.

Saving data to `.gwy` file also saves all color mapping settings: mapping type, range and gradient. Gradient is however not physically stored in the file, only referenced by name. In other words, color gradients of the same name are shared among files.

Color Gradient Editor

Color gradient editor can be invoked with Edit → Color Gradients. It consists of a gradient list similar to the full gradient selector, with an additional button panel, and the actual editor that can be invoked by double-clicking on a gradient you wish to edit or by activating the Edit button. Renaming is p Only user-created color gradients can be edited or deleted, system gradients installed with Gwyddion are immutable.

The last button in the gradient list control panel makes the currently selected gradient the default. It will be used for all newly displayed data that do not specify any particular color gradient.

Two editing modes are available:

Points The color gradient is defined by a set of points and their associated colors. The points are represented by triangular markers on the gradient displayed in the lower part of the editor window. Moving these markers moves the points, new points can be added by clicking into an empty space, existing points can be removed by dragging them away from the gradient.

Curve The color gradient is defined by red, green and blue curves. The curves are again segmented, but the segments of individual curves do not need to coincide.

3.8 Presentations and Masks

Presentations

Presentations can be used to show the height field in another way than as a false color map of the heights, for instance with shading or with highlighted edges. It is also possible to superimpose an arbitrary data field over another one as the presentation.

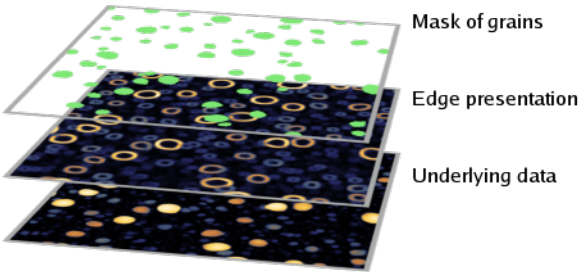
Note the superimposed presentation is really only a presentation, it is never used for calculations. In all data processing functions or tools the results are always computed from the original underlying data. Since presentations can be computationaly intensive to calculate, they are not automatically updated when the underlying data change. The various presentations available are described in section Presentations.

The presence of presentation over the data is indicated by flag P in the data browser and also by the empty false color map ruler on the right side of the data window that does not display any ticks nor the minimum and maximum value.

Masks

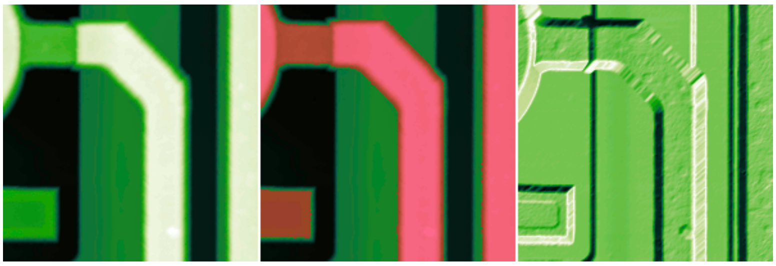
Masks are used for special areal selections, e.g. grains, defects or factes with certain orientation. Masks can have any shape and within the data window and they are visualized by a color overlayed over the data. The mask color and opacity can be changed in the right-click context menu of the data window.

Since grain marking is the most common use of masks, several functions that operate on marked areas are called ‘grain’ functions, e.g. Grain Statistics. Also, a contignuous part of mask is sometimes called grain in this guide. However, since a mask does not bear any information how it was created all mask functions can be used with masks of any origin.



Visualization of masks and presentations. If you look from above they can be imagined to be stacked as in the picture.

Both masks and presentations can be removed from the data by functions in the right-click menu of the data window, or with keyboard shortcuts.



Data in default false color representation (left), with superimposed mask visualized with a red color (centre) and with shading presentation (right).

Working with Masks

The mask-related functions can be divided into three main groups:

Creation Masks are created by various types of marking functions, namely grain marking functions (Mark by Threshold, Mark by Watershed), defect marking functions (Mask of Outliers, Mark Scars) and feature marking functions (Mask by Correlation, Facet Analysis, Certainty Map). In addition, some general mask editting functions provide means to create masks from scratch.

Masks are also used to mark invalid pixels in files imported from formats that distinguish between valid and invalid pixels since Gwyddion does not have a concept of invalid pixels.

Application In general, the mask-covered area is considered to be the area of interest, i.e. the area to operate on. This applies namely to statistical functions such as the Statstical Quantities tool. Function Remove Data Under Mask replaces the data under mask, while the Remove Grains tool can perform such replacement for individual grains. There are several functions for the examination of grain properties, see section Grain Statstics.

Some functions ask whether to consider the area under mask included or excluded (or ignore the mask), namely leveling functions. Such choice is offered only if a mask is present on the data.

Editting A few basic mask operations, such as inversion or complete removal, are available in Data Process → Mask menu. More advanced functions include the grain-oriented Remove Grains tool and Remove by Threshold that provide different means to remove parts of the mask, as well as Mask Editor tool and Mark With focused on general mask editting.

Mask Editor Tool

The Mask Editor is the basic mask modification tool. It provides two groups of functions: editing of the mask by drawing shapes directly in the data window and global operations with the mask such as inversion or growing and shrinking. The drawing operations are controlled by the buttons in the Editor group.

Buttons in the Mode row select how the shape drawn in the data window will modify the mask:

Set The mask is set to the drawn shape, discarding any mask already present.

Add The mask is extended by the drawn shape (if there is no mask yet a mask is created).

Subtract The drawn shape is cut out from the mask This function has no effect if there is no mask.

Intersect The mask is set to the intersection of the drawn shape and the already present mask. This function has no effect if there is no mask.

Buttons in the Shape row control which shape is drawn on the mask. The choices include rectangles, ellipses and thin lines.

The basic global operation with masks, i.e. inversion, removal and filling the entire data field area with a mask are available in the Actions row. Additional operations include:

Grow Extends the mask by Amount pixels on each side. More precisely, the mask is extended by one pixel on each side and this is repeated Amount times.

Normally, growing does not distinguish between individual parts of the mask. Parts that grow so much that they touch therefore merge. This can be prevented by Prevent grain merging by growing which makes individual parts of the mask stop growing once there is only one-pixel space between them.

Shrink Reduces the mask by Amount pixels from each side. More precisely, the mask is reduced by one pixel from each side and this is repeated Amount times.

The reduction may or may not occur from the data field borders. This is controlled by the Shrink from border check box.

Mark With

Data Process → Mask → Mark With

Mark With can create or modify masks using another mask or data of the same dimensions. The operations that can be applied to the current mask are the same as in the Mask Editor tool: creation, union, subtraction and intersection. The source of the other mask can be one of the following:

Mask This is the simplest case, a mask can be combined with another mask using the specified logical operations.

Data In the Data mode, another height field is used as the other mask source. The mask consists of pixels within a range of heights, specified as relative values within the total range. To use pixels outside a certain range for the masking, set the upper bound to a smaller value than the lower bound.

Presentation The Presentation mode differs from Data mode only in that a presentation is used instead of the data.

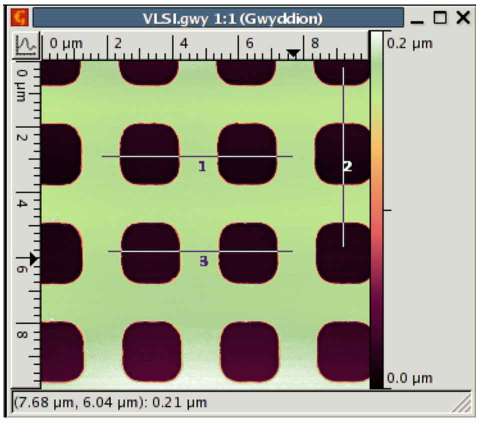
This is an exception to the rule stating that presentations are never used for further processing. Sometimes it can be useful to mark, for instance, edges found on the data even though the corresponding presentation visualizes a quantity weird from the physical point of view.

3.9 Selections

All interactive tools and some other processing methods allow to select geometrical shapes on data with mouse: points, lines, rectangles, circles/ellipses. Existing selections can be similarly modified by dragging corners, endpoints, or complete selections. When mouse cursor is moved near to an editable point of a selection, is changes its shape to indicate the possibility to edit this point.

Each tool typically uses only one type of selection and when it is activated on a data window, it sets the selection mode to this type. Selections of other types than currently displayed are remembered and they are recalled when a tool which uses them is activated again. E.g. when you select several lines with Profile extraction tool, then switch to Statistical quantities (the lines disappear) and select a rectangular area to calculate statistical characteristics of, and then switch back to Profile extraction, the rectangle disappears and the lines appear again.

Tools that use the same type of selection – e.g. both Statistical functions and Statistical quantities use rectangular selection – share it. To calculate height distribution of the same rectangle you have selected for statistical quantities, it is sufficient to switch the tool.



(7.68 µm, 6.04 µm): 0.21 µm

Data window with three selected lines, two horizontal and one vertical.

If you save data in Gwyddion native file format (.gwy), all selections are saved together with data and recalled the next time the file is opened and appropriate tool chosen.

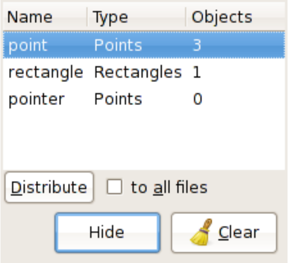
Pressing Shift during selection restricts the degrees of freedom of the shape, making it easier to draw shapes form a specific subset. Specifically, pressing Shift restricts

- rectanglular selections to perfect squares,
- elliptical selections to perfect circles,
- directions of line selections to multiples of 15°.

Selection Manager

The selection manager is a special tool that displays the list of all selections in a channel and enables to copy them to other channels.

For each selection, the selection shows the name, which is how the selection is identified in the .gwy file; the selection type and the number of objects (points, lines, rectangles, . . .) selected. Usually, there is at most one selection of any type because they are shared among the tools as described above. Nevertheless, sometimes there are special or private selections present as shown on the following figure displaying two point-wise selections.



Name	Type	Objects
point	Points	3
rectangle	Rectangles	1
pointer	Points	0

☐ to all files

Selection Manager showing several selections present in the data.

It is possible to delete individual selections by choosing them in the list and pressing Delete – this is equivalent to clearing the selection in the corresponding tool. The Clear button removes all selections.

However, the most interesting function of Selection Manager is selection copying. There are two ways to copy a selection to another channel:

- Dragging a row from the selection list onto a data window copies the selection to this data window.
- Clicking the Distribute button copies the selection to all other channels in the file. Or, if to all files is enabled, to all channels in all open files.

Selections are copied only to channels with compatible lateral units. This means that a selection in a normal channel with meters as the lateral units will not be distributed to a two-dimensional PSDF channel or a two-dimensional slope distribution.

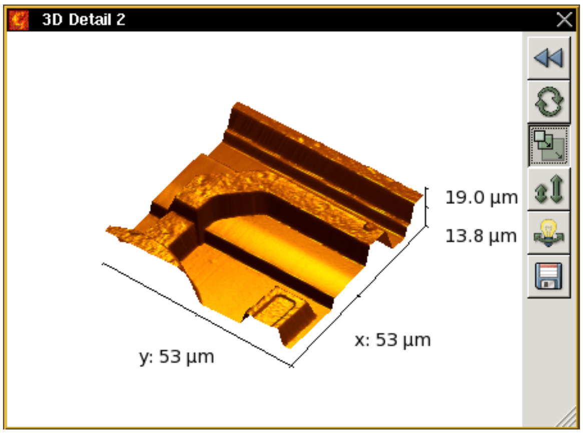
If the physical dimensions of the target data are not sufficient to contain all the objects of the copied selection then only those objects that fit are copied (this can also mean nothing is copied).

3.10 OpenGL 3D Data Display

Three-dimensional OpenGL display of the current data window can be invoked with the button with symbol of cube in View button row of main window.

This feature is optional, i.e. it can be disabled at compile time. It can also happen that while Gwyddion is capable of 3D data display your system does not support it. In both cases an attempt to invoke 3D view gives an error message explaining which of the two cases occured. In the former case you have to ask the producers of Gwyddion executables to build them with 3D support or build Gwyddion yourself from source code. If it is the latter case, refer to your operating system guide on how to enable OpenGL 3D capabilities.

The 3D window has two possible forms: with basic and expanded controls. It starts with basic controls only, this form is displayed on following figure. It can be switched to the expanded form (and back) with an expander button it the upper right corner. Clicking on the view with right mouse button brings a quick color gradient/GL material selector.



Three-dimensional OpenGL data display window with basic controls.

Basic Controls

Basic 3D window contains interaction mode controls at the right side of the view. By default, dragging the view with mouse rotates it horizontally and vertically. All possible modes are listed below:

- Rotation – this is the default. Dragging the view horizontally rotates it around z-axis, vertical drag rotates it around horizontal axis parallel with the plane of view.
- Scale – dragging the view right and down enlarges it, drag in the opposite direction makes it smaller.
- Z-scale – dragging the view up (down) increases (decreases) the z-scale, making the hills and valleys more or less pronounced.
- Light rotation – this possibility is available only in lighting visualization mode. Dragging the view changes position of light source similarly to rotation of data in normal rotation mode.

The basic controls also include an image export button.

When basic controls are shown it is possible to switch between the modes using keys **R** (rotation), **S** (scale), **V** (value scale) and **L** (light rotation).

Full Controls

In expanded controls the mode buttons are located in top row, however their function does not change. In addition, there are several tabs with options below them:

- Basic – controls to set rotations and scales numerically and to switch on an off axes, axis labels, and perspective projection.
- Light & Material – visualization settings. Gwyddion 3D view has two basic visualization modes: gradient, in which the data are simply colored with a false color scale exactly like in normal 2D view; and material, in which the data are presented as an OpenGL material rendered according to light position. This tab also contains controls to set light position numerically.
- Labels – fine tuning of sizes, positions, and other properties of axis labels.

Saving Images

The 3D view can be saved into a bitmap image with the Save button. The output is currently always a PNG (Portable Network Graphics) image with exactly the same size and contents as displayed on the screen. Entering a different file extensions than `.png` still produces an image in PNG format, albeit with a confusing extension.

Note due to the peculiarities of certain operating systems, graphics drivers and windowing environments, artefacts may sometimes appear on the exported image in parts corresponding to obscured parts of the 3D view. If you encounter this problem, make sure the 3D view is not obscured by other windows during the image export.

OpenGL Material Editor

OpenGL material editor can be invoked with Edit → GL Materials. The controls in the material list are the same as in the color gradient editor list and the material management works identically. The actual editor is of course different. It allows to edit four quantities defining the material:

- ambient color $k_{\mathrm{a},\alpha}$ (where $\alpha = \mathrm{red}, \mathrm{green}, \mathrm{blue}$), controlling the reflection of ambient light that is assumed come uniformly from all directions,
- diffuse color $k_{\mathrm{d},\alpha}$, describing the diffuse reflection which is independent on the direction of incident light and whose apparent brightness is independent of the viewing angle,
- specular color $k_{\mathrm{s},\alpha}$, controlling the specular reflection with reflected light intensity dependent on the angle between the observing direction and the direction of light that would be reflected by an ideal mirror with the same normal, and
- shininess s, a numeric exponent determining how much the specular reflection resembles an ideal mirror, smaller values mean rougher surfaces, higher values mean smoother surfaces.

If we denote **L** the normal vector pointing from the observed surface point to the light source, **V** the normal vector to the observer, **N** the normal vector to the surface **R** the normal vector in the direction of ideal mirror reflection, the observed light intensity in OpenGL lighting model can be expressed as

$$I_\alpha = k_{a,\alpha} I_{a,\alpha} + k_{d,\alpha} I_{d,\alpha} (\mathbf{N} \cdot \mathbf{L}) + k_{s,\alpha} I_{s,\alpha} (\mathbf{R} \cdot \mathbf{V})^s$$

where $I_{\mathrm{a},\alpha}$, $I_{\mathrm{d},\alpha}$ and $I_{\mathrm{s},\alpha}$ are the ambient, diffuse and specular light source intensities, respectively.

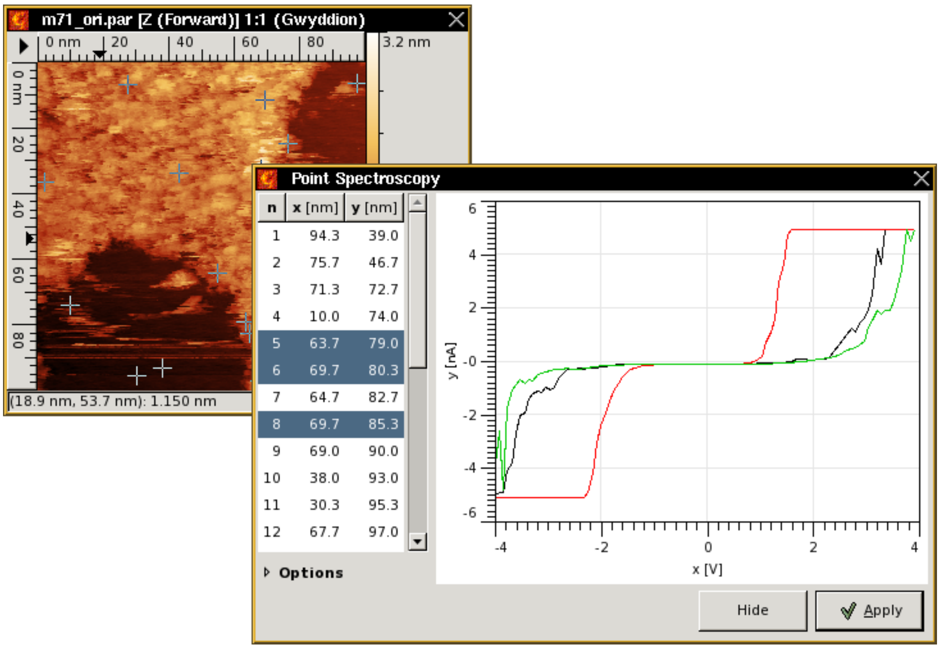
3.11 Single Point Spectra

Gwyddion currently offers some basic visualization and extraction means for single point spectroscopy data (we will generally refer to any curves measured in or otherwise attached to individual points of the sample as to ‘spectra’ here). If spectra import is supported for a file type, they will appear in the Spectra tab of the data browser. Standalone spectra files can be added to the two-dimensional data using file merging.

Point Spectroscopy Tool

The primary spectra visualization and extraction tool is the Point spectroscopy tool. It displays a list of measurement points and shows their positions on the data window. Individual curves can be selected either in the list on by selecting the corresponding crosses on the data window. If the file contains more than one spectrum set, one can choose among them by selecting the desired one in the Spectra tab list of the data browser.

The Apply button then extracts the selected set of curves into a graph that can be further analysed by graph functions, such as force-distance curve fitting.



n	x [nm]	y [nm]
1	94.3	39.0
2	75.7	46.7
3	71.3	72.7
4	10.0	74.0
5	63.7	79.0
6	69.7	80.3
7	64.7	82.7
8	69.7	85.3
9	69.0	90.0
10	38.0	93.0
11	30.3	95.3
12	67.7	97.0

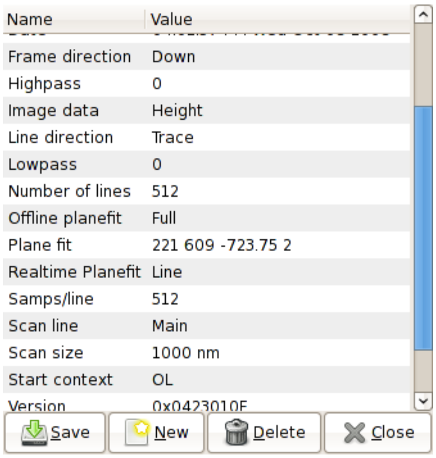
A data window with measurement points displayed and the point spectroscopy tool showing curves from three selected points.

3.12 Metadata

Auxiliary information and values describing certain data and the conditions it was measured on are called metadata in Gwyddion. They may include the SPM mode, tip bias, scanning frequency, measurement date and time or user comments.

Metadata are always per-channel. The metadata for the current channel can be displayed with Meta → Metadata Browser command. The browser lists all available metadata as Name, Value pairs. It also enables to modify and delete values or add new ones. It is possible to export all metadata of a channel to a text file with Save button.

The level of metadata support differs wildly between file formats. For file formats that are well documented and/or allow to import all metainformation generically lots of auxiliary data including obscure hardware settings can be listed. On the other hand it is possible that no metadata is imported from your files, for example when they contain no auxiliary data or it is not known how to read it.



Name	Value
Frame direction	Down
Highpass	0
Image data	Height
Line direction	Trace
Lowpass	0
Number of lines	512
Offline planefit	Full
Plane fit	221 609 -723.75 2
Realtime Planefit	Line
Samps/line	512
Scan line	Main
Scan size	1000 nm
Start context	OL
Version	0x0423010F

Metadata browser showing the metadata of a Nanoscope file.

3.13 Raw Data File Import

Both raw ASCII and binary data files and files in unsupported formats can be imported with rawfile module – with some effort. Raw data import can be explicitly invoked by selecting Raw data files type in the file open dialog. It can be also set to appear automatically when you try to open a file in an unknown format. This is controlled in the raw file dialog by option Automatically offer raw data import of unknown files.

Information

Its first tab, Information, allows to set basic file information:

Horizontal size, Vertical size Horizontal and vertical data resolution (number of samples).

Square sample Fixes horizontal and vertical resolution to the same value.

Width, Height Physical sample dimensions.

Identical measure Keeps the ratio between physical dimension and number of samples equal for horizontal and vertical direction, that is the data has square pixels.

Z-scale (per sample unit) The factor to multiply raw data with to get physical values.

Data Format

On the second tab, Data Format, particular data format can be chosen. There are two independent possibilities: Text data and Binary data.

Text files are assumed to be organized by lines, each line containing a one data row, data being represented by integers or floating point numbers in standard notation. Following options are available:

Start from line The line data starts at, that is the number of lines to ignore from file start. All types of end-of-line markers (Unix, MS-DOS, Macintosh) are recognized.

Each row skip The number of fields to ignore at the begining of each line.

Field delimiter, Other delimiter If delimiter is Any whitespace, then any nonzero number of whitespace characters counts as field delimiter. If a whitespace character is selected, the delimiter must be this character. Otherwise field are separated by specified character or string and all whitespace around delimiters is ignored.

Decimal separator is comma By default, floating point numbers are assumed to use decimal point. This option changes it to comma.

Following options are available for binary files:

Binary data You can either select one of predefined standard data formats, or User defined to specify a format with odd number of bits per sample or other peculiarities.

Byte swap pattern How bytes in samples are swapped. This option is only available for predefined formats larger than one byte. Its bits correspond to groups of bytes to swap: if j-th bit is set, adjacent groups of 2^j bits are swapped.

For example, value 3 means sample will be divided into couples (bit 1) of bytes and adjacent couples of bytes swapped, and then divided into single bytes (bit 0) and adjacent bytes swapped. The net effect is reversal of byte order in groups of four bytes. More generally, if you want to reverse byte order in groups of size 2^j, which is the common case, use byte swap pattern $j-1$.

Start at offset Offset in file, in bytes, the data starts at.

Sample size Size of one sample in bits for user defined formats. E.g., if you have a file with only 4 bits per sample, type 4 here. For predefined formats, their sample size is displayed, but it is not modifiable.

After each sample skip The number of bits to skip after each sample.

Usually, samples are adjacent to each other in the file. But sometimes there are unused bits or bytes between them, that can be speficified with this option. Note for predefined types the value must be a multiple of 8 (i.e., only whole bytes can be skipped).

After each row skip The number of bits to skip after each sample in addition to bits skipped after each sample.

Usually, rows are adjacent to each other in the file. But sometimes there are unused bits or bytes between them, that can be speficified with this option. Note for predefined types the value must be a multiple of 8 (i.e., only whole bytes can be skipped).

Reverse bits in bytes Whether the order of bits in each byte should be reversed.

Reverse bits in samples Whether the order bits in each sample should be reversed for user defined samples.

Samples are signed Whether samples are to be interpreted as signed numbers (as opposed to unsigned). For predefined formats, their signedness is displayed, but it is not modifiable.

Presets

Import settings can be saved as presets that allow to easily import the same file – or the same file type – later.

Button Store saves current import settings under the name in Preset name field. Rename renames currently selected preset to specified name, Delete deletes selected preset, and Load replaced current import setting with selected preset.

3.14 Specific Data Import

Import of several other types of data is not automatic and it requires human intervention.

Graphics Formats

Importing data from image formats such as PNG, TIFF, JPEG or BMP is similar to import from raw/unknown file formats, only simplier.

It is simplier because the file structure is known and the file format is automatically detected. Hence the file type does need to be selected explicitly. However, the data interpretation is still unknown and must be specified manually. The Pixmap import dialog therefore resembles the Information tab of raw data import, requiring you to set the physical dimensions and value scale.

Note the physical dimensions suggested there are not obtained from the file, they are simply the last values used. Some SPM data format are based on an image format (typically, TIFF is used as the base) and contain the information about physical scales and units, albeit stored in a manufacturer-specific way. In this case a separate import module can be written for this particular format to load the files automatically with correctly scaled values.

Graph Curves

Simple two-column text files containing curve data can be imported as graph curves. In some cases, these files are recognized automatically. They can also be explicitly selected as ASCII graph curve files in the file open dialog, causing the import module to try harder to load the file as a graph data.

The import dialog shows a preview of the graph and permits to set the units and labels.

XYZ Data

Three-column text files containing XYZ data are imported by selecting the XYZ data files file type. Again, they can be recognized automatically but requesting this format explicitly makes the module to try harder to load the file as XYZ data.

Since Gwyddion only works with data in a regular grid irregular XYZ data must be interpolated to a regular grid upon import. In fact, the XYZ data import module serves two different purposes:

- loading of data in a regular grid that were just saved as XYZ data – if the data is found to be in a regular grind only a very simple import dialog is presented where you can set the units because the import is straightforward;
- regularization and interpolation of irregular XYZ data – this case is much less straightforward and the rest of this section will discuss the options you have and some of the pitfalls.

The import dialog permits to set the basic parameters as the regularized data resolution and range and lateral and value units. However, the most important option is Interpolation type:

Round This interpolation is analogous to the Round interpolation for regular grids. The interpolated value in a point in the plane equals to the value of the nearest point in the XYZ point set. This means the Voronoi triangulation is performed and each Voronoi cell is ‘filled’ with the value of the nearest point.

Linear This interpolation is analogous to the Linear interpolation for regular grids. The interpolated value in a point is calculated from the three vertices of the Delaunay triangulation triangle containing the point. As the tree vertices uniquely determine a plane in the space, the value in the point is defined by this plane.

Field The value in a point is the weighted average of all the XYZ point set where the weight is proportional to the inverse fourth power of the mutual distance. Since all XYZ data points are considered for the calculation of each interpolated point this method can be very slow.

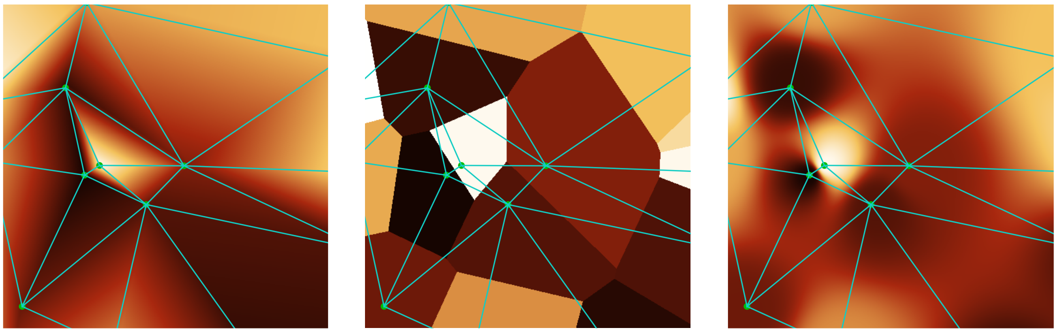
The former two interpolation types are based on Delaunay/Voronoi triangulation which is not well-defined for point sets where more than two points line on a line or more than three lie on a circle. If this happens the triangulation fails and the import module displays an error message.

The values outside the convex hull of the XYZ point set in the plane are influenced by Exterior type:

Border The point set is not amended in any way and the values on the convex hull simply extend to the infinity.

Mirror The point set is amended by points ‘reflected’ about the bounding box sides.

Periodic The point set is amended by periodically repeated points from around the opposite side of bounding box.



Delaunay triangulation displayed on linear (left), round (centre) and field (right) interpolation of a irregular set of points.

3.15 Plug-ins

Plug-ins are external programs that can be executed by Gwyddion to either perform some operation on the data or to read or write data in a third-party file format. In general, plug-ins are programe that can register itself within Gwyddion (for example printing something on standard output) to enable Gwyddion to create plugin menu choice and can be used for data processing (or IO operation).

Generally it is preferable to extend Gwyddion functionality by modules, because modules are dynamic libraries linked directly to Gwyddion at run-time allowing much more versatile interaction with the application, and they are also faster (for the same reason). For example, plug-ins generally cannot make use of existing Gwyddion data processing functions and cannot modify data in-place, a new window is always created for the result. Programming of modules is also no harder than programming of plug-ins, maybe it is even easier (assuming you know C).

Warning The plug-in mechanism is deprecated. It will remain supported in Gwyddion 2.x, however, it will not be exteneded or improved. The recommended method to extend Gwyddion by routines in another language is to use language bindings, at this moment a Python interface is available. The recommended method to run third-party programs is to write a small specialized C module that knows how to communicate with these programs.

Chapter 4

Data Processing and Analysis

The number and breadth of data manipulation and analysis functions is one of the Gwyddion main strenghts. The description of their principles and applications is the purpose of this chapter, with focus on the explanation of how they work and what they calculate or perform. Elements of their user interface are also occasionaly described where it seems useful, nevertheless, it is assumed the reader is familiar with the basic organization of data and controls in Gwydion, as described in the previous chapter.

4.1 Basic Operations

Value-reading and basic geometrical operations represent the core of any data processing program. Gwyddion offers a wide set of functions for data scaling, rotation, resampling or profile extraction. This section describes these simple but essential functions.

Basic 2D Data Operations

Within basic modules it is possible to perform the following operations with 2D data field:

- Resample the data to chosen dimensions or scale using selected interpolation method by Data Process → Basic Operations → Scale
- Crop the data using the Crop tool either in place or putting the result to a new channel (with option Create new channel). With Keep lateral offsets option enabled, the top left corner coordinates of the resulting image correspond to the top left corner of the selection, otherwise the top left corner coordinates are set to $(0,0)$.
- Rotate data by 90 degrees or by user-specified amount using some of the rotate functions: Data Process → Basic Operations → Rotate Clockwise, Rotate Anticlockwise or Rotate.
- Flip the data horizontally (i.e. about the vertical axis) and vertically (i.e. about the horizontal axis) with Data Process → Basic Operations → Flip Horizontally and Flip Vertically, respectively.
- Flip the data about the centre (i.e. about both axes) with Data Process → Basic Operations → Flip Both.
- Invert the data values using the Invert Value function: Data Process → Basic Operations → Invert Value. The values are inverted about the mean value which keeps the mean value unchanged.
- Upsample the data to make pixels square with Data Process → Basic Operations → Square Samples. Most scans have pixels with 1:1 aspect ratio, therefore this function has no effect on them.

Moreover, the recalibration module can be used for changing the physical dimensions, data value calibration and even to change the units of values and lateral dimensions: Data Process → Basic operations → Calibrate.

Reading Values

The simpliest value reading method is to place the mouse cursor over the point you want to read value of. The coordinates and/or value is then displayed in the data window or graph window status bar.

Read Value Tool

Tool Read Value offers more value reading posibilities: It displays coordinates and values of the last point of the data window the mouse button was pressed. It can avergae the value from a circular neighbourhood around the selected point, this is controlled by option Averaging radius. When the radius is 1, the value of a single pixel is displayed (as the simplest method does). Button Set Zero shifts the surface to make the current z the new zero level.

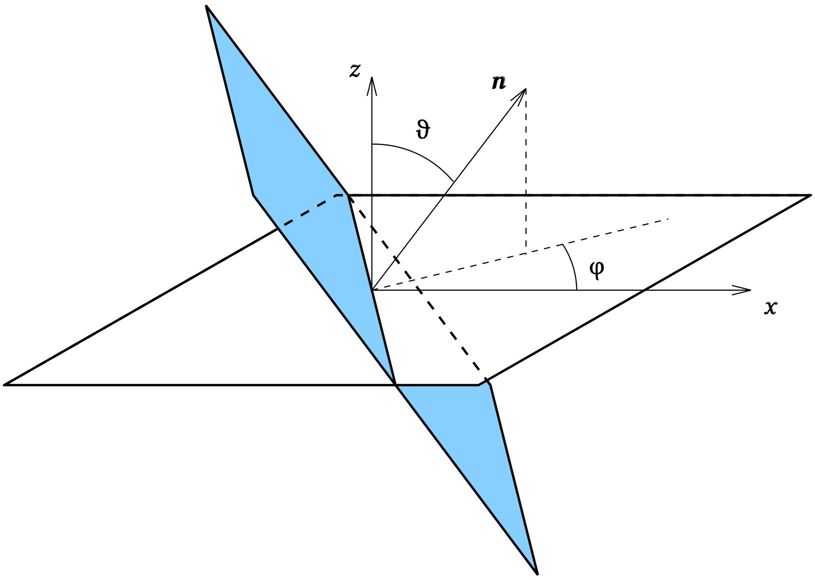
Read Value can also display the inclination of the local facet. Averaging radius again determines the radius of the area to use for the plane fit.

Inclinations

In all Gwyddion tools, facet and plane inclinations are displayed as the spherical angles (ϑ, φ) of the plane normal vector.

Angle ϑ is the angle between the upward direction and the normal, this means $\vartheta = 0$ for horizontal facets and it increases with the slope. It is always positive.

Angle φ is the counter-clockwise measured angle between axis x and the projection of the normal to the xy plane, as displayed on the following figure. For facets it means φ corresponds to the downward direction of the facet.

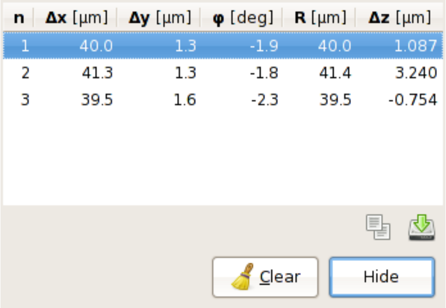


Surface facet (displayed blue) orientation measured as the counterclockwise angle from x-axis to the projection of facet normal vector **n** *to xy plane.*

Distance Tool

Distances and differences can be measured with the Distance tool. It displays the horizontal (Δx), vertical (Δy) and total planar (R) distances; the azimuth φ (measured identically to inclination φ) and the endpoint value difference (Δz) for a set of lines selected on the data.

The distances can be copied to the clipboard or saved to a text file using the buttons below the list.



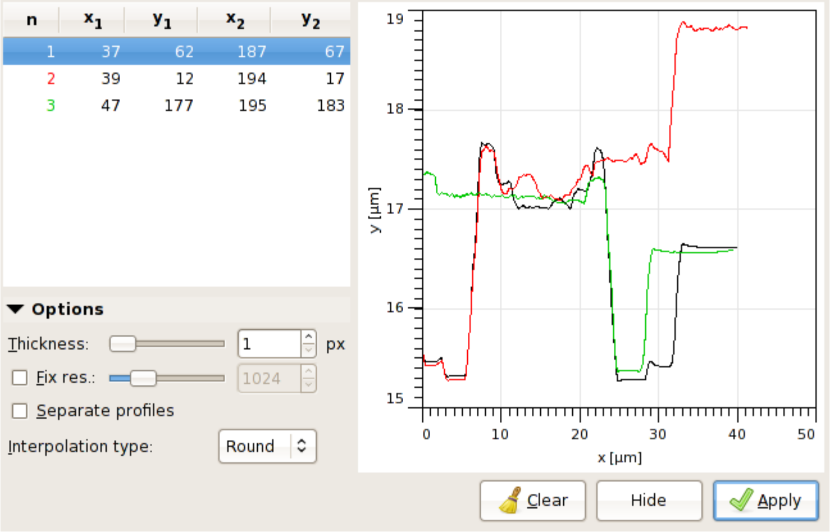
n	Δx [µm]	Δy [µm]	φ [deg]	R [µm]	Δz [µm]
1	40.0	1.3	-1.9	40.0	1.087
2	41.3	1.3	-1.8	41.4	3.240
3	39.5	1.6	-2.3	39.5	-0.754

Distance tool with three selected lines.

Profile Extraction

The profile extraction tool can be accessed from the toolbox. You can use mouse to draw several profiles in the image and they can be further moved and adjusted. The dialog includes a live profile graph preview. Profiles can be of different ‘thickness’ which means that more neighbour data perpendicular to profile direction are used for evaluation of one profile point for thicker profiles. This can be very useful for noise suppression while measuring regular objects.

After profiles are chosen, they can be extracted to graphs (separate or grouped in one Graph window) that can be further analysed using Graph functions.



n	x_1	y_1	x_2	y_2
1	37	62	187	67
2	39	12	194	17
3	47	177	195	183

Options

Thickness: 1 px

☐ Fix res.: 1024

☐ Separate profiles

Interpolation type: Round

Profile tool with three extracted profiles and expanded options.

The profile curve is constructed from data sampled at regular intervals along the selected line. Values in points that do not lie exactly at pixel centres (which normally occurs for oblique lines) are interpolated using the chosen interpolation mode. Unless an explicit number of samples to take is set using the Fix res. option, the number of samples corresponds to the line length in pixels. This means that for purely horizontal or purely vertical lines no interpolation occurs.

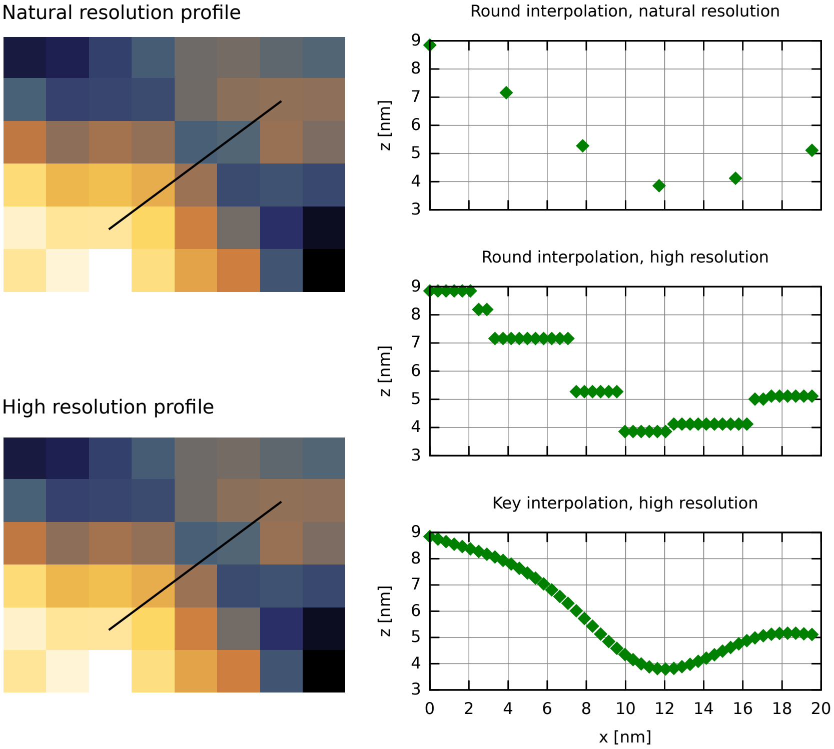


Illustration of data sampling in profile extraction for oblique lines. The figures on the left show the points along the line where the values are read for natural and very high resolution. The graphs on the right show the extracted values. Comparison of the natural and high resolution profiles taken with Round interpolation reveals that indeed natural-resolution curve points form a subset of the high-resolution points. The influence of the interpolation method on values taken in non-grid positions is demonstrated by the lower two graphs, comparing Round and Key interpolation at high resolution.

4.2 Interpolation

Most geometrical transformations, such as rotation, scaling or drift compensation utilize or depend on data interpolation. Also some other operations, e.g. profile extraction, can work with values between individual pixels and hence involve interpolation.

Since SPM data are relatively coarsely sampled compared to measured details (full images are typically only a few hundred pixels in width and height), the interpolation method used can become critical for proper quantitative analysis of data properties. Gwyddion implements several interpolation methods [1] and the user can choose which method to use for most of the modules using interpolation.

Here, we describe the principles and properties of one-dimensional interpolation methods. All implemented two-dimensional interpolation methods are separable and thus simply composed of the corresponding one-dimensional methods. The following interpolation method are currently available:

Round Round interpolation (also called nearest neighbourhood interpolation) is the simplest method – it just takes round value of the expected position and finds therefore the closest data value at integer position. Its polynomial degree is 0, regularity C^{-1} and order 1.

Linear Linear interpolation is a linear interpolation between the two closest data values. The value z at point of relative position x is obtained as

$$z = (1-x)z_0 + xz_1$$

where z_0 and z_1 are values at the preceding and following points, respectively. Its polynomial degree is 1, regularity C^0 and order 2. It is identical to the second-order B-spline.

Key Key interpolation (more precisely Key's interpolation with $a = -1/2$ which has the highest interpolation order) makes use also of values in the before-preceding and after-following points z_{-1} and z_2, respectively. In other words it has support of length 4, The value is then obtained as

$$z = w_{-1}z_{-1} + w_0 z_0 + w_1 z_1 + w_2 z_2$$

where

$$\begin{aligned} w_{-1} &= \big(-\tfrac{1}{2} + (1 - \tfrac{x}{2})x\big)x \\ w_0 &= 1 + (-\tfrac{5}{2} + \tfrac{3}{2}x)x^2 \\ w_1 &= \big(\tfrac{1}{2} + (2 - \tfrac{3}{2}x)x\big)x \\ w_2 &= (-\tfrac{1}{2} + \tfrac{x}{2})x^2 \end{aligned}$$

are the interpolation weights. Key's interpolation degree is 3, regularity C^1 and order 3.

Schaum Schaum interpolation (more precisely fourth-order Schaum) has also support of length 4. The interpolation weights are

$$\begin{aligned} w_{-1} &= -\tfrac{1}{6}x(x-1)(x-2) \\ w_0 &= \tfrac{1}{2}(x^2-1)(x-2) \\ w_1 &= -\tfrac{1}{2}x(x+1)(x-2) \\ w_2 &= \tfrac{1}{6}x(x^2-1) \end{aligned}$$

Its polynomial degree is 3, regularity C^0 and order 4.

NNA Nearest neighbour approximation is again calculated from the closest four data values but unlike all others it is not piecewise-polynomial. The interpolation weights are

$$w_k = \frac{\dfrac{1}{r_k^4}}{\displaystyle\sum_{j=-1}^{2} \frac{1}{r_j^4}} ,$$

for $k = -1, 0, 1, 2$, where $r_{-1} = 1 + x$, $r_0 = x$, $r_1 = 1 - x$, $r_2 = 2 - x$. Its order is 1.

B-spline B-spline was misimplemented up to version 2.1 (inclusive) and it blurred data. It should be avoided in these old versions. The weights are

$$\begin{aligned} w_{-1} &= \tfrac{1}{6}(1-x)^3 \\ w_0 &= \tfrac{2}{3} - x^2(1 - \tfrac{x}{2}) \\ w_1 &= \tfrac{1}{6} + \tfrac{1}{2}x\big(1 + x(1-x)\big) \\ w_2 &= \tfrac{1}{6}x^3 \end{aligned}$$

However, they are not used with directly function values as above, but with interpolation coefficients calculated from function values [1]. Its polynomial degree is 3, regularity C^2 and order 4.

O-MOMS O-MOMS was misimplemented up to version 2.1 (inclusive) and it blurred data. It should be avoided in these old versions. The weights are

$$\begin{aligned} w_{-1} &= \tfrac{4}{21} + \bigl(-\tfrac{11}{21} + (\tfrac{1}{2} - \tfrac{x}{6})x\bigr)x \\ w_0 &= \tfrac{13}{21} + \bigl(\tfrac{1}{14} + (-1 + \tfrac{x}{2})x\bigr)x \\ w_1 &= \tfrac{4}{21} + \bigl(\tfrac{3}{7} + (\tfrac{1}{2} - \tfrac{x}{2})x\bigr)x \\ w_2 &= (\tfrac{1}{42} + \tfrac{1}{6}x^2)x \end{aligned}$$

However, they are not used directly with function values as above, but with interpolation coefficients calculated from function values [1]. Its polynomial degree is 3, regularity C^0 and order 4.

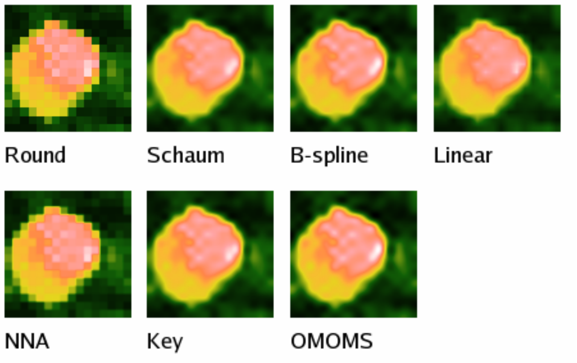


Illustration of the available interpolation types (the original pixels are obvious on the result of Round interpolation). All images have identical false color map ranges.

References

[1] P. Thévenaz, T. Blu, M. Unser: Interpolation revisited. IEEE Transactions on medical imaging, Volume 10, Number 7, July 2000, 739

4.3 Data Leveling and Background Subtraction

Leveling

The data obtained from SPM microscopes are very often not leveled at all; the microscope directly outputs raw data values computed from piezoscanner voltage, strain gauge, interferometer or other detection system values. This way of exporting data enables the user to choose his/her own method of leveling data.

The choice of leveling method should be based on your SPM system configuration. Basically, for systems with independent scanner(s) for each axis, plane leveling should be sufficient. For systems with scanner(s) moving in all three axes (tube scanners) 2nd order polynomial leveling should be used.

Of course, you can use higher order leveling for any data, however, this can supress real features on the surface (namely waviness of the surface) and therefore alter the statistical functions and quantities evaluated from the surface.

Fix Zero and Zero Mean Value

Data Process → Level → Fix Zero

Data Process → Level → Zero Mean Value

The simplest modules that are connected with data leveling are Fix Zero and Zero Mean Value that simply set the average height of the data to put the minimum to zero (Fix Zero) or mean value to zero (Zero Mean Value).

Plane Level

Data Process → Level → Plane Level

Plane leveling is usually one of the first functions applied to raw SPM data. The plane is computed from all the image points and is subtracted from the data.

If a mask is present plane leveling offers to use the data under mask for the plane fitting, exclude the data under mask or ignore the maks and use the entire data.

Tip You can quickly apply plane leveling by simply right-clicking on the image window and selecting Level.

Three Point Leveling Tool

The Three Point Leveling tool can be used for leveling very complicated surface structures. The user can simply mark three points in the image that should be at the same level, and then click Apply. The plane is computed from these three points and is subtracted from the data.

Facet Level

Data Process → Level → Facet Level

Facet Level levels data by subtracting a plane similarly to the standard Plane Level function. However, the plane is determined differently: it makes facets of the surface as horizontal as possible. Thus for surfaces with flat horizontal areas it leads to much better results than the standard Plane Level especially if large objects are present.

On the other hand, it is not suitable for some types of surface. These includes random surfaces, data with considerable fine noise and non-topographic images as the method does not work well if the typical lateral dimensions and 'heights' differ by many orders.

Similarly to Plane Level, Facet Level can include or exclude the data under mask. This choice is offered only if a mask is present.

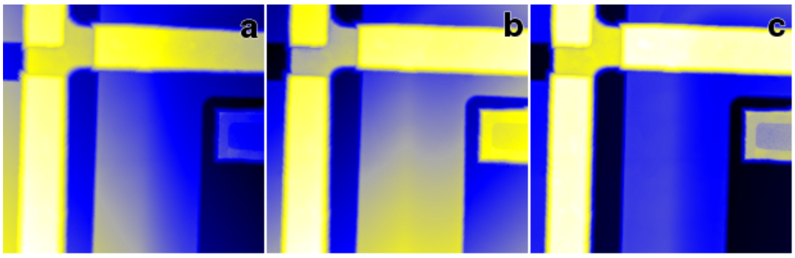
Finding the orientation of the facets is an iterative process that works as follows. First, the variation of local normals is determined:

$$\beta^2 = \frac{1}{N}\sum_{i=1}^{N} \mathbf{n}_i^2$$

where $\mathbf{n}_i$ is the vector of local facet normal (see inclination coordinates) in the i-th pixel. Then the prevalent normal is estimated as

$$\mathbf{n} = \frac{\sum_{i=1}^{N} \mathbf{n}_i \exp\left(-c\frac{\mathbf{n}_i^2}{\beta^2}\right)}{\sum_{i=1}^{N} \exp\left(-c\frac{\mathbf{n}_i^2}{\beta^2}\right)}$$

where $c = 1/20$ is a constant. Consequently, the plane corresponding to the prevalent normal $\mathbf{n}$ is subtracted and these three steps are repeated until the process converges. The gaussian weighting factors serve to pick a single set of similar local facet normals and converge to their mean direction. Without these factors, the procedure would obviously converge in one step to the overall mean normal – and hence would be completely equivalent to plain plane leveling.



Facet Level example: (a) uncorrected, sloping data; (b) data leveled by standard plane fitting (Plane Level); (c) data leveled by Facet Level.

Level Rotate

Data Process → Level → Level Rotate

Level Rotate behaves similarly to Plane Level, however it does not simply subtract the fitted plane from the data. Instead, this module takes the fitted plane parameters and rotates the image data by a calculated amount to make it lie in a plane. So unlike Plane Level, this module should therefore preserve angle data in the image.

Background Subtraction

Gwyddion has several special modules for background subtraction. All allow you to extract the subtracted background to a separate data window.

Tip For finer control, you can use any of Gwyddion's filtering tools on an image, and then use the Data Arithmetic module to subtract the results from your original image.

Polynomial Background

Data Process → Level → Polynomial Background

Fits data by a polynomial of the given order and subtracts this polynomial. In the Independent degree mode the horizontal and vertical polynomial orders can be generally set separately, i.e. the fitted polynomial is

$$\sum_{j=0}^{m}\sum_{k=0}^{n} a_{j,k}x^j y^k$$

where m and n are the selected horizontal and vertical polynomial degrees, respectively. In the Limited total degree mode the fitted polynomial is

$$\sum_{j+k\le n} a_{j,k}x^j y^k$$

where n is the selected total polynomial degree.

Similarly to Plane Level, polynomial background subtraction can include or exclude the data under mask. This choice is offered only if a mask is present.

Revolve Arc

Data Process → Level → Revolve Arc

Revolves virtual 'arc' of given radius horizontally or vertically over (or under) the data. The envelope of this arc is treated as a background, resulting in removal of features larger than the arc radius (approximately).

Median Level

Data Process → Level → Median Level

Filters data with a median filter using a large kernel and treats the result as background. Only features smaller than approximately the kernel size will be kept.

Note This method can be very slow.

Fit Sphere

Data Process → Level → Fit sphere

Fits part of sphere surface on the data. Sphere orientation (i.e. centre position) and initial fit values can be preset before fitting. Marquardt-Levenberg fitting routine is used to calculate the result.

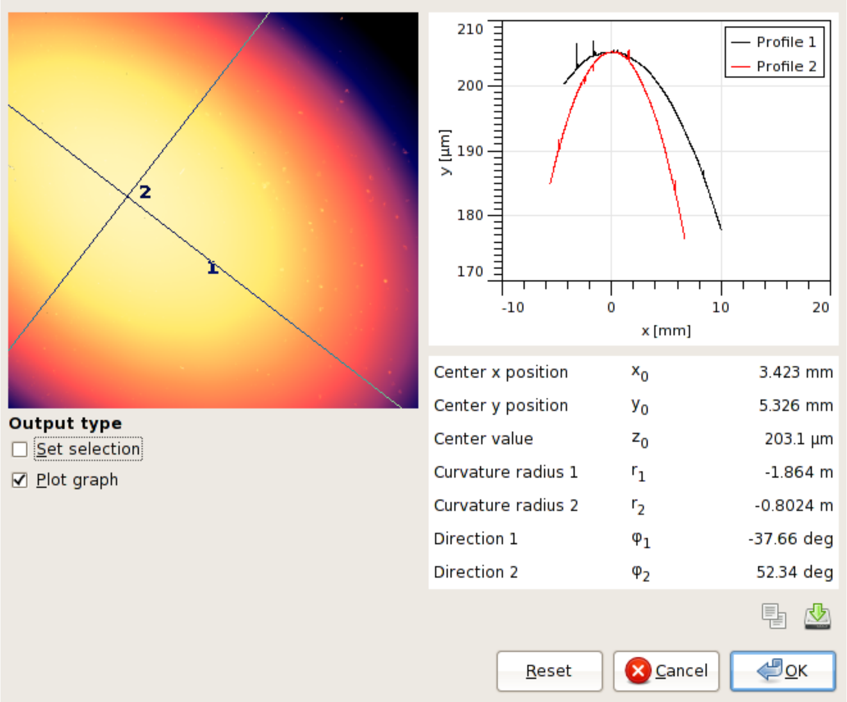
Curvature

Data Process → Level → Curvature

The global surface curvature parameters are calculated by fitting a quadratic polynomial and finding its main axes. Positive signs of the curvature radii correspond to a concave (cup-like) surface, whereas negative signs to convex (cap-like) surface, mixed signs mean a saddle-like surface.

Beside the parameter table, it is possible to set the line selection on the data to the fitted quadratic surface axes and/or directly read profiles along them. The zero of the abscissa is placed to the intersection of the axes.

Similarly to the background subtraction functions, if a mask is present on the data the module offers to include or exclude the data under mask.



Output type

□ Set selection

☑ Plot graph

Center x position	x_0	3.423 mm
Center y position	y_0	5.326 mm
Center value	z_0	203.1 µm
Curvature radius 1	r_1	-1.864 m
Curvature radius 2	r_2	-0.8024 m
Direction 1	φ_1	-37.66 deg
Direction 2	φ_2	52.34 deg

Curvature dialog screenshot showing the strong deflection of a glass plate with a thin film with compressive internal stress.

4.4 Filters

Basic Filters Tool

The Basic Filters tool lets you apply several simple filters to your image. This can be very useful for data denoising; however, the real measured data will get altered in the process, so great care should be taken not to destroy important features of the image.

- Mean filter – takes the mean value of neighborhood of the filtered value as the value.
- Median filter – takes the median value of neighborhood of the filtered value as the value.
- Conservative denoise filter – checks whether the value is not extreme within the neighborhood. If yes, filter substitutes the value by of the next highest (lowest) value.
- Kuwahara filter – is an edge-preserving smoothing filter.
- Minimum filter – also known as erode filter, replaces values by minimum found in neighborhood.
- Maximum filter – also known as dilate filter, replaces values by maximum found in neighborhood.
- Dechecker filter – a smoothing filter specially designed to remove checker pattern from the image while preserving other details. It is a convolution filter with kernel

$$w_{\text{dechecker}} = \begin{pmatrix} 0 & 1/144 & -1/72 & 1/144 & 0 \\ 1/144 & -1/18 & 1/9 & -1/18 & 1/144 \\ -1/72 & 1/9 & 7/9 & 1/9 & -1/72 \\ 1/144 & -1/18 & 1/9 & -1/18 & 1/144 \\ 0 & 1/144 & -1/72 & 1/144 & 0 \end{pmatrix}$$

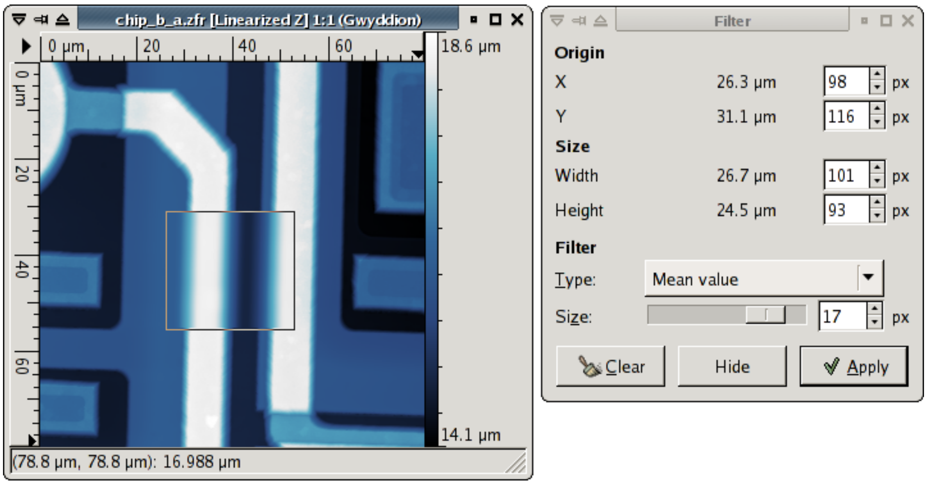
- Gaussian filter – a smoothing filter, the size parameter determines the FWHM (full width at half maximum) of the Gaussian. The relation between FWHM and σ is

$$\mathrm{FWHM} = 2\sqrt{2\ln 2}\,\sigma \approx 2.35482\sigma$$

Tip By default, these filters will be applied to the entire image. However, you can apply a filter to a specific region within your image by selecting it with the mouse. This can be useful for correcting badly measured areas within a good image. To apply a filter to the entire image again, just click once anywhere within the image window.

Moreover, there are more denoising functions in Gwyddion, for example DWT denoising and FFT filtering. For details see section Extended Data Edit.

If you need to only suppress some values in the SPM data that are obviously wrong, you can also try the Mask of Outliers module and the Remove Data Under Mask module. For details see section Data Edit.



(78.8 µm, 78.8 µm): 16.988 µm

Filter

Origin

X 26.3 µm 98 px

Y 31.1 µm 116 px

Size

Width 26.7 µm 101 px

Height 24.5 µm 93 px

Filter

Type: Mean value

Size: 17 px

Screenshot of filter tool with median filter applied to a rectangular selection

Convolution

Data Process → Integral Transforms → Convolution Filter

Convolutions with arbitrary kernels up to 9 × 9 can be performed with the Convolution Filter module.

The Divisor entry represents a common factor all the coefficients are divided before applying the filter. This allows to use denormalized coefficients that are often nicer numbers. The normalization can be also calculated automatically when automatic is checked. When the sum of the coefficients is nonzero, it makes the filter sum-preserving, i.e. it the factor normalizes the sum of coefficients to unity. When the sum of the coefficients is zero, the automatic factor is simply let equal to 1.

Since many filters used in practice exhibit various types of symmetry, the coefficients can be automatically completed according to the selected symmetry type (odd, even). Note the completion is performed on pressing **Enter** in the coefficient entry.

In a fresh installation only a sample Identity filter is present (which is not particularly useful as it does nothing). This filter cannot be modified, to create a new filter use the New button on the Presets page.

4.5 Presentations

Presentation modules do not modify the data, instead, they output their results into a separate layer displayed on top of the original data. The other data processing modules and tools will still operate on the underlying data. To remove a presentation, right-click on the data window, and select Remove Presentation.

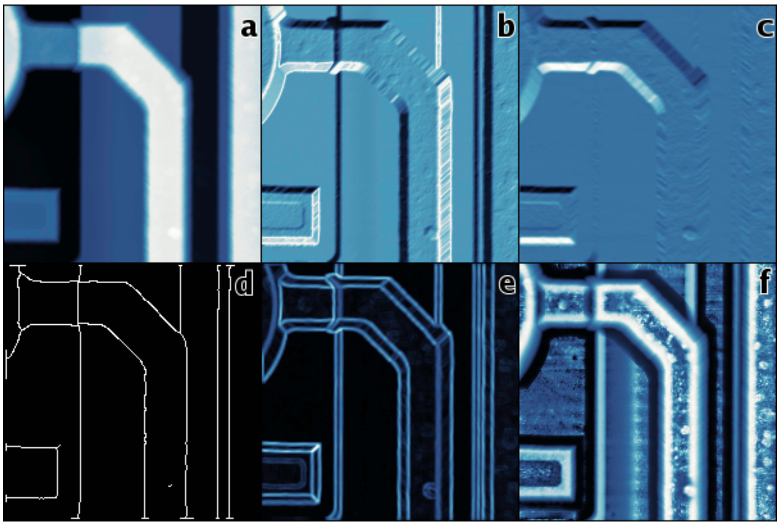
Basic Operations

The Data Process → Presentation menu contains a few basic presentation operations:

Attach Presentation Attaches another data field as a presentation to the current data. Note that this useful option can be particularly confusing while evaluating anything from the data as all the computed values are evaluated from the underlying data (not from the presentation, even if it looks like the data).

Remove Presentation Removes presentation from the current data window. This is an alternative to the right-click data window menu.

Extract Presentation Extracts presentation from the current data window to a a new channel in the same file. In this way one can get presentation data for further processing. Note, however, the extracted data have no absolute scale information as presentation often help to visualize certain features, but the produced values are hard or impossible to assign any physical meaning to. Hence the value range of the new channel is always $[0,1]$.



Presentation examples: (a) original data, (b) shading, (c) vertical Prewitt gradient, (d) Canny edge detection, (e) local nonlinearity edge detection, (f) local contrast improvement.

Shading Presentation

Data Process → Presentation → Shading

Simple and very useful way of seeing data as illuminated from some direction. The direction can be set by user. It is also possible to mix the shaded and original images for presentational purposes. Of course, the resulting image is meaningless from the physical point of view.

Gradient Detection Presentations

Data Process → Presentation → Gradient

Sobel horizontal and vertical gradient filter and Prewitt horizontal and vertical gradient filter create similar images as shading, however, they output data as a result of convolution of data with relatively standardized kernel. Thus, they can be used for further presentation processing for example. The kernels for horizontal filters are listed below, vertical kernels differ only by reflection about main diagonal.

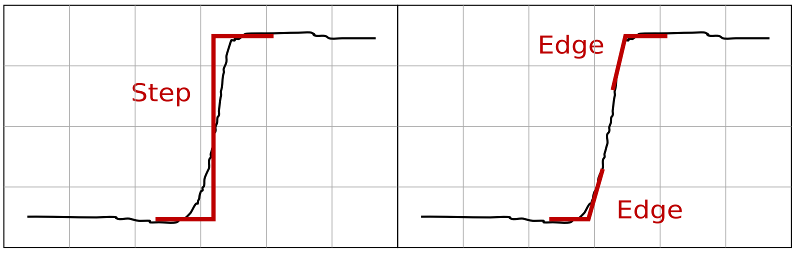
$$w_{\mathrm{prewitt}} = \begin{pmatrix} 1/3 & 0 & -1/3 \\ 1/3 & 0 & -1/3 \\ 1/3 & 0 & -1/3 \end{pmatrix}, \quad w_{\mathrm{sobel}} = \begin{pmatrix} 1/4 & 0 & -1/4 \\ 1/2 & 0 & -1/2 \\ 1/4 & 0 & -1/4 \end{pmatrix}$$

Edge Detection Presentations

Data Process → Presentation → Edge Detection

One is often interested in the visualization of the discontinuities present in the image, particularly in discontinuities in the value (zeroth order) and discontinuities in the derivative (first order). Although the methods of location of both are commonly referred to as ‘edge detection’ methods, these are actually quite different, therefore we will refer to the former as to step detection and to the latter as to edge detection. Methods for the detection of more specific features, e.g. corners, are commonly used too, these methods usually are of order zero.

The order of a discontinuity detection method can be easily seen on its output as edge detection methods produce typical double edge lines at value discontinuities as is illustrated in the following figure. While the positions of the upper and lower edge in an ideal step coincide, real-world data tend to actually contain two distinct edges as is illustrated in the picture. In addition, finding two edges on a value step, even an ideally sharp one, is often an inherent feature of edge detection methods.



Step versus edge in one dimension.

The following step and edge detection functions are available in Gwyddion (the later ones are somewhat experimental, on they other hand they usually give better results than the well-known algorithms):

Canny Canny edge detector is a well-known step detector can be used to extract the image of sharp value discontinuities in the data as thin single-pixel lines.

Laplacian of Gaussians Laplacian presents a simple convolution with the following kernel (that is the limit of discrete Laplacian of Gaussians filter for $\sigma \to 0$):

$$w_{\text{laplace}} = \begin{pmatrix} 0 & 1/4 & 0 \\ 1/4 & -1 & 1/4 \\ 0 & 1/4 & 0 \end{pmatrix}$$

Zero Crossing Zero crossing step detection marks lines where the result of Laplacian of Gaussians filter changes sign, i.e. crosses zero. The FWHM (full width half maximum) of the Gaussians determines the level of details covered. Threshold enables to exclude sign changes with too small absolute value of the neighbour pixels, filtering out fine noise. Note, however, that for non-zero threshold the edge lines may become discontinuous.

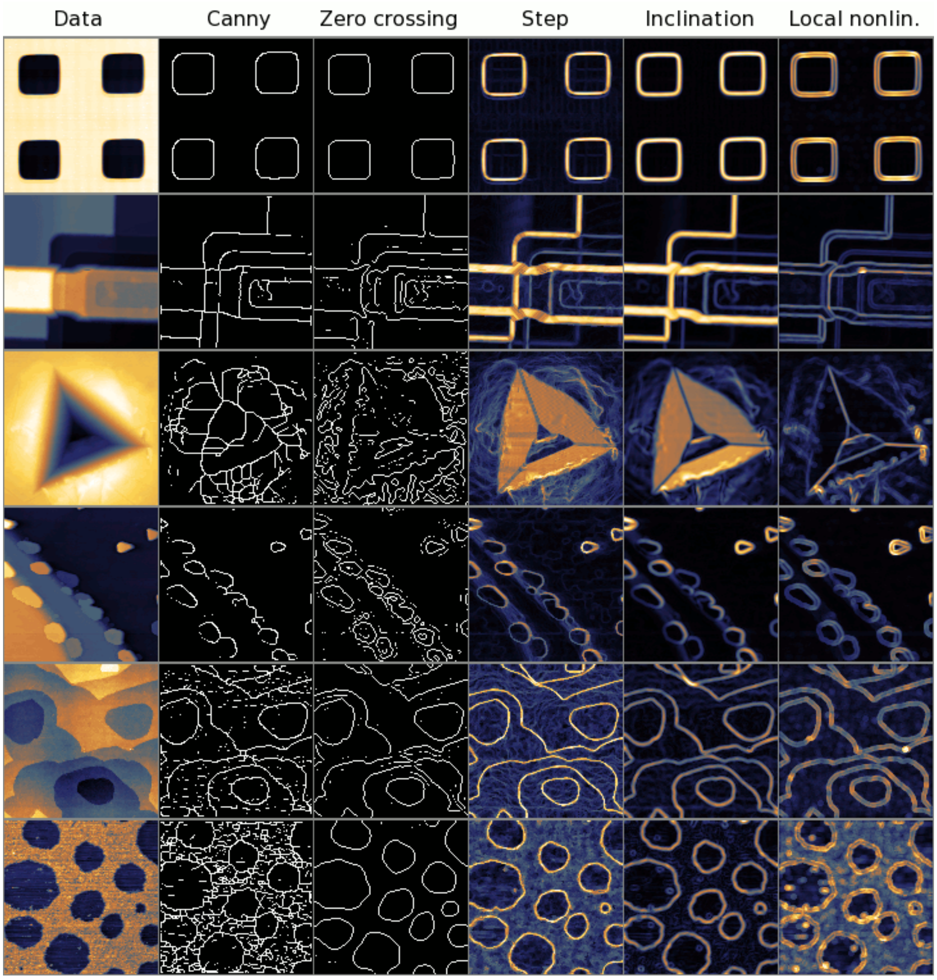
Step A step detection algorithm providing a good resolution, i.e. sharp discontinuity lines, and a good dynamic range while being relatively insensitive to noise. The principle is quite simple: it visualizes the square root of the difference between the 2/3 and 1/3 quantiles of the data values in a circular neighbourhood of radius 2.5 pixels centered around the sample.

RMS This step detector visualizes areas with high local value variation. The root mean square of deviations from the mean value of a circular neighbourhood of radius 2.5 pixels centered around each sample is calculated and displayed.

RMS Edge This function essentially postprocesses RMS output with a filter similar to Laplacian to emphasize boundaries of areas with high local value variation. Despite the name it is still a step detector.

Local Non-Linearity An edge detector which visualizes areas that are locally very non-planar. It fits a plane through a circular neighbourhood of radius 2.5 pixels centered around each sample and then calculates residual sum of squares of this fit reduced to plane slope, i.e. divided by $1 + b_x^2 + b_y^2$ where b_x and b_y are the plane coefficients in x and y directions, respectively. The square root is then displayed.

Inclination Visualizes the angle ϑ of local plane inclination. Technically this function belongs among step detectors, however, the accentuation of steps in its output is not very strong and it is more intended for easy visual comparison of different slopes present in the image.



Comparison of step and edge detection methods on several interesting, or typical example data. Canny and Zero crossing are step detectors that produce one pixel wide edge lines, Step and Inclination are step detectors with continous output, Local nonlinearity is an edge detector – the edge detection can be easily observed on the second and third row. Note zero crossing is tunable, it parameters were chosen to produce reasonable output in each example.

Local Contrast

Data Process → Presentation → Local contrast

A method to visualize features in areas with low and high value variation at the same time. This is achieved by calculation of local value range, or variation, around each data sample and stretching it to equalize this variation over all data.

Logscale

Data Process → Presentation → Logscale

Logarithmic scale is used for false colors data presentation.

4.6 Data Edit and Correction

There are several modules that enable direct or indirect editing of the SPM data. In principal, most of the data processing modules change the data in one way or another. However, in this section we would like to describe the modules and tools that are specifically designed to correct local defects in an image. The functions below remove 'bad' data from an image, and then fill it in using an interpolation algorithm.

Remove Spots Tool

The Remove Spots tool can be used for removing very small parts of the image that are considered a scanning error, dust particle or anything else that should not be present in the data. Note that doing so can dramatically alter the resulting statistical parameters of the surface, so be sure not to remove things that are really present on the surface.

While using this tool you can pick up position of the spot to magnify its neighbourhood in the tool window. Then, in the tool window, select a rectangle around the area that should be removed. You can then select one of several interpolation methods for creating data in place of the former 'spot':

- Hyperbolic flatten - uses information from selected area boundaries to interpolate the information inside area.
- Pseudo-Laplace and Laplace solver - solves Laplace equation to calculate data inside area; the boundary is treated as virtual source.
- Fractal correction - uses whole image to determine fractal dimension. Then tries to create randomly rough data that have the same fractal dimension and put them into the area.

Clicking Apply will execute the selected algorithm.

> **Note** Spot removal will only work for regions of size 64 × 64 pixels or smaller. To remove larger regions, create a mask using the Mask Editor tool, then use Data Process → Correct Data → Remove Data Under Mask.

Remove Grains Tool

This simple tool removes manually selected connected parts of mask or interpolates the data under them, or possibly both. The part of mask to remove is selected by clicking on it with left mouse button.

Remove Scars

Data Process → Correct Data → Remove Scars

Scars (or stripes, strokes) are parts of the image that are corrupted by a very common scanning error: local fault of the closed loop. Line defects are usually parallel to the fast scanning axis in the image. This function will automatically find and remove these scars, using neighbourhood lines to 'fill-in' the gaps. The method is run with the last settings used in Mark Scars.

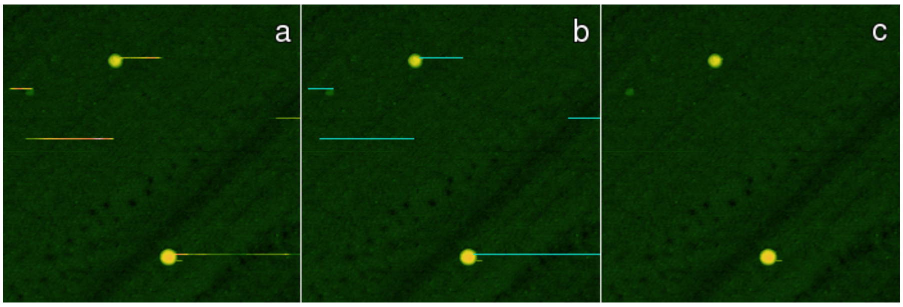
Mark Scars

Data Process → Correct Data → Mark Scars

Similarly, the `Mark Scars` module can create a mask of the points treated as scars. Unlike Remove Scars which directly interpolates the located defects, this module lets you interactively set several parameters which can fine-tune the scar selection process:

- Maximum width – only scars that are as thin or thinner than this value (in pixels) will be marked.
- Minimum length – only scars that are as long or longer than this value (in pixels) will be marked.
- Hard threshold – the minimum difference of the value from the neighbouring upper and lower lines to be considered a defect. The units are relative to image RMS.
- Soft threshold – values differing at least this much do not form defects themselves, but they are attached to defects obtained from the hard threshold if they touch one.
- Positive, Negative, Both – the type of defects to remove. Positive means defects with outlying values above the normal values (peaks), negative means defects with outlying values below the normal values (holes).

After clicking Ok the new scar mask will be applied to the image. Other modules or tools can then be run to edit this data.



Scars marking and removal example: (a) original data with defects, (b) data with marked deffects, (c) corrected data.

Remove Data Under Mask

Data Process → Correct Data → Remove Data Under Mask

This function substitutes the data under the mask by the solution of solving the Laplacian equation. The data values around the masked areas define the boundary conditions. The solution is calculated iteratively and it can take some time to converge.

Fractal Correction

Data Process → Correct Data → Fractal Correction

The Fractal Correction module, like the Remove Data Under Mask module, replaces data under the mask. However, it uses a different algorithm to come up with the new data: The fractal dimension of the whole image is first computed, and then the areas under the mask are substituted by a randomly rough surface having the same fractal dimension. The root mean square value of the height irregularities (roughness) is not changed by using this module.

Note This calculation can take some time, so please be patient.

Warning Running this module on data that do not have fractal properties can cause really unrealistic results and is strictly not recommended.

Mask of Outliers

Data Process → Correct Data → Mask of Outliers

This module creates mask of areas in the data that not pass the 3σ criterion. All the values above and below this confidence interval are marked in mask and can be edited or processed by other modules afterwards.

Line Correction

Profiles taken in the fast scanning axis (usually x-axis) can be mutually shifted by some amount or have slightly different slopes. The basic line correction functions deal with this type of discrepancy. Several functions can be used: The Polynomial and Path level tools and then several procedures under Data Process → Correct Data menu.

The Polynomial tool fits each horizontal or vertical line by a polynomial up to the third order and then subtracts the fitted polynomial – a very frequently used function in basic processing of raw SPM data. It also permits to exclude or include selected area from the fit. The inclusion or exclusion only applies to the lines interseting the selected area. Other lines are always fitted using all data values.

Line correction functions in Correct Data perform only horizontal line corrections, therefore one has to rotate the image to perform column-wise correction. They include:

- Match Line Correction,

- Median Line Correction,
- Modus Line Correction, and
- Median Difference Line Correction,
- Step Line Correction.

The first three are very similar, they all align rows of the data field to minimize some quantity. As the names indicate, Median Line Correction matches line medians while Modus Line Correction attempts to match line (pseudo)modus. Match Line Correction minimizes certain line difference function that gives more weight to flat areas and less weight to areas with large slopes. The effect of all three functions is often very similar, although some can be more suitable for certain type of data than others.

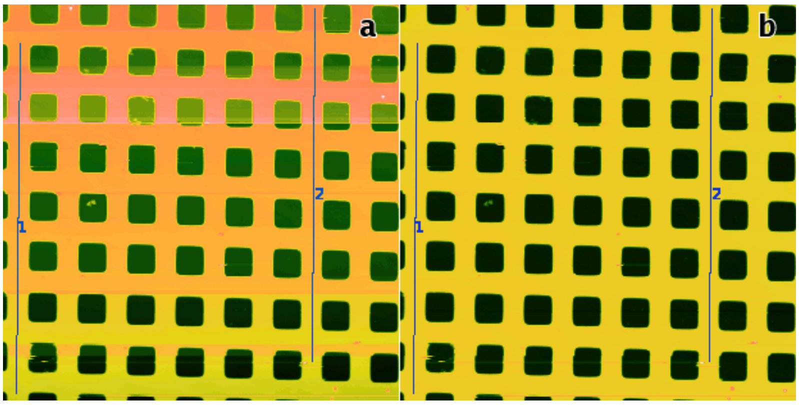
Function Median Difference Line Correction shifts the lines so that the median of differences (between vertical neighbour pixels) becomes zero, instead of the difference of medians. Therefore it better preserves large features while it is more sensitive to completely bogus lines.

Function Step Line Correction differs from the others. It attempts to identify misaligned segments within the rows and correct the height of each such segment individually. Therefore it is often able to correct data with discontinuities in the middle of a row. This function is rather experimental and the exact way it works can be subject of futher changes.

Path Leveling Tool

The Path Leveling tool can be used to correct the heights in an arbitrary subset of rows in complicated images.

First, one selects a number of straight lines on the data. The intersections of these lines with the rows then form a set of points in each row that is used for leveling. The rows are moved up or down to minimize the difference between the heights of the points of adjacent rows. Rows that are not intersected by any line are not moved (relatively to neighbouring rows).



Path Level example: (a) uncorrected data with steps that the automated method may fail to correct, two suitable leveling lines are selected; (b) the result of Path Level application with line width 5.

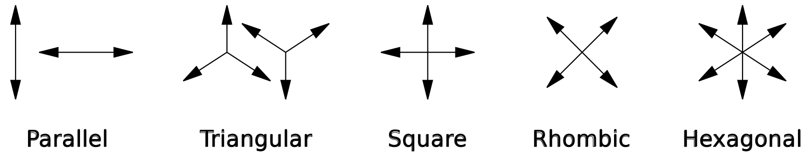
Unrotate

Data Process → Correct Data → Unrotate

Unrotate can automatically make principal directions in an image parallel with horizontal and/or vertical image edges. For that to work, the data need to have some principal directions, therefore it is most useful for scans of artifical and possibly crystallic structures.

The rotation necessary to straighten the image – displayed as Correction – is calculated from peaks in angular slope distribution assuming a prevalent type of structure, or symmetry. The symmetry can be estimated automatically too, but it is possible to select a particular symmetry type manually and let the module calculate only corresponding rotation correction. Note if you assume a structure type that does not match the actual structure, the calculated rotation is rarely meaningful.

It is recommended to level (or facet-level) the data first as overall slope can skew the calculated rotations.



Orientations of prevalent directions corresponding to Unrotate symmetry types.

The assumed structure type can be set with Assume selector. Following choices are possible:

Detected Automatically detected symmetry type, displayed above as Detected.

Parallel Parallel lines, one prevalent direction.

Triangular Triangular symmetry, three prevalent directions (unilateral) by 120 degrees.

Square Square symmetry, two prevalent directions oriented approximately along image sides.

Rhombic Rhombic symmetry, two prevalent directions oriented approximately along diagonals. The only difference from Square is the preferred diagonal orientation (as opposed to parallel with sides).

Hexagonal Hexagonal symmetry, three prevalent directions (bilateral) by 120 degrees.

4.7 Extended Data Edit

This section presents extended modules designed for editing (correcting) SPM data. Using simple data editing tools presented in chapter Data Edit and Correction it is possible to correct many local scanning defects that can be found on SPM images. There are also many error sources within SPM methods that lead to global errors, like low frequencies modulated on the data or data drift in the slow scanning axis.

Drift Compensation

Data Process → Correct Data → Compensate Drift

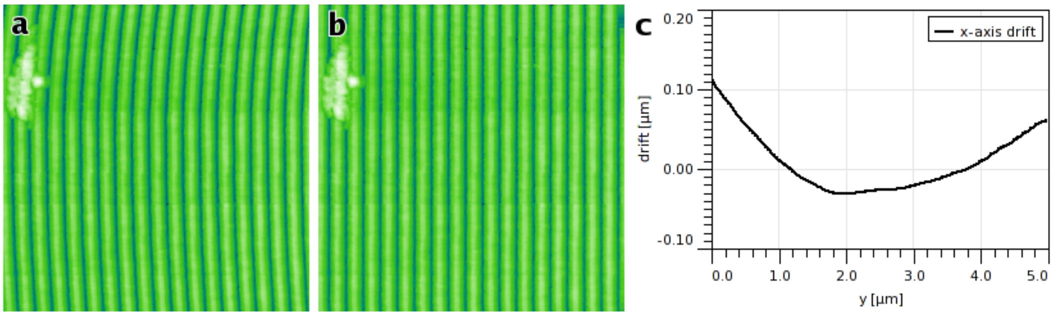
Compensate Drift calculates and/or corrects drift in the fast scanning axis (horizontal). This adverse effect can be caused by thermal effects or insufficient mechanical rigidity of the measuring device.

The drift graph, which is one of possible outputs, represents the horizontal shift of individual rows compared to a reference row (which could be in principle chosen arbitrarily, in practice the zero shift is chosen to minimize the amount of data sticking out of the image after compensation), with the row y-coordinate on the abscissa.

The drift is determined in two steps:

1. A mutual horizontal offset is estimated for each couple of rows not more distant than Search range. It is estimated as the offset value giving the maximum mutual correlation of the two rows. Thus a set of local row drift estimations is obtained (together with the maximum correlation scores providing an estimate of their actual similarity).
2. Global offsets are calculated from the local ones. At present the method is very simple as it seems sufficient in most cases: local drift derivatives are fitted for each row onto the local drift estimations and the global drift is then obtained by intergration (i.e. summing the local drifts).

Option Exclude linear skew subtracts the linear term from the calculated drift, it can be useful when the image is anisotropic and its features are supposed to be oriented in a direction not paralled to the image sides.



Drift correction example: (a) original data exhibiting strong drift in the fast scan axis, (b) corrected data, (c) calculated drift graph.

1D FFT Filter

Data Process → Correct Data → 1D FFT Filtering

One excellent way of removing frequency based of noise from an image is to use Fourier filtering. First, the Fourier transform of the image is calculated. Next, a filter is applied to this transform. Finally, the inverse transform is applied to obtain a filtered image. Gwyddion uses the Fast Fourier Transform (or FFT) to make this intensive calculation much faster.

Within the 1D FFT filter the frequencies that should be removed from spectrum (suppress type: null) or supressed to value of neighbouring frequencies (suppress type: suppress) can be selected by marking appropriate areas in the power spectrum graph. The selection can be inverted easily using the Filter type choice. 1D FFT filter can be used both for horizontal and vertical direction.

2D FFT Filter

Data Process → Correct Data → 2D FFT Filtering

2D FFT filter acts similarly as the 1D variant (see above) but using 2D FFT transform. Therefore, the spatial frequencies that should be filtered must be selected in 2D using mask editor. As the frequencies are related to center of the image (corresponding to zero frequency), the mask can snapped to the center (coordinate system origin) while being edited. There are also different display and output modes that are self-explanatory – image or FFT coefficients can be outputted by module (or both).

Note that the filter usually resamples the data to size that fits to the available FFT algorithm (FFTW or Gwyddion FFT). As this may affect results, the resampled image size information is stated in the module window.

Polynomial Distortion

Data Process → Correct Data → Polynomial Distortion

General distortion in the horizontal plane can be compensated, or created, with Polynomial distortion. It performs transforms that can be expressed as

$$x_{\mathrm{old}} = P_x(x_{\mathrm{new}}, y_{\mathrm{new}}),$$
$$y_{\mathrm{old}} = P_y(x_{\mathrm{new}}, y_{\mathrm{new}}),$$

where P_x and P_y are polynomials up to the third total order with user-defined coefficients. Note the direction of the coordinate transform – the reverse direction would not guarantee an unambiguous mapping.

The polynomial coefficients are entered as scale-free, i.e. as if the coordinate ranges were always [0, 1]. If Instant updates are enabled, pressing Enter in a coefficient entry (or just leaving moving keyboard focus elsewhere) updates the preview.

4.8 Statistical Analysis

While analyzing randomly rough surfaces we often need a statistical approach to determine some set of representative quantities. Within Gwyddion, there are several ways of doing this. In this section we will explain the various statistical tools and modules offered in Gwyddion, and also present the basic equations which were used to develop the algorithms they utilize.

Scanning probe microscopy data are usually represented as a two-dimensional data field of size $N \times M$, where N and M are the number of rows and columns of the data field, respectively. The real area of the field is denoted as $L_x \times L_y$ where L_x and L_y are the dimensions along the respective axes. The sampling interval (distance between two adjacent points within the scan) is denoted Δ. We assume that the sampling interval is the same in both the x and y direction. We assume that the surface height at a given point (x,y) can be described by a random function $\xi(x,y)$ that has given statistical properties.

Note that the AFM data are usually collected as line scans along the x axis that are concatenated together to form the two-dimensional image. Therefore, the scanning speed in the x direction is considerably higher than the scanning speed in the y direction. As a result, the statistical properties of AFM data are usually collected along the x profiles as these are less affected by low frequency noise and thermal drift of the sample.

Statistical Quantities Tool

Statistical quantities include basic properties of the height values distribution, including its variance, skewness and kurtosis. The quantities accessible within Gwyddion by means of the Statistical Quantities tool are as follows:

- Mean value, minimum, maximum and median.
- RMS value of the height irregularities: this quantity is computed from data variance.
- Ra value of the height irregularities: this quantity is similar to RMS value with the only difference in exponent (power) within the data variance sum. As for the RMS this exponent is $q = 2$, the Ra value is computed with exponent $q = 1$ and absolute values of the data (zero mean).
- Height distribution skewness: computed from 3rd central moment of data values.
- Height distribution kurtosis: computed from 4th central moment of data values.
- Projected surface area and surface area: computed by simple triangulation.
- Mean inclination of facets in area: computed by averaging normalized facet direction vectors.

Tip By default, the Statistical Quantities tool will display figures based on the entire image. If you would like to analyze a certain region within the image, simply click and drag a rectangle around it. The tool window will update with new numbers based on this new region. If you want you see the stats for the entire image again, just click once within the data window and the tool will reset.

More precisely, RMS (σ), skewness (γ_1), and kurtosis (γ_2) are computed from central moments of i-th order μ_i according to the following formulas:

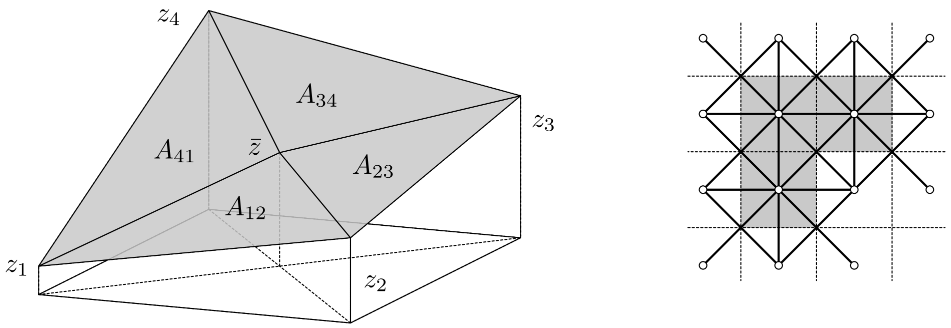
$$\sigma = \mu_2^{1/2}, \quad \gamma_1 = \frac{\mu_3}{\mu_2^{3/2}}, \quad \gamma_2 = \frac{\mu_4}{\mu_2^2} - 3$$

The surface area is estimated by the following method. Let z_i for $i = 1,2,3,4$ denote values in four neighbour points (pixel centres), and h_x and h_y pixel dimensions along corresponding axes. If an additional point is placed in the centre of the rectangle which corresponds to the common corner of the four pixels (using the mean value of the pixels), four triangles are formed and the surface area can be approximated by summing their areas. This leads to the following formulas for the area of one triangle (top) and the surface area of one pixel (bottom):

$$A_{12} = \frac{h_x h_y}{4} \sqrt{1 + \left(\frac{z_1 - z_2}{h_x}\right)^2 + \left(\frac{z_1 + z_2 - 2\bar{z}}{h_y}\right)^2}$$

$$A = A_{12} + A_{23} + A_{34} + A_{41}$$

The method is now well-defined for inner pixels of the region. Each value participates on eight triangles, two with each of the four neighbour values. Half of each of these triangles lies in one pixel, the other half in the other pixel. By counting in the area that lies inside each pixel, the total area is defined also for grains and masked areas. It remains to define it for boundary pixels of the whole data field. We do this by virtually extending the data field with a copy of the border row of pixels on each side for the purpose of surface area calculation, thus making all pixels of interest inner.



Surface area calculation triangulation scheme (left). Application of the triangulation scheme to a three-pixel masked area (right), e.g. a grain. The small circles represent pixel-center vertices z_i, thin dashed lines stand for pixel boundaries while thick lines symbolize the triangulation. The surface area estimate equals to the area covered by the mask (grey) in this scheme.

Statistical Functions Tool

One-dimensional statistical functions can be accessed by using the Statistical Functions tool. Within the tool window, you can select which function to evaluate using the selection box on the left labeled Output Type. The graph preview will update automatically. You can select in which direction to evaluate (x or y), but as stated above, we recommend using the fast scanning axis direction. You can also select which interpolation method to use. When you are finished, click Apply to close the tool window and output a new graph window containing the statistical data.

Tip Similar to the Statistical Quantities tool, this tool evaluates for the entire image by default, but you can select a sub-region to analyze if you wish.

Height and Angle Distribution Functions

The simplest statistical functions are the height and slope distribution functions. These can be computed as non-cumulative (i.e. densities) or cumulative. These functions are computed as normalized histograms of the height or slope (obtained as dreivatives in the selected direction – horizontal or vertical) values. In other words, the quantity on the abscissa in ‘angle distribution’ is the tangent of the angle, not the angle itself.

The normalization of the densities $\rho(p)$ (where p is the corresponding quantity, height or slope) is such that

$$\int_{-\infty}^{\infty} \rho(x)\,\mathrm{d}x = 1$$

Evidently, the scale of the values is then independent on the number of data points and the number of histogram buckets. The cumulative distributions are integrals of the densities and they have values from interval $[0,1]$.

First-Order vs. Second-Order Quantities

The height and slope distribution quantities belong to the first-order statistical quantities, describing only the statistical properties of the individual points. However, for the complete description of the surface properties it is necessary to study higher order functions. Usually, second-order statistical quantities observing mutual relationship of two points on the surface are employed. These functions are namely the autocorrelation function, the height-height correlation function, and the power spectral density function. A description of each of these follows:

Autocorrelation Function

The autocorrelation function is given by

$$\begin{aligned} G(\tau_x,\tau_y) &= \iint_{-\infty}^{\infty} z_1 z_2 w(z_1,z_2,\tau_x,\tau_y)\,\mathrm{d}z_1\,\mathrm{d}z_2 \\ &= \lim_{S\to\infty} \frac{1}{S} \iint_S \xi(x_1,y_1)\,\xi(x_1+\tau_x,y_1+\tau_y)\,\mathrm{d}x_1\,\mathrm{d}y_1 \end{aligned}$$

where z_1 and z_2 are the values of heights at points (x_1, y_1), (x_2, y_2); furthermore, $\tau_x = x_1 - x_2$ and $\tau_y = y_1 - y_2$. The function $w(z_1, z_2, \tau_x, \tau_y)$ denotes the two-dimensional probability density of the random function $\xi(x, y)$ corresponding to points (x_1, y_1), (x_2, y_2) and the distance between these points τ.

From the discrete AFM data one can evaluate this function as

$$G(m,n) = \frac{1}{(N-n)(M-m)} \sum_{l=1}^{N-n} \sum_{k=1}^{M-m} z_{k+m,l+n} z_{k,l}$$

where $m\tau_x/\Delta_x$, $m\tau_y/\Delta_y$. The function can thus be evaluated in a discrete set of values of τ_x and τ_y separated by the sampling intervals Δ_x and Δ_y, respectively. The two-dimensional autocorrelation function can be calculated with Data Process → Statistics → 2D Autocorrelation.

For AFM measurements, we usually evaluate the one-dimensional autocorrelation function based only on profiles along the fast scanning axis. It can therefore be evaluated from the discrete AFM data values as

$$G_x(m) = G(m,0) = \frac{1}{N(M-m)} \sum_{l=1}^{N} \sum_{k=1}^{M-m} z_{k+m,l} z_{k,l}$$

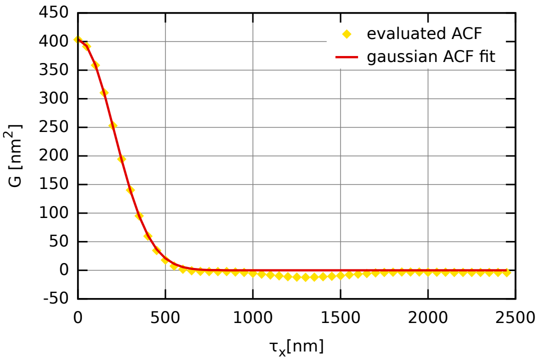
The one-dimensional autocorrelation function is often assumed to have the form of a Gaussian, i.e. it can be given by the following relation

$$G_x(\tau_x) = \sigma^2 \exp(-\tau_x^2/T^2)$$

where σ denotes the root mean square deviation of the heights and T denotes the autocorrelation length.

For the exponential autocorrelation function we have the following relation

$$G_x(\tau_x) = \sigma^2 \exp(-\tau_x/T)$$



Autocorrelation function obtained for simulated Gaussian randomly rough surface (i.e. with a Gaussian autocorrelation function) with $\sigma \approx 20\,\mathrm{nm}$ and $T \approx 300\,\mathrm{nm}$.

Note For optical measurements (e. g. spectroscopic reflectometry, ellipsometry) the Gaussian autocorrelation function is usually expected to be in good agreement with the surface properties. However, some articles related with surface growth and oxidation usually assume that the exponential form is closer to the reality.

Height-Height Correlation Function

The difference between the height-height correlation function and the autocorrelation function is very small. As with the autocorrelation function, we sum the multiplication of two different values. For the autocorrelation function, these values represented the different distances between points. For the height-height correlation function, we instead use the power of difference between the points.

For AFM measurements, we usually evaluate the one-dimensional height-height correlation function based only on profiles along the fast scanning axis. It can therefore be evaluated from the discrete AFM data values as

$$H_x(\tau_x) = \frac{1}{N(M-m)} \sum_{l=1}^{N} \sum_{n=1}^{M-m} (z_{n+m,l} - z_{n,l})^2$$

where $m = \tau/\Delta$. The function thus can be evaluated in a discrete set of values of τ separated by the sampling interval Δ.

The one-dimensional height-height correlation function is often assumed to be Gaussian, i.e. given by the following relation

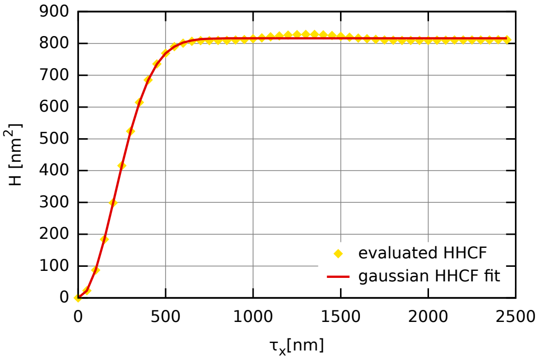
$$H_x(\tau_x) = 2\sigma^2 \left[1 - \exp\left(-\frac{\tau_x^2}{T^2}\right)\right]$$

where σ denotes the root mean square deviation of the heights and T

For the exponential height-height correlation function we have the following relation

$$H_x(\tau_x) = 2\sigma^2 \left[1 - \exp\left(-\frac{\tau_x}{T}\right)\right]$$

In the following figure the height-height correlation function obtained for a simulated Gaussian surface is plotted. It is fitted using the formula shown above. The resulting values of σ and T obtained by fitting the HHCF are practically the same as for the ACF.



Height-height correlation function obtained for simulated Gaussian randomly rough surface with $\sigma \approx 20\,\mathrm{nm}$ *and* $T \approx 300\,\mathrm{nm}$.

Power Spectral Density Function

The two-dimensional power spectral density function can be written in terms of the Fourier transform of the autocorrelation function

$$W(K_x, K_y) = \frac{1}{4\pi} \iint_{-\infty}^{\infty} G(\tau_x, \tau_y)\, \mathrm{e}^{-\mathrm{i}(K_x\tau_x + K_y\tau_y)}\, \mathrm{d}\tau_x\, \mathrm{d}\tau_y$$

Similarly to the autocorrelation function, we also usually evaluate the one-dimensional power spectral density function which is given by the equation

$$W_1(K_x) = \int_{-\infty}^{\infty} W(K_x, K_y)\, \mathrm{d}K_y$$

This function can be evaluated by means of the Fast Fourier Transform as follows:

$$W_1(K_x) = \frac{2\pi}{NMh} \sum_{j=0}^{N} |\hat{P}_j(K_x)|^2$$

where $P_j(K_x)$ is the Fourier coefficient of the j-th row, i.e.

$$\hat{P}_j(K_x) = \frac{h}{2\pi} \sum_{k=0}^{N} z_{kj} \exp(-\mathrm{i} K_x kh)$$

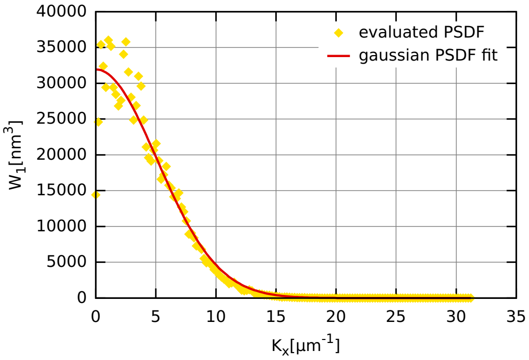
If we choose the Gaussian ACF, the corresponding Gaussian relation for the PSDF is

$$W_1(K_x) = \frac{\sigma^2 T}{2\sqrt{\pi}} \exp(-K_x^2 T^2/4)$$

For the surface with exponential ACF we have

$$W_1(K_x) = \frac{\sigma^2 T}{\pi} \frac{1}{1 + K_x^2 T^2}$$

In the following figure the resulting PSDF and its fit for the same surface as used in the ACF and HHCF fitting are plotted. We can see that the function can be again fitted by Gaussian PSDF. The resulting values of σ and T were practically same as those from the HHCF and ACF fit.



PSDF obtained for data simulated with Gaussian autocorrelation function.

We can also introduce radial PSDF $W_{\mathrm{r}}(K)$, which of course contains the same information as the one-dimensional PSDF for isotropic rough surfaces:

$$W_{\mathrm{r}}(K) = \int_0^{2\pi} W(K\cos\varphi, K\sin\varphi)\, K\, \mathrm{d}\varphi$$

For a surface with Gaussian ACF this function is expressed as

$$W_{\mathrm{r}}(K) = \frac{\sigma^2 T}{2} KT \exp(-K^2 T^2/4)$$

while for exponential ACF surface as

$$W_{\mathrm{r}}(K) = \sigma^2 T \frac{KT}{(1 + K^2 T^2)^{3/2}}$$

Tip Within Gwyddion you can fit all statistical functions presented here by their Gaussian and exponential forms. To do this, fist click Apply within the Statistical Functions tool window. This will create a new graph window. With this new window selected, click on Graph → Fit Graph.

Minkowski Functionals

The Minkowski functionals are used to describe global geometric characteristics of structures. Two-dimensional discrete variants of volume V, surface S, and connectivity (Euler-Poincaré Characteristic) χ are calculated according to following formulas:

$$V = \frac{N_{\text{white}}}{N}, \quad S = \frac{N_{\text{bound}}}{N}, \quad \chi = \frac{C_{\text{white}} - C_{\text{black}}}{N}$$

Here B denotes the total number of pixels, N_{white} denotes the number of ‘white’ pixels, that is pixels above the threshold. Pixels below the threshold are referred to as ‘black’. Symbol N_{bound} denotes the number of white-black pixel boundaries. Finally, C_{white} and C_{black} denote the number of continuous sets of white and black pixels respectively.

For an image with continuous set of values the functionals are parametrized by the height threshold value ϑ that divides white pixels from black, that is they can be viewed as functions of this parameter. And these functions $V(\vartheta)$, $S(\vartheta)$ and $\chi(\vartheta)$ are plotted.

Row/Column Statistics Tool

This tool calculates numeric characteristics of each row or column and plots them as a function of its position. This makes it kind of complementary to Statistical Functions tool. Available quantities include:

- Mean value, minimum, maximum and median.
- RMS value of the height irregularities computed from data variance R_q.
- Skewness and kurtosis of the height distribution.
- Surface line length. It is estimated as the total length of the straight segments joining data values in the row (column).
- Overall slope, i.e. the tangent of the mean line fitted through the row (column).
- Tangent of β_0. This is a characteristics of the steepnes of local slopes, closely related to the behaviour of autocorrelation and height-height correlation functions at zero. For discrete values it is calculated as follows:

$$\tan^2 \beta_0 = \frac{1}{(N-1)h^2} \sum_{i=1}^{N-1} (z_i - z_{i-1})^2$$

- Standard roughness parameters Ra, Rz, Rt.

In addition to the graph displaying the values for individual rows/columns, the mean value and standard deviation of the selected quantity is calculated from the set of individual row/column values.

Two-Dimensional Slope Statistics

Several functions in Data Process → Statistics operate on two-dimensional slope (derviative) statistics.

Slope Distribution calculates a plain two-dimensional distribution of derivatives, that is the horizontal and vertical coordinate on the resulting data field is the horizontal and vertical derivative, respectively. The slopes can be calculated as central derivatives (one-side on the borders of the image) or, if Use local plane fitting is enabled, by fitting a local plane through the neighbourhood of each point and using its gradient. Slope Distribution has also another mode operation called Per-angle graph. in which it plots the distribution of r^2 over φ where we introduced polar coordinates (r,φ) in the plane of derivatives. The relation between the derivative Cartesian coordinates of the two-dimensional slope distribution and the facet inclination angles are given by the following formula:

$$\vartheta = \operatorname{atan}\operatorname{hypot}\left(\frac{\mathrm{d}z}{\mathrm{d}x}, \frac{\mathrm{d}z}{\mathrm{d}y}\right) , \qquad \varphi = \operatorname{atan}_2\left(\frac{\mathrm{d}z}{\mathrm{d}y}, -\frac{\mathrm{d}z}{\mathrm{d}x}\right)$$

Angle Distribution function is a visualization tool that does not calculate a distribution in the strict sense. For each derivative v the circle of points satisfying

$$2\mathbf{r}\cdot\mathbf{v} = r^2$$

is drawn. The number of points on the circle is given by Number of steps.

Facet Analysis

Data Process → Statistics → Facet Analysis

Facet analysis enables to interactively study orientations of facets occuring in the data and mark facets of specific orientations on the image. The left view displays data with preview of marked facets. The right smaller view, called facet view below, displays two-dimensional slope distribution.

The centre of facet view always correspond to zero inclination (horizontal facets), slope in x-direction increases towards left and right border and slope in y-direction increases towards top and bottom borders. The exact coordinate system is a bit complex and it adapts to the range of slopes in the particular data displayed.

Facet plane size controls the size (radius) of plane locally fitted in each point to determine the local inclination. The special value 0 stands for no plane fitting, the local inclination is determined from symmetric x and y derivatives in each point. The choice of neighbourhood size is crucial for meaningful results: it must be smaller than the features one is interested in to avoid their smoothing, on the other hand it has to be large enough to suppress noise present in the image.

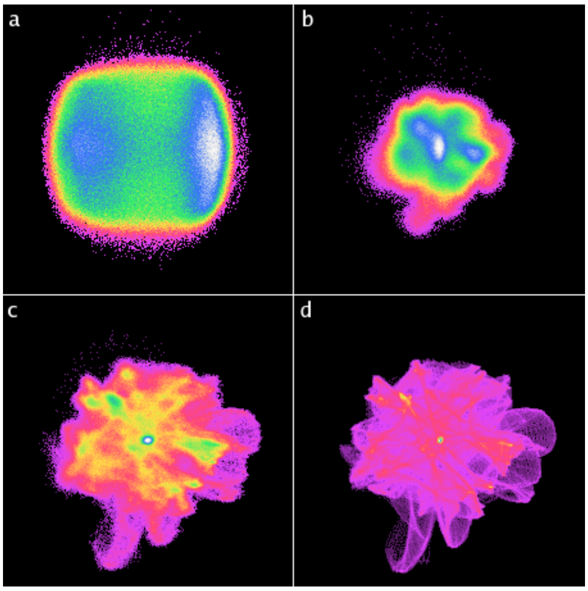


Illustration of the influence of fitted plane size on the distribution of a scan of a delaminated DLC surface with considerable fine noise. One can see the distribution is completely obscured by the noise at small plane sizes. The neighbourhood sizes are: (a) 0, (b) 2, (c) 4, (d) 7. The angle and false color mappings are full-scale for each particular image, i.e. they vary among them.

Both facet view and data view allow to select a point with mouse and read corresponding facet normal inclination value ϑ and direction φ under Normal. When you select a point on data view, the facet view selection is updated to show inclination in this point.

Button Find Maximum sets facet view selection to slope distribution maximum (the initial selection position).

Button Mark updates the mask of areas with slope similar to the selected slope. More precisely, of areas with slope within Tolerance from the selected slope. The facet view then displays the set of slopes corresponding to marked points (note the set of selected slopes may not look circular on facet view, but this is only due to selected projection). Average inclination of all points in selected range of slopes is displayed under Mean Normal.

4.9 One-Dimensional Roughness Parameters

Standardized one-dimensional roughness parameters can be evaluated with the roughness tool.

The one-dimensional texture is split to waviness (the low-frequency components defining the overall shape) and roughness (the high-frequency components) at the cut-off frequency. This frequency is specified in the units of the Nyquist frequency, that is value 1.0 corresponds to the Nyquist frequency.

In the following formulas we assume the mean value of r_j is zero, i.e.

$$r_j = z_j - \bar{z}$$

Roughness Amplitude Parameters

Roughness Average R_a Standards: ASME B46.1-1995, ASME B46.1-1985, ISO 4287-1997, ISO 4287/1-1997.

Arithmetical mean deviation. The average deviation of all points roughness profile from a mean line over the evaluation length

$$R_\mathrm{a} = \frac{1}{N}\sum_{j=1}^{N} |r_j|$$

An older means of specifying a range for R_a is RHR. This is a symbol on a drawing specifying a minimum and maximum value for R_a.

Root Mean Square Roughness R_q Standards: ASME B46.1-1995, ISO 4287-1997, ISO 4287/1-1997.

The average of the measured height deviations taken within the evaluation length and measured from the mean line

$$R_\mathrm{q} = \sqrt{\frac{1}{N}\sum_{j=1}^{N} r_j^2}$$

Maximum Height of the Profile R_t Standards: ASME B46.1-1995, ISO 4287-1997.

Maximum peak-to-peak-valley height. The absolute value between the highest and lowest peaks

$$R_\mathrm{t} = \left|\min_{1\le j\le N} r_j\right| + \left|\max_{1\le j\le N} r_j\right|$$

Maximum Profile Valley Depth R_v**,** R_m Standards: ASME B46.1-1995, ASME B46.1-1985, ISO 4287-1997, ISO 4287/1-1997.

Lowest valley. There is the depth of the deepest valley in the roghness profile over the evaluation length

$$R_\mathrm{v} = \left|\min_{1\le j\le N} r_j\right|$$

Maximum Profile Peak Height R_p Standards: ASME B46.1-1995, ASME B46.1-1985, ISO 4287-1997, ISO 4287/1-1997.

Highest peak. There is the height of the highest peak in the roughness profile over the evaluation length

$$R_\mathrm{p} = \left|\max_{1\le j\le N} r_j\right|$$

Average Maximum Height of the Profile $R_{\mathrm{t}m}$ Standards: ASME B46.1-1995, ISO 4287-1997.

Mean peak-to-valley roughness. It is determined by the difference between the highest peak ant the lowest valley within multiple samples in the evaluation length

$$R_{\mathrm{t}m} = R_{\mathrm{v}m} + R_{\mathrm{p}m}$$

where $R_{\mathrm{v}m}$ and $R_{\mathrm{p}m}$ are defined below.

For profile data it is based on five sample lengths (m = 5). The number of samples corresponded with the ISO standard.

Average Maximum Profile Valley Depth $R_{\mathrm{v}m}$ Standards: ISO 4287-1997.

The mean valley depth based on one peak per sampling length. The single deepest valley is found in five sampling lengths ($m = 5$) and then averaged

$$R_{\mathrm{v}m} = \frac{1}{m}\sum_{i=1}^{m} R_{\mathrm{v}i}$$

where

$$R_{\mathrm{v}i} = \left|\min r_j\right| \quad \text{for} \quad (i-1)\frac{N}{m} < j < i\frac{N}{m}$$

Average Maximum Profile Peak Height $R_{\mathrm{p}m}$ Standards: ISO 4287-1997.

The mean peak height based on one peak per sampling length. The single highest peak is found in five sampling lengths ($m = 5$) and then averaged

$$R_{\mathrm{p}m} = \frac{1}{m}\sum_{i=1}^{m} R_{\mathrm{p}i}$$

where

$$R_{\mathrm{p}i} = \left|\max r_j\right| \quad \text{for} \quad (i-1)\frac{N}{m} < j < i\frac{N}{m}$$

Base roughness depth R_{3z} Standards: ISO 4287-1997.

The distance between the third highest peak and the third lowest valley. A peak is a portion of the surface above the mean line crossings.

Base roughness profile depth $R_{3z\mathrm{ISO}}$ Standards: ISO 4287-1997.

The height of the third highest peak from the third lowest valley per sampling length. The base roughness depth is found in five sampling lengths and then averaged.

Ten-point height R_z Standards: ISO 4287-1997

The average absolute value of the five highest peaks and the five lowest valleys over the evaluation length.

Average peak-to-valley profile roughness $R_{z\mathrm{ISO}}$ Standards: ISO 4287-1997.

The average peak-to-valley roughness based on one peak and one valley per sampling length. The single largest deviation is found in five sampling lengths and then averaged. It is identical to $R_{\mathrm{t}m}$.

The Amplitude Distribution Function ADF Standards: ISO 4287-1997.

The amplitude distribution function s a probability function that gives the probability that a profile of the surface has a certain height z at any position x.

The Bearing Ratio Curve BRC Standards: ISO 4287-1997.

The Bearing Ratio Curve is related to the ADF, it is the corresponding cumulative probability distribution and sees much greater use in surface finish. The bearing ratio curve is the integral (from the top down) of the ADF.

Skewness R_{sk} Standards: ISO 4287-1997.

Skewness is a parameter that describes the shape of the ADF. Skewness is a simple measure of the asymmetry of the ADF, or, equivalently, it measures the symmetry of the variation of a profile about its mean line

$$R_{\mathrm{sk}} = \frac{1}{NR_q^3}\sum_{j=1}^{N} r_j^3$$

Kurtosis R_{ku} Standards: ISO 4287-1997.

Kurtosis is the ADF shape parameter considered. Kurtosis relates to the uniformity of the ADF or, equivalently, to the spikiness of the profile.

$$R_{\mathrm{ku}} = \frac{1}{NR_q^4}\sum_{j=1}^{N} r_j^4$$

4.10 Grain Analysis

There are several grain-related algorithms implemented in Gwyddion. First of all, simple thresholding algorithms can be used (height, slope or curvature thresholding). These procedures can be very efficient namely within particle analysis (to mark particles located on flat surface).

Thresholding methods can be accessed within Gwyddion as Data Process → Grains → Mark by Threshold. Height, slope and curvature thresholding is implemented within this module. The results of each individual thresholding methods can be merged together using several operators.

Similarly, the grains can be removed from the mask using Data Process → Grains → Remove Grains menu choice. Maximum height and/or size thresholding methods can be used to eliminate false grains occurred by noise or some dust particles, for example. You can use also interactive grain removal tool for doing this manually.

Watershed

For more complicated data structures the effectiveness of thresholding algorithms can be very poor. For these data a *watershed algorithm* can be used more effectively for grain or particle marking.

The watershed algorithm is usually employed for local minima determination and image segmentation in image processing. As the problem of determining the grain positions can be understood as the problem of finding local extremes on the surface this algorithm can be used also for purposes of grain segmentation or marking. For convenience in the following we will treat the data inverted in the z direction while describing the algorithm (i.e. the grain tops are forming local minima in the following text). We applied two stages of the grain analysis (see [1]):

1. At each point of the inverted surface the virtual water drop was placed. In the case that the drop was not already in a local minimum it followed the steepest descent path to minimize its potential energy. As soon as the drop reached any local minimum it stopped here and rested on the surface. In this way it filled the local minimum partially by its volume (see figure below and its caption). This process was repeated several times. As the result a system of lakes of different sizes filling the inverted surface depressions was obtained. Then the area of each of the lakes was evaluated and the smallest lakes were removed under assumption that they were formed in the local minima originated by noise. The larger lakes were used to identify the positions of the grains. In this way the noise in the AFM data was eliminated.

2. The grains found in the step 1 were marked (each one by a different number). The water drops continued in falling to the surface and filling the local minima. As the grains were already identified and marked after the first step, the next five situations could happen as soon as the drop reached a local minimum.

   (a) The drop reached the place previously marked as a concrete grain. In this case the drop was merged with the grain, i. e. it was marked as a part of the same grain.

   (b) The drop reached the place where no grain was found but a concrete grain was found in the closest neighbourhood of the drop. In this case the drop was merged with the grain again.

   (c) The drop reached the place where no grain was found and no grain was found even in the closest neighbourhood of the drop. In that case the drop was not marked at all.

   (d) The drop reached the place where no grain was found but more than one concrete grain was found in the closest neighbourhood (e. g. two different grains were found in the neighbourhood). In this case the drop was marked as the grain boundary.

   (e) The drop reached the place marked as grain boundary. In this case the drop was marked as the grain boundary too.

In this way we can identify the grain positions and then determine the volume occupied by each grain separately.

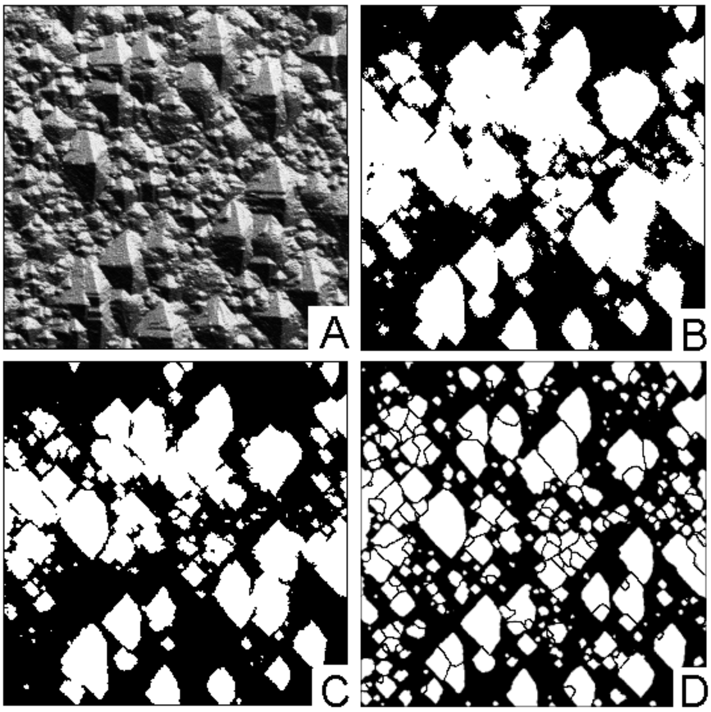


Image of grain-like surface structure (a) and corresponding results of height thresholding (b), curvature thresholding (c), and watershed (d) algorithm. Within watershed algorithm it is possible to segment image even further.

Statistics

Grain properties can be studied using several functions. The simplest of them is Grain Statistics

Grain Statistics

Data Process → Grains → Statistics

This function calculates the total number of marked grains, their total (projected) area both as an absolute value and as a fraction of total data field area, and the mean area and equivalent square size of one grain.

Overall characteristics of the marked area can be also obtained with Statistical Quantities tool when its Use mask option is switched on. By inverting the mask the same information can be obtained also for the non-grain area.

Grain Distributions

Data Process → Grains → Distributions

Grain Distributions is the most powerful and complex tool. It has two basic modes of operation: graph plotting and raw data export. In graph plotting mode selected characteristics of individual grains are calculated, gathered and summary graphs showing their distributions are plotted.

Raw data export is useful for experts who need for example to correlate properties of individual grains. In this mode selected grain characteristics are calculated and dumped to a text file table where each row corresponds to one grain and columns correspond to requested quantities. The order of the colums is the same as the relative order of the quantities in the dialog; all values are written in base SI units, as is usual in Gwyddion.

Grain Property Correlation

Data Process → Grains → Correlate

Grain correlation plots a graph of one selected graph quantity as the function of another grain quantity, visualizing correlations between them.

Grain Measurement Tool

The grain measurement tool is the interactive method to obtain the same information about individual grains as Grain Distributions in raw mode. After selecting a grain on the data window with mouse, all the available quantities are displayed in the tool window.

Beside physical characteristics this tool also displays the grain number. Grain numbers corresponds to row numbers (counting from 1) in files exported by Grain Distributions.

Grain Properties

Grain Distributions and Grain measurement tool can calculate the following grain properties:

Value-related properties

- Minimum, the minimum value (height) occuring inside the grain.
- Maximum, the maximum value (height) occuring inside the grain.
- Mean, the mean of all values occuring inside the grain, that is the mean grain height.
- Median the median of all values occuring inside the grain, that is the median grain height.
- Minimum on boundary, the maximum value (height) occuring on the inner grain boundary. This means within the set of pixels that lie inside the grain but at least one of their neighbours lies outside.
- Maximum on boundary, the maximum value (height) occuring on the inner grain boundary, defined similarly to the minimum.

Area-related properties

- Projected area, the projected (flat) area of the grain.
- Equivalent square side, the side of the square with the same projected area as the grain.
- Equivalent disc radius, the radius of the disc with the same projected area as the grain.
- Surface area, the surface area of the grain, see statistical quantities section for description of the surface area estimation method.

Boundary-related properties

- Projected boundary length, the length of the grain boundary projected to the horizontal plane (that is not taken on the real three-dimensional surface). The method of boundary length estimation is described below.
- Minimum bounding size, the minimum dimension of the grain in the horizontal plane. It can be visualized as the minimum width of a gap in the horizontal plane the grain could pass through.
- Minimum bounding direction, the direction of the gap from the previous item. If the grain exhibits a symmetry that makes several directions to qualify, an arbitrary direction is chosen.

- Maximum bounding size, the maximum dimension of the grain in the horizontal plane. It can be visualized as the maximum width of a gap in the horizontal plane the grain could fill up.
- Maximum bounding direction, the direction of the gap from the previous item. If the grain exhibits a symmetry that makes several directions to qualify, an arbitrary direction is chosen.

Volume-related properties

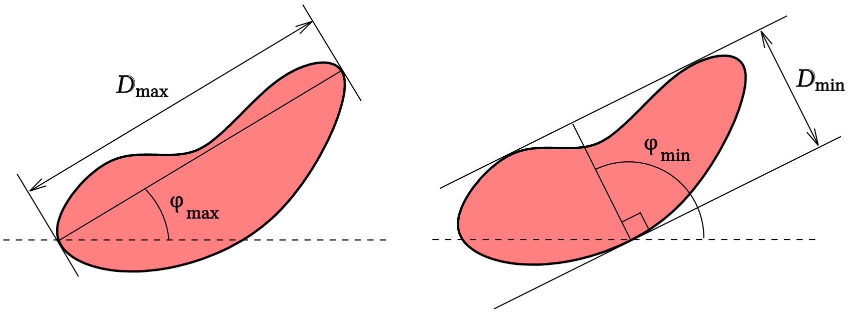
- Zero basis, the volume between grain surface and the plane $z = 0$. Values below zero form negative volumes. The zero level must be set to a reasonable value (often Fix Zero is sufficient) for the results to make sense, which is also the advantage of this method: one can use basis plane of his choice.
- Grain minimum basis, the volume between grain surface and the plane $z = z_{\text{min}}$, where z_{min} is the minimum value (height) occuring in the grain. This method accounts for grain surrounding but it typically underestimates the volume, especially for small grains.
- Laplacian backround basis, the volume between grain surface and the basis surface formed by laplacian interpolation of surrounding values. In other words, this is the volume that would disappear after using Remove Data Under Mask or Grain Remover tool with Laplacian interpolation on the grain. This is the most sophisticated method, on the other hand it is the hardest to develop intuition for.

Position-related properties

- Center x position, the horizontal coordinate of the grain centre. Since the grain area is defined as the area covered by the corresponding mask pixels, the centre of a single-pixel grain has half-integer coordinates, not integer ones. Data field origin offset (if any) is taken into account.
- Center y position, the verical coordinate of the grain centre. See above for the interpretation.

Slope-related properties

- Inclination ϑ, the deviation of the normal to the mean plane from the z-axis, see inclinations for details.
- Inclination φ, the azimuth of the slope, as defined in inclinations.

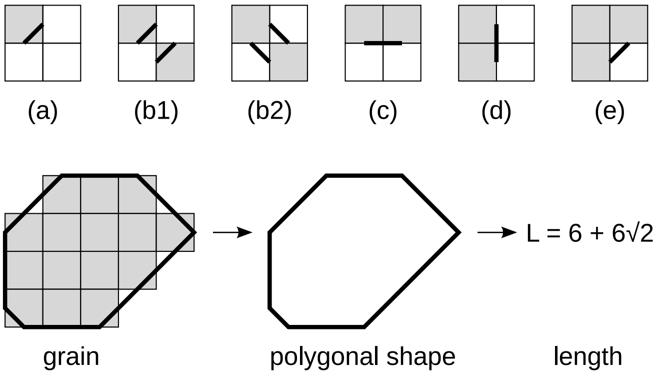


Maximum and minimum bounding dimensions and angles of a grain.

The grain boundary length is estimated by summing estimated contributions of each four-pixel configuration on the boundary. The contributions are displayed on the following figure for each type of configuration, where h_x and h_y are pixel dimension along corresponding axes and h is the length of the pixel diagonal:

$$h = \sqrt{h_x^2 + h_y^2}$$

The contributions correspond one-to-one to lenghts of segments of the boundary of a polygon approximating the grain shape. The construction of the equivalent polygonal shape can also be seen in the figure.



Contributions of pixel configurations to the estimated boundary length (top). Grey squares represent pixels inside the grain, white squares represent outside pixels. The estimated contribution of each configuration is: (a) $h/2$, (b1), (b2) h, (c) h_y, (d) h_x, (e) $h/2$. Cases (b1) and (b2) differ only in the visualization of the polygonal shape segments, the estimated boundary lengths are identical. The bottom part of the figure illustrates how the segments join to form the polygon.

The grain volume is, after subtracting the basis, estimated as the volume of exactly the same body whose upper surface is used for surface area calculation. Note for the volume between vertices this is equivalent to the classic two-dimensional trapezoid integration method. However, we calculate the volume under a mask centered on vertices, therefore their contribution to the integral is distributed differently as shown in the following figure.

$\frac{9}{16}$	$\frac{5}{48}$	$\frac{9}{16}$
$\frac{5}{48}$	$\frac{13}{24}$	$\frac{5}{48}$
$\frac{9}{16}$	$\frac{5}{48}$	$\frac{9}{16}$

Contributions of individual pixels to the volume of single pixel (grey).

References

[1] Petr Klapetek, Ivan Ohlídal, Daniel Franta, Alberto Montaigne-Ramil, Alberta Bonanni, David Stifter, Helmut Sitter: Acta Physica Slovaca, 3 (223-230), 2003

4.11 Fourier Transform

Two-dimensional Fourier transform can be accessed using Data Process → Integral Transforms → 2D FFT which implements the Fast Fourier transform (FFT). Fourier transform decomposes signal into its harmonic compoments, it is therefore useful while studying spectral frequencies present in the SPM data.

The 2D FFT module provides several types of output:

- Modulus – absolute value of the complex Fourier coefficient, proportional to the square root of the power spectrum density function (PSDF).
- Phase – phase of the complex coefficient (rarely used).
- Real – real part of the complex coefficient.
- Imaginary – imaginary part of the complex coefficient.

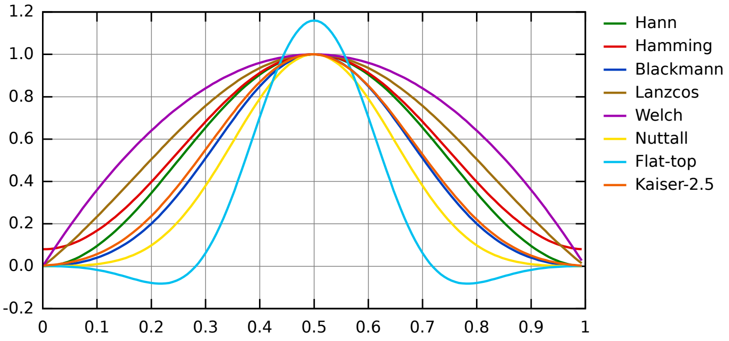
and some their combinations for convenience.

Radial sections of the two-dimensional PSDF can be conveniently obtained with Data Process → Statistics → PSDF Section. Several other functions producing spectral densities are described in section Statistical Analysis. It is also possible to filter images in the frequency domain using one-dimensional or two-dimensional FFT filters.

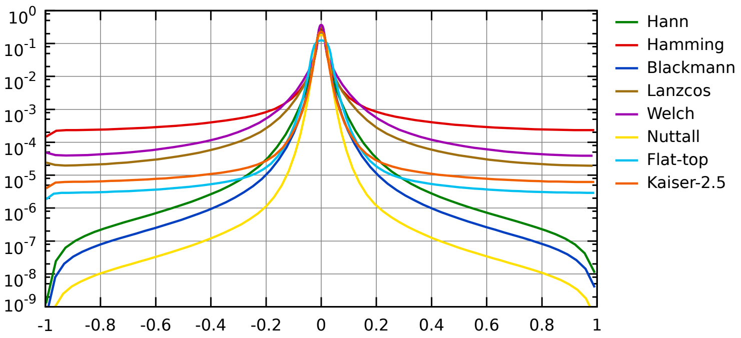
Note that the Fourier transform treats data as being infinite, thus implying some cyclic boundary conditions. As the real data do not have these properties, it is necessary to use some windowing function to suppress the data at the edgest of the image. If you do not do this, FFT treats data as being windowed by rectangular windowing function which has really bad Fourier image thus leading to corruption of the Fourier spectrum.

Gwyddion offers several windowing functions. Most of them are formed by some sine and cosine functions that damp data correctly at the edges. In the following windowing formula table the independent variable x is from interval $(0,1)$, which corresponds to the normalized abscissa; for simplicity variable $\xi = 2\pi x$ is used in some formulas. The available windowing types include:

Name	Formula
None	1
Rect	0.5 at edge points, 1 everywhere else
Hann	$w_{\mathrm{Hann}}(x) = 0.5 - 0.5\cos\xi$
Hamming	$w_{\mathrm{Hamming}}(x) = 0.54 - 0.46\cos\xi$
Blackmann	$w_{\mathrm{Blackmann}}(x) = 0.42 - 0.5\cos\xi + 0.08\cos 2\xi$
Lanczos	$w_{\mathrm{Lanczos}}(x) = \mathrm{sinc}\,\pi(2x-1)$
Welch	$w_{\mathrm{Welch}}(x) = 4x(1-x)$
Nutall	$w_{\mathrm{Nutall}}(x) = 0.355768 - 0.487396\cos\xi + 0.144232\cos 2\xi - 0.012604\cos 3\xi$
Flat-top	$w_{\mathrm{flattop}}(x) = 0.25 - 0.4825\cos\xi + 0.3225\cos 2\xi - 0.097\cos 3\xi + 0.008\cos 4\xi$
Kaiser α	$w_{\mathrm{Kaiser},\alpha}(x) = \dfrac{\mathrm{I}_0\left(\pi\alpha\sqrt{4x(1-x)}\right)}{\mathrm{I}_0(\pi\alpha)}$ where I_0 is the modified Bessel function of zeroth order and α is a parameter



Windowing functions: Hann, Hamming, Blackmann, Lanczos, Welch, Nutall, Flat-top, Kaiser 2.5.



Envelopes of windowing functions frequency responses: Hann, Hamming, Blackmann, Lanczos, Welch, Nutall, Flat-top, Kaiser 2.5.

Fourier transforms of data with sizes that are not factorable into small prime factors can be very slow – and many programs only implement FFT of arrays with dimensions that are powers of two.

In Gwyddion, however, the Fourier transform can be applied to data fields and lines of arbitrary dimensions, with no data resampling involved (at least since version 2.8). Fourier transforms are calculated either using the famous FFTW library or, if it is not available, using Gwyddion built-in routines that are slower but can also handle transforms of arbitrary size.

Nevertheless, if the data size is not factorable into small prime factors the transform is still considerably slower. Hence it is preferable to transform data fields of 'nice' sizes.

4.12 Wavelet Transform

The wavelet transform is a transform similar to the Fourier transform (or much more to the windowed Fourier transform) with a completely different merit function. The main difference is this: Fourier transform decomposes the signal into sines and cosinesm, i.e. the functions localized in Fourier space; in contrary the wavelet transform uses functions that are localized in both the real and Fourier space. Generally, the wavelet transform can be expressed by the following equation:

$$F(a,b) = \int_{-\infty}^{\infty} f(x)\, \psi^{*}_{(a,b)}(x)\, \mathrm{d}x$$

where the * is the complex conjugate symbol and function ψ is some function which can differ though it must obey certain rules.

As it is seen, the Wavelet transform is in fact an infinite set of various transforms, depending on the merit function used for its computation. This is the main reason, why we can hear the term 'wavelet transform' in very different situations and applications. There are also many ways how to sort the types of the wavelet transforms. Here we show only the division based on the wavelet orthogonality. We can use *orthogonal wavelets* for discrete wavelet transform development and *non-orthogonal wavelets* for continuous wavelet transform developement. These two transforms have the following properties:

1. The discrete wavelet transform returns a data vector of the same length as the input is. Usually, even in this vector many data are almost zero. This corresponds to the fact that it decomposes into a set of wavelets (functions) that are orthogonal to its translations and scaling. Therefore we decompose such a signal to a same or lower number of the wavelet coefficient spectrum as is the number of signal data points. Such a wavelet spectrum is very good for signal processing and compression, for example, as we get no redundant information here.

2. The continuous wavelet transform in contrary returns an array one dimension larger thatn the input data. For a 1D data we obtain an image of the time-frequecy plane. We can easily see the signal frequencies evolution during the duration of the signal and compare the spectrum with other signals spertra. As here is used the non-orthogonal set of wavelets, data are correlated highly, so big redundancy is seen here. This helps to see the results in a more humane form.

For more details on wavelet transorm see any of the thousands of wavelet resources on the Web, or for example [1].

Within Gwyddion data processing library, both these transforms are implemented and the modules using wavelet transforms can be accessed within Data Process → Integral Transforms menu.

Discrete Wavelet Transform

The discrete wavelet transform (DWT) is an implementation of the wavelet transform using a discrete set of the wavelet scales and translations obeying some defined rules. In other words, this transform decomposes the signal into mutually orthogonal set of wavelets, which is the main difference from the continuous wavelet transform (CWT), or its implementation for the discrete time series sometimes called discrete-time continuous wavelet transform (DT-CWT).

The wavelet can be constructed from a scaling function which describes its scaling properties. The restriction that the scaling functions must be orthogonal to its discrete translations implies some mathematical conditions on them which are mentioned everywhere, e.g. the dilation equation

$$\phi(x) = \sum_{k=-\infty}^{\infty} a_k \phi(Sx-k)$$

where S is a scaling factor (usually chosen as 2). Moreover, the area between the function must be normalized and scaling function must be ortogonal to its integer translates, i.e.

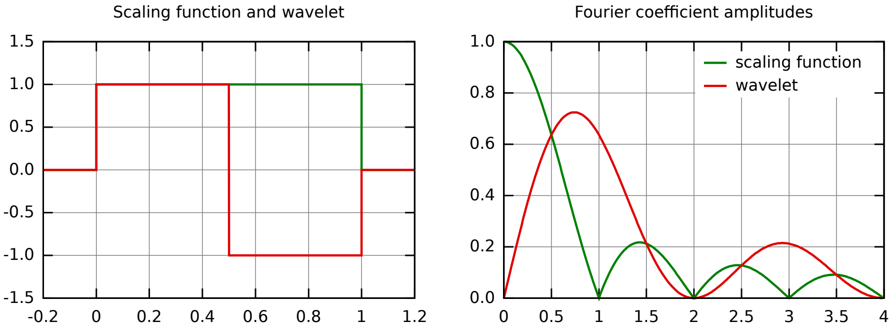
$$\int_{-\infty}^{\infty} \phi(x)\, \phi(x+l)\, \mathrm{d}x = \delta_{0,l}$$

After introducing some more conditions (as the restrictions above does not produce unique solution) we can obtain results of all this equations, i.e. the finite set of coefficients a_k which define the scaling function and also the wavelet. The wavelet is obtained from the scaling function as

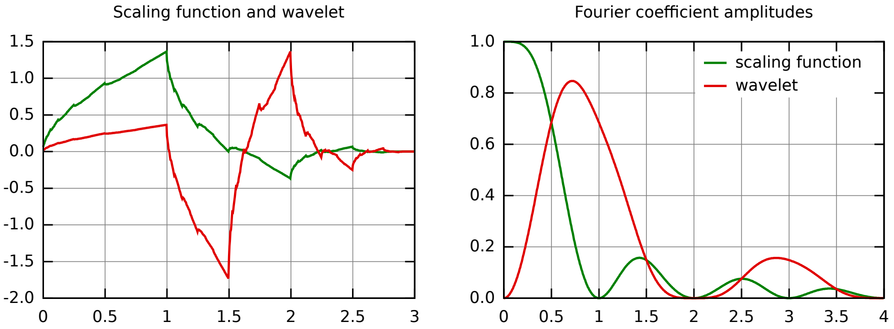
$$\psi(x) = \sum_{k=-\infty}^{\infty} (-1)^k a_{N-1-k} \psi(2x-k)$$

where N is an even integer. The set of wavelets than forms an orthonormal basis which we use to decompose signal. Note that usually only few of the coefficients a_k are nonzero which simplifies the calculations.

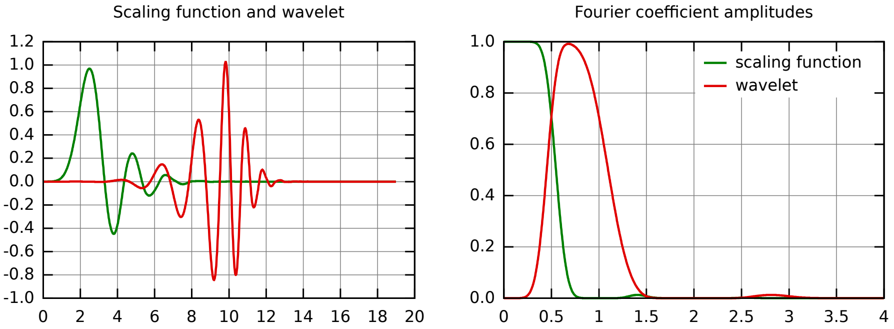
In the following figure, some wavelet scaling functions and wavelets are plotted. The most known family of orthonormal wavelets is a family of Daubechies. Her wavelets are usually denominated by the number of nonzero coefficients a_k, so we usually talk about Daubechies 4, Daubechies 6, etc. wavelets. Roughly said, with the increasing number of wavelet coeficients the functions become more smooth. See the comparison of wavelets Daubechies 4 and 20 below. Another mentioned wavelet is the simplest one, the Haar wavelet, which uses a box function as the scaling function.



Haar scaling function and wavelet (left) and their frequency content (right).



Daubechies 4 scaling function and wavelet (left) and their frequency content (right).



Daubechies 20 scaling function and wavelet (left) and their frequency content (right).

There are several types of implementation of the DWT algorithm. The oldest and most known one is the Malaat (pyramidal) algoritm. In this algorithm two filters – smoothing and non-smoothing one are constructed from the wavelet coefficients and those filters are recurrently used to obtain data for all the scales. If the total number of data $D = 2^N$ is used and signal length is L, first $D/2$ data at scale $L/2^{N-1}$ are computed, then $(D/2)/2$ data at scale $L/2^{N-2}$, $\ldots$ up to finally obtaining 2 data at scale $L/2$. The result of this algorithm is an array of the same length as the input one, where the data are usually sorted from the largest scales to the smallest ones.

Within Gwyddion the pyramidal algorithm is used for computing the discrete wavelet transform. Discrete wavelet transform in 2D can be accessed using DWT module.

Discrete wavelet transform can be used for easy and fast denoising of a noisy signal. If we take only a limited number of highest coefficients of the discrete wavelet transform spectrum, and we perform an inverse transform (with the same wavelet basis) we can obtain more or less denoised signal. There are several ways how to choose the coefficients that will be keeped. Within Gwyddion, the universal thresholding, scale adaptive thresholding [2] and scale and space adaptive thresholding [3] is implemented. For threshold determination within these methods we first determine the noise variance guess given by

$$\hat{\sigma} = \frac{\text{Median}\,|Y_{ij}|}{0.6745}$$

where Y_{ij} corresponds to all the coefficients of the highst scale subband of the decomposition (where most of the noise is assumend to be present). Alternatively, the noise variance can be obtained in an independent way, for example from the AFM signal variance while not scanning. For the highest frequency subband (universal thresholding) or for each subband (for scale adaptive thresholding) or for each pixel neighbourhood within subband (for scale and space adaptive thresholding) the variance is the computed as

$$\hat{\sigma}_Y^2 = \frac{1}{n^2} \sum_{i,j=1}^{n} Y_{ij}^2$$

Treshold value is finally computed as

$$T(\hat{\sigma}_X) = \hat{\sigma}^2 / \hat{\sigma}_X$$

where

$$\hat{\sigma}_X = \sqrt{\max(\hat{\sigma}_Y^2 - \hat{\sigma}^2, 0)}$$

When threshold for given scale is known, we can remove all the coefficients smaller than threshold value (hard thresholding) or we can lower the absolute value of these coefficients by threshold value (soft thresholding).

DWT denoising can be accessed with Data Process → Integral Transforms → DWT Denoise.

Continuous Wavelet Transform

Continuous wavelet transform (CWT) is an implementaion of the wavelet transform using an arbitrary scales and almost arbitrary wavelets. The wavelets used are not orthogonal and the data obtained by this transform are highly correlated. For the disctete time series we can uset this transform as well, with the limitation that the smallest wavelet translations must be equal to the data sampling. This is sometimes called Discrete Time Continuous Wavelet Transform (DT-CWT) and it is the mostly used way of computing CWT in real applications.

In principle the continuous wavelet transform works by using directly the definition of the wavelet transform, i.e. we are computing a convolution of the signal with the scaled wavelet. For each scale we obtain by this way an array of the same length N as the signal has. By using M arbitrarily chosen scales we obtain a field $N \times M$ that represents the time-frequency plane directly. The algoritm used for this computaion can be based on a direct convolution or on a convolution by means of multiplication in Fourier space (this is sometimes called Fast wavelet transform).

The choice of the wavelet that is used for time-frequency decomposition is the most important thing. By this choice we can inlfuence the time and frequency resolution of the result. We cannot change the main features of WT by this way (low frequencies have good frequecny and bad time resolution; high frequencies have good time and bad frequency resolution), but we can somehow increase the total frequency of total time resolution. This is directly proportional to the width of the used wavelet in real and Fourier space. If we use the Morlet wavelet for example (real part – damped cosine function) we can expect high frequency resolution as such a wavelet is very well localized in frequencies. In contrary, using Derivative of Gaussian (DOG) wavelet will result in good time localization, but poor one in frequencies.

CWT is implemented in the CWT module that can be accessed with Data Process → Integral Transforms → CWT.

References

[1] A. Bultheel: Bull. Belg. Math. Soc.: (1995) 2

[2] S. G. Chang, B. Yu, M. Vetterli: IEEE Trans. Image Processing, (2000) 9 p. 1532

[3] S. G. Chang, B. Yu, M. Vetterli: IEEE Trans. Image Processing, (2000) 9 p. 1522

4.13 Fractal Analysis

In practice objects exhibiting random properties are encountered. It is often assumed that these objects exhibit the self-affine properties in a certain range of scales. Self-affinity is a generalization of self-similarity which is the basic property of most of the deterministic fractals. A part of self-affine object is similar to whole object after anisotropic scaling. Many randomly rough surfaces are assumed to belong to the random objects that exhibit the self-affine properties and they are treated self-affine statistical fractals. Of course, these surfaces can be studied using atomic force microscopy (AFM). The results of the fractal analysis of the self-affine random surfaces using AFM are often used to classify these surfaces prepared by various technological procedures [1,2,3,4].

Within Gwyddion, there are different methods of fractal analysis implemented within Data Process → Statistics → Fractal analysis.

Cube counting method [1,2] is derived directly from a definition of box-counting fractal dimension. The algorithm is based on the following steps: a cubic lattice with lattice constant l is superimposed on the z-expanded surface. Initially $l$is set at $X/2$ (where X is length of edge of the surface), resulting in a lattice of $2 \times 2 \times 2 = 8$ cubes. Then $N(l)$ is the number of all cubes that contain at least one pixel of the image. The lattice constant l is then reduced stepwise by factor of 2 and the process repeated until l is equal to the distance between two adjacent pixels. The slope of a plot of $\log N(l)$ versus $\log 1/l$ gives the fractal dimension D_f directly.

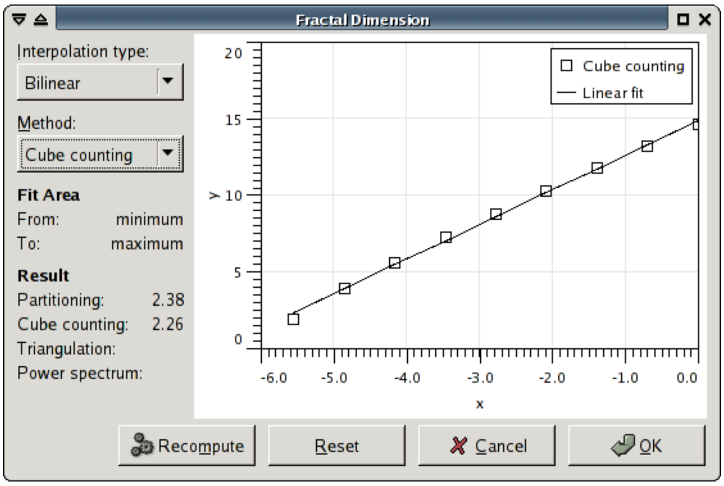
Triangulation method [1] is very similar to cube counting method and is also based directly on the box-counting fractal dimension definition. The method works as follows: A grid of unit dimension l is placed on the surface. This defines the location of the vertices of a number of triangles. When, for example, $l = X/4$, the surface is covered by 32 triangles of different areas inclined at various angles with respect to the xy plane. The areas of all triangles are calculated and summed to obtain an approximation of the surface area $S(l)$ corresponding to l. The grid size is then decreased by successive factor of 2, as before, and the process continues until l corresponds to distance between two adjacent pixel points. The slope of a plot of $S(l)$ versus $\log 1/l$ then corresponds to $D_\mathrm{f} - 2$.

Variance method [3,4] is based on the scale dependence of the variance of fractional Brownian motion. In practice, in the variance method one divides the full surface into equal-sized squared boxes, and the variance (power of RMS value of heights), is calculated for particular box size. Fractal dimension is evaluated from the slope β of a least-square regression line fit to the data points in log-log plot of variance as $D_\mathrm{f} = 3 - \beta/2$.

Power spectrum method [3,4,5] is based on the power spectrum dependence of fractional Brownian motion. In the power spectrum method, every line height profiles that forms the image is Fourier transformed and the power spectrum evaluated and then all these power spectra are averaged. Fractal dimension is evaluated from the slope In the power spectrum method, every line height profiles that forms the image is Fourier transformed and the power spectrum evaluated and then all these power spectra are averaged. Fractal dimension is evaluated from the slope β of a least-square regression line fit to the data points in log-log plot of power spectrum as $D_\mathrm{f} = 7/2 - \beta/2$.

The axes in Fractal Dimension graphs always show already logarithmed quantities, therefore the linear dependences mentioned above corresponds to straight lines there. The measure of the axes should be treated as arbitrary.

Note, that results of different methods differ. This fact is caused by systematic error of different fractal analysis approaches.



Interpolation type: Bilinear

Method: Cube counting

Fit Area
From: minimum
To: maximum

Result
Partitioning: 2.38
Cube counting: 2.26
Triangulation:
Power spectrum:

Fractal Dimension dialog.

Moreover, the results of the fractal analysis can be influenced strongly by the tip convolution. We recommned therefore to check the certainty map before fractal analysis. In cases when the surface is influenced a lot by tip imaging, the results of the fractal analysis can be misrepresented strongly.

Note, that algorithms that can be used within the fractal analysis module are also used in Fractal Correction module and Fractal Correction option of Remove Spots tool.

References

[1] C. Douketis, Z. Wang, T. L. Haslett, M. Moskovits: Fractal character of cold-deposited silver films determined by low-temperature scanning tunneling microscopy. Physical Review B, Volume 51, Number 16, 15 April 1995, 51

[2] W. Zahn, A. Zösch: The dependance of fractal dimension on measuring conditions of scanning probe microscopy. Fresenius J Analen Chem (1999) 365: 168-172

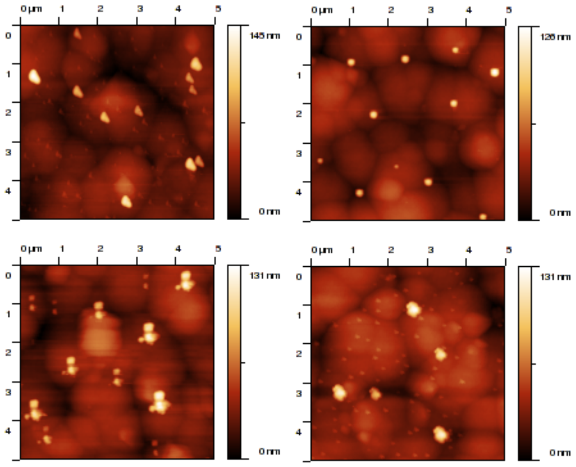
[3] A. Van Put, A. Vertes, D. Wegrzynek, B. Treiger, R. Van Grieken: Quantitative characerization of individual particle sutfaces by fractal analysis of scanning electron microscope images. Fresenius J Analen Chem (1994) 350: 440-447

[4] A. Mannelquist, N. Almquist, S. Fredriksson: Influence of tip geometry on fractal analysis of atomic force microscopy images. Appl. Phys. A 66,1998, 891-895

[5] W. Zahn, A. Zösch: Characterization of thin film surfaces by fractal geometry. Fresenius J Anal Chem (1997) 358: 119-121

4.14 Tip Convolution Artefacts

Tip convolution artefact is one of the most important error sources in SPM. As the SPM tip is never ideal (like delta function) we often observe a certain degree of image distortion due to this effect. We can even see some SPM tips imaged on the surface scan while sharp features are present on the surface.



Images of ZnSe surface measured with four different SPM tips (more or less broken ones).

We can fortunately simulate and/or correct the tip efects using algorithms of dilation and/or erosion, respectively. These algorithms were published by Villarubia (see [1]).

Obtaining the Tip Geometry

For studying the tip influence on the data we need to know tip geometry firts. In general, the geometry of the SPM tip can be determined in these ways:

1. use manufacturer's specifications (tip geometry, apex radiius and angle)
2. use scanning electron microscope of other independent technique to determine tip properties.
3. use known tip characterizer sample (with steep edges)

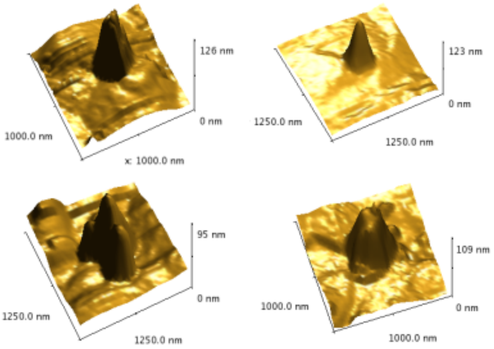
4. use blind tip estimation algorithm together with tip characterizers or other suitable samples

Within Gwyddion, we can use the first and the last approach of the mentioned ones. Using tip modelling (Data Process → Tip → Model Tip) most of the tips with simple geometries can be simulated. This way of tip geometry specification can be very efficient namely when we need to check only certainty map of perform tip convolution simulation.

To obtain more detailed (and more realistic) tip structure blind tip estimation algorithm can be used (Data Process → Tip → Blind Estimation).

Blind tip estimation algorithm is an extension of the well-known fact that on some surface data we can see images of certain parts of tip directly. The algortihm iterates over all the surface data and at each point tries to refine each tip point according to steepest slope in the direction between concrete tip point and tip apex.

We can use two modification of this algorithm within Gwyddion: *partial* tip estimation that uses only limited number of highest points on the image and *full* tip estimation taht uses full image (and is much slower therefore). Within Gwyddion tip estimation module we can use also partial tip estimation results as starting point for full estimation. This shlould improve the full tip estimation algorithm speed.

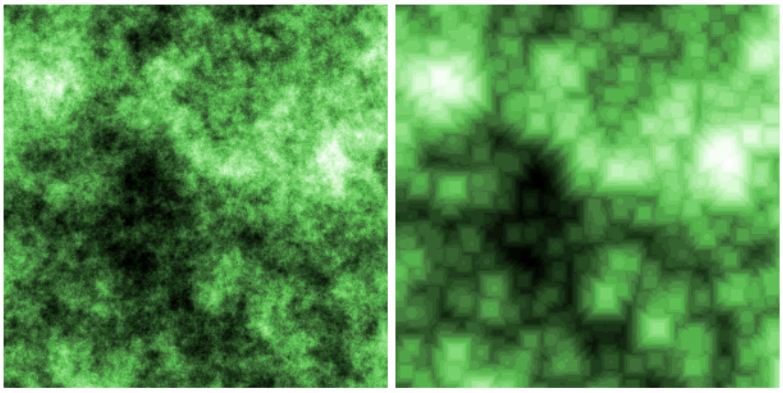


SPM tips obtained from data of previous figure using blind estimation algorithm.

Tip Convolution and Surface Reconstruction

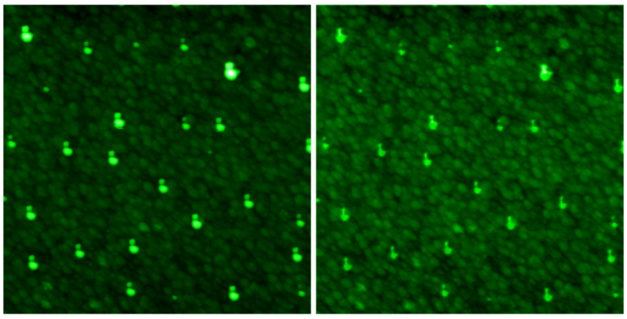
When we know tip geometry, we can use tip convolution (dilation) algorithm to simulate data acquisition process. For doing this use Dilation module (Data Process → Tip → Dilation). This can be in particular useful when working with data being result of some numerical modelling (see e.g. [2]).

Note this alrgorithms (as well as the following two) requires compatible scan and tip data, i.e. the physical dimensions of a scan pixel and of a tip image pixels have to be equal. This relation is automatically guaranteed for tips obtained by blind estimate when used on the same data (or data with an identical measure). If you obtained the tip image other means, you may need to resample it.



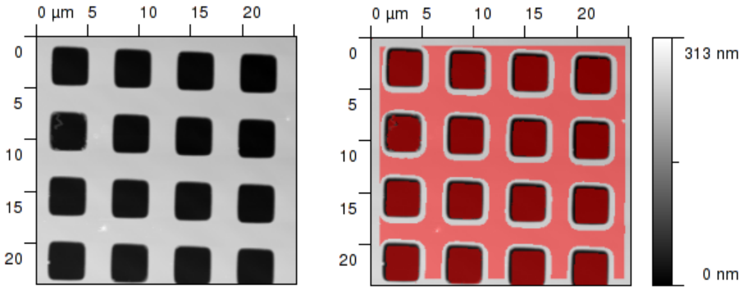
Simulated fractal surface before (left) and after (right) tip convolution.

The opposite of the tip convolution is surface reconstruction (erosion) that can be used to correct partially the tip influence on image data. For doing this, use Surface Reconstruction function (Data Process → Tip → Surface Reconstruction). Of course, the data corresponding to point in image not touched by tip (e. g. pores) cannot be reconstructed as there is no information about these points.



Original and reconstructed image of ZnSe imaged by broken SPM tip.

As it can be seen, the most problematic parts of SPM image are data points, where tip did not touch the surface in a single point, mut in multiple points. There is a loss of information in these points. Certainty map algorithm can mark point where surface was probably touched in a single point.



Certainty map obtained from standard grating. Note that the modelled tip parameters were taken from datasheet here for illustration purposes. (left) – sample, (right) – sample with marked certainty map.

Certainty map algortihm can be therefore used to mark data in the SPM image that are corrupted by tip convolution in an irreversible way. For SPM data analysis on surfaces with large slopes it is important to check always presence of these points. Within Gwyddion you can use Ceratinty Map function for creating these maps (Data Process → Tip → Certainty Map).

References

[1] J. S. Villarubia, J. Res. Natl. Inst. Stand. Technol. 102 (1997) 425.

[2] P. Klapetek, I. Ohlídal, Ultramicroscopy, 94 (19-29), 2003

4.15 Multiple Data

Arithmetic

Data Process → Multidata → Arithmetic

Data Arithmetic module makes possible to perform arbitrary point-wise operations on a single data field or corresponding points of several data fields (currently up to five). And although it is not its primary function it can be also used as a calculator with immediate expression evaluation. The expression syntax is described in section Expressions.

The data fields to operate on are called Operands and they are denoted **d1**, . . . , **d5**. In addition to values, local *x* and *y*-derivatives are denoted **bx1**, **by1**, **bx2**, . . . , **by5**.

The data fields that actually appear in the expression have to be compatible, i.e. their dimensions (both pixel and physical) have to be identical. Other data fields (i.e. those not actually entering the expression) are irrelevant. The result is always put into a newly created data field.

Examples: `-d1` performs value inversion – very similar to Invert Value, except that Invert Value reflects about the mean value while now we simply change all values to negative, `(d1 - d2)^2` calculates squared difference between two data fields.

In the calculator mode the expression is immediately evaluated as it is typed and the result is displayed below Expression entry. No special action is necessary to switch between data field expressions and calculator: expressions containing only numeric quantities are immediately evaluated, expressions referring to data fields are used to calculate a new data field.

Detail Immersion

Data Process → Multidata → Immerse

Immerse insets a detail, high-resolution image into a larger image. The image the function was run on forms the large, base image.

The detail can positioned manually on the large image with mouse. Button Improve can then be used to find the exact coordinates in the neighbourhood of the current position that give the maximum correlation between the detail and the large image. Or the best-match position can be searched through the whole image with Locate.

It should be noted the correlation search is insensitive to value scales and offsets, therefore the automated matching is based solely on data features, absolute heights play no role.

Result Sampling controls the size and resolution of the result image:

Upsample large image The resolution of the result is determined by the resolution of the inset detail. Therefore the large image is scaled up.

Downsample detail The resolution of the result is determined by the resolution of the large image. The detail is downsampled.

Detail Leveling selects the transform of the z values of the detail:

None No z value adjustment is performed.

Mean value All values of the detail image are shifted by a constant to make its mean value match the mean value of the corresponding area of the large image.

Merging

Data Process → Multidata → Merge

Images that form parts of a larger image can be merged together with Merge. The image the function was run on forms corresponds to the base image, the image selected with Merge with represents the second operand. The side of the base image the second one will be attached to is controlled with Put second operand selector.

If the images match perfectly, they can be simply placed side by side with no adjustments. This behaviour is selected by option None of alignment control Align second operand.

However, usually adjustments are necessary. Option Correlation selects automated alignment by correlation-based search of the best match. The search is performed both in the direction parallel to the attaching side and in the perpendicular direction. If a parallel shift is present, the result is expanded to contain both images fully (with undefined data filled with a background value).

Option Boundary treatment is useful only for the latter case of imperfectly aligned images. It controls the treatment of overlapping areas in the source images:

First operand Values in overlapping areas are taken from the first, base image.

Second operand Values in overlapping areas are taken from the second image.

Smooth A smooth transition between the first and the second image is made through the overlapping area by using a weighted average with a suitable weighting function.

Cross-Correlation

Data Process → Multidata → Cross-correlation

Module finds local correlations between details on two different images. As an ideal output, the shift of every pixel on the first image as seen on the second image is returned. This can be used for determining local changes on the surface while imaged twice (shifts can be for example due to some sample deformation or microscope malfunction).

For every pixel on the first operand (actual window), the module takes its neighbourhood and searches for the best correlation in the second operand within defined area. The postion of the correlation maximum is used to set up the value of shift for the mentioned pixel on the first operand.

Second operand Image to be used for comparison with the first operand - base image.

Search size Used to set the area whera algoritgm will search for the local neighbourhood (on the second operand). Should be larger than window size. Increase this size if there are big differences between the compared images.

Window size Used to set the local neighbourhood size (on the first operand). Should be smaller than search size. Increasing this value can improve the module functionality, but it will surely slow down the computation.

Output type Determines the output (pixel shift) format.

Add low score threshold mask For some pixels (with not very pronounced neighbourhood) the correlation scores can be small everywhere, but the algorithm anyway picks some maximum value from the scores. To see these pixels and possibly remove them from any further considerations you can let the module to set mask of low-score pixel shifts that have larger probability to be not accurately determined.

Mask by Correlation

Data Process → Multidata → Mask by Correlation

Module searches for a given correlation pattern within the actual image. The resulting pattern position is marked as a mask in the data window.

Correlation kernel Image to be found on the base image.

Output type There are several possibilities what to output: local correlation maxima (single points), masks of kernel size for each correlation maximum (good for presentation purposes), or simply the correlation score.

Correlation method Algorithm for computing correlation can be selected here.

Threshold Threshold for determining whether the local maximum will be treated as ‘correlation kernel found here’.

4.16 Graph Processing

Many of the Gwyddion data processing modules produce graph as a output. Graphs can be exported into text files or further analyzed within Gwyddion by several graph processing modules. These modules can be found in the Graph menu in the Gwyddion main window. Note that the number of graph modules is quite limited now and consists of basic modules for doing things that are very frequent within SPM data analysis. For more analytical tools you can use your favorite graph processing program.

In this section the graph modules present in Gwyddion are briefly presented.

Basic Operations

First of all zooming and data reading functions are available directly in the graph window:

- Logarithmic axes – horizontal and vertical axes can be switched between linear and logarithmic using the logscale buttons. Switching to logarithmic scale is possible only for positive values (either on abscissa or ordinate).
- Zoom in and zoom out – after selecting zoom in simply draw the area that should be zoomed by mouse. Zoom out restores the state when all data can be seen.
- Measure distances – enables user to select several points within the graph and displays their distances and angles between them.

Graph Level

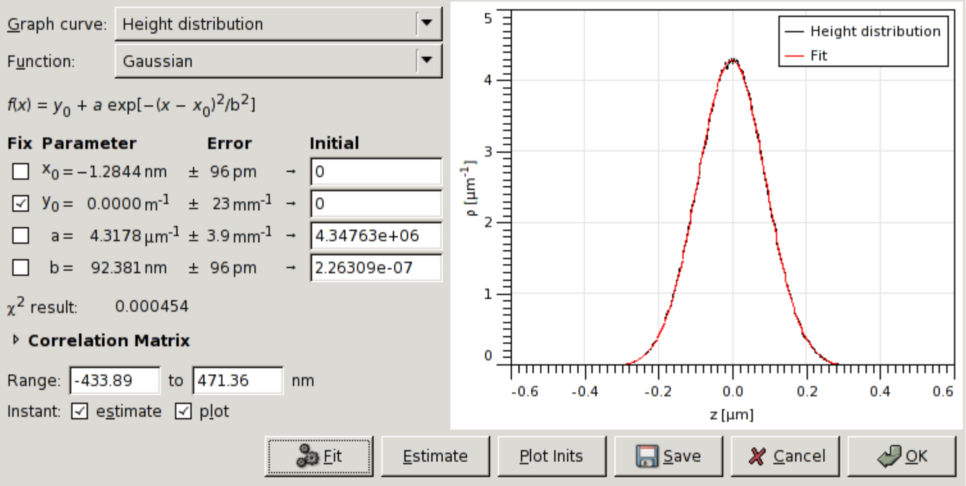
Graph level is a very simple module that currently performs linear fit of each graph curve and subtracts the fitted linear functions from them.

Function Fitting

The curve fitting is designed namely for fitting of statistical functions used in roughness parameters evaluation. Therefore most of the available functions are currently various statistical functions of surfaces with Gaussian or exponential autocorrelation functions. Nevertheless it also offers a handful of common general-purpose functions.

Within the fitting module you can select the area that should be fitted (with mouse or numerically), try some initial parameters, or let the module to guess them, and then fit the data using Marquardt-Levenberg algorithm.

As the result you obtain the fitted curve and the set of its parameters. The fit report can be saved into a file using Save button. Pressing OK button adds the fitted curve to the graph, if this is not desirable, quit the dialog with Cancel.



Graph curve: Height distribution

Function: Gaussian

$f(x) = y_0 + a \exp[-(x - x_0)^2/b^2]$

Fix	Parameter	Error		Initial
□	$x_0 = -1.2844$ nm	± 96 pm	→	0
☑	$y_0 =$ 0.0000 m^{-1}	± 23 mm^{-1}	→	0
□	a = 4.3178 µm^{-1}	± 3.9 mm^{-1}	→	4.34763e+06
□	b = 92.381 nm	± 96 pm	→	2.26309e-07

χ^2 result: 0.000454

▸ Correlation Matrix

Range: -433.89 to 471.36 nm

Instant: ☑ estimate ☑ plot

Curve fitting module dialog

Force-Distance Curve Fitting

The module for fitting of force-distance curves is very similar to the general curve fitting module, it is just specialized for force-distance curves. Currently, the module serves for fitting jump-in part of force-distance curve (representing attractive forces) using different models:

- van der Waals force between semisphere and half-space
- van der Waals force between pyramide and half-space
- van der Waals force between truncated pyramide and half-space
- van der Waals force between sphere and half-space
- van der Waals force between two spheres
- van der Waals force between cone and half-space
- van der Waals force between cylinder and half-space
- van der Waals force between paraboloid and half-space

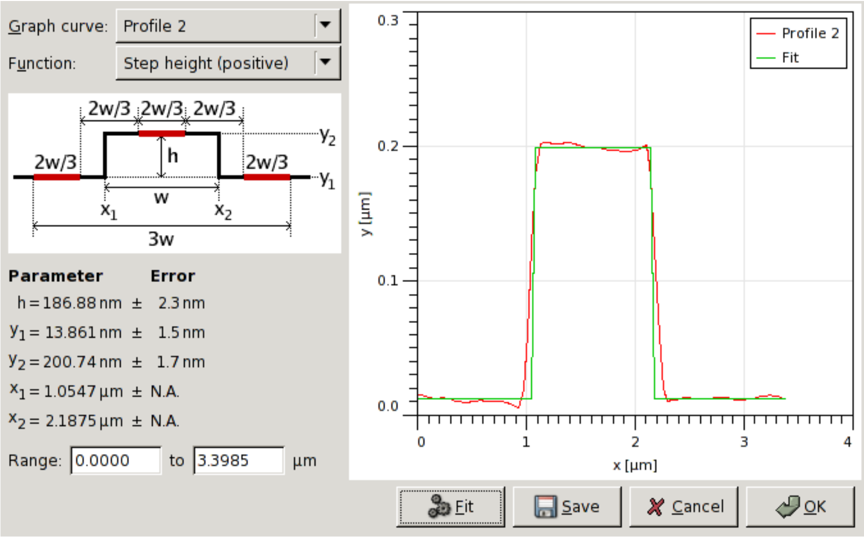
Note that the curve being fitted must be a real force-distance curve, not a displacement-distance or sensor-distance curve. Recalculation of cantilever deflection into force should be done before calling this module.

Also note that for small cantilever spring constants the amount of usable data in attractive region is limited by effect of jumping into contact.

Critical Dimension

Critical dimension module can be used to fit some ‘typical’ objects that are often found while analyzing profiles extracted from microchips and related surfaces. These objects are located in the graph and their properties are evaluated.

The user interface of this module is practically the same as of the graph fit module.



Graph curve: Profile 2

Function: Step height (positive)

Parameter	Error
h = 186.88 nm	± 2.3 nm
y_1 = 13.861 nm	± 1.5 nm
y_2 = 200.74 nm	± 1.7 nm
x_1 = 1.0547 µm	± N.A.
x_2 = 2.1875 µm	± N.A.

Range: 0.0000 to 3.3985 µm

Critical dimension module dialog.

4.17 Synthetic Surfaces

Beside functions for analysis of measured data, Gwyddion provides several generators of artificial surfaces that can be used for testing or simulations also outside Gwyddion.

All the surface generators share a certain set of parameters, determining the dimensions and scales of the created surface and the random number generator controls. These parameters are described below, the parameters specific to each generator are described in the corresponding subsections.

Image parameters:

Horizontal, Vertical size The horizontal and vertical resolution of the generated surface in pixels.

Square image This option, when enabled, forces the horizontal and vertical resolution to be identical.

Width, Height The horizontal and vertical physical dimensions of the generated surface in selected units. Note square pixels are assumed so, changing one causes the other to be recalculated.

Dimension, Value units Units of the lateral dimensions (Width, Height) and of the values (heights). The units chosen here also determine the units of non-dimensionless parameters of the individual generators.

Like Current Channel Clicking this button fills all the above parameters according to the current channel.

Note that while the units of values are updated, the value scale is defined by generator-specific parameters that might not be directly derivable from the statistical properties of the current channel. Hence these parameters are not recalculated.

Replace the current channel This option has two effects. First, it causes the dimensions and scales to be automatically updated each time the function is used as if Like Current Channel was clicked. Second, it makes the generated surface replace the current channel instead of creating a new channel.

Random generator controls:

All generated surfaces are periodic (i.e. perfectly tilable).

Random seed The random number generator seed. Choosing the same parameters and resolutions and the same random seed causes the same surface to be generated, even on different computers. Different seeds lead to different surfaces with the same overall characteristics given by the generator parameters.

New Replaces the seed with a random number.

Randomize Enabling this option makes the seed to be chosen randomly every time the generator is run. This permits to conveniently re-run the generator with a new seed simply by pressing **Ctrl-F** (see keyboard shortcuts).

Spectral

Spectral synthesis module creates randomly rough surfaces by constructing the Fourier transform of the surface according to specified parameters and then performing the inverse Fourier transform to obtain the real surface.

The Fourier image parameters define the shape of the PSDF, i.e. the Fourier coefficient modulus, the phases are chosen randomly. At present, all generated surfaces are isotropic, i.e. the PSDF is radially symmetric.

RMS The root mean square value of the heights (or of the differences from the mean plane which, however, always is the $z = 0$ plane).

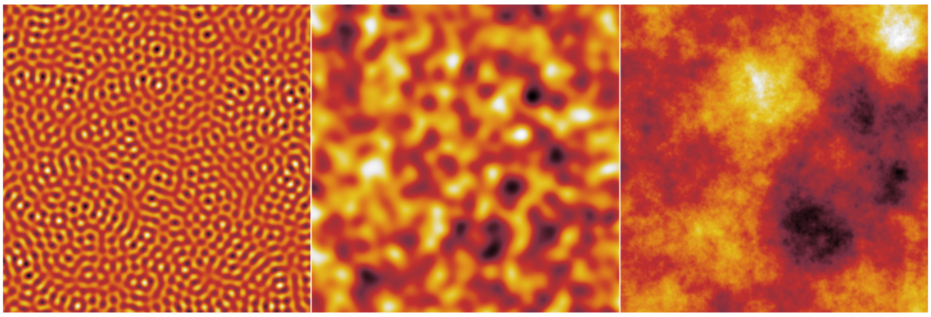
Minimum, maximum frequency The minimum and maximum spatial frequency. Increasing the minimum frequency leads to ‘flattening’ of the image, i.e. to removal of large features. Decreasing the maximum frequency limits the sharpness of the features.

Enable Gaussian multiplier Enables the multiplication of the Fourier coefficients by a Gaussian function that in the real space corresponds to the convolution with a Gaussian.

Autocorrelation length The autocorrelation length of the Gaussian (see section Statistical Analysis for the discussion of autocorrelation functions).

Enable power multiplier Enables multiplication by factor proportional to $1/k^p$, where k is the spatial frequency and p is the power. This permits to generate various fractal surfaces.

Power The power p.



Artificial surfaces generated by spectral synthesis: a narrow range of spatial frequencies (left), Gaussian random surface (centre) and a fractal surface generated with power multiplier of 1.5 (right).

Objects

The object placement method permits to create random surfaces composed of features of a particular shape. The algorithm is simple: the given number of objects is placed on random positions at the surface. For each object placed, the new heights are changed to $\max(z, z_0 + h)$, where z is the current height at a particular pixel, h is the height of the object at this pixel (assuming a zero basis) and z_0 is the current minimum height over the basis of the object being placed.

Shape The shape (type) of placed objects. At present the possibilities include half-spheres, boxes, pyramids, tetrahedrons and some more weird shapes.

Coverage The average number of times an object covers a pixel on the image. Coverage value of 1 means the surface would be exactly once covered by the objects provived that thay covered it uniformly. Larger values mean more layers of objects – and slower image generation.

Size The object size, usually the side of a containing square.

Aspect Ratio The ratio between the *x* and *y* dimensions of an object – with respect to same base proportions.

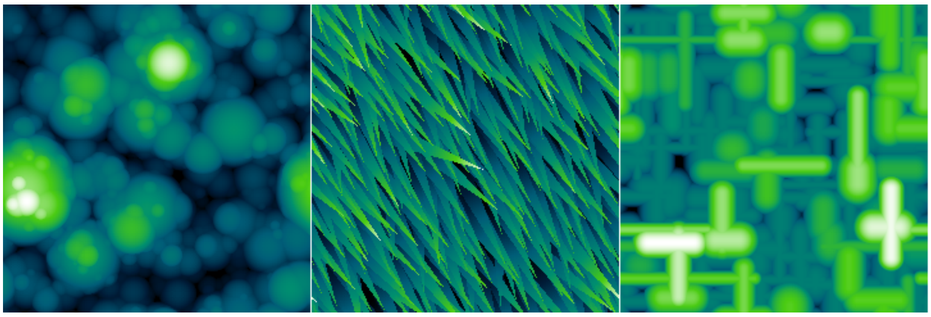
Changing the aspect ratio does not always imply mere geometrical scaling, e.g. objects called nuggets change between half-spheres and rods when the ratio is changed.

Height A quantity proportional to the height of the object, normally the height of the highest point.

Checking Scales with size makes unperturbed heights to scale proportionally with object size. Otherwise the height is independent on size.

Orientation The rotation of objects with respect to some base orientation, measured counterclockwise.

Each parameter can be randomized for individual objects, this is controlled by Variance. For multiplicative quantities (all except orientation), the distribution is log-normal with the RMS value of the logarithmed quantity given by Variance.



Artificial surfaces generated by object placement: spheres of varied size (left), narrow thatches of varied direction (centre), nuggets of varied aspect ratio (right).

Chapter 5

Summaries and Tables

This chapter provides reference for various formats, syntaxes and command options that you might find helpful. Most are related to advanced use of Gwyddion, except perhaps the table of common keyboard shortcuts and table of supported file formats.

5.1 gwyddion

Name

gwyddion – SPM data visualization and analysis

Synopsis

`gwyddion` [*OPTION*...] [*FILE*...]

Description

Gwyddion is a graphical SPM (Scanning Probe Microscope) data visualization and analysis program, using Gtk+.

Options

The program accepts all standard Gtk+, Gdk, and GtkGLExt options like `--display` or `--sync`. Please see documentation of these packages for description of toolkit options.

The behaviour of the remote-control options `--remote-*` is undefined when more than one instance of Gwyddion is running on the display. They can choose an arbitrary instance to communicate to.

Gwyddion options:

`--help` Prints a brief help and terminates.

`--version` Prints version information and terminates.

`--no-splash` Disables splash screen on program startup.

`--remote-new` Opens files given on the command line in an already running instance of Gwyddion on the display. Runs a new instance if none is running.

This is probably the most useful remote control option. File type associations are usually installed to run Gwyddion with this option.

`--remote-existing` Opens files given on the command line in an already running instance of Gwyddion on the display. Fails if none is running.

This is useful if you want to handle the case of Gwyddion not running differently than by starting it.

`--remote-query` Succeeds if an instance of Gwyddion is already running on the display and prints its instance identifier. Fails if none is running.

The instance identifier depends on the remote control backend in use. In some cases it is useful as a global window identifier, in some it is not. With libXmu this option prints the X11 Window, on Win32 HWND is printed, while with LibUnique the startup id is printed.

`--check` Instead of running the user interface and opening *FILE*s, it loads the files, performs a sanity check on them (printing errors to standard error output) and terminates.

--log-to-file Redirect messages from GLib, Gtk+, Gwyddion, etc. to `~/.gwyddion/gwyddion.log` or file given in GWYDDION_LOGFILE environment variable. Note messages are always redirected to a file on Win32 so, this option has not effect on Win32.

--debug-objects Prints list of objects created during run time, with creation and desctruction times or reference counts on program exit. Useful only for developers.

--startup-time Prints wall-clock time taken by various startup (and shutdown) tasks. Useful only for developers and people going to complain about too slow startup.

Environment

On Linux/Unix, following environment variables can be used to override compiled-in installation paths (MS Windows version always looks to directories relative to path where it was installed). Note they are intended to override system installation paths therefore they are not path lists, they can contain only a single path.

GWYDDION_DATADIR Base data directory where resources (color gradients, OpenGL materials, ...) were installed. Gwyddion looks into its `gwyddion` subdirectory for resources.

When it is unset, it defaults to compiled-in value of `${datadir}` which is usually `/usr/local/share`.

GWYDDION_LIBDIR Base library directory where modules were installed. Gwyddion looks into its `gwyddion/modules` subdirectory for modules.

When it is unset, it defaults to compiled-in value of `${libdir}` which is usually `/usr/local/lib` or `/usr/local/lib64`.

GWYDDION_LIBEXECDIR Base lib-exec directory where plug-ins were installed. Gwyddion looks into its `gwyddion/plugins` subdirectory for plug-ins.

When it is unset, it defaults to compiled-in value of `${libexecdir}` which is usually `/usr/local/libexec`.

GWYDDION_LOCALEDIR Locale data directory where message catalogs (translations) were installed.

When it is unset, it defaults to compiled-in value of `${datadir}/locale` which is usually `/usr/local/share/locale`.

Other variables that influence Gwyddion run-time behaviour include GLib+ variables and Gtk+ variables and some Gwyddion-specific variables:

GWYDDION_LOGFILE Name of file to redirect log messages to. On MS Windows, messages are always sent to a file as working with the terminal is cumbersome there. The default log file location, `gwyddion.log` in user's Documents and Settings, can be overriden with `GWYDDION_LOGFILE`. On Unix, messages go to the terminal by default and this environment variable has effect only if `--log-to-file` is given.

Files

~/.gwyddion/settings Saved user settings and tool states. Do not edit while Gwyddion is running, it will overwrite it at exit.

~/.gwyddion/glmaterials, ~/.gwyddion/gradients, ... User directories with various resources (OpenGL materials, color gradients, ...).

$GWYDDION_DATADIR/gwyddion/glmaterials, $GWYDDION_DATADIR/gwyddion/gradients ... The same for system-wide resources.

~/.gwyddion/pixmaps Directory to place user icons to. This is mainly useful for installation of modules to home.

$GWYDDION_DATADIR/gwyddion/pixmaps, The same for system-wide icons.

~/.gwyddion/modules Directory to place user modules to. They should be placed into `file`, `graph`, `process`, `layer`, and `tools` subdirectories according to their kind, though this is more a convention than anything else.

$GWYDDION_LIBDIR/gwyddion/modules, The same for system-wide modules.

~/.gwyddion/plugins Directory to place user plug-ins to. They should be placed into `file` and `process` subdirectories according to their kind.

$GWYDDION_LIBEXECDIR/gwyddion/plugins, The same for system-wide plug-ins.

~/.gwyddion/pygwy Directory to place user python modules or scripts to.

See also

gwyddion-thumbnailer(1), gxsm(1)

5.2 gwyddion-thumbnailer

Name

gwyddion-thumbnailer – Create thumbnails of SPM data files

Synopsis

`gwyddion-thumbnailer` --version | --help

`gwyddion-thumbnailer` [*OPTION*...] *MODE* [*ARGUMENT*...]

Description

Gwyddion-thumbnailer creates thumbnails of SPM (Scanning Probe Microscope) image files. Depending on the mode of operation, described below, the thumbnails are written to conform to various desktop standards so that they can be displayed in nautilus(1), thunar(1) and similar file managers.

Gwyddion-thumbnailer loads and renders files using gwyddion(1), libraries and modules, therefore, it can create thumbnails of all file formats supported by your Gwyddion installation. This also means it inherits Gwyddion settings, e.g. the default false color gradient, and that it is influenced by the same environment variables as Gwyddion.

Informative Options

--help Prints a brief help and terminates.

--version Prints version information and terminates.

Thumbnailing Options

--update Writes the thumbnail only if it does not exist yet or does not seem to be up-to-date. By default, gwyddion-thumbnailer overwrites existing thumbnails with fresh ones even if they seem up to date.

Mode

Three thumbnailing modes are available: `gnome2`, `tms` and `kde4`; and one special mode: `check`. They are described below.

Gnome 2

`gwyddion-thumbnailer` [*OPTION*...] gnome2 *MAX-SIZE INPUT-FILE OUTPUT-FILE*

In `gnome2` mode, gwyddion-thumbnailer creates PNG thumbnails according to the Gnome thumbnailer specification. Usings the convention from this specification, it should be run

```
gwyddion-thumbnailer gnome2 %s %i %o
```

Gwyddion installs the corresponding GConf schemas and enables thumbnailers for all file types it supports by default, so usually this should Just Work and should not need to be set up manually.

The thumbnails created in `gnome2` more are identical as in `tms` mode, including all the PNG auxiliary chunks (provided that the same *MAX-SIZE* as in `tms` mode is specified, of course).

TMS

`gwyddion-thumbnailer` [*OPTION*...] tms *MAX-SIZE* *INPUT-FILE*

In `tms` mode, gwyddion-thumbnailer creates PNG thumbnails according to the Thumbnail Managing Standard. Argument *MAX-SIZE* must be `128` or `normal` (both meaning 128 pixels) or `256` or `large` (both meaning 256 pixels).

Output file name is not given as it is prescribed by the TMS. The thumbnail is placed to the directory for normal or large thumbnails according to given *MAX-SIZE*.

This mode can also be useful for manual batch-creation of thumbnails. For instance, to create them for all `*.afm` files in directory `scans` and its subdirectories, you can run

```
find scans -type f -name '*.afm' -print0 \\
    | xargs -0 -n 1 gwyddion-thumbnailer --update tms normal
```

And then go make yourself a coffee because this will take some time.

KDE 4

`gwyddion-thumbnailer` kde4 *MAX-SIZE* *INPUT-FILE*

In `kde4` mode, gwyddion-thumbnailer creates PNG thumbnails that are intended to be consumed by gwythumbcreator KDE module. The thumbnail, again identical as in the other modes, is written to the standard output.

Do *not* use this mode from the command line. It is documented for completness, however, the protocol between gwythumbcreator and gwyddion-thumbnailer must be considered private and it can change any time.

Check

`gwyddion-thumbnailer` check *INPUT-FILE*

The `check` mode does not serve for thumbnail creation. Instead, gwyddion-thumbnailer prints information about available thumbnails of *INPUT-FILE* and cached failures to produce a thumbnail by individual applications, as described by the TMS.

If the normal-sized thumbnail exists and is up to date, the large version does not exist and there is one cached failure from gnome-thumbnail-factory, the output can be for instance:

```
File:   INPUT-FILE
URI:    file:///home/me/Pictures/naughty/broken-tip3/INPUT-FILE
Normal: /home/me/.thumbnails/normal/MD5.png
        status: OK
Large:  /home/me/.thumbnails/large/MD5.png
        status: Thumbnail does not exist or stat() fails on it.
Failed: /home/me/.thumbnails/fail/gnome-thumbnail-factory/MD5.png
```

URI is the canonical URI of the input file, *MD5* stands for the hex representation of MD5 sum of the URI, as described by the TMS. If there are no cached failures, no Failed lines are printed.

This function can be used to check thumbnails of any kind, not necessarily created by gwyddion or gwyddion-thumbnailer. In future, it might be reported as an error if the thumbnail does not contain Gwyddion-specific information though.

See also

gwyddion(1),

5.3 Keyboard Shortcuts

Shortcut	Menu equivalent	Context	Action
Ctrl-Q	File → Quit	toolbox, data window, 3D window, graph window, tool window	Quit Gwyddion.
Ctrl-O	File → Open	toolbox, data window, 3D window, graph window, tool window	Open a data file.

Shortcut	Menu equivalent	Context	Action
Ctrl-S	File → Save	toolbox, data window, 3D window, graph window, tool window	Save current data (you will be prompted for a file name if none is associated yet).
Ctrl-Shift-S	File → Save As	toolbox, data window, 3D window, graph window, tool window	Save current data under a different name. The file name associated with the data changes to the new name.
Ctrl-Shift-M	File → Merge	toolbox, data window, 3D window, graph window, tool window	Merge data from a file to the current file.
Ctrl-Z	Edit → Undo	toolbox, data window, 3D window, graph window, tool window	Undo the last processing step applied on current data.
Ctrl-Y	Edit → Redo	toolbox, data window, 3D window, graph window, tool window	Redo the last processing step applied on current data.
Ctrl-K	Edit → Remove Mask	toolbox, data window, 3D window, graph window, tool windows	Remove mask from current data window.
Ctrl-Shift-K	Edit → Remove Presentation	toolbox, data window, 3D window, graph window, tool windows	Remove presentation from current data window.
+		data window	Zoom current data window in.
=		data window	Zoom current data window in.
-		data window	Zoom current data window out.
Z		data window	Zoom current data window 1:1.
Ctrl-F	Data Process → Repeat Last	toolbox, data window, 3D window, graph window, tool windows	Repeat last data processing function with the last used parameters, on current data. Normally the operation is repeated silently, but if the processing step cannot be carried out without a human interaction, a dialog is shown.
Ctrl-Shift-F	Data Process → Re-Show Last	toolbox, data window, 3D window, graph window, tool windows	Re-show parameter dialog of the last data processing function. If the operation has no parameters to set, it is performed immediately.

5.4 Supported File Formats

File Format	Extensions	Module	Read	Write	SPS
APE Research DAT	.dat	apefile	Yes	No	No
Text matrix of data values	.txt	asciiexport	No	Yes	No
Assing AFM	.afm	assing-afm	Yes	Yes	No
Attocube Systems ASC	.asc	attocube	Yes	No	No
Image Metrology BCR, BCRF	.bcr, .bcrf	bcrfile	Yes	No	No
Burleigh BII	.bii	burleigh_bii	Yes	No	No
Burleigh IMG v2.1	.img	burleigh	Yes	No	No
Burleigh exported data	.txt, .bin	burleigh_exp	Yes	No	No
Createc DAT	.dat	createc	Yes	No	No
DME Rasterscope	.img	dmefile	Yes	No	No
ECS	.img	ecsfile	Yes	No	No
Nanosurf EZD, NID	.ezd, .nid	ezdfile	Yes	No	No

File Format	Extensions	Module	Read	Write	SPS
Gwyddion native data	.gwy	gwyfile	Yes	Yes	Yes
Psi HDF4	.hdf	hdf4file	Yes	No	No
Hitachi AFM	.afm	hitachi-afm	Yes	No	No
WaveMetrics IGOR binary wave v5	.ibw	igorfile	Yes	No	No
Intematix SDF	.sdf	intematix	Yes	No	No
JEOL	.tif	jeol	Yes	No	No
JPK Instruments	.jpk	jpkscan	Yes	No	No
MapVue	.map	mapvue	Yes	No	No
Zygo MetroPro DAT	.dat	metropro	Yes	No	No
MicroProf TXT	.txt	microprof	Yes	No	No
MicroProf FRT	.frt	microprof	Yes	No	No
Molecular Imaging MI	.mi	mifile	Yes	No	Limited[1]
Nanoeducator	.mspm, .stm, .spm	nanoeducator	Yes	No	No
Nanonics NAN	.nan	nanonics	Yes	No	No
Nanonis SXM	.sxm	nanonis	Yes	No	No
Nanoscan XML	.xml	nanoscan	Yes	No	No
Veeco Nanoscope III	.001, .002, etc.	nanoscope	Yes	No	No
Veeco Nanoscope II	.001, .002, etc.	nanoscope-ii	Yes	No	No
Nanotop SPM	.spm	nanotop	Yes	No	No
GSXM NetCDF	.nc	netcdf	Yes	No	No
NT-MDT	.mdt	nt-mdt	Yes	No	Yes
Olympus LEX 3000	.ols	ols	Yes	No	No
Omicron SCALA	.par, .tf*, .tb*, .sf*, .sb*	omicron	Yes	No	Yes
Omicron MATRIX	.mtrx	omicronmatrix	Yes	No	No
Wyko OPD	.opd	opdfile	Yes	No	No
Wyko ASCII	.asc	opdfile	Yes	No	No
Pixmap images	.png, .jpeg, .tiff, .tga, .pnm, .bmp	pixmap	Yes[2]	Yes[3]	No
Nanosurf PLT	.plt	pltfile	Yes	No	No
Pacific Nanotechnology PNI	.pni	pnifile	Yes	No	No
PSIA	.tiff	psia	Yes	No	No
Quesant AFM	.afm	quesant	Yes	No	No
Raw text files	any	rawfile	Yes	No	No
Raw binary files	any	rawfile	Yes	No	No
Graph text data (raw)	any	rawgraph	Yes[4]	No	No
XYZ data	.xyz, .dat	rawxyz	Yes[5]	No	No
RHK Instruments SM3	.sm3	rhk-sm3	Yes	No	Limited[??]
RHK Instruments SM4	.sm4	rhk-sm4	Yes	No	No
RHK Instruments SM2	.sm2	rhk-spm32	Yes	No	Limited[??]
Surfstand Surface Data File	.sdf	sdfile	Yes	Yes	No
Micromap SDFA	.sdfa	sdfile	Yes	No	No
Seiko SII	.xqb, .xqd, .xqt	seiko	Yes	No	No
Sensofar PLu v2000	.plu	sensofar	Yes	No	No
Sensolytics DAT	.dat	sensolytics	Yes	No	No
Shimadzu		shimadzu	Yes	No	No

File Format	Extensions	Module	Read	Write	SPS
IonScope SICM	.img	sicmfile	Yes	No	No
Surface Imaging Systems	.sis	sis	Yes	No	No
SPIP ASCII	.asc	spip-asc	Yes	No	No
Thermicroscopes SPMLab R4-R7	.tfr, .ffr, etc.	spmlab	Yes	No	No
Thermicroscopes SPMLab floating point	.flt	spmlabf	Yes	No	No
SPML (Scanning Probe Microscopy Markup Language)	.xml	spml	Yes	No	No
Omicron STMPRG	tp*, ta*	stmprg	Yes	No	No
Molecular Imaging STP	.stp	stpfile	Yes	No	No
Surf	.sur	surffile	Yes	No	No
Unisoku	.hdr, .dat	unisoku	Yes	No	No
WITec	.wit	witfile	Yes	No	No
Nanotec WSxM	.tom	wsxmfile	Yes	No	No

5.5 Expressions

Expressions used in Data Arithmetic module, grain quantity formulas and in graph function fitting have syntax similar to common programming languages.

All numbers are real (floating point), number literals use standard notation. Examples of valid numbers: `1`, `.707`, `2.661`, `8.2e-34`.

Function, constant, and variable names start with a letter and continue with zero or more letters, numbers, or underscores. Examples of valid identifiers: `pow10` (a function), `Pi` (a constant), `d2_2` (a variable).

The precedence of operations is summarized in following table.

Operation	Associativity	Examples
parentheses	N.A.	`(x)`
function call and unary operators	right to left	`-sqrt 3`
power operator	right to left	`2^16`
multiplication, division, and modulo operators	left to right	`9/2 * 8`
addition and subtraction operators	left to right	`3 - 4 + 5`

Note `-3^2` is 9, that is `(-3)^2`, like in **bc**, but unlike in Perl or Python.

Available operators and functions are listed in following table.

Operator	Meaning
+ (unary)	no op
− (unary)	negative value
~	negative value (equivalent to −)
+ (binary)	addition
− (binary)	subtraction
*	multiplication
/	division
%	floating point modulo
^	power
abs	absolute value
floor	rounding down to nearest integer
ceil	rounding up to nearest integer
sqrt	square root
cbrt	cubic root
sin	sine function
cos	cosine function
tan	tangent function
asin	arc sine function
acos	arc cosine function
atan	arc tangent function
exp	base-e exponential function
ln	base-e logarithm function
log	base-e logarithm function
pow10	base-10 exponential function
log10	base-10 logarithm function
sinh	hyperbolic sine function
cosh	hyperbolic cosine function
tanh	hyperbolic tangent function
asinh	inverse hyperbolic sine function
acosh	inverse hyperbolic cosine function
atanh	inverse hyperbolic tangent function
pow	power function, pow(x,y) equals to x^y
min	minimum of two values
max	maximum of two values
mod	floating point modulo, mod(x,y) equals to x % y
hypot	Euclidean distance function, hypot(x,y) equals to sqrt(x^2+y^2)
atan2	arc tangent function of two variables

Beside that, there are a few peculiarities that may make typing simple expression easier:

- Multiplication signs are optional, you can use spaces instead (or nothing, in some cases). E.g., 3/4 Pi and 5(4+3)(2+1) are valid expressions. However, 3a is not a valid expression, 3e-4 always means 0.0003, not 3*e - 4.
- There is no difference between function calls and unary operators, so parentheses can be often omitted. E.g, sqrt 5 and hypot hypot 3,4,5 are valid expression. The latter can be parenthesized as follows: hypot(hypot(3,4),5).

  Note however, function calls have higher priority than any other operator, thus sin Pi/2 is the same as (sin Pi)/2, not as sin(Pi/2).

If in doubt, write out expressions in full form.

5.6 Resources

Various bits of data, e.g. false color maps or raw file import presets, are stored in standalone files that are collectivelly called resource files. Gwyddion looks for resources in two different locations: system and user-specific.

System resources are installed along with the program and they are not modifiable. Typically, they are located under a directory such as `/usr/share/gwyddion` (Unix), `ProgramFiles\Gwyddion` (MS Windows) or other directory determined by GWYDDION_DATADIR.

User resources are located in a user's directory, this usually means under `~/.gwyddion` (Unix) or `DocumentsandSettings\gwyddion` (MS Windows).

All resource files are simple text files that can be easily examined and modified by text editors or sent to other users (if they are copied or created manually Gwyddion needs to be restarted to notice them). In most cases only characters of the ASCII can appear in the files. If international text can appear there it must be in the UTF-8 encoding.

Resources are organized in subdirectories according to their kind, e.g. color gradients reside in the subdirectory `gradients`. The name of the file determines the resource name – gradient Gray is found in file `gradients/Gray`. Modules can define their own resource types; the types described here are the most important types but the list may not be comprehensive.

Every resource file has the same structure. It starts with a line identifying the resource type:

```
Gwyddion resource GwyGradient
```

where GwyGradient is the type name in the type system (which is quite a low-level detail but so it is), followed by named parameters in the form

```
name value
```

and resource data. Some resource types may contain only named parameters, other may contain only data.

Gradients

Gradients, i.e. false color maps, reside in directory `gradients`, they are identified by GwyGradient and contain only data. They can be edited in the application using the gradient editor.

The gradient data consists of rows corresponding to individual points in the gradient:

```
position red green blue alpha
```

The position determines where the color defined by *`red`*, *`green`*, *`blue`* and *`alpha`* components is placed in the interval $[0,1]$ where 0 corresponds to the gradient start, 1 corresponds to the end. The color is interpolated linearly between the specified points.

The positions must form an increasing sequence from 0 to 1 (i.e. the minimum number of color points is two). The range of the color components is also $[0,1]$. Note the alpha value, corresponding to opacity, is unused and must be given as 1 (fully opaque).

For instance, the standard gradient Red going from black (0 0 0) to red (1 0 0) to white (1 1 1) is defined as follows:

```
Gwyddion resource GwyGradient
0.0 0 0 0 1
0.5 1 0 0 1
1.0 1 1 1 1
```

OpenGL Materials

OpenGL materials reside in directory `glmaterials`, they are identified by GwyGLMaterial and contain only data. They can be edited in the application using the OpenGL material editor.

The material data consists of four RGBA lines, similar to gradients that correspond in to the four OpenGL material components in the following order:

1. ambient,
2. diffuse,

3. specular,
4. emission.

See section OpenGL Material Editor for explanation of the components. They are followed by a line containing the shininess, again as a number from the interval $[0,1]$.

Note the emission component, while read and written by Gwyddion, is presently unused by the 3D view. It is recommended to set it to 0 0 0 1, i.e. black.

For instance, the standard material Red-Rubber with very dark red ambient color, grayish diffuse reflection, red specular reflection and low shininess is defined as follows:

```
Gwyddion resource GwyGLMaterial
0.05 0.0  0.0  1.0
0.5  0.4  0.4  1.0
0.7  0.04 0.04 1.0
0.0  0.0  0.0  1.0
.078125
```

Grain Values

Grain values reside in directory `grainvalues`, they are identified by GwyGrainValue and contain only named parameters. They can be used to define additional grain quantities, derived from the built-in quantities, that appear under User group in grain analysis functions. At the time of writing this, there is no editor in the application, new quantities must be created manually.

The named parameters are summarized in the following table:

Parameter	Required	Type	Description
`symbol`	required	identifier	Identifier to use in other expressions (but see below). It must be a valid identifier of ASCII letters, numbers and underscores, starting with a letter.
`expression`	required	free-form	Formula for calculation of this quantity from other grain quantities. The general expression syntax is described in section Expressions.
`symbol_markup`	optional	free-form	Fancy symbol that can include Greek letters or subscripts and superscripts expressed with the Pango markup language. It is used for presentation in the application so, while it is optional, it is recommended to at least define it identically to `symbol`.
`power_xy`	optional	integer	The power in which the lateral dimensions appear in the quantity. For instance, this is 1 for grain dimensions, 2 for areas and volumes. The default value is 0.
`power_z`	optional	integer	The power in which the ‘height’ dimension appears in the quantity. For instance, this is 1 for values and volumes, 0 for dimensions and areas. The default value is 0.
`same_units`	optional	0 or 1	Give as 1 if the quantity makes sense only for lateral and ‘height’ dimensions being the same physical quantities. For instance, this is required for the surface area. The default is 0.
`is_angle`	optional	0 or 1	Give as 1 if the quantity is an angle. The expression should calculate angles in radians. However, if `is_angle` is set Gwyddion knowns the value can be converted to degrees for presentation. The default is 0.

At present, user-defined grain quantities cannot depend on other user-defined grain quantities to avoid circular dependences. The built-in grain quantities are listed below:

Symbol	Group	Name
x_c	Position	Center x position
y_c	Position	Center y position
z_min	Value	Minimum value
z_max	Value	Maximum value
z_m	Value	Mean value
z_med	Value	Median value
b_min	Value	Minimum value on boundary
b_max	Value	Maximum value on boundary
A_0	Area	Projected area
A_s	Area	Surface area
a_eq	Area	Equivalent square side
r_eq	Area	Equivalent disc radius
A_h	Area	Area above half-height
V_0	Volume	Zero basis volume
V_min	Volume	Grain minimum basis volume
V_L	Volume	Laplacian background basis volume
L_b0	Boundary	Projected boundary length
D_min	Boundary	Minimum bounding size
phi_min	Boundary	Minimum bounding direction
D_max	Boundary	Maximum bounding size
phi_max	Boundary	Maximum bounding direction
theta	Slope	Inclination ϑ
phi	Slope	Inclination φ

For instance, a new grain value Height, measuing the grain height as the difference between the maximum and minimum value, can be defined as follows:

```
Gwyddion resource GwyGrainValue
symbol dz
symbol_markup Δz
power_xy 0
power_z 1
expression z_max - z_min
```

Raw File Presets

Raw file presents reside in directory `rawfile`, they are identified by GwyRawFilePreset and contain only named parameters. They are normally created and edited by the preset editor in the raw file import module.

The named parameters in the resource files correspond closely to the parameters in the user interface explained in detail in section Raw Data File Import. Hence, they will be described only briefly here.

Parameter	Type	Description
xres, yres	integer	horizontal and vertical size
xreal, yreal	number	physical dimensions, in units given by xyexponent and xyunit
xyexponent	multiple of 3	power of 10 to multiply xreal and yreal with
xyunit	string	base units of xreal and yreal, e.g. "m"
zscale	number	unit step in values
zexponent	multiple of 3	power of 10 to multiply zscale with
zunit	string	base units of zscale
format	0 or 1	0 means binary, 1 means text
builtin (binary)	integer	built-in data format id, see below
offset (binary)	integer	data offset in file, in bytes
size (binary)	integer	data value size, in bits
skip (binary)	integer	number of bits to skip after each value
rowskip (binary)	integer	number of additional bits to skip after each row
sign (binary)	0 or 1	0 means unsigned, 1 means signed
revsample (binary)	0 or 1	1 means reverse bits in values
revbyte (binary)	0 or 1	1 means reverse bits in bytes
byteswap (binary)	integer	byte swap pattern
lineoffset (text)	integer	lines to skip before starting to read the data
skipfields (text)	integer	fields to skip at the start of each line
delimiter (text)	string	field delimiter, empty string means arbitrary whitespace
decomma (text)	0 or 1	1 if decimal separator is comma, 0 for dot

Note the choice of a built-in binary format, i.e. nonzero builtin, implies the binary format to some extent. This means the options size, revbyte and sign are ignored as they are used only for detailed specification of user formats. The available formats are listed in the following table:

Type	Description
0	user-specified
1	signed 8bit integer
2	unsigned 8bit integer
3	signed 16bit integer
4	unsigned 16bit integer
5	signed 32bit integer
6	unsigned 32bit integer
7	IEEE float
8	IEEE double
9	signed 64bit integer
10	unsigned 64bit integer

5.7 Format of Gwyddion Files

Gwyddion native data files consists of a tree-like structure of serialized objects. Generally, these objects can be of various kind and contain other embedded objects (hence the tree-like structure). It can be instructive to play with gwydump, a simple file structure visualizer available in on the project's web, for a while and examine the contents of various files.

First of all, we will describe physical file structure without regard to possible interpretation of contained data.

Byte Order

All data is stored in little-endian (also known as LSB or Intel) byte order.

File Header

The file header consists of four bytes (magic number) with the values of ASCII characters `GWYP`.

This is the new file format, an older version of file format with magic header `GWYO` also exists. It will not be discussed here.

File Data

The rest of the file consists of a serialized GwyContainer object that contains all the data. It is stored exactly the same way as any other object, that is as described in the next section.

Object Layout

An object consists of three parts (in the following order):

- Type name, stored as a `NUL`-terminated string of ASCII characters. This is the type name in GObject type system.
- Serialized data size, stored as an unsigned 32bit integer. It does not include the size of the type name and the size of self.
- Component list. Components are named parts of object data, each of particular data type: an atomic type, an array of atomic types, or again an object. They are stored in no particular order.

Components

Each component consits of three parts (in the following order):

- Name, stored as a `NUL`-terminated string.
- Type, stored as a signle unsigned byte (character). The table of possible component types is presented below.
- Data, stored as whatever is appropriate for a particular type.

Data Types

Available atomic data types are listed in following table:

Type	Character	Note
boolean	`b`	Stored as a byte, zero is false, nonzero (normally 1) is true
character	`c`	
32bit integer	`i`	
64bit integer	`q`	
double	`d`	IEEE 754 double precession floating point number
string	`s`	`NUL`-terminated
object	`o`	Serialized object as described above

Each atomic type except boolean has its array counterpart. The type character of array types is the same as of the corresponding atomic type, except it is uppercase. Arrays are stored as unsigned 32bit array length (the number of items), followed by the item values. Array data types are listed in following table:

Type	Character	Note
array of characters	`C`	Not `NUL`-terminated
array of 32bit integers	`I`	
array of 64bit integers	`Q`	
array of doubles	`D`	
array of strings	`S`	
array of objects	`O`	Uppercase Oh, not zero

Particular Objects

To be written.

Chapter 6

Developing Gwyddion

You are encouraged to become a developer of Gwyddion.

If you want to become developer, we recommend you to start with some simple modules (see module tutorial), to see how the application works. If you write a module or plug-in, you are encouraged to share it here with other Gwyddion users. Let us know, so that we can link your modules or plug-ins to these pages or even include in it Gwyddion. You don't have to limit yourself to modules or plug-ins of course, but they should be easier to start with.

API References

There are many functions that can help you while developing your module. See API reference at Documentation section of the project web.

Bug reports

We will be very happy if you send as bug reports if you find errors in Gwyddion. For doing this, please, specify as much as possible the situation that led to error, operating system and Gwyddion version used. You can also send us the SPM data that were being processed when the problem was found, this is necessary namely for reporting bugs related to file loading and saving.

The preferred bug reporting method is to send an e-mail to klapetek@gwyddion.net.

Appendix A

GNU General Public License

A.1 Preamble

The licenses for most software are designed to take away your freedom to share and change it. By contrast, the GNU General Public License is intended to guarantee your freedom to share and change free software - to make sure the software is free for all its users. This General Public License applies to most of the Free Software Foundation's software and to any other program whose authors commit to using it. (Some other Free Software Foundation software is covered by the GNU Library General Public License instead.) You can apply it to your programs, too.

When we speak of free software, we are referring to freedom, not price. Our General Public Licenses are designed to make sure that you have the freedom to distribute copies of free software (and charge for this service if you wish), that you receive source code or can get it if you want it, that you can change the software or use pieces of it in new free programs; and that you know you can do these things.

To protect your rights, we need to make restrictions that forbid anyone to deny you these rights or to ask you to surrender the rights. These restrictions translate to certain responsibilities for you if you distribute copies of the software, or if you modify it.

For example, if you distribute copies of such a program, whether gratis or for a fee, you must give the recipients all the rights that you have. You must make sure that they, too, receive or can get the source code. And you must show them these terms so they know their rights.

We protect your rights with two steps:

1. copyright the software, and
2. offer you this license which gives you legal permission to copy, distribute and/or modify the software.

Also, for each author's protection and ours, we want to make certain that everyone understands that there is no warranty for this free software. If the software is modified by someone else and passed on, we want its recipients to know that what they have is not the original, so that any problems introduced by others will not reflect on the original authors' reputations.

Finally, any free program is threatened constantly by software patents. We wish to avoid the danger that redistributors of a free program will individually obtain patent licenses, in effect making the program proprietary. To prevent this, we have made it clear that any patent must be licensed for everyone's free use or not licensed at all.

The precise terms and conditions for copying, distribution and modification follow.

A.2 Terms And Conditions For Copying, Distribution And Modification

Section 0

This License applies to any program or other work which contains a notice placed by the copyright holder saying it may be distributed under the terms of this General Public License. The 'Program', below, refers to any such program or work, and a 'work based on the Program' means either the Program or any derivative work under copyright law: that is to say, a work containing the Program or a portion of it, either verbatim or with modifications and/or translated into another language. (Hereinafter, translation is included without limitation in the term 'modification'.) Each licensee is addressed as 'you'.

Activities other than copying, distribution and modification are not covered by this License; they are outside its scope. The act of running the Program is not restricted, and the output from the Program is covered only if its contents constitute a work based on the Program (independent of having been made by running the Program). Whether that is true depends on what the Program does.

Section 1

You may copy and distribute verbatim copies of the Program's source code as you receive it, in any medium, provided that you conspicuously and appropriately publish on each copy an appropriate copyright notice and disclaimer of warranty; keep intact all the notices that refer to this License and to the absence of any warranty; and give any other recipients of the Program a copy of this License along with the Program.

You may charge a fee for the physical act of transferring a copy, and you may at your option offer warranty protection in exchange for a fee.

Section 2

You may modify your copy or copies of the Program or any portion of it, thus forming a work based on the Program, and copy and distribute such modifications or work under the terms of Section 1 above, provided that you also meet all of these conditions:

1. You must cause the modified files to carry prominent notices stating that you changed the files and the date of any change.
2. You must cause any work that you distribute or publish, that in whole or in part contains or is derived from the Program or any part thereof, to be licensed as a whole at no charge to all third parties under the terms of this License.
3. If the modified program normally reads commands interactively when run, you must cause it, when started running for such interactive use in the most ordinary way, to print or display an announcement including an appropriate copyright notice and a notice that there is no warranty (or else, saying that you provide a warranty) and that users may redistribute the program under these conditions, and telling the user how to view a copy of this License.

> **Exception:**
> If the Program itself is interactive but does not normally print such an announcement, your work based on the Program is not required to print an announcement.)

These requirements apply to the modified work as a whole. If identifiable sections of that work are not derived from the Program, and can be reasonably considered independent and separate works in themselves, then this License, and its terms, do not apply to those sections when you distribute them as separate works. But when you distribute the same sections as part of a whole which is a work based on the Program, the distribution of the whole must be on the terms of this License, whose permissions for other licensees extend to the entire whole, and thus to each and every part regardless of who wrote it.

Thus, it is not the intent of this section to claim rights or contest your rights to work written entirely by you; rather, the intent is to exercise the right to control the distribution of derivative or collective works based on the Program.

In addition, mere aggregation of another work not based on the Program with the Program (or with a work based on the Program) on a volume of a storage or distribution medium does not bring the other work under the scope of this License.

Section 3

You may copy and distribute the Program (or a work based on it, under Section 2 in object code or executable form under the terms of Sections 1 and 2 above provided that you also do one of the following:

1. Accompany it with the complete corresponding machine-readable source code, which must be distributed under the terms of Sections 1 and 2 above on a medium customarily used for software interchange; or,
2. Accompany it with a written offer, valid for at least three years, to give any third party, for a charge no more than your cost of physically performing source distribution, a complete machine-readable copy of the corresponding source code, to be distributed under the terms of Sections 1 and 2 above on a medium customarily used for software interchange; or,
3. Accompany it with the information you received as to the offer to distribute corresponding source code. (This alternative is allowed only for noncommercial distribution and only if you received the program in object code or executable form with such an offer, in accord with Subsection b above.)

The source code for a work means the preferred form of the work for making modifications to it. For an executable work, complete source code means all the source code for all modules it contains, plus any associated interface definition files, plus the scripts used to control compilation and installation of the executable. However, as a special exception, the source code distributed need not include anything that is normally distributed (in either source or binary form) with the major components (compiler, kernel, and so on) of the operating system on which the executable runs, unless that component itself accompanies the executable.

If distribution of executable or object code is made by offering access to copy from a designated place, then offering equivalent access to copy the source code from the same place counts as distribution of the source code, even though third parties are not compelled to copy the source along with the object code.

Section 4

You may not copy, modify, sublicense, or distribute the Program except as expressly provided under this License. Any attempt otherwise to copy, modify, sublicense or distribute the Program is void, and will automatically terminate your rights under this License. However, parties who have received copies, or rights, from you under this License will not have their licenses terminated so long as such parties remain in full compliance.

Section 5

You are not required to accept this License, since you have not signed it. However, nothing else grants you permission to modify or distribute the Program or its derivative works. These actions are prohibited by law if you do not accept this License. Therefore, by modifying or distributing the Program (or any work based on the Program), you indicate your acceptance of this License to do so, and all its terms and conditions for copying, distributing or modifying the Program or works based on it.

Section 6

Each time you redistribute the Program (or any work based on the Program), the recipient automatically receives a license from the original licensor to copy, distribute or modify the Program subject to these terms and conditions. You may not impose any further restrictions on the recipients' exercise of the rights granted herein. You are not responsible for enforcing compliance by third parties to this License.

Section 7

If, as a consequence of a court judgment or allegation of patent infringement or for any other reason (not limited to patent issues), conditions are imposed on you (whether by court order, agreement or otherwise) that contradict the conditions of this License, they do not excuse you from the conditions of this License. If you cannot distribute so as to satisfy simultaneously your obligations under this License and any other pertinent obligations, then as a consequence you may not distribute the Program at all. For example, if a patent license would not permit royalty-free redistribution of the Program by all those who receive copies directly or indirectly through you, then the only way you could satisfy both it and this License would be to refrain entirely from distribution of the Program.

If any portion of this section is held invalid or unenforceable under any particular circumstance, the balance of the section is intended to apply and the section as a whole is intended to apply in other circumstances.

It is not the purpose of this section to induce you to infringe any patents or other property right claims or to contest validity of any such claims; this section has the sole purpose of protecting the integrity of the free software distribution system, which is implemented by public license practices. Many people have made generous contributions to the wide range of software distributed through that system in reliance on consistent application of that system; it is up to the author/donor to decide if he or she is willing to distribute software through any other system and a licensee cannot impose that choice.

This section is intended to make thoroughly clear what is believed to be a consequence of the rest of this License.

Section 8

If the distribution and/or use of the Program is restricted in certain countries either by patents or by copyrighted interfaces, the original copyright holder who places the Program under this License may add an explicit geographical distribution limitation excluding those countries, so that distribution is permitted only in or among countries not thus excluded. In such case, this License incorporates the limitation as if written in the body of this License.

Section 9

The Free Software Foundation may publish revised and/or new versions of the General Public License from time to time. Such new versions will be similar in spirit to the present version, but may differ in detail to address new problems or concerns.

Each version is given a distinguishing version number. If the Program specifies a version number of this License which applies to it and 'any later version', you have the option of following the terms and conditions either of that version or of any later version published by the Free Software Foundation. If the Program does not specify a version number of this License, you may choose any version ever published by the Free Software Foundation.

Section 10

If you wish to incorporate parts of the Program into other free programs whose distribution conditions are different, write to the author to ask for permission. For software which is copyrighted by the Free Software Foundation, write to the Free Software Foundation; we sometimes make exceptions for this. Our decision will be guided by the two goals of preserving the free status of all derivatives of our free software and of promoting the sharing and reuse of software generally.

NO WARRANTY Section 11

BECAUSE THE PROGRAM IS LICENSED FREE OF CHARGE, THERE IS NO WARRANTY FOR THE PROGRAM, TO THE EXTENT PERMITTED BY APPLICABLE LAW. EXCEPT WHEN OTHERWISE STATED IN WRITING THE COPYRIGHT HOLDERS AND/OR OTHER PARTIES PROVIDE THE PROGRAM 'AS IS' WITHOUT WARRANTY OF ANY KIND, EITHER EXPRESSED OR IMPLIED, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE. THE ENTIRE RISK AS TO THE QUALITY AND PERFORMANCE OF THE PROGRAM IS WITH YOU. SHOULD THE PROGRAM PROVE DEFECTIVE, YOU ASSUME THE COST OF ALL NECESSARY SERVICING, REPAIR OR CORRECTION.

Section 12

IN NO EVENT UNLESS REQUIRED BY APPLICABLE LAW OR AGREED TO IN WRITING WILL ANY COPYRIGHT HOLDER, OR ANY OTHER PARTY WHO MAY MODIFY AND/OR REDISTRIBUTE THE PROGRAM AS PERMITTED ABOVE, BE LIABLE TO YOU FOR DAMAGES, INCLUDING ANY GENERAL, SPECIAL, INCIDENTAL OR CONSEQUENTIAL DAMAGES ARISING OUT OF THE USE OR INABILITY TO USE THE PROGRAM (INCLUDING BUT NOT LIMITED TO LOSS OF DATA OR DATA BEING RENDERED INACCURATE OR LOSSES SUSTAINED BY YOU OR THIRD PARTIES OR A FAILURE OF THE PROGRAM TO OPERATE WITH ANY OTHER PROGRAMS), EVEN IF SUCH HOLDER OR OTHER PARTY HAS BEEN ADVISED OF THE POSSIBILITY OF SUCH DAMAGES.

END OF TERMS AND CONDITIONS

A.3 How to Apply These Terms to Your New Programs

If you develop a new program, and you want it to be of the greatest possible use to the public, the best way to achieve this is to make it free software which everyone can redistribute and change under these terms.

To do so, attach the following notices to the program. It is safest to attach them to the start of each source file to most effectively convey the exclusion of warranty; and each file should have at least the 'copyright' line and a pointer to where the full notice is found.

```
      <one line to give the program's name and a brief idea of what it does.>
      Copyright (C) <year>    <name of author>
      This program 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 2 of the License, or
      (at your option) any later version.

      This program 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.

      You should have received a copy of the GNU General Public License along
      with this program; if not, write to the Free Software Foundation, Inc.,
      51 Franklin Street, Fifth Floor, Boston, MA  02110-1301, USA
```

Also add information on how to contact you by electronic and paper mail.

If the program is interactive, make it output a short notice like this when it starts in an interactive mode:

```
Gnomovision version 69, Copyright (C) year name of author Gnomovision
comes with ABSOLUTELY NO WARRANTY; for details type show w.
This is free software, and you are welcome to redistribute it under
certain conditions; type show c for details.
```

The hypothetical commands ‘show w’ and ‘show c’ should show the appropriate parts of the General Public License. Of course, the commands you use may be called something other than ‘show w’ and ‘show c’; they could even be mouse-clicks or menu items--whatever suits your program.

You should also get your employer (if you work as a programmer) or your school, if any, to sign a ‘copyright disclaimer’ for the program, if necessary. Here is a sample; alter the names:

```
Yoyodyne, Inc., hereby disclaims all copyright interest in the
program ‘Gnomovision’ (which makes passes at compilers) written
by James Hacker.

<signature of Ty Coon>, 1 April 1989
Ty Coon, President of Vice
```

This General Public License does not permit incorporating your program into proprietary programs. If your program is a subroutine library, you may consider it more useful to permit linking proprietary applications with the library. If this is what you want to do, use the GNU Library General Public License instead of this License.

Appendix B

GNU Free Documentation License

B.1 Preamble

The purpose of this License is to make a manual, textbook, or other functional and useful document ‘free’ in the sense of freedom: to assure everyone the effective freedom to copy and redistribute it, with or without modifying it, either commercially or noncommercially. Secondarily, this License preserves for the author and publisher a way to get credit for their work, while not being considered responsible for modifications made by others.

This License is a kind of ‘copyleft’, which means that derivative works of the document must themselves be free in the same sense. It complements the GNU General Public License, which is a copyleft license designed for free software.

We have designed this License in order to use it for manuals for free software, because free software needs free documentation: a free program should come with manuals providing the same freedoms that the software does. But this License is not limited to software manuals; it can be used for any textual work, regardless of subject matter or whether it is published as a printed book. We recommend this License principally for works whose purpose is instruction or reference.

B.2 Applicability And Definitions

This License applies to any manual or other work, in any medium, that contains a notice placed by the copyright holder saying it can be distributed under the terms of this License. Such a notice grants a world-wide, royalty-free license, unlimited in duration, to use that work under the conditions stated herein. The ‘Document’, below, refers to any such manual or work. Any member of the public is a licensee, and is addressed as ‘you’. You accept the license if you copy, modify or distribute the work in a way requiring permission under copyright law.

A ‘Modified Version’ of the Document means any work containing the Document or a portion of it, either copied verbatim, or with modifications and/or translated into another language.

A ‘Secondary Section’ is a named appendix or a front-matter section of the Document that deals exclusively with the relationship of the publishers or authors of the Document to the Document’s overall subject (or to related matters) and contains nothing that could fall directly within that overall subject. (Thus, if the Document is in part a textbook of mathematics, a Secondary Section may not explain any mathematics.) The relationship could be a matter of historical connection with the subject or with related matters, or of legal, commercial, philosophical, ethical or political position regarding them.

The ‘Invariant Sections’ are certain Secondary Sections whose titles are designated, as being those of Invariant Sections, in the notice that says that the Document is released under this License. If a section does not fit the above definition of Secondary then it is not allowed to be designated as Invariant. The Document may contain zero Invariant Sections. If the Document does not identify any Invariant Sections then there are none.

The ‘Cover Texts’ are certain short passages of text that are listed, as Front-Cover Texts or Back-Cover Texts, in the notice that says that the Document is released under this License. A Front-Cover Text may be at most 5 words, and a Back-Cover Text may be at most 25 words.

A ‘Transparent’ copy of the Document means a machine-readable copy, represented in a format whose specification is available to the general public, that is suitable for revising the document straightforwardly with generic text editors or (for images composed of pixels) generic paint programs or (for drawings) some widely available drawing editor, and that is suitable for input to text formatters or for automatic translation to a variety of formats suitable for input to text formatters. A copy made in an otherwise Transparent file format whose markup, or absence of markup, has been arranged to thwart or discourage subsequent modification by readers is not Transparent. An image format is not Transparent if used for any substantial amount of text. A copy that is not ‘Transparent’ is called ‘Opaque’.

Examples of suitable formats for Transparent copies include plain ASCII without markup, Texinfo input format, LaTeX input format, SGML or XML using a publicly available DTD, and standard-conforming simple HTML, PostScript or PDF designed for human modification. Examples of transparent image formats include PNG, XCF and JPG. Opaque formats include proprietary formats that can be read and edited only by proprietary word processors, SGML or XML for which the DTD and/or processing tools are not generally available, and the machine-generated HTML, PostScript or PDF produced by some word processors for output purposes only.

The ‘Title Page’ means, for a printed book, the title page itself, plus such following pages as are needed to hold, legibly, the material this License requires to appear in the title page. For works in formats which do not have any title page as such, ‘Title Page’ means the text near the most prominent appearance of the work’s title, preceding the beginning of the body of the text.

A section ‘Entitled XYZ’ means a named subunit of the Document whose title either is precisely XYZ or contains XYZ in parentheses following text that translates XYZ in another language. (Here XYZ stands for a specific section name mentioned below, such as ‘Acknowledgements’, ‘Dedications’, ‘Endorsements’, or ‘History’.) To ‘Preserve the Title’ of such a section when you modify the Document means that it remains a section ‘Entitled XYZ’ according to this definition.

The Document may include Warranty Disclaimers next to the notice which states that this License applies to the Document. These Warranty Disclaimers are considered to be included by reference in this License, but only as regards disclaiming warranties: any other implication that these Warranty Disclaimers may have is void and has no effect on the meaning of this License.

B.3 Verbatim Copying

You may copy and distribute the Document in any medium, either commercially or noncommercially, provided that this License, the copyright notices, and the license notice saying this License applies to the Document are reproduced in all copies, and that you add no other conditions whatsoever to those of this License. You may not use technical measures to obstruct or control the reading or further copying of the copies you make or distribute. However, you may accept compensation in exchange for copies. If you distribute a large enough number of copies you must also follow the conditions in section 3.

You may also lend copies, under the same conditions stated above, and you may publicly display copies.

B.4 Copying In Quantity

If you publish printed copies (or copies in media that commonly have printed covers) of the Document, numbering more than 100, and the Document’s license notice requires Cover Texts, you must enclose the copies in covers that carry, clearly and legibly, all these Cover Texts: Front-Cover Texts on the front cover, and Back-Cover Texts on the back cover. Both covers must also clearly and legibly identify you as the publisher of these copies. The front cover must present the full title with all words of the title equally prominent and visible. You may add other material on the covers in addition. Copying with changes limited to the covers, as long as they preserve the title of the Document and satisfy these conditions, can be treated as verbatim copying in other respects.

If the required texts for either cover are too voluminous to fit legibly, you should put the first ones listed (as many as fit reasonably) on the actual cover, and continue the rest onto adjacent pages.

If you publish or distribute Opaque copies of the Document numbering more than 100, you must either include a machine-readable Transparent copy along with each Opaque copy, or state in or with each Opaque copy a computer-network location from which the general network-using public has access to download using public-standard network protocols a complete Transparent copy of the Document, free of added material. If you use the latter option, you must take reasonably prudent steps, when you begin distribution of Opaque copies in quantity, to ensure that this Transparent copy will remain thus accessible at the stated location until at least one year after the last time you distribute an Opaque copy (directly or through your agents or retailers) of that edition to the public.

It is requested, but not required, that you contact the authors of the Document well before redistributing any large number of copies, to give them a chance to provide you with an updated version of the Document.

B.5 Modifications

You may copy and distribute a Modified Version of the Document under the conditions of sections 2 and 3 above, provided that you release the Modified Version under precisely this License, with the Modified Version filling the role of the Document, thus licensing distribution and modification of the Modified Version to whoever possesses a copy of it. In addition, you must do these things in the Modified Version:

GNU FDL Modification Conditions

A. Use in the Title Page (and on the covers, if any) a title distinct from that of the Document, and from those of previous versions (which should, if there were any, be listed in the History section of the Document). You may use the same title as a previous version if the original publisher of that version gives permission.

B. List on the Title Page, as authors, one or more persons or entities responsible for authorship of the modifications in the Modified Version, together with at least five of the principal authors of the Document (all of its principal authors, if it has fewer than five), unless they release you from this requirement.

C. State on the Title page the name of the publisher of the Modified Version, as the publisher.

D. Preserve all the copyright notices of the Document.

E. Add an appropriate copyright notice for your modifications adjacent to the other copyright notices.

F. Include, immediately after the copyright notices, a license notice giving the public permission to use the Modified Version under the terms of this License, in the form shown in the Addendum below.

G. Preserve in that license notice the full lists of Invariant Sections and required Cover Texts given in the Document's license notice.

H. Include an unaltered copy of this License.

I. Preserve the section Entitled ‘History’, Preserve its Title, and add to it an item stating at least the title, year, new authors, and publisher of the Modified Version as given on the Title Page. If there is no section Entitled ‘History’ in the Document, create one stating the title, year, authors, and publisher of the Document as given on its Title Page, then add an item describing the Modified Version as stated in the previous sentence.

J. Preserve the network location, if any, given in the Document for public access to a Transparent copy of the Document, and likewise the network locations given in the Document for previous versions it was based on. These may be placed in the ‘History’ section. You may omit a network location for a work that was published at least four years before the Document itself, or if the original publisher of the version it refers to gives permission.

K. For any section Entitled ‘Acknowledgements’ or ‘Dedications’, Preserve the Title of the section, and preserve in the section all the substance and tone of each of the contributor acknowledgements and/or dedications given therein.

L. Preserve all the Invariant Sections of the Document, unaltered in their text and in their titles. Section numbers or the equivalent are not considered part of the section titles.

M. Delete any section Entitled ‘Endorsements’. Such a section may not be included in the Modified Version.

N. Do not retitle any existing section to be Entitled ‘Endorsements’ or to conflict in title with any Invariant Section.

O. Preserve any Warranty Disclaimers.

If the Modified Version includes new front-matter sections or appendices that qualify as Secondary Sections and contain no material copied from the Document, you may at your option designate some or all of these sections as invariant. To do this, add their titles to the list of Invariant Sections in the Modified Version's license notice. These titles must be distinct from any other section titles.

You may add a section Entitled ‘Endorsements’, provided it contains nothing but endorsements of your Modified Version by various parties–for example, statements of peer review or that the text has been approved by an organization as the authoritative definition of a standard.

You may add a passage of up to five words as a Front-Cover Text, and a passage of up to 25 words as a Back-Cover Text, to the end of the list of Cover Texts in the Modified Version. Only one passage of Front-Cover Text and one of Back-Cover Text may be added by (or through arrangements made by) any one entity. If the Document already includes a cover text for the same cover, previously added by you or by arrangement made by the same entity you are acting on behalf of, you may not add another; but you may replace the old one, on explicit permission from the previous publisher that added the old one.

The author(s) and publisher(s) of the Document do not by this License give permission to use their names for publicity for or to assert or imply endorsement of any Modified Version.

B.6 Combining Documents

You may combine the Document with other documents released under this License, under the terms defined in section 4 above for modified versions, provided that you include in the combination all of the Invariant Sections of all of the original documents, unmodified, and list them all as Invariant Sections of your combined work in its license notice, and that you preserve all their Warranty Disclaimers.

The combined work need only contain one copy of this License, and multiple identical Invariant Sections may be replaced with a single copy. If there are multiple Invariant Sections with the same name but different contents, make the title of each such section unique by adding at the end of it, in parentheses, the name of the original author or publisher of that section if known, or else a unique number. Make the same adjustment to the section titles in the list of Invariant Sections in the license notice of the combined work.

In the combination, you must combine any sections Entitled 'History' in the various original documents, forming one section Entitled 'History'; likewise combine any sections Entitled 'Acknowledgements', and any sections Entitled 'Dedications'. You must delete all sections Entitled 'Endorsements'.

B.7 Collections Of Documents

You may make a collection consisting of the Document and other documents released under this License, and replace the individual copies of this License in the various documents with a single copy that is included in the collection, provided that you follow the rules of this License for verbatim copying of each of the documents in all other respects.

You may extract a single document from such a collection, and distribute it individually under this License, provided you insert a copy of this License into the extracted document, and follow this License in all other respects regarding verbatim copying of that document.

B.8 Aggregation With Independent Works

A compilation of the Document or its derivatives with other separate and independent documents or works, in or on a volume of a storage or distribution medium, is called an 'aggregate' if the copyright resulting from the compilation is not used to limit the legal rights of the compilation's users beyond what the individual works permit. When the Document is included in an aggregate, this License does not apply to the other works in the aggregate which are not themselves derivative works of the Document.

If the Cover Text requirement of section 3 is applicable to these copies of the Document, then if the Document is less than one half of the entire aggregate, the Document's Cover Texts may be placed on covers that bracket the Document within the aggregate, or the electronic equivalent of covers if the Document is in electronic form. Otherwise they must appear on printed covers that bracket the whole aggregate.

B.9 Translation

Translation is considered a kind of modification, so you may distribute translations of the Document under the terms of section 4. Replacing Invariant Sections with translations requires special permission from their copyright holders, but you may include translations of some or all Invariant Sections in addition to the original versions of these Invariant Sections. You may include a translation of this License, and all the license notices in the Document, and any Warranty Disclaimers, provided that you also include the original English version of this License and the original versions of those notices and disclaimers. In case of a disagreement between the translation and the original version of this License or a notice or disclaimer, the original version will prevail.

If a section in the Document is Entitled 'Acknowledgements', 'Dedications', or 'History', the requirement (section 4) to Preserve its Title (section 1) will typically require changing the actual title.

B.10 Termination

You may not copy, modify, sublicense, or distribute the Document except as expressly provided for under this License. Any other attempt to copy, modify, sublicense or distribute the Document is void, and will automatically terminate your rights under this License. However, parties who have received copies, or rights, from you under this License will not have their licenses terminated so long as such parties remain in full compliance.

B.11 Future Revisions Of This License

The Free Software Foundation may publish new, revised versions of the GNU Free Documentation License from time to time. Such new versions will be similar in spirit to the present version, but may differ in detail to address new problems or concerns. See http://www.gnu.org/copyleft/.

Each version of the License is given a distinguishing version number. If the Document specifies that a particular numbered version of this License 'or any later version' applies to it, you have the option of following the terms and conditions either of that specified version or of any later version that has been published (not as a draft) by the Free Software Foundation. If the Document does not specify a version number of this License, you may choose any version ever published (not as a draft) by the Free Software Foundation.

B.12 ADDENDUM: How to use this License for your documents

To use this License in a document you have written, include a copy of the License in the document and put the following copyright and license notices just after the title page:

> SAMPLE INVARIANT SECTIONS LIST
>
> Copyright (c) YEAR YOUR NAME. Permission is granted to copy, distribute and/or modify this document under the terms of the GNU Free Documentation License, Version 1.2 or any later version published by the Free Software Foundation; with no Invariant Sections, no Front-Cover Texts, and no Back-Cover Texts. A copy of the license is included in the section entitled 'GNU Free Documentation License'.

If you have Invariant Sections, Front-Cover Texts and Back-Cover Texts, replace the 'with...Texts.' line with this:

> SAMPLE INVARIANT SECTIONS LIST
>
> with the Invariant Sections being LIST THEIR TITLES, with the Front-Cover Texts being LIST, and with the Back-Cover Texts being LIST.

If you have Invariant Sections without Cover Texts, or some other combination of the three, merge those two alternatives to suit the situation.

If your document contains nontrivial examples of program code, we recommend releasing these examples in parallel under your choice of free software license, such as the GNU General Public License, to permit their use in free software.

Appendix C

Index