Gwyddion user guide

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This guide is a work in progress.

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Chapter 1

Introduction

The latest version of this guide is available on-line at http://gwyddion.net/documentation/user-guide-en/. This guide is available in several languages, namely English, French and Russian. All language versions are listed on-line 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 varies depending on the operating system and the various installation methods will be described in the following sections.

Gwyddion needs or can utilise various software libraries, described in section Build Dependencies. If you install binary packages you usually do not need to concern yourself with the required components as the packager has taken care of it and ensured that all are present. However, it is important if you compile Gwyddion from source code.

To play with Gwyddion you might also want to download the sample Gwyddion files. They are in native Gwyddion format and represent typical AFM data.

2.1 Linux/Unix Packages

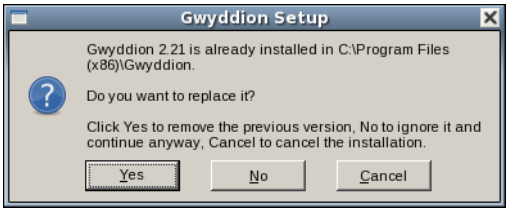
Some GNU/Linux and Unix systems provide binary packages of Gwyddion. The download page of the project also tracks known packages and packaging efforts. For instance, Debian, Ubuntu, Gentoo, openSuSE or FreeBSD offer Gwyddion packages. If your operating system provides such a package and it is recent 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

Note The packaging of MS Windows executables has changed substantially in version 2.23. So, if you upgrade from a pre-2.23 version to version 2.23 or newer, please read the description of the changes.

If you have already installed Gwyddion the installer asks if you want to replace the previous version.



The question what to do with the previous Gwyddion version.

You have three options:

Yes (replace) The already installed version will be replaced. This is the normal upgrade method.

No (keep) The already installed version will be ignored and the installation will proceed as a fresh one. Generally, this is a bad idea as both versions will share settings and registry keys and if you uninstall one the other will be affected. In some cases, though, you can find this option useful.

Cancel The installation will be aborted and the old version will be kept untouched.

In the following steps the installer reminds you of the software components included in the package and their licenses (that are all Free Software), lets you change the installation directory and offers a choice of languages to use for the user interface.

The installer creates the following useful keys under `HKEY_LOCAL_MACHINE\Software\Gwyddion\2.0`:

InstallDir Installation directory, e.g. `C:\Program Files\Gwyddion`. Reading this key can be useful for determining where to install extensions.

Version Full Gwyddion version as a string.

Locale Language of Gwyddion user interface chosen during the installation (more precisely, a locale specification that, among other things, defines the language). You can modify it using **regedit** to choose another language as described below.

The list of available languages and corresponding `Locale` values include:

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)

If you want to uninstall Gwyddion go to *Start* → *Control Panel* → *Add or Remove Programs* and choose Gwyddion. Note that this is valid for Windows XP. The path to the *Add/Remove* window may be slightly different on other Windows OS.

2.3 Build Dependencies

The following table lists packages required to build Gwyddion from source code. If your operating system has separate development packages for libraries you need them too. The table does not include common software compilation prerequisites like the C compiler or the **make** utility. Operating system specifics are described in following sections dedicated to building on particular operating systems.

BUILD DEPENDENCIES

GTK+ ≥ **2.8.0** *Required.*

This includes the dependencies of GTK+ such as GLib, Pango or Cairo.

pkg-config ≥ **0.16** *Required.*

GtkGLExt ≥ **1.0** *Optional.*

Enables OpenGL 3D data views.

LibXML2 ≥ **2.x** *Optional.*

Enables import of SPML files.

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

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

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 modularisation of X in Xorg 7.0 it is distributed separately and therefore you might not have its development files installed.

Zlib *Optional.*

Enables compression support in some file formats (Createc, NRRD).

Bzip2 *Optional.*

Enables compression support in some file formats (NRRD).

Minizip *Optional.*

Enables the import of some compressed formats (NanoObserver).

Libpng *Optional.*

Enables export of heightfields to 16bit greyscale PNG images and import of 16bit PNG images.

OpenEXR *Optional.*

Enables import and export of OpenEXR HDR images.

PyGTK2, including codegen *Optional.*

Enables pygwy, the Gwyddion Python scripting interface.

Note that pygwy is not really 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 Compilation on Linux/Unix

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.

Quick Instructions

If you know the drill:

```
tar -jxvf gwyddion-2.26.tar.xz
cd gwyddion-2.26
./configure
make install
```

Source Unpacking

Unpack the source code tarball with

```
tar -Jxvf gwyddion-2.26.tar.xz
```

replacing 2.26 with the actual version number. It will create directory `gwyddion-2.26` (again, with the actual version number in place of 2.26), **cd** to this directory. All other compilation actions will take place there.

If your operating system does not come with xz you might want to download `gwyddion-2.26.tar.gz` (compressed with gzip) instead and unpack it with

```
tar -zxvf gwyddion-2.26.tar.gz
```

However, modern Unix and Unix-like systems come with both xz and gzip so, the considerably smaller `gwyddion-2.26.tar.xz` 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. At the end, **configure** also prints a summary of enabled/disabled optional features, including the reasons why features were disabled.

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/fftw3/lib/pkgconfig
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 set:

```
CPPFLAGS=-I/usr/local/include
export CPPFLAGS
LDFLAGS=-L/usr/local/lib
export LDFLAGS
```

Option `--prefix` of **configure** sets the base installation directory. Program components will be installed into its `bin`, `lib`, `share`, etc. subdirectories (that 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 into your home directory you may want to use for instance

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

If you install Gwyddion for personal use it is recommended to use a similar installation directory as no steps need to be performed as root in this case.

Configuration tweaks

Optional features can be enabled/disabled with options such as `--with-foo`/`--without-foo` or `--enable-foo`/`--disable-foo`. For instance compilation with FFTW3 can be disabled with:

```
./configure --without-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.

The complete list of **configure** options and important variables can be obtained with:

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

Certain auxiliary installation actions can be disabled in **configure**: Updating of Freedesktop files can be disabled with **--disable-desk** 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**.

If you intend to patch or otherwise modify Gwyddion source code pass option `--enable-maintainer-mode` to **configure** to enable various update and rebuild rules that are not used in mere compilation. Depending on the nature of the modifications, some of the additional tools described in section Subversion Checkout, Development may be necessary.

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

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

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. This is the *only* command that you might have to run as root during the installation. For example using **sudo**:

```
sudo make install
```

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. 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.

If you install Gwyddion into `/usr/local` and get error message that `libgwyapp.so.0` cannot be found your system probably lacks standard library directories in the dynamic linker configuration. Notably, this happens on Ubuntu. Edit file `/etc/ld.so.conf` and add the line

```
/usr/local/lib
```

there.

Running

Running Gwyddion does not normally require any additional setup.

The misfeatures of some desktop environments, however, may render Gwyddion unusable and need to be disabled. The hijacking of program main menu in Unity makes most of Gwyddion menus inaccessible. It can be disabled by by unsetting `UBUNTU_MENUPROXY` while running Gwyddion:

```
UBUNTU_MENUPROXY= gwyddion
```

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-2.26.tar.xz
```

where 2.26 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 localed 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 summarises 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 little 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 gwyddion (e.g. /usr/local/bin/gwyddion) as *Command*. After this you can choose gwyddion from the X11 menu.

2.6 Cross-Compiling for MS Windows

Cross-compiling Gwyddion for MS Windows under Linux is quite similar to normal Unix compilation with certain additional setup and extra steps. Although the process is quite smooth the initial setup may seem a bit complicated. If, in addition, you are not familiar with the normal Unix compilation you might wish to start with that and attempt cross-compilation once you familiarise yourself with the basic procedure.

These instructions describe compilation under Fedora using its MinGW cross-compilation support as this is what Gwyddion developers use. Instructions for openSUSE are also provided. Compilation in other distributions or in native MinGW should be also possible – reports of success (or failure) and additions to these instructions for other systems are welcome.

Full cross-compilation has the following steps:

- configuration for mingw32,
- compilation,
- installation into a staging area,
- creation of an installer using NSIS.

A script is available that automatically performs all the steps, as described below.

Setup

Before the first compilation you must set up the cross-compilation environment. This has to be done only once.

Base MinGW32 Packages

On Fedora, everything is in the default 'Everything' repository. On openSUSE, it is necessary to add additional package repositories `windows:mingw:win32/openSUSE_11.3` and `devel:tools/openSUSE_11.3`, where 11.3 is of course to be replaced with the actual openSUSE version. In unsure, you can also look up the packages in the on-line openSUSE package search.

Run as root:

```
# Fedora
yum install mingw32-{gcc-c++,gtk2,libxml2}

# openSUSE
zypper install mingw32-cross-{gcc,gcc-c++,pkg-config} \
               mingw32-{gtk2,expat,libxml2,fftw3,libjasper,libcairo2} \
               mingw32-{gtk2,libxml2,fftw3,libjasper,libcairo2}-devel
```

to install the necessary mingw32 packages (several more packages will be installed as dependencies of those explicitly given here).

Wine

Wine is the MS Windows compatibility layer/emulator for Unix. It is used to run NSIS that creates the executable Gwyddion Windows installer. Wine can also be used to run and test the cross-compiled Gwyddion, as described below.

Run

```
# Fedora
yum install wine

# openSUSE
zypper install wine
```

to install Wine.

NSIS

Nullsoft scriptable install system (NSIS) is used to create the Gwyddion installer. This is a MS Windows program, therefore, it is installed *under Wine*.

Download NSIS from its web page and run

```
wine nsis-2.46-setup.exe
```

replacing 2.46 with the actual version. Version 2.46 of NSIS is the oldest that has been tested.

Extra MinGW32 Packages

The official Gwyddion packages utilise additional libraries that are not available in the Fedora and/or openSUSE MinGW environment, namely GtkGLExt and FFTW. They can be omitted though you will have to modify some scripts if you do so. At the time of writing this, Fedora lacks both packages while openSuSE lacks only GtkGLExt. In addition, the default Bzip2 package is built to use the stdcall calling convention and is not found by configure.

The source packages `mingw32-fftw`, `mingw32-gtkglext` and `mingw32-bzip2-cdecl` can be downloaded from Gwyddion SourceForge pages. Build binary packages using **rpmbuild**:

```
rpmbuild --rebuild mingw32-fftw-3.2.2-1.src.rpm
```

replacing the file name with the name of the downloaded file. If the **rpmbuild** command complains about missing dependences install them using **yum install** as before. The created package can then be installed as root:

```
#Fedora
yum localinstall --nogpgcheck ~/rpmbuild/RPM/RPMS/noarch/mingw32-3.2.2-1.noarch.rpm

# openSUSE
zypper install ~/rpmbuild/RPM/RPMS/noarch/mingw32-3.2.2-1.noarch.rpm
```

The same applies to the other source packages (all built RPMs can be installed at once with a single **yum** or **zypper** invocation).

If you have never built any RPM the package building support has to be installed and initialised first. Run as root:

```
# Fedora
yum install rpm-build rpmdevtools

# openSUSE
zypper install rpmdevtools
```

and then as a normal user (who is going to build the RPMs):

```
rpmdev-setuptree
```

This creates a directory tree in `~/rpmbuild` where the RPM package building will take place.

Support scripts

Support scripts and data are available in `mingw32-cross-compile` module in the Gwyddion subversion repository. Run

```
svn checkout https://gwyddion.svn.sourceforge.net/svnroot/gwyddion/trunk/mingw32-cross-comp
```

to check it out from the repository.

The most important tool you obtain is the **cross-build** script that automates all the cross-compilation steps. Before you use it for the first time, review file `setup` that defines where various things are located. The default contents looks as follows:

```
source_dir=$HOME/Projects/Gwyddion/gwyddion-mingw32
mingw32_prefix=/usr/i686-pc-mingw32/sys-root/mingw
target_prefix=$HOME/opt/gwyddion-mingw32
nsis_compiler=C:\\Program\ Files\ \(x86\)\\NSIS\\makensis.exe
```

Variable `source_dir` specifies the location of the untarred or checked-out Gwyddion source code and it will likely need to be adjusted. Variable `target_prefix` specifies the installation directory (staging area) for the cross-compiled Gwyddion. The default value should be reasonable and you do not need to change it unless you want to. The remaining two variables, `mingw-32_prefix` and `nsis_compiler`, specify the location of MinGW files and NSIS compiler, respectively. They do not need to be changed from the default values under normal circumstances although NSIS can be installed in either `Program Files (x86)` or `Program Files` by default depending on Wine configuration. Note `setup` is read by shell so there must not be any spaces around =.

Compilation

The setup was tedious but it was worth it because the compilation is then extremely simple. Run

```
./cross-build
```

in `mingw32-cross-compile` directory. That's all. If it succeeds an executable Gwyddion Windows installer with bundled GTK+ and everything will be created in `$target_prefix`.

You can make a coffee meanwhile – or study the `cross-build` script (it is actually quite short and clear).

Running Under Wine

Compiled Gwyddion can be run under Wine. Assuming the default value of `target_prefix`:

```
wine ~/opt/gwyddion-mingw32/bin/gwyddion.exe
```

To run `gwyddion.exe` the dynamic linker must be able to find all the necessary DLLs. This is ensured in a somewhat crude way by script **copysysfiles** that copies all necessary MinGW files from system to `$target_prefix`. Since **copysysfiles** is executed by **cross-build** you normally do not need to execute it manually.

The second step that might be necessary is setting registry key

`HKEY_LOCAL_MACHINE\Software\Microsoft\Windows\CurrentVersion\App Paths\gwyddion.exe`

to point to `gwyddion.exe` and the value `Path` to point to the `bin` subdirectory.

2.7 Subversion Checkout, Development

Gwyddion uses Subversion version control system for source code revision management. The organisation 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 repository does not contain any generated files, no matter how exotic tools may be necessary to generate them. Therefore, additional packages are required for building from a fresh checkout. There are also certain platform limitations. The additional tools and packages required for development are essentially the same as for compilation from Subversion checkout. More precisely, to build from a fresh checkout all the additional tools are necessary, whereas development may require only a subset of them or even none, depending on the type and extent of the changes in the source code.

ADDITIONAL DEVELOPMENT BUILD DEPENDENCIES

- GNU autoconf $\geq$ 2.60
- GNU automake $\geq$ 1.11
- GNU libtool $\geq$ 1.4
- Python $\geq$ 2.2
- Perl5
- gtk-doc $\geq$ 1.12
- GNU gettext $\geq$ 0.12, including development stuff
- probably GNU versions of most tools: the compiler, binutils, ...

After a fresh checkout, run **`./autogen.sh`** with any arguments you would give to **configure**. Note it automatically adds options `--enable-maintainer-mode` and `--enable-gtk-doc` to ensure the rules for creation and updates of various files are active. Generally, you should always use `--enable-maintainer-mode` if you intend to change the program source code in a non-trivial way.

On some systems, **autogen.sh** can fail even if you have sufficient versions of autotools installed. These systems do not install general **autoconf** or **automake** commands, only versioned commands such as **autoconf261** or **automake19**. This makes it particularly difficult to find for example '**automake** 1.9 or newer' with no limit on how newer it can be. Therefore, **autogen.sh** does not attempt this 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.

MS Windows

Since the standard method to create MS Windows executables is cross-compilation in Linux the recommended method to develop for MS Windows is also to compile in Linux. This can be done either on a different physical computer using **ssh** or in a virtual machine running on the same computer as the host MS Windows system. In both cases the Gwyddion build directory (and other directories) can be shared between the Linux and MS Windows systems using either Samba or a shared directory mechanism of the virtual machine and the compiled executables thus can be directly tested in MS Windows without having to transfer files back and forth.

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.

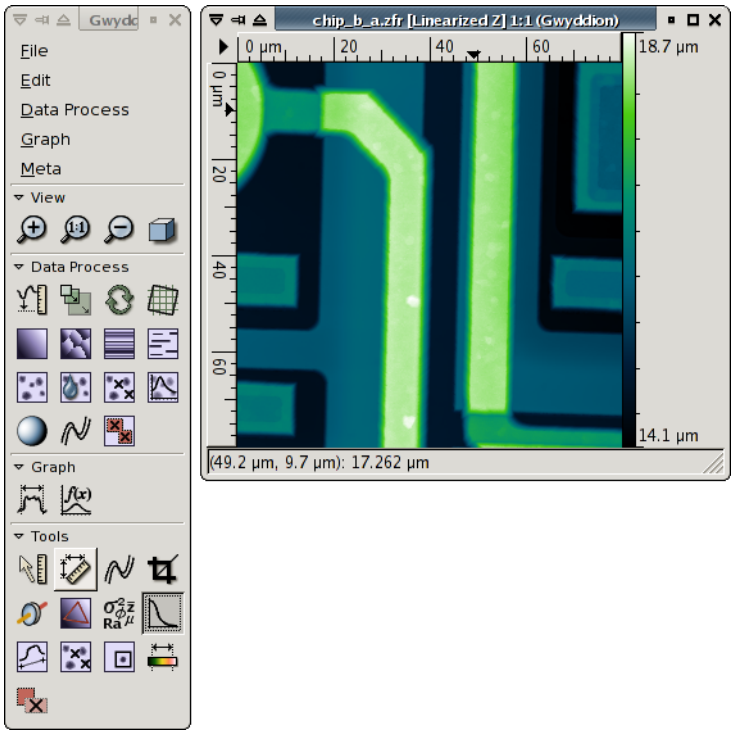
Data Process is built automatically from all data processing modules available in the Gwyddion module directory (depending on the operating system). This menu together with *Tools* panel of buttons contain most of the commands you will need at analyzing your SPM data. A subset of these functions is also 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.



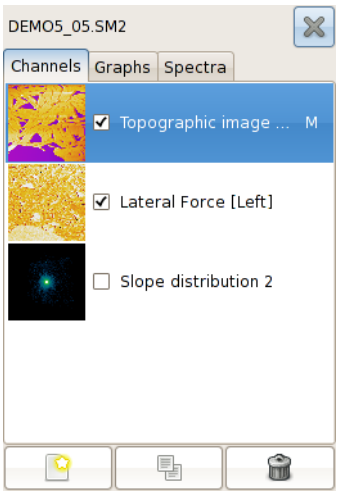
Main window and a data window showing microchip surface (Gwyddion sample file `chip.gwy`*).*

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.



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.

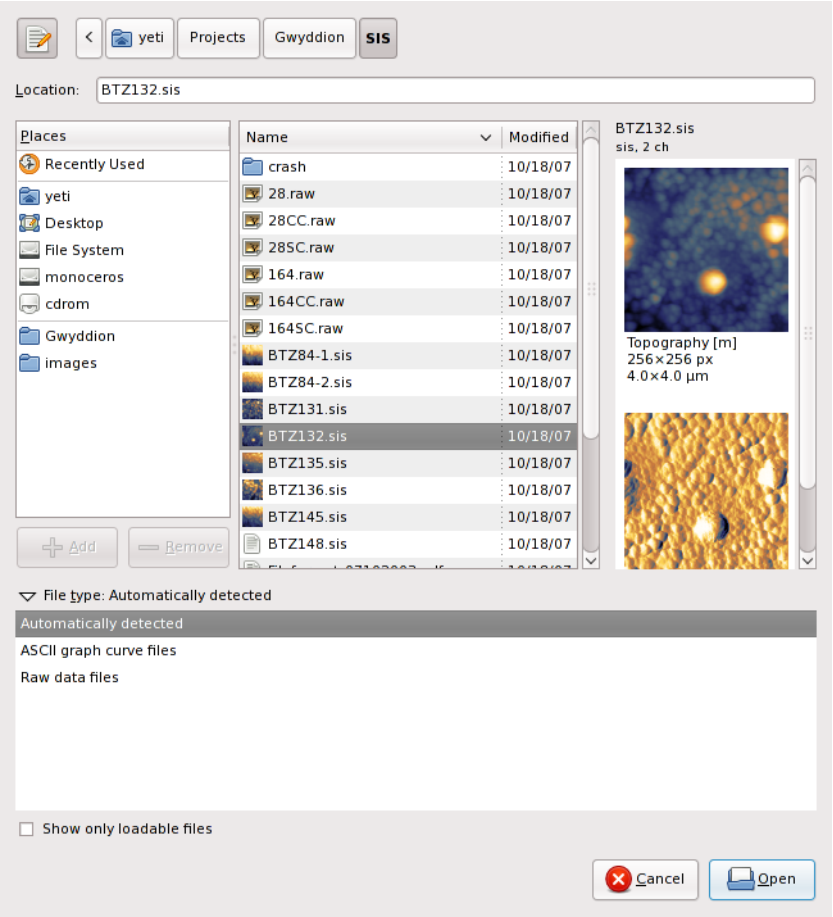
The list of all supported file formats can be found in chapter Summaries and Tables.

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.



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* → *Merge*, 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.

File → Save as... can also be used to export channels to image formats. Just enter `foo.png` as the file name to export a PNG image the current channel, similarly for other formats.

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.

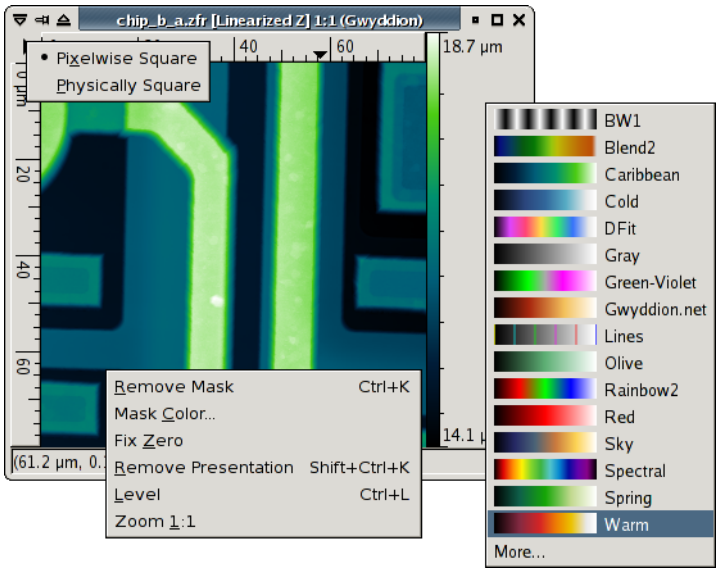
3.4 Data Window

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.

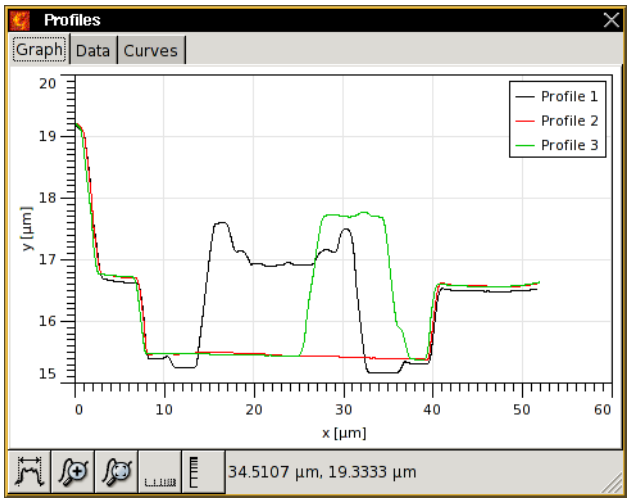


Data window with all three available context menus shown.

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.

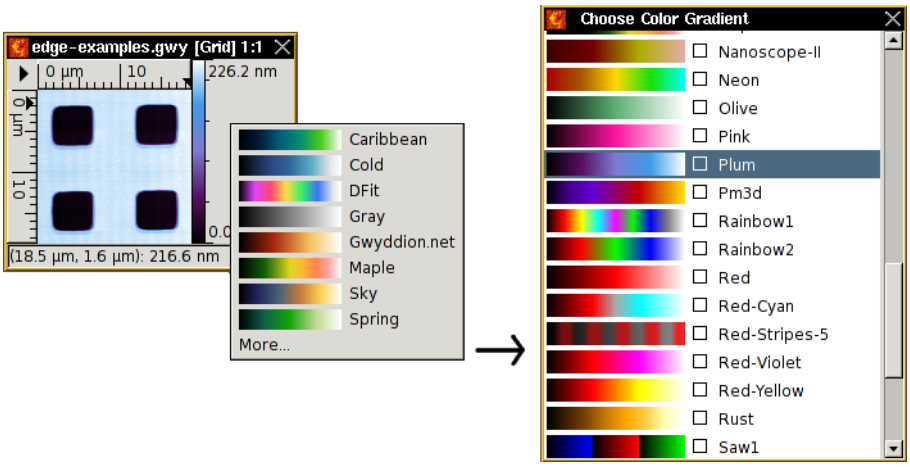
Tool dialogs can be closed (or more precisely hidden, as the current tool is still active even if its dialog is not visible), beside activating the *Hide* button, by pressing **Esc** or clicking the tool's button in the toolbox again.

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.

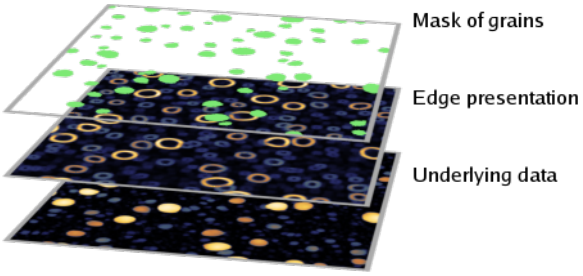
Note the superimposed presentation is really only a presentation, it is never used for calculations. In all data processing functions or tools the results are always computed from the original underlying data. Since presentations can be computationaly intensive to calculate, they are not automatically 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 contiguous 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 universal mask modification tool. It provides two groups of functions: editing of the mask by drawing directly in the data window and global operations with the mask such as inversion or growing and shrinking.

The direct mask modification is controlled by the buttons in the *Editor* group. It can be done in two ways: by selecting geometrical shapes that are subsequently filled or erased (using the *Shapes* option), and by freehand drawing operations using drawing tools (option *Drawing Tools*).

Buttons in the *Mode* row select how the geometrical 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.

Freehand drawing tools are selected by buttons in the *Tool* row:

Pencil Freehand drawing with a pencil of radius speficied by parameter *Radius*. Note this may be slow on slow computers and/or large data fields.

Eraser Freehand erasing with an eraser of radius speficied by parameter *Radius*. Note this may be slow on slow computers and/or large data fields.

Fill Bucket-filling of a contiguous unmasked area.

Unfill Bucket-unfilling of a contiguous masked area.

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.

Fill Voids Makes the grains single-connected, i.e. without any holes, by filling the holes in grains.

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.

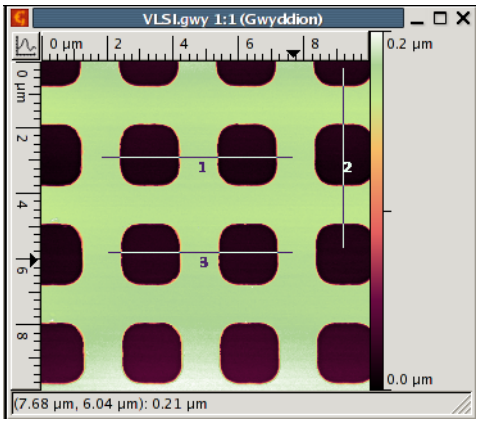
This is an exception to the rule stating that presentations are never used for further processing. Sometimes it can be useful to mark, for instance, edges found on the data even though the corresponding presentation visualizes a quantity weird from the physical point of view.

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.



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.

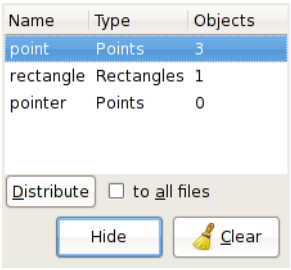
Pressing Shift during selection restricts the degrees of freedom of the shape, making it easier to draw shapes form a specific subset. Specifically, pressing Shift restricts

- 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.



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.

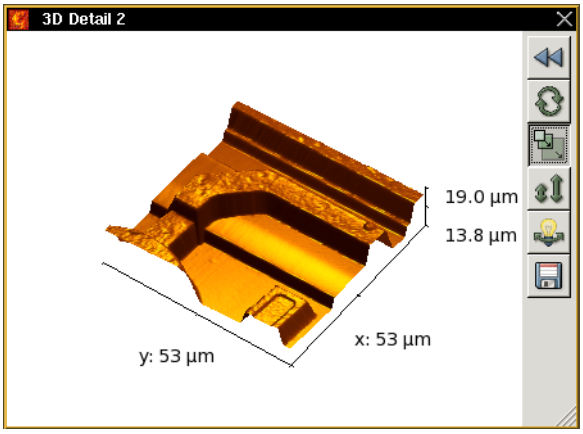
If the physical dimensions of the target data are not sufficient to contain all the objects of the copied selection then only those objects that fit are copied (this can also mean nothing is copied).

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 $\mathbf{L}$ the normal vector pointing from the observed surface point to the light source, $\mathbf{V}$ the normal vector to the observer, $\mathbf{N}$ the normal vector to the surface and $\mathbf{R}$ 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.

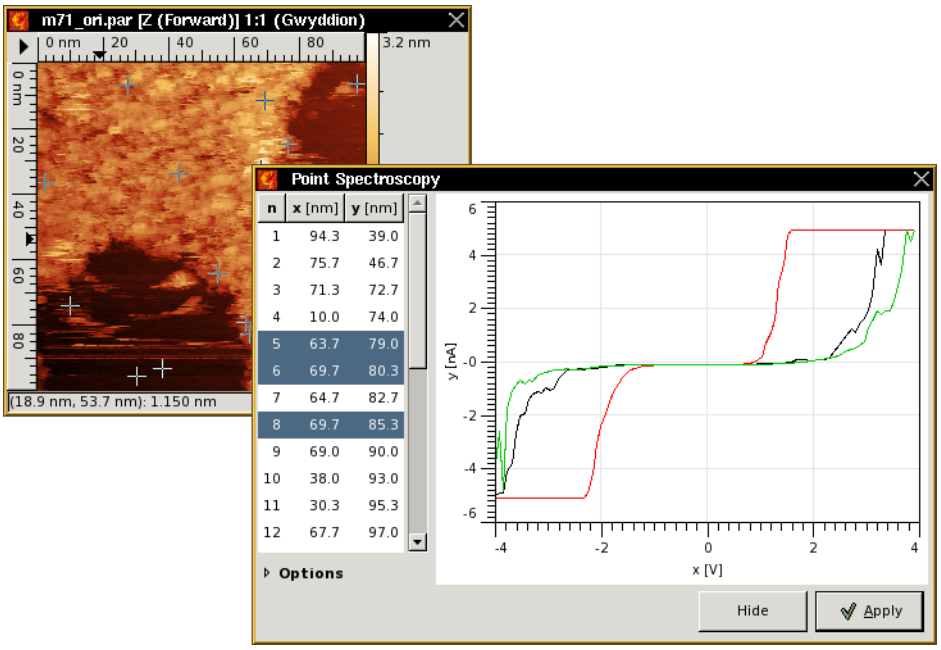
3.11 Single Point Spectra

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.



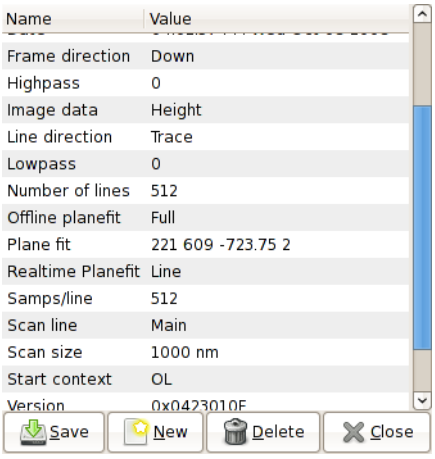
A data window with measurement points displayed and the point spectroscopy tool showing curves from three selected points.

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.



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 the 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.

See the reference section High-Depth Image Formats for the details of support for high-depth images and the possibility of using them for data representations.

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.

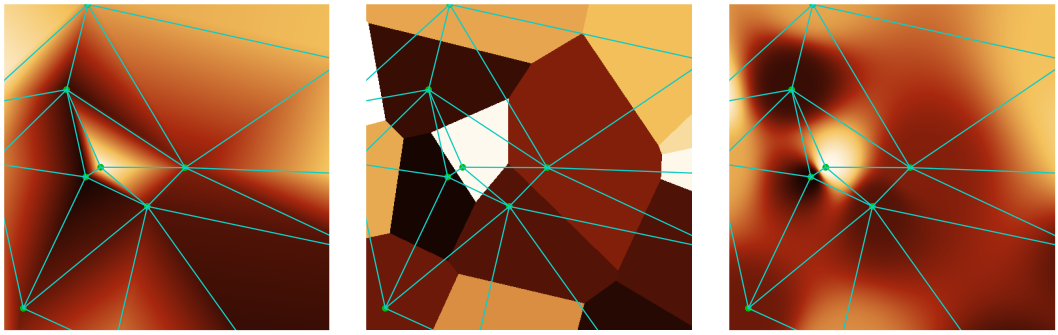
The former two interpolation types are based on Delaunay/Voronoi triangulation which is not well-defined for point sets where more than two points line on a line or more than three lie on a circle. If this happens the triangulation fails and the import module displays an error message.

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.
- Limit the data range by cutting values outside a specified range by *Data Process* → *Basic Operations* → *Limit Range*. The range can be set numerically or taken from the false colour map range previously set using the Color range tool and it is also possible to cut off outliers farther than a chosen multiple of RMS from the mean value.
- 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.
- Tilt the data by specified gradient or angle using *Data Process* → *Basic Operations* → *Tilt*.
- Change physical dimensions, units or value scales and also lateral offsets using *Data Process* → *Basic operations* → *Dimensions and Units*. This is useful to correct raw data that have been imported with wrong physical scales or as a simple manual recalibration of dimensions and values.

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.

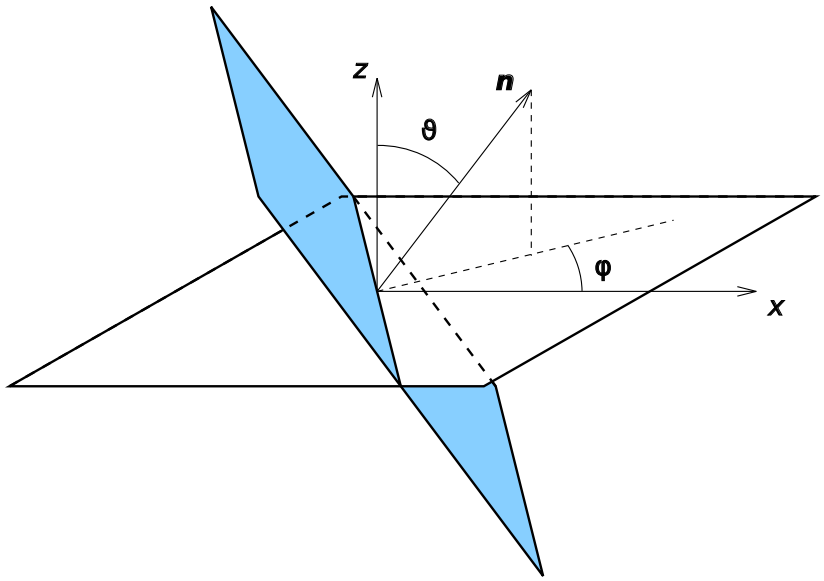
Read Value can also display the inclination of the local facet. *Averaging radius* again determines the radius of the area to use for the plane fit.

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 that $\vartheta = 0$ 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

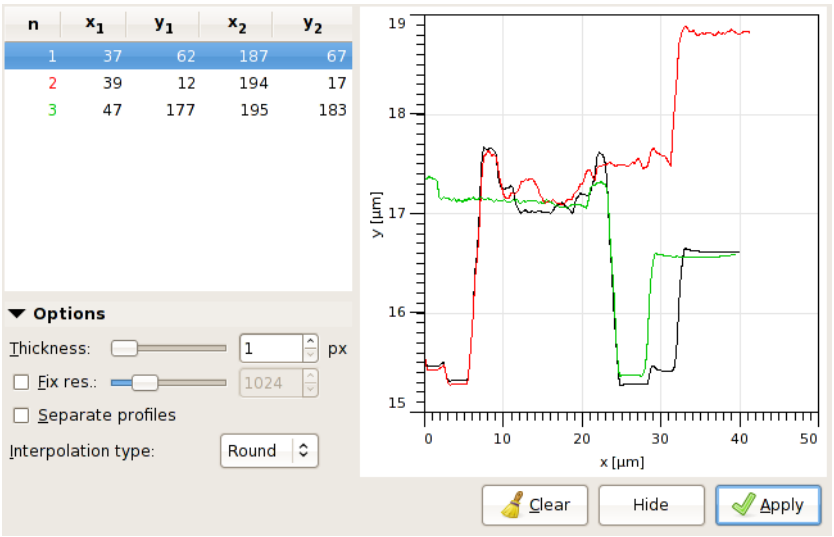
Clear Hide

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.



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.

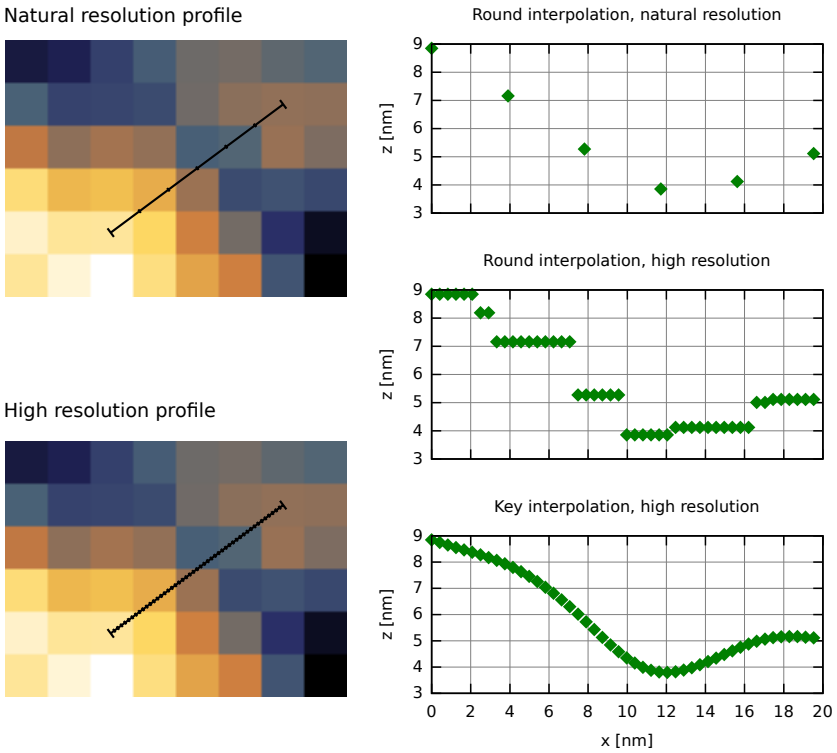


Illustration of data sampling in profile extraction for oblique lines. The figures on the left show the points along the line where the values are read for natural and very high resolution. The graphs on the right show the extracted values. Comparison of the natural and high resolution profiles taken 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 rounded 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

$$z = w_{-1}z_{-1} + w_0z_0 + w_1z_1 + w_2z_2$$

where

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

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

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

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 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 The weights are

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

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.

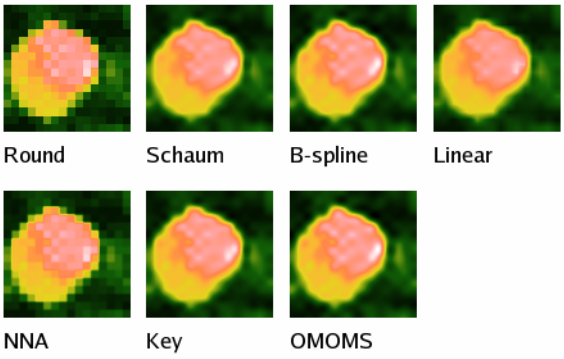


Illustration of the available interpolation types (the original pixels are obvious on the result of Round interpolation). All images have identical false color map ranges.

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.

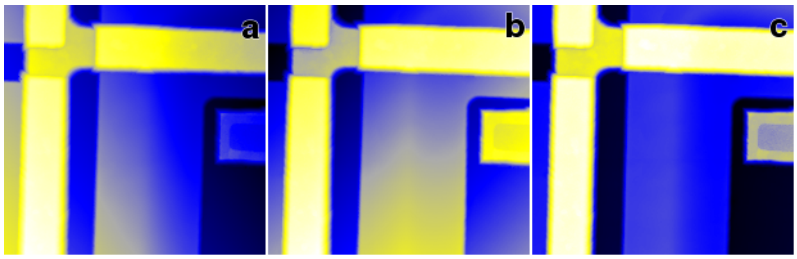
Finding the orientation of the facets is an iterative process that works as follows. First, the variation of local normals is determined:

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

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. Subsequently, 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.

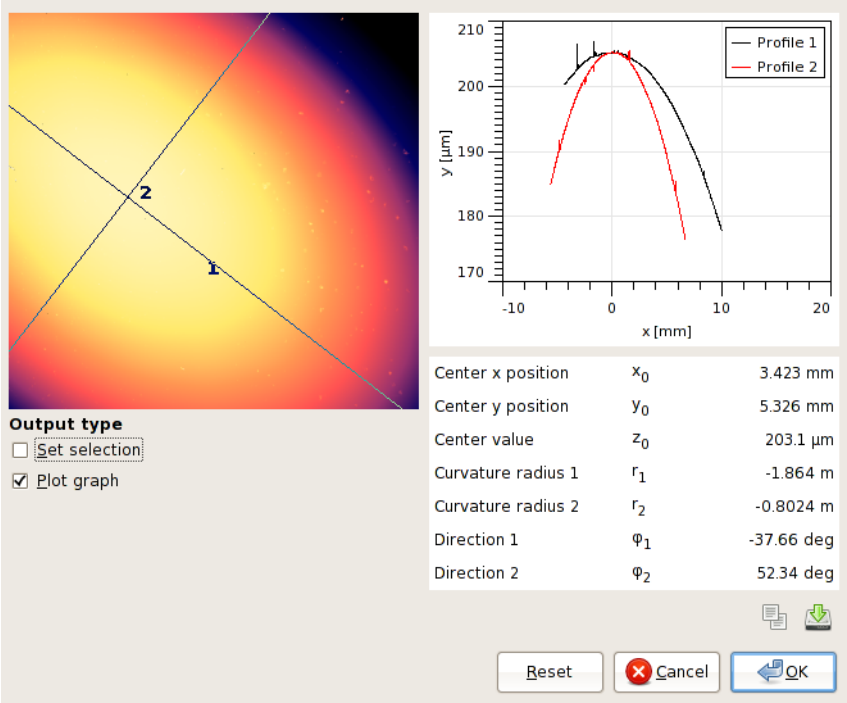
Curvature

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.



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

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

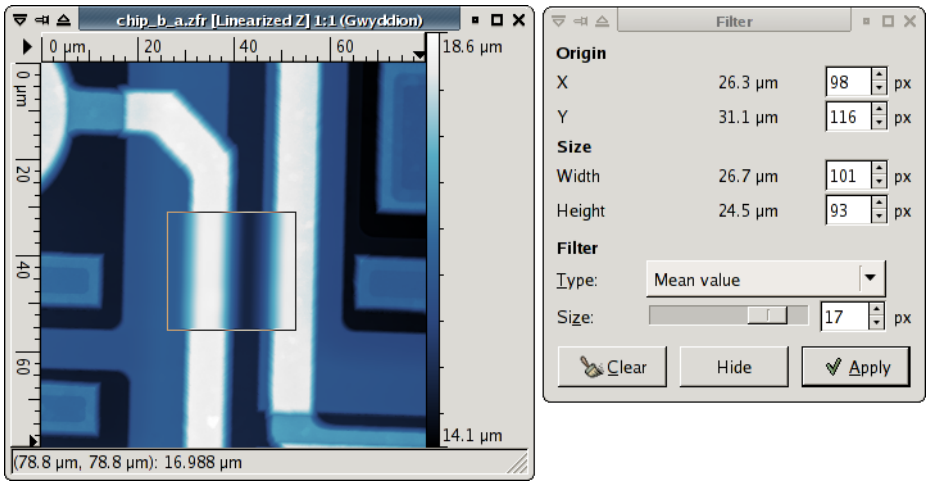
- Gaussian filter – a smoothing filter, the size parameter determines the FWHM (full width at half maximum) of the Gaussian. The relation between FWHM and σ is

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

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.



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*.

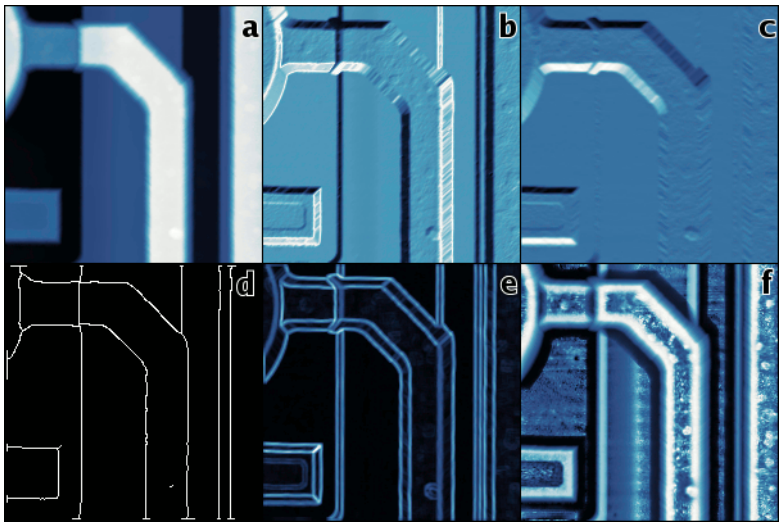
Basic Operations

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 non-linearity 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.

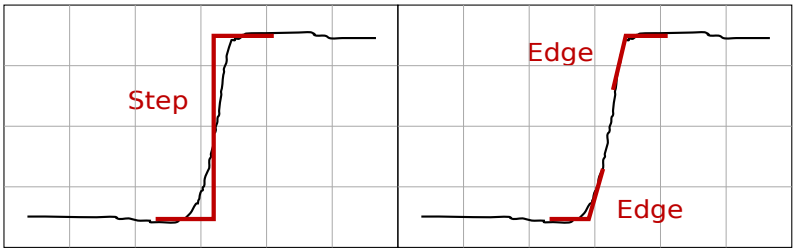
$$w_{\text{Prewitt}} = \begin{pmatrix} 1/3 & 0 & -1/3 \\ 1/3 & 0 & -1/3 \\ 1/3 & 0 & -1/3 \end{pmatrix}, \quad w_{\text{Sobel}} = \begin{pmatrix} 1/4 & 0 & -1/4 \\ 1/2 & 0 & -1/2 \\ 1/4 & 0 & -1/4 \end{pmatrix}$$

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.

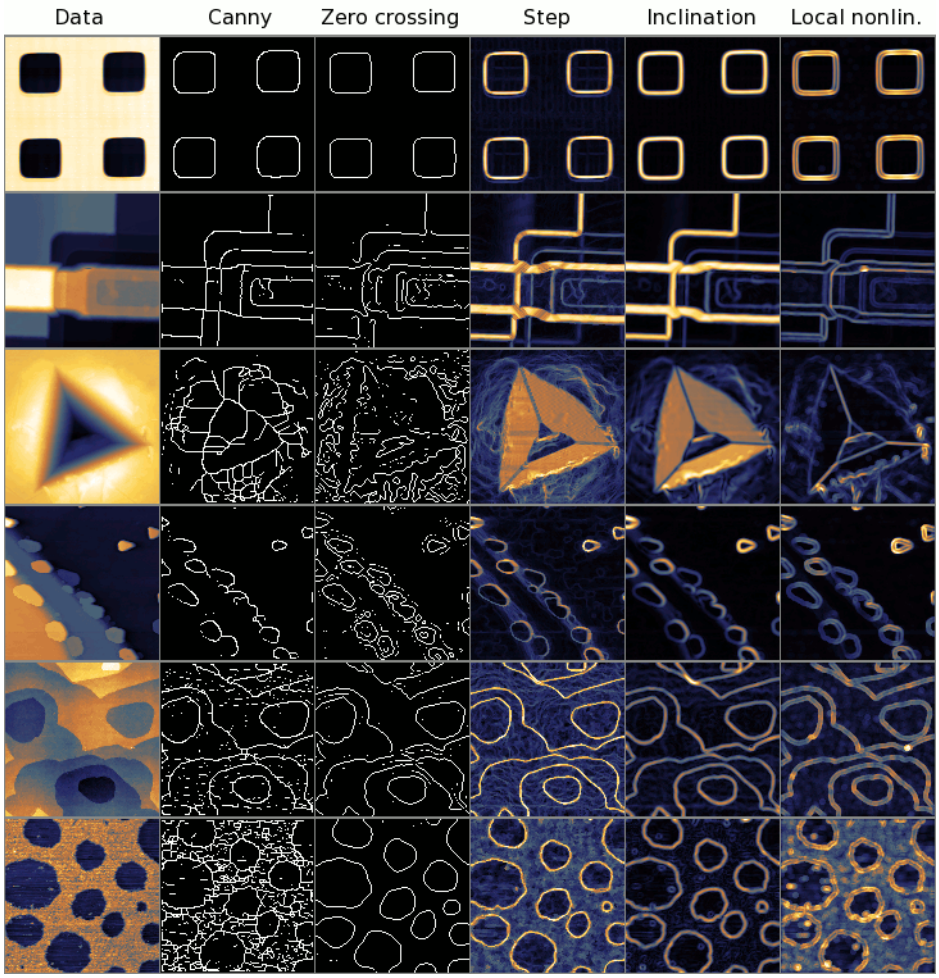
Step A step detection algorithm providing a good resolution, i.e. sharp discontinuity lines, and a good dynamic range while being relatively insensitive to noise. The principle is quite simple: it visualizes the square root of the difference between the 2/3 and 1/3 quantiles of the data values in a circular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

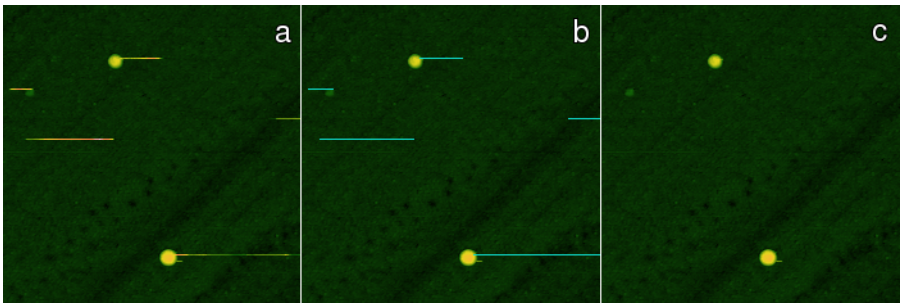
Data Process → *Correct Data* → *Mark Scars*

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.

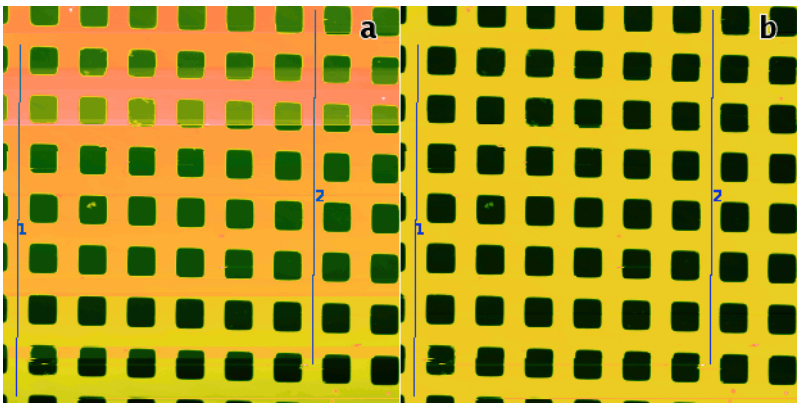
Function *Median Difference Line Correction* shifts the lines so that the median of differences (between vertical neighbour pixels) becomes zero, instead of the difference of medians. Therefore it better preserves large features while it is more sensitive to completely bogus lines.

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.

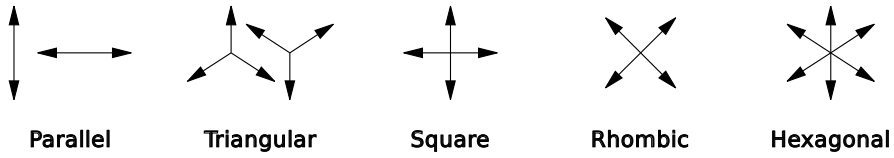
Unrotate

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.

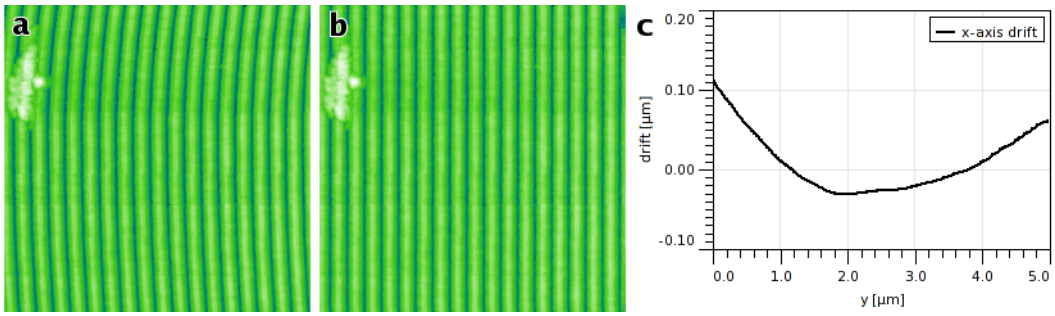
The drift graph, which is one of possible outputs, represents the horizontal shift of individual rows compared to a reference row (which could be in principle chosen arbitrarily, in practice the zero shift is chosen to minimize the amount of data sticking out of the image after compensation), with the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

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

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 and 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.
- R_a 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 R_a 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:

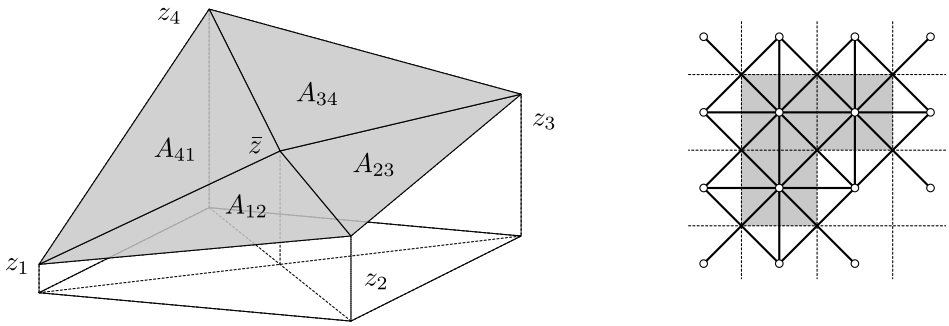
$$\sigma = \mu_2^{1/2}, \quad \gamma_1 = \frac{\mu_3}{\mu_2^{3/2}}, \quad \gamma_2 = \frac{\mu_4}{\mu_2^2} - 3$$

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 (horizontal or vertical), 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

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

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 $m = \tau_x/\Delta x$, $n = \tau_y/\Delta y$. The function can thus be evaluated in a discrete set of values of τ_x and τ_y separated by the sampling intervals Δx and Δy, 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

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

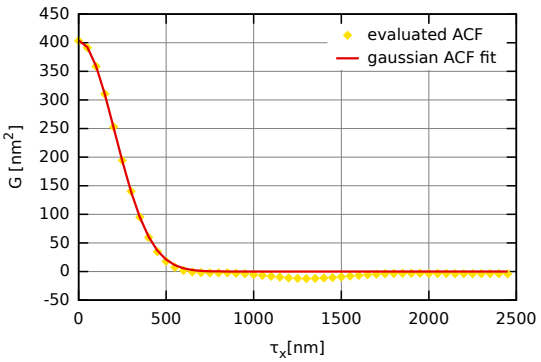
The one-dimensional autocorrelation function is often assumed to have the form of a Gaussian, i.e. it can be given by the following relation

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

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* $T \approx 300\,\mathrm{nm}$.

We can also introduce the radially averaged ACF $G_r(\tau)$ which of course contains the same information as the one-dimensional ACF for isotropic surfaces:

$$G_r(\tau) = \int_0^{2\pi} W(\tau\cos\varphi, \tau\sin\varphi)\,\mathrm{d}\varphi$$

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 $m = \tau_x/\Delta x$. The function thus can be evaluated in a discrete set of values of τ_x separated by the sampling interval Δx.

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

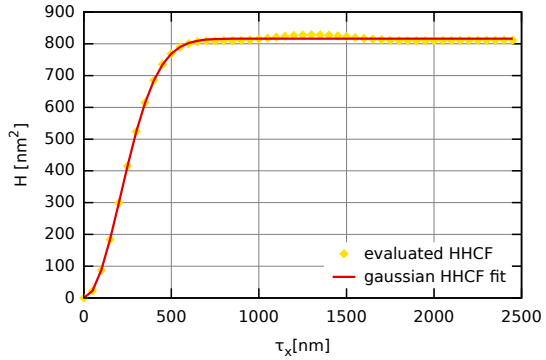
$$H_x(\tau_x) = 2\sigma^2 \left[1 - \exp\left(-\frac{\tau_x^2}{T^2}\right)\right]$$

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

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.

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

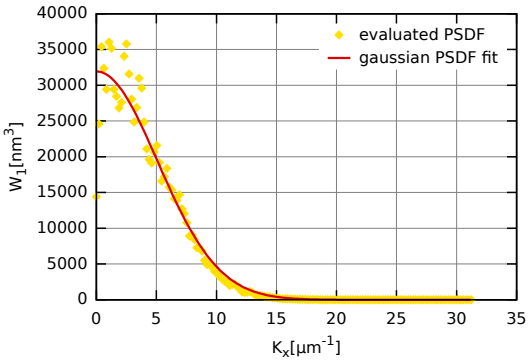
If we choose the Gaussian ACF, the corresponding Gaussian relation for the PSDF is

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

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 the 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

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

while for exponential-ACF surface as

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

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 the following formulas:

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

Here N 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:

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

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 x-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.

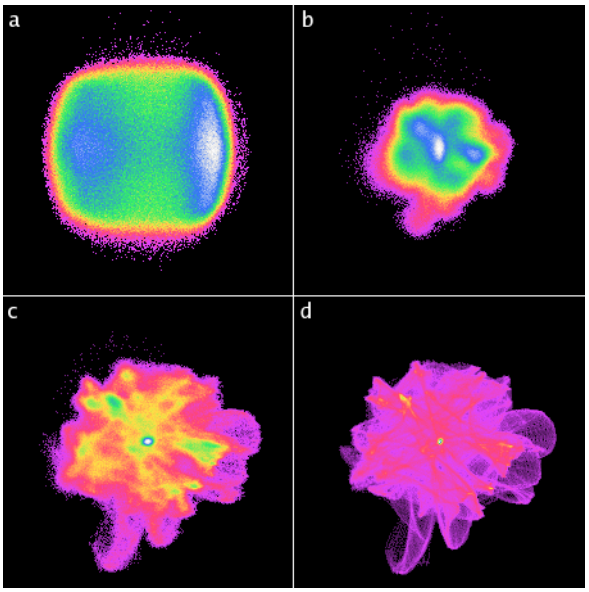


Illustration of the influence of fitted plane size on the distribution of a scan of a delaminated DLC surface with considerable fine noise. One can see the distribution is completely obscured by the noise at small plane sizes. The neighbourhood sizes are: (a) 0, (b) 2, (c) 4, (d) 7. The angle and false 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. it holds

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

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

$$R_a = \frac{1}{N}\sum_{j=1}^{N} |r_j|$$

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

$$R_q = \sqrt{\frac{1}{N}\sum_{j=1}^{N} r_j^2}$$

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

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

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

$$R_v = \left|\min_{1\le j\le N} r_j\right|$$

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

$$R_p = \left|\max_{1\le j\le N} r_j\right|$$

Average Maximum Height of the Profile R_{tm} 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

$$R_{tm} = R_{vm} + R_{pm}$$

where R_{vm} and R_{pm} are defined below.

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

Average Maximum Profile Valley Depth R_{vm} 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

$$R_{vm} = \frac{1}{m}\sum_{i=1}^{m} R_{vi}$$

where

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

Average Maximum Profile Peak Height R_{pm} 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

$$R_{pm} = \frac{1}{m}\sum_{i=1}^{m} R_{pi}$$

where

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

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_{3zISO} 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_{tm}.

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.

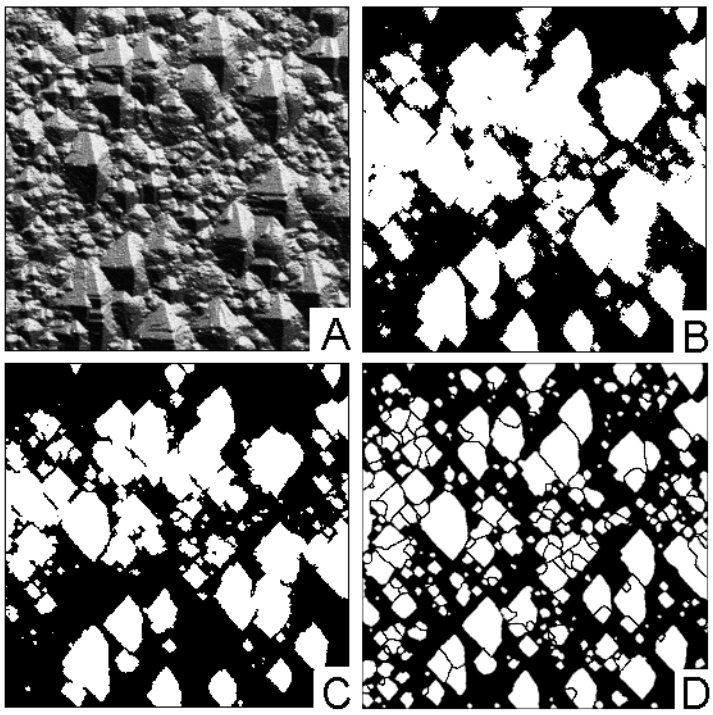


Image of grain-like surface structure (a) and corresponding results of height thresholding (b), curvature thresholding (c), and watershed (d) algorithm. Within watershed algorithm it is possible to segment image even further.

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 minimum 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 $z = z_{\min}$, 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

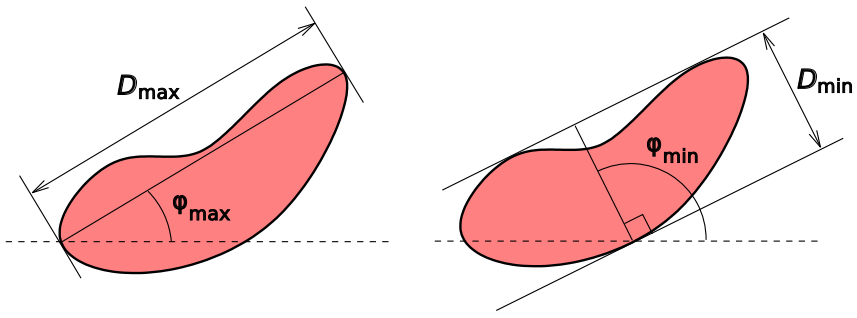
- *Center x position*, the horizontal coordinate of the grain centre. Since the grain area is defined as the area covered by the corresponding mask pixels, the centre of a single-pixel grain has half-integer coordinates, not integer ones. Data field origin offset (if any) is taken into account.
- *Center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

Curvature-related properties

- *Curvature center x*, the horizontal position of the center of the quadratic surface fitted to the grain surface.
- *Curvature center y*, the vertical position of the center of the quadratic surface fitted to the grain surface.
- *Curvature center z*, the value at the center of the quadratic surface fitted to the grain surface. Note this is the value at the fitted surface, not at the real grain surface.
- *Curvature 1*, the smaller curvature (i.e. the inverse of the curvature radius) at the center.
- *Curvature 2*, the larger curvature (i.e. the inverse of the curvature radius) at the center.
- *Curvature angle 1*, the direction corresponding to *Curvature 1*.
- *Curvature angle 2*, the direction corresponding to *Curvature 2*.

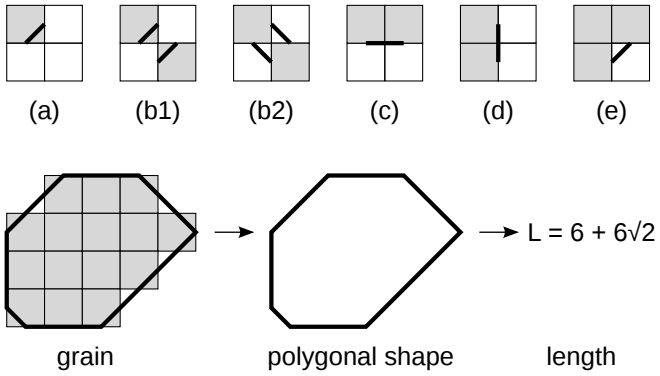


Maximum and minimum bounding dimensions and angles of a grain.

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.

$\frac{1}{96}$	$\frac{5}{48}$	$\frac{1}{96}$
$\frac{5}{48}$	$\frac{13}{24}$	$\frac{5}{48}$
$\frac{1}{96}$	$\frac{5}{48}$	$\frac{1}{96}$

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

Curvature-related properties of individual grains are calculated identically to the global curvature calculated by Curvature. See its description for some discussion.

Grain Levelling

Grains can be aligned vertically using *Data Process* → *Grains* → *Level Grains*. This function vertically shifts each grain to make a certain height-related quantity of all grains equal. Typically, the grain minimum values are aligned but other choices are possible.

Data between grains are also vertically shifted. The shifts are interpolated from the grain shifts using the Laplace equation, leading to a smooth transition of the shifts between the grains (though with no regard to other possible surface features).

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.

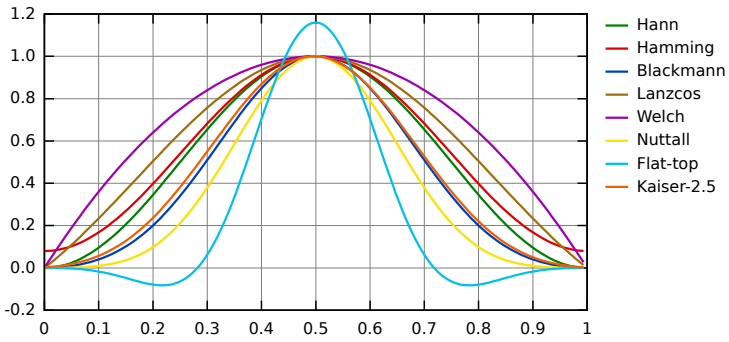
and some their combinations for convenience.

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.

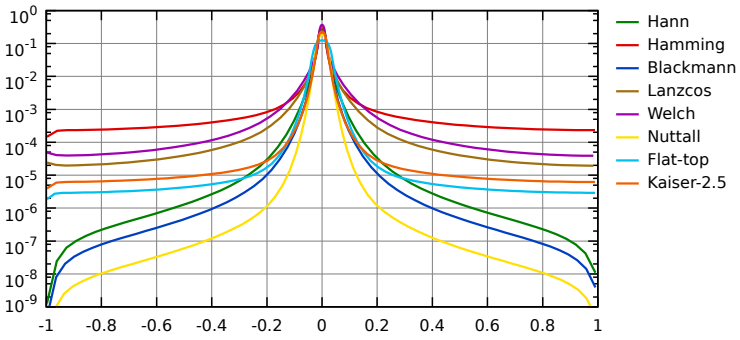
Note that the Fourier transform treats data as being infinite, thus implying some cyclic boundary conditions. As the real data do not have these properties, it is necessary to use some windowing function to suppress the data at the edgest of the image. If you do not do this, FFT treats data as being 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	$w_{\text{Hann}}(x) = 0.5 - 0.5\cos\xi$
Hamming	$w_{\text{Hamming}}(x) = 0.54 - 0.46\cos\xi$
Blackmann	$w_{\text{Blackmann}}(x) = 0.42 - 0.5\cos\xi + 0.08\cos 2\xi$
Lanczos	$w_{\text{Lanczos}}(x) = \operatorname{sinc}\pi(2x-1)$
Welch	$w_{\text{Welch}}(x) = 4x(1-x)$
Nutall	$w_{\text{Nutall}}(x) = 0.355768 - 0.487396\cos\xi + 0.144232\cos 2\xi - 0.012604\cos 3\xi$
Flat-top	$w_{\text{flattop}}(x) = 0.25 - 0.4825\cos\xi + 0.3225\cos 2\xi - 0.097\cos 3\xi + 0.008\cos 4\xi$
Kaiser α	$w_{\text{Kaiser},\alpha}(x) = \dfrac{\mathrm{I}_0\left(\pi\alpha\sqrt{4x(1-x)}\right)}{\mathrm{I}_0(\pi\alpha)}$, 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. This function can be chosen arbitrarily provided that obeys 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

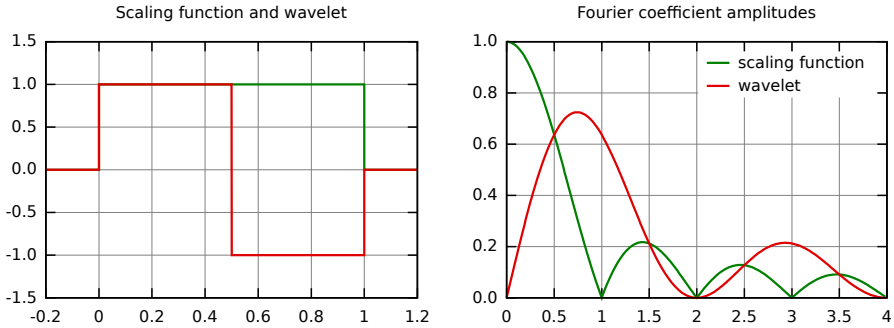
$$\phi(x) = \sum_{k=-\infty}^{\infty} a_k \phi(Sx - k)$$

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.

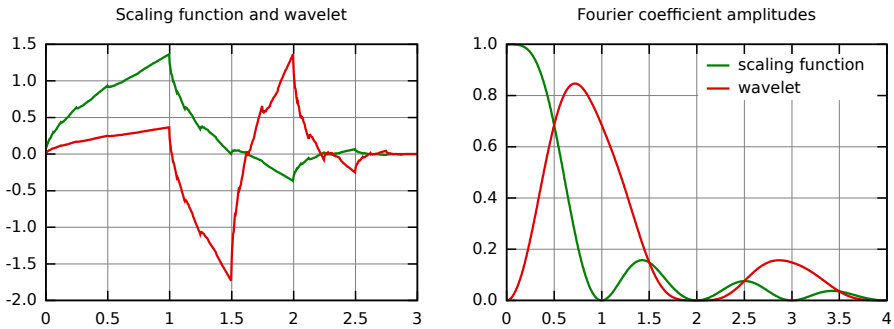
$$\int_{-\infty}^{\infty} \phi(x)\,\phi(x+l)\,\mathrm{d}x = \delta_{0,l}$$

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 that define the scaling function and also the wavelet. The wavelet is obtained from the scaling function as N 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.

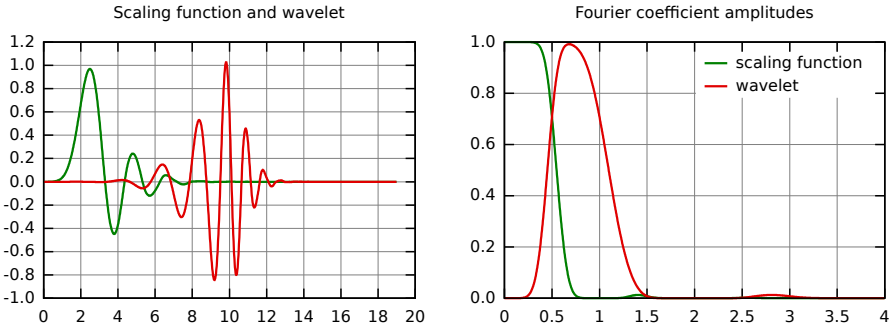
In the following figure, some wavelet scaling functions and wavelets are plotted. The most known family of orthonormal wavelets is a family of Daubechies. Her wavelets are usually denominated by the number of nonzero coefficients a_k, so we usually talk about Daubechies 4, Daubechies 6, etc. wavelets. 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 the signal length is L, first $D/2$ data at scale $L/2^{N-1}$ are computed, then $(D/2)/2$ data at scale $L/2^{N-2}$, ... 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 equals 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.

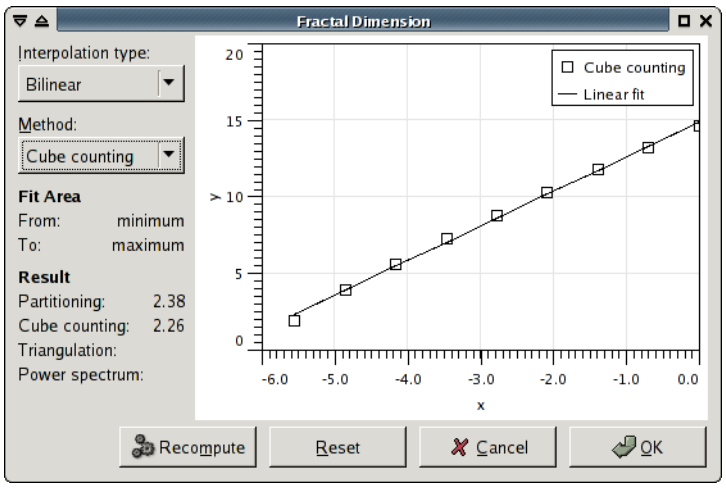
Triangulation method [1] is very similar to cube counting method and is also based directly on the box-counting fractal dimension definition. The method works as follows: A grid of unit dimension l is placed on the surface. This defines the location of the vertices of a number of triangles. When, for 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.



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

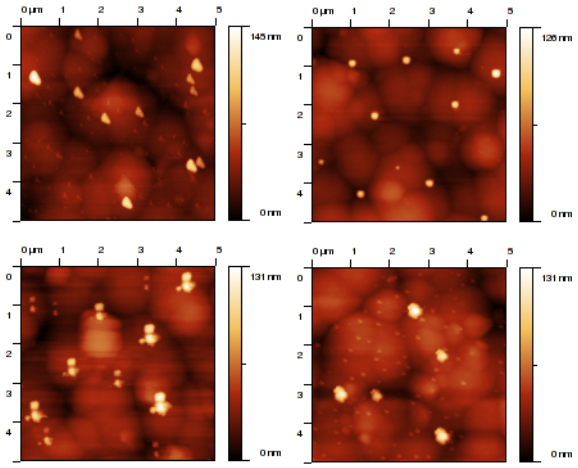
[3] A. Van Put, A. Vertes, D. Wegrzynek, B. Treiger, R. Van Grieken: Quantitative characerization of individual particle sutfaces by fractal analysis of scanning electron microscope images. Fresenius J Analen Chem (1994) 350: 440-447

[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:

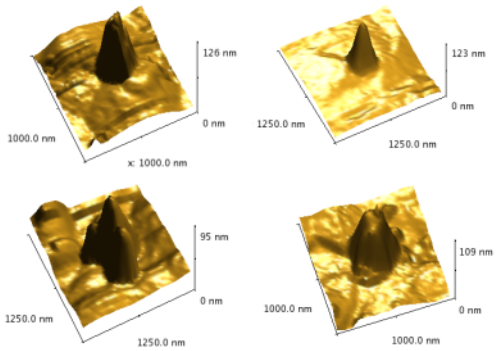
1. use manufacturer's specifications (tip geometry, apex radiius and angle)
2. use scanning electron microscope of other independent technique to determine tip properties.
3. use known tip characterizer sample (with steep edges)
4. use blind tip estimation algorithm together with tip characterizers or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

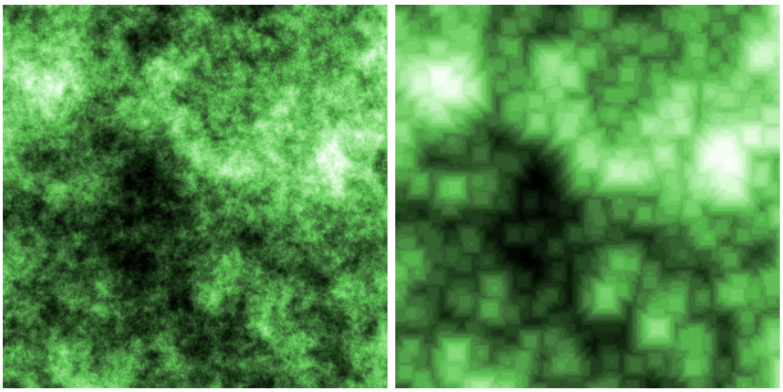


SPM tips obtained from data of previous figure using blind estimation algorithm.

Tip Convolution and Surface Reconstruction

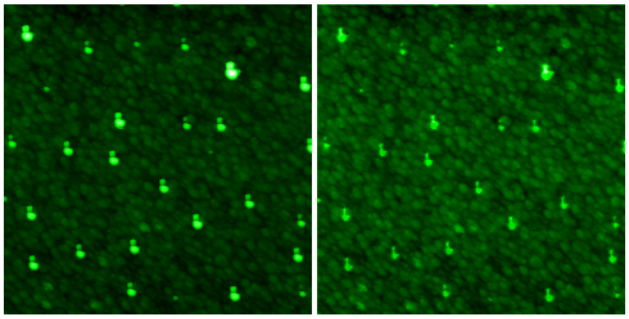
When we know tip geometry, we can use tip convolution (dilation) algorithm to simulate data acquisition process. For doing this use Dilation module (*Data Process → Tip → Dilation*). This can be in particular useful when working with data being result of some numerical modelling (see e.g. [2]).

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.



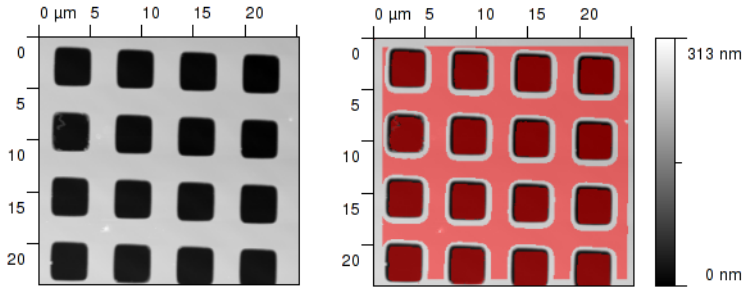
Simulated fractal surface before (left) and after (right) tip convolution.

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 enables to perform arbitrary point-wise operations on a single data field or on the corresponding points of several data fields (currently up to eight). And although it is not its primary function it can be also used as a calculator with immediate expression evaluation if a plain numerical expression is entered. The expression syntax is described in section Expressions.

The expression can contain the following variables representing values from the individual input data fields:

Variable	Description
`d1`, ..., `d8`	Data value at the pixel. The value is in base physical units, e.g. for height of 233 nm, the value of `d1` is 2.33e-7.
`m1`, ..., `m8`	Mask value at the pixel. The mask value is either 0 (for unmasked pixels) or 1 (for masked pixels). The mask variables can be used also if no mask is present; the value is then 0 for all pixels.
`bx1`, ..., `bx8`	Horizontal derivative at the pixel. Again, the value is in physical units. The derivative is calculated as standard symmetrical derivative, except in edge pixels where one-side derivative is taken.
`by1`, ..., `by8`	Vertical derivative at the pixel, definied similarly to the horizontal derivative.

In addition, the constant π is available and can be typed either as π or **`pi`**.

All data fields that appear in the expression have to be compatible. This means 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 in the current file (which may be different from the files of all operands).

Since the evaluator does not automatically infer the correct physical units of the result the units have to be explicitly specified.

This can be done by two means: either by selecting a data field that has the same value units as the result should have, or by choosing option *Specify units* and typing the units manually.

The following table lists several simple expression examples:

Expression	Meaning
`-d1`	Value inversion. The result is very similar to Invert Value, except that Invert Value reflects about the mean value while here we simply change all values to negative.
`(d1 - d2)^2`	Squared difference between two data fields.
`d1 + m1*1e-8`	Modification of values under mask. Specifically, the value 10^{-8} is added to all masked pixels.
`d1*m3 + d2*(1-m3)`	Combination of two data fields. Pixels are taken either from data field 1 or 2, depending on the mask on field 3.

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. The preview showing the result of an operation with fields is not immediately updated as you type; you can update it either by clicking *Update* or just pressing **Enter** in the expression entry.

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.

Mutual Crop

Data Process → Multidata → Mutual Crop

Two slightly different images of the same area (for example, before and after some treatment) can be croped to intersecting area (or non-intersecting parts can be removed) with this module.

Intersecting part is determined by correlation of larger image with center area of smaller image. Images resolution (pixels per linear unit) should be equal.

The only parameter now is *Select second operand* - correlation between it and current image will be calculated and both data fields will be cropped to remove non-intersecting near-border parts.

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

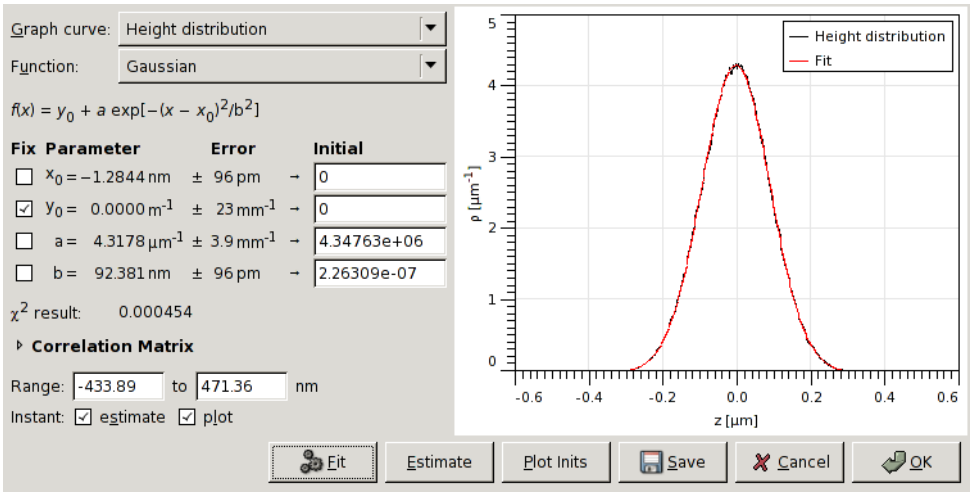
Graph level is a very simple module that currently performs linear fit of each graph curve and subtracts the fitted linear functions from them.

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*.



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

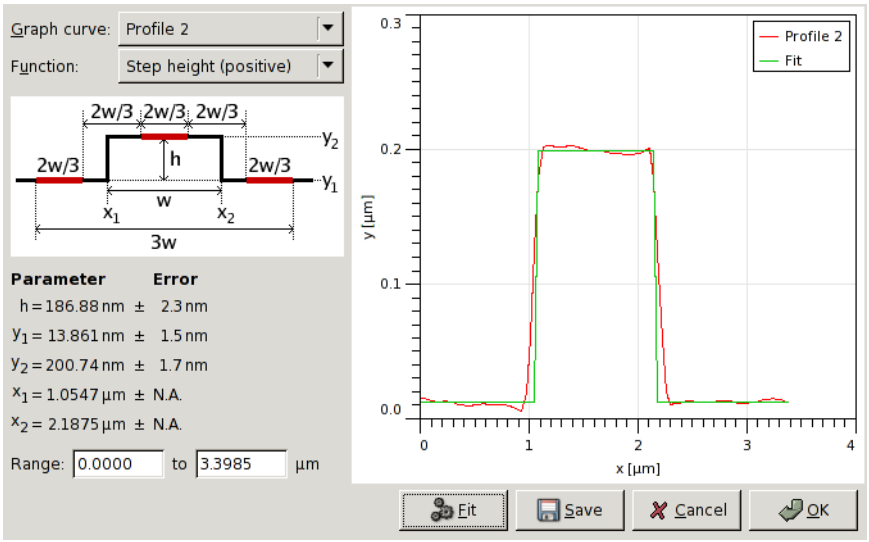
Note that the curve being fitted must be a real force-distance curve, not a displacement-distance or sensor-distance curve. Recalculation of cantilever deflection into force should be done before calling this module.

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.



Critical dimension module dialog.

DOS spectrum

DOS spectrum module intended to obtain Density-of-States spectra from I-V STM spectroscopy. It calculates

$$\left| \frac{\frac{\mathrm{d}I}{\mathrm{d}U}}{\frac{I}{U}} \right| (U)$$

and plots it as graph.

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.

Take Dimensions from 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 set to those of the current channel. Second, it makes the generated surface replace the current channel instead of creating a new channel.

Start from the current channel This option has two effects. First, it causes the dimensions and scales to be automatically set to those of the current channel. Second, it makes the generator to start from the surface contained in the current channel and modify it instead of starting from a flat surface. Note this does not affect whether the result actually goes to the current channel or a new channel is created.

Random generator controls:

Random seed The random number generator seed. Choosing the same parameters and resolutions and the same random seed leads to the same surface, 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 generated surfaces are periodic (i.e. perfectly tilable).

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). Button *Like Current Channel* sets the RMS value to those of the current channel.

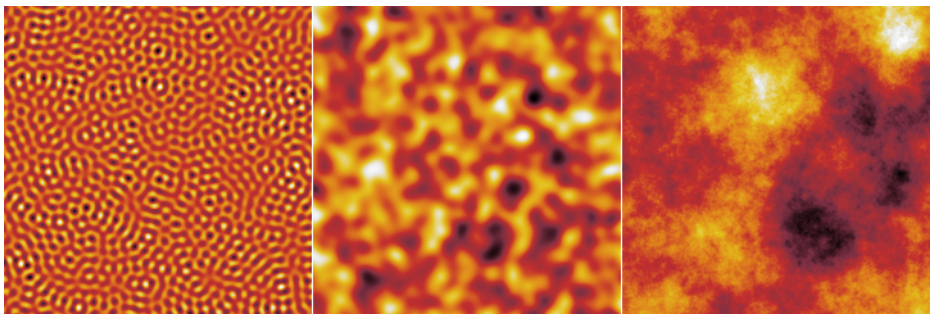
Minimum, maximum frequency The minimum and maximum spatial frequency. Increasing the minimum frequency leads to 'flattening' of the image, i.e. to removal of large features. Decreasing the maximum frequency limits the sharpness of the features.

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 and p equal to 1.5 (right).

Objects

The object placement method permits to create random surfaces composed of features of a specific 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 specific 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. The algorithm consideres the horizontal plane to be filled with identical copies of the surface, hence, the generated surfaces are also periodic (i.e. perfectly tilable).

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 assuming that they covered it uniformly. Larger values mean more layers of objects – and slower image generation.

Size The lateral 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 some default 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.

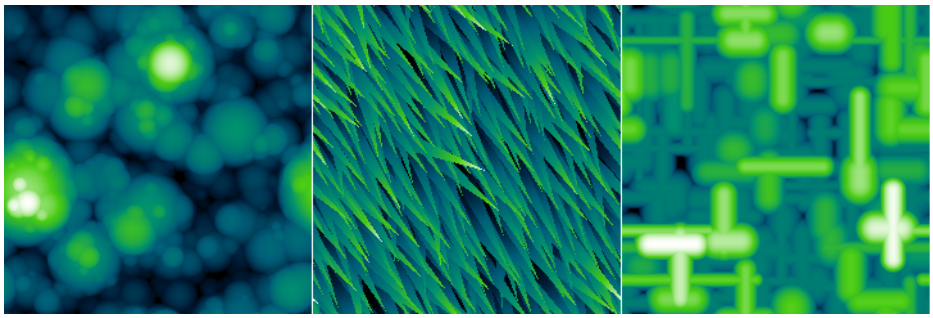
Checking *Scales with size* makes unperturbed heights to scale proportionally with object size. Otherwise the height is independent on size.

Button *Like Current Channel* sets the height value to a value based on the RMS of the current channel.

Orientation The rotation of objects with respect to some base orientation, measured counterclockwise.

Truncate The shapes can be truncated at a certain height, enabling creation of truncated cones, pyramids, etc. The truncation height is given as a proportion to the total object height. Unity means the shape is not truncated, zero would mean complete removal of the object.

Each parameter can be randomized for individual objects, this is controlled by *Variance*. For multiplicative quantities (all except orientation and truncation), 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).

Noise

Random uncorrelated point noise is generated independently in each pixel. Several distributions are available.

Distribution The distribution of the noise value. The possibilities include Gaussian, exponential, uniform and triangular distributions.

Direction The noise can be generated as symetrical or one-sided. The mean value of the distribution of a symmetrical noise is zero, i.e. the mean value of data does not change when a symmetrical noise is added. One-sided noise only increases (if positivie) or decreases (if negative) the data values.

RMS Root mean square value of the noise distribution. More precisely, it is the RMS of the corresponding symmetrical distribution in the case the distribution is one-sided.

Line Noise

Line noise represents noise with non-negligible duration that leads to typical steps or scars (also called strokes) in the direction of the fast scanning axis. Parameters *Distribution*, *Direction* and *RMS* have the same meaning as in Point noise. Other parameters control the lateral characteristics of the noise.

Two basic line defect types are available: steps and scars. Steps represent abrupt changes in the value that continue to the end of the scan (or until another step occurs). Scars are changes of the value with a finite duration, i.e. the values return to the original level after some time.

Steps have the following parameters:

Density Average number of defects per scan line, including any dead time (as determined by parameter *Within line*).

Within line Fraction of the time to scan one line that corresponds to actual data acquisition. The rest of time is a dead time. Value 1 means there is no dead time, i.e. all steps occur within the image. Value 0 means the data acquisition time is negligible to the total line scan time, consequently, steps only occur between lines.

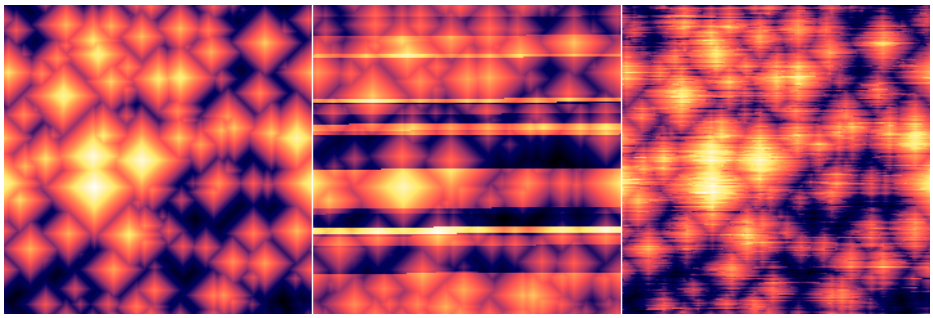
Cumulative For cumulative steps the random step value is always added to the current value offset; for non-cumulative steps the new value offset is directly equal to the random step value.

Scars have the following parameters:

Coverage The fraction of the the image covered by defect if they did not overlap. Since the defect may overlap coverage value of 1.0 does not mean the image is covered completely.

Length Scar length in pixels.

Variance Variance of the scar length, see Objects for description of variances.



Different types of line noise added to an artificial pyramidal surface: unmodified surface (left); with relatively unfrequent non-cumulative steps (centre); with scars of mean length of 16 px and high coverage (right).

Pattern

Regular geometrical patterns represent surfaces often encountered in microscopy as standards or testing samples such as ridges, steps or holes. Each type of pattern has its own set of geometrical parameters determining the shape and dimensions of various part of the pattern. Each parameter has a variance control, similar to Object synthesis, that permits to make the pattern irregular in some aspects.

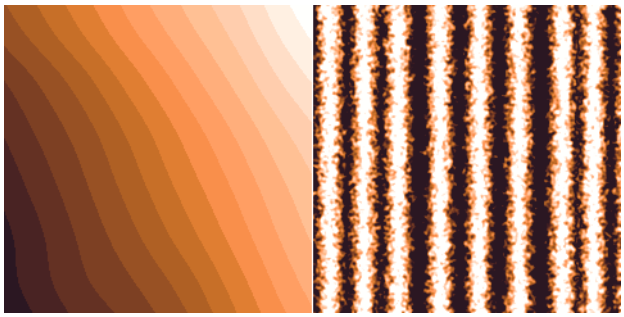
The placement of the pattern in the horizontal plane is controlled by parameters in tab *Placement*, common to all pattern types:

Orientation The rotation of the pattern with respect to some base orientation, measured counterclockwise.

This tab also contains the deformation parameters. While enabling the variation of geometrical parameters makes the generated surface somewhat irregular the shape of its features is maintained. *Deformation* is complementary method to introduce irregularity, specifcially by distorting the pattern in the *xy* plane. It has two parametres:

Amplitude The magnitude of the lateral deformation. It is a relative numerical quantity essentially determining how far the deformation can reach.

Lateral scale The characteristic size of the deformations. It descrbies not how far the features are moved but how sharply or slowly the deformation itself changes within the horizontal plane.



Artificial pattern surfaces: sharp steps oriented at 30 deg, deformed with a deformation with a large autocorrelation length (left); non-unofrmly spaced ridges with moderate slopes between the top and bottom planes, defomed with a deformation with a small autocorrelation length (right).

4.18 Calibration and uncertainties

Calibration data

Calibration data can be used to provide correction of measured data or perform uncertainty calculations. Generally, calibration data can be of different type and different level of complexity. For most of the cases user acquires error in each axis, e. g. using a calibrated standard. This value can be used for data correction. Similarily, the value of uncertainty is mosttly determined for each axis from calibrated standard certificate and from measurement process uncertainty budget.

In more complex case, calibration data can be determined locally. Scanner error cannot always be described by only three parameters (one for each axis) and its uncertainty is not necessarily the same in whole range. For precise measurements it is

therefore practical to determine local errors and namely local uncertainties that can be used for further calculations. By mean "local" we mean here uncertainties that are related to certain location in the complete volume that can be reached scanner.

To obtain local errors and uncertainties, one can use a calibration standard again or use a more complex instrument, like interferometer for scanning stange calibration. This is usually done in metrology institutes.

In Gwyddion, there is a set of tools helping local uncertainty processing. Primary calibration data, related to a scanning stage, can be determined or loaded. They can be assigned to a certain SPM measurement data creating a set of calibrations. These are used automatically in tools and modules where uncertainty propagation calculation can be performed in order to provide measurement uncertainty.

Calibration data acquisition

Data Process → Calibration → 3D calibration

Calibration data can be acquired in the following ways: The module *3D calibration → Create...* can be used for creating simplest primary calibration data - based only on knowledge of xyz errors and uncertainties and on scanner volume geometry. We also need to specify calibration name. Primary calibration data will be accesible under this name module for its data application to SPM measurements.

Using *3D calibration → Get simple error map...* module, we can determine primary xyz calibration data from a set of calibration grating measurements. Here we need to provide several measurements of calibration grating for different z-levels of the scanner. This forms several cross-sections of the full scanner volume. Providing single grating detail, nominal grating pitch and assuming that the grating planarity and orthogonality is much higher than that of scanning stage we can determine primary calibration data on the basis of correlation. Note that this way of calibrating an microscope is only very approximate and its use for metrology purposes is very limited. However, it can provide a lot of useful information about our scanner properties if we are unable to perform more complex analysis.

Finally, using *3D calibration → Load from file...* we can load any primary 3D calibration data determined by an external device, like set of interferometers. Data should be a plain text file containing number of calibration sets and sets (x, y, z, x_err, y_err, z_err, x_unc, y_unc, z_unc).

Calibration data application and further use

Data Process → Calibration → 3D calibration

Primary calibration data obtained in previous steps are related to a scanning stage, not to concrete SPM measurements. We can use primary calibration data for different measurements. To use primary calibration data for our measured data processing, we need to apply them first. Using module *3D calibration → Apply to data...* we can review and select calibration data applied on our height field measurements. After applying calibration data a set of calibration datafields is created and attached to selected data. A 'C' character appears in data browser as a sign of data with attached calibration. Note that the calibration attached to SPM measurement is no more related with primary calibration data (that were used for its creation).

When there is calibration attached to data, data reading and statistical quantities evaluation modules and tools recognize it automatically. Measurement uncertainty is then added to the measurement results. Uncertainty is calculated using uncertainty propagation law.

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

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.

If a directory is given as *FILE* argument the program opens a file chooser in this directory.

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.

--disable-gl Disables OpenGL entirely, including any checks whether it is available. This option, of course, has any effect only if Gwyddion was built with OpenGL support and one of the most visible effects is that 3D view becomes unavailable. However, you may find it useful if you encounter a system so broken that even checking for OpenGL capabilities leads to X server errors.

--log-to-file Redirect messages from GLib, Gtk+, Gwyddion, etc. to `~/.gwyddion/gwyddion.log` or file given in GWYDDION_LOGFILE environment variable. This option is most useful on Unix as on Win32 messages are redirected to a file by default.

--no-log-to-file Prevents redirection of messages from GLib, Gtk+, Gwyddion, etc. to a file. This is most useful on Win32 (where messages are redirected to a file by default) provided that stdout and stderr go somewhere you can see them.

--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 overridden 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

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.
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-H	*File → Open Recent → Document History*	toolbox, data window, 3D window, graph window, tool window	Open the document history browser (or bring it forward if it is already displayed).
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.

Shortcut	Menu equivalent	Context	Action
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.

You can assign your own keyboard shortcuts to all functions in the menus and it is also possible to invoke tools with keyboard shortcuts.

To change the keyboard shortcut of a menu item simply select the item using the mouse or arrow keys, press the key combination you want to assing to it and it will be immediately assigned. The shortcut must be either a special key, e.g. **F3**, or a key combination including modifiers, e.g. **Ctrl-Shift-D**. It is not possible to assign bare keys such as **Q**.

To prevent inadvertent modification of shortcuts, they can be changed only if *Edit → Keyboard Shortcuts* is enabled. Modifications are disabled by default which is also the recommended setting during normal use.

All keyboard shortcuts are stored in file `ui/accel_map` in the user's directory, which usually means `~/.gwyddion` (Unix) or `Documents and Settings\gwyddion` (MS Windows). Assigning shortcuts to tools can be only done by editting this file. Each line corresponds to an action that can be invoked with a shortcut. For instance the Mask Editor tool's line is by default:

```
; (gtk_accel_path "<tool>/GwyToolMaskEditor" "")
```

Semicolons represents comments, i.e. lines starting with a seimicolon are inactive. Hence, to assign the combo **Ctrl-Shift-E** to the Mask Editor tool, remove the semicolon to make the line active and fill the desired shortcut in the empty quotes:

```
(gtk_accel_path "<tool>/GwyToolMaskEditor" "<Control><Shift>e")
```

5.4 Supported File Formats

File Format	Extensions	Module	Read	Write	SPS
AIST-NT	.aist	aistfile	Yes	No	No
Alicona Imaging AL3D data	.al3d	alicona	Yes	No	No
Ambios AMB	.amb	ambfile	Yes	No	No
Anfatec	.par, .int	anfatec	Yes	No	No
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 IMG v2.1	.img	burleigh	Yes	No	No
Burleigh BII	.bii	burleigh_bii	Yes	No	No
Burleigh exported data	.txt, .bin	burleigh_exp	Yes	No	No
Code V interferogram data	.int	codevfile	Yes	No	No
Createc DAT	.dat	createc	Yes	No	No
Benyuan CSM	.csm	csmfile	Yes	No	No
DME Rasterscope	.img	dmefile	Yes	No	No
Gwyddion dumb dump data	.dump	dumbfile	Yes	No	No
ECS	.img	ecsfile	Yes	No	No
Nanosurf EZD, NID	.ezd, .nid	ezdfile	Yes	No	No
DME GDEF	.gdf	gdeffile	Yes	No	No

File Format	Extensions	Module	Read	Write	SPS
Gwyddion Simple Field	.gsf	gsffile	Yes	Yes	No
Gwyddion native data	.gwy	gwyfile	Yes	Yes	Yes
Psi HDF4	.hdf	hdf4file	Yes	No	No
Hitachi AFM	.afm	hitachi-afm	Yes	No	No
Hitachi S-3700 and S-4800 SEM data	.txt, +, image	hitachi-sem	Yes	No	No
WaveMetrics IGOR binary wave v5	.ibw	igorfile	Yes	No	No
Intematix SDF	.sdf	intematix	Yes	No	No
ISO 28600:2011 SPM data transfer format	.spm	iso28600	Yes	Yes	Limited[1]
JEOL	.tif	jeol	Yes	No	No
JPK Instruments	.jpk	jpkscan	Yes	No	No
Olympus LEXT 4000	.lext	lextfile	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
DME MIF	.mif	miffile	Yes	No	No
Molecular Imaging MI	.mi	mifile	Yes	No	Limited[??]
Aarhus MUL	.mul	mulfile	Yes	No	No
Nanoeducator	.mspm, .stm, .spm	nanoeducator	Yes	No	Yes
Nanonics NAN	.nan	nanonics	Yes	No	No
Nanonis SXM	.sxm	nanonis	Yes	No	No
NanoObserver	.nao	nanoobserver	Yes	No	No
Nanoscan XML	.xml	nanoscan	Yes	No	No
Veeco Nanoscope II	.001, .002, etc.	nanoscope-ii	Yes	No	No
Veeco Nanoscope III	.001, .002, etc.	nanoscope	Yes	No	Limited[??]
Nanotop SPM	.spm	nanotop	Yes	No	No
GSXM NetCDF	.nc	netcdf	Yes	No	No
Nearly raw raster data (NRRD)	.nrrd	nrrdfile	Yes[2]	Yes[3]	No
NT-MDT	.mdt	nt-mdt	Yes	No	Yes
oldmda	.sxml, .dat	oldmda	Yes	No	No
Olympus LEXT 3000	.ols	ols	Yes	No	No
Omicron SCALA	.par, .tf*, .tb*, .sf*, .sb*	omicron	Yes	No	Yes
Omicron flat format	.*_flat	omicronflat	Yes	No	No
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[4]	Yes[5]	No
Nanosurf PLT	.plt	pltfile	Yes	No	No
Pacific Nanotechnology PNI	.pni	pnifile	Yes	No	No
Park Systems	.tiff,, .tif	psia	Yes	No	No
SymPhoTime TTTR v2.0 data	.pt3	pt3file	Yes	No	No

File Format	Extensions	Module	Read	Write	SPS
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[6]	No	No
XYZ data	.xyz, .dat	rawxyz	Yes[7]	No	No
RHK Instruments SM3	.sm3	rhk-sm3	Yes	No	Limited[??]
RHK Instruments SM4	.sm4	rhk-sm4	Yes	No	Limited[??]
RHK Instruments SM2	.sm2	rhk-spm32	Yes	No	Limited[??]
Automation and Robotics Dual Lens Mapper	.mcr, .mct, .mce	robotics	Yes	No	No
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
IonScope SICM	.img	sicmfile	Yes	No	No
Surface Imaging Systems	.sis	sis	Yes	No	No
SPIP ASCII	.asc	spip-asc	Yes	No	No
SPML (Scanning Probe Microscopy Markup Language)	.xml	spml	Yes	No	No
Thermicroscopes SPMLab R4-R7	.tfr, .ffr, etc.	spmlab	Yes	No	No
Thermicroscopes SPMLab floating point	.flt	spmlabf	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
WIPfile	.wip	wipfile	Yes	No	Yes
WITec ASCII export	.dat	witec-asc	Yes	No	No
WITec	.wit	witfile	Yes	No	No
WSF ASCII data	.wsf	wsffile	Yes	No	No
Nanotec WSxM	.tom	wsxmfile	Yes	No	No
Carl Zeiss SEM scans	.tif	zeiss	Yes	No	No

5.5 High-Depth Image Formats

Gwyddion can export data to 16bit greyscale PNG, PNM and TIFF images and to OpenEXR images with half, float and 32bit data types. In case of 16bit images the full data range is always stretched to the full greyscale range; OpenEXR export permits to specify the value scaling factor.

When data are exported to a high-depth image additional information is stored to the file to enable automated loading back to Gwyddion without having to specify the dimensions and scales manually. By storing this additional information to image files you create you can also make them directly loadable to Gwyddion with correct dimensions and scales. The information is organised as key-value pairs, stored using individual format-specific means for each format, described in the following table.

	Format	Method
	PNG	`tEXt` chunks
	OpenEXR	named attributes
	PNM	header comments of the form `# key: value`

Most keys are identical to those used in Gwyddion Simple Fields, except for the added `Gwy::` prefix, so see also GSF description for more details. Floating point values are stored directly if the format permits it (OpenEXR), otherwise a text representation of the number is used (in the C format). The keys are listed below.

Key	Type	Meaning
`Gwy::XReal`	floating point	Horizontal size in physical units (given by `XYUnits`), a positive floating point number.
`Gwy::YReal`	floating point	Vertical size in physical units (given by `XYUnits`), a positive floating point number.
`Gwy::XOffset`	floating point	Horizontal offset in physical units (given by `XYUnits`).
`Gwy::YOffset`	floating point	Vertical offset in physical units (given by `XYUnits`).
`Gwy::ZScale`	floating point	Value scaling factor. Image data are to be multiplied by this factor to obtain physical values. This parameter is usually used with limited-range floating point formats such as half. For integer data, `Gwy::ZMin` and `Gwy::ZMax` is usually used.
`Gwy::ZMin`	floating point	Value in physical units corresponding to the minimum value representable in the image (normally 0).
`Gwy::ZMax`	floating point	Value in physical units corresponding to the maximum value representable in the image.
`Gwy::XYUnits`	string	Lateral units, i.e. units of physical sizes and offsets.
`Gwy::ZUnits`	string	Value units, i.e. units of data values.
`Gwy::Title`	string	Data/channel title.

In case of PNG, the scaling information is also stored in the standard `sCAL` and `pCAL` chunks (with linear scaling formula). Conversely, if these chunks are present (and the Gwyddion-specific are absent) the information from them is used in import. See the PNG speficiation for the chunk description.

5.6 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.

5.7 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), `Program Files\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 `Documents and Settings\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. Numerical values are represented in the standard POSIX format, i.e. with decimal point, independently on what decimal separator is usual in the user's language.

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
x_0	Curvature	Curvature center x position
y_0	Curvature	Curvature center y position
z_0	Curvature	Curvature center z value
kappa_1	Curvature	Curvature 1
kappa_2	Curvature	Curvature 2
phi_1	Curvature	Curvature angle 1
phi_2	Curvature	Curvature angle 2

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

5.8 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`	finite IEEE 754 double precision floating point number, i.e. files must not contain infinities and not-a-numbers
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

Top-Level GwyContainer

The names (keys) of data objects in a GwyContainer representing a Gwyddion file strongly resemble UNIX file names, i.e. they have the form of /-separated paths and form a sort of tree-like structure. For instance the title of the first channel, numbered 0, is stored under they key /0/data/title. Note some data or information is found under keys that do not seem logical; the reason is usually historical.

The following sections describe the organisation of interesting data and information in the GwyContainer. The list is not necessarily complete. However, since all data items in the file specify consistently their name, type and size in bytes it is always possible to skip unknown data types or data you are not interested in and extract only the desired data items.

Channels

The following table summarises the common keys of channel-related data in the top-level container for channel number 0. For other channels, the number 0 has to be replaced with the corresponding channel number. Note that channels are often numbered sequentially, starting from 0, however, they can have any numbers and the set of channels numbers does not have to be contiguous.

Key	Type	Meaning
/0/data	GwyDataField	Channel data.
/0/data/title	string	Channel title, as shown in the data browser.
/0/data/visible	boolean	Whether the channel should be displayed in a window when the file is loaded.
/0/base/palette	string	Name of the false colour gradient used to display the channel.
/0/base/range-type	32bit integer	False colour mapping type (as set by the Color range tool), the value is from GwyLayerBasicRangeType enum.
/0/base/min	double	Minimum value for user-set display range.
/0/base/max	double	Maximum value for user-set display range.
/0/mask	GwyDataField	Mask data. The pixel dimensions of this data field must match those of the channel data.
/0/mask/red	double	Red component of the mask colour.
/0/mask/green	double	Green component of the mask colour.
/0/mask/blue	double	Blue component of the mask colour.
/0/mask/alpha	double	Alpha (opacity) component of the mask colour.
/0/show	GwyDataField	Presentation data. The pixel dimensions of this data field must match those of the channel data.
/0/meta	GwyContainer	Channel metadata. The keys are directly the names as displayed in the metadata browser and the string values are the values.
/0/select/*foo*	a GwySelection subclass	Selection data. Each kind of selection has (usually) a different object type and is stored under a different name; the specific name *foo* is the same as shown in the selection manager.

Channels are represented as GwyDataField objects. The components of a GwyDataField are summarised in the following table:

Component	Type	Meaning
xres	32bit integer	Horizontal size in pixels.
yres	32bit integer	Vertical size in pixels.
xreal	double	Horizontal dimension in physical units.
yreal	double	Vertical dimension in physical units.
xoff	double	Horizontal offset of the top-left corner in physical units. It usually occurs only if non-zero.
yoff	double	Vertical offset of the top-left corner in physical units. It usually occurs only if non-zero.
si_unit_xy	GwySIUnit	Unit of lateral dimensions.
si_unit_z	GwySIUnit	Unit of data values.
data	array of doubles	Field data, stored as a flat array of size xres×yres, from top to bottom and from left to right.

Graphs

The following table summarises the common keys of graph-related data in the top-level container for graph number 1. For other graphs, the number 1 has to be replaced with the corresponding graph number. Note that graphs are often numbered sequentially, starting from 1, however, they can have any numbers positive and the set of graph numbers does not have to be contiguous. The number 0 in the prefix of graph keys is a historical relict that does not mean anything and it is always 0.

Key	Type	Meaning
/0/graph/graph/1	GwyGraphModel	Graph model object data.
/0/graph/graph/1/visible	boolean	Whether the graph should be displayed in a window when the file is loaded.

Graphs are represented as GwyGraphModel objects. The components of a GwyGraphModel are summarised in the following table:

Component	Type	Meaning
curves	array of GwyGraphCurveModels	Individual graph curves.
title	string	Graph title as displayed in the data browser.
x_unit	GwySIUnit	Unit of the abscissa.
y_unit	GwySIUnit	Unit of the ordinate.
top_label	string	Label on the top axis.
bottom_label	string	Label on the bottom axis.
left_label	string	Label on the left axis.
right_label	string	Label on the right axis.
x_is_logarithmic	boolean	Whether the abscissa has a logarithmic scale.
y_is_logarithmic	boolean	Whether the ordinate has a logarithmic scale.
x_min	double	User-set minimum value of the abscissa.
x_min_set	boolean	Whether user-set minimum value of the abscissa should be used (otherwise the range is determined automatically).
x_max	double	User-set maximum value of the abscissa.
x_max_set	boolean	Whether user-set maximum value of the abscissa should be used (otherwise the range is determaxed automatically).
y_min	double	User-set minimum value of the ordinate.

Component	Type	Meaning
y_min_set	boolean	Whether user-set minimum value of the ordinate should be used (otherwise the range is determined automatically).
y_max	double	User-set maximum value of the ordinate.
y_max_set	boolean	Whether user-set maximum value of the ordinate should be used (otherwise the range is determaxed automatically).
grid-type	32bit integer	Type of grid shown. The value is from GwyGraphGridType enum.
label.has_frame	boolean	Whether the graph key has a frame.
label.frame_thickness	32bit integer	Width of graph key frame.
label.reverse	boolean	Whether to reverse the graph key.
label.visible	boolean	Whether the graph key is visible.
label.position	32bit integer	The position (corner) where the graph key is places. The value is from GwyGraphLabelPosition enum.

Graph curves are represented as GwyGraphCurveModel objects. The components of a GwyGraphCurveModel are summarised in the following table:

Component	Type	Meaning
xdata	array of doubles	Abscissa points. The number of point must match ydata.
ydata	array of doubles	Ordinate points. The number of point must match xdata.
description	string	Curve description (name).
type	32bit integer	Curve mode (points, lines, etc.) The value is from GwyGraphCurveType enum.
color.red	double	Red component of the curve colour.
color.green	double	Green component of the curve colour.
color.blue	double	Blue component of the curve colour.
point_type	32bit integer	Type of symbols representing data points. The value is from GwyGraphPointType enum.
point_size	32bit integer	Size of symbols representing data points.
line_type	32bit integer	Type of lines connecting data points. The value is from GwyGraphLineType enum.
line_size	32bit integer	Width of lines connecting data points.

Spectra

The following table summarises the common keys of spectra-related data in the top-level container for spectra set number 0. For other spectra, the number 0 has to be replaced with the corresponding spectra set number. Note that spectra sets are often numbered sequentially, starting from 0, however, they can have any numbers and the set of spectra set numbers does not have to be contiguous.

Key	Type	Meaning
/sps/0	GwySpectra	Spectra data.

Sets of spectra of one kind are represented as GwySpectra objects. The components of a GwySpectra are summarised in the following table:

Component	Type	Meaning
title	string	Spectra title as displayed in the data browser.
si_unit_xy	GwySIUnit	Unit of spectrum position coordinates.
coords	array of doubles	Coordinates of points where the spectra were taken, in physical units. Each spectrum takes two items: for the horizontal and vertical coodrdinate. The number of coordinates must match the number of curves in data.
data	array of GwyDataLines	Individual spectra curves.
selected	array of 32bit integers	Indices of selected spectra curves.

Individual curves in spectra are represented as GwyDataLine objects. The components of a GwyDataLine are summarised in the following table:

Component	Type	Meaning
res	32bit integer	Number of data points.
real	double	Length in physical units.
off	double	Offset of the begining in physical units. It usually occurs only if non-zero.
si_unit_x	GwySIUnit	Unit of abscissa.
si_unit_y	GwySIUnit	Unit of data values.
data	array of doubles	Line data, stored as an array of res, from left to right.

Auxiliary Objects

The components of a GwySIUnit are summarised in the following table:

Component	Type	Meaning
unitstr	string	Textual representation of the unit, e.g. "A" or "m^-1" (as base SI unit, prefixes are ignored).

The components of a GwySelection are summarised in the following table. Some selection types can have other data members; refer to the documentation of specific selection classes for how to interpret the data.

Component	Type	Meaning
max	32bit integer	Maximum number of objects the selection can hold (this is the number set by gwy_selection_set_max_objects()).
data	array of doubles	Selection data. The number of items that form one selection object is determined by the selection type.

5.9 Simple Field Files

The Gwyddion native file format captures all the information and state Gwyddion needs to save and consequently it is quite complex. Often it is not practical to save files in .gwy format in custom programs and scripts creating input for Gwyddion.

The Gwyddion Simple Field file format (.gsf) can be used in these situations instead. It is a single-channel format for 2D data that was designed to be easy and efficient to read and write, with human-readable header, reasonably expressive, and avoiding instrument or application specific fields (though it can optionally bear them).

GSF can be read and written by Gwyddion version 2.20 or later.

Overall structure

A GSF file consists of four parts, in the following order:

magic line Files begin with a ‘magic line’ identifying the file type.

text header The header consists of lines of the form

```
name = value
```

defining individual parameters.

NUL padding The header is terminated by one to four NUL bytes, aligning the data start to a multiple of 4.

binary data Binary data is in 32bit floating-point format.

Magic line

GSF files start with the line

```
Gwyddion Simple Field 1.0
```

terminated by a linefeed character (`\n`, ASCII 0x0a).

Text header

Each header line has the form

```
name = value
```

where any whitespace before the name, around the equal sign and at the end of value is ignored. Field names are case-sensitive and follow the usual rules for identifiers in programming languages.

Similarly to the magic line, the lines in the text header are terminated by a linefeed character as is usual on Unix. This means the header must be read and written in binary mode to ensure preservation of end-of-line characters on other systems (and not changing the header size e.g. by LF → CRLF transformation).

Any non-ASCII characters, that can occur for example in the channel title, are represented in UTF-8 encoding. The NUL character may not occur in the header.

Header fields:

Name	Type	Value
`XRes`	Mandatory	The horizontal size in pixels, a positive integer.
`YRes`	Mandatory	The vertical size in pixels, a positive integer.
`XReal`	Optional	Horizontal size in physical units (given by `XYUnits`), a positive floating point number. It defaults to 1.0 if not given.
`YReal`	Optional	Vertical size in physical units (given by `XYUnits`), a positive floating point number. It defaults to 1.0 if not given.
`XOffset`	Optional	Horizontal offset in physical units (given by `XYUnits`), a floating point number. It defaults to 0.0 if not given.
`YOffset`	Optional	Vertical offset in physical units (given by `XYUnits`), a floating point number. It defaults to 0.0 if not given.
`Title`	Optional	Data/channel title. It has no default, applications might display ‘Unknown’ or something similar if not given.
`XYUnits`	Optional	Lateral units, i.e. units of physical sizes and offsets. They must be given as base units, that is `m` or `A` with no power-of-10 prefix (Gwyddion could deal with it but it might present a problem for other software). The default is no units. This means in SPM data, you normally wish to specify `XYUnits` as `m` because the lateral dimensions are in metres.
`ZUnits`	Optional	Value units, i.e. units of data values. See `XYUnits` above for details.

Floating point numbers can be in the scientific format, e.g. `1.23e-4`. They are represented in the standard C/POSIX locale, i.e. decimal dot is used (not comma or other separators).

The header may contain other fields beside those listed above. Gwyddion will load them into metadata. Common informational fields can include `Comment`, `Date` or `Direction`.

Fields may occur in any order, nevertheless, it is recommended to start with mandatory fields, continue with optional fields and put custom fields last.

A simple header example (also including the magic line):

```
Gwyddion Simple Field 1.0
XRes = 400
YRes = 400
XReal = 5e-05
YReal = 5e-05
XYUnits = m
ZUnits = V
Title = ADC2
```

NUL padding

The text header is followed by one to four NUL (`\0`, ASCII 0x00) bytes that (a) terminate it and (b) align the data start to an offset from the begining of file that is a multiple of 4. More precisely, denoting N the total lenght of the magic line and the text header, the data starts at the nearest multiple of 4 larger than N.

This padding to a multiple of 4 ensures aligned memory access when mapping the the file directly to memory. The number of NUL bytes is uniquely determined by the remainder of the length modulo four (N mod 4):

Remainder	Number of padding NULs
0	4
1	3
2	2
3	1

Binary data

Data values are stored as IEEE 32bit single-precision floating point numbers, in little-endian (LSB, or Intel) byte order. Values are stored by row, from top to bottom, and in each row from left to right.

The physical units of these values are `ZUnits`.

The size of the image data is exactly `4*XRes*YRes` and there is no data after it in the file.

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.

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```

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```

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Chapter 7

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