Power Spectrum 2015

Multiscale Consulting

Manual / Instructions

"God made the bulk; surfaces were invented by the devil."

- Wolfgang Pauli

*The software module **Power Spectrum 2015** calculates (a) the two-dimensional (2D) power spectrum $C(\boldsymbol{q}) = C(q_x, q_y)$ from any surface roughness topography measured over a square (or rectangular) surface area or (b) the one-dimensional (1D) power spectrum from the surface topography measured along a line. For the latter case it also calculates the 2D power spectrum assuming that the surface roughness is isotropic [so that $C(\boldsymbol{q})$ only depends on the magnitude q of the wave vector $\boldsymbol{q} = (q_x, q_y)$], or for the case where the surface is perfectly anisotropic (with the groves aligned along one direction and the surface roughness is measured along the direction orthogonal to the groves). For the 2D case, where the surface topography is measured over a square (or rectangle), the code also gives information about the anisotropy, e.g., the Peklenik and Tripp anisotropy numbers.*

Contents

What is the Power Spectrum?

The surface roughness power spectrum is the only input needed for the contact mechanics theory developed by Persson[1]. It basically contains all necessary information about the roughness properties of the surface studied. By decomposing measured or mathematically generated topography data into sinusoidal waves using the Fourier transform, this quantity describes how height fluctuations (or the power of the signal) are distributed with frequency or wave vector q. From the surface roughness power spectrum all parameters characterizing the surface roughness, like amplitude parameter or slope, spacing, and counting parameters, can be calculated. For more information on the power spectrum please also view the online lectures on our homepage `http://www.multiscaleconsulting.com/index.php/online-lectures.com`. The 2D power spectrum is calculated as described in Appendix D of [2] and Appendix B of [3] (both papers can be found at `http://www.multiscaleconsulting.com`). That is,

$$C(\mathbf{q}) = \frac{(2\pi)^2}{A} \langle |h(\mathbf{q}|^2 \rangle,$$

where $A = L^2$ is the surface area (here assumed to be a square with side L) and $h(\mathbf{q})$ the Fourier transform of the surface height profile $h(\mathbf{x}) = h(x,y)$:

$$h(\mathbf{q}) = \frac{1}{(2\pi)^2} \int_A d^2x \ h(\mathbf{x}) e^{-\mathbf{q} \cdot \mathbf{x}}.$$

If it is assumed that $h(\mathbf{x})$ is given over a square with $N \times N$ grid points and lattice constant a, so that $L = Na$, then $C(\mathbf{q})$ will be given over a square area in $\mathbf{q}$ space: $-\pi/a < q_x < \pi/a$, $-\pi/a < q_y < \pi/a$ on a grid with lattice constant $a^* = 2\pi/L$ where the smallest wave vector will be $a^*/2 = \pi/L$. For surfaces with anisotropic properties the following matrix is of importance:

$$D(q) = \frac{\int_0^{2\pi} d\phi \ C(\mathbf{q}) \mathbf{q} \mathbf{q}/q^2}{\int_0^{2\pi} d\phi \ C(\mathbf{q})},$$

where $\mathbf{q} = q(\cos\phi, \sin\phi)$. This matrix is diagonalizable. In the coordinate system where it is diagonal it is defined that $D_{11} = 1/[1 + \gamma(q)]$. Here one denotes $\gamma(q)$ as the LOCAL Tripp gamma parameter which depends on the wave vector q. The rotation angle relative to the q_x-axis of the coordinate system where D is diagonal is denoted as the Tripp angle and depends also on q in general. In a similar way the EXTENDED Tripp gamma parameter and angle (which also depends on q) from the matrix

$$\tilde{D}(q) = \frac{\int_{q'>q} d^2q' \ C(\mathbf{q'}) \mathbf{q'} \mathbf{q'}/q'^2}{\int_{q'>q} d^2q' \ C(\mathbf{q'})}$$

are defined. The Tripp gamma parameter and angle are important for fluid flow at interfaces between contacting solids.

General Information

Please note that due to memory limitations of the computer and the operating system, there is also a limit on the maximum size of the input file for calculating the surface roughness power spectrum. For a 2D input file the highest possible number of points along the x-axis is 4000 data points. The same is true also for the y-axis so that the biggest topography able to analyze is 4000×4000 points. For 1D input files the maximum number of points along the measured axis is limited to 500.000 data points. However it is possible to analyze up to 32 individual lines put one after another in the same input file. How to prepare the input files properly is described in greater detail below.

All output is calculated in SI-units if not explicitly stated else! Also the input data should be given in SI-units or at least the corresponding factor to convert the data to SI-units should be given in the input file. Please see below for further details how this is done.

A lot of the output given in the different files is on a logarithmic scale. Unless explicitly stated otherwise, all logarithms are with 10 as basis!

Installation

This section explains briefly how to install the software on your computer. There are two possibilities to install the Power Spectrum program. The first one is, if you have received a zipped file, to unzip the zip archive to your hard disk. The program inside this folder is already prepared to run and should work directly after unzipping it. If you have instead received an installer, start the installer and please follow the steps through the install process.

Please note: All programs from Multiscale Consulting have to be installed in a folder with short path names. The reason is that under Windows, due to the length of some file names, the calculation could get stopped by the OS (program crashes). It is recommended to install all programs directly under **"C:\Multiscale\..."** for example.

> Warning:
>
> Please note that some of the output file names are very long because they contain information about the data inside the file. This can cause trouble in Windows as their is a limitation on the total length of a file name including its path. If the program is not working properly this may be the reason and it is therefore highly suggested to put all the MultiscaleConsulting software tools directly on **"C:\"**! If there are problems with the calculations, an error message is shown with a short description of the error. It is suggested to carefully check again the format and the specifications of/for the input file and repeat the calculation.

Windows Version / First Steps

In order to do calculations under Windows, a GUI (Graphical User Interface) version of the software has been developed. Note that the functionality of the program as described in the Linux section has not been changed. The input data needed, possible options for the calculation as well as the results are identical with the Linux program.

The following instruction has been written to explain the difference in using the GUI Windows version compared to the CLI (Command-Line Interface) Linux version. To calculate the surface roughness power spectrum of a given (measured or generated) topography file a couple of information need to be specified, e.g., about the type of input. By changing the options in the software different properties are being calculated. Below we will now go through the software step by step and explain the procedure how to calculate the power spectrum and the meaning of all the different options. First start the program by executing the **PowerSpectrum2015.exe** file in the folder where our power spectrum software is located. This will open the main user interface as shown in Fig. 1.

Step1 - Project Name

Before starting a calculation, first some information about the system which should be analyzed need to be specified. The first step is to supply a project name for the calculation. The project name is entered into the input field which can be found at the top of the interface as shown in Fig. 1. After the calculation
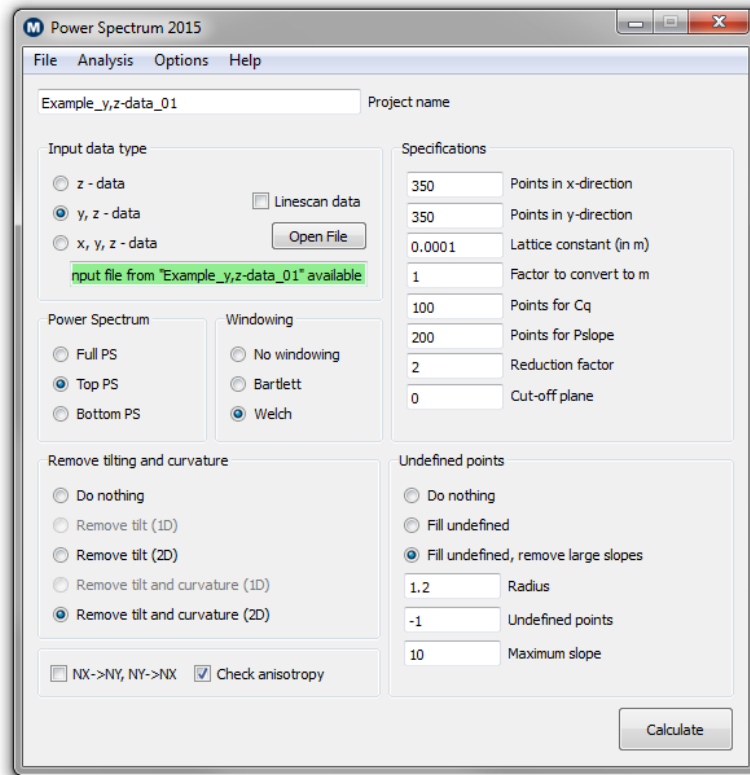
Figure 1: Graphical user interface of the Windows software.

is finished, all the results will be stored inside a separate folder which will have the name according to the project name as follows: "C:\Multiscale\data* Projectname*". For the case in Fig. 1, e.g., all the results will be stored in "C:\Multiscale\data\Example__y,z-data__01". Inside this folder there will also be some additional folders where the input data (e.g., the topography file and the logfile) is archived and additional, not so important information are stored. Please note that the output in this folder differs depending on the type of calculation and the different options chosen. The output files will be discussed at a later point in this manual in the results section.

> Choose a meaningful project name under which all the results will be stored in "C:\Multiscale\data* Projectname*".

Step 2 - Choosing the Input Format

Assuming that the surface roughness measurement of a given surface was successful, please export the results as ASCI files without any preprocessing of the data. This means, do not filter or smoothen nor flatten the results in the instrument software. Depending on the measurement technique, the instrument used and the company producing the device, the format of the topography information may differ. Hence the file needs to be prepared properly so that it can be used as an input file for the Power Spectrum program. Here the software requires as input an ASCII file with the measured height information given in columns and without any header prior to the topography input or any footer in the bottom. Usually it is necessary to delete the additional information from the measurement at the beginning of the file (header) as well as in the end (footer). The file type of the input has to be "*.txt". In case the ASCII file

has a different file extension it can easily be renamed to "*.txt" without further problems. Concerning the format of the input data type, the three following cases can be handled:

x - data
The height information are plotted in a single column ($z = h$) as shown in Fig. 2 left.

x, y - data
The height information and the position are plotted in two columns ($y, h(y)$) as shown in Fig. 2 center.

x, y, z - data
The height information and the position are plotted in three columns ($x, y, h(x, y)$) as shown in Fig. 2 right.
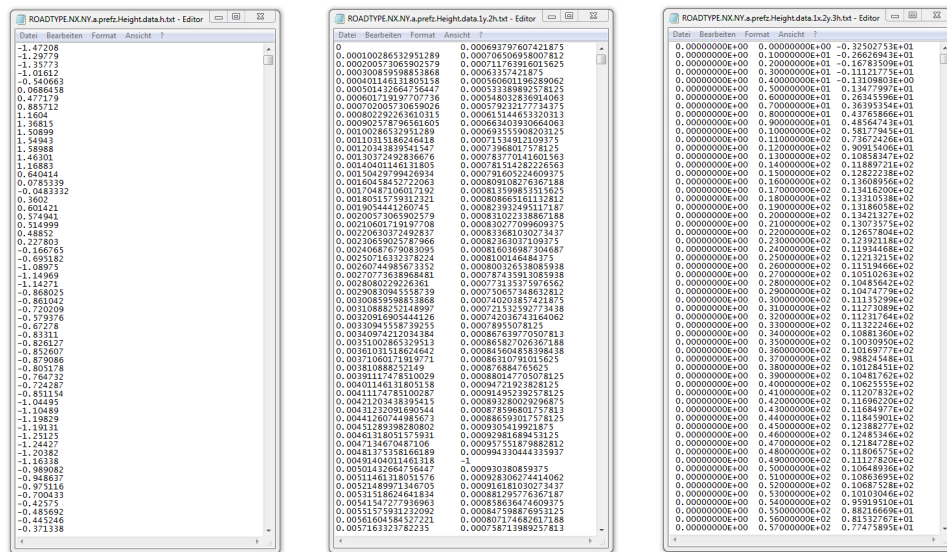

Figure 2: Possible input data formats. Left: x - data, height information in a single column ($z = h$). Center: x, y - data, height information in two columns ($y, h(y)$). Right: x, y, z - data, height information in three columns ($x, y, h(x, y)$). Note that there should be **no** header or other information before or after the input data!

Depending on the format of the actual input file, the input data type has to be chosen according to the explanation above. In case the topography has been measured over a square or rectangular area, the flag "Linescan data" should not be checked. However there are some measurement techniques, e.g., stylus instruments, which make it possible to measure surface roughness profiles only along a single line. This can be taken into account by checking the "Linescan data" option. As already mentioned in the beginning of this manual, then the 1D instead of the 2D power spectrum will be calculated. The 2D power spectrum is then approximated by assuming that the surface roughness is isotropic. Consider that for linescan input data there will be no additional information available about, e.g., anisotropy of the surface roughness.

Note that it is possible to also take into account multiple line scans all performed on the same surface. If the surface roughness is randomly rough and isotropic (e.g., road surfaces or sandblasted surfaces), the results and hence also the power spectrum does not depend on the direction of the experiment. Usually one can do several scans and add them one after another in a single file by simply copying them all together. However, to indicate to the program that the different individual data sets or scans are not related to each other and that they therefore need to be treated differently compared to input information that have been measured over a square or rectangular surface region, the "Linescan data" option has to be checked. This option is at the moment available only for "x - data" or for "x, y - data" input files.

Remove the header and footer in the topography file and prepare an appropriate input file. Specify then the type of format depending on how many data columns the file has. For the analysis of line scan results, please select the option "Linescan data".

Step 3 - Specifications

After specifying the topography input file for calculating the power spectrum, it is now necessary to provide the following, additional information about the data in the input file:

Points in x-direction
Specify how many measurement points in the x-direction in the input file exist.

Points in y-direction
Specify how many measurement points in the y-direction in the input file exist.

These two parameters basically determine the number of measurement points inside the topography file. Usually when measuring over a square area, the data in this file is ordered, so that there is one long column where the position along the x-direction is changed while the y-direction is kept fixed and the height is measured. When the endpoint of the x-direction is reached, the x value is reset and starts at 0 again. The following information in the column are now after increasing the y value by one step. So the first variable which is changed in the file is referred to as the x-direction while the other variable, which gets changed only when the x value has been changed until its final value, is called the y-direction.
In case of linescan data input, which has been produced by copying multiple line scan results into one file, the points in x-direction would be the total number of points along the scan direction while points in y-direction would be the number of how many individual line scans are inside the input file. Please note that all the line scans need to have the same number of points along the scan direction!
The total number of points is checked after specifying the input file and must match the number of points when multiplying the input from points in x-direction with points in y-direction. If this number is not consistent the code will give an error message. Please check the numbers again carefully.
Also note, that all measurement points need to be included in the input file. There are some measurement techniques which, depending on the surface measured, are not able to measure the height for all points. Usually the instrument then puts a "-1" or "NaN" in the file. However there are also instruments which simply leave out these points. This is not allowed! The missing points then need to be specified by pre-processing the data and including the empty spaces with "-1" as height value.

Lattice constant (in m)
Specify the distance between each measurement point in units of meter. If the lateral resolution was 1μm, one has to put "1.0E-06" as lattice constant. Please note that the lattice constant along the y-direction has to be the same as along the x-direction.

For illustration: if the surface region has been measured over a square area of 10×5mm with a lateral resolution of 1μm, the topography will consist of 1000×500 points. In this case one has to put the numbers 1000 in "Points in x-direction" and 500 in "Points in y-direction". The resolution of the measurement, or the step length between individual measurement points, is called the lattice constant. In the example above one would have to put 1μm ("1.0E-06") as lattice constant. Please note that the lattice constant in x- and y-direction needs to be the same. Because of the 2D Fourier transform it is not possible to have different lattice constants in the two directions!

Factor to convert to m
If the data in the input file is not in SI units (which would be meter), one has to specify here the factor which is needed to convert, when multiplying the result with this factor, the input information into meter. Atomic Force Microscopy (AFM) results are usually in nanometer. For this case one would have to put "1.0E-09" as the correct convert factor here.

The following settings are usually not modified, however it is sometimes useful to change them.

Points for $C(\mathbf{q})$

One important result from the calculation using this software is the surface roughness power spectrum which will be calculated as a function of wave vector q. Here one can specify for how many points (resolution in q-space) this result will be calculated. In case this number is too small, the power spectrum may lack important information about roughness on a particular length scale. In some sense this value specifies the "resolution" of the power spectrum. However if this number is too high, which depends on the total number of points in the input file, it can also happen that due to not enough information, the result becomes noisy. For most cases a number of order 100 is appropriate.

Points for Pslope

Another result for most calculations is the probability distribution for slopes. The number of points chosen here, similar as explained above for $C(\mathbf{q})$, will specify of how many points this curve consists. Here one has to think about similar problems as explained above. Usually a number of order 200 is good enough.

Reduction factor

The output file from a topography measurement can become very large in size when measuring over large surface areas with high resolution. This results in files with many data points, e.g., 4096×4096 or higher. Hence it is rather complicated to handle files that large, e.g., when trying to plot the topography file. One output file which gets created when running the software is a reduced topography file with reduced number of points. If one puts 2 as reduction factor, a reduced topography file with, e.g., only 2048×2048 points instead of 4096×4096 will be created. This can dramatically reduce the size of the file and hence improve its handleability.

Cut-off plane

When calculating the top power spectrum they surface roughness profile below the average plane is replaced by something which has the same statistical properties as above the average plane. The same is true for calculating the bottom power spectrum only the other way around. However it is sometimes very useful to change the position of the mean plane, or the cut-off plane for calculating top and bottom power spectra. The reason is, that, e.g., a tire on a road only makes contact with a few percent of the nominal contact area. Depending on the surface the rubber therefore does not penetrate deep enough into the rough substrate to experience the full top power spectrum which has been cut-off at the mean plane. With this option the position of the cut-off plane for calculating the top and bottom power spectra can be changed. Note that this number gives the position (or height) of the cut-off plane relative to the mean plane in units of the rms roughness value.

> Specify here the total number of points in x- and y-direction of the input file and also the distance between each point (lattice constant) and the conversion factor needed to convert the input information into SI units.

Step 4 - Specify the Input File

In this step one has to specify the input file used to calculate the power spectrum. Note again that the input file needs to be prepared in a special way so that the software can read it in. Remove any other information from the file than the raw topography information which has to be given in columns (see Step 2 again for further information). To specify the input file, click on the button "Open File" in the upper left part of the interface. In the file dialog window choose the file which should be used in the analysis.

After opening the file, the program will check that the format of the input is correct, e.g., number of columns or total number of points. If there are problems with the file, the software will show an error message and dismiss the file while the name display will change to red. One then has to carefully check if the format is correct, that there is no header or footer left in the file and that the information given under "Specification" are all correct and consistent. In case that the input file is okay, the name of the file will be displayed in the name display with green background.

> Select the input file which will be used for the calculation by clicking on the "Open File" button. Please make sure that the file is prepared correctly.

Step 5 - Power Spectrum

After selecting the input file one has to specify if the full power spectrum or the top or bottom power spectra should be calculated. The difference is the following: the full power spectrum takes into account all the information inside the input file. This is what is usually done when calculating the power spectrum. However for further analysis using, e.g., the contact mechanics or the rubber friction codes it is sometimes necessary to calculate the top power spectrum. Doing so, the software calculates the mean plane of the topography and takes into account only data points which are above this mean plane. A randomly rough surface should not exhibit any difference between the roughness components above compared to below the mean plane. However a road surface for example which has been used for some time will be smoother on top of the roughness asperities due to polishing processes. When a rubber block slides on this road surface it will usually only be in contact with these smoothened regions as the contact area is usually just a few percent of the nominal contact area. Therefore the "rougher" valleys will not be probed by the rubber so that one would like to exclude them from further analysis. Here one has the option to calculate the top power spectrum which only takes into account the roughness components above the mean plane which is an approximate approach to take the problem mentioned above into account.
It is recommended to carefully check the height probability distribution and the skewness parameters as they will give information on if a surface is randomly rough. It is also suggested to calculate both, the full as well as the top and bottom power spectra and compare them with each other to check if the results are consistent.
The bottom power spectrum is the counterpart of the top power spectrum. It takes into account only the roughness components below the average plane. For some applications this can be of certain importance. For example if it is not possible (for whatever reason) to bring the surface to the measurement instrument, one solution is to take a negative of the surface sample (e.g., using silicone rubber) which can be handled much easier and hence be brought to the lab and measured. The results, when measuring the negative, are now actually mirrored so that if one wants to calculate the top power spectrum, one actually has to calculate the bottom power spectrum.
For more information on the top and bottom power spectra please read [2] which can be found on our homepage `http://www.multiscaleconsulting.com`. Here one can also find some online video lectures explaining this in greater detail.

> Choose to calculate the full, top or bottom power spectrum. Note that it is recommended to compare the different results with each other for consistency.

Step 6 - Windowing

The next step is that the windowing method which should be used in the Fourier transform needs to be specified. In the Fourier analysis, the information are treated as infinitely repeating data segments and to

avoid edge effects windowing is often used. This means that both ends of a single line in the topography file are modified so that they will have the same height giving a smooth transition for the sinus waves in the Fourier analysis. Here one can choose between two different approaches to smoothen the edges which are called "Bartlett" and "Welch" (see [5, 6, 7] for further information). It is usually found that these two methods give basically the same result in our application here. In addition it is also possible to do no windowing before calculating the power spectrum.

Note that "no windowing" can result, depending on the topography input, in high local changes in the height at the edges. This will be represented by a large power spectrum at small length scales or large wave vectors q. Hence, no windowing will typically affect the quality of the power spectrum at the highest wave vectors. On the other hand when the profile is smoothened, by using one of the two methods described above, the power spectrum at large length scales or small wave vectors will be affected. Here the power spectrum is usually a little bit smaller due to the windowing of the edges.

It is recommended that both options are tested and compared to each other to check its influence on the power spectrum. However usually the difference is very small here.

> A windowing method has to be selected for the Fourier transform. Selecting the windowing option will usually give slightly smaller power spectra for small wave vectors while no windowing gives higher results for large wave vectors.

Step 7 - Remove tilting and curvature

When measuring the topography of a surface, the sample is usually not completely horizontal and the profile therefore tilted. As only the surface roughness is of interest in this study, and not the macroscopic shape of the sample, it is recommended to remove tilting. This will also affect the impact of the windowing on the power spectrum. It is in addition possible to remove curvature in case the measured surface is curved, e.g., the barrel of a syringe or a ball from a ball bearing. The option "Remove tilting and curvature" takes these two cases into account by removing tilting and curvature from the input file before calculating the power spectrum.

> Removing tilt and curvature from the input information will avoid that the surface roughness power spectrum is influenced by the macroscopic shape of our sample.

Step 8 - Undefined points

Some measurement techniques have problems to measure the height at some coordinates during the experiment. If the instrument fails to measure the correct height, usually a "-1" or a "NaN" is put instead of the height value into the output file. There are different reasons why the instrument might not be able to measure the height correctly, depending on the technique but also on the settings in the experiment or the surface sample itself. The problems will not be further discussed at this point in the manual. They must be solved individually depending on instrument, system under study and conditions. If the number of undefined points is small compared to the total number of points, it is possible to remove these empty coordinates and replace them with height information which are interpolated from the points closest to the location of the undefined point. To do so, one simply selects "Fill undefined", provides the radius for the interpolation and the symbol for an undefined point. The radius basically describes how many neighboring coordinates are considered in the interpolation process. Note that the value for the radius is in units of lattice constants! Choosing a value < 1 will result in no interpolation as the closest

neighbors are 1 lattice away from the location of interest. The bigger this value is chosen, the more points will be considered.

Most instruments will provide a "-1" if there is any undefined point (see Fig 2 center for example). The software needs to be informed about this so that it knows when there is this value in the input file, that it actually is not a valid data point. The symbol which can be entered here has to be a number! In case that there are characters like "NaN", they have to be globally replaced using, e.g., the windows text editor before calculating the power spectrum.

Not replacing undefined points usually leads to large and abrupt roughness changes with high amplitudes. The power spectrum of such a surface would look very unusual.

Another error which can happen in the roughness experiment is, that very high slopes can be observed. This is usually also unphysical and should not occur. If there are regions with very high surface slopes they are usually also errors from the measurement which need to be removed prior to the analysis. This can be done by choosing "Fill undefined, remove large slopes" and specifying the highest slope which should be allowed. The software will then smoothen these points by comparing the height value with those of the nearest neighbors which are given by the radius (which was discussed before already). It is usually found that choosing 1.2 as radius and 10 as maximum slope gives good results.

> Choose one of these options to remove undefined points and points with very high surface slopes from the input file. Note that the input file needs to be prepared in the correct form.

Step 9 - Additional options

There are in the bottom left corner of the interface two additional options which can be selected for the analysis and which will provide additional information:

Nx->Ny, Ny->Nx

This will rotate the input file by 90 degrees by simply switching Nx and Ny. Doing so one can check if a rotation of the input file will give the same power spectrum as compared to before rotating it. This should actually be always the case.

Check anisotropy

Choosing this option, the software will calculate additional information about surface roughness anisotropy which can then be found as output files in the project folder. This is for example important for further analysis of contact mechanics problems, rubber friction and fluid flow between interfaces as this will depend on how surface roughness is distributed depending on direction.

> Choose these additional options (which can be useful for further calculations) to check the results by rotating the input file and calculate additional information on surface roughness anisotropy.

Step 10 - Calculate

After choosing the correct options and providing the necessary information about the input file, the calculation can be started. To do so simply click on the "Calculate" button. Depending on the size of the input file and the options chosen, the computational time may differ. It can take up to a minute before the calculation is finished. Please do not quit the program before!

> After completing the settings as explained above and providing the input file, click on "Calculate" to start the analysis.

Results / Output Files

When the calculation of the power spectrum is finished successfully, all the important output files can be found inside the project folder. All the relevant information for further calculations and results can be found in the ASCII files generated. But before going into detail and explaining these files, lets first have a look at the plotting functionality of the software. The most important output can be plotted directly from the software to have a quick check if the results look consistent before proceeding with the analysis of the output files. There are usually four different output results (depending on the options) which one might want to check after the calculation. They can be found under "Analysis" in the upper menu of the program.

Show Data Out

All options chosen for a particular calculation are stored in a file which is called `DATA.OUT.PowerSpectrum.txt` and which can be found in the project folder. Here the upper half of this file contains the options and input information while in the lower half the most important results are summarized. In the power spectrum program this includes the important roughness parameters and information on anisotropy. The file can be accessed under "Analysis - Show Data Out" as shown in Fig. 3. Note that this file is one of the most important files which is always produced. Also in all the other programs there will be a "DATA.OUT.***.txt" file basically summarizing the project.
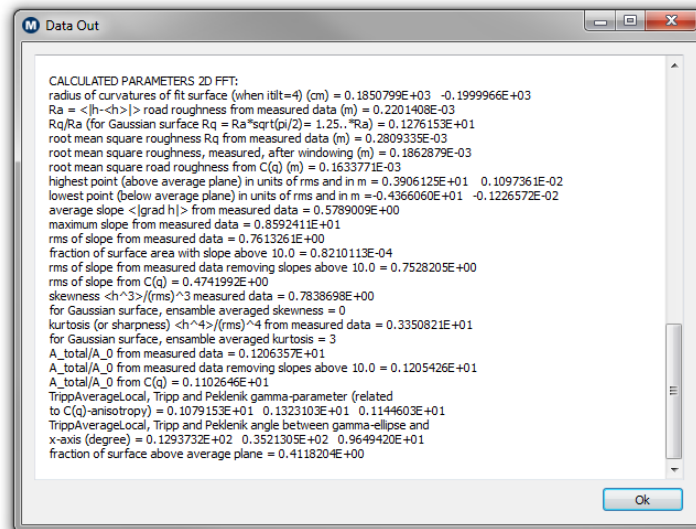

Figure 3: The DATA.OUT file contains a summary of the input parameters and the options chosen for the calculation. In the lower half of this file the most important results, e.g., roughness parameters, are shown.

> Depending on calculating the full, top or bottom power spectrum, the name of the Data Out file might slightly vary (with an added "*.T" or "*.B" in the end of the file name). This is in fact true for all other important files as well.

Plot Power Spectrum

Here the calculated surface roughness power spectrum as calculated from the input file can be found (under "Analysis - Plot Power Spectrum"). Fig. 4 shows the result from the project Example_y,z-data_01. The power spectrum is plotted on a logarithmic scale (with 10 as basis) with wave vector q on the abscissa (or x-axis) and the power spectrum $C(\mathbf{q})$ on the ordinate (y-axis). The shape of the power spectrum of the example here is very typical. One can see a roll-off region for small wave vectors and a linear relation between the power spectrum and the wave vector for larger wave vectors when plotting both quantities on a logarithmic scale. For further information on the power spectrum please visit our homepage `http://www.multiscaleconsulting.com` where an online lecture on this topic can be found explaining the power spectrum in greater detail. This lecture is also available on our YouTube channel `http://www.youtube.com/user/MultiscaleConsulting`.
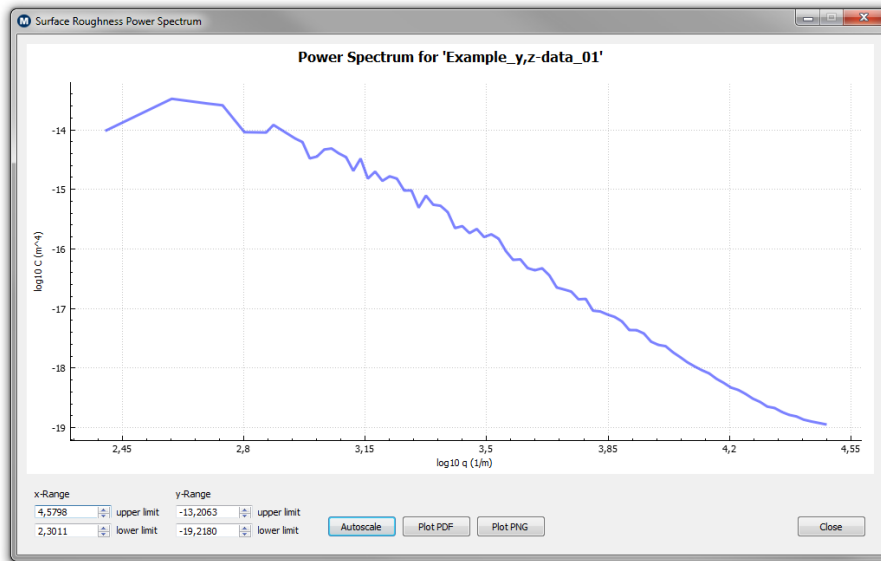

Figure 4: The surface roughness power spectrum $C(\mathbf{q})$ plotted over the wave vector q. Both axes are on a log scale with 10 as basis. Please notice the clear roll-off region far smaller wave vectors and the linear relation for larger wave vectors which is very typical.

Note that in the plotting window which pops up and shows the power spectrum, one can use the mouse wheel to zoom in and out and move the curve by drag and drop (simply click in the plot window, hold the mouse button and move the graph). The scale of both axis can also be adjusted directly by changing the numbers in the input fields for the lower and upper limits for the two axis shown in the lower left corner. The button "Autoscale" will bring back the initial plot of the curve, fitting it to the window size. If needed, the plot can be saved as a separate file by either printing it to a Portable Document Format (PDF) or a Portable Network Graphics (PNG) image file. Simply click either "Plot PDF" or "Plot PNG" will create a file in the project folder where all the results are stored.

The results shown in Fig. 4 can be found in the file `IN_ROADTYPE.q0.qr.q1.h0.H.1logWavevector.2logPowerSpectrum` inside the project folder. The file name usually gives information on what can be found inside the file. Opening the file will show a header followed by the the power spectrum which is given in two columns. In the header there are the project name, the long-distance roll-off wave vector $q0$, qr, the short-distance cut-off wave vector $q1$, $h0$ and the Hurst exponent H. From the file name one can deduce that the 1st column is the logarithm of the wave vector and the 2nd column the logarithm of the power spectrum $C(\mathbf{q})$.

When calculating the power spectrum for a line scan measurement, the extension of the file name changes to `.from.1D.linescan`. This file is actually the most important output of the power spectrum software and is further used as input describing the surface properties in the contact mechanics and the rubber friction software. As explained already above, please note that depending on calculating the full, top or

bottom power spectrum the file name might slightly change.

Plot Height Probability

"Analysis - Plot Height Probability" plots the probability distribution of the relative height compared to the mean plane of the topography. For an ideal, randomly rough surface, this curve should look like a Gaussian function centered at 0. However, it is usually never be a perfectly Gaussian but typically differs slightly also exhibiting noise from the measurement itself. The better the measurement is, in terms of resolution and size of the surface region which has been measured, the smoother this curve should become. This means, that when measuring only small surface regions the probability distribution can depend on the location of the measurement. Only when measured over large enough surface regions (which should be larger then the macroscopic roughness components) enough data is available so that the statistics of the surface are averaged correctly. This means, that a large enough roll-off region should show up in the power spectrum. Hence the shape of the height probability curve will actually no longer depend on the position of the measurement.

If the calculated probability distribution can not be fitted nicely with a Gaussian function even when covering enough roughness information, as shown in Fig. 5, one speaks of a "skewed" surface. Here the maximum is not positioned at 0 and one can observe that the curve also extends to either larger positive or negative heights. For the first case, this would mean that the surface measured is rather flat with few larger particles sticking out. This is the case, e.g., for sandpaper where one finds corundum particles glued with a polymer onto a paper substrate. Here the bottom of the valleys of the surface would be rather smooth while the particles glued to the smooth paper would extend to larger heights as seen in Fig. 12.

The height probability distribution is an important curve as it gives information on the skewness of the surface measured as well as on the quality of the experiment. Therefore this curve should be checked always after the calculation has successfully finished. The results can be found in the file `1h.2Ph.micrometer.txt`.
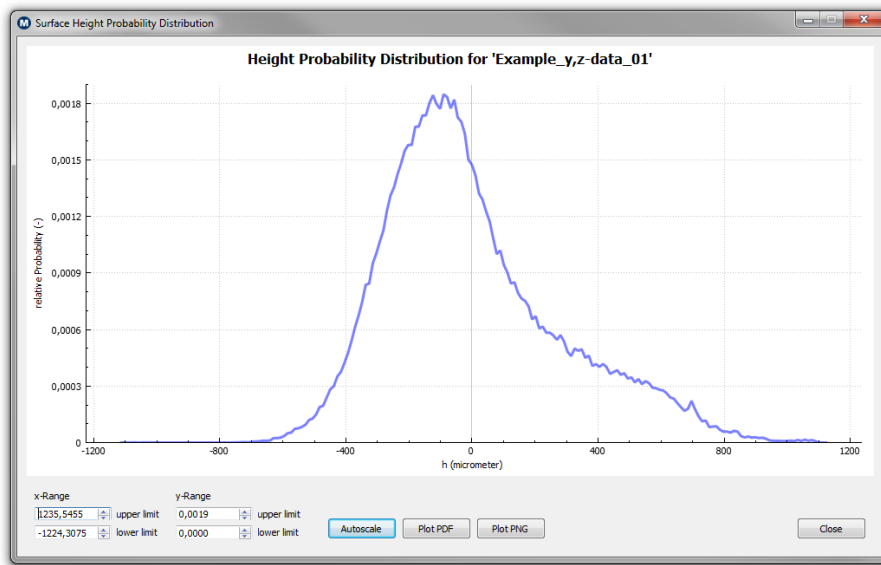

Figure 5: The height probability distribution. This figure shows the relative probability for a certain height or distance h (in μm) away from the mean plane of the surface. For a randomly rough surface this curve should look like a Gaussian function centered at 0.

Plot Slope Probability

Selecting "Analysis - Plot Slope Probability" will show a plot of the probability function for local slopes. Here the y-axis shows the relative probability as a function of the local slope on the x-axis (see Fig. 6). The curve shown here is also very typical for a randomly rough surface. There is a maximum at slopes below 1 with a tail going up to higher slopes. As shown in Fig. 6 the highest slope is of order 2.9 in this example. Note that these high slopes occur very rarely as reflected by the very small probability here. The local surface slope should not be too large as this usually reflects measurement problems as very high surface slopes (sharp and abrupt local deviations of the topography) do not occur. If the slopes in the analysis are too large, it is then suggested to smoothen the input file before calculating the power spectrum by removing high slopes as explained in "Step 8 - Undefined points".

Integrating the curve shown in Fig. 6 will give the root mean square (rms) slope of the measured surface. Note that plotting the slope probability curve is only possible when using topography input files. This function is not calculated for line scan input data. The results can be found in the file `1slope.2Pslope.txt`.
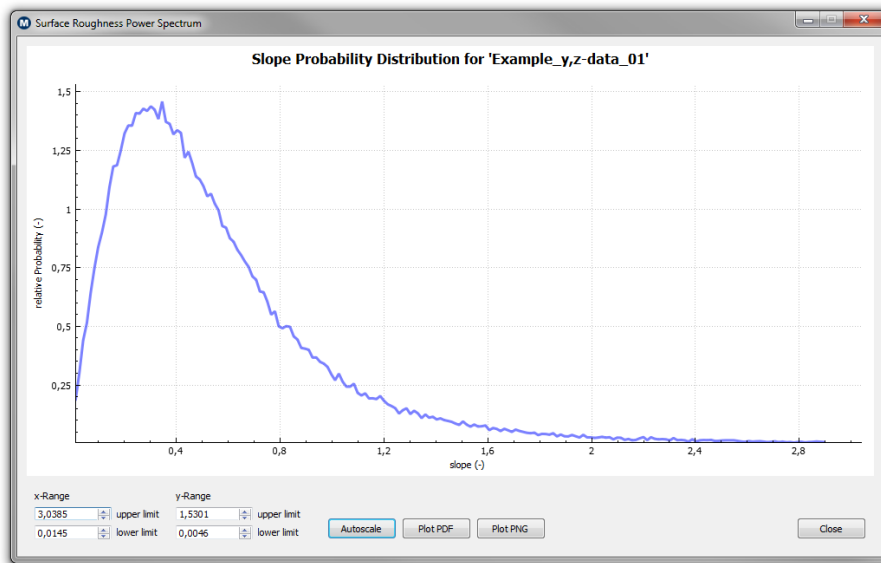

Figure 6: The slope probability distribution. This figure shows the relative probability on the y-axis for a particular surface slope. This curve usually has a maximum at smaller slopes and a tail to higher slopes. Note that the highest slope should not be too large. By definition the slope can only be positive.

Output Files

All results shown here can be found in the project folder. Please note that from the file name the content of the file can be deduced. The file `1slope.2Pslope.txt` for example contains two columns with the local slope in column 1 and the probability for this slope in column 2. For further information on the different files please read the description in the Linux section of this manual or see the following summary of the most important output files. Please note that the file name might slightly vary depending on the options chosen for the calculation (e.g., DATA.OUT.txt gets renamed to DATA.OUT.T.txt when calculating the top power spectrum). Below the symbols *** indicate when and where the name might vary:

   main files

- `DATA.OUT.PowerSpectrum.***.txt -` is the summary of the calculation done containing information on the options chosen and the most important results like characteristic roughness parameters.

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- `IN_ROADTYPE.q0.qr.q1.h0.H.1logWavevector.2logPowerSpectrum.***` - contains the surface roughness power spectrum with some information in the header and the logarithm of the wave vector q in the first column and the logarithm of the power spectrum C_q in the second column. Note that when calculating the power spectrum from linescan input data, the file name changes to `IN_ROADTYPE.q0.qr.q1.h0.H.1logWavevector.2logPowerSpectrum.from.1D.linescan`.

- `1slope.2Pslope.***.txt` - contains the surface slope probability distribution as explained above already.

- `1h.2Ph.micrometer.***.txt` - contains the height probability distribution as explained above already.

input

- `logfileParameters.para` - is a logfile which can be used to repeat an earlier calculation. Please read the section "Repeating a Calculation / The Logfile" below for further information.

- `ROADTYPE.NX.NY.a.prefz.Height.data.***.txt` - this is the original input file used in the calculation.

additional_results

- `1logq.2logC.meter.***.txt` - contains the power spectrum again.

- `accumulated.decrease.q.1log.q.2rms.3slope.4Area` - contains information on how rms roughness, slope and the surface area divided by the projected area depend on the logarithm of q. This shows how roughness are distributed with length scale when decreasing q.

- `accumulated.increase.q.1log.q.2rms.3slope.4Area` - contains information on how rms roughness, slope and the surface area divided by the projected area depend on the logarithm of q. This shows how roughness are distributed with length scale when increasing q.

- `NEW.ROADTYPE.NX.NY.a.prefz.Height.data.h` - contains the input data after removing tilting and curvature and filling out undefined points and removing large slopes. Note that the format has changed and the data is now with only height information in one column.

- `out.2D.Height.Topography.original.for.plotting.h.mum.txt` - the topography input data with reduced number of points according to the reduction factor chosen. The file has not been changed compared to the original input file.

- `out.2D.Height.Topography.removed.curvature.for.plotting.h.mum.txt` - the topography input data with reduced number of points according to the reduction factor chosen. Here the macroscopic curvature has been subtracted away. Plot this file together with the original topography file to see the influence of removing curvature.

- `out.2D.Height.Topography.smoothed.for.plotting.h.mum.txt` - the topography input data with reduced number of points according to the reduction factor chosen. Here undefined points and large slopes have been removed. Plot this file together with the original topography file to see the influence of removing undefined points and large slopes.

- `out.2D.Height.Topography.with.CutPlane.for.plotting.h.mum.txt` - the topography input data with reduced number of points according to the reduction factor chosen. Here the location of the mean plane for calculating the top and bottom power spectra has been changed according to the number chosen as "cut-off plane". Plot this file together with the original topography file to see the new location of the mean plane.

- `out.FILL.1FractionUndefined.2FractionUndefinedAfter.3nit.txt -` this file contains information about the procedure to remove undefined points and large slopes. Here one can see how big fraction of the input data was undefined before and after interpolating undefined points as a function of the number of iterations.

- `out.1D.logq.2logCq1D.yDirec.3logCq2D.for.1D.roughness.Ang.aver.4logCq2D.for.isotropic.` `roughness.txt -` this file contains the 1D power spectrum calculated directly from linescan input data when ploting column 1 as x-axis and column 2 as y-axis (logarithmic scale). One can also plot 3 over 1 or 4 over 1 showing the, from the 1D power spectrum, calculated 2D power spectrum for 1D roughness and the angular averaged power spectrum assuming isotropic roughness, respectively.

- `out.Radius.Curvature.for.1D.fit.function.txt -` contains the macroscopic, curved profile which has been subtracted from the input data when removing curvature and tilt is activated.

anisotropy_results

- `1logq.2Peklenik.3angle.degree.txt -` c.

- `EXTENDED.1logq.2ellipsegamma.3ellipsepsi.4rms.5slope.txt -` c.

- `full.height.profile.2D.dry.txt -` c.

- `height.profile.1D.dry.txt -` c.

- `IN.2D.1angev.1NZ.1NX.1dq.1qx.2qy.3logCq.REDUCED3.txt -` c.

- `IN.2D.1angev.1NZ.1NX.1dq.1qx.2qy.3logCq.REDUCED5.txt -` c.

- `IN.2D.1angev.1NZ.1NX.1dq.1qx.2qy.3logCq.txt -` c.

- `in.2D.logCq.REDUCED3.txt -` c.

- `in.2D.logCq.REDUCED5.txt -` c.

- `LOCAL.1logq.2ellipsegamma.3ellipsepsi.4delta.rms.0.5q.to.2q.txt -` c.

- `out.2D.logCq.txt -` c.

- `Peklenik.Elippse.1qx.2qy.txt -` c.

- `reduced.height.profile.2D.dry.txt -` c.

- `RubberFrictionAnisotropicCq.1logq.2logCqx.3logCqy.4logCqaverage.bad.txt -` c.

- `RubberFrictionAnisotropicCq.1logq.2logCqx.3logCqy.4logCqaverage.good.txt -` c.

Additional Files

As explained already above, the results of every calculation will be stored as a number of different output files in the project folder. In case that not all the files are of interest, it is possible to suppress these files so that they are not generated. To do this, click on "Options" in the menu bar and select "Additional Files". This will bring up a window showing most of the output files (see Fig. 7). Not storing all the output files can help saving some hard disk space as some of the files, depending on the size of the input file, might be very large in size.
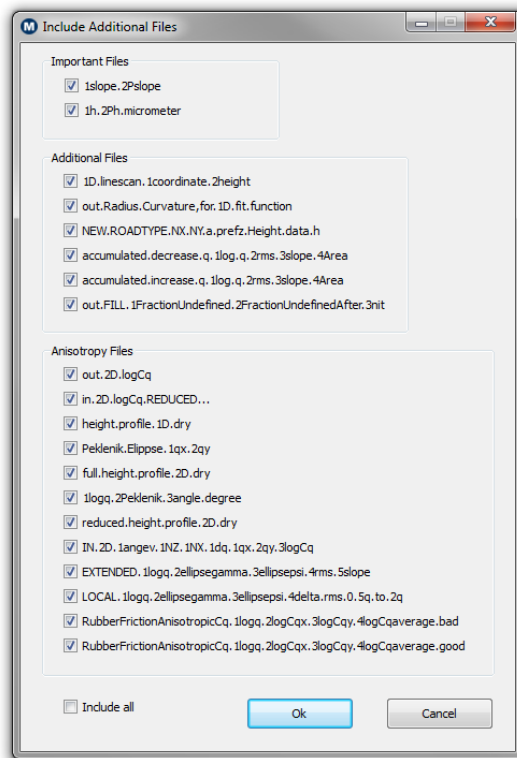
Figure 7: Removing unnecessary files from the calculation output by deselecting them. This might help in saving storage space on the hard disk.

Repeating a Calculation / The Logfile

After successfully finishing a calculation, the input files, as well as the settings used for the calculation, are stored in a separate folder named `input` inside the project folder which is always generated. In case that one wants to repeat an earlier calculation again, one can simply load the file `logfileParameters.para` to set up the program with the old settings and choose the input file `ROADTYPE.NX.NY.a.prefz.Height.data...` from the `input` folder. The file `logfileParameters.para` can be selected when clicking in the menu on "File" and then on "Load Logfile". A file dialog window will appear on the screen in which the correct logfile can be selected.

This functionality can also be used if a set of specific measurements should be done routinely to analyze the measurement results. Instead of changing the settings for each calculation, one can instead set up the program for a specific standard measurement and save the logfile. Whenever one would like to analyze data which has been measured in the same way, simply load the logfile, select the input topography file and start the calculation immediately after.

> **Warning:**
>
> Note that old logfiles might be incompatible with updated versions of the code. If this is the case, please create a new logfile for future applications.

Batch Mode

In case it is necessary to analyze many different measurements which have all been done in the same way, one can run the program in "batch mode" to calculate the power spectrum for each measurement. To do this, the program needs to be set up in the correct way with the right settings for the particular input file type used for this calculation and the correct options to calculate what one is interested in. It is strongly recommended to check if everything is okay by performing a test calculation for one of the input files. If this calculation is successful and without any problems, simply click on "File" in the Menu and select "Batch Mode".

To run the program in batch mode, it is necessary that all the input files which should be analyzed are in one common folder. Note that the input files need to be prepared so that the program can access and read all necessary information. As first step, the program will ask for the folder where the files which should be analyzed using the batch mode are located. Note again that all the files need to be in the same folder for this and that one has to specify the path for this folder, not the individual files! As a second step, a dialog opens up displaying all the files which the program could find in the selected folder (see Fig. 8). In case one doesn't want to use all the files, simply remove them from the list by selecting these files and exclude them from the analysis by clicking on the button "Remove from List".

To start the batch mode, click on the button "Run" in the lower left corner of the dialog window. The program will then automatically calculate the power spectrum of all the input files which are in the list. The results will be saved in the data folder with the name of the input file as folder name. The progress of the analysis is shown during the calculation which can be stopped at any point. Please note that when clicking "Stop" it may take some time before the process is canceled as the program will have to finish to calculate the power spectrum of the input file which it started with last.

Linux Version

Input Files

The input data to the code are the following 3 data files:
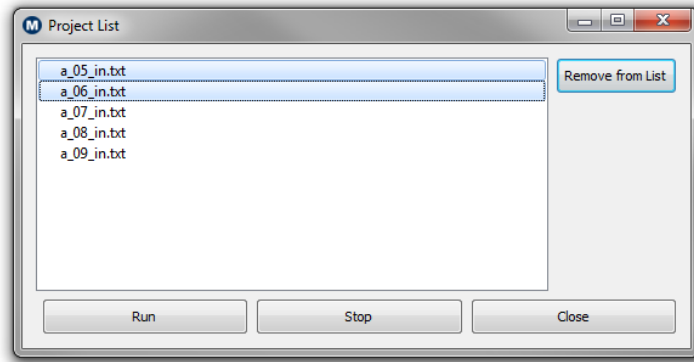
`IN.flagparameters` - A flag parameter file.

Figure 8: The Batch mode window. Here all the files found in the selected folder are shown. Files can be excluded from the analysis by selecting them and clicking on "Remove from List". To start the patch mode simply click on "Run".

`IN.PrepareData.FillUndefined.ReduceSlope` - A file with parameters used to specify undefined data points (if any) and to smoothen the height profile (if necessary):

`ROADTYPE.NX.NY.a.prefz.Height.data.1x.2y.3h` - The height profile which can be given on 3 different forms, either as $x, y, h(x, y)$ data.

`ROADTYPE.NX.NY.a.prefz.Height.data.1y.2h` - or as $y, h(y)$ data as typical for 1D line scan data.

`ROADTYPE.NX.NY.a.prefz.Height.data.h` - or as a single row of height $z = h$ data (typical Atomic Force Microscopy data).

The data file `IN.flagparameters` contains the following parameters:

iflag1
= 1 no WINDOWING
= 2 WINDOWING with Bartlett
= 3 WINDOWING with Welch
Windowing is a procedure to get the height profile continuous at its boundaries which is necessary to calculate good power spectra for large wave vectors. So usually use iflag1 = 2 or 3. However windowing will effect the smallest wave vectors so sometimes using iflag1 = 1 can also be useful if the small wave vector region is most important.

iflag2
= 1 if the input height data consists of h - data (one single row, usually AFM data)
= 2 then y, h - data (two column)
= 3 then x, y, h - data (three column)

iflag3
= 1 gives C(q)
= 2 gives CT(q) (top power spectrum)
= 3 gives CB(q) (bottom power spectrum)
Note, the top power spectrum is the power spectrum resulting when the surface profile below the average plane is the mirror of the surface roughness above the average plane, and similar for the bottom power spectrum. For randomly rough surfaces C(q) = CT(q) = CB(q) but sometimes the surface exhibits, e.g., skewness, and in this case the different power spectra differ. In many applications two interacting solids only experience the upper part of the roughness profile and in this case CT(q) may be more relevant than C(q).

iflag4
= 1 (and iflag3 = 1) implies a wet surface where the power spectrum is obtained for a wet surface profile. This is only useful in a few cases.

iflag5
= 1 gives the height correlation functions $G(r) = \langle h^2 \rangle - \langle h(r)h(0) \rangle$ and $G3(r) = \langle h(r)h(0) \rangle - \langle h \rangle^2$.

iflag6
= 1 calculates power spectrum from 1D-data
Typically with NX=1, NY=N, N=number of point. Suppose the line profile has been measured at several places (say N' different times) one can average over all the measurements by putting all the data after each other (no spacing) in the height profile input data file, and in this case Nx=N' in the height profile input data file (see below).

iswitch
= 1 will switch rows and columns (transpose) in the height data file h(i,j)→h(j,i); NX→NY, NY→NX (particular useful when iflag6 = 1)

ido
= 1 or 2, fill out undefined data points hfill, see below

ireduce
= 1 reduces the number of output data files by removing (very large) anisotropy and topography files.

itilt
= 0 remove nothing
= 1 remove tilt of line
= 2 remove tilt of surface plane
= 3 remove tilt and curvature of line
= 4 remove tilt and curvature of surface

Cqpoints
equals the number of points for which C(q) is given, typically use of order 100.

Phpoints
equals the number of points for which the distribution of heights P(h) and slopes P(slope) are given, typically use of order 200.

nreduce1
integer reducing size of height data for plotting with Gnuplot, use, e.g., 1 (no reduction) or 2 or 4 or 8

The data file `IN.PrepareData.FillUndefined...` contains the following parameters: ido, hfill, radius and slopemax and are used as follows:
If ido=1, fill undefined points which may exist in the height input data file. Such undefined data points often occur in optically measured height profiles (maybe where the surface slope is too high). The undefined points in the input height data file should be denoted by hfill. The undefined data points are defined by using the average height from within a circular region centered at the undefined point. The radius (in units of the lattice or grid spacing) of the circle is denoted as radius and is also given in this input file. If ido=2 the code first fills undefined points, then replaces points where the surface slope is larger than slopemax with undefined points, and then fills undefined points again. Everything is repeated until all points with slope higher than slopemax have been removed. So using ido=2 will result in some smoothing of the surface topography.
The data file `ROADTYPE.NX.NY.a.prefz.Height.data.1x.2y.3h` contains:

ROADTYPE
is the name of the surface

NX
number of height data points in x-direction

NY
number of height data points in y-direction

a

the lattice or grid spacing (assumed to be the same in the x- and y-directions) in meter

prefz

the number with which the height coordinate must be multiplied in order to convert it into meter

1x.2y.3h

three columns with the x, y and $z = h$ (height) coordinates. Only the z=h coordinate is used as the lattice spacing is already defined before.

`ROADTYPE.NX.NY.a.prefz.Height.data.1y.2h` and `*.Height.data.h` contains similar information as `*.Height.data.1x.2y.3h` but giving either only the y and z=h coordinates as typical for 1D line scan (stylus) data or just the height coordinate z=h as a single long row as is typical for Atomic Force Microscopy (AFM) data.

Output

OUTPUT FILES when ireduce = 0, iflag6 = 0:

Lets first discuss the output files obtained when ireduce = 0 and iflag6 = 0. When ireduce = 1, a large number of additional files are generated which relate to surface anisotropy and also some (reduced) height topography data sets convenient for plotting. When iflag6 = 0 one calculates the 2D power spectrum. In this case the output files are:

`1logq.2logC.meter`, first column: log (with 10 as basis) of the wave vector (in 1/meter), second column: log of power spectrum (in meter^4)

`IN_ROADTYPE.q0.qr.q1.h0.H.1log.wavevector.m-1.2log.RoadPowerSpectrum.m+4`, the first 5 lines contain the smallest wavevector q0 for which the surface power spectrum has been calculated, followed by a roll-off wavevector qr (here put equal to q0), the smallest wavevector q1 for which the surface power spectrum has been calculated, the root-mean-square roughness amplitude h0, and the Hurst exponent (here put equal to H=0.8). After this follows the calculated surface roughness power spectrum just as in the file `1logq.2logC.meter`. This data file has the form necessary for being direct input into contact mechanics and rubber friction codes although the parameters q0,qr,q1,h0 and H may need to be changed.

`1h.2Ph.meter`, the probability distribution of surface heights (h = surface height (in meter) from the average surface plane, Ph = relative probability (in 1/meter))

`1slope.2Pslope`, the probability distribution of surface slopes (slope = surface slope, Ph = relative probability)

`accumulated.increase.q.1log.q.2rms.3slope.4Area` gives the cumulative (or accumulated) values for the root-mean-square roughness (second column), the slope (third column) and the surface area as all the surface roughness components from q0 to the wavevector q given in the first column are included in the calculation (the first column is the logarithm of q).

`accumulated.decrease.q.1log.q.2rms.3slope.4Area` gives the same as for the `accumulated.increase.q...` file just mentioned, but instead including all the roughness between q and the largest wavevector q1.

`DATA.OUT.PowerSpectrum` summarize many input and output data.

OUTPUT FILES when ireduce = 0, iflag6 = 1:

This creates the files `1h.2Ph.meter` and `DATA.OUT.PowerSpectrum` like above, and in addition the following files:

`out.1D.logq.2logCq1D.3logCq2D.for.1D.roughness.4logCq2D.for.isotropic.roughness` This file gives the logarithm of the 1D power spectrum (second column) (in meter^3) as a function of the logarithm of the wavevector (first column) (in 1/meter). For two special cases one can calculate the 2D power

spectrum (in meter^4) from the 1D power spectrum, namely when the surface roughness is one dimensional and the topography has been measured orthogonal to the groves of the rough surface, and for the case when the surface has isotropic statistical properties. The resulting power spectra are given by column 3 (for uni-axial roughness) and column 4 (for isotropic roughness). Even when the surface is anisotropic, the angular averaged power spectrum (which enters in many contact mechanics calculations) will usually be close to the result presented in column 4.

The data file `1logq.2logC.meter.from.1D.linescan` gives again the results contained in column 1 and 4 in the data file presented above.

The data file `IN_ROADTYPE.q0.qr.q1.h0.H.1logWavevector.2logPowerSpectrum.from.1D.linescan` contains the same information as discussed above when iflag6 = 0, but the power spectrum is now calculated from the 1D power spectrum assuming isotropic statistical properties, i.e., it is the same as in the file `1logq.2logC.meter.from.1D.linescan`.

OUTPUT FILES when ireduce = 1, iflag6 = 0:

In this case the code produce additional output related to surface topography and surface anisotropy.

`reduced.height.profile.2D.dry` is the surface topography on a grid with larger lattice constant suitable for plotting using Gnuplot (Gnuplot; set pm3d; splot "reduced.height.profile.2D.dry" w pm3d).

`height.profile.1D.dry` is the surface topography along a line.

`out.2D.logCq` is the 2D power spectrum on a form suitable for plotting with Gnuplot (Gnuplot; set pm3d; splot "out.2D.logCq" w pm3d).

`out.2D.logCq.REDUCED3` is the surface power spectrum on a grid with 3 times larger lattice constant suitable for plotting using Gnuplot.

`out.2D.logCq.REDUCED5` is the surface power spectrum on a grid with 5 times larger lattice constant suitable for plotting using Gnuplot.

`IN.2D.1angev.1NZ.1NX.1dq.1qx.2qy.3logCq` is the surface power spectrum on a form used as input for anisotropic rubber friction.

`IN.2D.1angev.1NZ.1NX.1dq.1qx.2qy.3logCq.REDUCED3` is the surface power spectrum on a reduced form used as input for anisotropic rubber friction.

`IN.2D.1angev.1NZ.1NX.1dq.1qx.2qy.3logCq.REDUCED5` is the surface power spectrum on a reduced form used as input for anisotropic rubber friction.

`Peklenik.Elipse.1qx.2qy` are the contour lines (denoted "ellipse" but in general not an ellipse) in the (qx,qy)-plane of the cut between the power spectrum surface z = C(qx,qy) and a plane z = constant for 1000 planes at different z uniformly distributed between Max C and Min C on a log scale.

`1logq.2Peklenik.3angle.degree` is the ratio between the major and minor axis of the Peklenik ellipse and the rotation angle relative to the qx-axis as a function of the logarithm of the wavevector q. The Peklenik number can roughly be interpreted as the ratio between the major and minor axis of the asperities observed at the length scale 1/q.

`EXTENDED.1logq.2ellipsegamma.3ellipsepsi.4rms.5slope` - the second column gives the Tripp gamma parameter as a function of the logarithm of the wavevector using an extended definition (see below). The third column gives the Tripp rotation angle and column 4 and 5 the rms roughness and rms slope as a function of q including only the roughness with wavevector between q and the large wavevector cut-off $q1$. The Tripp gamma parameter enters in the calculation of fluid flow at interfaces in the contact mechanics code. The Tripp gamma parameter and angle are defined in [4] which can be found on `www.multiscaleconsulting.com`

`LOCAL.1logq.2ellipsegamma.3ellipsepsi.4delta.rms.0.5q.to.2q` - the second column gives the Tripp number as a function of the logarithm of the wavevector using a local definition (see below).

The other quantities are defined the same way as for EXTENDED.

`RubberFrictionAnisotropicCq.1logq.2logCqx.3logCqy.4logCqaverage.good` gives information about the anisotropy of the viscoelastic contribution to rubber friction. Here Cqx is the angular average (in **q**-space) between the product of C(qx,qy) and qx/q = cos (theta) where theta is the angle between the vector **q** and the qx-axis. Similar for Cqy. Also given (column 4) is the angular average of the power spectrum. All on a log-scale.

`RubberFrictionAnisotropicCq.1logq.2logCqx.3logCqy.4logCqaverage.bad` contains the same information as in the file above but calculated in a different way.

A Note About Surface Anisotropy

Information about surface anisotropy can also be deduced from 1D line-scan measurements if they are performed in two orthogonal directions, one along the groves (one principle direction of the matrix D defined above), and one orthogonal to the groves (the other principle direction of the matrix D). This can be illustrated with the following example, consider a surface with isotropic roughness which is self-affine fractal with the Hurst exponent H. For this case the 1D power spectrum in the x-direction will scale as

$$C_x = \frac{1}{2\pi} \int dx \ \langle h(x)h(0) \rangle e^{iqx} \sim q^{-1-2H}$$

and the same result holds in the y-direction, $C_x(q) = C_y(q)$. Now suppose that the surface is stretched in the x-direction by a factor of $\gamma > 1$. In this case the power spectrum in the y-direction will be unchanged, $\bar{C}_y(q) = C_y(q)$, while the power spectrum in the x-direction can be calculated as follows: The height profile of the stretched surface $\bar{h}(x) = h(x/\gamma)$ so that

$$\bar{C}_x = \frac{1}{2\pi} \int dx \ \langle \bar{h}(x)\bar{h}(0) \rangle e^{iqx}$$

$$= \frac{1}{2\pi} \int dx \ \langle h(x/\gamma)h(0) \rangle e^{iqx}$$

$$= \frac{1}{2\pi} \int dx \ \gamma \langle h(x)h(0) \rangle e^{iq\gamma x} = \gamma C_x(\gamma q) = \gamma^{-2H} C_x(q)$$

Thus $\bar{C}_x(q) = \gamma^{-2H} \bar{C}_y(q)$ and at least if the surface is self-affine fractal one can deduce the Peklenik number γ from the 1D power spectrum measured in two orthogonal directions, one along the groves and one perpendicular to the groves! This is illustrated in Fig. 16 which shows the 1D surface roughness power spectrum along the x and y-directions (red and green lines), of a randomly rough self-affine fractal surface with the Peklenik factor $\gamma = 3$. Note that they differ by exactly a factor $-2H \times \log_{10}\gamma$ as expected on the log-log scale. Also shown is the power spectrum of a randomly rough surface with the same Hurst exponent and rms roughness but with isotropic statistical properties (blue line) which is almost identical to the 1D power spectrum along the rough direction (green line) for the $\gamma = 3$ case. Since the root-mean-square roughness amplitude $h_{\rm rms}$ is determined from the 1D line-scan measurements (note: $h_{\rm rms}$ is the same along the x or y-directions), and since the statistical properties of the surface are fully defined by the parameters H, γ and $h_{\rm rms}$, for a self-affine fractal surface with anisotropic statistical properties, obtained by stretching one direction, from 1D line-scan measurements in two orthogonal directions the full 2D power spectrum can be easily calculated. Real surfaces may be more complex but one should at least be able to approximately calculate the 2D power spectrum from 1D measurements using the procedure described above.
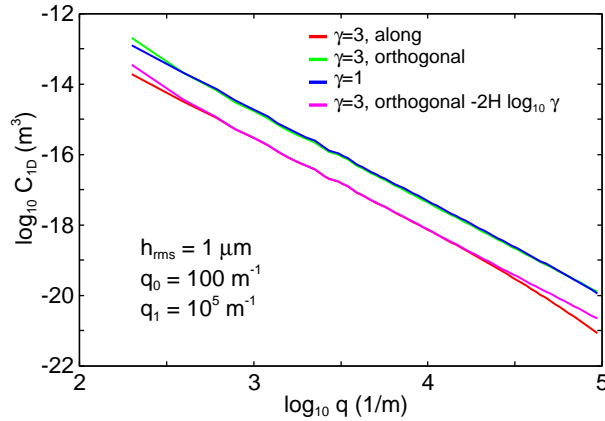
Figure 9: The 1D power spectra of a randomly rough, self affine fractal surface with anisotropic roughness with the Peklenik number $\gamma = 3$, along the x and y-directions (red and green lines). Note that they differ by exactly a factor $-2H \times \log_{10}\gamma$ (as indicated by the pink line, which is the green line shifted downwards by $-2H \times \log_{10}\gamma$) as expected on the log-log scale. Also shown is the power spectrum of a randomly rough surface with the same Hurst exponent and rms roughness, but with isotropic statistical properties (blue line) which is almost identical to the 1D power spectrum along the rough direction (green line) for the $\gamma = 3$ case.

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