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Reference software for calculating areal surface texture parameters: User manual

P M Harris and I M Smith

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P M Harris and I M Smith
Mathematics and Scientific Computing Group

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ABSTRACT

This report constitutes a *user manual* for reference software developed at the National Physical Laboratory for calculating S–F and S–L areal surface texture parameters. The reference software is used as a benchmark against which software in a measuring instrument can be compared. A data set is used as input to both the software under test and the reference software, and the results delivered by the software under test are compared with those provided by the reference software. The software is provided with a simple-to-use graphical user interface and the calculated parameter values are written to an output text file.

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National Physical Laboratory,
Hampton Road, Teddington, Middlesex, United Kingdom TW11 0LW

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Approved on behalf of NPLML by Dr Bajram Zeqiri,
Knowledge Leader for the Acoustics and Ionizing Radiation team

Contents

1 Introduction

1.1 Background

Knowledge of the topography of a machined surface is necessary in order to understand the functional performance of the surface, and is consequently essential to the manufacturing process [1, 2, 3]. As with the instruments used in many other areas of metrology, those that measure surface texture generally interface to a computer that collects and analyses numerical data. As part of the data analysis, surface texture parameters are evaluated. The use of a surface texture parameter to characterise numerically the measured topography was proposed many years ago [4], and a number of parameters have been adopted by standards bodies and are used in industry for this purpose. Whereas it is commonplace to use physical artefacts to calibrate surface measuring instruments, such artefacts do not allow validation and verification in isolation of the software components of the instrument.

ISO 5436–2 [5] introduced into international standardisation the concept of the *software measurement standard* in the context of the measurement of surface texture. The standard defines Type F1 (reference data) and Type F2 (reference software) software measurement standards for testing the numerical correctness of software used in surface texture measurement. Reference software is used as a benchmark against which software in a measuring instrument can be compared. A data set is used as input to both the software under test and the reference software, and the results delivered by the software under test are compared with those provided by the reference software. The most important consideration in the design and development of reference software is its numerical correctness. This is in contrast to the considerations for production software, for which the requirements on numerical correctness are generally more modest, but issues of efficiency, such as computing time and memory, and usability are of concern.

This report is a user manual for reference software developed at the National Physical Laboratory (NPL) for the calculation of S–F and S–L areal surface texture parameters. The software is supplemented by two papers: the first [6] describes the software, focusing on the definition of the surface parameters and describing the numerical algorithms employed in the software to implement those definitions; the second [7] presents a comparison of the results returned by the reference software with those obtained using proprietary software for surface texture measurement.

The report is organised as follows. The remainder of this section describes the main functions of the software, including the conditions for its use. Section 2 gives information on installing and uninstalling the software. Section 3 describes how to use the software. Finally, appendices to the report contain background technical information on the algorithms implemented in the reference software, including definitions of the areal surface texture parameters considered.

1.2 Software User Licence Agreement

The software is provided with a Software User Licence Agreement (Ref: MSC/L/11/003) and the use of the software is subject to the terms laid out in that agreement. By installing and running the software, the user accepts the terms of the agreement.

To run the software, the user must first install MATLAB's Component Runtime (MCR) libraries (section 2). The MCR installer file is not included in the software distribution, but it may be obtained by contacting NPL. Information on how to obtain the MCR installer file is given in the file `README.txt` included in the software distribution. The user must accept the terms of the MCR Library License as part of the installation of the MCR libraries.

1.3 Main functions of the software

The main functions of the reference software are as follows:

- Read data defining an *S–F surface* [8, clause 3.1.5], i.e., a surface that has been S–filtered (to remove small scale components) and from which form has been removed (using an F–operator);
- Apply a Gaussian areal filter to the data defining an S–F surface to obtain data defining the corresponding *S–L surface* [8, clause 3.1.6] (appendix A);
- Remove points from the data defining an S–L surface, i.e., 'trim' the data, to produce a surface defined on an area which has sides with lengths that are integer multiples of the cut-off wavelength for the Gaussian areal filter used to obtain the surface (appendix B);
- Apply surface interpolation to the data defining the S–F and S–L surfaces to obtain continuous representations of those surfaces (appendix C);
- Evaluate areal surface texture parameters in terms of these continuous representations of the S–F and S–L surfaces (appendix D);
- Write the values of the areal surface texture parameters to an output file.

The areal surface texture parameters to be evaluated are from the S–parameter set and include height parameters[1]

- root mean square height S_{q},

[1]For clarity, and to ensure the notation is mathematically unambiguous, the notation S_{q}, etc., is used throughout to denote areal surface texture parameters in place of the (more familiar) notation Sq, etc., used in practice.

- skewness S_{sk},
- kurtosis S_{ku},
- maximum peak height S_{p},
- maximum pit height S_{v},
- maximum height S_{z}, and
- arithmetical mean height S_{a},

spatial parameters

- autocorrelation length S_{al}, and
- texture aspect ratio S_{tr},

and hybrid parameters

- root mean square gradient S_{dq}, and
- developed interfacial area ratio S_{dr}.

The following conditions are assumed to apply:

1. The input data is provided in X3P format [9], a format for defining surface data that allows the smooth interchange of data between different measuring systems. Software implementing the data format has been developed by the 'openGPS' consortium as freeware [10];
2. The input data has a uniform sampling inverval $\Delta x > 0$ in the x–direction and a uniform sampling interval $\Delta y > 0$ in the y–direction with, in general, $\Delta x \neq \Delta y$;
3. For an S–F surface, the *evaluation area* [8, clause 3.1.10], i.e., the area used to specify the part of the surface under evaluation, is a rectangle with sides of lengths L_x in the x–direction and L_y in the y–direction containing all the surface heights;
4. For Gaussian areal filtering, the same cut-off wavelength $\lambda > 0$ is applied in the x– and y–directions;
5. The cut-off wavelength λ is an integer multiple of the sampling intervals Δx and Δy;
6. In order to minimise any distortion of the filtered surface due to the finite extent of the surface, the lengths L_x and L_x are at least three times the cut-off wavelength;

7. In order to minimise any distortion of the filtered surface due to the finite number of data points per cut-off wavelength, there should be at least fifty points per cut-off wavelength in each direction;

8. For an S–L surface, the evaluation area is a rectangle of largest area with sides having lengths equal to integer multiples of λ that is contained within the rectangle obtained from the evaluation area for the corresponding S–F surface by removing λ from each side. The evaluation area for an S–L surface is generally not uniquely defined. A particular choice is made by requiring that it is positioned 'centrally' with respect to the evaluation area for the corresponding S–F surface (appendix B).

For an S–F surface, the input data consists of matrices $\boldsymbol{X}$, $\boldsymbol{Y}$ and $\boldsymbol{Z}$, each of dimension $m_x \times m_y$, containing, respectively, the x–coordinates $x_{ij} = x_0 + (i-1)\Delta_x$, y–coordinates $y_{ij} = y_0 + (j-1)\Delta_y$ and surface heights (z–coordinates) z_{ij}, $i = 1, \ldots, m_x$, $j = 1, \ldots, m_y$, i.e., z_{11} is the height at the origin (x_0, y_0) of the xy–coordinate system and $z_{m_x m_y}$ is the height at the point 'diagonally opposed' to the origin. For an S–L surface, the input data consists of that for an S–F surface together with the cut-off wavelength λ.

It is assumed that the x–, y– and z–coordinates, together with the cut-off wavelength λ, are provided in the same unit of measurement, which then determines the units of measurement of the calculated surface texture parameters. For example, if the data is provided with $\mu\mathrm{m}$ as the unit of measurement, then the calculated surface texture parameters have the following units of measurement:

- $S_{\mathrm{q}}/\mu\mathrm{m}$;
- $S_{\mathrm{sk}}/1$;
- $S_{\mathrm{ku}}/1$;
- $S_{\mathrm{p}}/\mu\mathrm{m}$;
- $S_{\mathrm{v}}/\mu\mathrm{m}$;
- $S_{\mathrm{z}}/\mu\mathrm{m}$;
- $S_{\mathrm{a}}/\mu\mathrm{m}$;
- $S_{\mathrm{al}}/\mu\mathrm{m}$;
- $S_{\mathrm{tr}}/1$;
- $S_{\mathrm{dq}}/1$;
- $S_{\mathrm{dr}}/1$.

2 Installing and uninstalling the software

The software takes the form of an application program called `Areal_SOFTGAUGES.exe`, generated by compiling (using the MATLAB compiler) software implemented in the MATLAB programming language [11], together with the associated files:

- `ISO5436_2_XML.dll`;
- `xerces-c_2_7_vc80.dll`;
- `openX3P.mexw32`;
- `writeX3P.mexw32`;
- `iso5436_2.xsd`;
- `RomIntWeights.mat`;
- `npl_logo_black_large.jpg`;
- `ArealSoftgaugesSoftware-R1.pdf`;
- `ArealSoftgauges-MSC_L_11_003.pdf`;
- `cos_512_1um_512_2um_ls.x3p`;
- `cos_512_1um_512_2um_ls.txt`;
- `README.txt`.

The program has been created and tested on a personal computer running the Microsoft Windows XP Professional operating system.

To install the software, undertake the following steps:

1. Copy the application program and the above associated files to a working folder;
2. Create the User Environment Variable `OPENGPS_LOCATION` and set its value to the path of the working folder containing the application program and its associated files;
3. Install MATLAB's Component Runtime (MCR) libraries. This is done by running the MCR installation program

   ```
   MCRInstaller.exe
   ```

once on the target machine, i.e., the machine on which it is intended to run the application program. It is necessary to have administrative privileges for the target machine because both the system registry and system path are modified as part of the installation process. The MCR installation program installs the MCR libraries, registers the components as needed, and updates the system path to point to the MCR binary folder. The installation process takes some time due to the number of files that are installed. The MCR installation program is about 173 MB in size, and the installed libraries require about 456 MB of disk space.

The software is uninstalled by

- running the MCR installation program `MCRInstaller.exe` and selecting 'Remove' to uninstall the MCR libraries, and
- deleting the application program and its associated files.

3 Using the software

3.1 General

The application program may be run in either of two ways:

(a) Double-clicking on the executable file (with the extension `.exe`) in Windows Explorer. An MS-DOS window opens and the main graphical user interface (GUI) is displayed;

(b) Opening an MS-DOS window, navigating to the folder containing the program, typing the name of the program (without the extension `.exe`), and pressing `Return`. The main GUI is displayed (and the MS-DOS command line may not be accessed again until the user has exited the software).

It may take several seconds for the GUI to be displayed.

The GUI is divided into a number of parts that allow the user to perform the following operations:

1. Select X3P file;
2. Select (surface texture) parameters;
3. Select output file;
4. Process data;

5. Exit.

Each of these operations is described in the sections below.

3.2 Select X3P file

The user must first select an X3P file. This is done by pressing the `BROWSE...` button in part 1 of the GUI, navigating to the folder in which the required X3P file is located and either double-clicking on that file or clicking on the file and pressing `Open`. If no file is selected before pressing `Open`, a warning message is displayed.

3.3 Select surface texture parameters

Once the user has selected an X3P file (section 3.2), the check boxes for the S–F and S–L parameters in part 2 of the GUI become active.

The S–F parameters to be calculated are selected by clicking on the check boxes corresponding to those parameters. The `ALL/NONE` check box provides a shortcut to selecting all or none of the parameters (repeated clicking on this check box toggles between all parameters and no parameter being selected).

A number of the parameters require a tolerance to be provided (section 3.4). When the check box for a parameter that requires a tolerance is ticked the corresponding text box for the tolerance becomes active. In addition, the parameters S_{al} and S_{tr} require the user to enter a value for the autocorrelation function (section 3.5).

The S–L parameters to be calculated are selected similarly. In addition to providing values for any tolerances and the autocorrelation function, a value of the cut-off wavelength for an areal Gaussian filter must also be entered (section 3.6).

3.4 Set tolerances

S_{q} The user is not required to provide a tolerance value.

S_{sk} The user is not required to provide a tolerance value.

S_{ku} The user is not required to provide a tolerance value.

S_{a} The user is required to provide a tolerance value ϵ_{a}.

Approximations $\widehat{S}_{\mathrm{a}}(K)$ to S_{a} are calculated for a sequence of increasing values of K (from $K = 3$ to a maximum value of $K = 8$) until the relative difference in

successive approximations is less than the tolerance, i.e.,

$$\left|\widehat{S}_{\mathrm{a}}(K) - \widehat{S}_{\mathrm{a}}(K-1)\right| < \epsilon_{\mathrm{a}}\widehat{S}_{\mathrm{a}}(K-1), \tag{1}$$

and S_{a} is set to the value $\widehat{S}_{\mathrm{a}}(K)$.

The default value for the tolerance is $\epsilon_{\mathrm{a}} = 1 \times 10^{-3}$.

A check is made that the value ϵ_{a} entered by the user is greater than zero.

S_{p}, S_{v}, S_{z} The user is required to provide a tolerance value ϵ_{h}.

Values for the parameters are obtained from the solutions to a set of linearly constrained optimisation problems that are solved iteratively using MATLAB's `fmincon` optimisation function. The tolerance ϵ_{h} is used as a termination tolerance for changes in the objective function value and for the length of the step between successive solution estimates.

The default value for the tolerance is $\epsilon_{\mathrm{h}} = 1 \times 10^{-3}$.

A check is made that the value ϵ_{h} entered by the user is greater than zero.

S_{al}, S_{tr} The user is required to provide a tolerance value ϵ.

The calculation of S_{al} and S_{tr} requires the solution of two non-linear equality constrained optimisation problems. These problems are solved iteratively using MATLAB's `fmincon` optimisation function. The tolerance ϵ is used as a termination tolerance for changes in the objective function value, for the length of the step between successive solution estimates and on the violation of the equality constraints.

The default value for the tolerance is $\epsilon = 1 \times 10^{-3}$.

A check is made that the value ϵ entered by the user is greater than zero.

S_{dq} The user is not required to provide any tolerance value.

S_{dr} The user is required to provide a tolerance value ϵ_{dr}.

Approximations $\widehat{S}_{\mathrm{dr}}(K)$ to S_{dr} are calculated for a sequence of increasing values of K (from $K = 3$ to a maximum value of $K = 8$) until the relative difference in successive approximations is less than the tolerance, i.e.,

$$\left|\widehat{S}_{\mathrm{dr}}(K) - \widehat{S}_{\mathrm{dr}}(K-1)\right| < \epsilon_{\mathrm{dr}}\widehat{S}_{\mathrm{dr}}(K-1), \tag{2}$$

and S_{dr} is set to the value $\widehat{S}_{\mathrm{dr}}(K)$.

The default value for the tolerance is $\epsilon_{\mathrm{dr}} = 1 \times 10^{-3}$.

A check is made that the value ϵ_{dr} entered by the user is greater than zero.

3.5 Set value of autocorrelation function

For the calculation of S_{al} and S_{tr}, the user is required to provide a value s for the autocorrelation function.

The default value for the autocorrelation function is $s = 0.2$.

A check is made that the value s entered by the user lies in the open interval $(0, 1)$.

3.6 Set cut-off wavelength

For the calculation of S–L parameters, the user is required to provide a value λ of the cut-off wavelength of an areal Gaussian filter.

The default value for the tolerance is $\lambda = 1 \times 10^{-4}$, which corresponds to 0.1 mm when the x–, y– and z–coordinates are provided in units of metres.

Checks are made that:

- λ is greater than zero;
- $\lambda/\Delta x$ is an integer greater than or equal to 50, where Δx is the uniform sampling interval in the x-direction;
- $\lambda/\Delta y$ is an integer greater than or equal to 50, where Δy is the uniform sampling interval in the y-direction;
- L_x/λ is greater than or equal to 3, where L_x is the length of the definition area in the x-direction;
- L_y/λ is greater than or equal to 3, where L_y is the length of the definition area in the y-direction.

3.7 Select output file

Once the user has selected an X3P file (section 3.2), a default output file path appears in the edit box in part 3 of the GUI. The default output file is located in the same folder as the X3P file and has the same name but the `.txt` extension. The user may edit the default output file path, including the extension of the file name, which is not required to be `.txt`. If the file does not exist, it will be created. If it does exist, results will be appended to the end of the file.

3.8 Process data

When a parameter check box in part 2 of the GUI has been ticked, the CALCULATE button in part 4 of the GUI becomes active.

To calculate the selected parameters, press the CALCULATE button. A 'progress' text box appears that indicates the current calculation being undertaken. When this text box disappears, all calculations have been completed.

3.9 Exit

Pressing the EXIT button in part 5 of the GUI terminates the program and closes the GUI. Alternatively, the user may click on 'File' in the main menu of the GUI and then click on 'Exit'.

If a parameter has been calculated, an 'Application Error' message appears. This message can be ignored. Click on OK to exit the software completely. If the application program was run by double-clicking on the executable file (section 3.1, (a)), the MS-DOS window closes. If it was run from within an MS-DOS window (section 3.1, (b)), the user may now access the MS-DOS command line again.

It may take several seconds for the 'Application Error' message to be displayed.

3.10 Help

Clicking on 'Help' in the main menu of the GUI and then clicking on 'About Areal SOFTGAUGES' causes a message box displaying information about the software to be displayed. Click on 'OK' to close this message box.

Clicking on 'Help' in the main menu of the GUI and then clicking on 'Help Documentation' causes the user manual (this document) to be opened (using the default program for viewing PDF files).

Clicking on 'Help' in the main menu of the GUI and then clicking on 'Licence Agreement' causes the licence agreement to be opened (using the default program for viewing PDF files).

3.11 Output file

Each time the CALCULATE button is pressed, the following information is written to the output file:

- Details (name, release number and date of release) of the software;
- The date and time at which the software was run;
- The path to the X3P file being processed;
- S–F surface parameter values (if any are calculated);
- S–L surface parameter values (if any are calculated).

Output of S–F parameter values is accompanied by any corresponding tolerance and autocorrelation values provided by the user. Output of S–L parameter values is accompanied by the value of the cut-off wavelength and any corresponding tolerance and autocorrelation values provided by the user. For each parameter, the time taken to undertake the calculation of that parameter is also written to the output file.

Since S_{sk} (appendix D.2) and S_{ku} (appendix D.3) depend on S_{q}, S_{q} is calculated even if it has not been selected by the user. The value of S_{q} (and the time taken to undertake the calculation) is written to the output file.

For those parameters that are calculated using an iterative procedure, additional information may be written to the output file as follows:

S_{a} If inequality (1) is not satisfied for any $K \leq 8$, S_{a} is set to the final calculated value $\widehat{S}_{\mathrm{a}}(8)$. A message informing the user that the tolerance has not been satisfied and the relative error

$$\left|\widehat{S}_{\mathrm{a}}(8) - \widehat{S}_{\mathrm{a}}(7)\right| / \widehat{S}_{\mathrm{a}}(7)$$

for the final value are written to the output file.

S_{p}, S_{v}, S_{z} For the calculation of S_{p} (and similarly for S_{v}), the optimisation algorithm is applied for each of a (potentially very large) number N of rectangular regions within the evaluation area (section 1.3). If the number N_0 of regions for which the optimisation algorithm has not terminated successfully is non-zero, both N_0 and N are written to the output file. For a large value of N_0 (relative to N), doubt may be placed on the value of S_{p} (S_{v}) and subsequently on the value of S_{z}.

S_{al}, S_{tr} For the calculation of S_{al} (and similarly for the denominator of S_{tr}, appendix D.9), the optimisation algorithm is applied over the evaluation area. A flag is returned whose value indicates the reason for termination of the optimisation algorithm as follows:

- A value of 1 indicates that the tolerance on both the objective function and equality constraint values was satisfied. In this case, the solution obtained in the final iteration is used.

- A value of 2 indicates that the tolerance on both the parameter estimate and equality constraint values was satisifed. In this case, the solution obtained in the final iteration is used.
- A value of zero indicates that a solution was not found within the permitted maximum number of iterations or function evaluations. In this case, the solution obtained in the final iteration is used.
- A value of -1 or -2 indicates that a solution was not found. In this case, the initial estimate of the solution is used.

$S_{\rm dr}$ If inequality (2) is not satisfied for any $K \leq 8$, $S_{\rm dr}$ is set to the final calculated value $\widehat{S}_{\rm dr}(8)$. A message informing the user that the tolerance has not been satisfied and the relative error

$$\left|\widehat{S}_{\rm dr}(8) - \widehat{S}_{\rm dr}(7)\right| / \widehat{S}_{\rm dr}(7)$$

for the final value are written to the output file.

3.12 Timings

Table 1 gives values (in seconds) that are indicative of the elapsed times for the calculation of S–F surface texture parameters using the software running on a desktop personal computer for data sets of sizes (a) 256×256, (b) 512×512, and (c) 1024×1024. The timings are intended to help users estimate how long the calculation of parameters may take for their own data sets.

The results suggest that for most parameters (all except $S_{\rm a}$, $S_{\rm al}$ and $S_{\rm tr}$), the time to calculate a parameter is proportional to the size of the data set. For those parameters, if the number of sampled points is doubled, say, in both the x– and y–directions, so that the total number of points increases by a factor of four, the calculation times increase (approximately) by a factor of four. Alternatively, halving the number of sampled points in both directions leads to the calculation times decreasing (approximately) by a factor of four. It would be expected that similar timings would be obtained when calculating these parameters for data sets of the same size but containing different data.

The calculations of $S_{\rm a}$, $S_{\rm dr}$, $S_{\rm al}$ and $S_{\rm tr}$ involve an iterative approach so that the calculation times for these parameters depend not only on the time taken for a single iteration but also on the number of iterations implemented, which is bounded. It is therefore more difficult to predict the calculation times for these parameters, even for data sets of the same size as considered here. Nevertheless, it is clear that the time to calculate $S_{\rm al}$ and $S_{\rm tr}$ dominates that for any other parameter. A discussion of the calculation times is available [7].

The calculation times associated with the operations of forming a bicubic spline interpolant to the data and areal Gaussian filtering (not given here) are short compared to those for calculating the surface texture parameters.

Parameter	Size of data set		
	256×256	512×512	1024×1024
S_{q}	0.9	3.7	14.6
S_{sk}	7.1	28.6	113.8
S_{ku}	45.8	198.1	716.7
S_{p}, S_{v}, S_{z}	12.8	52.4	205.0
S_{a}	30.5	64.8	531.0
S_{al}, S_{tr}	397.3	1 907.7	14 216.3
S_{dq}	1.8	7.1	28.6
S_{dr}	5.6	22.3	89.7

Table 1: Timings (in seconds) for the calculation of S–F surface texture parameters for data sets of sizes (a) 256×256, (b) 512×512, and (c) 1024×1024.

3.13 Example files

The example X3P file

```
cos_512_1um_512_2um_ls.x3p
```

is provided as part of the software distribution. Also included is the example output file

```
cos_512_1um_512_2um_ls.txt
```

which was generated by processing the example X3P file, calculating all S–F and S–L parameters using the default values for the cut-off wavelength, tolerances and autocorrelation function.

Having installed the software, users may run it on the example X3P file to check that installation has been successful. The values of the parameters should agree with those in the example output file. The timings obtained may vary because they are dependent on a number of factors, e.g., specification of the computer used, additional programs running concurrently, etc.

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A Gaussian areal filter

The Gaussian areal filter is defined by the weighting function

$$s_{x,y}(\xi,\eta) = \frac{1}{\alpha^2\lambda^2}\exp\left[-\pi\left(\frac{\xi}{\alpha\lambda}\right)^2 - \pi\left(\frac{\eta}{\alpha\lambda}\right)^2\right],$$

with $\alpha = \sqrt{\log 2/\pi}$, and λ denoting the cut-off wavelength in the x– and y–directions [12]. Given a continuous surface $z(x,y)$, the Gaussian filtered surface $w(x,y)$ is defined by the convolution integral

$$w(x,y) = \int\int z(\xi,\eta)s_{x,y}(x-\xi,y-\eta)\,\mathrm{d}\xi\mathrm{d}\eta.$$

Due to the separability of the weighting function

$$w(x,y) = \int\left[\int z(\xi,\eta)s(x-\xi)\,\mathrm{d}\xi\right]s(y-\eta)\,\mathrm{d}\eta,$$

where

$$s(\xi) = \frac{1}{\alpha\lambda}\exp\left[-\pi\left(\frac{\xi}{\alpha\lambda}\right)^2\right]$$

is the weighting function for a Gaussian profile filter with cut-off wavelength λ [13, 14]. It follows that Gaussian filtration for an areal surface can be undertaken by applying profile Gaussian filtration in the x–direction followed by profile Gaussian filtration in the y–direction (or *vice versa*).

In practice, knowledge of the surface $z(x,y)$ takes the form of surface heights z_{ij} at finitely-many points (x_{ij},y_{ij}) (section 1.3). Then, the calculation of w_{ij}, an approximation to $w(x_{ij},y_{ij})$, is implemented using the discrete convolution

$$w_{ij} = \sum_{\ell=j-n_y}^{j+n_y}\left[\sum_{k=i-n_x}^{i+n_x} z_{k\ell}s(x_{ij}-x_{k\ell})\right]s(y_{ij}-y_{k\ell})$$

for $i = 1+n_x,\ldots,m_x-n_x$, $j = 1+n_y,\ldots,m_y-n_y$, and integers $n_x = \lambda/\Delta_x$ and $n_y = \lambda/\Delta_y$. Finally, the S–L surface derived from the S–F surface by Gaussian areal filtration is defined by surface heights r_{ij} with

$$r_{ij} = z_{ij} - w_{ij}, \quad i = 1+n_x,\ldots,m_x-n_x, \quad j = 1+n_y,\ldots,m_y-n_y.$$

B Evaluation area for an S–L surface

Following application of a Gaussian areal filter, the S–L surface is defined by surface heights r_{ij}, $i = 1+n_x,\ldots,m_x-n_x$, $j = 1+n_y,\ldots,m_y-n_y$, corresponding to points (x_{ij},y_{ij}) in

a rectangle with sides of lengths $L_x - 2\lambda$ in the x–direction and $L_y - 2\lambda$ in the y–direction. In general, the lengths are not integer multiples of λ (section 1.3), and it is necessary to trim the data set (x_{ij}, y_{ij}, r_{ij}).

Consider first the x–direction. Let $H_x = p_x\lambda$, where p_x is chosen to be the largest integer for which $H_x \leq L_x - 2\lambda$. Since $\lambda = n_x\Delta x$ for integer n_x (appendix A), $H_x = p_x n_x \Delta x$. Consequently, the length $L_x - 2\lambda$ contains $m_x - 2n_x$ points and the length H_x contains $p_x n_x + 1$ points. Define

$$r_x = (m_x - 2n_x) - (p_x n_x + 1) = m_x - (2 + p_x)n_x - 1.$$

If r_x is even, then $r_x/2$ points x_{ij} are removed from the left- and right-hand ends of the sets $x_{ij},\ i = 1 + n_x, \ldots, m_x - n_x$. If r_x is odd, then int$(r_x/2)$ points are removed from the left-hand end, and int$(r_x/2) + 1$ points from the right-hand end, where int(q) denotes the integer part of q.

Similar considerations apply to the y–direction. After removing points in this way, the resulting set of heights r_{ij} defines the S–L surface for which areal surface texture parameters are calculated, and the corresponding set of points (x_{ij}, y_{ij}) defines the evaluation area for that S–L surface, which is a rectangle with sides of lengths H_x in the x–direction and H_y in the y–direction.

C Surface interpolation

The surface heights z_{ij} and r_{ij} defining, respectively, the S–F and S–L surfaces are used to construct continuous representations $z(x, y)$ and $r(x, y)$ of the unknown underlying surfaces. These continuous representations are then used as the basis for evaluating surface texture parameters that are defined in standards (e.g., [8]) in terms of such representations.

For this purpose, a bicubic spline interpolant to the surface height data is used, which is a generalisation of cubic spline interpolation applied to (tabulated) data describing a curve. The interpolant provides an 'empirical' continuous representation of the unknown underlying surface when the only knowledge of that surface comprises the values z_{ij} or r_{ij}. The choice of interpolant constitutes a compromise that can be applied generally: it is smoother than, for example, a bilinear interpolant, since it is continuous in value and first and second derivatives, but not as smooth as high order polynomial interpolants, which can introduce distortions. In the presence of additional information about the underlying surface, alternative forms for the interpolant may be expected to perform better. For example, a Fourier series may better represent a surface that is known to be periodic, and one that includes a step may be better represented by a function that is not smooth in the region of the step. However, it is assumed in this work that such additional information is not available.

The bicubic spline interpolant $z(x, y)$ is constructed to 'reproduce' (i.e., interpolate) the surface height z_{ij} at the point (x_{ij}, y_{ij}). It comprises a set of polynomial surfaces, each

defined on a rectangular region, that reduce to a cubic polynomial in x (for a fixed value of y) and a cubic polynomial in y (for a fixed value of x). At the boundaries of the regions the polynomial surfaces join in such a way that $z(x, y)$ is continuous in value, and first and second order derivatives at points on the boundaries.

D Definitions of areal surface texture parameters

In the following, $f(x, y) \equiv z(x, y)$ for an S–F surface or $f(x, y) \equiv r(x, y)$ for an S–L surface. For both S–F and S–L surfaces, the function $f(x, y)$ takes the form of a bicubic spline surface defined over a *definition area* [8, clause 3.1.9], i.e., the area used to specify the part of the surface for defining surface texture parameters, which is denoted by A. For an S–F surface, the definition area equals its evaluation area. For an S–L surface, it also generally equals its evaluation area. However, for certain height parameters (viz., S_{p}, S_{v} and S_{z}), the definition area is a square of side λ. Values for these parameters are determined as the arithmetic mean of values calculated over each definition area within the evaluation area. The definition area is expressed as the union of rectangular regions A_{ij} defined by the knots of $f(x, y)$. The function $f(x, y)$ reduces to a (smooth) bicubic *polynomial* surface defined on each rectangular region A_{ij}.

D.1 Root mean square height

The parameter S_{q} [8, clause 4.1.1] is defined by

$$S_{\mathrm{q}} = \sqrt{\frac{1}{A}\int_{(x,y)\in A} f^2(x, y)\,\mathrm{d}x\mathrm{d}y}.$$

D.2 Skewness

The parameter S_{sk} [8, clause 4.1.2] is defined by

$$S_{\mathrm{sk}} = \frac{1}{S_{\mathrm{q}}^3}\left[\frac{1}{A}\int_{(x,y)\in A} f^3(x, y)\,\mathrm{d}x\mathrm{d}y\right].$$

D.3 Kurtosis

The parameter S_{ku} [8, clause 4.1.3] is defined by

$$S_{\mathrm{ku}} = \frac{1}{S_{\mathrm{q}}^4}\left[\frac{1}{A}\int_{(x,y)\in A} f^4(x, y)\,\mathrm{d}x\mathrm{d}y\right].$$

D.4 Maximum peak height

The parameter S_{p} [8, clause 4.1.4] is defined as the largest peak height:

$$S_{\mathrm{p}} = \max_{(x,y)\in A} f(x,y).$$

D.5 Maximum pit height

The parameter S_{v} [8, clause 4.1.5] is defined as the largest absolute pit height:

$$S_{\mathrm{v}} = \left| \min_{(x,y)\in A} f(x,y) \right|.$$

D.6 Maximum height

The parameter S_{z} [8, clause 4.1.6] is defined as the sum of the maximum peak and maximum pit heights:

$$S_{\mathrm{z}} = S_{\mathrm{p}} + S_{\mathrm{v}}.$$

D.7 Arithmetical mean height

The parameter S_{a} [8, clause 4.1.7] is defined by

$$S_{\mathrm{a}} = \frac{1}{A} \int_{(x,y)\in A} |f(x,y)| \, \mathrm{d}x\mathrm{d}y.$$

D.8 Autocorrelation length

The parameter S_{al} [8, clause 4.2.1] is defined by

$$S_{\mathrm{al}} = \min_{(t_x,t_y)\in R} \sqrt{t_x^2 + t_y^2},$$

where

$$R = \{(t_x, t_y) : \mathrm{ACF}(t_x, t_y) \leq s\}$$

and $\mathrm{ACF}(t_x, t_y)$, the autocorrelation function, is defined by

$$\mathrm{ACF}(t_x, t_y) = \frac{\int_{(x,y)\in A} f(x,y) f(x - t_x, y - t_y) \, \mathrm{d}x\mathrm{d}y}{\int_{(x,y)\in A} f(x,y) f(x,y) \, \mathrm{d}x\mathrm{d}y} \tag{3}$$

in terms of 'lags' t_x in the x–direction and t_y in the y–direction. For an S–F surface, $-L_x \leq t_x \leq L_x$ and $-L_y \leq t_y \leq L_y$; for an S–L surface, $-H_x \leq t_x \leq H_x$ and $-H_y \leq t_y \leq H_y$. The value $0 < s < 1$ is set by the user; the default value is $s = 0.2$.

D.9 Texture aspect ratio

The parameter S_{tr} [8, clause 4.2.2] is defined by

$$S_{\mathrm{tr}} = \frac{\min_{(t_x,t_y)\in R}\sqrt{t_x^2+t_y^2}}{\max_{(t_x,t_y)\in Q}\sqrt{t_x^2+t_y^2}},$$

where

$$R = \{(t_x,t_y) : \mathrm{ACF}(t_x,t_y) \leq s\}$$

and

$$Q = \{(t_x,t_y) : \mathrm{ACF}(t_x,t_y) \geq s\}.$$

The function $\mathrm{ACF}(t_x,t_y)$ is defined by expression (3). The value $0 < s < 1$ is set by the user; the default value is $s = 0.2$.

D.10 Root mean square gradient

The parameter S_{dq} [8, clause 4.3.1] is defined by

$$S_{\mathrm{dq}} = \sqrt{\frac{1}{A}\int_{(x,y)\in A}\left(\frac{\partial f(x,y)}{\partial x}\right)^2 + \left(\frac{\partial f(x,y)}{\partial y}\right)^2 \mathrm{d}x\mathrm{d}y}.$$

D.11 Developed interfacial area ratio

The parameter S_{dr} [8, clause 4.3.2] is defined by

$$S_{\mathrm{dr}} = \frac{1}{A}\int_{(x,y)\in A}\sqrt{1+\left(\frac{\partial f(x,y)}{\partial x}\right)^2 + \left(\frac{\partial f(x,y)}{\partial y}\right)^2} - 1\ \mathrm{d}x\mathrm{d}y.$$