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How to characterize the regularity of surface topographies?

G GUILLEMOT¹, M BIGERELLE², J ANTONI² and K ANSELME³

¹Laboratoire de Mécanique de Lille, UMR CNRS 8107, Arts et Métiers ParisTech - Lille, 8, boulevard Louis XIV 59046 Lille Cedex, France.

E-mail: gildas.guillemot@ensam.eu

Abstract. In this paper, a new parameter is proposed to characterize the regularity of a surface topography. The regularity of the surface with scaling invariance both in amplitude and position allows us to quantify the organization of surfaces by a number lying between 0 and 100%. This parameter is used to quantify the influence of different processes on the topography of the surface and calibrated on noisy periodical surface topography.

1. Introduction

Current literature does not provide su any parameter to quantify the regularity of the surface with scaling invariance both in amplitude and position. Consequently, we created a new original scale invariant roughness parameter to quantify the organization of surfaces. This parameter is used to quantify the influence of different processes on the topography of the surface.

2. The regularity parameter

The main idea is to find a parameter without resorting to Fourier's analysis because spectrum parameters have little robustness and sin-cosine basis is not always appropriate to characterize surface roughness. This parameter must have a upper limit value (100%) if surfaces are periodic, a medium value if surfaces get a non neglected first order autocorrelation and lower limit null value for uncorrelated random surfaces (white noise). First, we define a normalized autocorrelation function such that:

$$R(x_i) = \frac{1}{Rq^2(N-i)} \sum_{j=1}^{N-i} y_j y_{j+i}$$
 (1)

where $(x_i,y_i)_{1 \le i \le N}$ are the N equidistant discretized points of the roughness profile and Rq is the standard deviation of the amplitude. The autocorrelation length, L, corresponds to the first point x_i (L = x_i), such that $R(x_i) \le \lambda$, where λ is a chosen threshold. A threshold value of 0.1 is usually chosen. Secondly, we define a correlation integral J such that:

² Laboratoire Roberval, UMR 6253, UTC/CNRS, UTC Centre de Recherches de Royallieu BP 20529, 60205 Compiègne, France.

³ Institut De Sciences Des Matériaux De Mulhouse, CNRS LRC 7228, 15, rue Jean Starcky, Université De Haute-Alsace, BP 2488, 68057 Mulhouse, France

¹ To whom any correspondence should be addressed.

$$J = \int_{x=0}^{x=L} R(x) dx \tag{2}$$

This integral represents a kind of fundamental for the autocorrelation function.

Thirdly, we define the series of integrals I_K :

$$I_{\kappa} = \int_{x=kL}^{x=(k+1)L} |R(x)| dx$$
These integrals represent the successive harmonics. Finally, the regularity parameter is defined as:

$$Regularity = \frac{100}{KJ} \sum_{k=1}^{K} I_k$$
 (4)

This parameter lies between 0 (white noise profiles) and 100 (perfect periodic profiles without noise). The main advantage of this parameter is to be mathematically independent of the amplitude parameter and of the autocorrelation length, L, of the surface. This parameter could be extended in two dimensions and used to measure the anisotropy of surfaces. We intensively used this parameter in profile analysis. Moreover it can be linked to the information of surfaces via Shannon's theory.

To test the relevance of this parameter to measure regularity, some simulated profiles have been defined. These profiles are noised with a stationary uncorrelated Gaussian noise (ie. white Gaussian noise) with a given standard deviation. Various shapes of periodical function have been retained: a sinusoidal function ('Sinus'), a triangular function ('Triangular'), a square function ('Square'), an shifted absolute sinusoidal function ('Abs Sinus'), and finally A white noise (see figure 1, left). Profiles have 10000 points and are normalized in the range [-1:1]. Then the effect of the added Gaussian noise is analyzed (see figure 1, right). 100 profiles are simulated for each calculation.

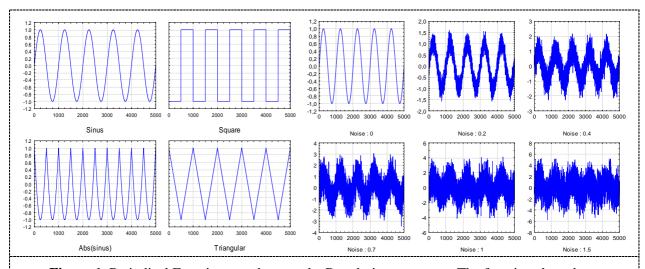


Figure 1. Periodical Functions used to test the Regularity parameter. The functions have been represented in the range [0...5000] (left) and Sinus Functions test with added white Gaussian noise at various amplitude levels. The 'Noise' value corresponds to the standard deviation of the added noise (right).

Figure 2 represents the Autocorrelation Function (AF) of the sinus function for different values of the noise (Fig. 1). The AF of the unnoised sinusoid is the sinusoid function itself. The amplitude of the AF for x>0 decreases by a constant factor when the amplitude of the added Gaussian noise increases. Nevertheless AF(x=0) is always equal to 1.

To compute the regularity parameters, the Autocorrelation Length (AL) must be defined. The definition of the autocorrelation length is still under debate. Its value is often affected to the fact that the value of the lag length at which the AF drop to 1/e of its value at zero lag and will be called the Inverse Lag Length λ (IAL). This value depends of the threshold value used to equal the autocorrelation function. This threshold value will further be called the Inverse Lag Length (IAL), λ . Sometimes, authors take the IAL as equalled to 0.1 or 0.4. The only justification to the value of 1/e (ie. 1/2.71828~0.4) is that AF follows an exponential form and then analytical computation will be simplified in a high number of scientific fields. The value of the regularity parameters depends on the autocorrelation length and it will be of major interest to compute the value of this parameter for various AL and corresponding IAL threshold values.

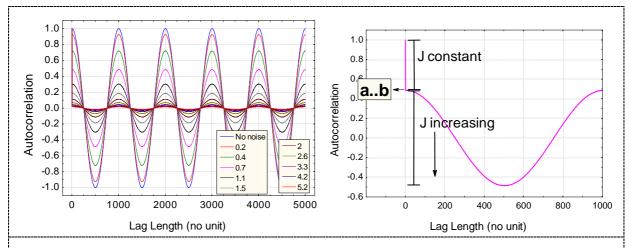


Figure 2. Autocorrelation function of sinus functions test with white noise at different amplitude level (left) and an zoom of Autocorrelation function of a noisy sinus function (right) with notations used in the text.

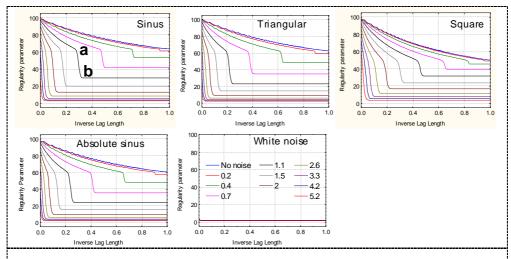


Figure 4. Value of the regularity parameters versus the inverse lag length for the six functions with different Gaussian noise amplitudes

Figure 3 represents the value of the regularity parameters versus the λ that determines the autocorrelation length allowing the computation of the regularity parameter for the six functions with various Gaussian noise amplitudes (Fig. 1). Let now analyze the various results:

Regularity functions always decrease or stay constant for a given noise when λ increases.

For all unnoised periodical functions, for $\lambda = 0$, the regularity is equals to 100%.

For noised periodical functions, it can be observed three stages, $\lambda \in [0,a], \lambda \in [a,b]$ and $\lambda \in [b,1]$:

Stage 1, $\lambda \in [0,a]$: A decrease until reaching $\lambda = a$. For $\lambda = 0$, the regularity decreases with an increase of noise amplitude until reaches the value of the noise regularity (regularity = 1.9 +/- 0.001). The regularity is maximal for $\lambda = 0$, because the integration of J and I_K is computed on the ½ period of the functions. For $\lambda > 0$, the regularity decreases with an increase of λ . This decrease is due to the fact that taking a value of $\lambda > 0$ will decrease the I_K value.

Stage 2, $\lambda \in [a,b]$: The a value depends on the noise amplitude and decreases when noise amplitude increases. The value of regularity (a) is a noise-amplitude independent for a given function and is equals to regularity (1) of the unnoised function. This fact can be explained as follow: while $\lambda > b$, the J integral is constant and measures the noise (figure 2, left). When $\lambda < a$, then J is integrated on the part of period of the autocorrelation function increasing then the regularity. The interval [a,b] is due to stochastic sampling by increasing the number of points in the profile, the difference a-b decreases.

Stage 3, $\lambda \in [b, I]$: Regularity function is constant because J is always constant and I_K . As I_K decreases when noise increases, regularity function decreases.

We have explained why regularity function depends on the choice of the Inverse Autocorrelation Length (IAF) value, λ . However, the choice of the value is still under debate. As consequence, the relevance of the choice must be shown. It is stated that the best choice of λ value will enable the best discrimination in change of the profile. In our case, the change of profile regularity is given by the noise amplitude and then we have to find the λ value which will give the best discrimination between the various noises. Consequently, an analysis of variance will be performed on the regularity parameter at each λ value for all classes of noise amplitudes. The Fisher statistics $F(\lambda)$ is then computed. The greater $F(\lambda)$ is, the better regularity parameters discriminate noise effect on the profiles. Figure 4, (left) represents the F values for the five periodical signals, versus the IAF λ . Some results are shown on these curves:

- The relevance depends on the IAF and consequently this value can not be randomly chosen.
- The relevance is very poor for the low IAF value (typically λ <0.1). This result is quite surprising because for IAF equals to zero, the integrations are computed on $\frac{1}{4}$ of the period and would decrease the variance of the estimator. In fact, the variance of the auto correlation length is maximal and increase the variance of the regularity parameter.
- Even if curves seem similar, regularity better discriminate the sinus, triangular and absolute sinus than square and triangular one. The both last periodical function presents the well known Gibbs phenomena (discontinuity) that increases the variance of the estimator of the regularity.
- When AIF is estimated near the unity, the regularity parameter well discriminates the noise influence.
- The curves possesses some local decrease of relevance: at some particular values of the AIF, due to the fact that for some particular noise, the autocorrelation length can be change from small value (noise) to a ¼ period (function) that increases variance of the regularity estimation.

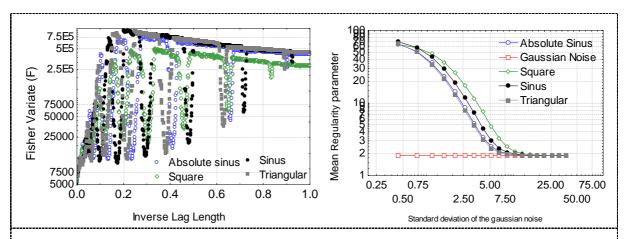


Figure 5. Value of Fisher variate (Anova analysis) versus the inverse lag length to test the relevance of the regularity parameter to discriminate the effect of noise on test functions (left). Autocorrelation function of sinus functions test with white noise at different amplitude level(right).

As a consequence, due to the difficulty to find accuracy the autocorrelation length, we propose to avoid the use of a single IAF and a correspondingly single autocorrelation length. We then propose to retain the average of the regularity parameter computed for all autocorrelation length (given at different level from 0 to 1 of the autocorrelation function). Then the new Mean Regularity roughness parameter \overline{O} is proposed:

$$\overline{O} = \int_{0}^{I} 100 \sum_{k=1}^{K} \int_{x=kL(y)}^{x=(k+I)L(y)} |R(x)| dx / \left(K \int_{x=0}^{x=L(y)} R(x) dx\right) dy$$
 (5)

with L(y) is defined such that y = R(L(y)) is the autocorrelation length taken at the value y of the autocorrelation function. Figure 4 (right) represents the evolution of the mean regularity parameter \overline{O} versus the intensity of the Gaussian noise. This parameter discriminates for all periodical functions the effect of the noise: higher is the noise intensity, lower is the regularity of profiles. To test the accuracy, the analysis of variance is computed to quantify how this new parameter discriminate the effect of the noise. Table 1 represents the F values for the five periodical functions. As it can be observed, Values of the F is quiet less than the maximal value corresponding to the most relevant correlation length but is better in mean than choosing randomly the Autocorrelation length. This step validates the relevancy of the mean regularity parameter applied on periodical function.

Table 1. Value of Fisher variate (Anova analysis) for the mean regularity parameter to test the relevance to discriminate the effect of noise on test functions. The max F and Mean F respectively represent the maximal values obtained from the figure 5.

	Absolute	Sinus	Triangular	Triangular	Square
	sinus			one	
\overline{o}	$6.54\ 10^5$	$6.78 ext{ } 10^5$	$6.64\ 10^5$	$4.73 \ 10^5$	$4.88\ 10^5$
Max F	7.58 10 ⁵	9.21 10 ⁵	9.11 10 ⁵	$3.44 \ 10^{5}$	4.99 10 ⁵
Mean F	$4.01\ 10^{5}$	4.39 10 ⁵	9.11 10⁵	$4.41 \ 10^{5}$	$2.63 \ 10^{5}$

This methodology was applied on various surface topographies and demonstrates that the most relevant roughness parameters are frequencies ones rather than amplitude ones to characterize cell adhesion. It is also proves that periodicity of the surface decrease cell adhesion [1].

3. Conclusion

By this new parameter used to characterize the morphological properties of a surface, it was shown that the effect of quality of the periodicity a profile can be determined by an unscale parameter. We works actually on weighting the autocorrelation function according to its variance to introduce a corrected Regularity parameter that will certainly diminish its standard error. Other aspects are still under discussions such analyzing the scale effect on fractal curves and the effect of autocorrelated noise on periodical signals.

4. References

[1] Anselme K, and Bigerelle M, 2005 Acta Biomaterialia 1(2) 211

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