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Evolution of the free volume between rough surfaces in contact

M. Paggi [a,b,*], Q.-C. He [a]

[a] *Université Paris Est, Laboratoire Modélisation et Simulation Multi Echelle, MSME UMR 8208 CNRS, 5 Bd Descartes, 77454 Marne-la-Vallée Cedex 2, France*
[b] *IMT Institute for Advanced Studies Lucca, Piazza San Francesco 19, 55100 Lucca, Italy*

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ABSTRACT

The free volume comprised between rough surfaces in contact governs the fluid/gas transport properties across networks of cracks and the leakage/percolation phenomena in seals. In this study, a fundamental insight into the evolution of the free volume depending on the mean plane separation, on the real contact area and on the applied pressure is gained in reference to fractal surfaces whose contact response is solved using the boundary element method. Particular attention is paid to the effect of the surface fractal dimension and of the surface resolution on the predicted results. The free volume domains corresponding to different threshold levels are found to display fractal spatial distributions whose bounds to their fractal dimensions are theoretically derived. A synthetic formula based on the probability distribution function of the free volumes is proposed to synthetically interpret the numerically observed trends.

1. Introduction

Contact mechanics between rough surfaces is a topic of paramount importance in engineering and physics, since surface phenomena in nature and technology strongly depend on the topological properties of interfaces. Real surfaces are never ideally flat and roughness is present at different scales, from the specimen size down to the interatomic distance. Hence, when two bodies are pressed against each other, contact takes place at the asperities (the 3D maxima of the surfaces) and the real contact area is a fraction of the nominal one.

In the context of rough surfaces, the scientific community has paid particular attention to the relation between the real contact area and the applied pressure [1–7], the contact stiffness [8–13] which is proportional to the electric and thermal contact conductances [14–17], frictional phenomena [18,19], adhesion [20,21], and hydrophobic properties of surfaces [22,23]. Recent studies on rough surfaces are also relative to elasto-plastic contact [24,25], adhesive contact [26], and lubrication [27].

Another important topic regards the transport properties of rough surfaces in contact. Below the full contact limit, a free volume between the contacting bodies is always present due to roughness. Such a free volume constitutes a fractal network whose properties are important for flow and transport of hydrothermal fluids, water, and contaminants in groundwater systems, but also of oil and gas in petroleum reservoirs [28]. For instance, the transport properties of proppant through fracture networks are relevant for hydraulic fracturing [29]. At a much smaller scale, welded surfaces in micro-electro-mechanical systems (MEMS) may present a free volume forming channels and capillaries of random distribution. Such channels are critical for gas leakage that may penetrate the soldered joint and affect the reliability of the system [30]. These problems are also relevant in materials for energy applications, such as in solid oxide fuel cells [31] and in photovoltaic modules where humidity can diffuse along the interface between the textured surface of solar cells and the encapsulating polymer, promoting a chemical degradation of electric contacts. The topological features of roughness in seal contacts are also very important for the onset of wear, see [32].

Attempts to predict the transport properties across these finite thickness interface regions composed of voids and contact areas are relatively recent and rely on the theory of fractal porous media [33,34]. Based on this modelling assumption, simplified theories are put forward where the free volumes are treated as pores of spherical shape with diameter obeying a power-law distribution. Pioneering analytical models have been proposed in [35–37] by examining the evolution of the contact area depending on the surface resolution. For a flat surface, the full contact regime takes place and no percolation channels are present. By refining the surface resolution, roughness comes into play and the real contact area becomes a fraction of the nominal one. For a given critical

* Corresponding author at: IMT Institute for Advanced Studies Lucca, Piazza San Francesco 19, 55100 Lucca, Italy. Tel.: +39 0583 4326 604; fax: +39 0583 4326 565.
E-mail addresses: marco.paggi@imtlucca.it (M. Paggi), qi-chang.he@univ-paris-est.fr (Q.-C. He).

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resolution, a first percolating channel will be originated. Further surface refinements will lead to other percolation channels that may contribute to the global leakage rate. Such contributions have been neglected in [35–37]. Due to such a simplifying assumption, predictions were found in good agreement with experimental results only in the low pressure regime.

A rigorous computational approach to predict the contact area and the transmissivity and diffusivity of the network of the created free channels was recently proposed in [38], where the problem was tackled from the numerical point of view by using the boundary element method (BEM). However, the analysis was restricted to two specific surface topologies created by lapping or sand blasting treatments and general trends were not discussed.

In the present study we propose an extensive numerical investigation of the evolution of the free volume between fractal rough surfaces in contact with an elastic half plane as a function of the main contact variables, i.e., the mean plane separation, the contact force and the real contact area. A computational approach based on BEM, analogous to that described in [38], is used. A deep analysis of the morphological properties of the free volume domains is performed, without making simplifying assumptions *a priori* on their shape and distribution, as in previous models based on the percolation theory. Moreover, all the channels are considered without any approximation apart from that arising from the spatial discretization intrinsic in the method. The obtained numerical trends and their interpretation are expected to provide useful hints for the development of further semi-analytical models taking into account the observed scaling laws, or to refine the existing ones.

The paper is structured as follows. In Section 2, the numerical method used to generate the rough surfaces is outlined and the fundamental equations of the boundary element method used to solve the contact problem are described. In Section 3, numerical results are presented and focus on the scaling of the free volume and on the multi-scale characterization of its network pattern. Further theoretical considerations on the statistical distribution of the free volumes are provided in Section 4, along with a synthetic formula for the computation of the free volume and for a deeper understanding of the observed numerical trends. Conclusions and outlook on the relevance of the proposed methodology for the study of wear in seal applications complete the study.

2. Numerical method

Rough surfaces with fractal properties are numerically generated according to the random midpoint displacement (RMD) algorithm [39]. This method allows generating rough surfaces with a power spectral density function of power-law type, characterized by a given fractal dimension D $(2 < D < 3)$. Applications of the method to contact mechanics can be found in [3,6,40]. Square surfaces with different resolutions can be generated by successively refining an initial mesh by a successive addition of a series of intermediate heights. In the algorithm, the number of successive refinements is defined by the parameter m, which is related to the number of heights per side of the squared generated grid, $2^m + 1$. Given L the lateral size of the surface, the grid spacing is $\delta = L/2^m$ and the resolution can be defined as $s = 1/\delta$. The method generates surfaces with higher m that are finer representations of the coarser ones, i.e., the height field of a surface with $m = i$, $i \in \mathbb{N}$, contains the height field of the coarser realizations with $m < i$.

A sketch showing how the RMD algorithm operates is provided in Fig. 1. Starting with $m = 1$, the elevation of the four corner nodes of the grid, nodes o, p, j, s in Fig. 1, are set equal to zero. Afterwards, the elevation of the central point of the grid, l, is determined by the average value of the elevations of the corner nodes, plus a random number extracted from a Gaussian distribution with zero mean and variance $\sigma_1^2 = \sigma_0^2/2^{(3-D)/2}$, where σ_0^2 is a free parameter set equal to $1/\sqrt{0.09}$. The elevations of the nodes i, k, q, r are then assigned by averaging over three elevations, those of the two corner nodes and that of the central node, plus a random number extracted from a Gaussian distribution with zero mean and reduced variance $\sigma_2^2 = \sigma_1^2/2^{(3-D)/2}$. This procedure is further iterated at the next refinement, $m = 2$. This version differs from the original RMD algorithm detailed in [39] by the fact that the elevations of the four initial corner nodes are set equal to zero rather than randomly assigned. The reason is to avoid to create topologies dominated by these initial values, which might constitute a bias especially at low resolution.

The most accurate solution of the contact problem between the generated rough surfaces and a smooth plane by keeping as minimum as possible the simplifying assumptions on the surface geometry can be achieved by using the boundary element method for contact mechanics [41]. By imposing a far-field closing displacement Δ to the bodies in contact, the displacement at each point of the contact area is related to the contact pressures as follows [42]:

$$u(\mathbf{x}) = \int_S H(\mathbf{x}, \mathbf{y}) p(\mathbf{y})\, \mathrm{d}S, \tag{1}$$

where $u(\mathbf{x})$ is the displacement at the surface point defined by the position vector $\mathbf{x}$, $H(\mathbf{x}, \mathbf{y})$ is the displacement at $\mathbf{x}$ due to a unit pressure acting at $\mathbf{y}$, and S is the apparent contact area. Assuming linear elastic isotropic materials, the influence coefficients are given by [41,42]

$$H(\mathbf{x}, \mathbf{y}) = \frac{1-\nu^2}{\pi E} \frac{1}{\|\mathbf{x}-\mathbf{y}\|}, \tag{2}$$

where E and ν denote, respectively, the composite Young's modulus and Poisson's ratio of the materials of the bodies in contact, respectively. Upon discretization of the surface as a grid where

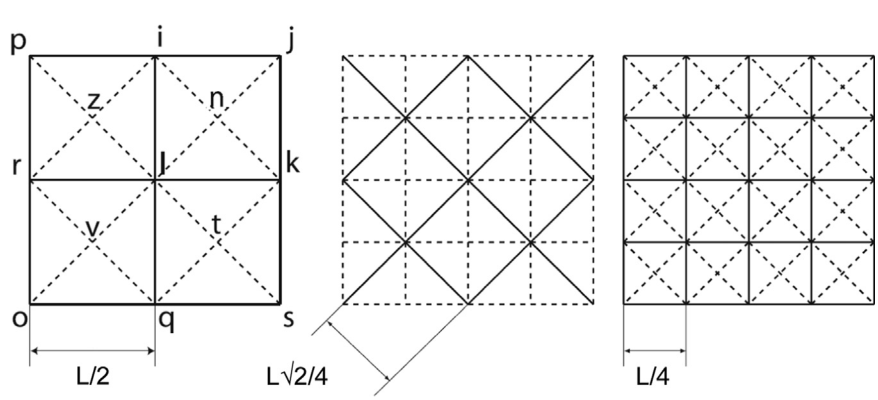

Fig. 1. Recursive steps for the generation of rough surfaces using the RMD algorithm.