MATH0488 Assignment — Rough surface adhesion

Maarten Arnst, Jérémy Xhardez, and Vinh Hoang Truong.

Organization

- Guidelines for the preparation of your report for this project:
  - The report should collect your solutions to all the questions that you worked on. Please include enough guiding discussion, as well as the main equations that you used.
  - This project is a group assignment. Please work in groups of either 2 or 3 people. Please send the first and last names of all the group members, as well as their email addresses, by email to M. Arnst (maarten.arnst@ulg.ac.be) before/on Monday March 24, 2014.
  - The report must be neat and well organized. You may write in either French or English. Indicate the last names of all the group members, the page number, and the total number of pages on each page of your report. Pay attention to spelling and grammar: use a spell checker! Pay attention to the clarity of your figures: all figures must be computer plots with adequate ranges, ticks, and scales; axes and ticks must be adequately labeled; and proper units must be included in labels and legends where appropriate.
  - If you should consult any references, you must list them at the end of your report.
  - The report must be sent in PDF format by email to M. Arnst before/on Wednesday May 7, 2014. Late reports will not be accepted unless the lateness can be appropriately justified or prior arrangements were made. Please attach to your email your Matlab code.
- Guidelines for the preparation of your presentation for this project:
  - The presentation (Tuesday 13/05) should collect only those solutions that you consider to be the most important ones. It should emphasize the understanding that you gained.
  - The presentation must be neat and well organized. You may present in either French or English. Pay attention to the clarity of your figures: for the sake of readability, axis and tick labels might have to be larger in your presentation than in your report.
  - Length of 10 slides, namely, 1 title slide that includes the group members names, 1 slide that provides a general overview, 4 slides that describe the model (data, from data to random-field model, from random-field model to random-collection-of-spheres model, traction-distance curve), 2 slides for the analysis of the results (interpretation of the p.s.d., scatter of results), 1 slide for the open question, and 1 slide with conclusions.
- If you should need some help:
  - Introductory lecture on Tuesday 18/03, B4 A204.
  - Discussion sessions on Tuesdays 25/03, 01/04, 22/04, 29/04, and 06/05, B4 A204.
  - You are welcome to contact by email J. Xhardez (jxhardez@ulg.ac.be), V. Hoang Truong (v.hoangtruong@ulg.ac.be), or M. Arnst to ask questions and ask for feedback.
  - You are welcome to ask J. Xhardez, V. Hoang Truong, or M. Arnst for an appointment.
- Please regularly check the errata list to correct potential errors in the slides/assignment.
- This project (report + presentation) will count for 65% of your grade.

1 Part 1: Implementation of model in Matlab

This first part of the project will guide you in implementing in Matlab a model of adhesion between a smooth and a rough silicon surface.

1.1 Data

We will not base our study on an experimentally measured real rough silicon surface. Instead, we will base our study on a numerically simulated surface that mimics a real rough silicon surface.

We consider a random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ indexed by $\mathbb{R}^2$, with values in $\mathbb{R}$, of the second order, mean-square stationary, Gaussian, zero-mean, and of power spectral density function

$$s_Z(\boldsymbol{\xi}) = \begin{cases} \dfrac{s_0}{(\xi_\mathrm{l}/\xi_0)^\alpha} & \text{if } \|\boldsymbol{\xi}\| \leq \xi_\mathrm{l}, \\ \dfrac{s_0}{(\|\boldsymbol{\xi}\|/\xi_0)^\alpha} & \text{if } \xi_\mathrm{l} \leq \|\boldsymbol{\xi}\| \leq \xi_\mathrm{h}, \\ 0 & \text{if } \|\boldsymbol{\xi}\| \geq \xi_\mathrm{h}; \end{cases}$$

here, the constant s_0, the exponent α, and the wavenumbers ξ_l, ξ_h, and ξ_0 are parameters to be chosen such that the random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ mimics roughness of real rough silicon surfaces.

To numerically simulate a realization of this random field, we apply a numerical method based on the spectral representation of this random field. Fully describing this numerical method is beyond the scope of this project; for details, please refer to [2]. Suffice it to say that for a fixed positive real scalar ξ_L and a fixed integer μ, to be chosen in a manner discussed later, this numerical method allows an approximation of a realization of this random field to be obtained as follows:

$$z^\mu(\boldsymbol{x}) = \sqrt{2\Delta\xi^2}\ \mathrm{Re}\Big(\sum_{\ell_1=1}^{\mu}\sum_{\ell_2=1}^{\mu}\sqrt{\frac{1}{(2\pi)^2}s_Z(\xi_{\ell_1},\xi_{\ell_2})}\ \zeta_{(\ell_1,\ell_2)}\ \exp\left(ix_1\xi_{\ell_1} + ix_2\xi_{\ell_2} + i\phi_{(\ell_1,\ell_2)}\right)\Big);$$

- the values $\{(\xi_{\ell_1},\xi_{\ell_2}),\ 1 \leq \ell_1,\ell_2 \leq \mu\}$ are a sampling of the wavenumber domain such that $(\xi_{\ell_1},\xi_{\ell_2}) = (-\xi_\mathrm{L} + (\ell_1 - 1/2)\Delta\xi, -\xi_\mathrm{L} + (\ell_2 - 1/2)\Delta\xi)$, $1 \leq \ell_1,\ell_2 \leq \mu$, with $\Delta\xi = 2\xi_\mathrm{L}/\mu$;
- the values $\{\phi_{(\ell_1,\ell_2)},\ 1 \leq \ell_1,\ell_2 \leq \mu\}$ are $\mu \times \mu$ independent realizations of a uniform random variable with values in $[0, 2\pi]$;
- the values $\{\zeta_{(\ell_1,\ell_2)},\ 1 \leq \ell_1,\ell_2 \leq \mu\}$ are such that $\zeta_{(\ell_1,\ell_2)} = \sqrt{-\log(\psi_{(\ell_1,\ell_2)})}$, $1 \leq \ell_1,\ell_2 \leq \mu$, where the values $\{\psi_{(\ell_1,\ell_2)},\ 1 \leq \ell_1,\ell_2 \leq \mu\}$ are $\mu \times \mu$ independent realizations of a uniform random variable with values in $[0, 1]$.

Here, Re is the function that associates to any complex number its real part, and the superscript μ in $z^\mu(\boldsymbol{x})$ is not an exponent but serves only to emphasize the dependence of $z^\mu(\boldsymbol{x})$ on μ.

We can observe that the previous equation is consistent with the interpretation of the power spectral density function as indicating the distribution of the variance of the random field over harmonic components of different wavenumbers. In fact, the previous equation provides an approximation of a realization of the random field as a linear combination of harmonic components of different wavenumbers, each with a random phase shift and a random amplitude proportional to the square root of the value taken by the power spectral density function at the corresponding wavenumber.

Upon introducing a corresponding sampling of the spatial domain, we obtain

$$z^\mu(x_{k_1},x_{k_2}) = \sqrt{2\Delta\xi^2}\ \mathrm{Re}\Big(\sum_{\ell_1=1}^{\mu}\sum_{\ell_2=1}^{\mu}\sqrt{\frac{1}{(2\pi)^2}s_Z(\xi_{\ell_1},\xi_{\ell_2})}\ \zeta_{(\ell_1,\ell_2)}\ \exp\left(ix_{k_1}\xi_{\ell_1} + ix_{k_2}\xi_{\ell_2} + i\phi_{(\ell_1,\ell_2)}\right)\Big);$$

- the values $\{(x_{k_1}, x_{k_2}),\ 1 \leq k_1, k_2 \leq \mu\}$ are a sampling of the spatial domain such that $(x_{k_1}, x_{k_2}) = (-\chi/2 + (k_1-1)\Delta x, -\chi/2 + (k_2-1)\Delta x)$, $1 \leq k_1, k_2 \leq \mu$, with $\Delta x = \chi/\mu$;
- this sampling of the spatial domain is made to correspond to the sampling of the wavenumber domain by setting $\Delta x = \pi/\xi_{\mathrm{L}}$ and therefore $\chi = \mu\pi/\xi_{\mathrm{L}}$;
- it follows from this correspondence that $\Delta x = 2\pi/(2\xi_{\mathrm{L}})$, that is, the step in the spatial domain is inversely proportional to the size of the sampled portion of the wavenumber domain, and $\chi = 2\pi/\Delta\xi$, that is, the size of the sampled portion of the spatial domain is inversely proportional to the step in the wavenumber domain.

Owing to the correspondence $\Delta x = \pi/\xi_{\mathrm{L}}$, the previous equation can be written equivalently as

$$z^\mu(x_{k_1}, x_{k_2}) = \sqrt{2\Delta\xi^2}\,\mathrm{Re}\bigg(\exp\Big(i\pi(\mu-1) + i(k_1-1)\pi(-1+1/\mu) + i(k_2-1)\pi(-1+1/\mu)\Big)\sum_{\ell_1=1}^{\mu}\sum_{\ell_2=1}^{\mu}\sqrt{\frac{1}{(2\pi)^2}s_Z(\xi_{\ell_1}, \xi_{\ell_2})}$$
$$\zeta_{(\ell_1,\ell_2)}\,\exp\Big(-i\pi(\ell_1-1) - i\pi(\ell_2-1) + i\phi_{(\ell_1,\ell_2)}\Big)\exp\Big(i(k_1-1)\frac{2\pi}{\mu}(\ell_1-1) + i(k_2-1)\frac{2\pi}{\mu}(\ell_2-1)\Big)\bigg),$$

thus enabling the computation of the summation by means of the discrete Fourier transform, hence, if μ is a power of two, by means of the fast Fourier transform algorithm (FFT/IFFT).

Let us now return to the choice of the values of ξ_{L} and μ which determine the sampling of the wavenumber domain. If the size χ of the sampled portion of the spatial domain is given, then, owing to the correspondence of the sampling of the spatial domain and that of the wavenumber domain, the step in the wavenumber domain must be $\Delta\xi = 2\pi/\chi$. To fully fix the sampling of the wavenumber domain, the value of μ should be chosen such that (i) μ is a power of two to enable the use of the fast Fourier transform and (ii) $\xi_{\mathrm{L}} = \mu\Delta\xi/2 \geq \xi_{\mathrm{h}}$ to ensure that the sampled portion of the wavenumber domain encompasses the support of the p.s.d. (Nyquist criterion).

This numerical simulation can be implemented in Matlab as follows:

```
function [zmu] = smltrf(s0,xil,xih,xi0,alpha,xiL,mu);

Dxi=2*xiL/mu;
xi=-xiL+([0:mu-1]+0.5)*Dxi;

s=zeros(length(xi),length(xi));
for m1=1:length(xi)
   for m2=1:length(xi)
     if norm([xi(m1);xi(m2)])<=xil
       s(m1,m2)=s0/(xil/xi0)^alpha;
     elseif norm([xi(m1);xi(m2)])<=xih
       s(m1,m2)=s0/(norm([xi(m1);xi(m2)])/xi0)^alpha;
     end
   end
end

zmu=sqrt(2*Dxi^2)*real(mu^2*(exp(i*pi*(mu-1))*exp(i*[0:mu-1]'*pi*(-1+1/mu))*...
   exp(i*[0:mu-1]*pi*(-1+1/mu))).*ifft2(sqrt(s/(2*pi)^2).*...
   (exp(i*[0:mu-1]'*(-pi))*exp(i*[0:mu-1]*(-pi))).*...
   sqrt(-log(rand(mu,mu))).*exp(i*2*pi*rand(mu,mu))));
```

In order for the random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ to mimic roughness of real rough silicon surfaces, let us set $s_0 = 7.0 \times 10^{-6}\,\mu\mathrm{m}^4$, $\alpha = 1.8$, $\xi_{\mathrm{l}} = 2.5\,\mu\mathrm{m}^{-1}$, $\xi_{\mathrm{h}} = 75\,\mu\mathrm{m}^{-1}$, and $\xi_0 = 1\,\mu\mathrm{m}^{-1}$. It can be shown that for these values of the constant s_0, the exponent α, and the wavenumbers ξ_{l}, ξ_{h}, and ξ_0, the key statistical descriptors of the local maxima of the random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ are in agreement with those of roughness of real rough silicon surfaces reported in [1, 3].

- **Question 1:** Please plot the power spectral density function s_Z as a function of the components ξ_1 and ξ_2 of $\boldsymbol{\xi}$.
- **Question 2:** Please plot the power spectral density function s_Z as a function of $\|\boldsymbol{\xi}\|$, first on a linear-linear scale and then on a log-log scale (Hint: Matlab function `loglog`).
- **Question 3:** Please simulate a realization of the random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ restricted to the subset $[-\chi/2, \chi/2] \times [-\chi/2, \chi/2]$ of space with $\chi = 40\,\mu\mathrm{m}$. Plot the surface height as a function of the components x_1 and x_2 of $\boldsymbol{x}$.

1.2 From data to random-field model

- **Question 4:** Please split the numerically simulated surface into $\nu = 8 \times 8$ subsurfaces of equal size and transform each subsurface into the wavenumber domain. For one of these subsurfaces, first plot the surface height as a function of the components x_1 and x_2 of $\boldsymbol{x}$ and then plot the amplitude of the transformed surface height as a function of the components ξ_1 and ξ_2 of $\boldsymbol{\xi}$.
- **Question 5:** Please deduce an estimate $s_Z^{\chi,\nu}$ of the power spectral density function s_Z from the $\nu = 8 \times 8$ subsurfaces of equal size which you transformed into the wavenumber domain. Plot $s_Z^{\chi,\nu}$ as a function of the components ξ_1 and ξ_2 of $\boldsymbol{\xi}$. Plot $s_Z^{\chi,\nu}$ as a function of the component ξ_1 while keeping the component ξ_2 fixed equal to 0. Compare these figures with those that you made under Questions 1 and 2 to verify your results.
- **Question 6:** Please deduce estimates $\mu_0^{\chi,\nu}$, $\mu_2^{\chi,\nu}$, and $\mu_4^{\chi,\nu}$ of the spectral moments μ_0, μ_2, and μ_4 from the estimate $s_Z^{\chi,\nu}$ of the power spectral density function s_Z.

1.3 From random-field model to random-collection-of-spheres model

- **Question 7:** Please deduce estimates $\overline{n}^{\chi,\nu}$, $(\sigma_H^{\chi,\nu})^2$, and $\overline{\rho}^{\chi,\nu}$ of the mean number of local maxima per unit area $\overline{n}$, the variance of the height of a local maximum σ_H^2, and the mean of the radius of curvature of a local maximum $\overline{\rho}$.

1.4 Traction-distance curve

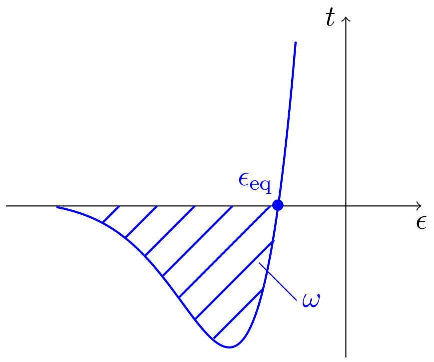

Figure 1: Definition of equilibrium distance ϵ_{eq} and adhesive energy density ω.

The adhesive-contact-of-spheres model requires the Young's modulus, the Poisson coefficient, and the surface energy of the considered material to be specified. For silicon, we use in this project values of $y = 130 \times 10^{-3}\,\mathrm{N\,\mu m^{-2}}$, $\nu = 0.23$, and $\gamma = 2.54 \times 10^{-6}\,\mathrm{N\,\mu m^{-1}}$, respectively.

- **Question 8:** Please implement the adhesive-contact-of-spheres model for the case of a sphere of radius $\overline{\rho}^{\chi,\nu}$. Plot first the relationship between the contact radius a and the contact force f and then the relationship between the contact force f and the contact displacement δ.
- **Question 9:** Putting everything together, please consider the contact between a smooth silicon surface and a rough silicon surface (with properties $\overline{n}^{\chi,\nu}$, $(\sigma_H^{\chi,\nu})^2$, and $\overline{\rho}^{\chi,\nu}$). Plot the relationship between the average contact force per unit area t and the distance ϵ between the smooth silicon surface and the reference plane in the rough silicon surface.
- **Question 10:** Following the definitions on Fig. 1, deduce from the traction-distance curve the equilibrium distance $\epsilon_{\mathrm{eq}}^{\chi,\nu}$ and adhesive energy density $\omega^{\chi,\nu}$. Interpret your results.

2 Part 2: Analysis of results

This second part involves the application of concepts from stochastic processes and statistics to analyze the results obtained using the present rough surface adhesion model.

- **Question 11:** This question concerns a study of the interpretation and impact of the constant s_0 and the exponent α that control the shape of the power spectral density function s_Z of the random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$. Please repeat your work under Part 1 first for a changed value of s_0 and then for a changed value of α. From among all your results, include in your report only those that highlight best the interpretation and the impact of s_0 and α and discuss.
- **Question 12:** Please repeat your work under Part 1 three times (for the values $\alpha = 1.8$ and $s_0 = 7.0 \times 10^{-6}\,\mathrm{\mu m^4}$ and without resetting Matlab's random number generator between these repetitions). Report the values that you obtain as estimates of the spectral moments, the equilibrium distance, and the adhesive energy density. Interpret your results.

3 Part 3: Open question

This third part of the project is an open question that invites you to use your Matlab code to study a question of your own choice, which you find interesting. Please do not hesitate to discuss with J. Xhardez, V. Hoang Truong, or M. Arnst for feedback on the question that you study.

References

[1] V. Hoang Truong. Capillary effect on stiction in MEMS. Master's thesis, Université de Liège, Belgium, 2013.

[2] F. Poirion and C. Soize. Numerical methods and mathematical aspects for simulation of homogeneous and non homogeneous Gaussian vector fields. In P. Krée and W. Wedig, editors, *Probabilistic Methods in Applied Physics*, volume 451 of *Lecture Notes in Physics*, pages 17–53. Springer, Berlin Heidelberg, Germany, 1995. doi: 10.1007/3-540-60214-3_50.

[3] L. Wu, L. Noels, V. Rochus, M. Pustan, and J.-C. Golinval. A micro-macroapproach to predict stiction due to surface contact in microelectromechanical systems. *Journal of Microelectromechanical Systems*, 20:976–991, 2011. doi: 10.1109/JMEMS.2011.2153823.