MATH0488 – Elements of stochastic processes

Rough surface adhesion

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Vinh Hoang Truong, and Jérémy Xhardez

March 18, 2014

Agenda

- We will be meeting in building B4 room A204 at the following dates:

1	2	3	4	5	6	D
18/03	25/03	01/04	22/04	29/04	06/05	13/05
introductory lecture	Q&A	Q&A	Q&A	Q&A	Q&A	defense
A+X+H	X+H	X+H	A+X+H	A+X+H	A+X+H	A+X+H

- Your presence is mandatory for the introductory lecture:
  - Tuesday March 18, 10h45–12h45.

- If you should need some help, please attend the Q&A sessions or contact M. Arnst, J. Xhardez, or V. Hoang Truong by email to ask a question by email or schedule an appointment.

- Please send the first and last names of all the group members (2 or 3 people), as well as their email addresses, by email to M. Arnst before/on Monday March 24, 2014.

- The project report must be sent in PDF format by email to M. Arnst before/on Wednesday May 7.

- Project presentations will be scheduled on Tuesday May 13 at a time and location to be set later.

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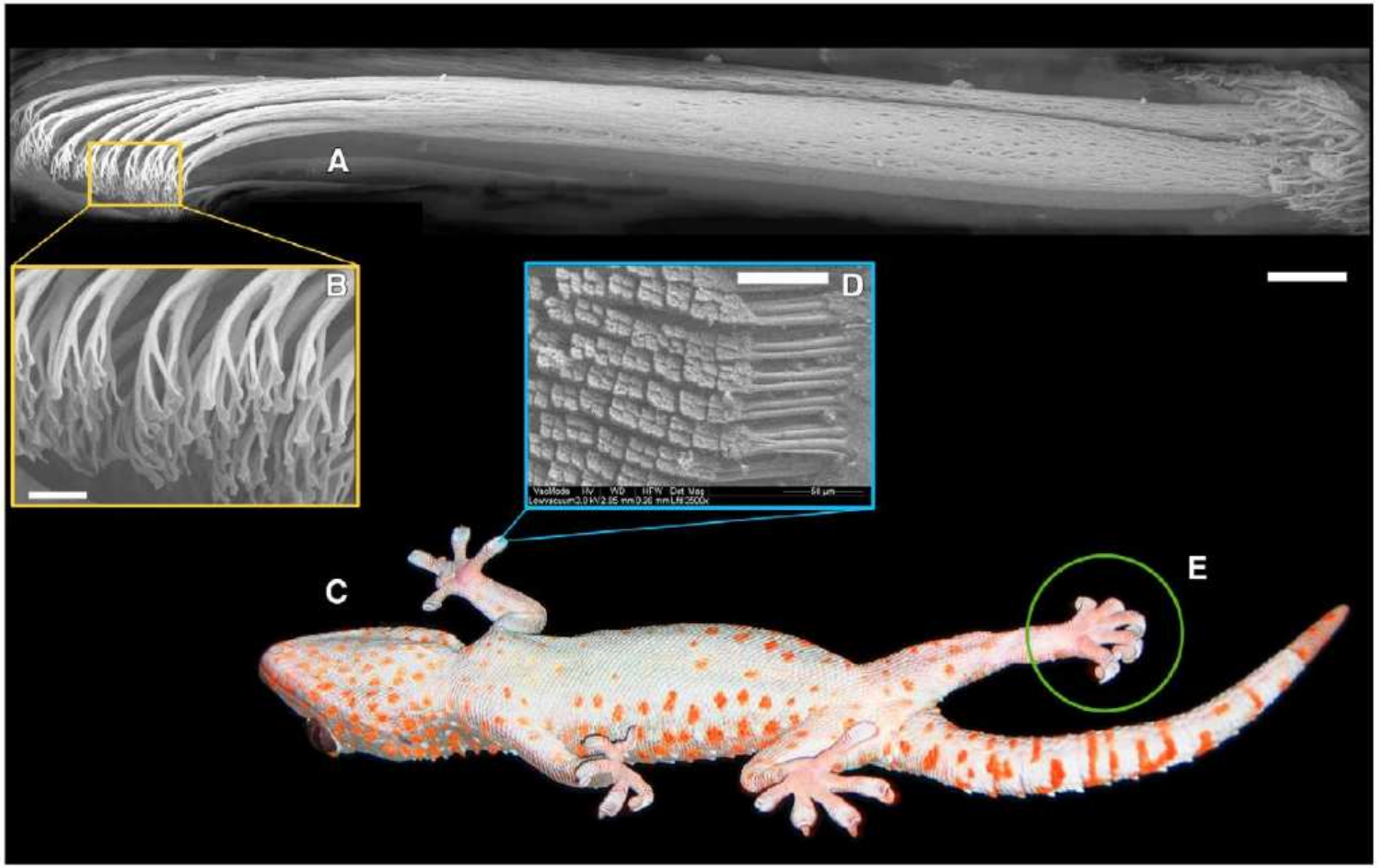
Motivation

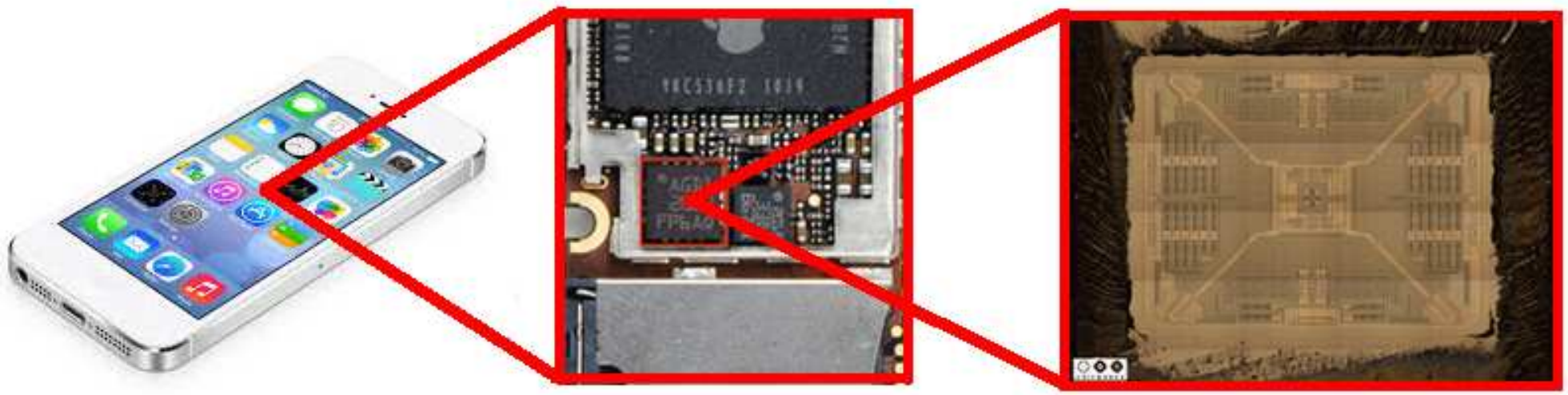
Gecko lizzards can climb stones, plants, and other steep natural surfaces.

Motivation



A complex hierarchical lamellae structure on their feet allows gecko lizzards
to exploit intermolecular adhesion forces at micrometer length scales to stick to natural surfaces.

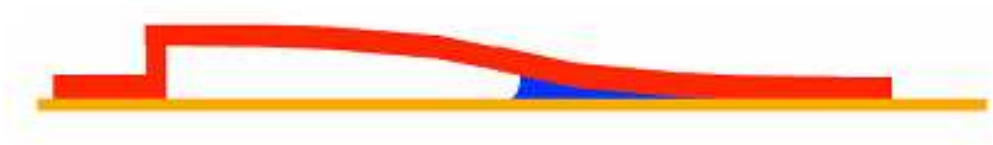
Motivation

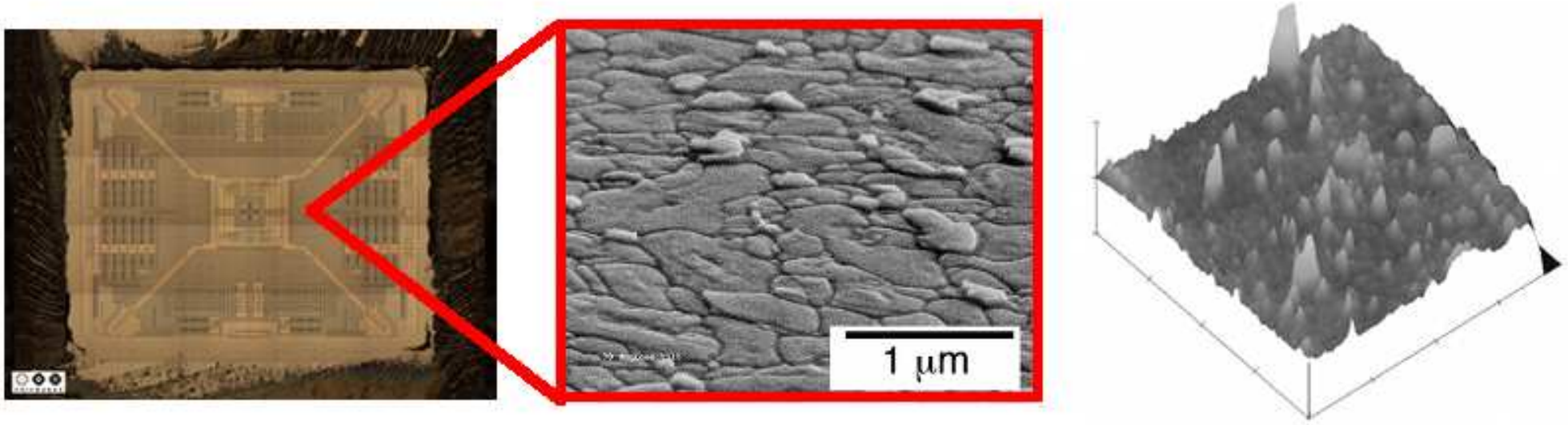


Smartphones have micrometer scale gyroscopes that allow them to sense rotation.

Shocks can bring freely moving parts close to the enclosure, where intermolecular adhesion forces can cause these freely moving parts to stick to this enclosure, thus leading to failure.

Motivation

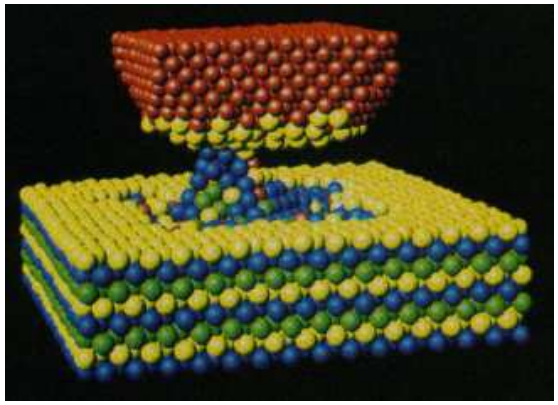




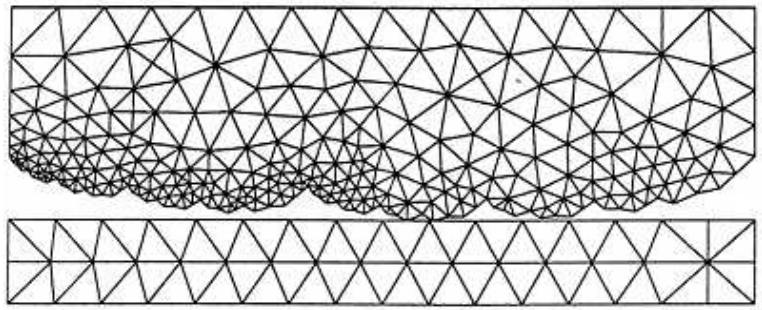
Silicon surfaces are rough at micrometer and nanometer length scales.

Roughness significantly affects adhesion between surfaces.

Motivation



Atomistic modeling.



Continuum modeling
using finite elements.

Analytical modeling.

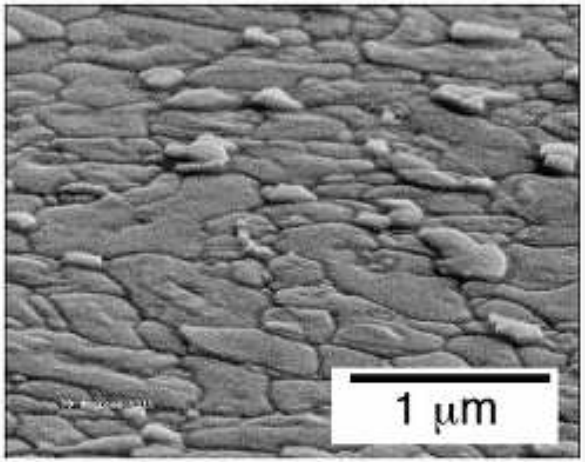
We will carry out an analytical study of rough surface adhesion,
whereby we will represent surface roughness using stochastic processes.

If two rough surfaces, or a rough surface and a smooth surface, are placed in contact, actual contact between the surfaces will occur only wherever “hills” of one surface touch the “hills” of the other surface.

These “hills,” also called “**asperities**,” are located around **local maxima**.
They play a key role in rough surface adhesion.

Methodology

Experimental data
Atomic Force Microscopy



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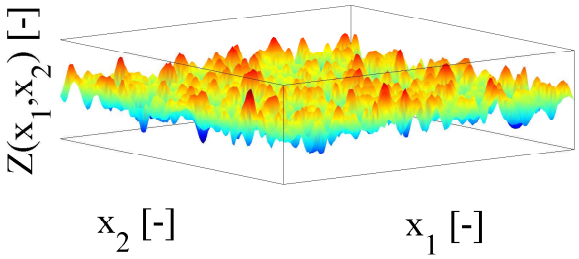
Random field model
of surface roughness



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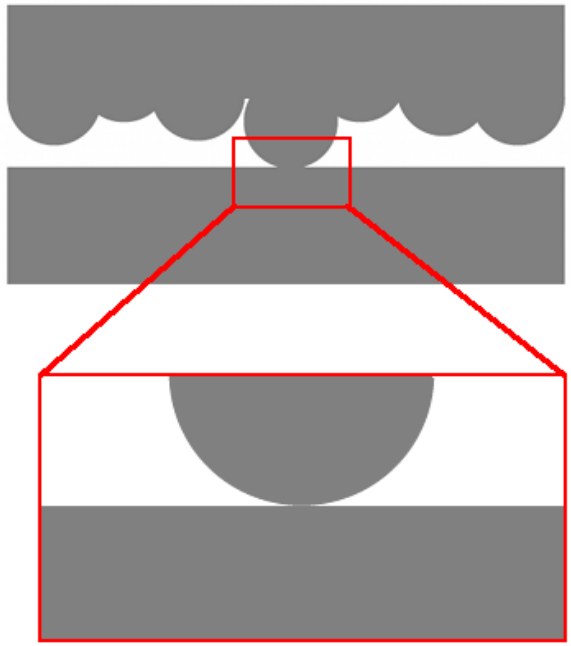
Equivalent model
as random collection of spheres



Adhesive contact
of spheres

To facilitate analytical calculations, we will replace the model of the rough surface as a random field with an **“equivalent” model of the rough surface as a random collection of spheres**.

Locally, the contact of each sphere will be treated by means of analytical models from elasticity theory.

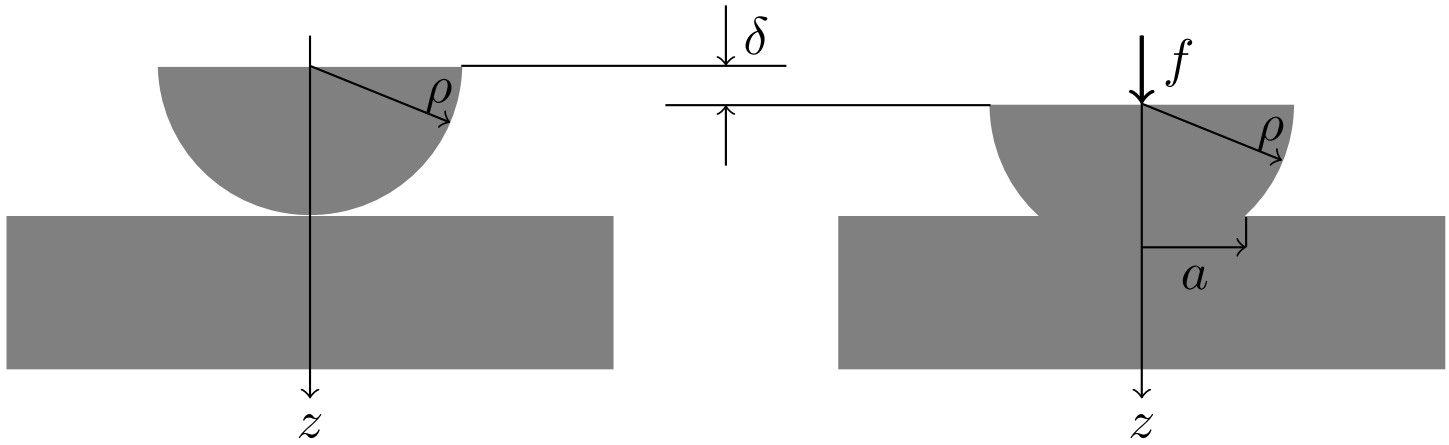
Plan

- Agenda.
- Contact.
- Motivation.
- Methodology.
- Plan.
- Adhesive contact of spheres.
- Random field model of surface roughness.
- Random collection of spheres.
- From data to random field.
- Conclusion.
- References.

Adhesive contact of spheres

Adhesive contact of spheres

- Deformation of elastic spherical punch pressing the surface of an elastic halfspace:



Linear elasticity equations (with Young modulus y_1 and Poisson coefficient ν_1) are imposed in the sphere. Contact develops over a contact zone bounded by a circle of radius a, where it is imposed that there be no penetration, adhesion (with surface energy γ), only pressure/ traction where contact, and no friction. Linear elasticity equations (y_2, ν_2) are imposed in the halfspace.

- An analytical solution exists for this problem: the vertical displacement δ of the center of the sphere is related to the contact force f as

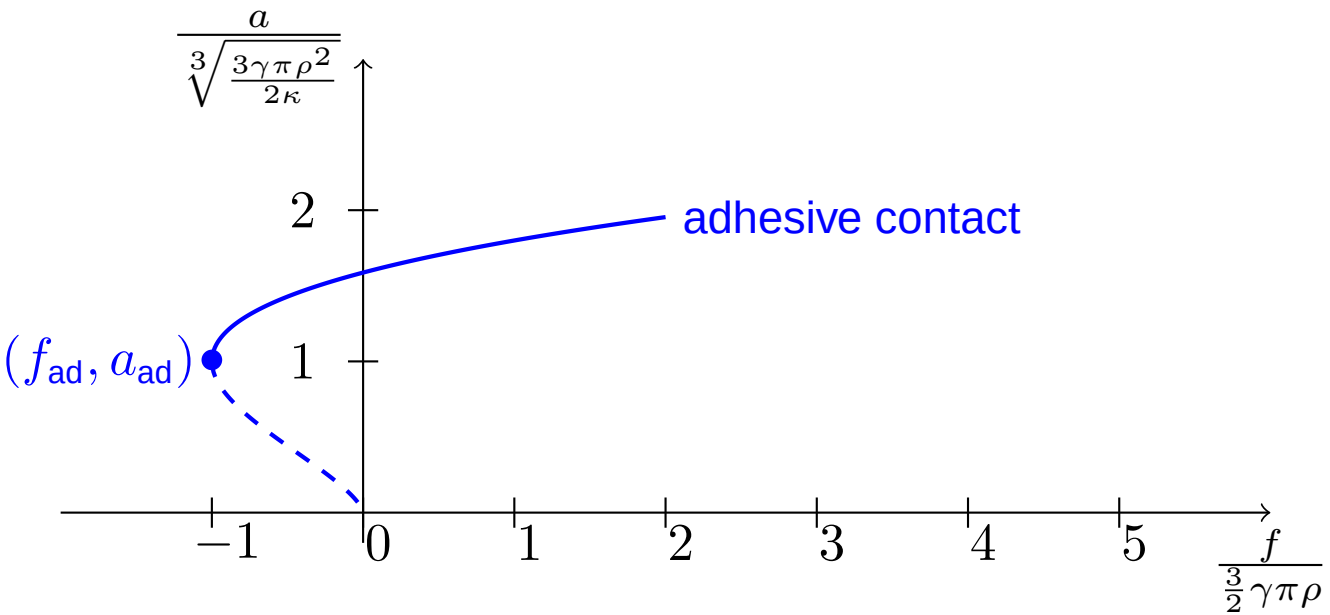
$$\delta = \frac{1}{3}\frac{a^2}{\rho} + \frac{2}{3}\frac{f}{\kappa a},$$

where $\frac{1}{\kappa} = \frac{3}{4}\left(\frac{1-\nu_1^2}{y_1} + \frac{1-\nu_2^2}{y_2}\right)$, and the radius a of the circle that bounds the contact zone satisfies

$$a^3 = \frac{\rho}{\kappa}\left(f + 3\gamma\pi\rho + \sqrt{6\gamma\pi\rho f + (3\gamma\pi\rho)^2}\right).$$

Adhesive contact of spheres

- Force-radius relationship:

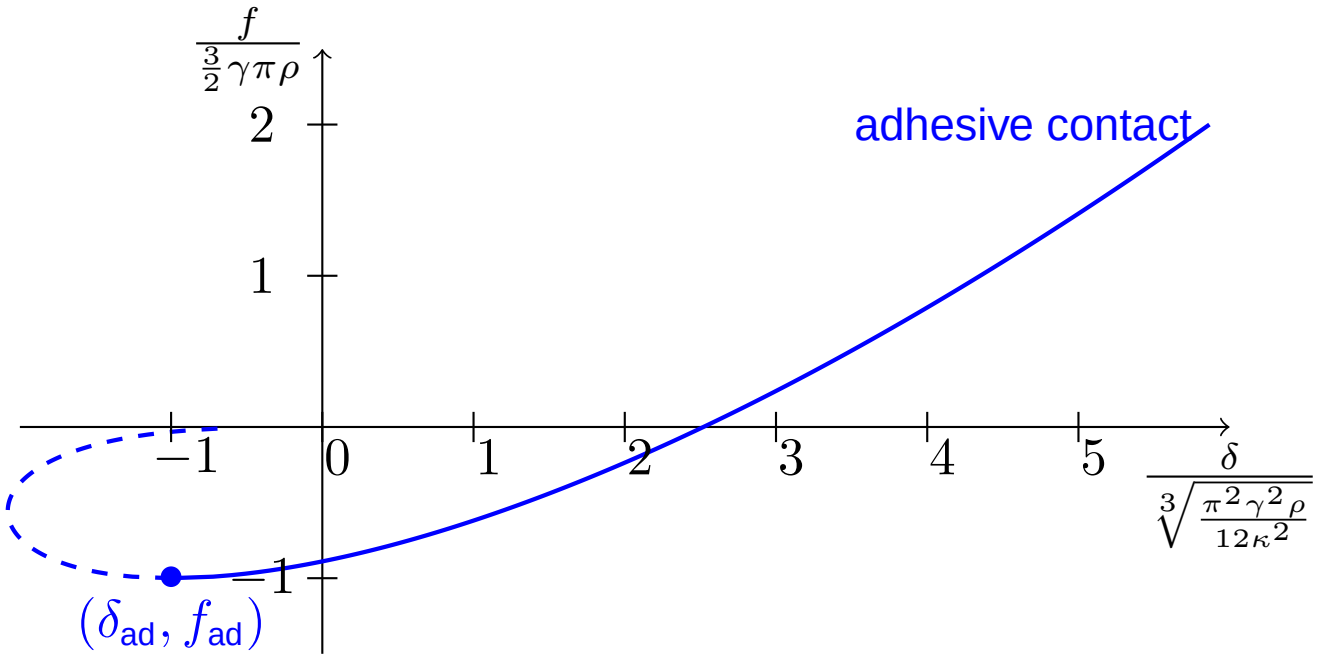


Here, the solid line corresponds to stable equilibrium configurations (determined by Eqns. on previous slide); conversely, the dashed line corresponds to unstable equilibrium configurations.

This adhesive-contact-of-spheres model indicates that in a force-controlled experiment, upon decreasing the contact force f, separation will occur when this contact force f is equal to the so-called adhesion force $f_{\text{ad}} = -\frac{3}{2}\gamma\pi\rho$. The radius at separation is equal to $a_{\text{ad}} = \sqrt[3]{\frac{3\gamma\pi\rho^2}{2\kappa}}$.

Adhesive contact of spheres

- Force-displacement relationship:



The displacement corresponding to the adhesion force $f_{\text{ad}} = -\frac{3}{2}\gamma\pi\rho$ is equal to $\delta_{\text{ad}} = -\sqrt[3]{\frac{\pi^2\gamma^2\rho}{12\kappa^2}}$.

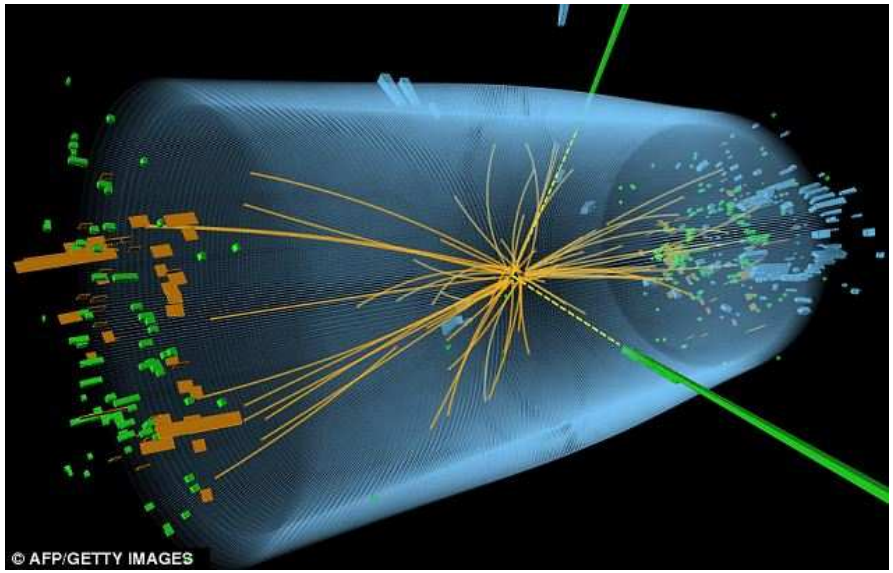
Adhesive contact of spheres

- Matlab code used to generate these figures:

```
f1=[-1:0.01:2];
a1=((f1+2)+2*sqrt(f1+1)).^(1/3);

f2=[-1:0.01:0];
a2=((f2+2)-2*sqrt(f2+1)).^(1/3);

figure;hold on;
plot(f1,a1,'b-');
plot(f2,a2,'b--');
set(gca,'XLim',[-2 6]);
set(gca,'YLim',[0 4]);

f1=[-1:0.01:2];
d1=((f1+2)+2*sqrt(f1+1)).^(2/3)+8^(1/3)*f1.*((f1+2)+2*sqrt(f1+1)).^(-1/3);

f2=[-1:0.01:0];
d2=((f2+2)-2*sqrt(f2+1)).^(2/3)+8^(1/3)*f2.*((f2+2)-2*sqrt(f2+1)).^(-1/3);

figure;hold on;
plot(-d1,f1,'b-');
plot(-d2,f2,'b--');
set(gca,'YLim',[-1.5 1.5]);
```

More details: The four forces of nature

- There are four distinct forces in nature:
  - strong nuclear force.
  - electromagnetic force.
  - weak nuclear force.
  - gravitation force.



More details: Intermolecular forces

- Intermolecular forces are attraction and repulsion forces acting between atoms or molecules.

- Intermolecular forces can be subdivided into the following types:
  - ionic (Coulomb attraction between ions of opposite charge).
  - covalent (sharing one or more pairs of electrons to form molecules).
  - metallic (due to electrons moving freely between positive ions).
  - hydrogen bond (linking molecules through a hydrogen atom belonging to one of them).
  - Van der Waals forces.

- These intermolecular forces are all electromagnetic.

More details: Van der Waals forces between molecules

- Three types of intermolecular force are collectively referred to as Van der Waals forces:
  - forces between permanent dipoles (Keesom orientation forces).
  - forces between permanent and induced dipoles (Debye induction).
  - attraction forces between nonpolar molecules (London dispersion).

- Intermolecular forces can be adequately modeled as conservative forces. Thus, one can always find an intermolecular potential, from which the intermolecular forces can be obtained by differentiation.

- The Lennard-Jones potential, the simplest example of such an intermolecular potential, models the potential energy $\phi(r)$ between two molecules as a function of the distance r between them as

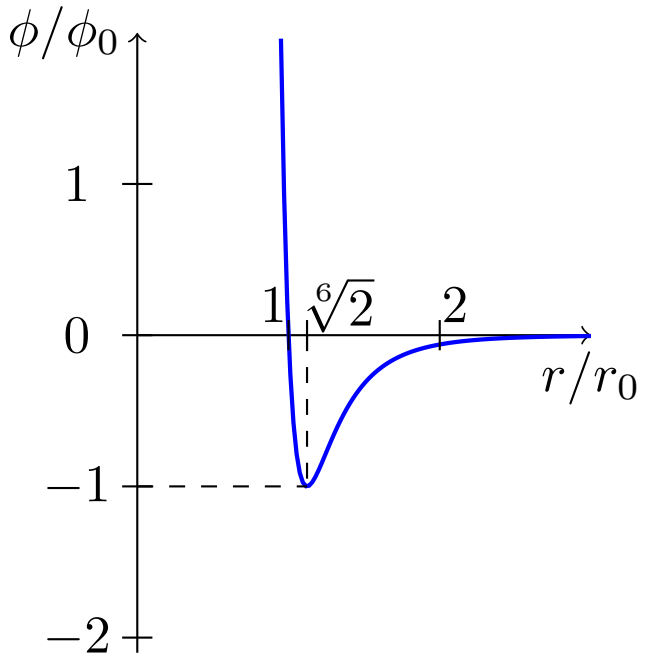
$$\phi(r) = 4\phi_0 \left(\left(\frac{r_0}{r} \right)^{12} - \left(\frac{r_0}{r} \right)^{6} \right);$$

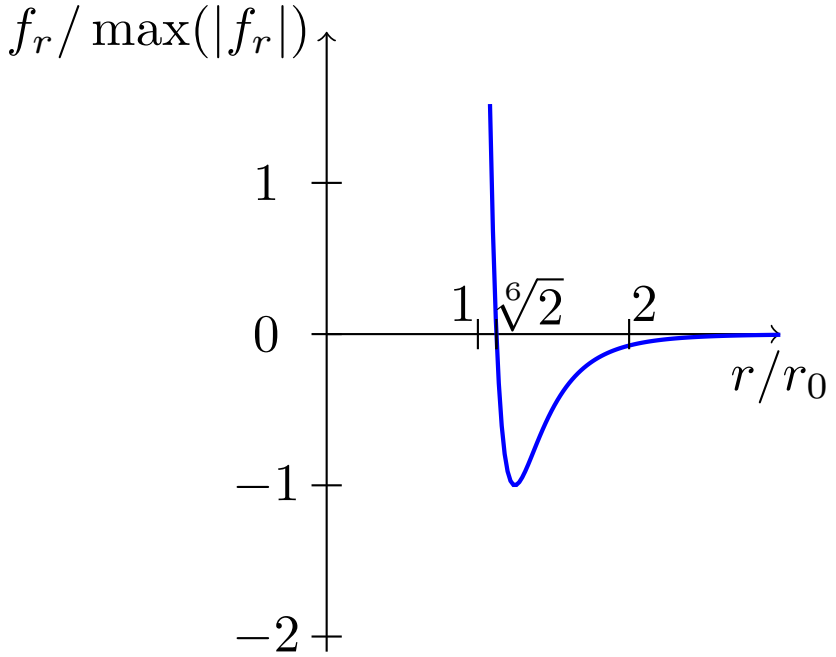
here, ϕ_0 and r_0 are parameters that can be fitted to experimental data.

- Alternative, but more complicated, expressions for intermolecular potentials have been proposed in the literature, which can often reproduce experimental data more accurately.

More details: Van der Waals forces between molecules

- The Lennard-Jones potential consists of a repulsive potential (repulsion when electronic clouds begin to overlap) and an attractive potential (Van der Waals forces). The repulsive potential varies with $1/r^{12}$, corresponding to a repulsive force that varies with $1/r^{13}$, and the attractive potential varies with $1/r^6$, corresponding to an attractive force that varies with $1/r^7$.





$$\phi(r) = 4\phi_0 \left(\left(\frac{r_0}{r} \right)^{12} - \left(\frac{r_0}{r} \right)^{6} \right).$$

$$f_r(r) = -\frac{d\phi}{dr}(r) = 4\phi_0 \left(12 \frac{r_0^{12}}{r^{13}} - 6 \frac{r_0^6}{r^7} \right).$$

- In fact, the more general relation $\boldsymbol{f} = -\boldsymbol{\nabla}\Phi$ simplifies here to $\boldsymbol{f} = f_r \boldsymbol{i}_r$ with $f_r(r) = -\frac{d\phi}{dr}(r)$ because of the spherical symmetry of the Lennard-Jones potential.

More details: Attractive Van der Waals forces between two molecules

- Taking into account only the attractive part of the aforementioned Lennard-Jones potential, we can model the attractive potential energy between two molecules separated by a distance r as

$$\phi(r) = -\frac{c}{r^6} \quad \text{with} \quad c = 4\phi_0 r_0^6,$$

  which corresponds to an attractive force given by

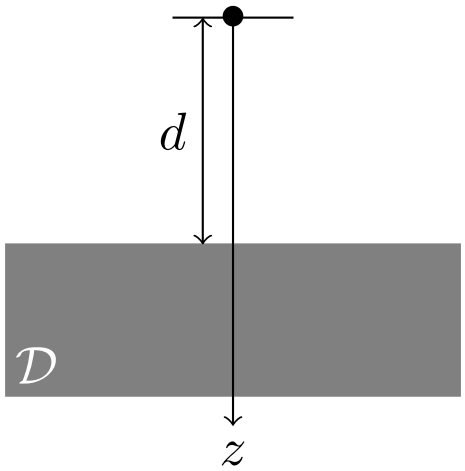
$$f_r(r) = -\frac{d\phi}{dr}(r) = -\frac{6c}{r^7};$$

  here, the coefficient c in the attractive potential is sometimes called the London constant.

- Assuming that Van der Waals forces are additive, we can use this formula to determine the resultant Van der Waals force between a molecule and a halfspace, between a sphere and a halfspace, and between two halfspaces, as shown next.

More details: Attractive Van der Waals forces between a molecule and a halfspace

- Consider a molecule at a distance d from a halfspace with n molecules per unit volume.



molecule

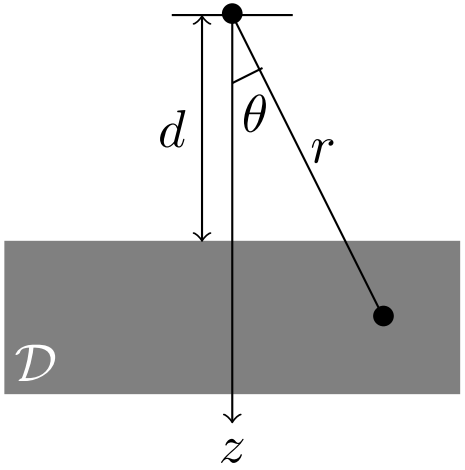
halfspace with n molecules per unit volume

- Then, by integration, the attractive force between the molecule and the halfspace is given by

$$f = \iint_{\mathcal{D}} -\boldsymbol{\nabla}\phi \cdot \boldsymbol{i}_z n dV = \frac{\pi n c}{2d^4},$$

as proved on the next slide.

Proof: Attractive Van der Waals forces between a molecule and a halfspace



molecule

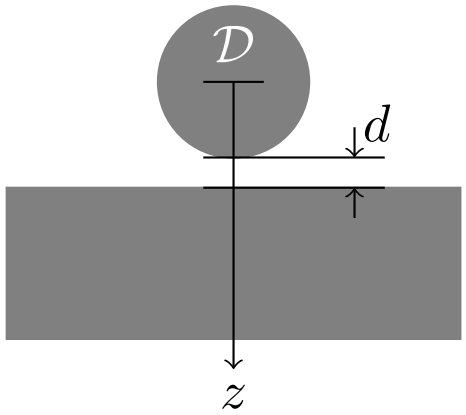
halfspace with n molecules per unit volume

- The vertical component of the attractive force between the molecule and a molecule located at a distance r in the plane of ordinate z is given by $6c\cos(\theta)/r^7$.
- By integration, followed by a change of variables to spherical coordinates with jacobian $r^2\sin(\theta)$ and with $r = z/\cos(\theta)$, the attractive force between the molecule and the half space is obtained as

$$\begin{aligned} f = \iint_{\mathcal{D}} -\boldsymbol{\nabla}\phi \cdot \boldsymbol{i}_z n dV &= \int_d^{+\infty} \int_0^{\pi/2} \frac{6c\cos(\theta)}{r^7} n 2\pi z^2 \frac{\sin(\theta)}{(\cos(\theta))^3} d\theta dz \\ &= 12\pi nc \int_d^{+\infty} \frac{dz}{z^5} \int_0^{\pi/2} (\cos(\theta))^5 \sin(\theta) d\theta \\ &= \frac{\pi nc}{2d^4}. \end{aligned}$$

More details: Attractive Van der Waals force between a sphere and a halfspace

- Consider a sphere of radius ρ at a distance d from a halfspace with n molecules per unit volume.



sphere with n molecules per unit volume

halfspace with n molecules per unit volume

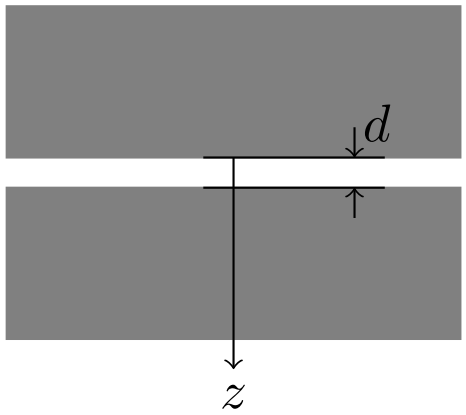
- Then, by integration, the attractive force between the sphere and the halfspace is given by

$$f = \iint_{\mathcal{D}} \frac{\pi n c}{2z^4} n dV = \int_{d-\rho}^{d+\rho} \frac{\pi n c}{2z^4} n\pi\big(\rho^2 - (d+\rho-z)^2\big)dz \overset{\rho \gg d}{\approx} \frac{h\rho}{6d^2};$$

here, the coefficient $h = \pi^2 n^2 c$ in the attractive force is sometimes called the Hamaker constant.

More details: Attractive Van der Waals force per unit area between two halfspaces

- Consider two halfspaces at a distance d from each other, both with n molecules per unit volume.



halfspace with n molecules per unit volume

halfspace with n molecules per unit volume

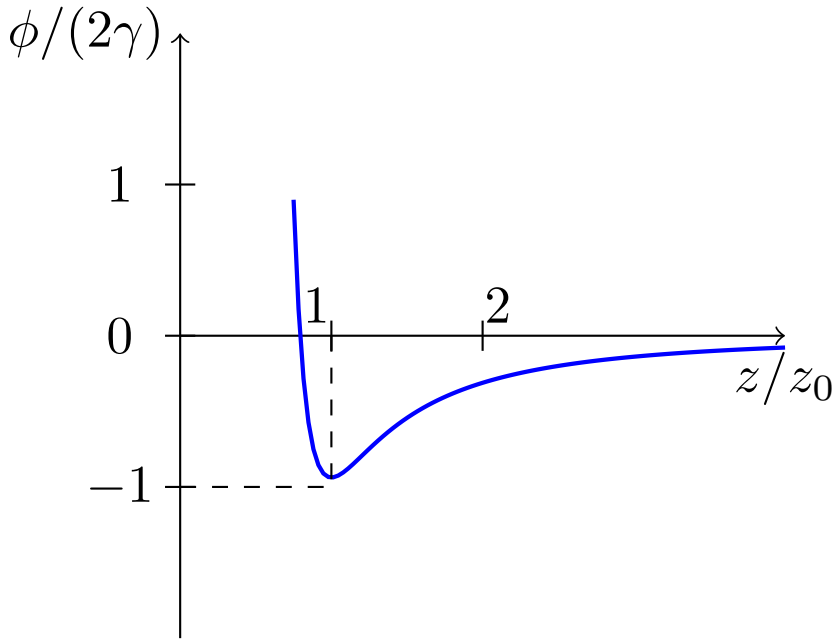
- Then, by integration, the attractive force per unit area between the halfspaces is given by

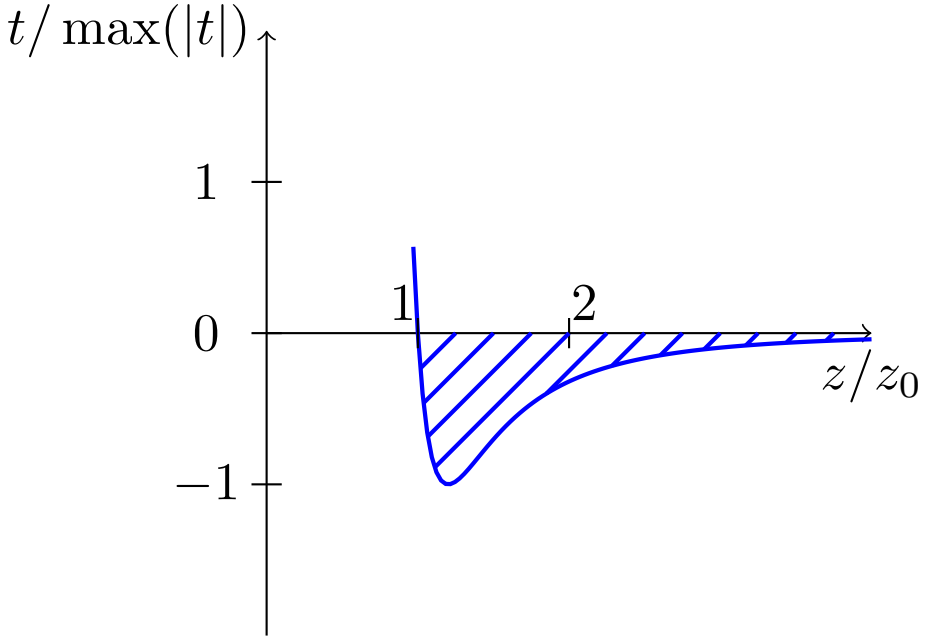
$$t = \int_d^{+\infty} \frac{\pi n c}{2z^4} n dz = \frac{h}{6\pi d^3};$$

here, the coefficient $h = \pi^2 n^2 c$ in the attractive force is still the Hamaker constant.

More details: Surface energy density

- The surface energy density γ of a solid determines the energy γdS needed to create (reversibly and isothermally) an elementary area dS of new surface.
- If we imagine cutting a solid along a plane and separating the two surfaces, work must be done to overcome the attractive forces which provide the cohesion of the solid. The work thus required to create a unit area of new surface is the surface energy density.





$$\phi(z) = \frac{4}{3} 2\gamma \left(\frac{1}{4} \left(\frac{z_0}{z} \right)^8 - \left(\frac{z_0}{z} \right)^2 \right).$$

$$t(z) = \frac{3\sqrt{3}}{2} \max(|t|) \left(\left(\frac{z_0}{z} \right)^9 - \left(\frac{z_0}{z} \right)^3 \right).$$

More details: Surface energy density

- After calculating the repulsive force per unit area between two hafspaces in a manner analogous to that for the attractive one, we find that the force per unit area between two Lennard-Jones halfspaces at a distance d from each other, both with n atoms per unit volume, is given by

$$t(z) = \frac{b}{z^9} - \frac{h}{6\pi z^3}.$$

- With z_0 the equilibrium distance such that $t(z_0) = 0$, we obtain $b = \frac{hz_0^6}{6\pi}$ and thus

$$t(z) = \frac{h}{6\pi z_0^3}\left(\left(\frac{z_0}{z}\right)^9 - \left(\frac{z_0}{z}\right)^3\right).$$

- The surface energy density is obtained as

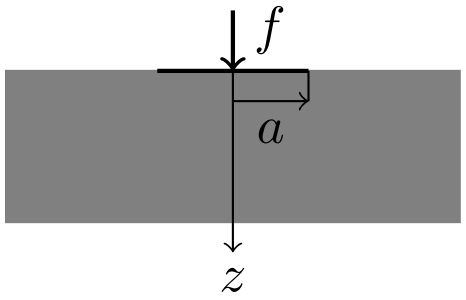
$$2\gamma = -\int_{z_0}^{+\infty} t(z)dz = -\int_{z_0}^{+\infty} -\frac{d\phi}{dz}dz = \phi(+\infty) - \phi(z_0) = -\phi(z_0),$$

where $\phi(z) = \frac{h}{12\pi z_0^2}\left(\frac{1}{4}\left(\frac{z_0}{z}\right)^8 - \left(\frac{z_0}{z}\right)^2\right)$ is the potential such that $t(z) = -\frac{d\phi}{dz}(z)$, and thus

$$2\gamma = -\frac{h}{12\pi z_0^2}\left(\frac{1}{4} - 1\right) = \frac{h}{16\pi z_0^2}.$$

More details: Boussinesq model

- Deformation of an elastic halfspace due to a rigid and circular flat punch pressing the surface:



Linear elasticity equations in halfspace:

$$
\begin{aligned}
&\mathbf{div}\boldsymbol{\sigma} = \mathbf{0}, && \text{in } \mathbb{R}^2 \times \mathbb{R}_0^+ \quad \text{(equilibrium eqn.)},\\
&\boldsymbol{\sigma} = \lambda \mathrm{tr}(\boldsymbol{\epsilon})\boldsymbol{I} + 2\mu\boldsymbol{\epsilon}, && \text{in } \mathbb{R}^2 \times \mathbb{R}_0^+ \quad \text{(constitutive eqn.)},\\
&\boldsymbol{\epsilon} = \frac{1}{2}\left(\mathbf{D}\boldsymbol{u} + \mathbf{D}\boldsymbol{u}^{\mathrm{T}}\right) && \text{in } \mathbb{R}^2 \times \mathbb{R}_0^+ \quad \text{(strain-displacement)},\\
&\boldsymbol{\sigma}(-\boldsymbol{i_z}) = (\boldsymbol{\sigma}(-\boldsymbol{i_z}) \cdot \boldsymbol{i}_z)\boldsymbol{i}_z, && \text{in } \{0 \le r \le a\} \times \{z = 0\}\\
&\boldsymbol{u} \cdot \boldsymbol{i}_z = \delta && \text{in } \{0 \le r \le a\} \times \{z = 0\} \quad \text{(b.c.)}.\\
&\boldsymbol{\sigma}(-\boldsymbol{i_z}) = \mathbf{0} && \text{on } \{r > a\} \times \{z = 0\}
\end{aligned}
$$

- Boussinesq deduced for this problem an analytical solution; he found that the vertical displacement δ of the rigid and circular flat punch is related to the contact force f as follows:

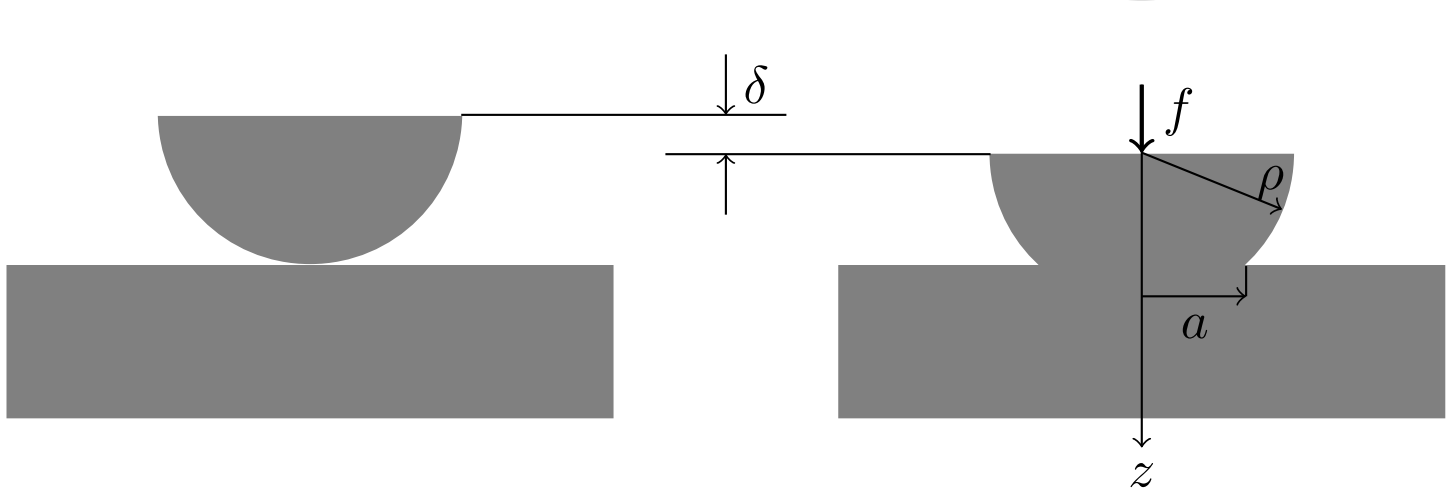
$$
\delta = \frac{1-\nu^2}{2y}\frac{f}{a}, \qquad \begin{cases} y\text{: Young's modulus,} \\ \nu\text{: Poisson coefficient,} \end{cases}
$$

and he found that the pressure exerted by the rigid and circular flat punch on the halfspace reads as

$$
\boldsymbol{\sigma}(\boldsymbol{i}_z) \cdot \boldsymbol{i}_z = \frac{f}{2\pi a^2}\frac{1}{\sqrt{1-r^2}} \quad \text{on } \{0 \le r \le a\} \times \{z = 0\}.
$$

More details: Hertz nonadhesive contact model

- Deformation of an elastic halfspace and an elastic spherical punch pressing the surface:



Linear elasticity eqns. (y_1, ν_1) in the sphere. Contact develops over a contact zone bounded by a circle of radius a, where it is imposed that there be no penetration, no adhesion, only pressure where contact, and no friction. Linear elasticity eqns. (y_2, ν_2) in the halfspace.

- Hertz deduced for this problem an analytical solution; he found that the vertical displacement δ of the center of the sphere is related to the contact force f as

$$\delta = \sqrt[3]{\frac{f^2}{\kappa^2 \rho}} \quad \text{(vertical displacement } \delta \text{ varies with } f^{2/3}\text{)},$$

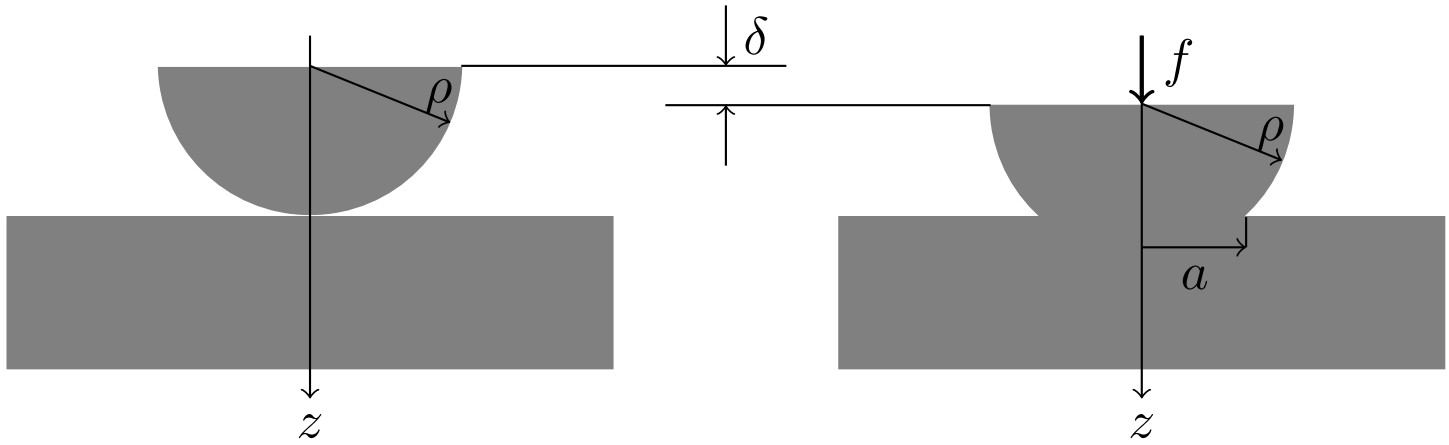
where $\frac{1}{\kappa} = \frac{3}{4}\left(\frac{1-\nu_1^2}{y_1} + \frac{1-\nu_2^2}{y_2}\right)$, and the radius a of the circle that bounds the contact zone satisfies

$$a^3 = \frac{\rho}{\kappa} f \quad \text{(radius } a \text{ varies with } f^{1/3}\text{)}.$$

Adhesive contact of spheres

More details: Johnson-Kendall-Roberts adhesive contact model

- Deformation of an elastic halfspace and an elastic spherical punch pressing the surface:



Linear elasticity eqns. (y_1, ν_1) in the sphere. Contact develops over a contact zone bounded by a circle of radius a, where it is imposed that there be no penetration, adhesion (γ), only pressure/ traction where contact, and no friction. Linear elasticity eqns. (y_2, ν_2) in the halfspace.

- Johnson, Kendall, and Roberts deduced for this problem an analytical solution; they found that the vertical displacement δ of the center of the sphere is related to the contact force f as

$$\delta = \frac{1}{3}\frac{a^2}{\rho} + \frac{2}{3}\frac{f}{\kappa a},$$

where $\frac{1}{\kappa} = \frac{3}{4}\left(\frac{1-\nu_1^2}{y_1} + \frac{1-\nu_2^2}{y_2}\right)$, and the radius a of the circle that bounds the contact zone satisfies

$$a^3 = \frac{\rho}{\kappa}\left(f + 3\gamma\pi\rho + \sqrt{6\gamma\pi\rho f + (3\gamma\pi\rho)^2}\right).$$

Proof: Johnson-Kendall-Roberts adhesive contact model

- The deformed configuration is determined by using the principle of minimum total energy: the deformed configuration is the one that minimizes the total energy

$$u_{\mathsf{T}} = u_{\mathsf{E}} + u_{\mathsf{M}} + u_{\mathsf{S}}, \quad \begin{cases} u_{\mathsf{E}}\text{: stored elastic energy,} \\ u_{\mathsf{M}}\text{: potential energy of the contact force,} \\ u_{\mathsf{S}}\text{: surface energy.} \end{cases}$$

- The stored elastic energy is obtained by considering the deformed configuration to be the superposition of a Hertz loading to a radius a corresponding to an contact force g such that $a^3 = \frac{\rho g}{\kappa}$ and a Boussinesq unloading at constant radius a from the contact force g to the contact force f:

$$\begin{aligned} u_{\mathsf{E}} &= \int_0^g \frac{h_z^{2/3}}{\kappa^{2/3}\rho^{1/3}} dh_z - \int_f^g \frac{2}{3}\frac{h_z}{\kappa a} dh_z \\ &= \frac{2}{5}\frac{g^{5/3}}{\kappa^{2/3}\rho^{1/3}} - \frac{1}{3\kappa a}(g^2 - f^2) \\ &= \frac{1}{\kappa^{2/3}\rho^{1/3}} \left(\frac{1}{15} g^{5/3} + \frac{1}{3} f^2 g^{-1/3} \right). \end{aligned}$$

Adhesive contact of spheres

Proof: Johnson-Kendall-Roberts adhesive contact model

- The potential energy of the contact force reads as

$$u_{\mathsf{M}} = -f\left(\frac{g^{2/3}}{\kappa^{2/3}\rho^{1/3}} - \frac{2}{3}\frac{g-f}{\kappa a}\right) = -\frac{f}{\kappa^{2/3}\rho^{1/3}}\left(\frac{1}{3}g^{2/3} + \frac{2}{3}fg^{-1/3}\right).$$

- The surface energy reads as

$$u_{\mathsf{S}} = -\gamma\pi a^2 = -\gamma\pi\left(\frac{\rho g}{\kappa}\right)^{2/3}.$$

- Stationarity of the total energy reads as $\frac{du_{\mathsf{T}}}{da} = 0$, which is equivalent to $\frac{du_{\mathsf{T}}}{dg} = 0$, that is,

$$\frac{du_{\mathsf{T}}}{dg} = \frac{g^{-4/3}}{9\kappa^{2/3}\rho^{2/3}}\left(g^2 - f^2 - 2fg + 2f^2 - 6\gamma\pi\rho g\right) = 0;$$

  therefore,

$$g = (f + 3\gamma\pi\rho) \pm \sqrt{(f+3\gamma\pi\rho)^2 - f^2}.$$

  By examining the second derivative of the total energy, it can be shown that the positive sign corresponds to a stable equilibrium (solid line on Slides 12 and 13) whereas the negative sign corresponds to an unstable equilibrium (dashed line on Slides 12 and 13). Inserting the expression for the stable equilibrium in $a^3 = \frac{\rho g}{\kappa}$, we obtain the asserted expressions.

More details: Conclusion

- On the basis of a simple model of the force exerted between two molecules, we obtained by integration the force exerted between a molecule and a halfspace, between a sphere and a halfspace, and between two halfspaces.

  This allowed us to understand the notion of surface energy density, which we defined as the work that must be done to overcome attractive forces to create a unit area of new surface.

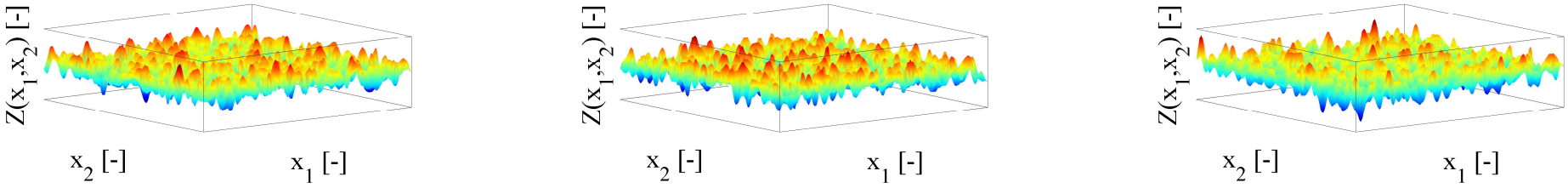
- We considered the contact between a sphere and a halfspace, first without adhesion (Hertz), then with adhesion (JKR). In the JKR case, adhesion is taken into account through the notion of surface energy density. For both the Hertz case and the JKR case, relationships were obtained which link the contact force to the displacement of the sphere center and to the radius of the contact zone.

- The force-radius relationship and the force-displacement relationship are important in designing devices that can fail due to adhesion, such as MicroElectroMechanical Systems (MEMS).

Random field model of surface roughness

Random field model of surface roughness

- We model the surface roughness as a Gaussian random field (=2D stochastic process).



- Specifically, we model the surface roughness as 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 (=wide-sense) stationary, Gaussian, zero-mean, and of autocorrelation function r_Z with corresponding power spectral density function s_Z.

- A Gaussian random field is fully defined once its mean function and either its autocorrelation function or the corresponding power spectral density function have been specified. Here, only the specification of either the autocorrelation function or the corresponding power spectral density function is required because the Gaussian random field has zero mean.

  Later, we will see how the power spectral density function can be estimated from experimental data.

Random field model of surface roughness

More details: Notations and conventions

- A lowercase letter, for example, x, is a real deterministic variable.
- A boldface lowercase letter, for example, $\boldsymbol{x} = [x_1, \ldots, x_d]^{\mathrm{T}}$, is a real deterministic column vector.
- An uppercase letter, for example, X, is a real random variable.
  Exceptions: E (mathematical expectation) and P (probability).
- A boldface uppercase letter, for example, $\boldsymbol{X} = [X_1, \ldots, X_d]^{\mathrm{T}}$, is a real random column vector.
- An uppercase letter between square brackets, for example, $[A]$, is a real deterministic matrix.
- A boldface uppercase letter between square brackets, for example, $[\boldsymbol{A}]$, is a real random matrix.

More details: Notations and conventions

- Let $f : \mathbb{R} \to \mathbb{R}$ be an **integrable function**, that is, $\int_{\mathbb{R}} |f(t)|dt < +\infty$. Then, the **Fourier transform** $\hat{f}$ of f is the bounded, continuous function $\hat{f}$ from $\mathbb{R}$ into $\mathbb{C}$ such that

$$\hat{f}(\omega) = \mathcal{F}f(\omega) = \int_{\mathbb{R}} \exp(-i\omega t) f(t) dt.$$

  The Fourier transform of an integrable function is not necessarily integrable itself.

- Let $f : \mathbb{R} \to \mathbb{R}$ be a **square-integrable function** , that is, $\int_{\mathbb{R}} |f(t)|^2 dt < +\infty$. Then, the **Fourier transform** $\hat{f}$ of f is the square-integrable function $\hat{f}$ from $\mathbb{R}$ into $\mathbb{C}$ such that

$$\begin{cases} \hat{f}(\omega) = \mathcal{F}f(\omega) = \displaystyle\int_{\mathbb{R}} \exp(-i\omega t) f(t) dt, \\ f(t) = \mathcal{F}^{-1}\hat{f}(t) = \dfrac{1}{2\pi} \displaystyle\int_{\mathbb{R}} \exp(i\omega t) \hat{f}(\omega) d\omega. \end{cases}$$

- These definitions indicate that one cannot take the Fourier transform of any function: these definitions provide the Fourier transform only for integrable and square-integrable functions.
- We include the minus sign in the forward transform and the factor $\frac{1}{2\pi}$ in the inverse transform.

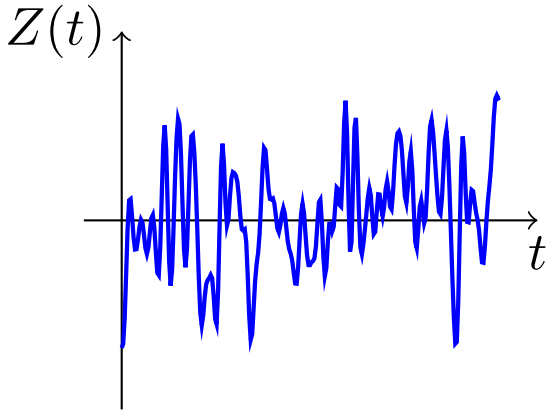
Random field model of surface roughness

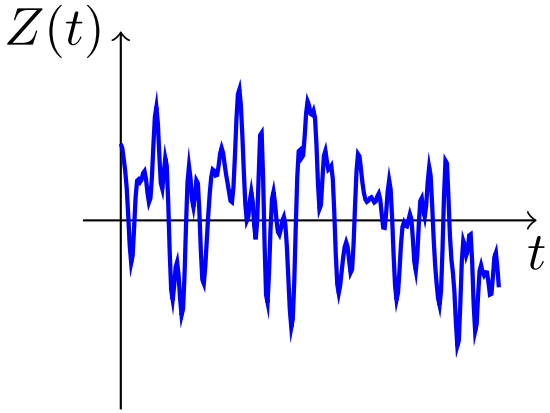
More details: Outlook

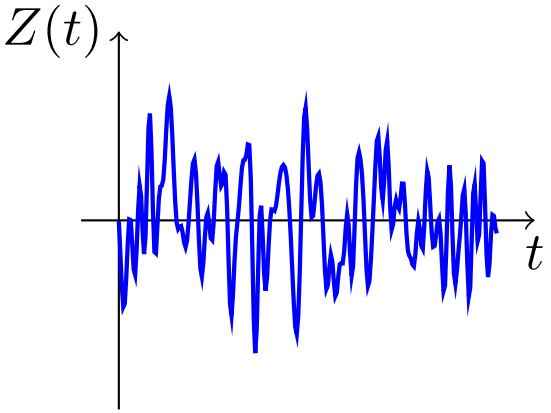
- **Random variables** (samples are scalars, vectors, matrices,. . .):



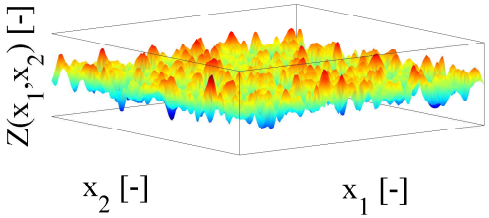
- **Stochastic processes** (samples are functions of one variable):

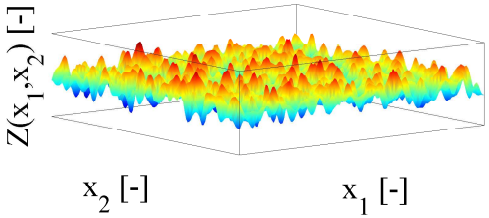


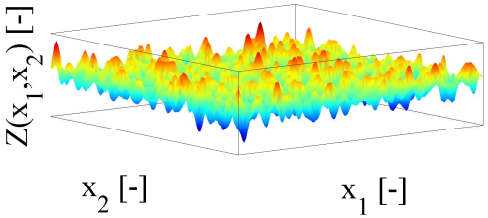




- **Random fields** (samples are functions of two or more variables):







More details: Random variables

- The **probability distribution** P_Z of a random variable Z with values in $\mathbb{R}$ is the function that associates to any meaningful subset $\mathcal{B}$ of $\mathbb{R}$ the probability that the value taken by Z is in $\mathcal{B}$, that is,

$$P_Z(\mathcal{B}) = P(Z \in \mathcal{B}).$$

- The **probability density function** ρ_Z of a probability distribution P_Z with respect to dz, if it exists, is the function from $\mathbb{R}$ into $\mathbb{R}^+$ such that for any meaningful subset $\mathcal{B}$ of $\mathbb{R}$, we have

$$P_Z(\mathcal{B}) = \int_{\mathcal{B}} \rho_Z(z) dz.$$

  The probability density function is normalized in that $P_Z(\mathbb{R}) = \int_{\mathbb{R}} \rho_Z(z) dz = 1$.

- A random variable Z with values in $\mathbb{R}$ is a **Gaussian** random variable with mean $\overline{z}$ and variance σ_Z^2 if it admits the probability density function

$$\rho_Z(z) = \frac{1}{\sqrt{2\pi}\sigma_Z} \exp\left(-\frac{(z-\overline{z})^2}{2\sigma_Z^2}\right).$$

More details: Random variables

- A random variable Z with values in $\mathbb{R}$ is of the **second order** if

$$E(Z^2) = \int_{\mathbb{R}} z^2 \rho_Z(z) dz < +\infty.$$

- The **mean** $\overline{z}$ of a second-order random variable Z with values in $\mathbb{R}$ is defined by

$$\overline{z} = E(Z) = \int_{\mathbb{R}} z \rho_Z(z) dz.$$

- The **variance** σ_Z^2 of a second-order random variable Z with values in $\mathbb{R}$ is defined by

$$\sigma_Z^2 = E\big((Z - \overline{z})^2\big) = \int_{\mathbb{R}} (z - \overline{z})^2 \rho_Z(z) dz.$$

- Please note that $\sigma_Z^2 = E\big((Z - \overline{z})^2\big) = E(Z^2) - \overline{z}^2$.

More details: Stochastic processes

- A **stochastic process** $\{Z(t),\ t \in \mathcal{T}\}$ indexed by a subset $\mathcal{T}$ of $\mathbb{R}$ and with values in $\mathbb{R}$ is a collection of random variables $Z(t)$ with values in $\mathbb{R}$ indexed by t in $\mathcal{T}$.

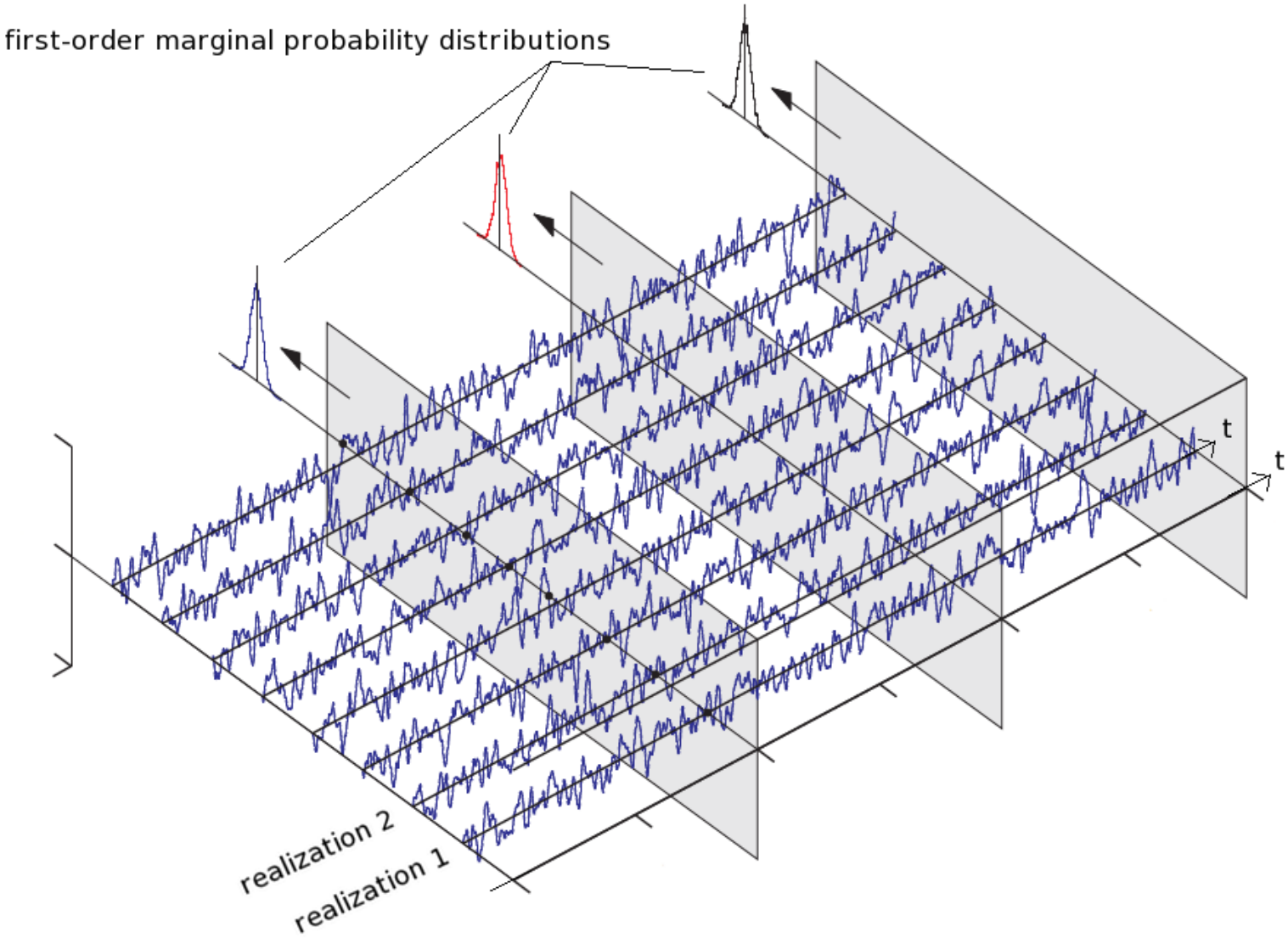
- For any nonempty finite subset $\{t_1, \ldots, t_m\}$ of $\mathcal{T}$, where m denotes the number of elements in this subset, the joint probability distribution $P_{(Z(t_1),\ldots,Z(t_m))}$ of $(Z(t_1), \ldots, Z(t_m))$ is called a **(m-th order) marginal probability distribution** of the stochastic process $\{Z(t),\ t \in \mathcal{T}\}$.

  The collection of all the marginal probability distributions of a stochastic process is called the **system of marginal probability distributions**.

- A stochastic process $\{Z(t),\ t \in \mathcal{T}\}$ indexed by $\mathcal{T}$ and with values in $\mathbb{R}$ is **Gaussian** if each probability distribution in its system of marginal probability distributions is Gaussian.

Random field model of surface roughness

More details: Stochastic processes



More details: Stochastic processes

- A stochastic process $\{Z(t),\ t \in \mathcal{T}\}$ indexed by $\mathcal{T}$ with values in $\mathbb{R}$ is of the **second order** if

$$E\big(Z(t)^2\big) = \int_{\mathbb{R}} z^2 \rho_{Z(t)}(z) dz < +\infty, \quad \forall t \in \mathcal{T}.$$

- The **mean function** of a second-order stochastic process $\{Z(t),\ t \in \mathcal{T}\}$ indexed by $\mathcal{T}$ with values in $\mathbb{R}$ is the function $\overline{z}$ from $\mathcal{T}$ into $\mathbb{R}$ such that

$$\overline{z}(t) = E\big(Z(t)\big) = \int_{\mathbb{R}} z \rho_{Z(t)}(z) dz.$$

- The **autocorrelation function** of a second-order stochastic process $\{Z(t),\ t \in \mathcal{T}\}$ indexed by $\mathcal{T}$ with values in $\mathbb{R}$ is the function r_Z from $\mathcal{T} \times \mathcal{T}$ into $\mathbb{R}$ such that

$$r_Z(t,\tilde{t}) = E\big(Z(t)Z(\tilde{t})\big) = \int_{\mathbb{R}\times\mathbb{R}} z\tilde{z} \rho_{(Z(t),Z(\tilde{t}))}(z,\tilde{z}) dz d\tilde{z}.$$

- The **covariance function** of a second-order stochastic process $\{Z(t),\ t \in \mathcal{T}\}$ indexed by $\mathcal{T}$ with values in $\mathbb{R}$ is the function c_Z from $\mathcal{T} \times \mathcal{T}$ into $\mathbb{R}$ such that

$$c_Z(t,\tilde{t}) = E\Big(\big(Z(t)-\overline{z}(t)\big)\big(Z(\tilde{t})-\overline{z}(\tilde{t})\big)\Big) = \int_{\mathbb{R}\times\mathbb{R}} \big(z-\overline{z}(t)\big)\big(\tilde{z}-\overline{z}(\tilde{t})\big) \rho_{(Z(t),Z(\tilde{t}))}(z,\tilde{z}) dz d\tilde{z}.$$

- Please note that $c_Z(t,\tilde{t}) = E\Big(\big(Z(t) - \overline{z}(t)\big)\big(Z(\tilde{t}) - \overline{z}(\tilde{t})\big)\Big) = r_Z(t,\tilde{t}) - \overline{z}(t)\overline{z}(\tilde{t})$.

More details: Stochastic processes

- A second-order stochastic process $\{Z(t),\ t \in \mathbb{R}\}$ indexed by $\mathbb{R}$ with values in $\mathbb{R}$ is **mean-square stationary** if $\overline{z}(t) = \overline{z}$ is independent of t and $r_Z(t, \tilde{t}) = r_Z(t - \tilde{t})$ depends on only $t - \tilde{t}$.

- The **power spectral density function** of a zero-mean, mean-square stationary, second-order stochastic process $\{Z(t),\ t \in \mathbb{R}\}$ indexed by $\mathbb{R}$ with values in $\mathbb{R}$, if it exists, is the function s_Z from $\mathbb{R}$ into $\mathbb{R}^+$ such that

$$r_Z(t - \tilde{t}) = \frac{1}{2\pi} \int_{\mathbb{R}} s_Z(\omega) \exp\big(i\omega(t - \tilde{t})\big) d\omega.$$

  The power spectral density function s_Z has the following properties:

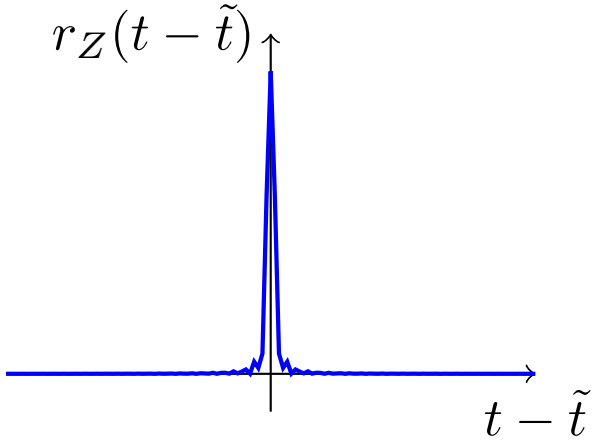
  - it is even because of the evenness of r_Z,
  - it is positive owing to Bochner's theorem,
  - it is integrable because $E\big(Z(t)^2\big) = r_Z(0) = \frac{1}{2\pi} \int_{\mathbb{R}} s_Z(\omega) d\omega < +\infty$.

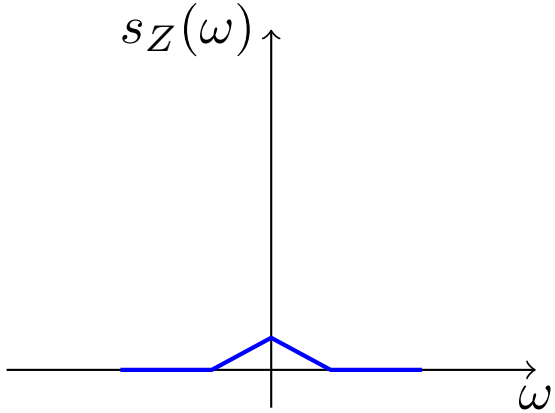
- If α is an integer, the **spectral moment of order α**, denoted by m_α, if it exists, is the integral

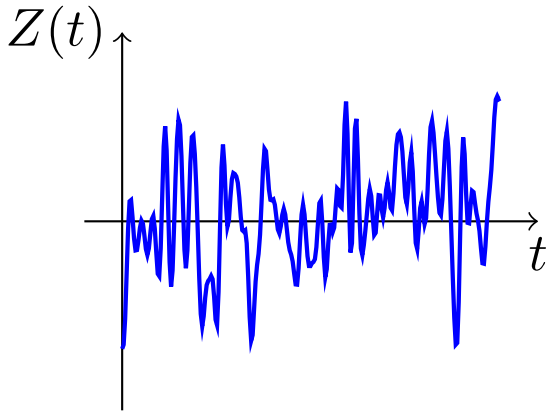
$$m_\alpha = \frac{1}{2\pi} \int_{\mathbb{R}} \omega^\alpha s_Z(\omega) d\omega.$$

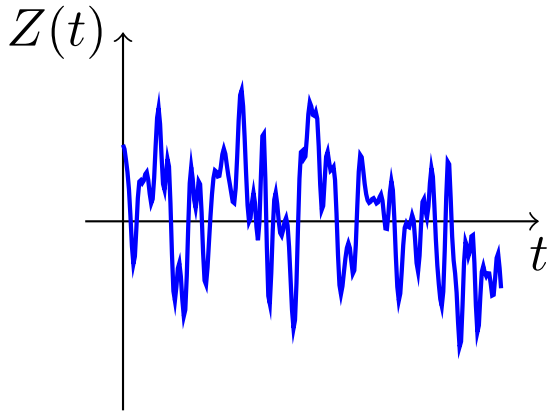
Random field model of surface roughness

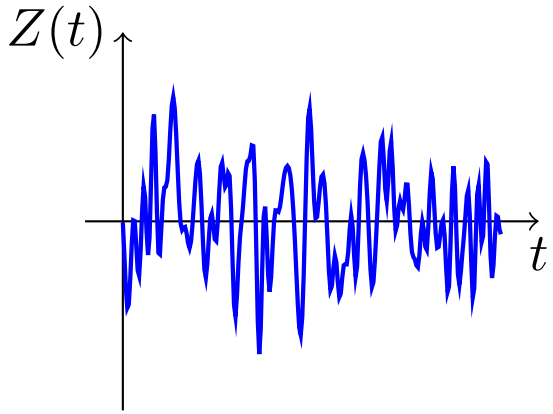
More details: Stochastic processes





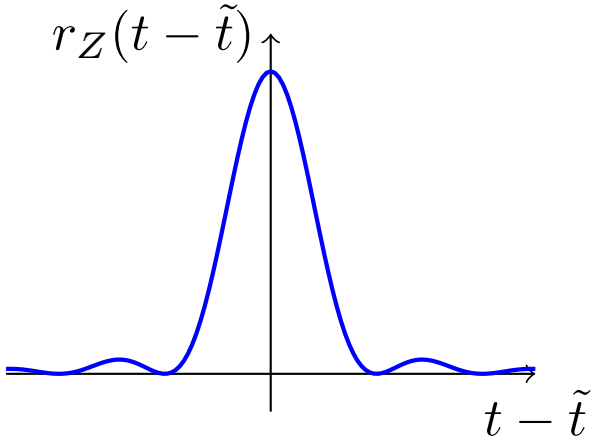


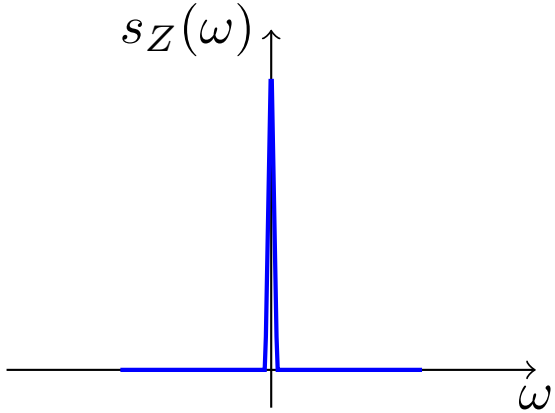


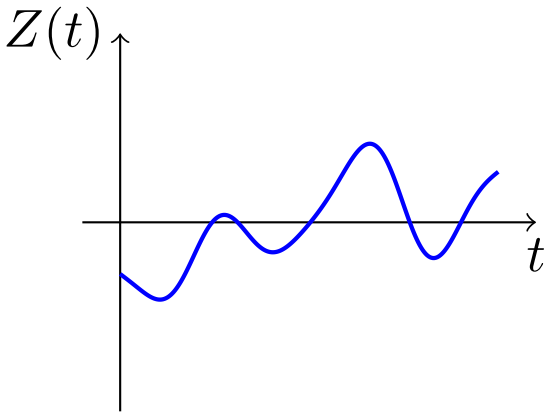


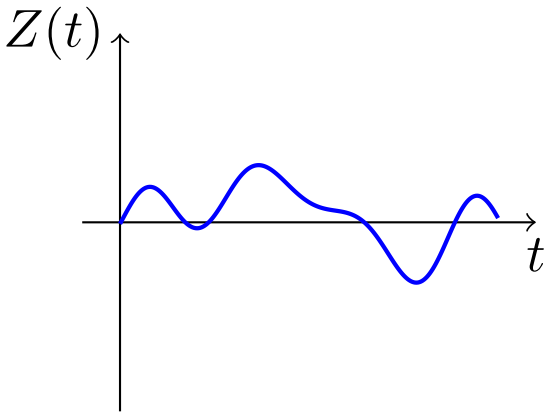
Random field model of surface roughness

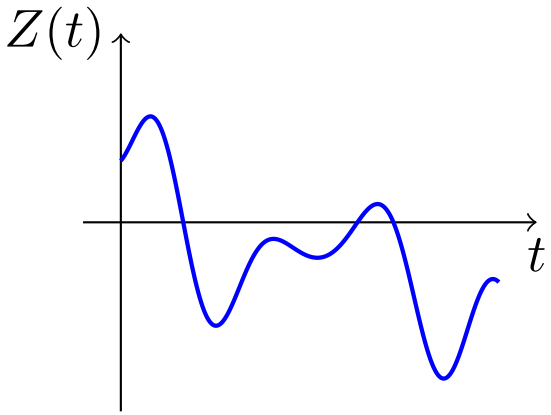
More details: Stochastic processes











More details: Stochastic processes

- The **mean-square derivative** of a second-order stochastic process $\{Z(t),\ t \in \mathcal{T}\}$ indexed by $\mathcal{T}$ with values in $\mathbb{R}$, if it exists, is the second-order stochastic process $\{\dot{Z}(t),\ t \in \mathcal{T}\}$ such that

$$\dot{Z}(t) = \lim_{\tau \to 0} \frac{Z(t+\tau) - Z(t)}{\tau}, \quad \forall t \in \mathcal{T},$$

where the limit is defined in the sense of the mean-square convergence of second-order r. v.

Provided that all the derivatives in the expressions to follow exist, the second-order statistical descriptors of $\{\dot{Z}(t),\ t \in \mathcal{T}\}$ are related to those of $\{Z(t),\ t \in \mathcal{T}\}$ as follows:

$$\overline{\dot{z}}(t) = E\big(\dot{Z}(t)\big) = \dot{\overline{z}}(t), \qquad r_{\dot{Z}}(t,\tilde{t}) = E\big(\dot{Z}(t)\dot{Z}(\tilde{t})\big) = \frac{\partial^2 r_Z}{\partial t \partial \tilde{t}}(t,\tilde{t}).$$

- In the case of a zero-mean, mean-square stationary, second-order stochastic process $\{Z(t),\ t \in \mathbb{R}\}$, and provided that all the derivatives in the expressions to follow exist, the second-order statistical descriptors of $\{\dot{Z}(t),\ t \in \mathbb{R}\}$ are related to those of $\{Z(t),\ t \in \mathbb{R}\}$ as follows:

$$\overline{\dot{z}} = 0, \qquad r_{\dot{Z}}(t-\tilde{t}) = -\frac{d^2 r_Z}{d(t-\tilde{t})^2}(t-\tilde{t}),$$

$$s_{\dot{Z}}(\omega) = \omega^2 s_Z(\omega), \qquad E\big(\dot{Z}(t)^2\big) = r_{\dot{Z}}(0) = \frac{1}{2\pi}\int_{\mathbb{R}} \omega^2 s_Z(\omega) d\omega = m_2.$$

Proof: Second-order statistical descriptors of mean-square derivative

- Because of the triangle inequality and the Cauchy-Schwartz inequality, we have

$$\begin{aligned}
&\left| E\left(\dot{Z}(t)\dot{Z}(\tilde{t}) - \frac{Z(t+\tau)-Z(t)}{\tau}\frac{Z(\tilde{t}+\tilde{\tau})-Z(\tilde{t})}{\tilde{\tau}} \right) \right| \\
&\quad \leq \sqrt{E\left(\left(\dot{Z}(t) - \frac{Z(t+\tau)-Z(t)}{\tau} \right)^2 \right)} \sqrt{E\left(\dot{Z}(\tilde{t})^2 \right)} \\
&\quad + \sqrt{E\left(\left(\frac{Z(t+\tau)-Z(t)}{\tau} \right)^2 \right)} \sqrt{E\left(\left(\dot{Z}(\tilde{t}) - \frac{Z(\tilde{t}+\tilde{\tau})-Z(\tilde{t})}{\tilde{\tau}} \right)^2 \right)}.
\end{aligned}$$

- Because the right-hand side tends to 0 as a whole when τ and $\tilde{\tau}$ tend to 0, we have

$$\begin{aligned}
r_{\dot{Z}}(t,\tilde{t}) &= \lim_{\tau,\tilde{\tau}\to 0} E\left(\frac{Z(t+\tau)-Z(t)}{\tau}\frac{Z(\tilde{t}+\tilde{\tau})-Z(\tilde{t})}{\tilde{\tau}} \right) \\
&= \lim_{\tau,\tilde{\tau}\to 0} \frac{r_Z(t+\tau,\tilde{t}+\tilde{\tau}) - r_Z(t+\tau,\tilde{\tau}) - r_Z(t,\tilde{t}+\tilde{\tau}) + r_Z(t,\tilde{t})}{\tau\tilde{\tau}}.
\end{aligned}$$

- If r_Z is twice continuously differentiable, then the limit equals $r_{\dot{Z}}(t,\tilde{t}) = \frac{\partial^2 r_Z}{\partial t \partial \tilde{t}}(t,\tilde{t})$, as asserted.

More details: Stochastic processes

- In the case of a zero-mean, mean-square stationary, second-order stochastic process $\{Z(t), t \in \mathbb{R}\}$, the spectral moment $m_{2\alpha}$, if it exists, provides the variance of the α-th mean-square derivative of this stochastic process, that is,

$$\sigma^2_{\frac{d^\alpha Z}{dt^\alpha}} = E\left(\left(\frac{d^\alpha Z}{dt^\alpha}(t) - \underbrace{\frac{d^\alpha \overline{z}}{dt^\alpha}}_{=0}\right)^2\right) = E\left(\left(\frac{d^\alpha Z}{dt^\alpha}(t)\right)^2\right) = r_{\frac{d^\alpha Z}{dt^\alpha}}(0) = \frac{1}{2\pi}\int_{\mathbb{R}} \omega^{2\alpha} s_Z(\omega) d\omega = m_{2\alpha}.$$

- For example, the spectral moments m_0, m_2, and m_4, if they exist, provide the variances of a zero-mean, mean-square stationary, second-order stochastic process $\{Z(t), t \in \mathbb{R}\}$, its first mean-square derivative, and its second mean-square derivative:

$$\sigma^2_Z = E\left(\left(Z(t) - \underbrace{\overline{z}}_{=0}\right)^2\right) = E\left(\left(Z(t)\right)^2\right) = r_Z(0) = \frac{1}{2\pi}\int_{\mathbb{R}} s_Z(\omega) d\omega = m_0,$$

$$\sigma^2_{\dot{Z}} = E\left(\left(\dot{Z}(t) - \underbrace{\dot{\overline{z}}}_{=0}\right)^2\right) = E\left(\left(\dot{Z}(t)\right)^2\right) = r_{\dot{Z}}(0) = \frac{1}{2\pi}\int_{\mathbb{R}} \omega^2 s_Z(\omega) d\omega = m_2,$$

$$\sigma^2_{\ddot{Z}} = E\left(\left(\ddot{Z}(t) - \underbrace{\ddot{\overline{z}}}_{=0}\right)^2\right) = E\left(\left(\ddot{Z}(t)\right)^2\right) = r_{\ddot{Z}}(0) = \frac{1}{2\pi}\int_{\mathbb{R}} \omega^4 s_Z(\omega) d\omega = m_4.$$

Random field model of surface roughness

More details: Random fields

- For $d \geq 2$, a **random field** $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ indexed by a subset $\mathcal{D}$ of $\mathbb{R}^d$ and with values in $\mathbb{R}$ is a collection of random variables $Z(\boldsymbol{x})$ with values in $\mathbb{R}$ indexed by $\boldsymbol{x}$ in $\mathcal{D}$.

- For any nonempty finite subset $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m\}$ of $\mathcal{D}$, where m denotes the number of elements in this subset, the joint probability distribution $P_{(Z(\boldsymbol{x}_1),\ldots,Z(\boldsymbol{x}_m))}$ of $(Z(\boldsymbol{x}_1), \ldots, Z(\boldsymbol{x}_m))$ is called a **(m-th order) marginal probability distribution** of the random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$.

  The collection of all the marginal probability distributions of a random field is called the **system of marginal probability distributions**.

- A random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ indexed by $\mathcal{D}$ and with values in $\mathbb{R}$ is **Gaussian** if each probability distribution in its system of marginal probability distributions is Gaussian.

More details: Random fields

- A random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ indexed by $\mathcal{D}$ with values in $\mathbb{R}$ is of the **second order** if

$$E\big(Z(\boldsymbol{x})^2\big) = \int_{\mathbb{R}} z^2 \rho_{Z(\boldsymbol{x})}(z) dz < +\infty, \quad \forall \boldsymbol{x} \in \mathcal{D}.$$

- The **mean function** of a second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ indexed by $\mathcal{D}$ with values in $\mathbb{R}$ is the function $\overline{z}$ from $\mathcal{D}$ into $\mathbb{R}$ such that

$$\overline{z}(\boldsymbol{x}) = E\big(Z(\boldsymbol{x})\big) = \int_{\mathbb{R}} z \rho_{Z(\boldsymbol{x})}(z) dz.$$

- The **autocorrelation function** of a second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ indexed by $\mathcal{D}$ with values in $\mathbb{R}$ is the function r_Z from $\mathcal{D} \times \mathcal{D}$ into $\mathbb{R}$ such that

$$r_Z(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = E\big(Z(\boldsymbol{x}) Z(\tilde{\boldsymbol{x}})\big) = \int_{\mathbb{R}\times\mathbb{R}} z\tilde{z} \rho_{(Z(\boldsymbol{x}), Z(\tilde{\boldsymbol{x}}))}(z, \tilde{z}) dz d\tilde{z}.$$

- The **covariance function** of a second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ indexed by $\mathcal{D}$ with values in $\mathbb{R}$ is the function c_Z from $\mathcal{D} \times \mathcal{D}$ into $\mathbb{R}$ such that

$$c_Z(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = E\Big(\big(Z(\boldsymbol{x}) - \overline{z}(\boldsymbol{x})\big)\big(Z(\tilde{\boldsymbol{x}}) - \overline{z}(\tilde{\boldsymbol{x}})\big)\Big) = \int_{\mathbb{R}\times\mathbb{R}} \big(z - \overline{z}(\boldsymbol{x})\big)\big(\tilde{z} - \overline{z}(\tilde{\boldsymbol{x}})\big) \rho_{(Z(\boldsymbol{x}), Z(\tilde{\boldsymbol{x}}))}(z, \tilde{z}) dz d\tilde{z}.$$

- Please note that $c_Z(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = E\Big(\big(Z(\boldsymbol{x}) - \overline{z}(\boldsymbol{x})\big)\big(Z(\tilde{\boldsymbol{x}}) - \overline{z}(\tilde{\boldsymbol{x}})\big)\Big) = r_Z(\boldsymbol{x}, \tilde{\boldsymbol{x}}) - \overline{z}(\boldsymbol{x})\overline{z}(\tilde{\boldsymbol{x}})$.

More details: Random fields

- A second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^d\}$ indexed by $\mathbb{R}^d$ with values in $\mathbb{R}$ is **mean-square stationary** if $\overline{z}(\boldsymbol{x}) = \overline{z}$ is independ of $\boldsymbol{x}$ and $r_Z(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = r_Z(\boldsymbol{x} - \tilde{\boldsymbol{x}})$ depends on only $\boldsymbol{x} - \tilde{\boldsymbol{x}}$.

- The **power spectral density function** of a zero-mean, mean-square stationary, second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^d\}$ indexed by $\mathbb{R}^d$ with values in $\mathbb{R}$, if it exists, is the function s_Z from $\mathbb{R}^d$ into $\mathbb{R}^+$ such that

$$r_Z(\boldsymbol{x} - \tilde{\boldsymbol{x}}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} s_Z(\boldsymbol{\xi}) \exp\big(i\boldsymbol{\xi} \cdot (\boldsymbol{x} - \tilde{\boldsymbol{x}})\big) d\boldsymbol{\xi}.$$

  The power spectral density function s_Z has the following properties:

  - it is even because of the evenness of r_Z,
  - it is positive owing to Bochner's theorem,
  - it is integrable because $E\big(Z(\boldsymbol{x})^2\big) = r_Z(\boldsymbol{0}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} s_Z(\boldsymbol{\xi}) d\boldsymbol{\xi} < +\infty$.

- For $\boldsymbol{\alpha}$ in $\mathbb{N}^d$, the **spectral moment of order $\boldsymbol{\alpha}$**, denoted by $m_{\boldsymbol{\alpha}}$, if it exists, is the integral

$$m_{\boldsymbol{\alpha}} = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \boldsymbol{\xi}^{\boldsymbol{\alpha}} s_Z(\boldsymbol{\xi}) d\boldsymbol{\xi}, \quad \text{where} \quad \boldsymbol{\xi}^{\boldsymbol{\alpha}} = \xi_1^{\alpha_1} \times \ldots \times \xi_d^{\alpha_d}.$$

More details: Random fields

- The **mean-square partial derivative with respect to x_k** of a second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ indexed by $\mathcal{D} \subset \mathbb{R}^d$ with values in $\mathbb{R}$, where $1 \leq k \leq d$, if it exists, is the second-order stochastic process $\{\frac{\partial Z}{\partial x_k}(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ such that

$$\frac{\partial Z}{\partial x_k}(\boldsymbol{x}) = \lim_{h \to 0} \frac{Z(\boldsymbol{x} + h\boldsymbol{i}_k) - Z(\boldsymbol{x})}{h}, \quad \forall \boldsymbol{x} \in \mathcal{D},$$

  where the limit is defined in the sense of the mean-square convergence of second-order r. v.

  Provided that all the derivatives in the expressions to follow exist, the second-order statistical descriptors of $\{\frac{\partial Z}{\partial x_k}(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ are related to those of $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathcal{D}\}$ as follows:

$$\overline{\frac{\partial Z}{\partial x_k}}(\boldsymbol{x}) = \frac{\partial \overline{z}}{\partial x_k}(\boldsymbol{x}), \qquad r_{\frac{\partial Z}{\partial x_k}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \frac{\partial^2 r_Z}{\partial x_k \partial \tilde{x}_k}(\boldsymbol{x}, \tilde{\boldsymbol{x}}).$$

- In the case of a zero-mean, mean-square stationary, second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^d\}$, and provided that all the derivatives in the expressions to follow exist, the second-order statistical descriptors of $\{\frac{\partial Z}{\partial x_k}(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^d\}$ are related to those of $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^d\}$ as follows:

$$\overline{\frac{\partial Z}{\partial x_k}} = 0, \qquad r_{\frac{\partial Z}{\partial x_k}}(\boldsymbol{x} - \tilde{\boldsymbol{x}}) = -\frac{d^2 r_Z}{d(x_k - \tilde{x}_k)^2}(\boldsymbol{x} - \tilde{\boldsymbol{x}}),$$

$$s_{\frac{\partial Z}{\partial x_k}}(\boldsymbol{\xi}) = \xi_k^2 s_Z(\boldsymbol{\xi}), \quad E\left(\left(\frac{\partial Z}{\partial x_k}(\boldsymbol{x})\right)^2\right) = r_{\frac{\partial Z}{\partial x_k}}(\boldsymbol{0}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \xi_k^2 s_Z(\boldsymbol{\xi}) d\boldsymbol{\xi} = m_{(\underbrace{0, \ldots, 0}_{k-1 \text{ zeros}}, 2, \underbrace{0, \ldots, 0}_{d-k \text{ zeros}})}.$$

More details: Random fields

- In the case of a zero-mean, mean-square stationary, second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^d\}$, the spectral moment $m_{2\boldsymbol{\alpha}}$, if it exists, provides the variance of the $\boldsymbol{\alpha}$-th mean-square derivative of this random field, that is,

$$\sigma^2_{\frac{\partial^{\boldsymbol{\alpha}} Z}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}}}} = E\left(\left(\frac{\partial^{\boldsymbol{\alpha}} Z}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}}}(\boldsymbol{x}) - \underbrace{\frac{\partial^{\boldsymbol{\alpha}} \overline{z}}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}}}}_{=0}\right)^2\right) = E\left(\left(\frac{\partial^{\boldsymbol{\alpha}} Z}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}}}(\boldsymbol{x})\right)^2\right) = r_{\frac{\partial^{\boldsymbol{\alpha}} Z}{\partial \boldsymbol{x}^{\boldsymbol{\alpha}}}}(\mathbf{0}) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^d} \boldsymbol{\xi}^{2\boldsymbol{\alpha}} s_Z(\boldsymbol{\xi}) d\boldsymbol{\xi} = m_{2\boldsymbol{\alpha}}.$$

- For example, the spectral moments $m_{(0,0)}$ and $m_{(2,0)}$, if they exist, provide the variances of a zero-mean, mean-square stationary, second-order two-dimensional random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ and its first mean-square derivative:

$$\sigma^2_Z = E\Big(\big(Z(\boldsymbol{x}) - \underbrace{\overline{z}}_{=0}\big)^2\Big) = E\Big(\big(Z(\boldsymbol{x})\big)^2\Big) = r_Z(\mathbf{0}) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^d} s_Z(\boldsymbol{\xi}) d\boldsymbol{\xi} = m_{(0,0)},$$

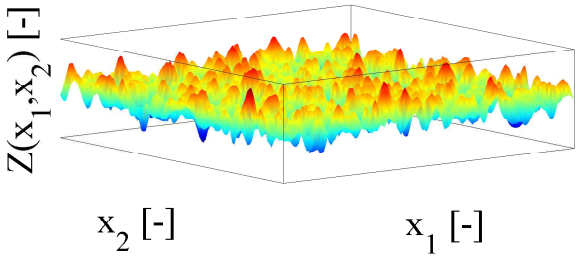
$$\sigma^2_{\frac{\partial Z}{\partial x_1}} = E\left(\left(\frac{\partial Z}{\partial x_1}(\boldsymbol{x}) - \underbrace{\frac{\partial \overline{z}}{\partial x_1}}_{=0}\right)^2\right) = E\left(\left(\frac{\partial Z}{\partial x_1}(\boldsymbol{x})\right)^2\right) = r_{\frac{\partial Z}{\partial x_1}}(\mathbf{0}) = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} \xi_1^2 s_Z(\boldsymbol{\xi}) d\boldsymbol{\xi} = m_{(2,0)}.$$

Random collection of spheres

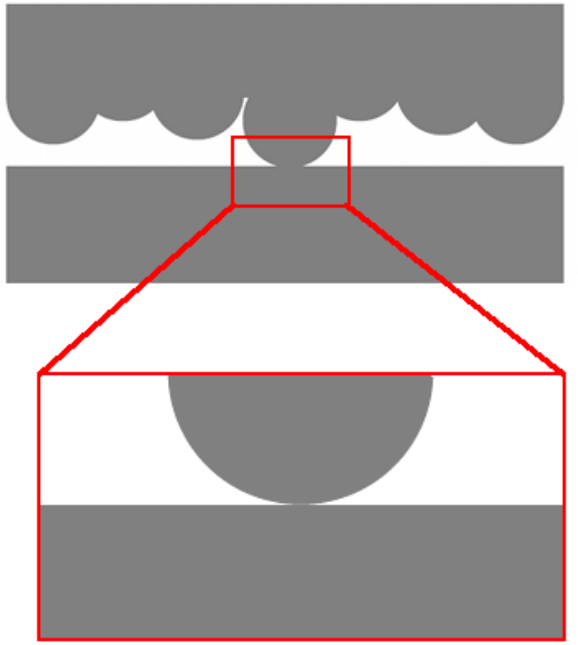
Random collection of spheres

- To facilitate analytical calculations, we will replace the model of the rough surface as a random field with an **“equivalent” model of the rough surface as a random collection of spheres**.

Random field model
of surface roughness



Equivalent model
as random collection of spheres



Adhesive contact
of spheres

- Locally, we will treat the contact of each sphere by means of analytical models from elasticity theory.

Random collection of spheres

- If two rough surfaces, or a rough surface and a smooth surface, are placed in contact, actual contact will occur only wherever “hills” of one surface touch the “hills” of the other surface:

- These “hills,” also called “**asperities**,” are located around **local maxima**.

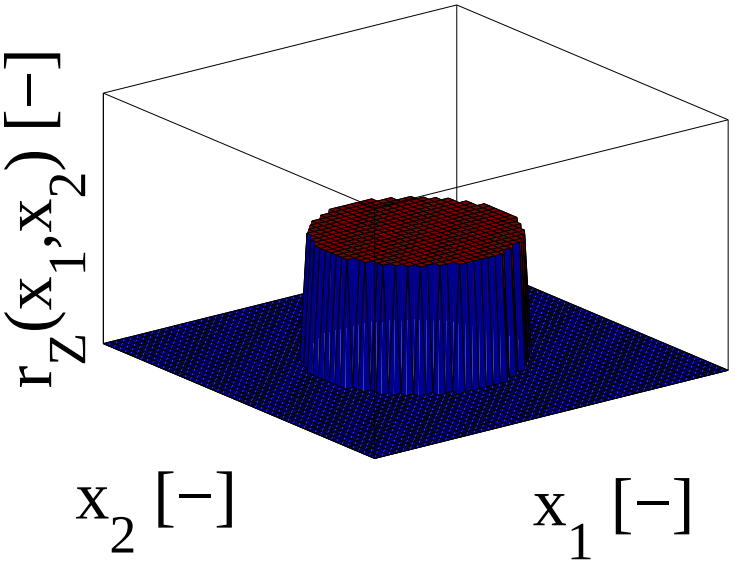
- Thus, to replace the model of the rough surface as a random field with an “equivalent” model of the rough surface as a random collection of spheres, we will strive to **mimic the properties of the local maxima of the random field** (the number of local maxima per unit area, the local structure of the local maxima, . . .) in the properties of the spheres in the random collection of spheres.

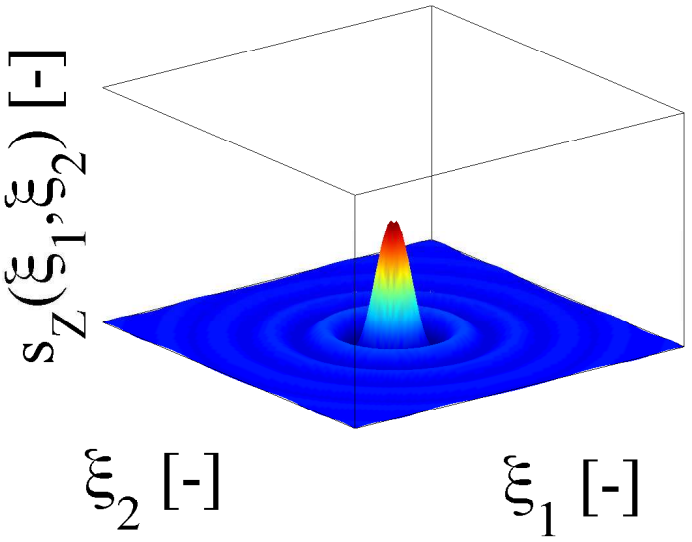
- Consequently, in preparation of our construction of the “equivalent” model of the rough surface as a random collection of spheres, we will first study properties of local maxima of random fields.

- Interestingly, for zero-mean, isotropic, mean-square stationary, Gaussian two-dimensional random fields, statistical descriptors (mean number per unit area, local structure,. . .) of the local maxima can be deduced from only the first few spectral moments, as shown next.

Random collection of spheres

- A mean-square stationary second-order random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^d\}$ is **isotropic** if its autocorrelation function is circularly symmetric, that is, $(\boldsymbol{x} - \tilde{\boldsymbol{x}}) \mapsto r_Z(\boldsymbol{x} - \tilde{\boldsymbol{x}}) = r_Z(\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|)$ depends on only $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|$. Circular symmetry of the autocorrelation function implies circular symmetry of the p.s.d., if it exists, that is, $\boldsymbol{\xi} \mapsto s_Z(\boldsymbol{\xi}) = s_Z(\|\boldsymbol{\xi}\|)$ depends on only $\|\boldsymbol{\xi}\|$.





- For zero-mean, isotropic, mean-square stationary, second-order two-dimensional random fields, many spectral moments vanish and simple relations exist between the remaining ones, if they exist:
  - $m_{(2,0)} = m_{(0,2)} \equiv \mu_2$.
  - $m_{(1,1)} = m_{(1,3)} = m_{(3,1)} = 0$.
  - $m_{(0,0)} \equiv \mu_0$.
  - $3m_{(2,2)} = m_{(4,0)} = m_{(0,4)} \equiv \mu_4$.

(These relations are proved later on Slide 62).

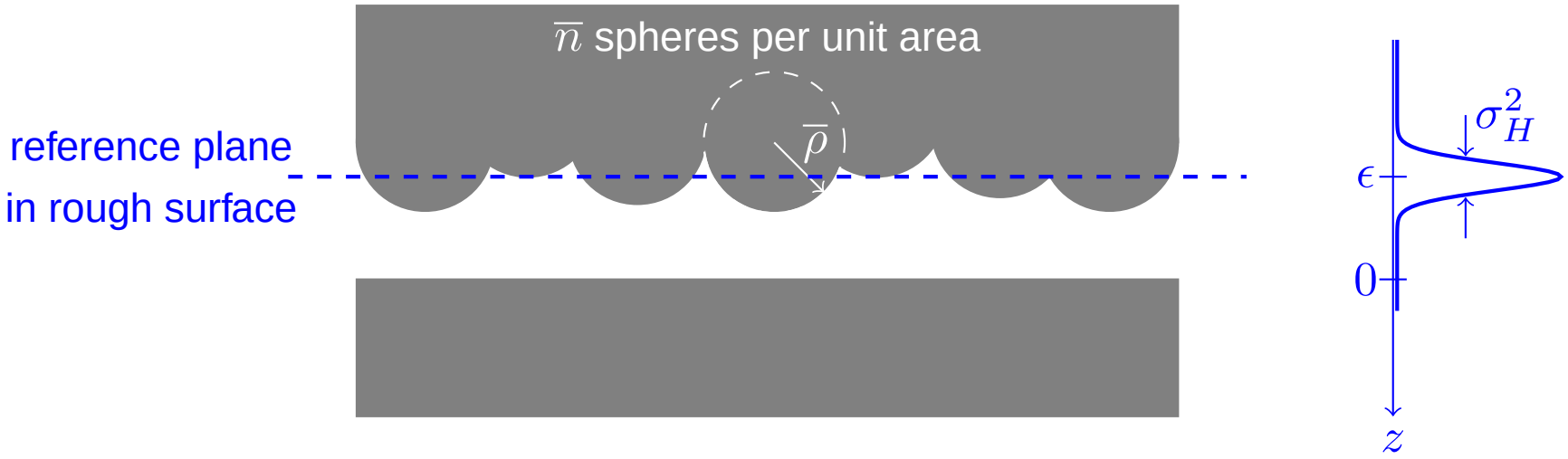
Random collection of spheres

- For zero-mean, isotropic, mean-square stationary, Gaussian two-dimensional random fields, statistical descriptors of the local maxima can be deduced from μ_0, μ_2, and μ_4, if they exist:
  - the **mean number of local maxima per unit area** is given by
$$\overline{n} = \frac{1}{6\pi\sqrt{3}} \frac{\mu_4}{\mu_2},$$
  - the **mean of the height of a local maximum** is given by
$$\overline{h} = \frac{4}{\sqrt{\pi\alpha}},$$
  - the **variance of the height of a local maximum** is given by
$$\sigma_H^2 = \left(1 - \frac{0.8968}{\alpha}\right) \mu_0,$$
  - the **mean of the radius of curvature of a local maximum** is given by
$$\overline{\rho} = \frac{3}{8}\sqrt{\frac{\pi}{\mu_4}},$$

  where $\alpha = \mu_0\mu_4/\mu_2^2$. Because local maxima appear wherever the first derivatives vanish and the matrix made up of the second derivatives is negative definite, the interpretation of spectral moments in terms of variances of derivatives intuitively explains the appearance of spectral moments in these relations, which we will prove more rigorously later on Slides 63–67.

Random collection of spheres

- To replace the model of the rough surface as a random field with an “equivalent” model of the rough surface as a random collection of spheres, we strive to **mimic the properties of the local maxima of the random field** (the number of local maxima per unit area, the local structure of the local maxima, . . .) in the properties of the spheres in the random collection of spheres.

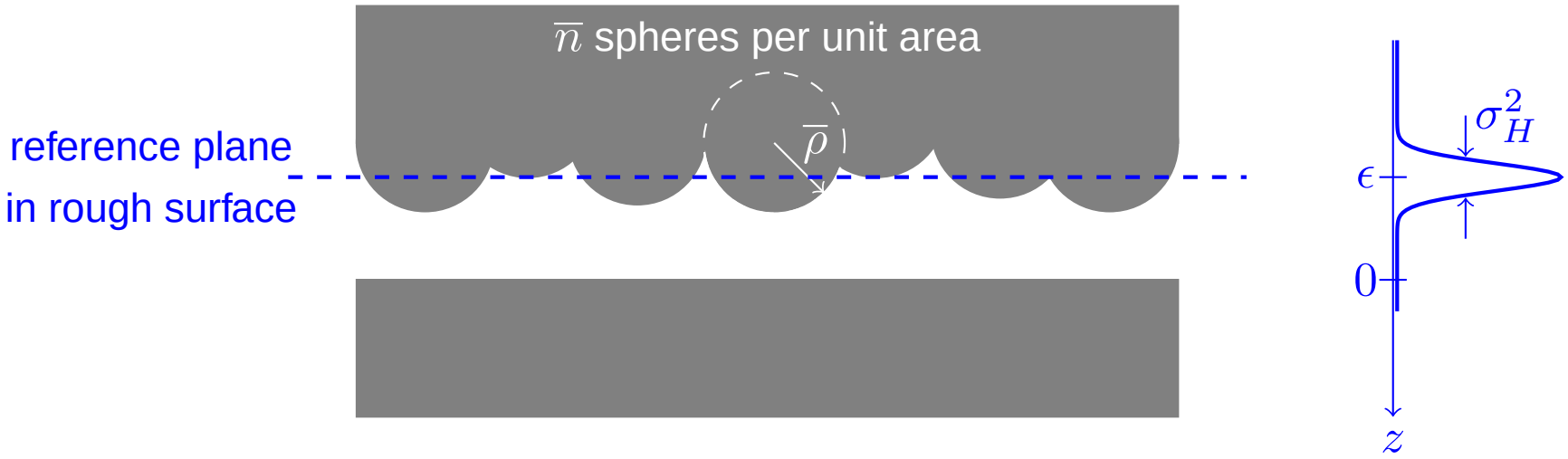


We follow the work of Greenwood and Williamson and of McCool in assuming that there are $\overline{n}$ spheres per unit area, that the spheres all have the same radius equal to $\overline{\rho}$, and that the heights of the sphere summits admit a Gaussian p.d.f. with variance σ_H^2.

- The distance ϵ is the distance between the smooth surface and the reference plane in the rough surface that is located at the mean height of a local maximum. In the literature, this distance ϵ is sometimes also referred to as the interference ϵ.
- Locally, we treat the contact of each sphere by means of analytical models from elasticity theory. Specifically, we use the Johnson-Kendall-Roberts adhesive contact model.

Random collection of spheres

- Assuming that a large number of asperities is involved in the contact, we can then obtain an approximation of the average contact force per unit area as follows



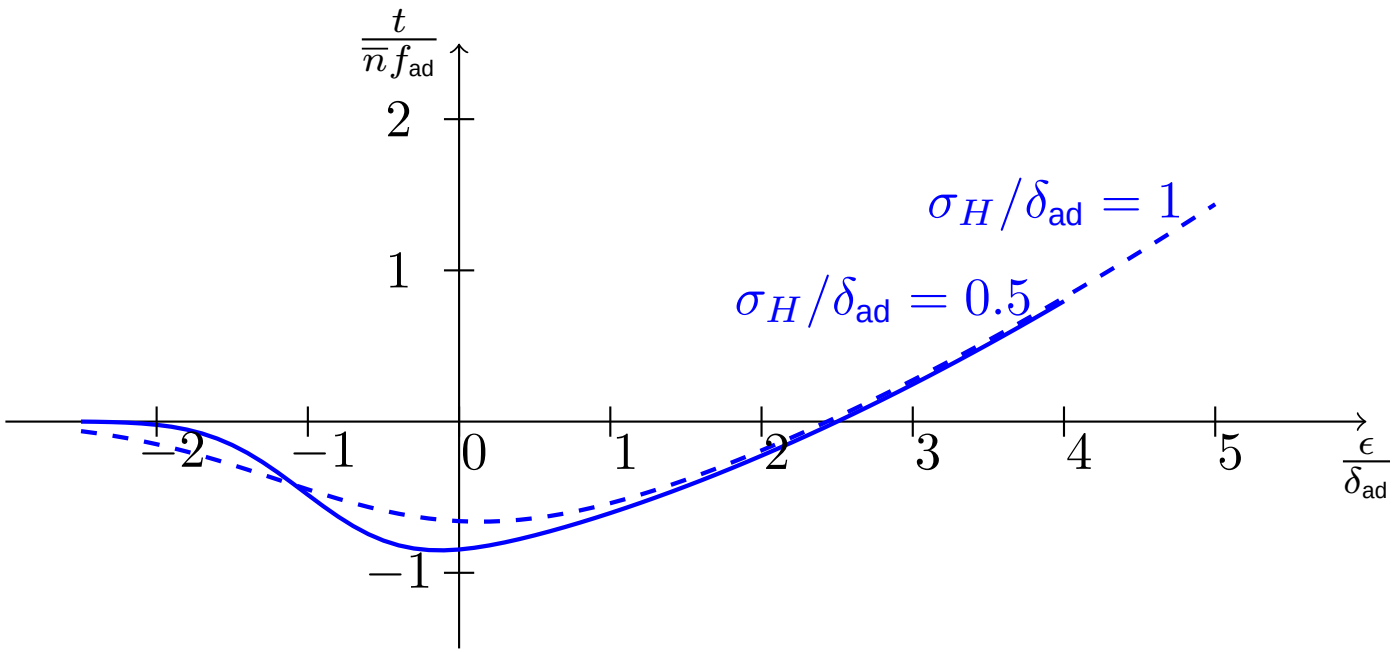
$$\underbrace{t(\epsilon)}_{\substack{\text{average contact force}\\ \text{per unit area}}} \approx \underbrace{\overline{n}}_{\substack{\text{average number of spheres}\\ \text{per unit area}}} \underbrace{\int_{\delta_{\text{ad}}}^{+\infty} f(z;\overline{\rho}) \frac{1}{\sqrt{2\pi}\sigma_H} \exp\left(-\frac{(z-\epsilon)^2}{2\sigma_H^2}\right) dz}_{\substack{\text{average contact force}\\ \text{per sphere}}}.$$

- Here, $f(z;\overline{\rho})$ is determined by means of the Johnson-Kendall-Roberts model, that is, by solving

$$\begin{cases} z = \dfrac{1}{3}\dfrac{a^2}{\overline{\rho}} + \dfrac{2}{3}\dfrac{f(z;\overline{\rho})}{\kappa a}, \\ a^3 = \dfrac{\overline{\rho}}{\kappa}\left(f(z;\overline{\rho}) + 3\gamma\pi\overline{\rho} + \sqrt{6\gamma\pi\overline{\rho}f(z;\overline{\rho}) + (3\gamma\pi\overline{\rho})^2}\right). \end{cases}$$

Random collection of spheres

- Traction-distance relationship:



Here, $f_{\text{ad}} = -\frac{3}{2}\gamma\pi\overline{\rho}$ and $\delta_{\text{ad}} = -\sqrt[3]{\frac{\pi^2\gamma^2\overline{\rho}}{12\kappa^2}}$ are the adhesion force and the displacement corresponding to the adhesion force for $\overline{\rho}$, respectively.

Random collection of spheres

- Matlab code used to generate this figure:

```
sigma=0.5;

f=[-1:0.01:10];
d=((f+2)+2*sqrt(f+1)).^(2/3)+8^(1/3)*f.*((f+2)+2*sqrt(f+1)).^(-1/3);

epsilon=[-2.5:0.1:5];
t=zeros(length(epsilon),1);
for m1=1:length(epsilon)
  t(m1)=quad(@(z)interp1(d,f,z).*normpdf(z,epsilon(m1),sigma),-1,epsilon(m1)+3*sigma);
end

figure;
plot(epsilon,t,'b-');
```

Proof: Relationships between spectral moments:

- The first three relationships on Slide 56 follow trivially from the circular symmetry of the p.s.d.

- In order to prove the fourth relationship on Slide 56, let us introduce a function $\tilde{r}_Z$ from $\mathbb{R}$ into $\mathbb{R}$ such that $r_Z(\boldsymbol{x}) = r_Z(\|\boldsymbol{x}\|) = \tilde{r}_Z(\|\boldsymbol{x}\|^2)$. Then, the spectral moments can be easily obtained by evaluating derivatives of $\tilde{r}_Z$ at the origin. In fact,

$$\frac{\partial^4 r_Z}{\partial x_1^4}(\boldsymbol{x}) = 12\ddot{\tilde{r}}_Z(\|\boldsymbol{x}\|^2) + 48x_1^2\dddot{\tilde{r}}_Z(\|\boldsymbol{x}\|^2) + 16x_1^4\ddddot{\tilde{r}}_Z(\|\boldsymbol{x}\|^2),$$

$$\frac{\partial^4 r_Z}{\partial x_1^2 \partial x_2^2}(\boldsymbol{x}) = 4\ddot{\tilde{r}}_Z(\|\boldsymbol{x}\|^2) + 8x_1^2\dddot{\tilde{r}}_Z(\|\boldsymbol{x}\|^2) + 8x_1^2\dddot{\tilde{r}}_Z(\|\boldsymbol{x}\|^2) + 16x_1^2x_2^2\ddddot{\tilde{r}}_Z(\|\boldsymbol{x}\|^2),$$

so that

$$m_{(4,0)} = \frac{\partial^4 r_Z}{\partial x_1^4}(\mathbf{0}) = 12\ddot{\tilde{r}}_Z(0),$$

$$m_{(2,2)} = \frac{\partial^4 r_Z}{\partial x_1^2 \partial x_2^2}(\mathbf{0}) = 4\ddot{\tilde{r}}_Z(0);$$

hence, $3m_{(2,2)} = m_{(4,0)} = m_{(0,4)}$, as asserted.

Proof: Statistical descriptors of local maxima:

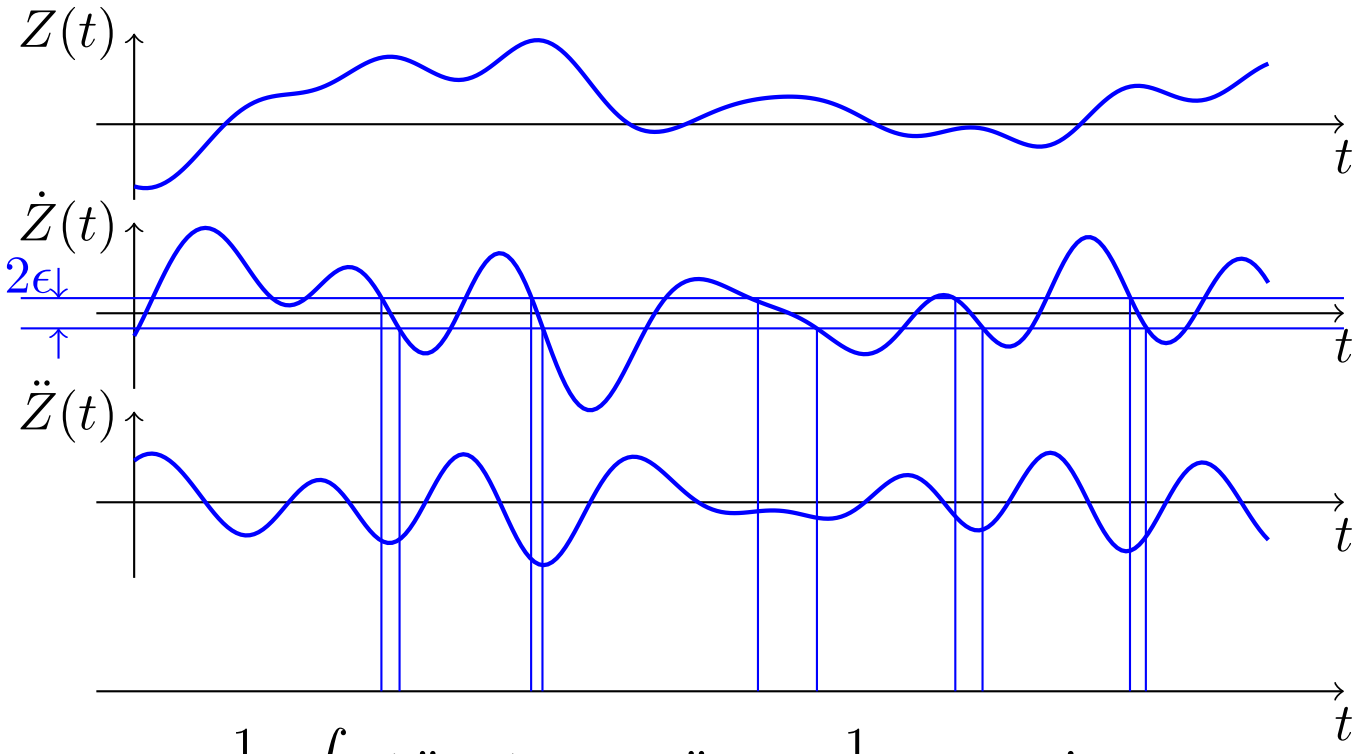
- The proof of the expression for the mean number of local maxima per unit area is based on writing this number of local maxima per unit area in an integral form more amenable to analytical calculation. The proofs of the expressions for the mean of the height, the variance of the height, and the mean of the radius of curvature of a local maximum are based on a study of the behavior of the random field near a local maximum by using notions of conditional probability and ergodicity.

- These proofs are quite technical. You may find details in the following references:
  - R. Adler. The geometry of random fields. John Wiley & Sons, 1981. Chapter 6.
  - R. Adler and J. Taylor. Random fields and geometry. Springer, 2007. Chapter 11.

- We will limit ourselves here to the proof of the expression for the mean number of local maxima per unit area. We will omit all technicalities and provide only the main ideas.

Proof: Statistical descriptors of local maxima (continued):

- The proof is based on writing the number of local maxima per unit area in an integral form more amenable to analytical calculation. We will deduce this integral form for the simpler case of a stochastic process and then generalize to the case of a random field.



$$N = \frac{1}{|\mathcal{T}|} \int_{\mathcal{T}} \underbrace{|\ddot{Z}(t)|}_{\text{jacobian}} \; 1_{\mathbb{R}_0^-}\big(\ddot{Z}(t)\big) \; \frac{1}{2\epsilon} 1_{]-\epsilon,\epsilon[}\big(\dot{Z}(t)\big) \; dt.$$

Here, $\mathcal{T}$ is a finite interval, $|\mathcal{T}|$ the length of $\mathcal{T}$, N the number of local maxima per unit length in $\mathcal{T}$, and for a set $\mathcal{B}$, the function $1_{\mathcal{B}}$ is equal to 1 if the argument is in $\mathcal{B}$ and 0 otherwise.

Proof: Statistical descriptors of local maxima (continued):

- Because the left-hand side of the previous equation is independent of ϵ, we can take the limit as ϵ tends to zero to obtain

$$N = \lim_{\epsilon \to 0} \frac{1}{|\mathcal{T}|} \int_{\mathcal{T}} \left|\ddot{Z}(t)\right| \; 1_{\mathbb{R}_0^-}\left(\ddot{Z}(t)\right) \; \frac{1}{2\epsilon} 1_{]-\epsilon,\epsilon[}\left(\dot{Z}(t)\right) \; dt.$$

- Taking the mathematical expectation, we find the mean number of local maxima per unit length

$$\overline{n} = E(N) = E\left(\lim_{\epsilon \to 0} \frac{1}{|\mathcal{T}|} \int_{\mathcal{T}} \left|\ddot{Z}(t)\right| \; 1_{\mathbb{R}_0^-}\left(\ddot{Z}(t)\right) \; \frac{1}{2\epsilon} 1_{]-\epsilon,\epsilon[}\left(\dot{Z}(t)\right) \; dt \right).$$

- Assuming that integrals and limits can be interchanged (the justification is quite technical), we obtain

$$\overline{n} = \frac{1}{|\mathcal{T}|} \int_{\mathcal{T}} \int_{\mathbb{R}} \int_{\mathbb{R}} |v| 1_{\mathbb{R}_0^-}(v) \lim_{\epsilon \to 0} \int_{\mathbb{R}} 1_{]-\epsilon,\epsilon[}(y) \rho_{\left(Z(t),\dot{Z}(t),\ddot{Z}(t)\right)}(z,y,v) dy dz dv dt.$$

- Evaluating the limit and using the fact that if $\{Z(t),\ t \in \mathbb{R}\}$ is a mean-square stationary Gaussian stochastic process, then $\rho_{\left(Z(t),\dot{Z}(t),\ddot{Z}(t)\right)}$, if it exists, is independent of t, we obtain

$$\overline{n} = \int_{\mathbb{R}} \int_{\mathbb{R}_0^-} |v| \rho_{\left(Z(t),\dot{Z}(t),\ddot{Z}(t)\right)}(z,0,v) dz dv.$$

Proof: Statistical descriptors of local maxima (continued):

- We now turn our attention to the case of a zero-mean, isotropic, mean-square stationary, Gaussian two-dimensional random field $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$.

- We introduce the following shorthand notation:

$$G_1 = Z(\boldsymbol{x}), \qquad G_4 = \frac{\partial^2 Z}{\partial x_1^2}(\boldsymbol{x}),$$

$$G_2 = \frac{\partial Z}{\partial x_1}(\boldsymbol{x}), \qquad G_5 = \frac{\partial^2 Z}{\partial x_1 \partial x_2}(\boldsymbol{x}),$$

$$G_3 = \frac{\partial Z}{\partial x_2}(\boldsymbol{x}), \qquad G_6 = \frac{\partial^2 Z}{\partial x_2^2}(\boldsymbol{x}).$$

- Then, extending the previously obtained expression to the case of a random field, we find the mean number of local maxima per unit area

$$\overline{n} = \int_{\mathbb{R}} \int_{\mathcal{V}} |g_4 g_6 - g_5^2| \rho_{(G_1,G_2,G_3,G_4,G_5,G_6)}(g_1, 0, 0, g_4, g_5, g_6) dg_1 dg_4 dg_5 dg_6,$$

where $\mathcal{V} = \{(g_4, g_5, g_6)\ :\ g_4 < 0,\ g_6 < 0,\ \text{and}\ g_4 g_6 - g_5^2 > 0\}$.

Proof: Statistical descriptors of local maxima (continued):

- Because of the relationships that exist between the statistical descriptors of $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ and those of its mean-square partial derivatives, if they exist, the mean $\boldsymbol{g} = E(\boldsymbol{G})$ and the covariance matrix $[C_{\boldsymbol{G}}] = E((\boldsymbol{G} - \overline{\boldsymbol{g}})(\boldsymbol{G} - \overline{\boldsymbol{g}})^{\mathrm{T}})$ of $\boldsymbol{G} = (G_1, G_2, G_3, G_4, G_5, G_6)$ read as

$$\overline{\boldsymbol{g}} = \boldsymbol{0} \quad \text{and} \quad [C_{\boldsymbol{G}}] = \begin{bmatrix} \mu_0 & 0 & 0 & -\mu_2 & 0 & -\mu_2 \\ 0 & \mu_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mu_2 & 0 & 0 & 0 \\ -\mu_2 & 0 & 0 & \mu_4 & 0 & \mu_4/3 \\ 0 & 0 & 0 & 0 & \mu_4/3 & 0 \\ -\mu_2 & 0 & 0 & \mu_4/3 & 0 & \mu_4 \end{bmatrix}.$$

- If $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ is a Gaussian random field, then $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ and its mean-square partial derivatives, if they exist, are jointly Gaussian random fields. This property follows from the fact that mean-square convergence of random variables implies convergence in distribution. Hence, the joint probability distribution of $\boldsymbol{G} = (G_1, G_2, G_3, G_4, G_5, G_6)$ reads as:

$$\rho_{\boldsymbol{G}}(\boldsymbol{g}) = \frac{1}{\sqrt{(2\pi)^6 \det([C_{\boldsymbol{G}}])}} \exp\left(-\frac{1}{2}\boldsymbol{g}^{\mathrm{T}}[C_{\boldsymbol{G}}]^{-1}\boldsymbol{g}\right).$$

- After inserting this expression for $\rho_{\boldsymbol{G}}$ into the expression for $\overline{n}$ and after a tedious analytical calculation of the integral (see Nayak, 1971), we obtain $\overline{n} = \frac{1}{6\pi\sqrt{3}}\frac{\mu_4}{\mu_2}$, as asserted.

More details: Conclusion

- The theory of stochastic processes affords a natural extension to random fields. As for stochastic processes, various statistical descriptors can be defined for random fields, such as the mean function, the autocorrelation function, the power spectral density function, and spectral moments.

- For zero-mean, isotropic, mean-square stationary, Gaussian two-dimensional random fields, statistical descriptors (mean number per unit area, local structure,. . .) of the local maxima can be deduced from only the first few spectral moments.

- Greenwood/Williamson and McCool use these statistical descriptors of the local maxima to replace a given representation of a rough surface as a random field with an “equivalent” representation of the rough surface as a random collection of spheres, thus allowing an average contact force per unit area to be calculated by using analytical contact theories for the contact of spheres.

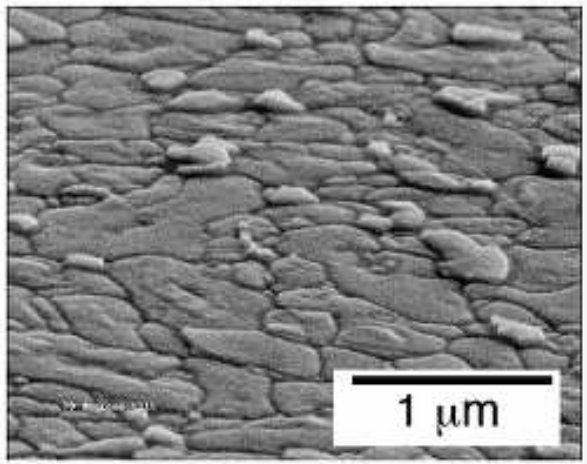
- The traction-distance curve and other relationships are important in designing devices, involving rough surfaces, which can fail due to adhesion, such as MicroElectroMechanical Systems (MEMS).

From data to random field

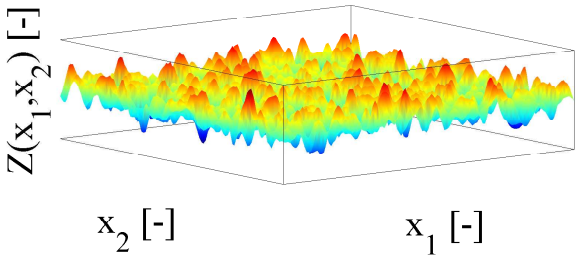
From data to random field

- Now, we will see how the power spectral density function can be estimated from experimental data:

Experimental data
Atomic Force Microscopy



Random field model
of surface roughness

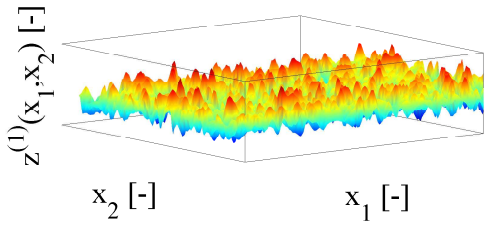


- A Gaussian random field is fully defined once its mean function and either its autocorrelation function or the corresponding power spectral density function have been specified. Here, only either the autocorrelation function or the corresponding power spectral density function is required because we model the surface roughness as a Gaussian random field that has zero mean.

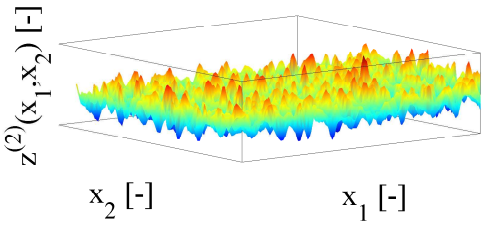
From data to random field

- **Context**:
  Let $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ be a zero-mean, mean-square stationary, second-order random field indexed by $\mathbb{R}^2$ with values in $\mathbb{R}$. Let $\{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^2\}$ admit a power spectral density function s_Z that is continuous and has a bounded support $\text{supp}(s_Z) = [-\xi_L, \xi_L] \times [-\xi_L, \xi_L]$.

- **Available information**:
  Let ν realizations $\{z^{(j)}(\boldsymbol{x}),\ -\frac{\chi}{2} \leq x_1, x_2 \leq \frac{\chi}{2}\}$ with domain $[-\frac{\chi}{2}, \frac{\chi}{2}] \times [-\frac{\chi}{2}, \frac{\chi}{2}]$ be available:

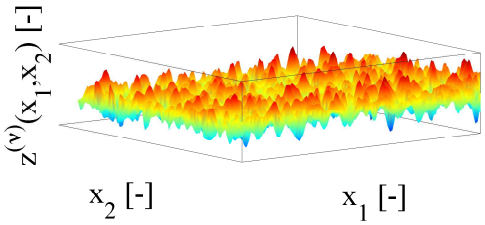


$\{z^{(1)}(\boldsymbol{x}), -\frac{\chi}{2} \leq x_1, x_2 \leq \frac{\chi}{2}\}$.



$\{z^{(2)}(\boldsymbol{x}), -\frac{\chi}{2} \leq x_1, x_2 \leq \frac{\chi}{2}\}$.

$\ldots$



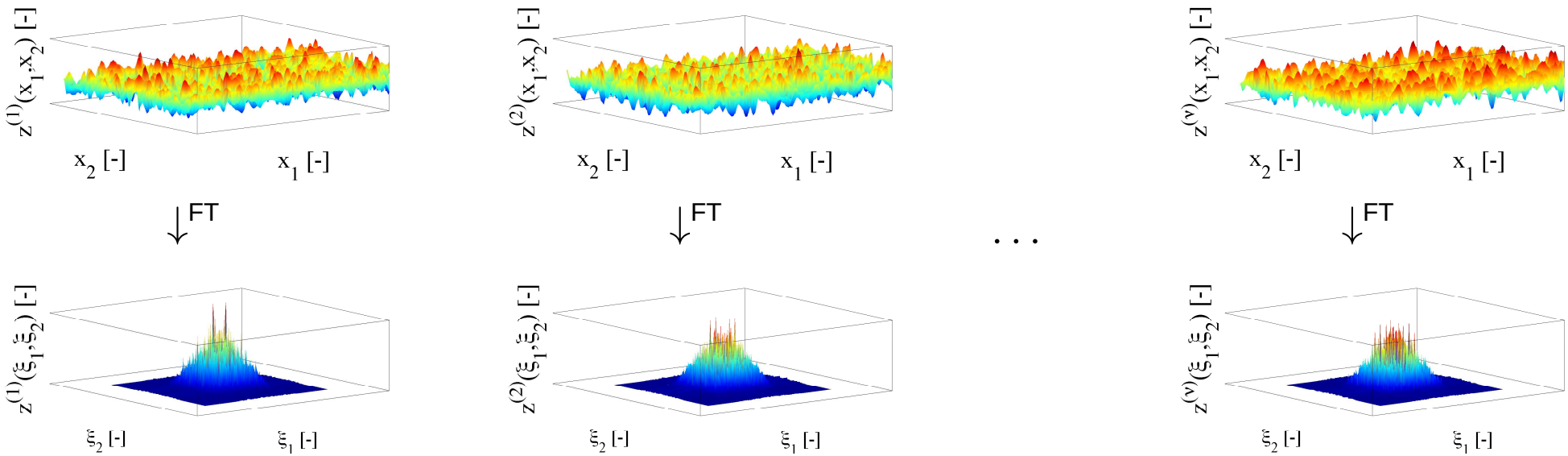
$\{z^{(\nu)}(\boldsymbol{x}), -\frac{\chi}{2} \leq x_1, x_2 \leq \frac{\chi}{2}\}$.

- **Objective of the estimation**:
  We will consider the inference of an estimate $s_Z^{\chi,\nu}$ of the power spectral density function s_Z from the available information $\left\{\{z^{(j)}(\boldsymbol{x}),\ -\frac{\chi}{2} \leq x_1, x_2 \leq \frac{\chi}{2}\},\ 1 \leq j \leq \nu\right\}$.

- **Available estimation methods**:
  - Indirect method: estimate first the autocorrelation and then the p.s.d. function therefrom.
  - Direct method: let's look at this method in more detail!

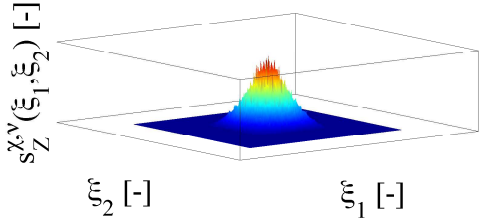
From data to random field

- **Step 1**: Transform each realization into the wavenumber domain by using the FT, assuming that this realization vanishes outside of the domain $[-\frac{\chi}{2}, \frac{\chi}{2}] \times [-\frac{\chi}{2}, \frac{\chi}{2}]$:



- **Step 2**: Compute the estimate $s_Z^{\chi,\nu}$ of s_Z as follows:

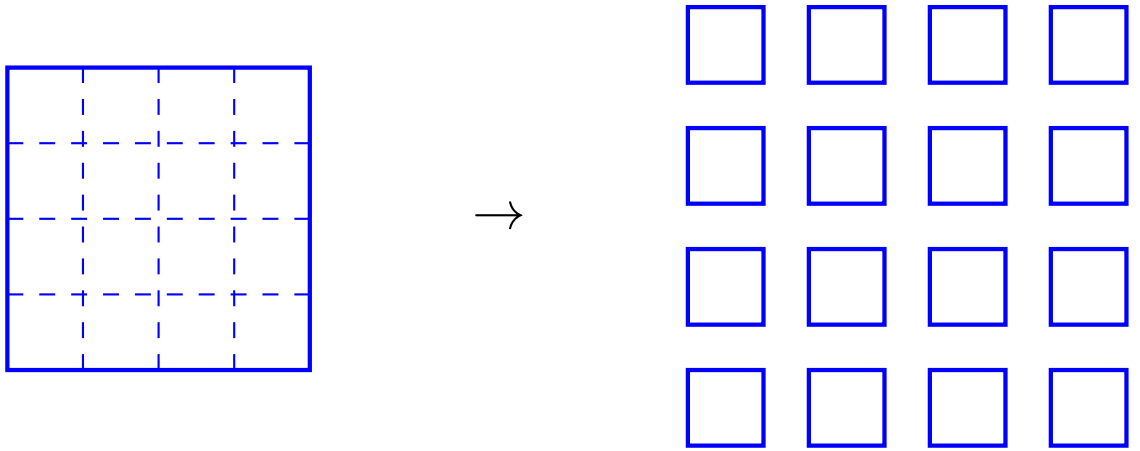
$$s_Z(\boldsymbol{\xi}) \approx s_Z^{\chi,\nu}(\boldsymbol{\xi}) = \frac{1}{\chi^2}\,\frac{1}{\nu}\sum_{j=1}^{\nu} |\hat{z}^{(j)}(\boldsymbol{\xi})|^2, \quad \forall \boldsymbol{\xi} \in \mathbb{R}^2,$$



- Here, the FT can be approximated by DFT (see Slides 79–80).

From data to random field

- What if the available information consists of only a single realization?
- **Step 0**: Split the realization into ν subrealizations of equal domain:



- **Step 1**: Transform each subrealization into the wavenumber domain by using the FT.
- **Step 2**: Compute the estimate $s_Z^{\chi,\nu}$ of s_Z using the equation mentioned previously.
- Determine ν and χ such that a suitable bias/variance tradeoff is achieved (see Slides 75–78). As a rule of thumb, a splitting into $\nu = 8 \times 8$ subrealizations is often used.

From data to random field

- Matlab code used to generate the previous figures:

```
% simulation of one realization of Gaussian random field with triangular p.s.d.

a=0.1; % spatial correlation length along one dimension
mu=1024; % number of discretization points along one dimension
chi=50; % size of spatial domain along one dimension

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

Dx=chi/mu;

z=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((a/pi)^2*tripuls(xi'*a/pi/2)*tripuls(xi*a/pi/2)/(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))));

% estimation of power spectral density function given z and Dx

mu=length(z);

nutilde=8; % number of subrealizations along one dimension

sZ=zeros(mu/nutilde,mu/nutilde);
for m1=1:nutilde
  for m2=1:nutilde
    zmuhat=Dx^2*fft2(z((m1-1)*mu/nutilde+1:m1*mu/nutilde,(m2-1)*mu/nutilde+1:m2*mu/nutilde).*...
      (exp(i*[-mu/nutilde/2:mu/nutilde/2-1]'*pi)*exp(i*[-mu/nutilde/2:mu/nutilde/2-1]*pi))./...
      (exp(-i*[0:mu/nutilde-1]'*pi)*exp(-i*[0:mu/nutilde-1]*pi));
    sZ=sZ+(1/nutilde)^2*(nutilde/mu/Dx)^2*abs(zmuhat).^2;
  end
end

figure;surf([-pi/Dx:2*pi/mu/Dx*nutilde:pi/Dx-2*pi/mu/Dx*nutilde],[-pi/Dx:2*pi/mu/Dx*nutilde:pi/Dx-2*pi/mu/Dx*nutilde],abs(zmuhat));

figure;surf([-pi/Dx:2*pi/mu/Dx*nutilde:pi/Dx-2*pi/mu/Dx*nutilde],[-pi/Dx:2*pi/mu/Dx*nutilde:pi/Dx-2*pi/mu/Dx*nutilde],sZ);
```

More details: Bias and variance of estimators of mean and variance

- Let us recall the following elements from statistics...
- Let Z be a second-order r.v. with values in $\mathbb{R}$. Its mean $\overline{z}$ and variance σ_Z^2 are given by

$$\overline{z} = \int_{\mathbb{R}} z \rho_Z(z) dz \quad \text{and} \quad \sigma_Z^2 = \int_{\mathbb{R}} z \rho_Z (z - \overline{z})^2 dz.$$

- Let $z^{(1)}, \ldots, z^{(\nu)}$ be ν independent realizations of Z. Their sample mean $\overline{z}^\nu$ and sample variance $(s_Z^\nu)^2$ are given by

$$\overline{z}^\nu = \frac{1}{\nu} \sum_{j=1}^{\nu} z^{(j)} \quad \text{and} \quad (s_Z^\nu)^2 = \frac{1}{\nu - 1} \sum_{j=1}^{\nu} \left(z^{(j)} - \overline{z}^\nu \right)^2.$$

- To show the adequacy of these statistical estimates, we can study the bias and variance of the corresponding estimators. Given ν independent and identically distributed copies $Z^{(1)}, \ldots, Z^{(\nu)}$ of Z, the estimators $\overline{Z}$ and $(S_Z^\nu)^2$ of the mean and the variance of Z, respectively, are given by

$$\overline{Z}^\nu = \frac{1}{\nu} \sum_{j=1}^{\nu} Z^{(j)} \quad \text{and} \quad (S_Z^\nu)^2 = \frac{1}{\nu - 1} \sum_{j=1}^{\nu} \left(Z^{(j)} - \overline{Z}^\nu \right)^2.$$

More details: Bias and variance of estimators of mean and variance (continued)

- It can be easily shown that the estimators $\overline{X}$ and $(S_X^\nu)^2$ are unbiased, that is,

$$E\big(\overline{Z}^\nu\big) = \overline{z} \quad \text{and} \quad E\big(S_Z^\nu\big)^2 = \sigma_Z^2,$$

and that the variance of the the estimators $\overline{X}$ and $(S_X^\nu)^2$ decreases with the square root of ν:

$$E\Big(\big(\overline{Z}^\nu - \overline{z}\big)^2\Big) = \frac{\sigma_Z^2}{\nu} \quad \text{and} \quad E\Big(\big(S_Z^\nu\big)^2 - \sigma_Z^2\big)^2\Big) \approx \frac{E\big((Z-\overline{z})^4\big) - \sigma_Z^4}{\nu}.$$

- Hence, provided that $E\big((Z-\overline{z})^4\big) < +\infty$, the accuracy of statistical estimates of the mean and variance improves with the square root of the number of samples ν.

- More generally, to show the adequacy of statistical estimates, we can study the bias and variance of the corresponding estimators. We will do this for the aforementioned estimator of the p.s.d. next.

More details: Bias and variance of estimator of p.s.d.

- The mean of the estimator of the power spectral density function reads as follows:

$$E\big(S_Z^{\chi,\nu}(\boldsymbol{\xi})\big) = \frac{1}{\chi^2} E\big(|\widehat{Z}(\boldsymbol{\xi})|^2\big), \quad \text{where} \quad \widehat{Z}(\boldsymbol{\xi}) = \int_{\mathbb{R}^2} 1_{[-\frac{\chi}{2},\frac{\chi}{2}]\times[-\frac{\chi}{2},\frac{\chi}{2}]}(\boldsymbol{x}) Z(\boldsymbol{x}) \exp(-i\boldsymbol{\xi}\cdot\boldsymbol{x}) d\boldsymbol{x}.$$

- Elaborating and then using the expression for the autocorrelation function, we obtain

$$\begin{aligned} E(S_Z^{\chi,\nu}(\boldsymbol{\xi})) &= \frac{1}{\chi^2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} 1_{[-\frac{\chi}{2},\frac{\chi}{2}]\times[-\frac{\chi}{2},\frac{\chi}{2}]}(\boldsymbol{x}) 1_{[-\frac{\chi}{2},\frac{\chi}{2}]\times[-\frac{\chi}{2},\frac{\chi}{2}]}(\tilde{\boldsymbol{x}}) r_Z(\boldsymbol{x}-\tilde{\boldsymbol{x}}) \exp\big(-i\boldsymbol{\xi}\cdot(\boldsymbol{x}-\tilde{\boldsymbol{x}})\big) d\boldsymbol{x} d\tilde{\boldsymbol{x}}, \\ &= \frac{1}{\chi^2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} 1_{[-\frac{\chi}{2},\frac{\chi}{2}]\times[-\frac{\chi}{2},\frac{\chi}{2}]}(\boldsymbol{x}) 1_{[-\frac{\chi}{2},\frac{\chi}{2}]\times[-\frac{\chi}{2},\frac{\chi}{2}]}((\boldsymbol{x}-\tilde{\boldsymbol{x}})-\boldsymbol{x}) r_Z(\boldsymbol{x}-\tilde{\boldsymbol{x}}) \exp\big(-i\boldsymbol{\xi}\cdot(\boldsymbol{x}-\tilde{\boldsymbol{x}})\big) d\boldsymbol{x} d(\boldsymbol{x}-\tilde{\boldsymbol{x}}). \end{aligned}$$

- Using the relationships between the convolution, product, and Fourier transform, we obtain

$$E\big(S_Z^{\chi,\nu}(\boldsymbol{\xi})\big) = \frac{1}{\chi^2}\left(\frac{1}{(2\pi)^2}|\hat{1}_{[-\frac{\chi}{2},\frac{\chi}{2}]\times[-\frac{\chi}{2},\frac{\chi}{2}]}|^2 \star s_Z\right)(\boldsymbol{\xi}).$$

  In the limit as the domain size χ of the realizations increases to infinity, we obtain

$$\lim_{\chi\to+\infty} \frac{1}{\chi^2}\frac{1}{(2\pi)^2}|\hat{1}_{[-\frac{\chi}{2},\frac{\chi}{2}]\times[-\frac{\chi}{2},\frac{\chi}{2}]}|^2 = \delta_{\mathbf{0}}, \quad \text{hence,} \quad \lim_{\chi\to+\infty} E\big(S_Z^{\chi,\nu}(\boldsymbol{\xi})\big) = s_Z(\boldsymbol{\xi}).$$

  Thus, for finite domain size χ, there is **leakage**, that is, local averaging of wavenumber components. As the domain size χ increases, leakage decreases. The estimator is asymptotically unbiased.

- We conclude that the **wavenumber resolution improves with increasing domain size χ**.

More details: Bias and variance of estimator of p.s.d. (continued)

- The variance of the estimator of the power spectral density function reads as follows:

$$E\Big(S_Z^{\chi,\nu}(\boldsymbol{\xi}) - E\big(S_Z^{\chi,\nu}(\boldsymbol{\xi})\big)^2\Big) = E\big(|S_Z^{\chi,\nu}(\boldsymbol{\xi})|^2\big) - \Big(E\big(S_Z^{\chi,\nu}(\boldsymbol{\xi})\big)\Big)^2.$$

- Using $S_Z^{\chi,\nu}(\boldsymbol{\xi}) = \frac{1}{\chi^2}\,\frac{1}{\nu}\sum_{j=1}^{\nu}|\widehat{Z}^{(j)}(\boldsymbol{\xi})|^2$, where $\widehat{Z}^{(j)}(\boldsymbol{\xi}) = \int_{\mathbb{R}^2} 1_{[-\frac{\chi}{2},\frac{\chi}{2}]\times[-\frac{\chi}{2},\frac{\chi}{2}]}(\boldsymbol{x}) Z^{(j)}(\boldsymbol{x}) \exp(-i\boldsymbol{\xi}\cdot\boldsymbol{x}) d\boldsymbol{x}$,

$$E\Big(S_Z^{\chi,\nu}(\boldsymbol{\xi}) - E\big(S_Z^{\chi,\nu}(\boldsymbol{\xi})\big)^2\Big) = \frac{1}{\chi^4}\,\frac{1}{\nu}\Big(E\big(|\widehat{Z}(\boldsymbol{\xi})|^4\big) - \big|E\big(|\widehat{Z}(\boldsymbol{\xi})|^2\big)\big|^2\Big).$$

  Thus, provided that the additional condition that $E\big(|\widehat{Z}(\boldsymbol{\xi})|^4\big) < +\infty$ is fulfilled, the error introduced by the use of only a finite number of realizations decreases with increasing number of realizations ν.

- We conclude that the **error introduced by the use of only a finite number of realizations decreases with increasing number of realizations ν.**

More details: Computation of Fourier transform by using the DFT

- The Fourier transform can be approximated numerically by using the DFT as follows.
- Let us consider a smooth function z from $\mathbb{R}^2$ into $\mathbb{R}$ whose Fourier transform $\hat{z}$ vanishes outside a bounded interval $[-\xi_{\mathsf{L}}, \xi_{\mathsf{L}}] \times [-\xi_{\mathsf{L}}, \xi_{\mathsf{L}}]$.
- To numerically approximate the Fourier transform $\hat{z}$ of z by using the DFT, we require corresponding samplings of the spatial domain and the wavenumber domain, respectively:

$$\left\{ \boldsymbol{x}_{(k_1,k_2)} = \left(\left(k_1 - \frac{\mu}{2} - 1\right)\Delta x, \left(k_2 - \frac{\mu}{2} - 1\right)\Delta x \right), 1 \leq k_1, k_2 \leq \mu \right\} \text{ with space step } \Delta x,$$

$$\left\{ \boldsymbol{\xi}_{(\ell_1,\ell_2)} = \Big(-\xi_{\mathsf{L}} + (\ell_1 - 1)\Delta\xi, -\xi_{\mathsf{L}} + (\ell_2 - 1)\Delta\xi \Big), 1 \leq \ell_1, \ell_2 \leq \mu \right\} \text{ with wavenumber step } \Delta\xi = 2\xi_{\mathsf{L}}/\mu.$$

We say that these samplings of the spatial domain and the wavenumber domain correspond if the spatial step is chosen as $\Delta x = \pi/\xi_{\mathsf{L}}$ (Nyquist criterion). We then obtain

$$\hat{z}(\boldsymbol{\xi}_{(\ell_1,\ell_2)}) \approx \exp\big(i\pi(\ell_1-1)+i\pi(\ell_2-1)\big) \underbrace{\sum_{k_1=1}^{\mu}\sum_{k_2=1}^{\mu} \tilde{z}_{(k_1,k_2)} \exp\Big(-i(k_1-1)\frac{2\pi}{\mu}(\ell_1-1) - i(k_2-1)\frac{2\pi}{\mu}(\ell_2-1)\Big)}_{\text{DFT}},$$

where

$$\tilde{z}_{(k_1,k_2)} = \Delta x^2 z\big(\boldsymbol{x}_{(k_1,k_2)}\big) \exp\left(i\left(k_1 - \frac{\mu}{2} - 1\right)\pi + i\left(k_2 - \frac{\mu}{2} - 1\right)\pi \right).$$

- If μ is a power of 2, this can be implemented efficiently by using the fast Fourier transform (FFT).

More details: Computation of Fourier transform by using the DFT (continued)

- In summary, we consider the following samplings of the spatial and wavenumber domains:

spatial domain

size of sampled portion $\mu\Delta x$

step Δx

$$\boxed{\Delta x = \frac{\mu\Delta x}{\mu}}$$

$$x_k = \big(k - \tfrac{\mu}{2} - 1\big)\Delta x,\ 1 \le k \le \mu.$$

wavenumber domain

size of sampled portion $2\xi_{\mathsf{L}}$

step $\Delta\xi$

$$\boxed{\Delta\xi = \frac{2\xi_{\mathsf{L}}}{\mu}}$$

$$\xi_\ell = -\xi_{\mathsf{L}} + (\ell - 1)\Delta\xi,\ 1 \le k \le \mu.$$

- These samplings of the spatial domain and the wavenumber domain correspond in that

$$\boxed{\begin{aligned} \Delta x &= \frac{\pi}{\xi_{\mathsf{L}}} = \frac{2\pi}{2\xi_{\mathsf{L}}}, \\ \mu\Delta x &= \frac{\mu\pi}{\xi_{\mathsf{L}}} = \frac{2\pi}{\Delta\xi}. \end{aligned}}$$

- This correspondence indicates that the step Δx in the spatial domain is inversely proportional to the size $2\xi_{\mathsf{L}}$ of the sampled portion of the wavenumber domain and that the size $\mu\Delta x$ of the sampled portion of the spatial domain is inversely proportional to the step $\Delta\xi$ in the wavenumber domain.

Proof: Computation of Fourier transform by using the DFT

- We begin by representing the Fourier transform using the Shannon/Poisson formula

$$\hat{z}(\boldsymbol{\xi}) = 1_{[-\xi_{\mathsf{L}},\xi_{\mathsf{L}}]\times[-\xi_{\mathsf{L}},\xi_{\mathsf{L}}]}(\boldsymbol{\xi})\Delta x^2 \sum_{\tilde{k}_1=-\infty}^{+\infty}\sum_{\tilde{k}_2=-\infty}^{+\infty} f(\tilde{k}_1\Delta x, \tilde{k}_2\Delta x)\exp(-i\tilde{k}_1\Delta x\xi_1 - i\tilde{k}_2\Delta x\xi_2),$$

  which we approximate by

$$\hat{z}^{\mu}(\boldsymbol{\xi}) = 1_{[-\xi_{\mathsf{L}},\xi_{\mathsf{L}}]\times[-\xi_{\mathsf{L}},\xi_{\mathsf{L}}]}(\boldsymbol{\xi})\Delta x^2 \sum_{\tilde{k}_1=-\mu/2}^{\mu/2-1}\sum_{\tilde{k}_2=-\mu/2}^{\mu/2-1} f(\tilde{k}_1\Delta x, \tilde{k}_2\Delta x)\exp(-i\tilde{k}_1\Delta x\xi_1 - i\tilde{k}_2\Delta x\xi_2).$$

- At the sampling points in the wavenumber domain, we obtain

$$\hat{z}^{\mu}(\boldsymbol{\xi}_{(\ell_1,\ell_2)}) = \Delta x^2 \sum_{\tilde{k}_1=-\mu/2}^{\mu/2-1}\sum_{\tilde{k}_2=-\mu/2}^{\mu/2-1} f(\tilde{k}_1\Delta x, \tilde{k}_2\Delta x)\exp\Big(-i\tilde{k}_1\Delta x\big(-\xi_{\mathsf{L}}+(\ell_1-1)\Delta\xi\big)-i\tilde{k}_2\Delta x\big(-\xi_{\mathsf{L}}+(\ell_1-1)\Delta\xi\big)\Big).$$

- Because $\Delta x\xi_{\mathsf{L}} = \pi$ and therefore $\Delta x\Delta\xi = 2\pi/\mu$, we obtain

$$\hat{z}^{\mu}(\boldsymbol{\xi}_{(\ell_1,\ell_2)}) = \sum_{\tilde{k}_1=-\mu/2}^{\mu/2-1}\sum_{\tilde{k}_2=-\mu/2}^{\mu/2-1} \Delta x^2 f(\tilde{k}_1\Delta x, \tilde{k}_2\Delta x)\exp(i\tilde{k}_1\pi+i\tilde{k}_2\pi)\exp\Big(-i\tilde{k}_1\frac{2\pi}{\mu}(\ell_1-1)-i\tilde{k}_2\frac{2\pi}{\mu}(\ell_2-1)\Big).$$

- Finally, by the changes of variables $k_1 = \tilde{k}_1 + \mu/2 + 1$ and $k_2 = \tilde{k}_2 + \mu/2 + 1$, we find the asserted equation.

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