Micromechanical modeling of rough interface behavior

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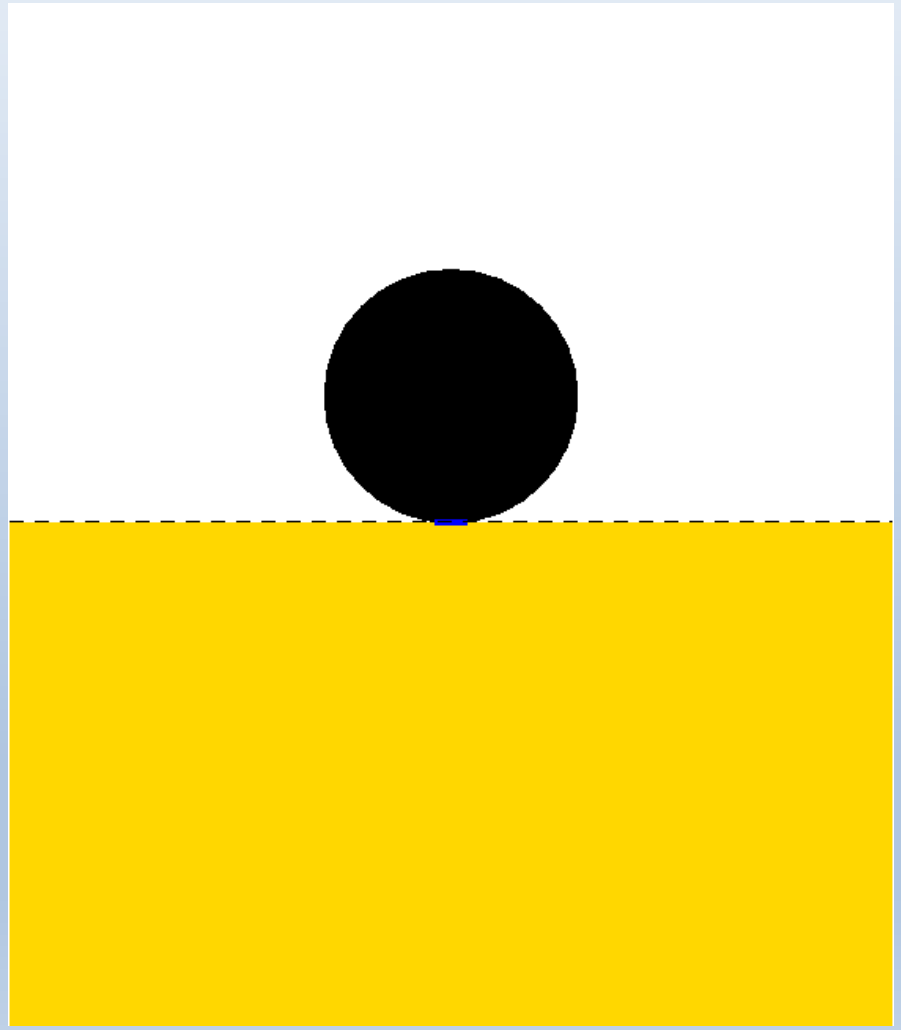
Associate professor in South China University of Technology in civil engineering.
Ph.D. degree in civil engineering at the University of Kansas in 2011,USA.
Postdoctoral fellow at John's Hopkins University from 2014 to 2016,USA.

research interests>computational mechanics and experimental mechanics. My group currently has 9 master students.

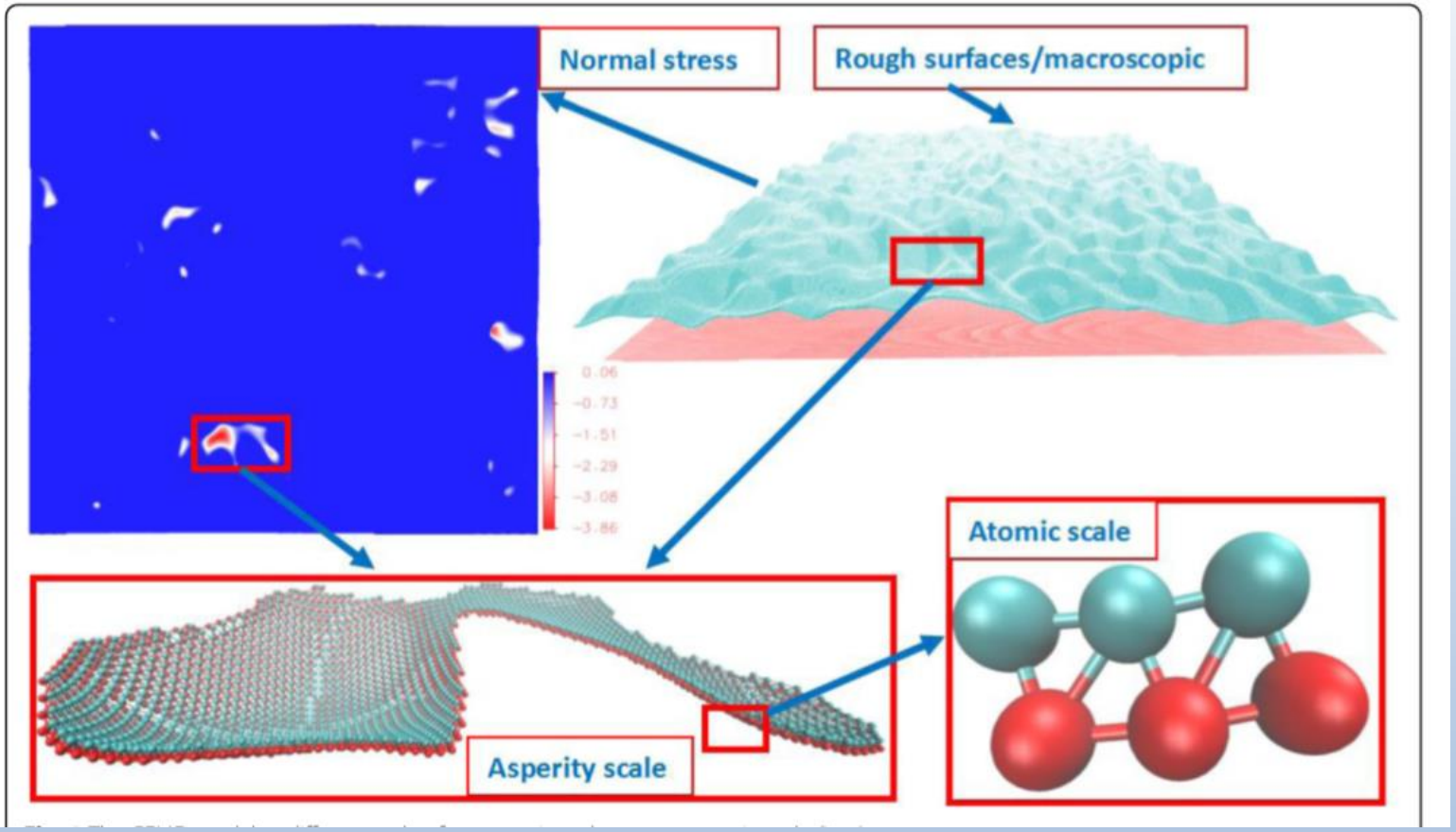
From September 2019 to February 2021, I am supported by NSFC-ERC project and will be a Visiting Professor at the ERC Advanced Grant project DyCon under the supervision of Prof. Enrique Zuazua (FAU, University of Deusto and UAM).

Contact mechanics is the study of the deformation of solids that touch each other at one or more points.

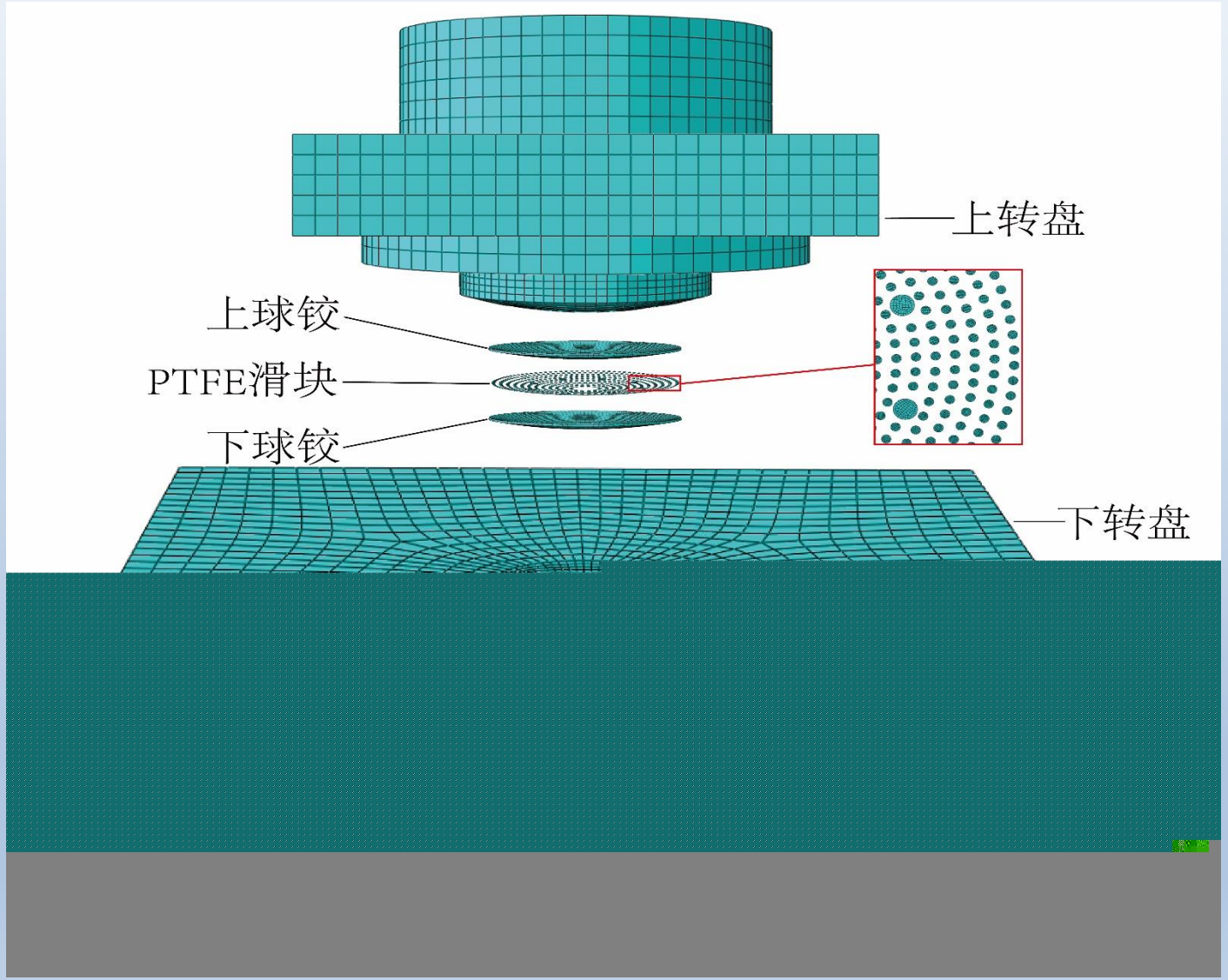


From Wikipedia

Atomic simulation



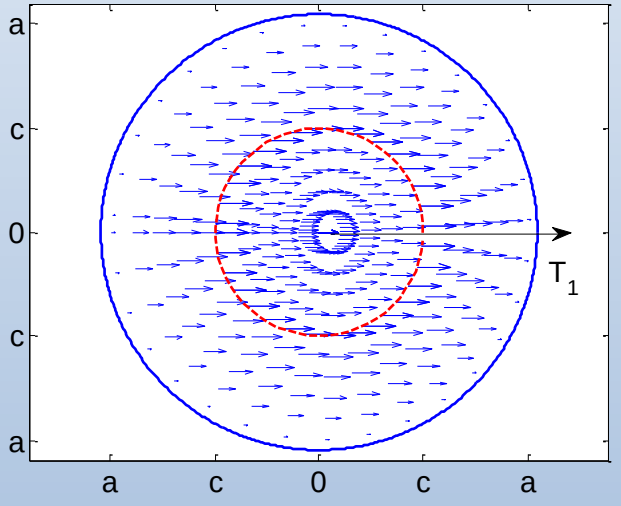
Finite element simulation based on Continuum mechanics

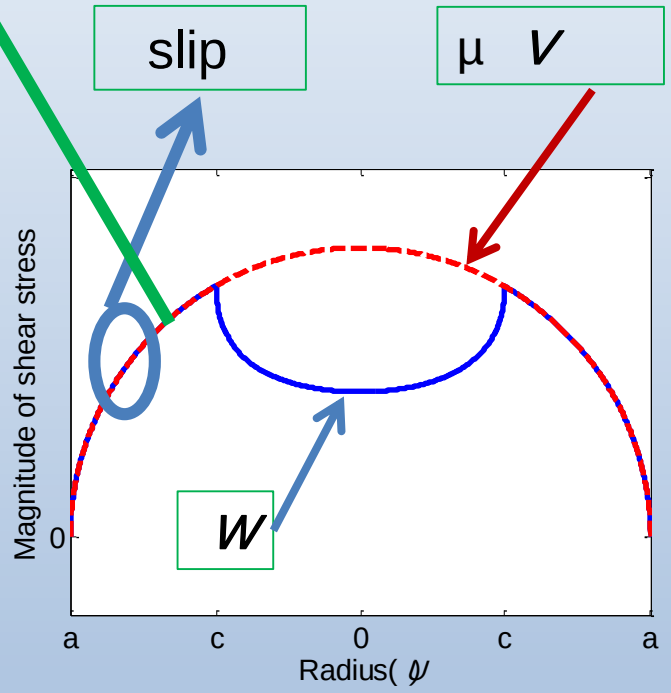


Asperity Mechanics
Basic formulation for Hertz-Mindlin system

Energy dissipation

Tangential traction on the contact area under shear





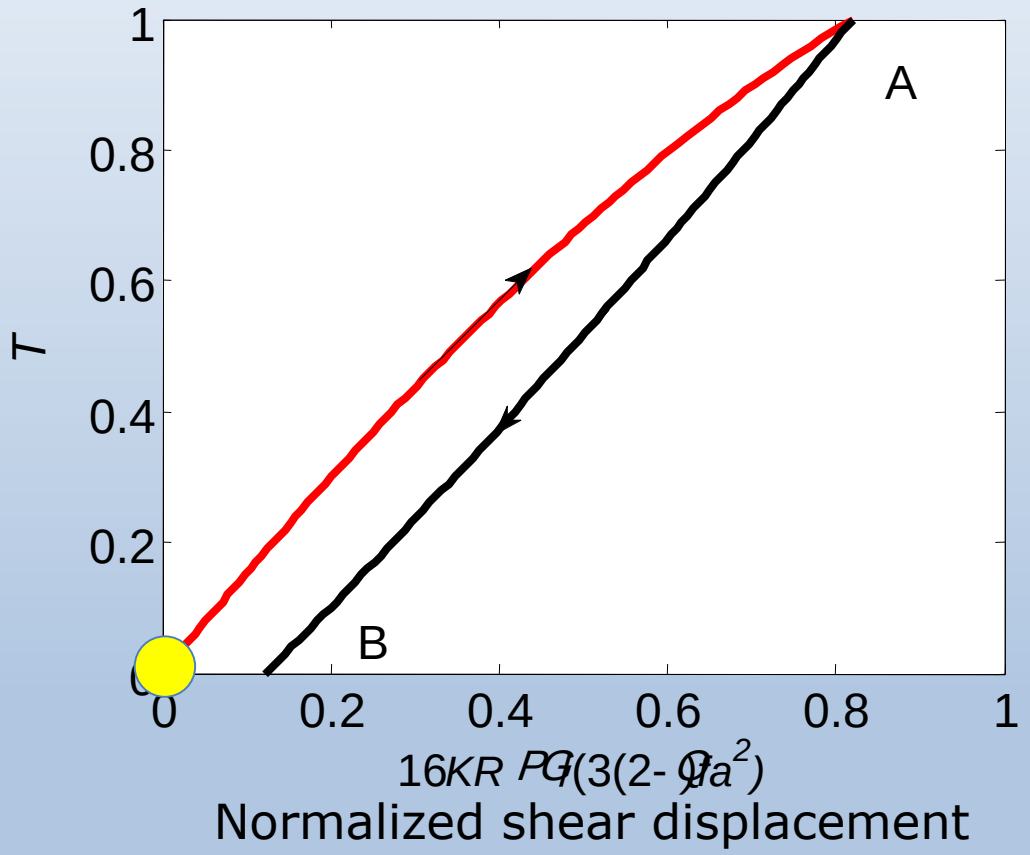
$$W \frac{3fN}{2Sa^3}(a^2 \quad {}^2)^{1/2}, c \; d \quad da$$

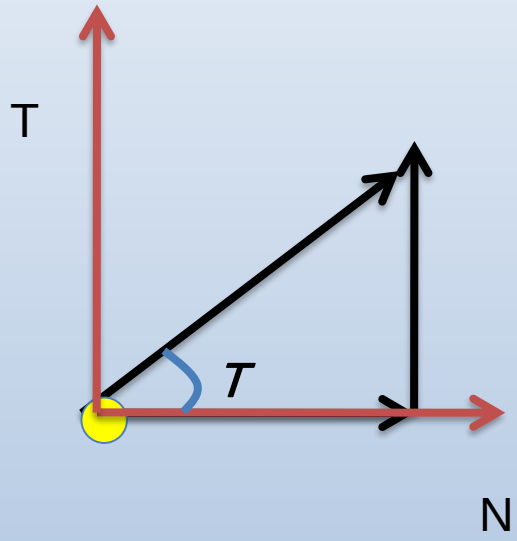
$$W \frac{3fN}{2Sa^3}(a^2 \quad {}^2)^{1/2} \; (c^2 \quad {}^2)^{1/3a}, \quad d\alpha$$

$$c \quad a(1 \quad \frac{T}{AN})^{1/3}$$

Cross section of the tangential traction

Asperity contact behavior Path dependent



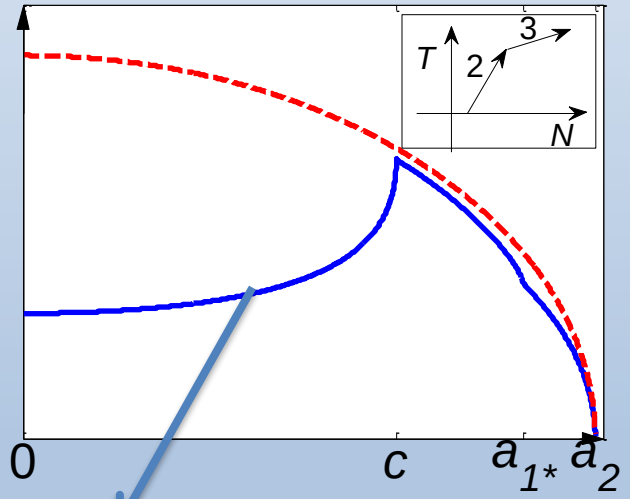


If tan T < P

The cause of path dependency

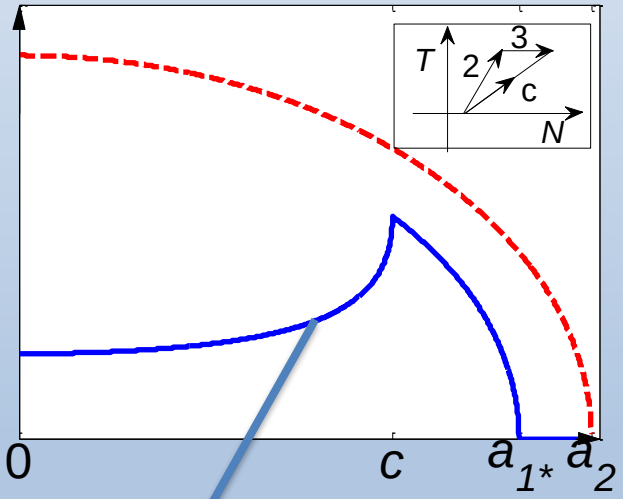
Different loading path may cause different tangential traction

(c)



Tangential traction

(d)



Tangential traction

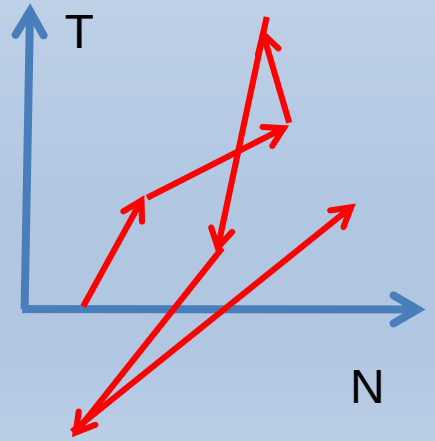
Extension of Hertz-Mindlin Theory

Only the shear behavior is path dependent, affected by loading ratio and loading history.

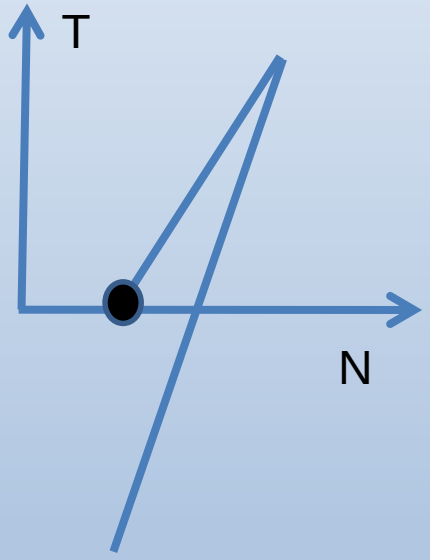
We derived a general procedure to get the tangential traction by superposition of the basic solution, which records all the loading history.

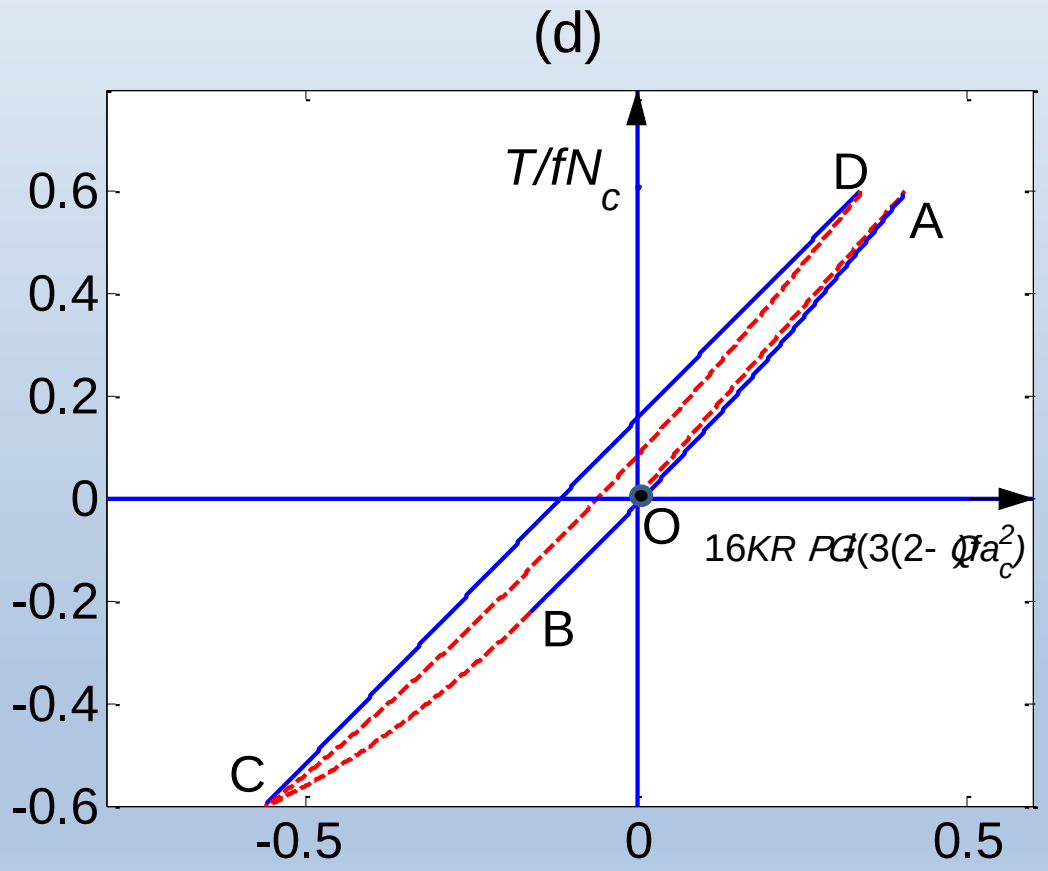
Based on the traction obtained, displacement, stiffness and energy dissipation can be determined.

This procedure allows us to solve any loading conditions in-plane

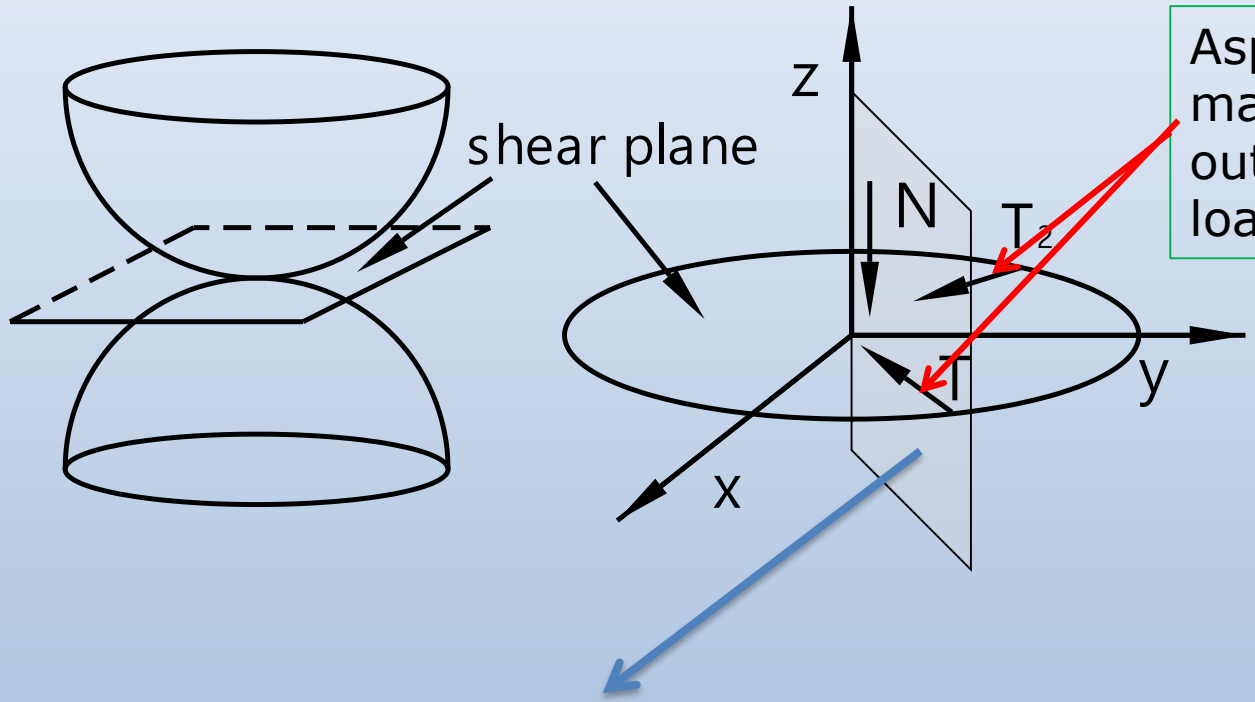


Extension of Hertz-Mindlin Theory: Example





Asperity contact mechanics: Out-of-plane loading

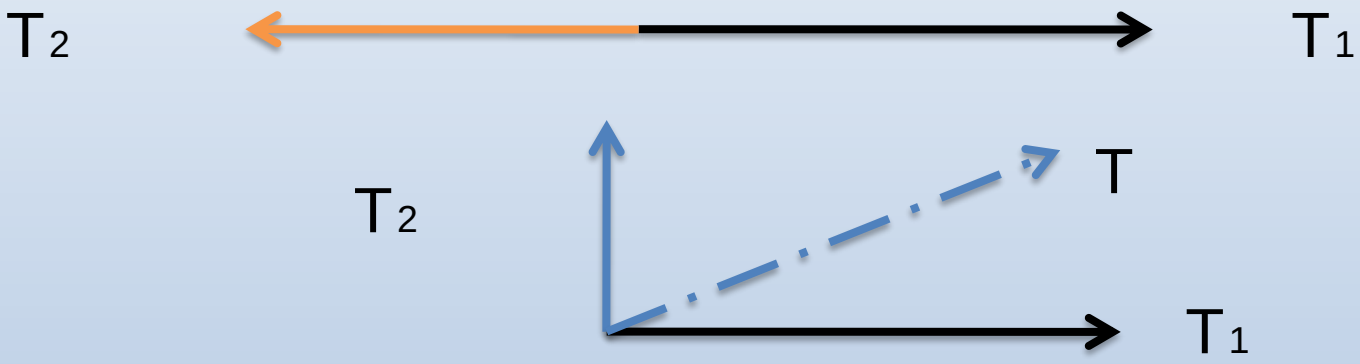


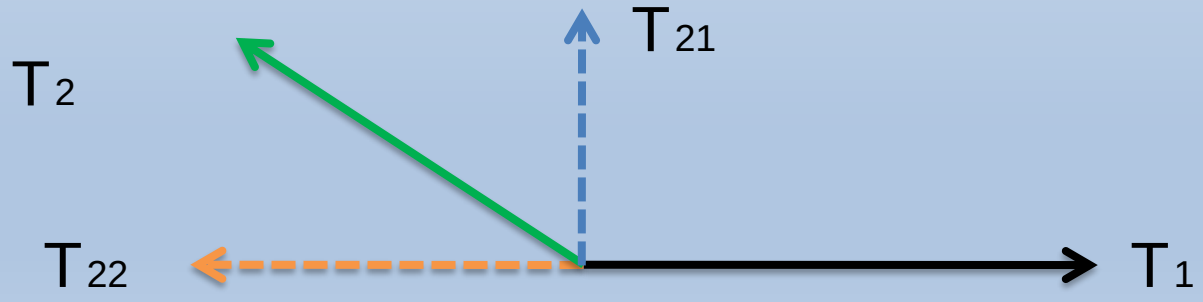
Asperity contact may experience out-of-plane loading

Hertz - Mindlin theory only concerned with in - plane loading

Difference between in-plane and out-of-plane loading

T_1 and T_2 are in shear plane, apply T_1 first, T_2 second





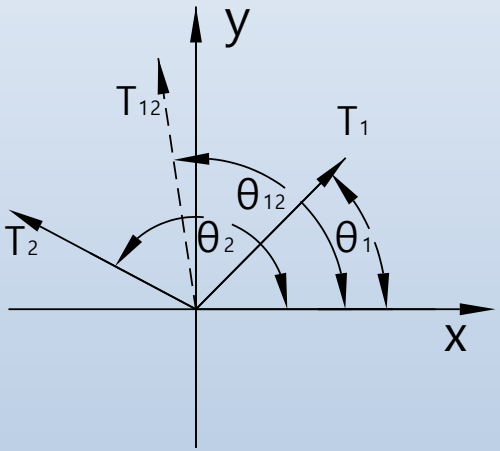
Solutions for the out-of-plane loading

Satisfy the Amonton Law

Has the same slip annulus

Equilibrium and boundary condition

T_1 and T_2 are in shear plane, apply T_1 first, T_2 second.



$$G_{x2} = \frac{3(2-\nu)(f\cos T_1 - k\cos_2 T)N}{16Ea}\left(1 - \frac{k\cos_2 T}{f\cos T_1 - k\cos_2 T}\frac{b^2}{a^2} - \frac{f\cos_1 T}{f\cos_1 T - k\cos_2 T}\frac{c^2}{a^2}\right)$$

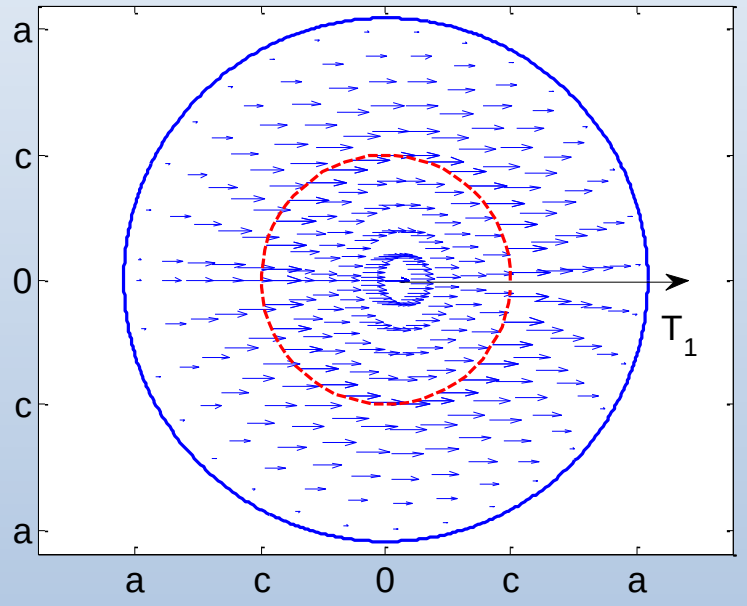
$$\frac{3(2-\nu)(f\cos T_1 - k\cos_2 T)N}{16Ea}\left(1 - \frac{k\cos_2 T}{f\cos T_1 - k\cos_2 T}\left(1 - \frac{T_2}{kN}\right)^{2/3} - \frac{f\cos_1 T}{f\cos_1 T - k\cos_2 T}\left(1 - \frac{T_1}{fN}\right)^{2/3}\right)$$

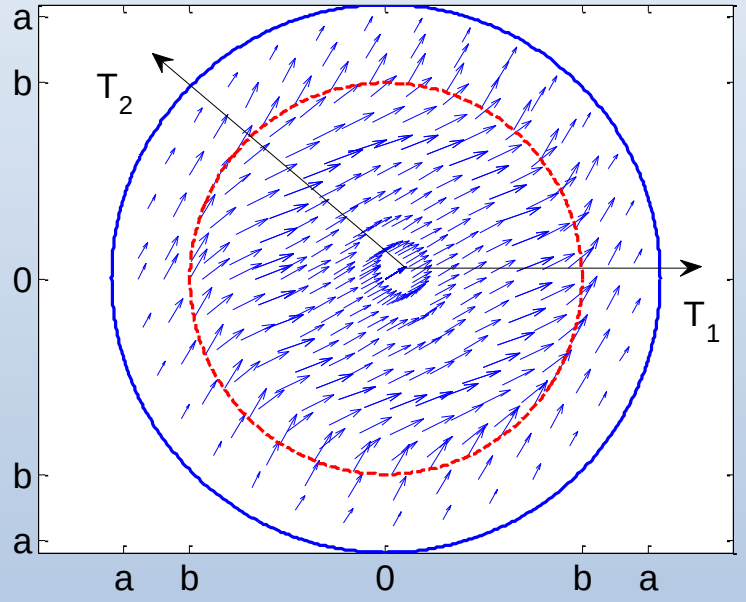
$$k = 2f\cos(\theta_1 - \theta_2)$$

G_{x2} is the shear displacement in x direction

Comparison in plane and out-of-plane loading

Tangential tractions

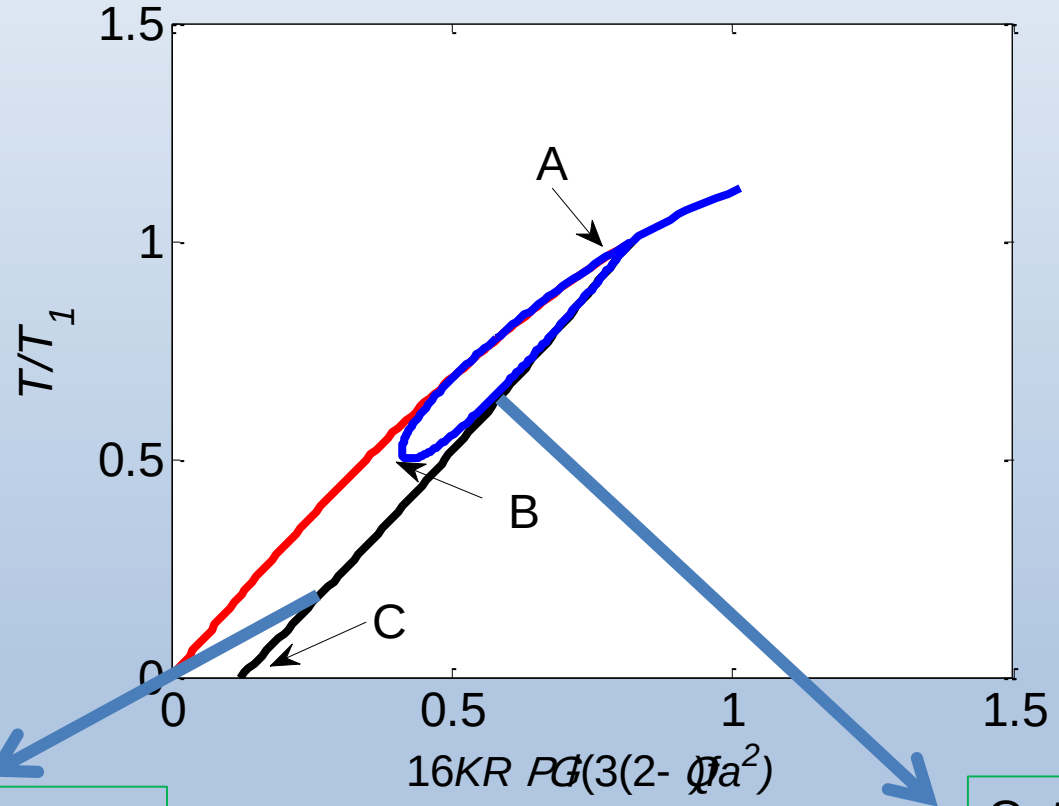




In - plane loading

Out - of - plane loading

Comparison in plane and out-of-plane loading



In - plane(Mindlin) (A - C curve)

Out - of - plane (A - B - A curve)

Conclusion from asperity contact mechanics

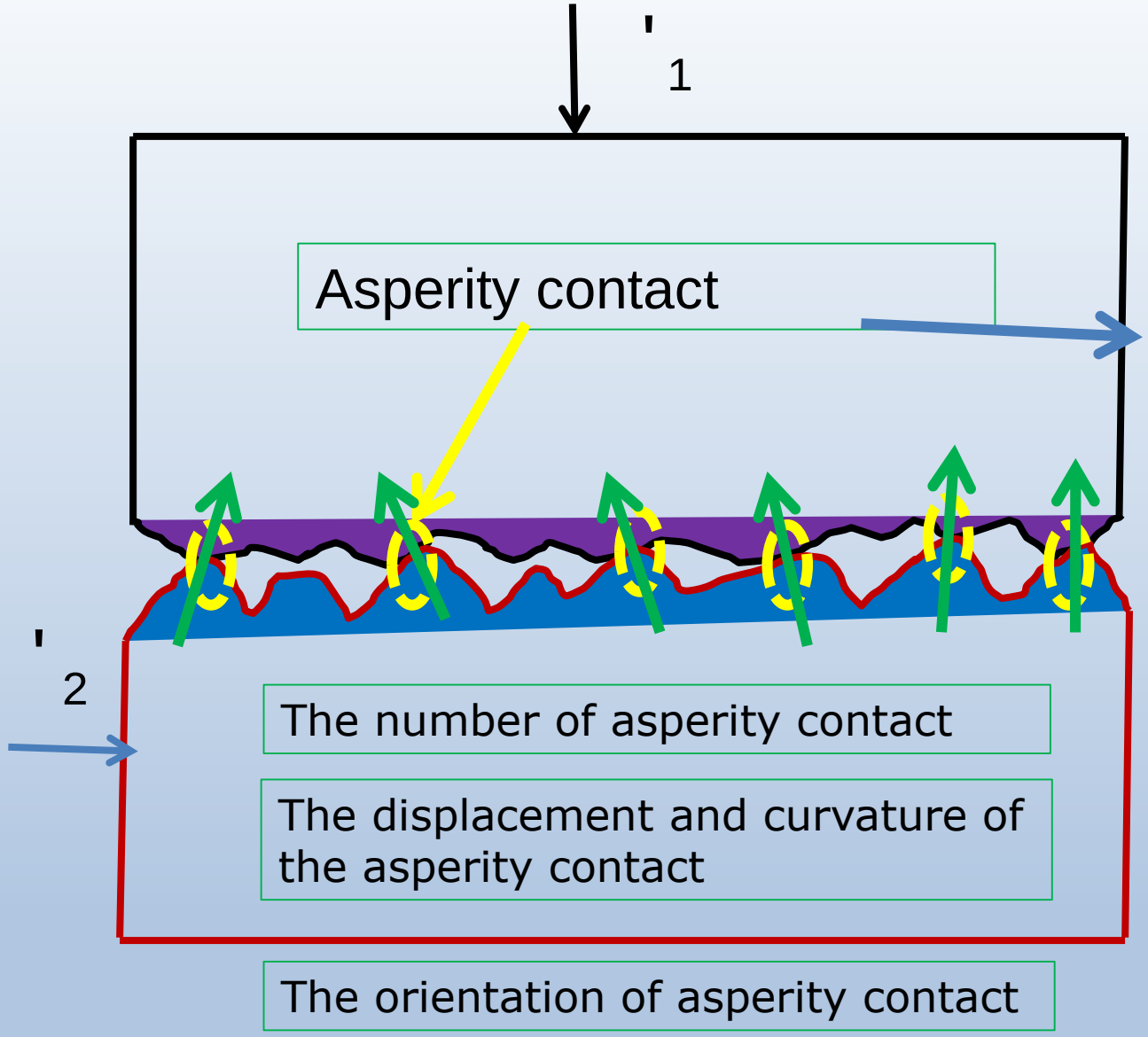
Tangential traction is path dependent

Out-of-plane loading may cause loading and unloading simultaneously

Energy dissipation could be avoided by choosing the path

The upper bound energy dissipation can be determined by in-plane loading, loading the normal direction first, shear second.

However, for engineering applications, the path dependency can be ignored because dissipation is small


'
1
Asperity contact
'
2
The number of asperity contact
The displacement and curvature of the asperity contact
The orientation of asperity contact

Why statistical method

We have N=100000000 asperity contact points

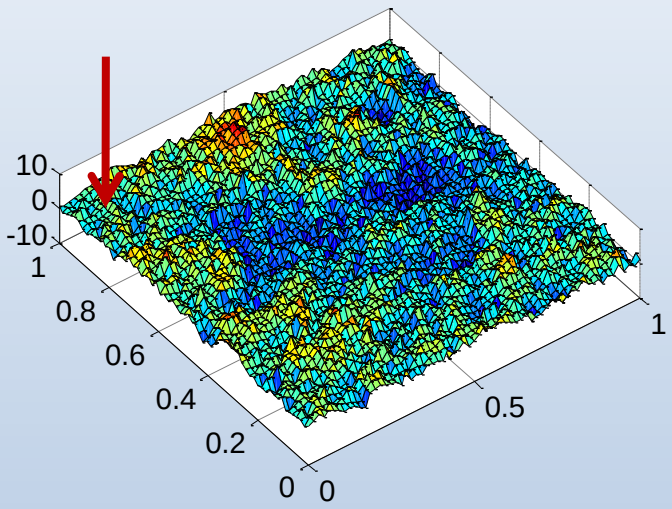
the probability of the following conditions is:
displacement($G = G_0$)
Radius of curvature($R = R_0$)
Contact orientation($T = 0$)
p=1/100000

N_0 = Np =1000 points have the same behavior

One calculation for 1000 asperity contacts=Efficiency

The key is to get the probability distribution

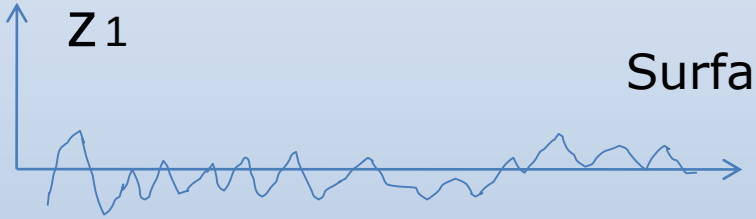
Statistical description of the rough interface- Fundamental equations



$$z_1(x,y) = \sum_{n1} c_{n1}\cos(xk_{xn1} + yk_{yn1} + H_{n1})$$

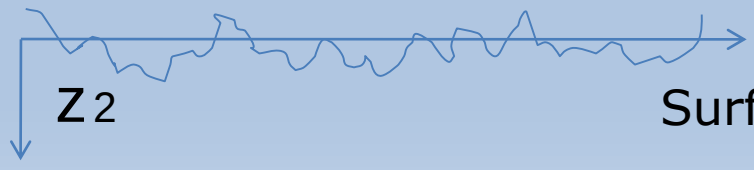
where k_{xn}, k_{yn} are component wavenumbers

H_n is a uniformly distributed random phase $(0, 2\pi)$



Similarly:

$$z_2(x,y) = \sum_{n2} c_{n2}\cos(xk_{xn2} + yk_{yn2} + H_{n2})$$



Statistical description of the rough interface – Fundamental equations

$$z(x,y) = z_1 + z_2 = \sum_{n1} c_{n1}\cos(x k_{xn1} + y k_{yn1} + \varphi_{n1}) + \sum_{n2} c_{n2}\cos(x k_{xn2} + y k_{yn2} + \varphi_{n2})$$

$$m_{00} = \sigma^2 = \frac{1}{A}\int_{dA} z(x,y)^2\,dx\,dy \quad \Rightarrow \quad \sigma^2 = \frac{1}{2}\left(\sum_{n1} c_{n1}^2 + \sum_{n2} c_{n2}^2\right)$$

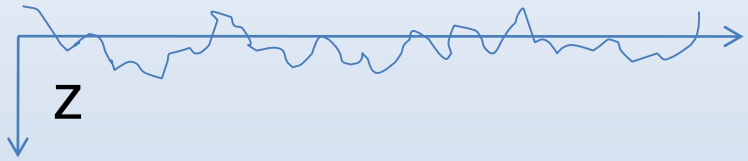
Alternatively

$$\sigma^2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Phi(k_{xn}, k_{yn})\,dk_x\,dk_y = \frac{1}{2}\left(\sum_{n1} c_{n1}^2 + \sum_{n2} c_{n2}^2\right)$$

$$m_{pq} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} k_{xn}^p k_{yn}^q \Phi(k_{xn}, k_{yn})\,dk_x\,dk_y = \frac{1}{2}\left(\sum_{n} c_{n1}^2 k_{xn}^p k_{yn}^q + \sum_{n} c_{n2}^2 k_{xn}^p k_{yn}^q\right) \quad m_{pq1} + m_{pq2}$$

$$m_{pq} = \frac{1}{A}\int_{dA} \frac{\partial^{p+q} z(x,y)}{\partial x^p \partial y^q}\,dx\,dy$$

Statistical parameters for the profile vs surface



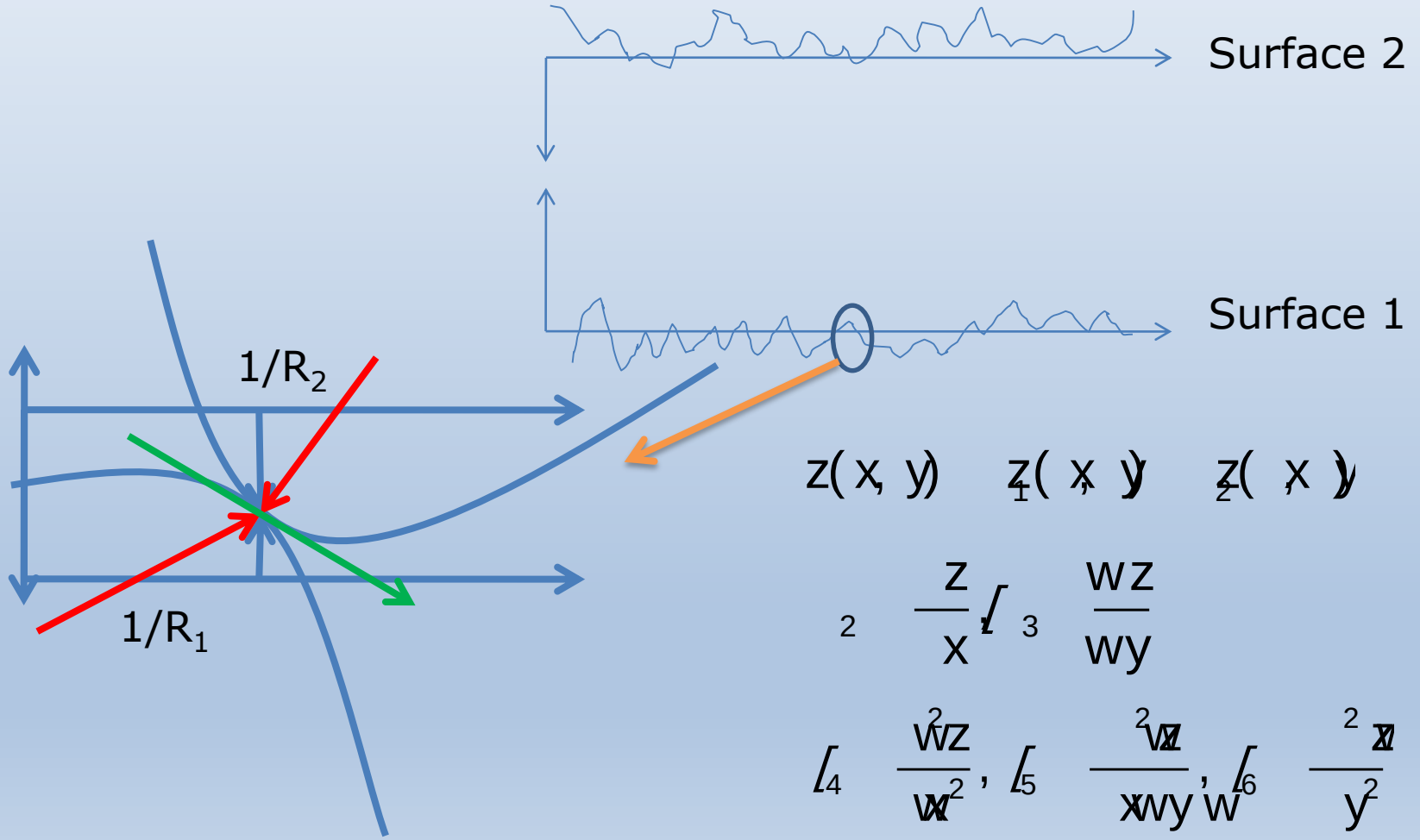
$$m_p(\ell) \quad \int_{-\infty}^{\infty} z^p \, \rho(z) \, dz$$

$$m_n(\ell) \quad m_{n,0}\cos^n \ell + C_1^n m_{n-1,1}\cos^{n-1}\ell \sin\ell + \ldots + m_{0,n}\sin^n \ell$$

For isotropic surface m_n is independent of ℓ:

$$\begin{cases} m_{20} \quad m_{02} \quad m_2; \; m_{11} \quad m_{33} \quad m_{31} \quad 0 \\ m_{00} \quad m_0; 3\, m_{22} \quad m_{40} \quad m_{04} \quad m_4 \end{cases}$$

Statistical description of the rough interface- Fundamental equations



Surface description of contact surface

$$\begin{matrix} \xi_1 = z & \xi_4 = \frac{\partial^2 z}{\partial x^2} \\ \xi_2 = \frac{\partial z}{\partial x} & \xi_5 = \frac{\partial^2 z}{\partial x \partial y} \\ \xi_3 = \frac{\partial z}{\partial y} & \xi_6 = \frac{\partial^2 z}{\partial y^2} \end{matrix}$$

Joint probability of these variables

$$p(\xi_1 \ldots \xi_6) \quad 2\pi^{-\frac{n}{2}} |\Sigma|^{-\frac{n}{2}} \exp\left(-\frac{1}{2} M_{ij} \xi_i \xi_j\right)$$

Where M_{ij} the inverse of the convariance matrix N_{ij}

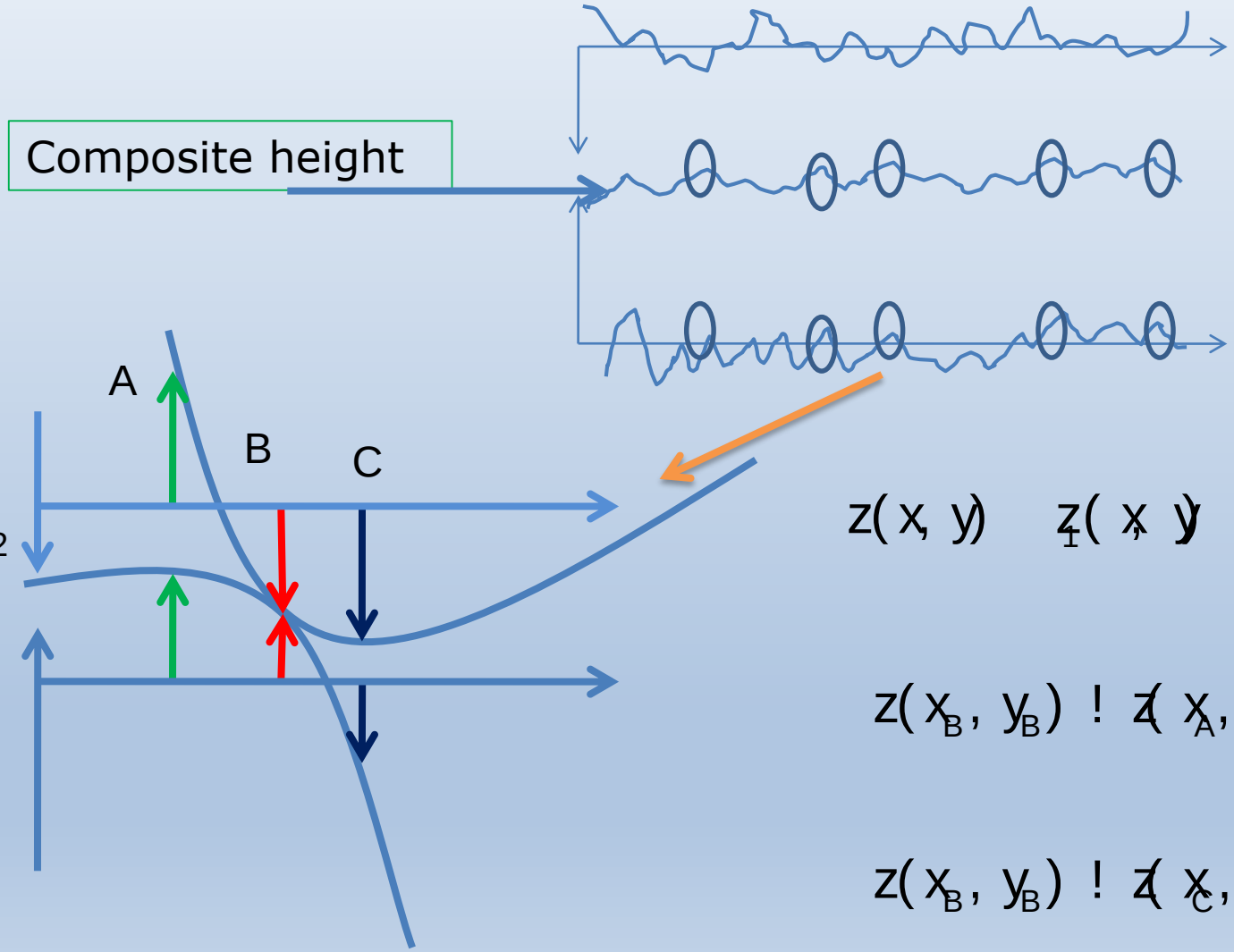
$$N_{ij} = \begin{matrix} m_{00} & 0 & 0 & m_{20} & m_{11} & m_{02} \\ 0 & m_{20} & m_{11} & 0 & 0 & 0 \\ 0 & m_{11} & m_{02} & 0 & 0 & 0 \\ m_{20} & 0 & 0 & m_{40} & m_{31} & m_{22} \\ m_{11} & 0 & 0 & m_{31} & m_{22} & m_{13} \\ m_{02} & 0 & 0 & m_{22} & m_{13} & m_{04} \end{matrix}$$

Slope is independent of height and curvature

Alternatively

$$p(\xi_1 \ldots \xi_6) \quad 2\pi^{-3} |\Sigma|^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \begin{matrix} \frac{2m_4}{\Delta} \xi_1^2 & \frac{9\sigma_4}{4m'_{4\,1}} (\xi_4^2 \quad \xi_6^2) & \frac{3}{m_4} \xi_5^2 & , \\ \frac{3m_2}{\Delta} \xi_1 (\xi_4 \quad \xi_6) & \frac{3\sigma_3}{2m'_{4\,1}} \xi_4 \xi_6 & \frac{1}{m_2} (\xi_2^2 \quad \xi_3^2) \end{matrix}\right)$$

Statistical description of the rough interface- Fundamental equations



$$z(x, y) \quad z_1(x, y) \quad z_2(x, y)$$

$$z(x_B, y_B) \neq z(x_A, y_A)$$

$$z(x_B, y_B) \neq z(x_C, y_C)$$

Interface description of contact surface

Criteria for an asperity contact: find the summit of composite surface

$$\begin{cases} \zeta_2 \quad \zeta_{21} \quad \zeta_{22} \quad 0 \\ \zeta_3 \quad \zeta_{31} \quad \zeta_{31} \quad 0 \\ \zeta_4 \quad 0, \zeta_6 \quad 0, \zeta_4 \zeta_6 \quad \zeta_5^2 \end{cases}$$

Probability distribution of asperity contact height:

$$p_{ac}(\zeta_1)d\zeta_1 \quad d\zeta_1 \quad \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \beta(\zeta_1, 0, 0, \zeta_4, \zeta_5, \zeta_6)d\zeta_4 d\zeta_5 d\zeta_6$$

$$p_{ac}(\zeta_1) \quad \frac{\exp(-m_4\zeta_1^2/2)}{2\pi^{3/2}} \int_0^{\infty}\int_0^{\infty}\int_{-\infty}^{\infty} \left|\zeta_5^2\right| \exp\left[\frac{9}{9m_4^2}(\zeta_4^2+\zeta_6^2) - \frac{3}{2m_4}\zeta_5^2 - \frac{3m_2}{2}\zeta_1(\zeta_4+\zeta_6) - \frac{3}{4m_4^2}\zeta_4\zeta_6\right] d\zeta_4 d\zeta_5 d\zeta_6$$

Interface description of contact surface

Define:

Mean curvature

$$(s, r\cos T, r\sin T) \quad \frac{3}{m_4}^{1/2} \quad 1/2(\quad _4 \quad _6), \quad _5, \quad 1/2(\quad _4 \quad _6)$$

Substitute in probability distribution of asperity contact height:

$$p_{ac}(\ _1, s, r) \quad \frac{m_4\sqrt{C}}{24m_2 V S} \exp(\ C_1 \ ^2_{1\ 2}) \ s^2 \quad r^2 \ r \exp \ \frac{1}{2}(C_1 s^2 \quad r^2 \quad C_2 s \ )$$

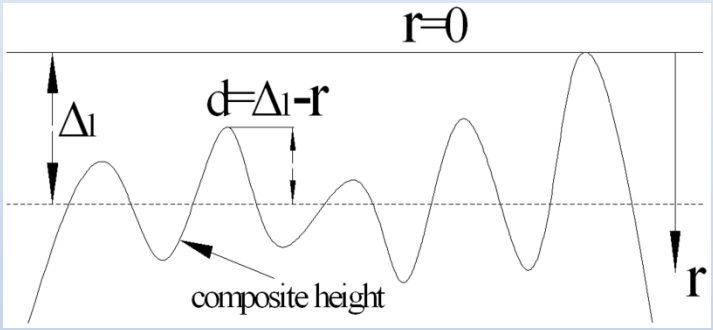
Joint probability distribution of height and curvature:

$$p_{ac}(\ _1, s) \quad \frac{m_4\sqrt{C_1}}{12m_2 V^2 S} \exp(\ C_1 \ ^2_{1\ 2}) \ s^2 \quad 2 \quad 2\exp(\frac{1}{2} s^2) \exp \ \frac{1}{2}(C_1 s^2 \quad C_2 s$$

$$N \quad \frac{m_4}{6 S\sqrt{3}m_2}$$

Interface description of contact surface

Consider shifted asperity contact height $r=r_m-l_1$ and radius of curvature R :



Joint probability distribution of height and radius of curvature:

$$H(r,R)\quad \frac{3\sqrt{C_1}}{2\,V\,R^2\sqrt{m_4}}\quad \exp\left(-C_1\frac{(r_m-r)^2}{V^2}\right)\quad \frac{3}{m_4R^2}\quad 2\quad 2\exp\left(-\frac{3}{2m_4R^2}\right)\quad \exp\left(\frac{\sqrt{3C_2}}{2R\sqrt{m_4}}\frac{r_m-r}{V}-\frac{3C_1}{2m_4R^2}\right)$$

Asperity contact orientation distribution

Slope is independent of height and curvature

Probability distribution of asperity contact slope for surface 1:

$$p_1(\xi_{21}, \xi_{31}) \quad \frac{1}{2 S_2^{1/2}} \exp \quad m_{02} \xi_{21} \quad 2m_{11} \xi_2 \xi \quad m_{20} \xi_3 \quad / 2' \; {}_{2\neg}^{a}$$

After simplification for isotropic surface:

$$p_1(\xi_{21}, \xi_{31}) \quad \frac{1}{2 S M_{21}} \exp \quad \xi_{21} \quad \xi_{31} \quad / M_{21\neg}^{a}$$

Similarly for surface 2:

$$p_2(\xi_{22}, \xi_{32}) \quad \frac{1}{2 S M_{22}} \exp \quad \xi_{22} \quad \xi_{32} \quad / M_{22\neg}^{a}$$

Asperity contact orientation distribution

Probability distribution of asperity contact orientation:

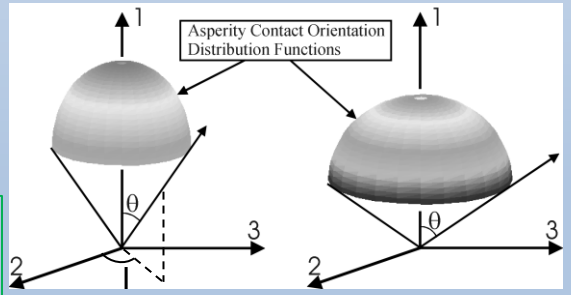
$$p(\xi_2 \mid \xi_{21} \quad \xi_{22}, \xi_3 \mid \xi_{31} \quad \xi_{32}) \quad \frac{p_1 p_2(\xi_{22} \quad \xi_{21}, \xi_{32} \quad \xi_{31})}{\int\int p_1 p_2 \, d\xi_{21} d\xi_{31}}$$

Upon simplification:

$$p(\xi_2, \xi_3) \quad \frac{M_{22} \quad M_{21}}{\pi M_{22} M_{21}} \exp \quad \xi_2^2 \quad \xi_3^2 / M_{22} \quad \xi_2^2 \quad \xi_3^2 / M_{21}$$

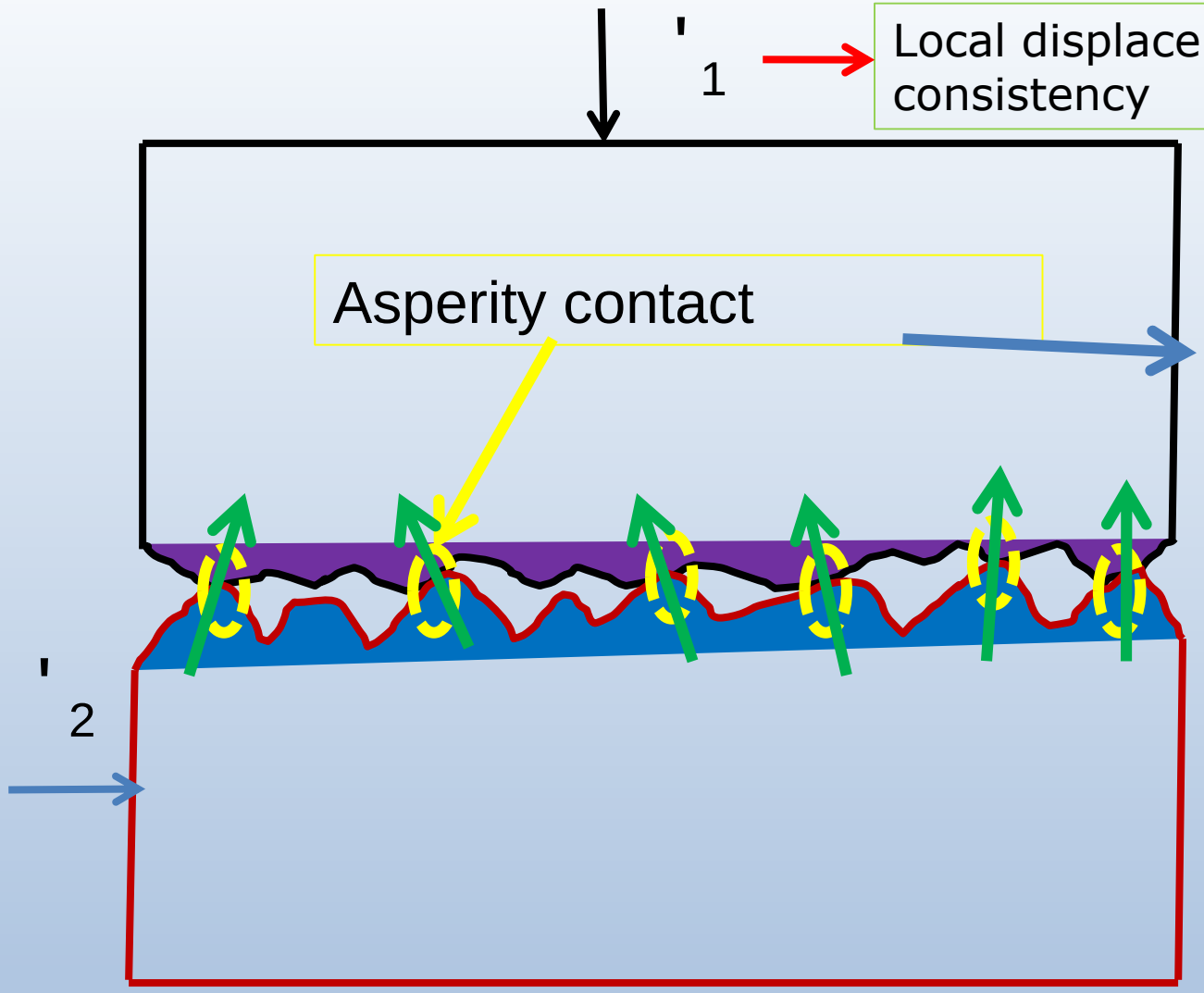
Using the coordinate transformation:

$$\xi_2 \quad \tan \tau \cos \psi, \quad \xi_3 \quad \tan \tau \sin \psi$$



Probability distribution of asperity contact orientation in spherical coordinates:

$$f(\tau, \psi) \quad \frac{\tan}{F \cos^2 \tau} \exp\left(-\frac{\tan^2 \tau}{F}\right) \qquad \text{where: } F \quad \frac{M_{22} M_{21}}{M_{22} \quad M_{21}}$$



Local displacement -displacement consistency

Homogenization method

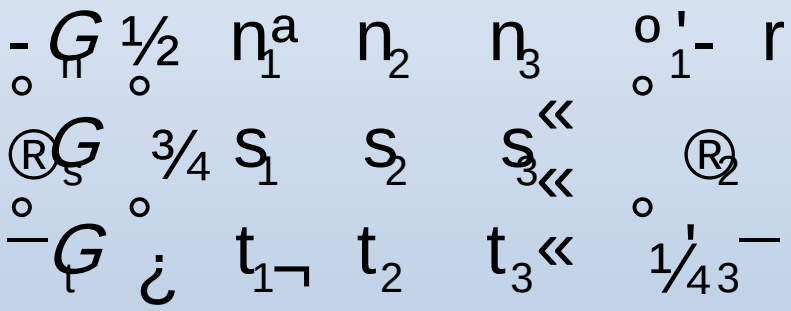
The number of asperity contact

Height and curvature distribution

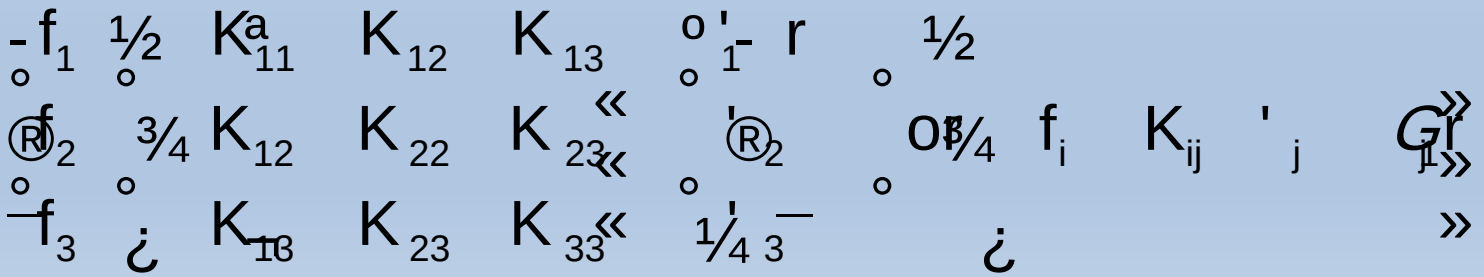
The orientation distribution

Micromechanical stress-displacement relationship

Global-local displacement relationship (displacement consistency)



Asperity contact mechanics



Interface stress-displacement relationship

Integrate asperity forces to obtain the interface stress as follows

$$F_i = N \left[\int_{r^{el}} \int_{R^{el}} \int_{\Omega^{el}} f_i^{el}(\theta, \phi)\, d\theta\, d\phi\, H(r,R)\, dr\, dR + \int_{r^{p}} \int_{R^{p}} \int_{\Omega^{p}} f_i^{p}(\theta, \phi)\, d\theta\, d\phi\, H(r,R)\, dr\, dR \right]$$

Since closed-form inverse of F_i is not possible, thus linearization of the equation above is needed to get σ_i

Newton-Raphson method for linearization

¾Define the residual force vector as

$$R_i(\theta_i) = N \int_{r^{el}} \int_{R^{el}} \int_{\Omega^{el}} B_i^{el}(r,R)\, T\, H^{el}(r,R)\, dr\, dR - \int_{r^{p}} \int_{R^{p}} \int_{\Omega^{p}} B_i^{p}(r,R)\, T\, H^{p}(r,R)\, dr\, dR \Big] - F_i^E = 0$$

¾Expand in Taylor's series

$$R_j(\theta_i) = R_j(\theta_i^{n-1}) + \left[\frac{\partial R_j}{\partial \theta_i}\right]^{n-1} d\theta_i + \ldots$$

¾Iteration procedure

$$d\theta_i = \frac{R_j(\theta_i^{n-1})}{T_{ji}^{n-1}} \qquad T_{ji}^{n-1} = \left[\frac{\partial R_j}{\partial \theta_i}\right]^{n-1}$$

$$\Rightarrow \quad (\theta_i)^n = \theta_i^{n-1} + d\theta_i$$

Interface behavior - Results

¾Sliding boundary

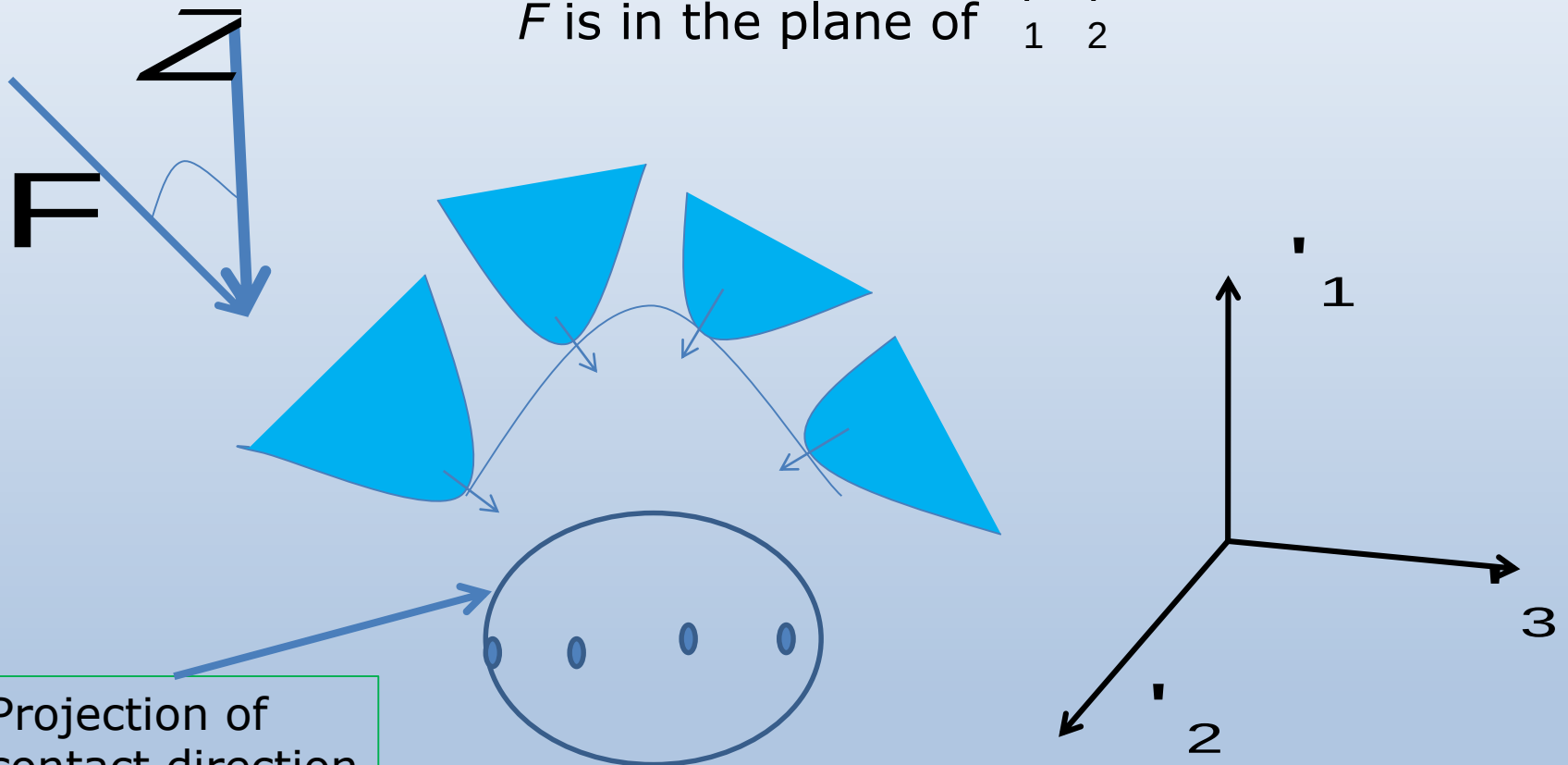
¾Normal contact behavior

¾Shear behavior

¾Coupling effect between shear and normal loading

Sliding behavior

F is in the plane of $'_1$ $'_2$

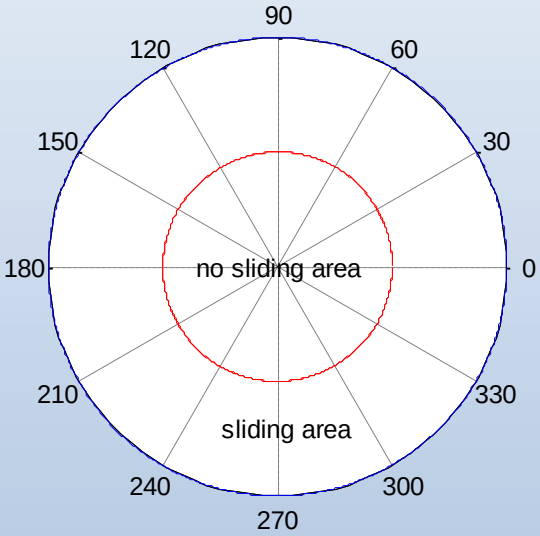


Projection of contact direction in $'_2$ $'_3$ plane.

Using the Amonton-Coulomb law for sliding criteria: $O P_n \cdot \cdot G_{st}$

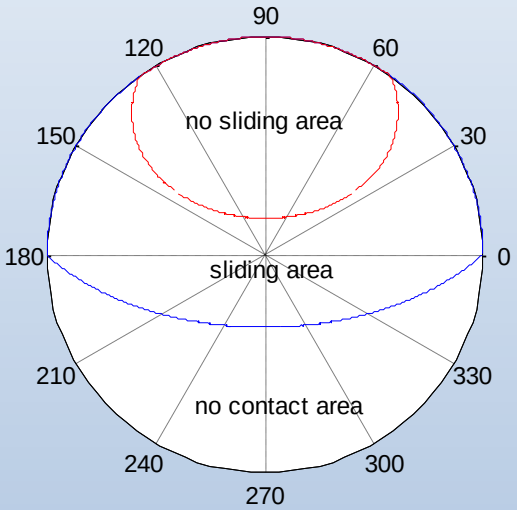
Sliding behavior

Zeffect



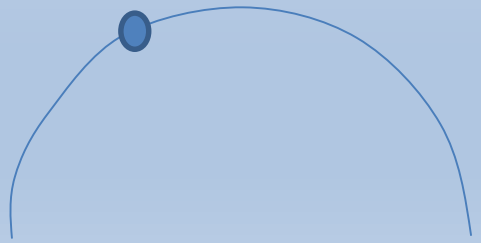
$Z \quad 0$

$P \; O1$



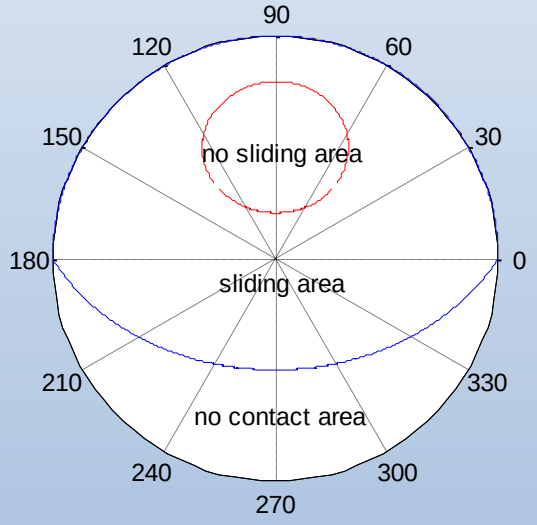
$Z \quad /3$

$P \; O1$



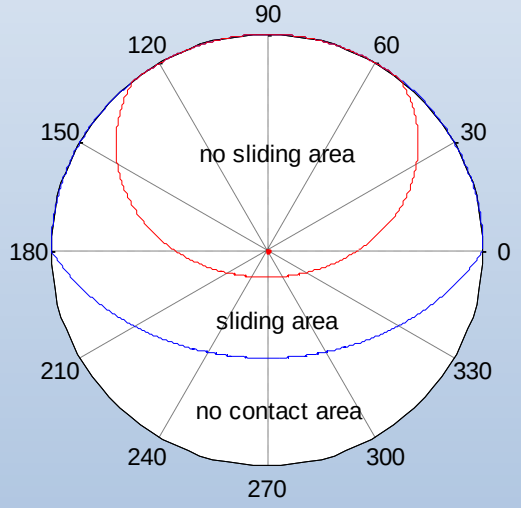
Sliding behavior

μ Oeffect



$Z\ /4$

$P\ O0.5$

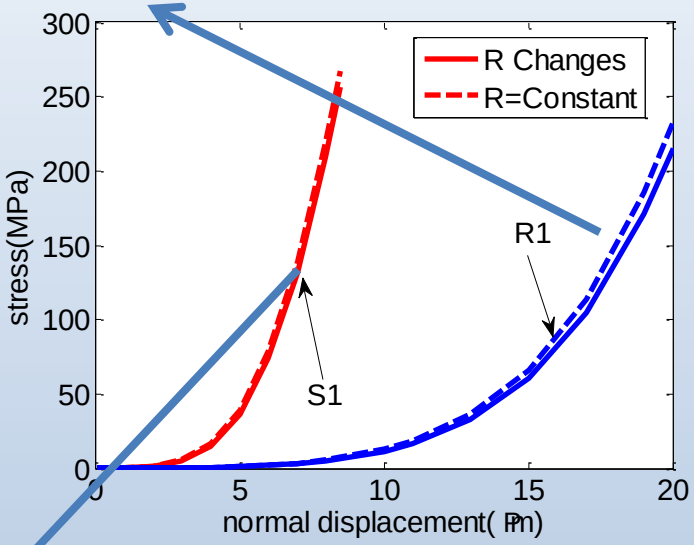


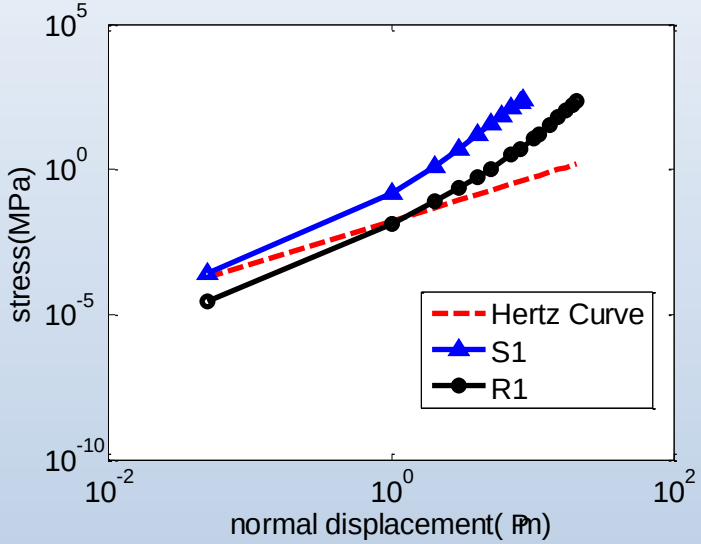
$Z\ /4$

$P\ O1.5$

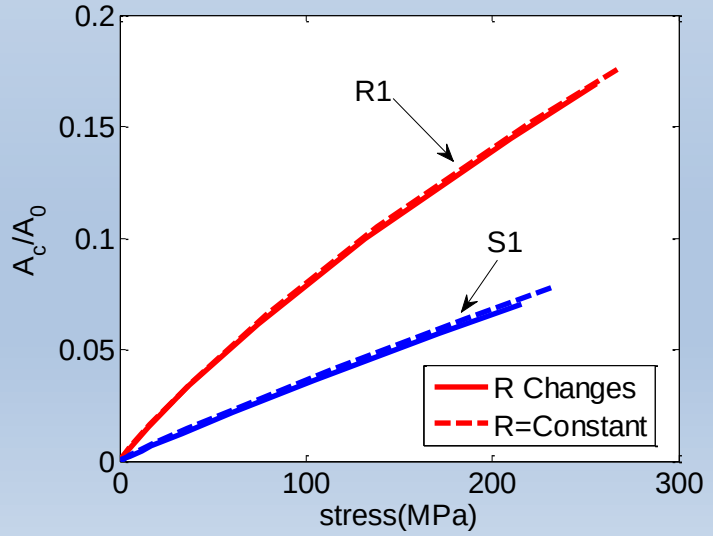
Normal behavior

Rough interface



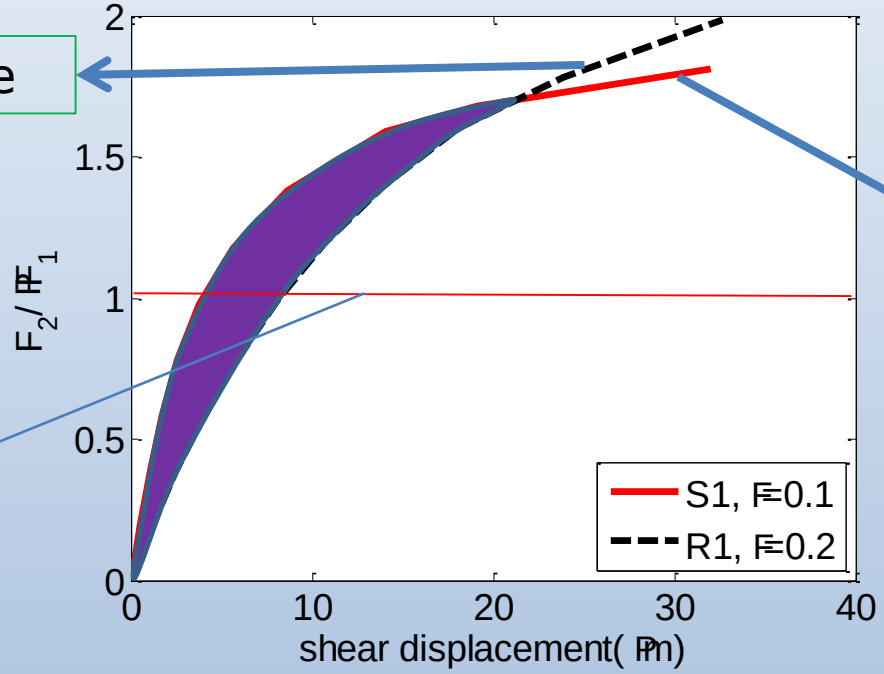


Smooth interface



Shear behavior

Interface sheared in 2-direction keeping normal stress F_1 constant.



Rough interface

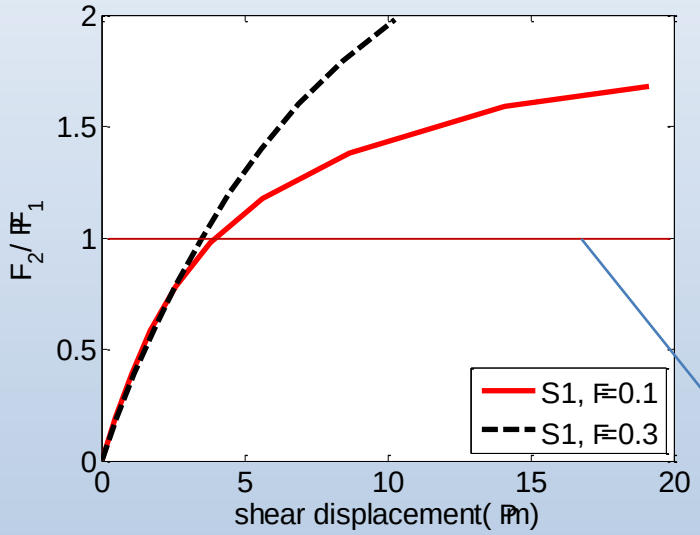
Smooth interface

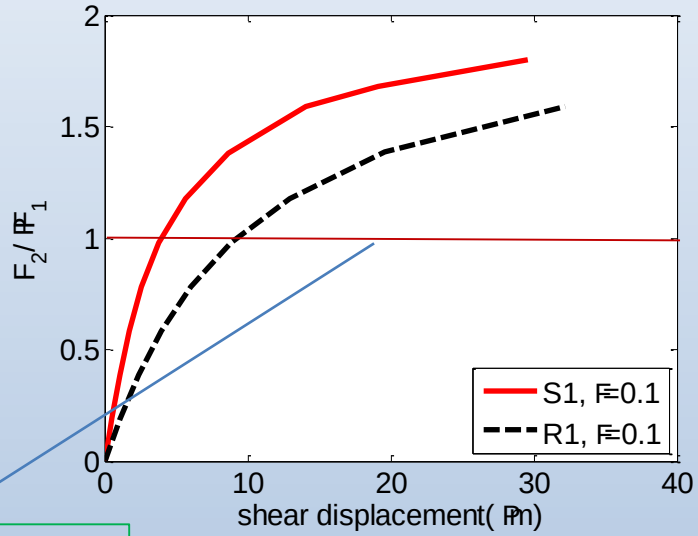
Amonton law failure

The cross-over behavior of smooth and rough interfaces caused by the difference in asperity contact orientation distributions

Shear behavior

Interface sheared in 2-direction keeping normal stress F_1 constant.





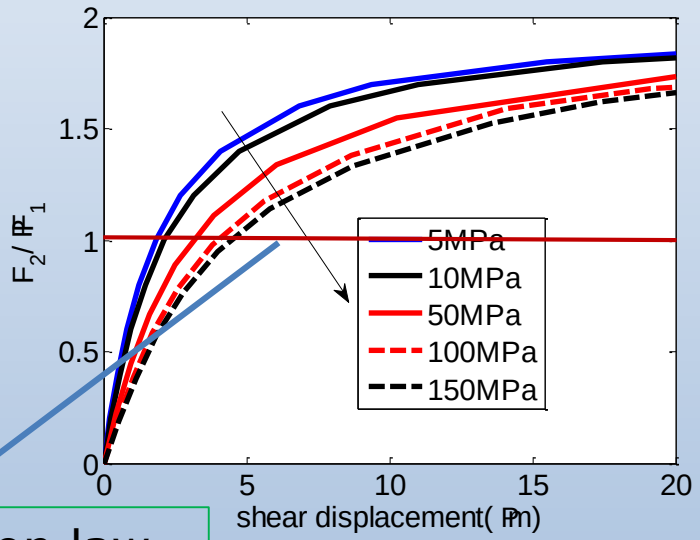
Amonton law failure

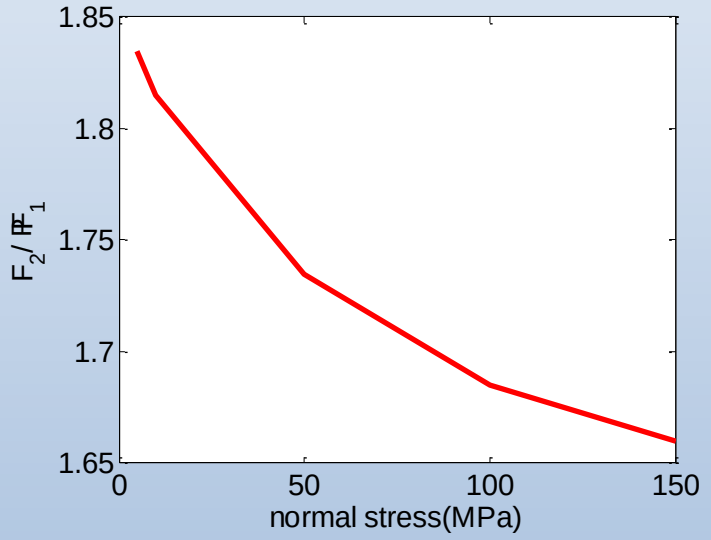
Cross-over behavior is observed by the difference in asperity contact orientation distributions

Cross-over behavior is not observed by the difference only height distribution

Shear behavior

Interface sheared in 2-direction keeping normal force F_1 constant.

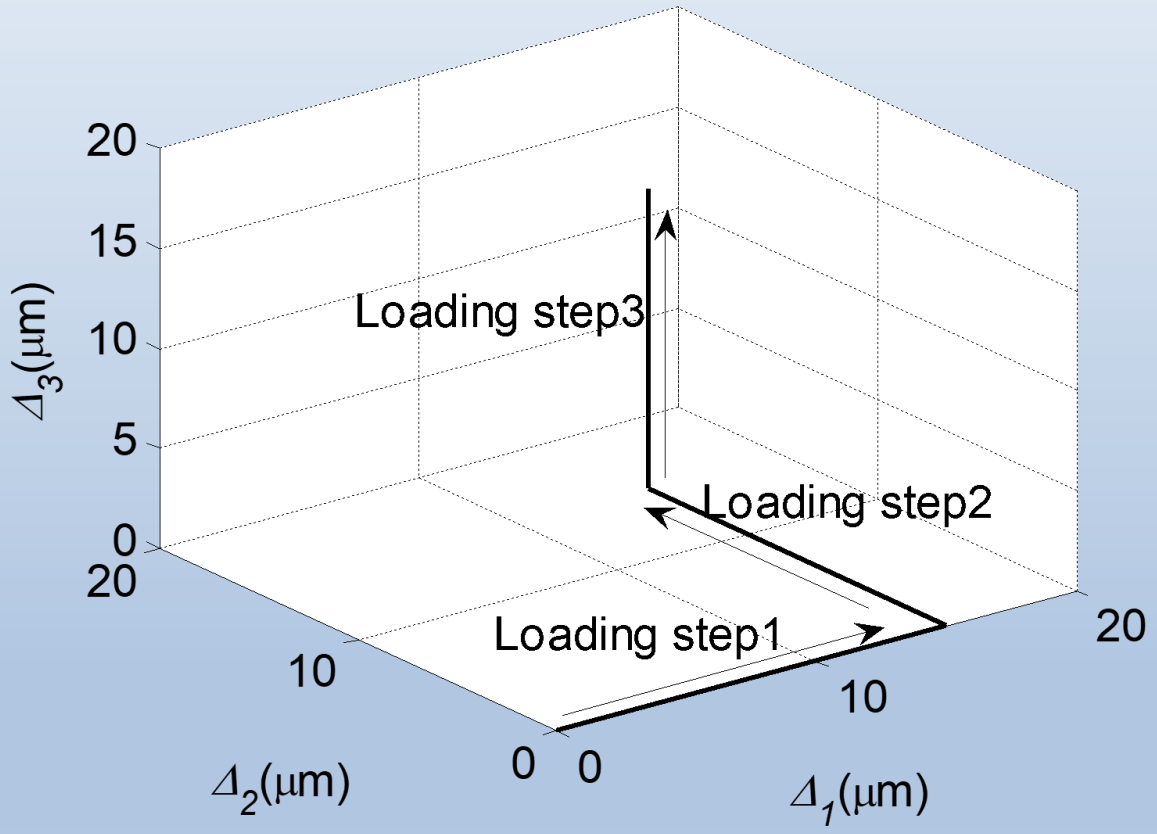




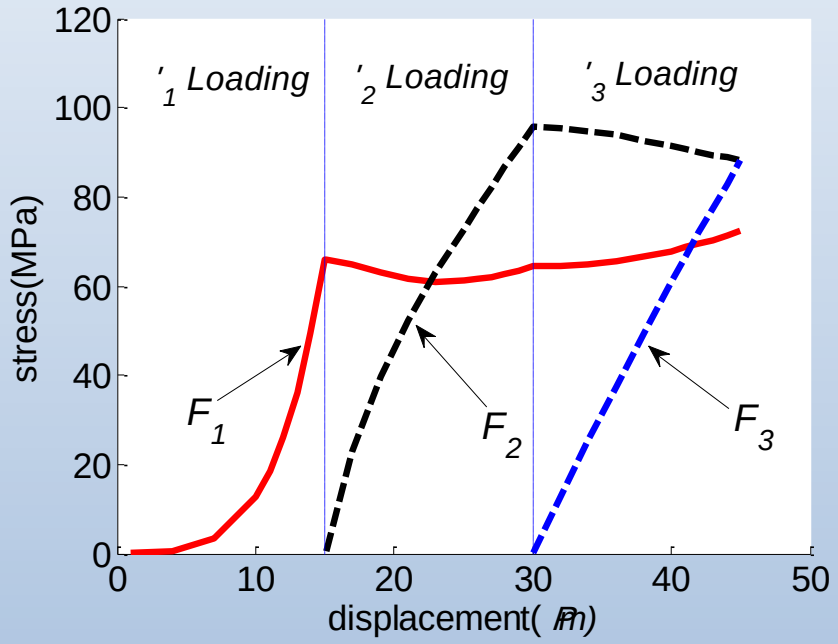
Amonton law failure

Effect of normal stress F_1 on shear behavior.

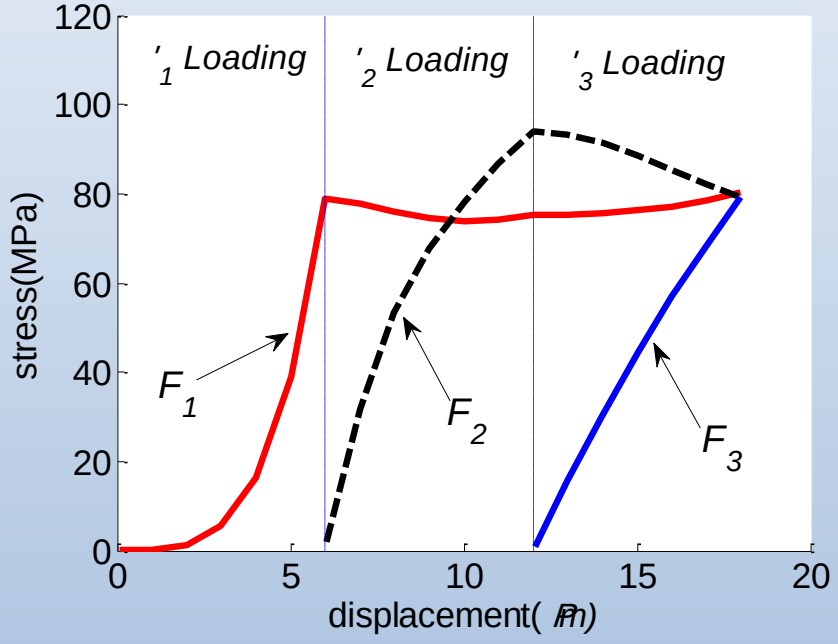
Coupling effect between normal and tangential loading



Coupling effect between normal and shear

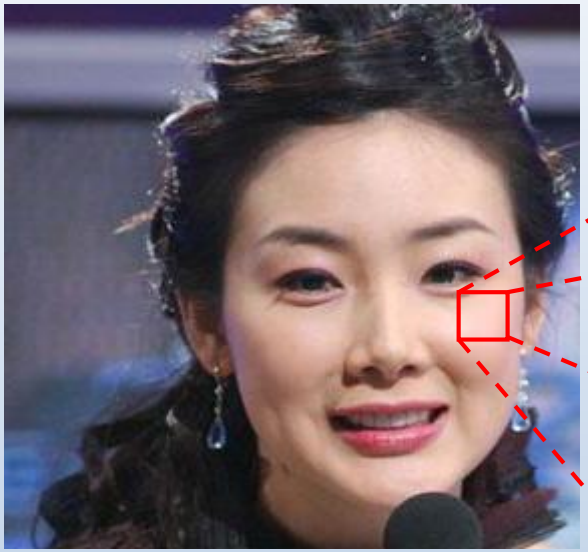


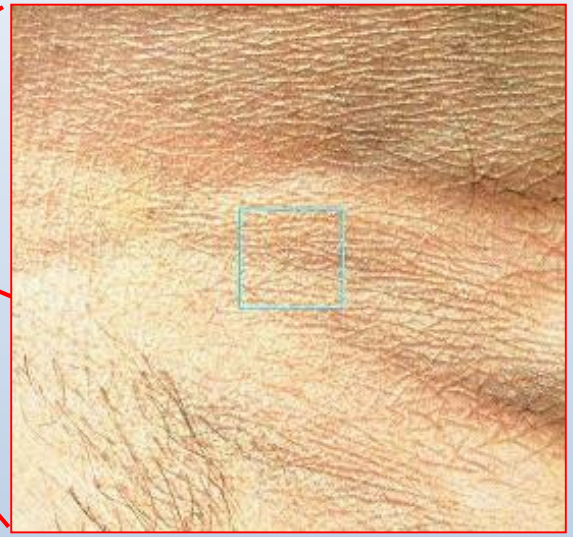
Rough interface



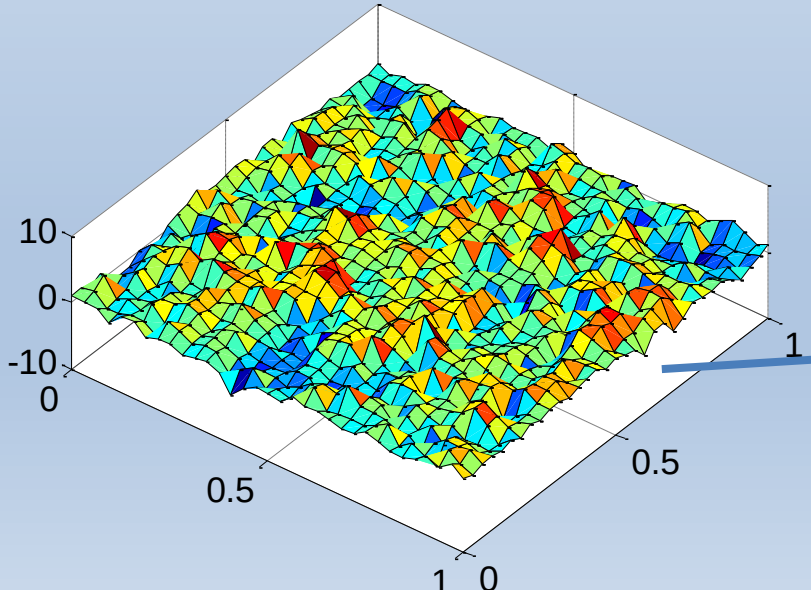
Smooth interface

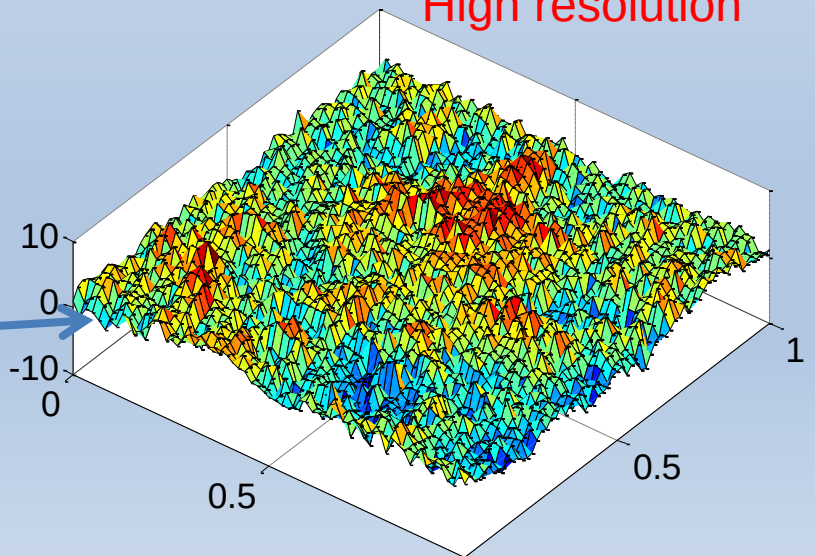
Scale dependency of rough contact





High resolution





Scale dependency of rough contact

The moments of a profile are scale-dependent:

$$m_n = \int_{-\infty}^{\infty} z^n P(z)\,dz \qquad P(f) = Bf^{(5-2D)}$$

The PSD of surface profile is a power law function (Sayles and Thomas 1978)

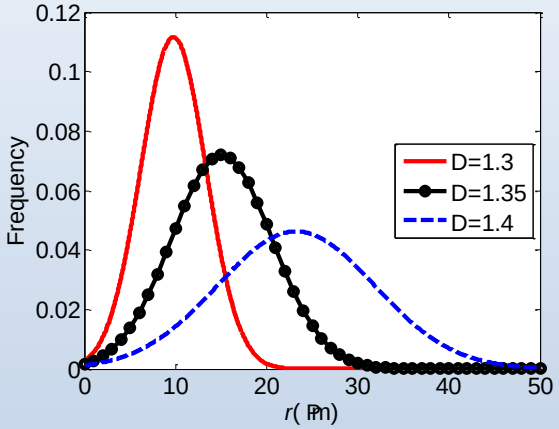
$$\begin{cases} -\infty & \dfrac{2S}{L} \\ \circledR & \\ \circ & \dfrac{2S}{G} \end{cases}$$

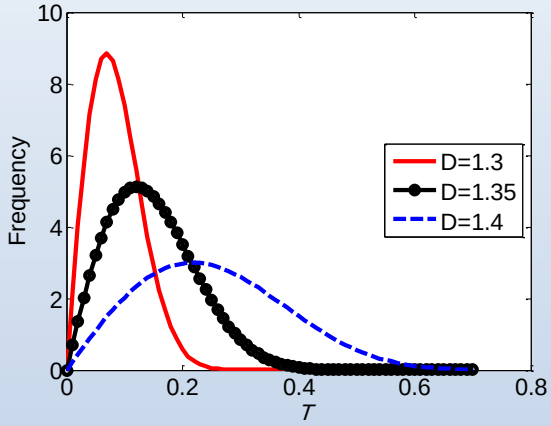
Where L=sample size, G=resolution,

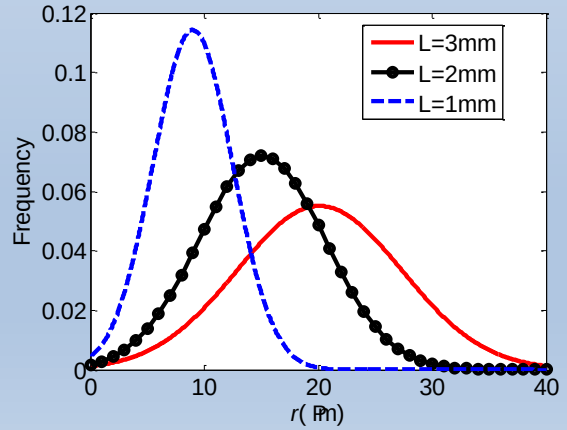
$$m_0 \# \frac{B}{2D-4}\left(\frac{2S}{L}\right)^{2D-4} \qquad m_2 \# \frac{B}{2D-2}\left(\frac{2S}{G}\right)^{2D-2} \qquad m_4 \# \frac{B}{2D}\left(\frac{2S}{G}\right)^{2D}$$

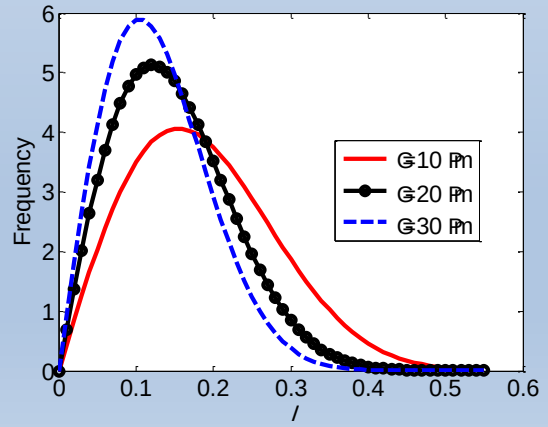
Statistical parameters are dependent on sample size, resolution and fractal dimension

Scale dependency of rough interface distributions

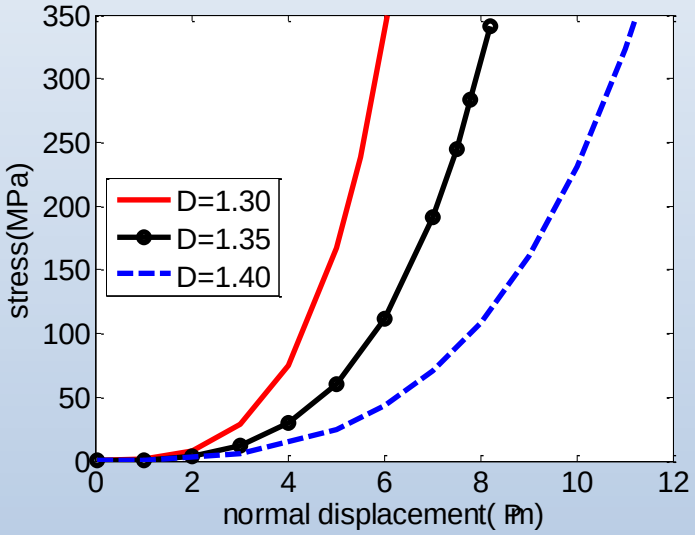


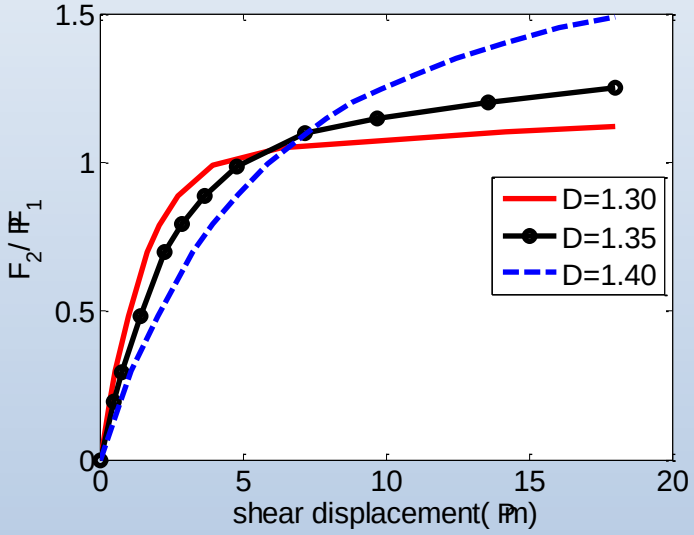




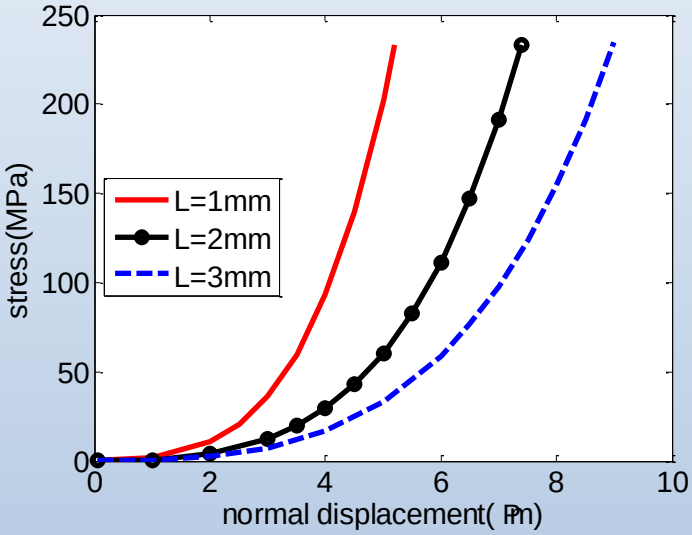


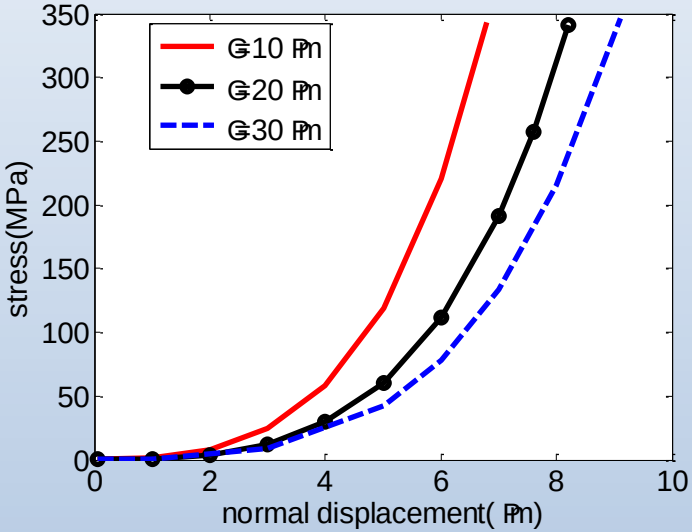
Effect of fractal dimension: Normal and shear behavior



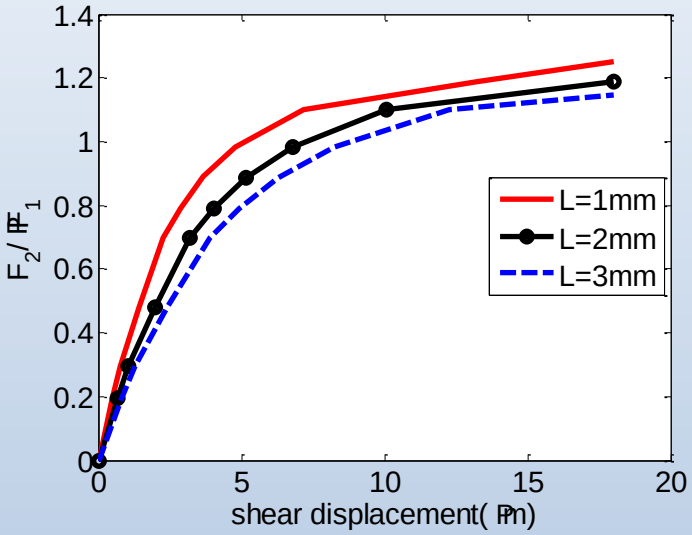


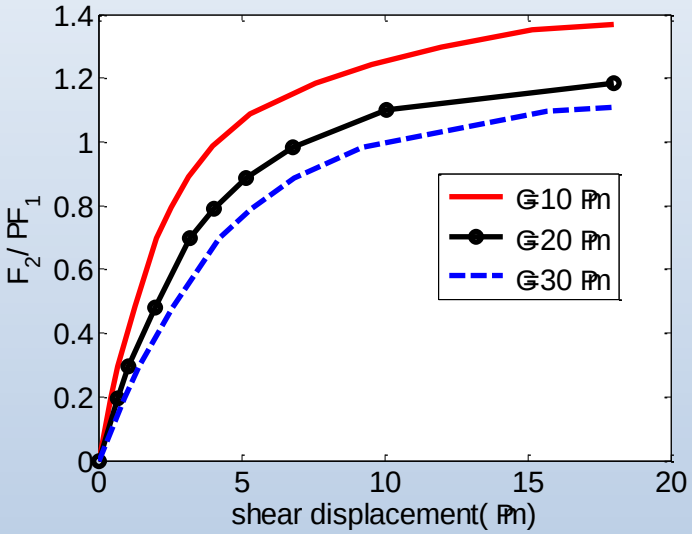
Effect of sample size and resolution : Normal behavior





Effect of sample size and resolution: Shear behavior





Conclusion

Summary of main contributions:

- Further developed asperity contact mechanics for changing oblique loading and out-of-plane loading.
- Developed statistical description of rough interfaces (formed by two rough surfaces) using random process theory. The asperity contact orientation was considered for the first time in rough contact mechanics.
- Refined the micromechanical theory of rough contact using the developed statistical descriptions and asperity contact mechanics. Introduced numerical method for evaluating the resultant stress-displacement relationship
- Investigated scale-dependency of interface behavior using the developed rough contact theory.

Thank you very much!