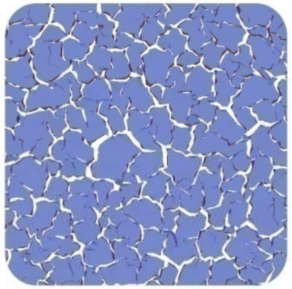
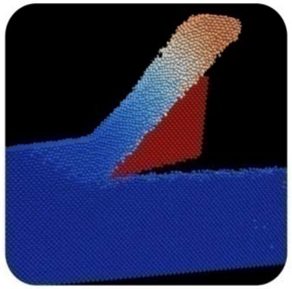
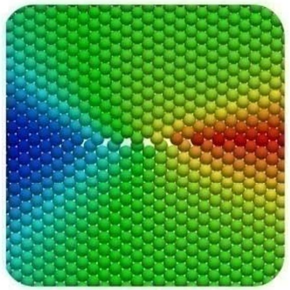
Numerical modeling of sliding contact

J.F. Molinari

1) Atomistic modeling of sliding contact; P. Spijker, G. Anciaux
2) Continuum modeling; D. Kammer, V. Yastrebov, P. Spijker

ICTP/FANAS Conference on Trends in Nanotribology, 2011

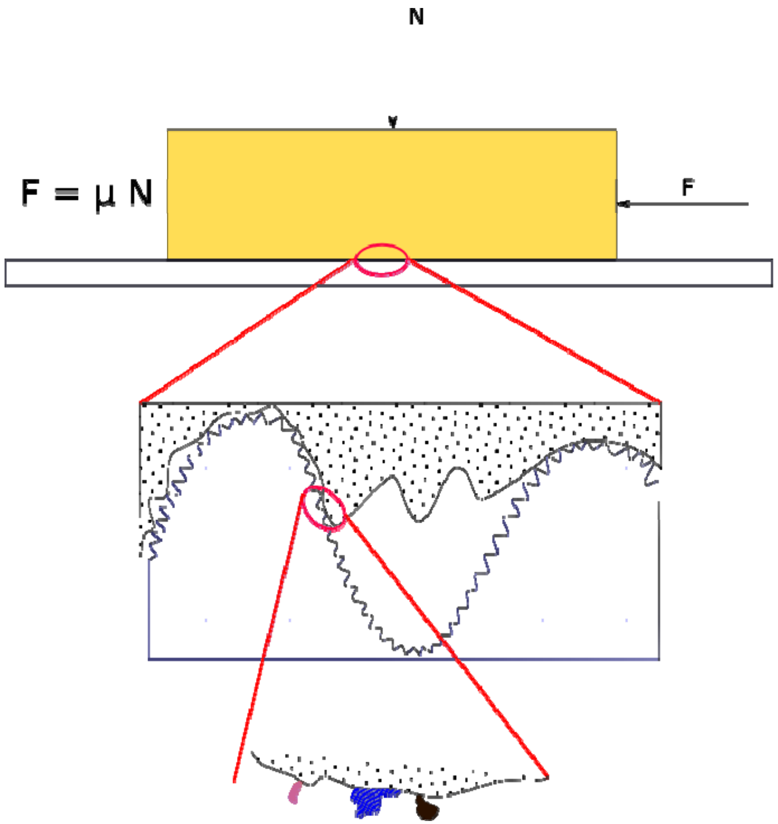






Motivation

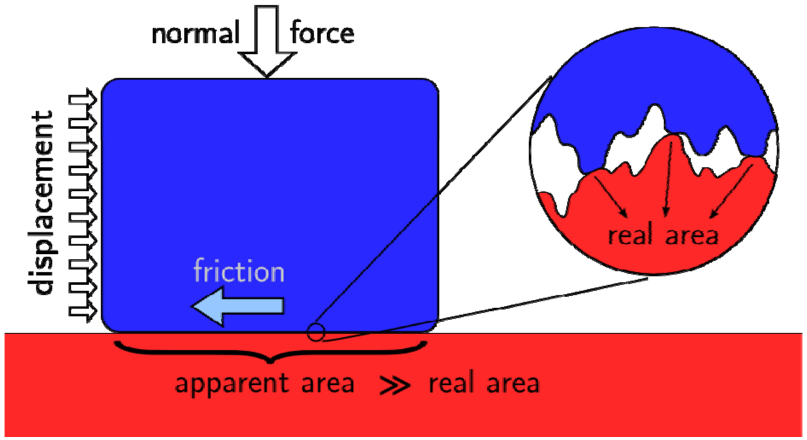
Friction: one of the great unsolved mystery

- Can we explain the microscopic origins of friction ? (nm)
- What happens inside an earthquake ? (km) (rated by livescience as top mystery)
- Challenge of scales (time and length)
- Complex physics (plasticity, surface roughness, third body interactions, adhesion, chemistry…)



A quick introduction

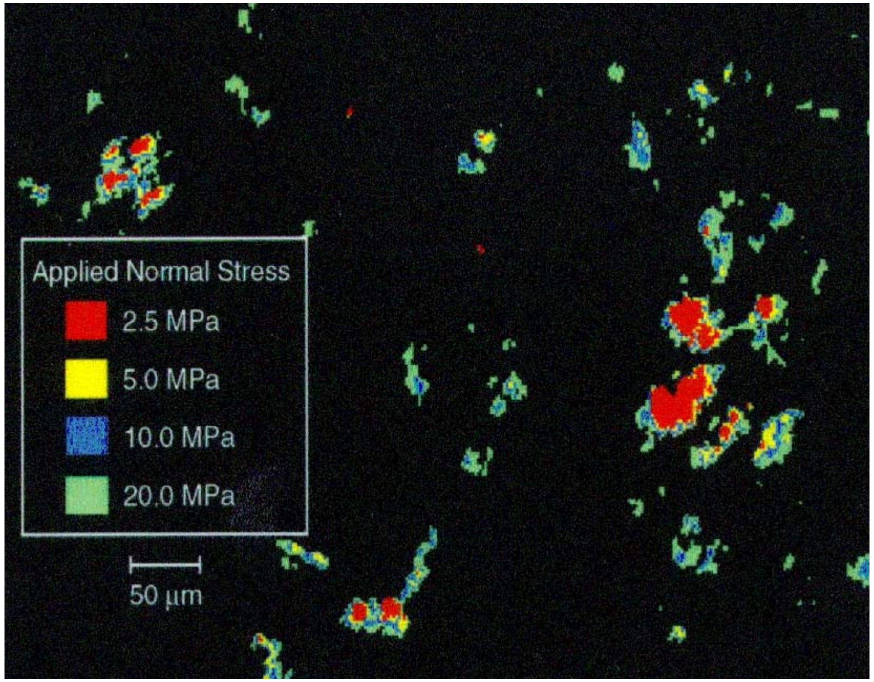
Historical notes on friction research



According to Da Vinci, Amontons, and Coulomb, **friction** is ...

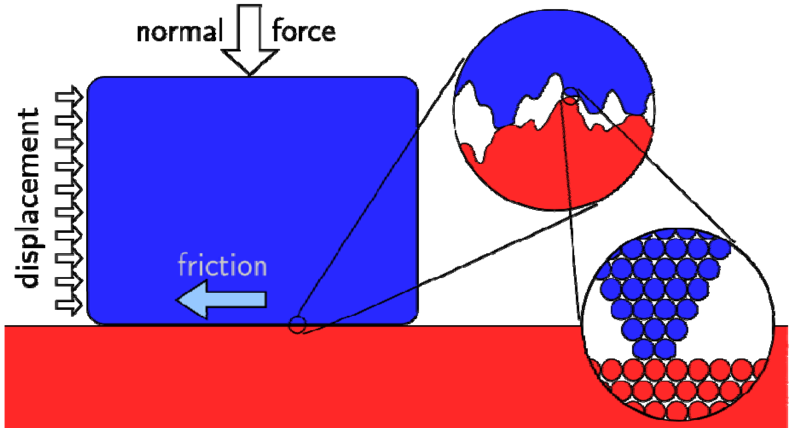
- ... proportional to load
- ... independent of contact area
- ... independent of sliding speed

- Bowden and Tabor (1950)
  - real vs. apparent contact area
  - contact surface is rough
  - number of contacting asperities increases with load (confirmed by Dieterich)
- Theoretical models:
  - Greenwood and Williamson
  - Persson

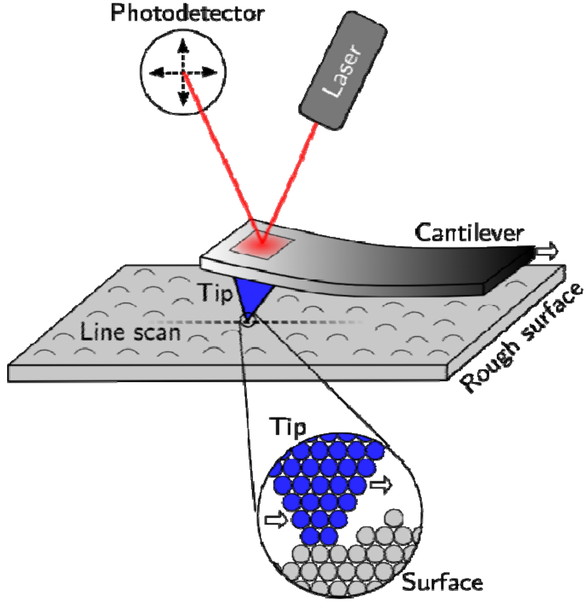


Toward the atomistic scale

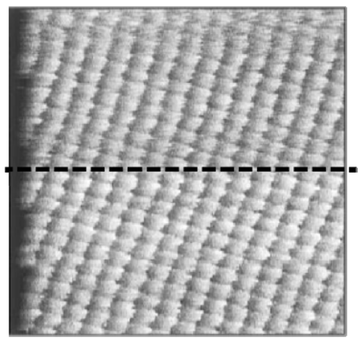
Nanotribology



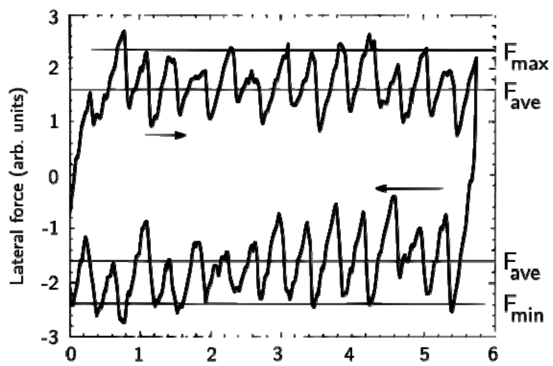
- Magnification until atomic level
- Domain of nanotribology
- Elucidate molecular origins of friction



- Experimental techniques include AFM



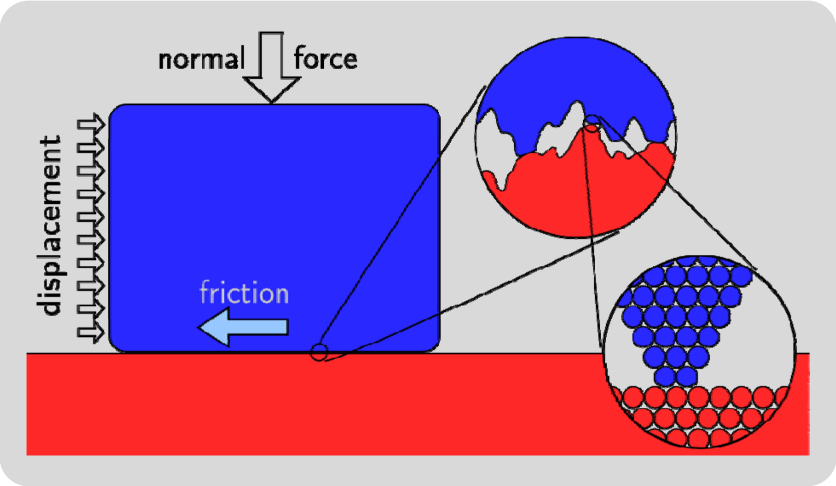
Lateral force image (6x6 nm)

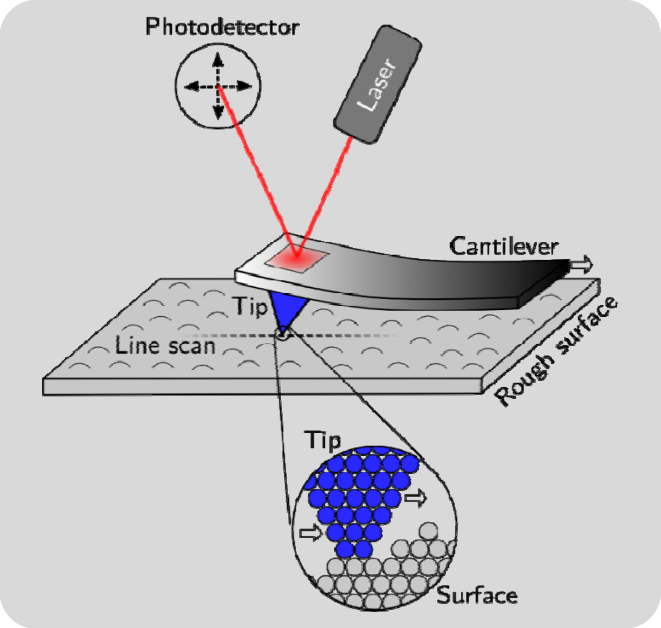


Friction loop (line scan)

Influence of roughness

Open questions…



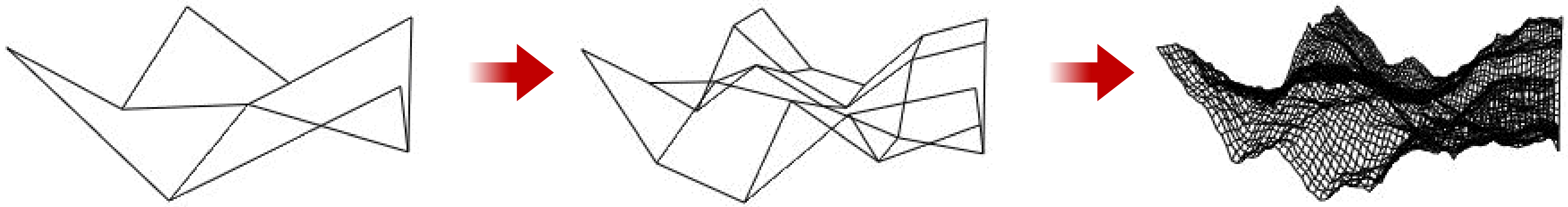


- Roughness generally not included in Molecular Dynamics modeling (flat on flat, or single tip on flat)
- Computed friction coefficients tend to be low
- Roughness, plasticity (wear) dominate at the engineering scale
- Objective: investigate atomic scale roughness
- Existence ?
- How does it influence friction?

Self-affine fractal surfaces

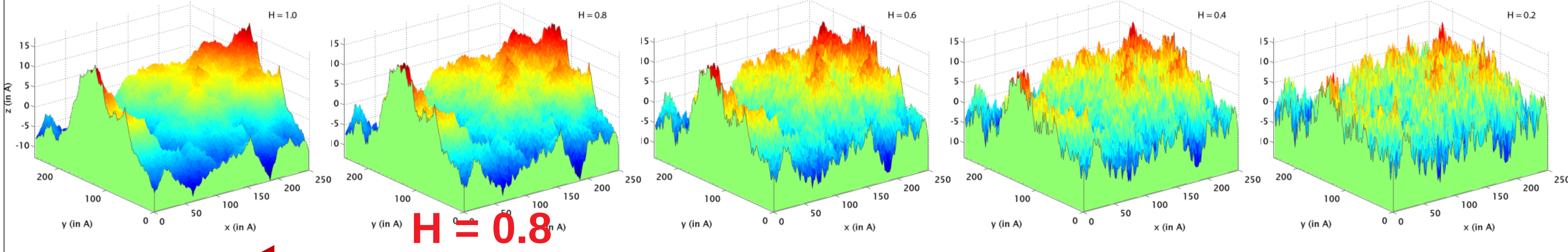
Random mid-point displacement algorithm with different Hurst exponents

- Random mid-point displacement algorithm



(also known as Voss algorithm, diamond-square algorithm, plasma fractal)

$$C(\mathbf{q}) = \frac{1}{2\pi} \int h(\mathbf{x}) h(\mathbf{0}) \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{x}} \mathrm{d}\mathbf{x} \qquad C(\mathbf{q}) \sim \mathbf{q}^{-2(H+1)}$$



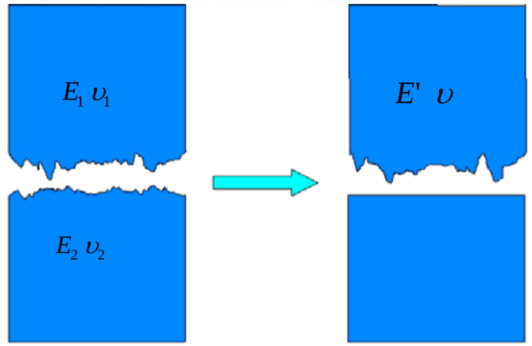
Increasing Hurst exponent
smoother surface / larger asperities / less asperities

Continuum Mechanics

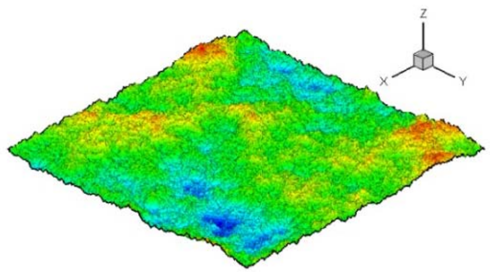
Finite Element Simulations

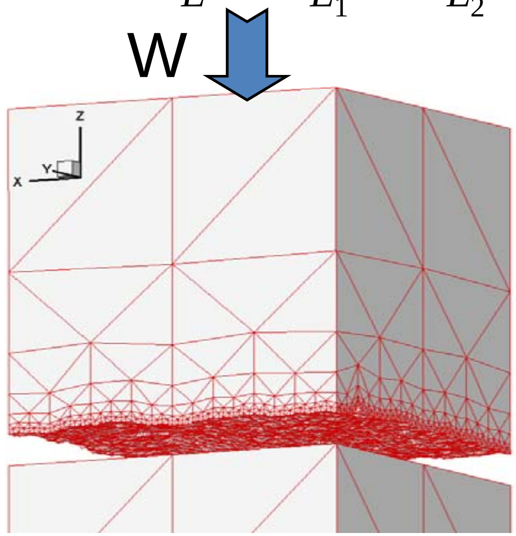
Elastic or J2 elasto/perfectly-plastic solid with a rough surface contacting a rigid surface
L = 512 nodes per side; periodic BCs
Full range of H and roughness amplitude

No Frictional Force
No plasticity
(Johnson, 1985)



$$\frac{1-\upsilon^2}{E'} = \frac{1-\upsilon_1^2}{E_1} + \frac{1-\upsilon_2^2}{E_2}$$

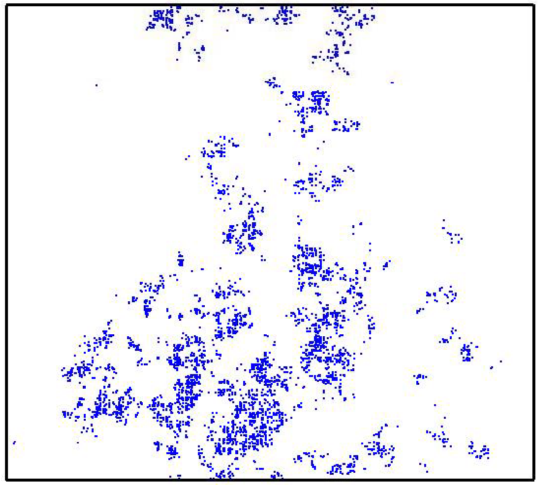




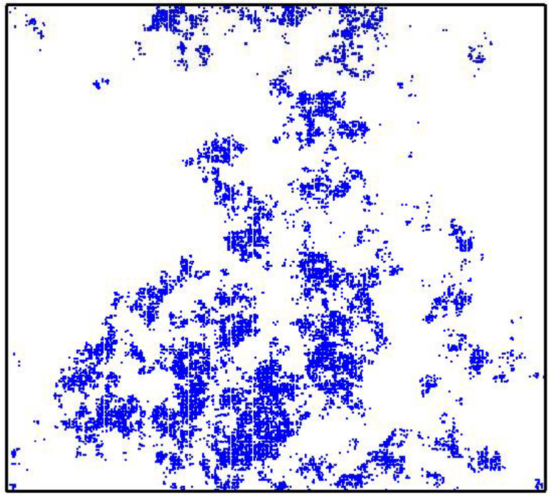
H=0.7 (D = 3 - H = 2.3), 256x256 grid; generated by successive Random Addition Rule (RF Voss)

• S. Hyun, L. Pei, J.F. Molinari, and M.O. Robbins, “Finite-element analysis of contact between elastic self-affine surfaces”, *Phys. Rev. E*, 2004
• L. Pei, S. Hyun, J.F. Molinari, and M.O. Robbins, “Finite-element analysis of contact between elasto-plastic self-affine surfaces”, *Journal of the Mechanics and Physics of Solids, 2006*

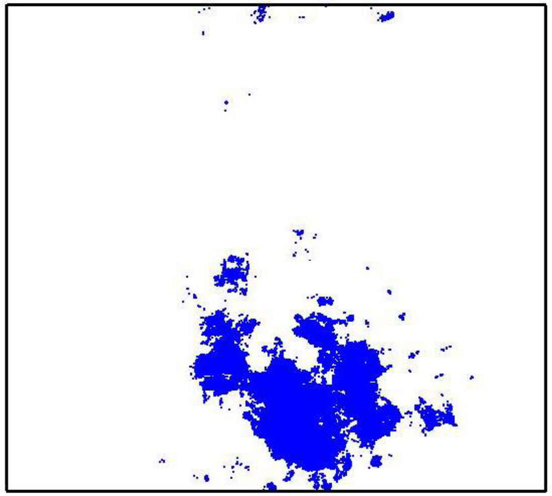
Complex contact morphology



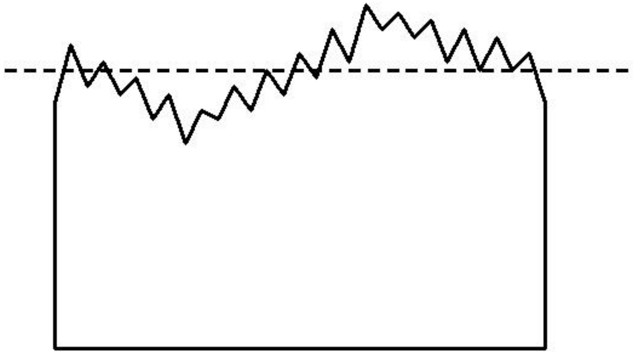
Elastic contact with A=0.0125



Elasto-plastic contact,
A=0.0335
Perfectly plastic (more contact area for fixed W)



Overlap or cut-off model,
A=0.03

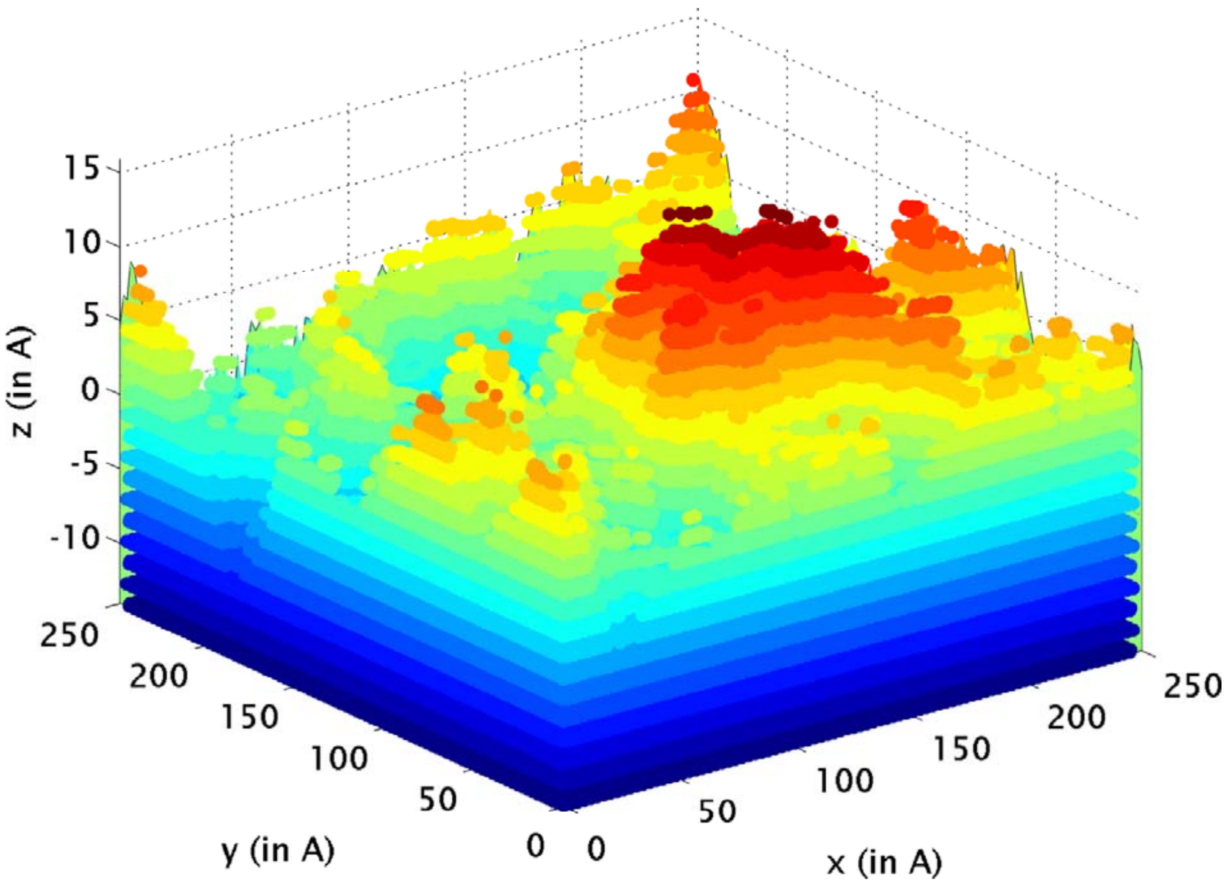


Overlap model way off:
asperities elastic (long range) interactions matter!

Morphology dominated by small contact clusters

Atomic rough surfaces

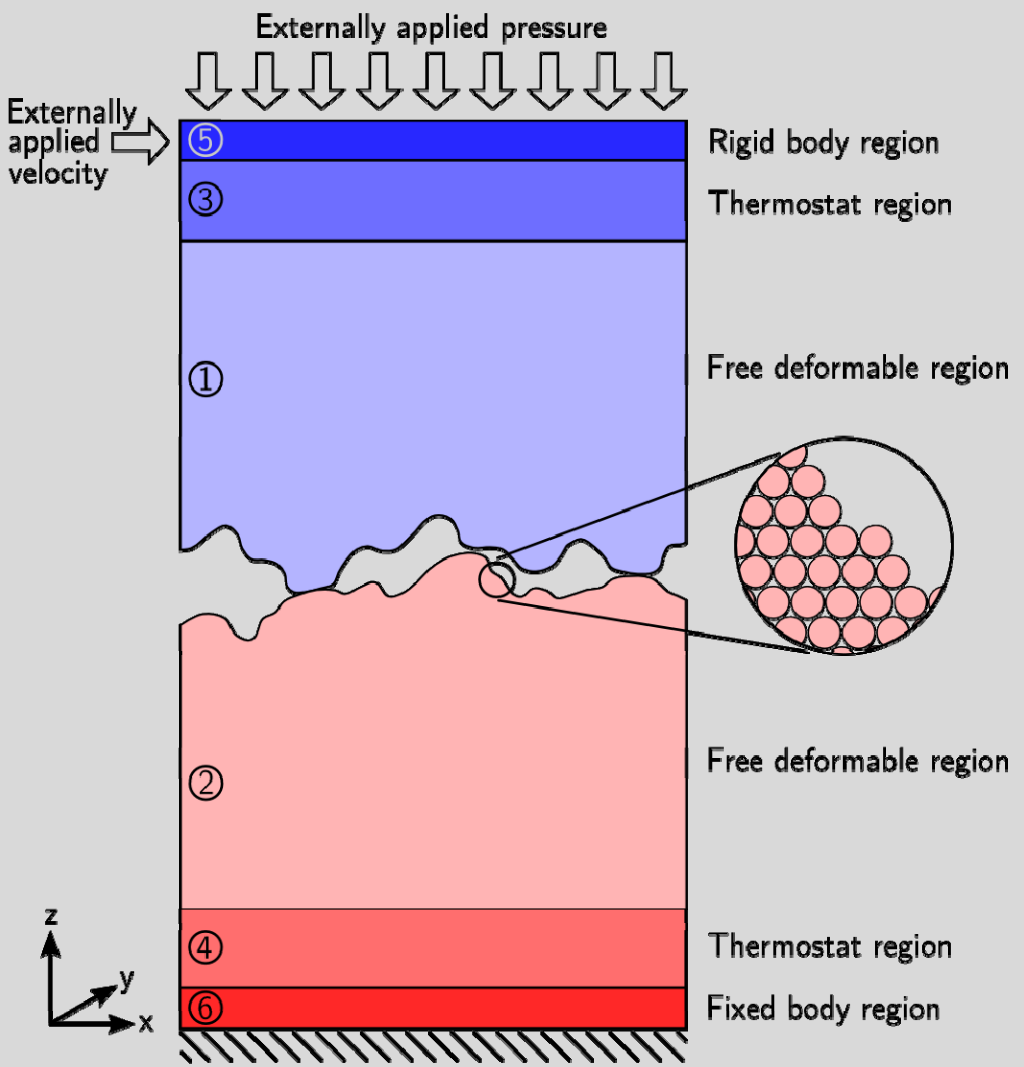
Top a mesoscale asperity



Characteristics:
- Hurst = 0.5
- Grid size = 128
- Peak-valley = 30 Å
- R_A = 3.92 Å
- RMS = 4.96 Å

Atom representation:
- N_{atoms} = 485,368
- r_{atom} = 1.0 Å
- dims. = 250 x 250 Å

MD simulation set-up



Material

- aluminium (FCC structure)
- diameter: 0.291 nm / mass: 27 g/mol
- Young's modulus: 68 GPa / *v*: 0.35

Potential

- Lennard-Jones
- bulk-energy: 10.3 kJ/mol
- gap-energy: 0.103 kJ/mol (**weak adhesion**)

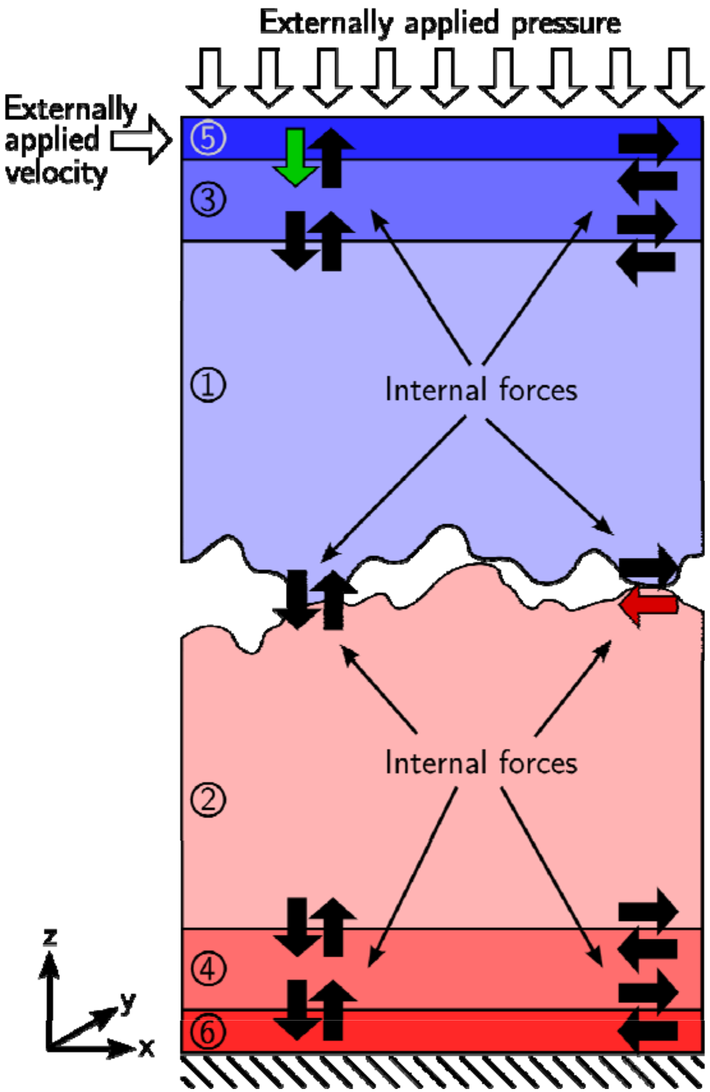
System set-up

- 6 different regions
- dimensions: 13 x 13 x 26 nm (**periodic**)
- 185,000 to 240,000 particles
- top domain rotated by 21 degrees
- Langevin thermostat close to 0 K

Simulations (all 10 ns with 5 fs time step)

- 3 rough surfaces (0.2, 0.5, 1.0 nm)
- for every RMS 3 different surfaces
- 5 applied pressures (0.05 – 0.25 GPa)
- 3 **high** sliding speeds (2, 10, 50 m/s)

Simulation analysis



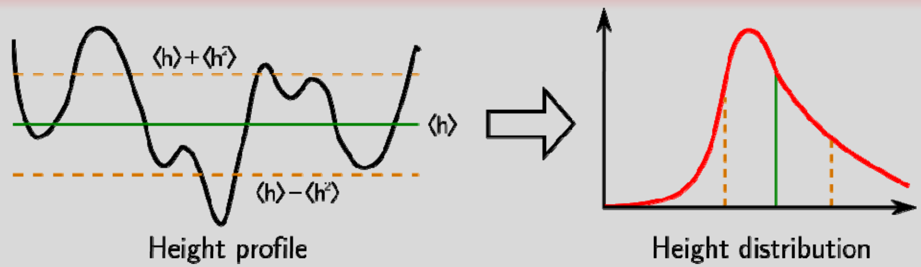
Global forces

- decompose forces per region
- allows to compute global μ = F/F_N

Change of surface characteristics

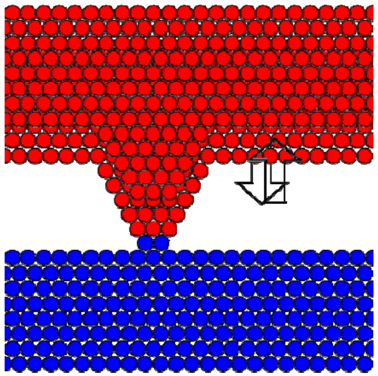
- RMS roughness / RMS slope
- Skewness, flatness

Statistics and height distribution

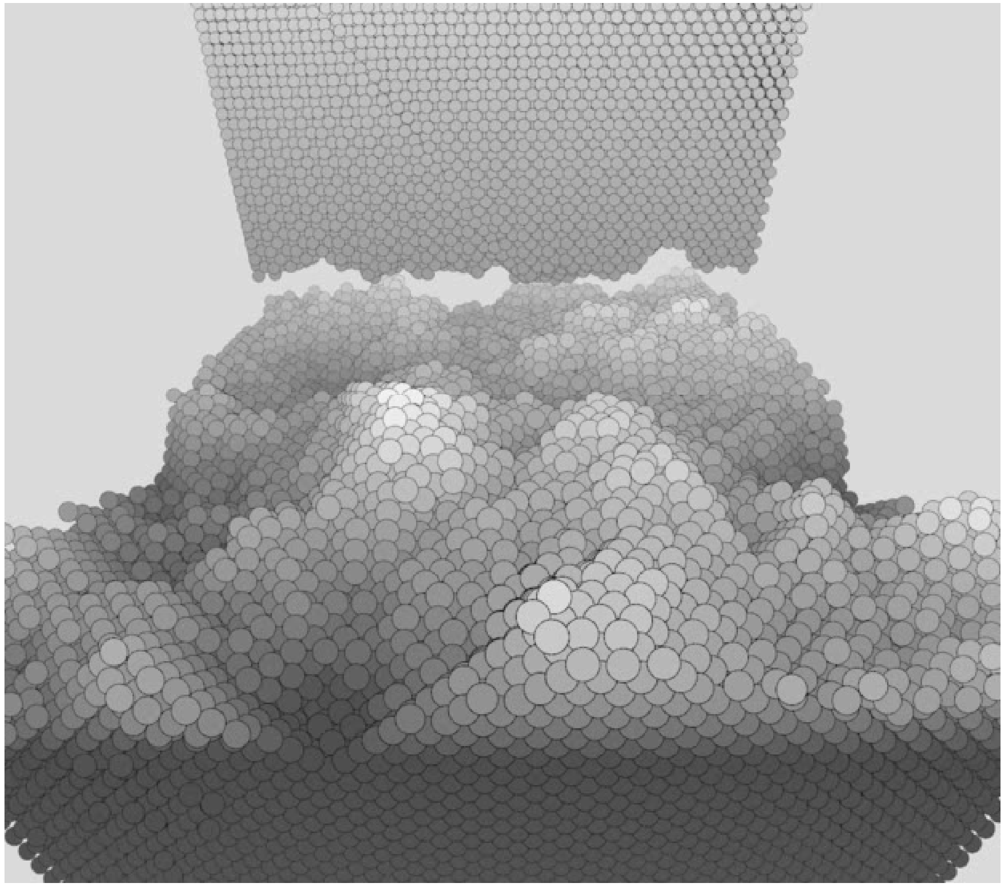


Contact area

- retype particles if necessary
- projected on *xy*-plane
- compute `true' contact area

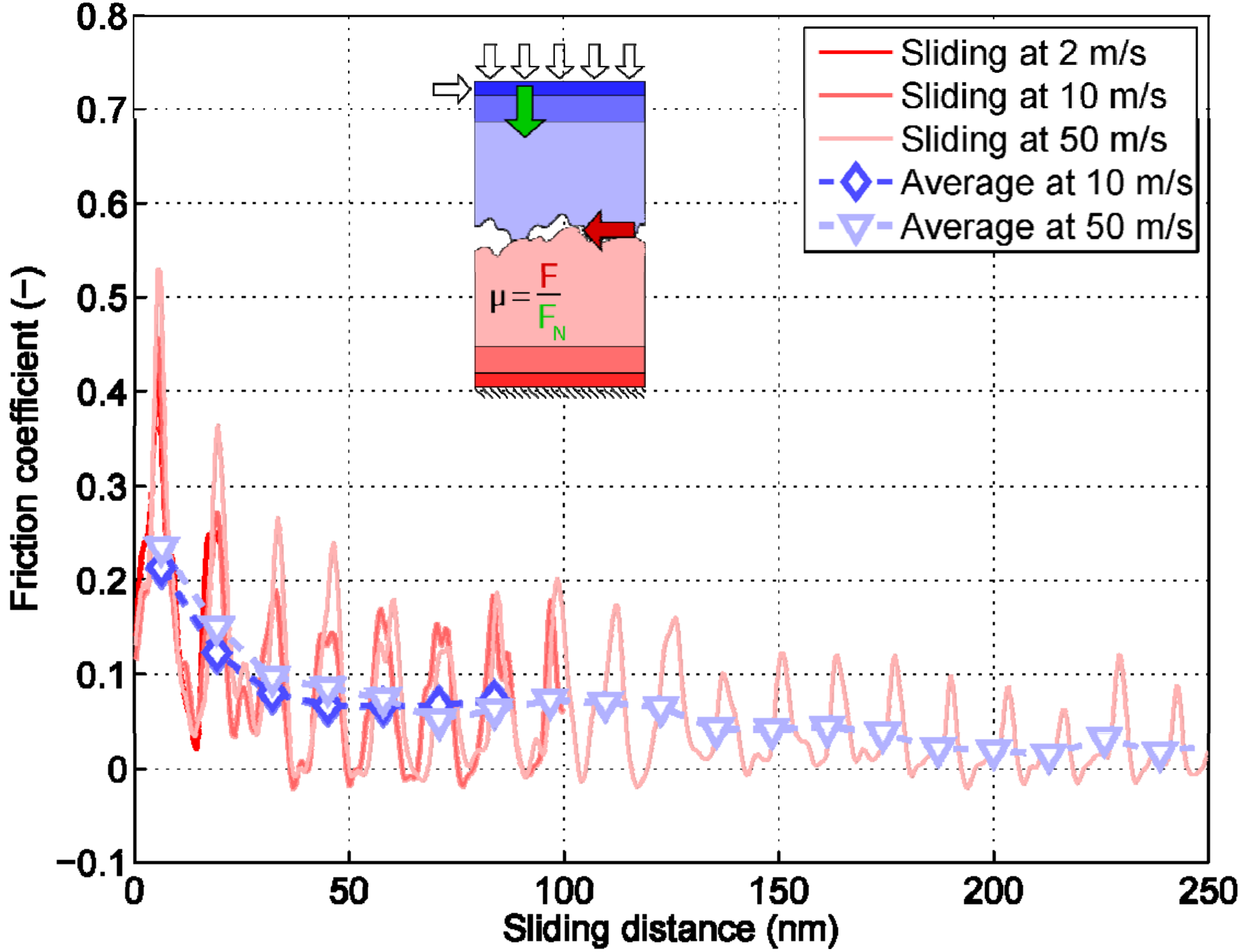


Animation



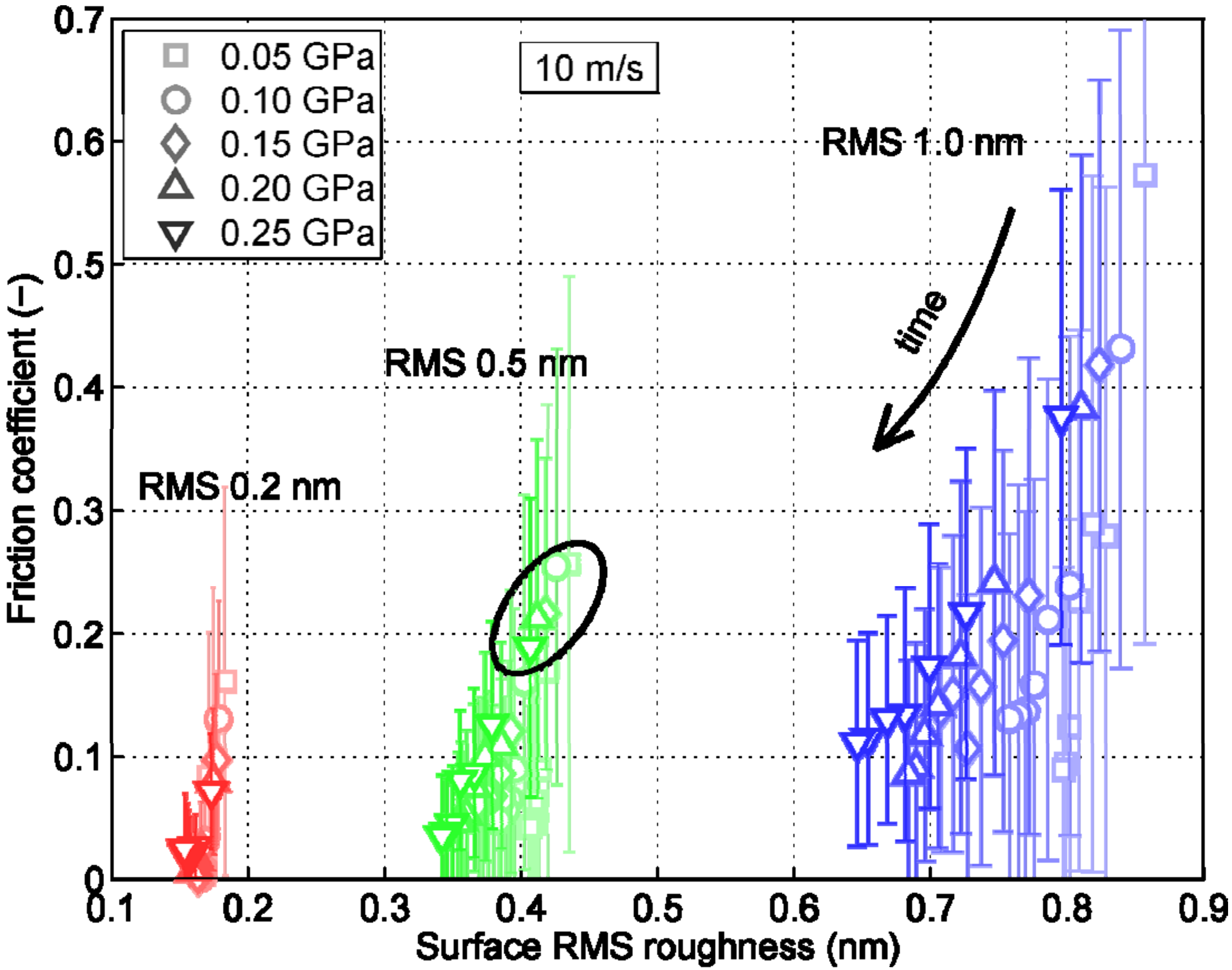
Simulation results

Friction coefficient vs. time (RMS roughness 0.5 nm / load 0.20 GPa)



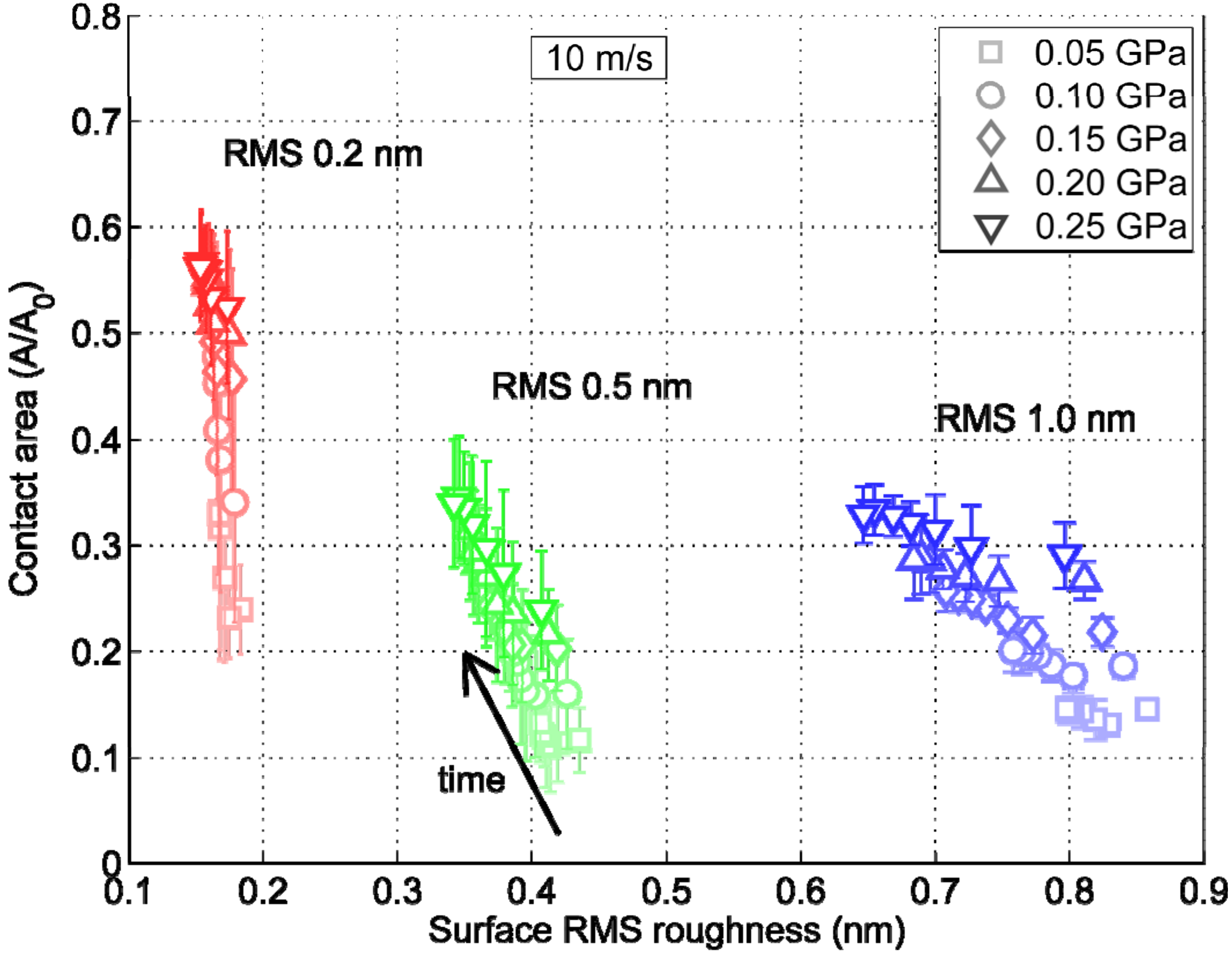
Simulation results

Friction coefficient vs. roughness



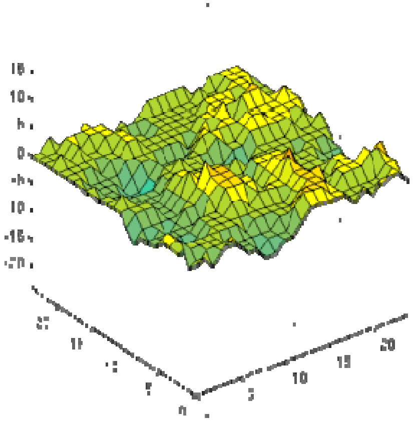
Simulation results

Surface roughness vs. contact area

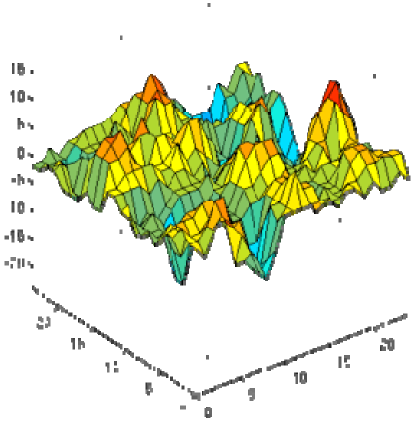


Simulation results

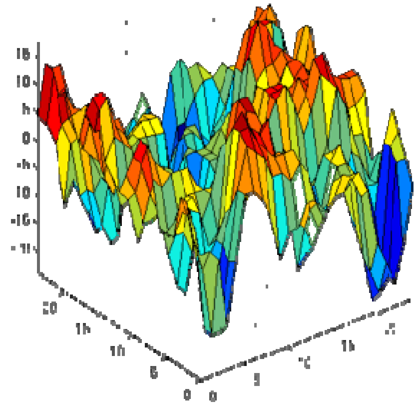
Flattening of surfaces; threshold = 20% difference in height between points



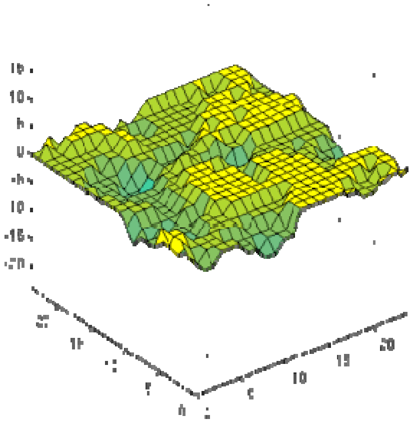
RMS 0.2 nm



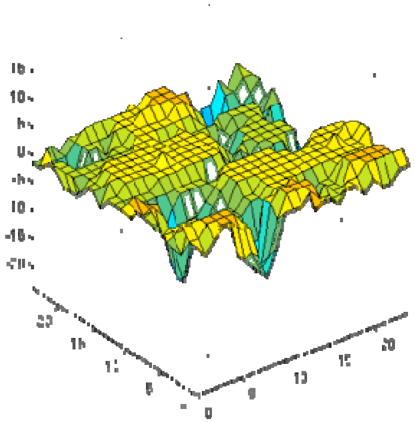
RMS 0.5 nm



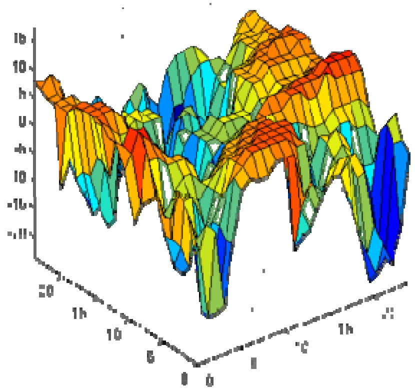
RMS 1.0 nm



RMS 0.2 nm



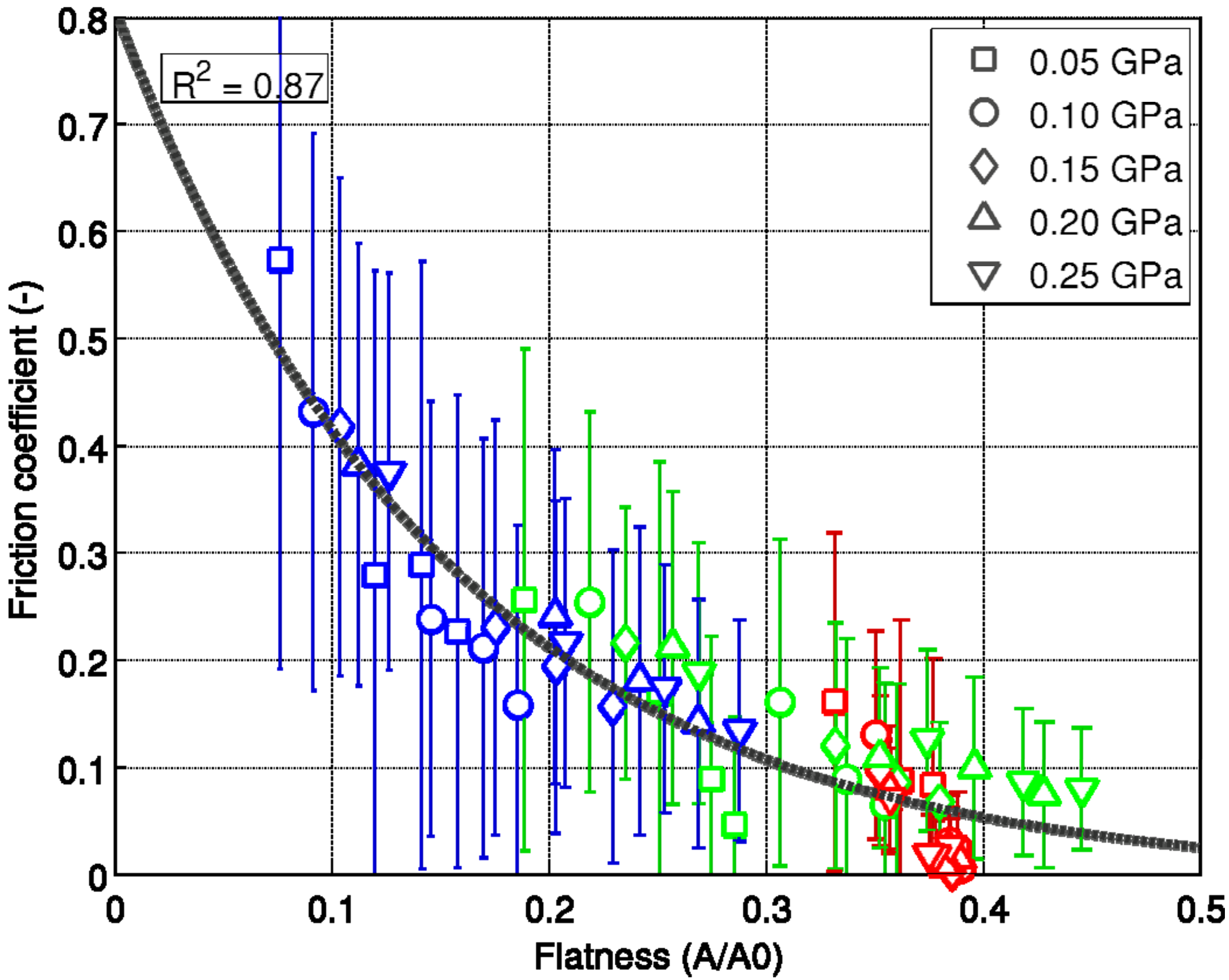
RMS 0.5 nm



RMS 1.0 nm

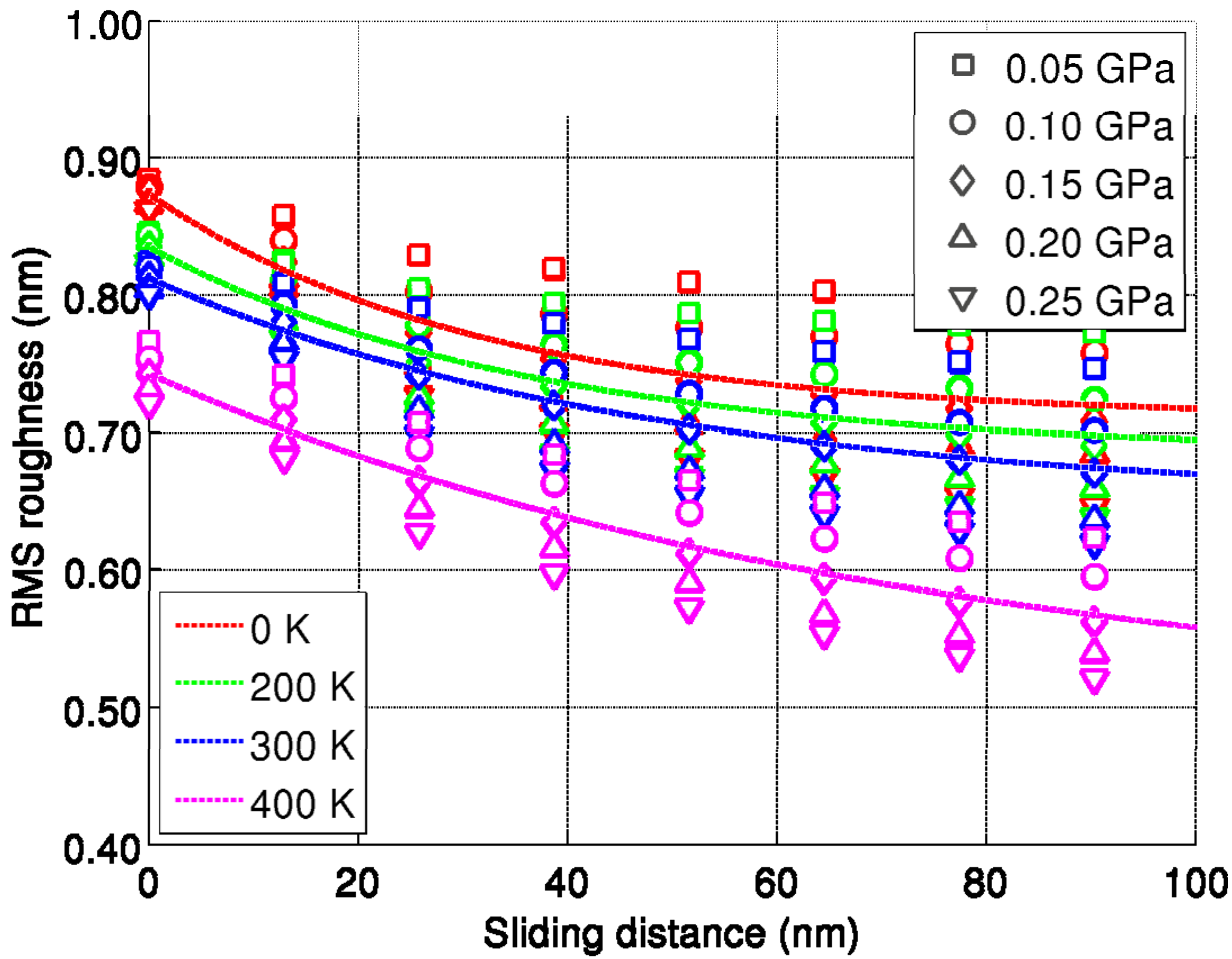
Simulation results

Flatness vs. friction; exponential decay



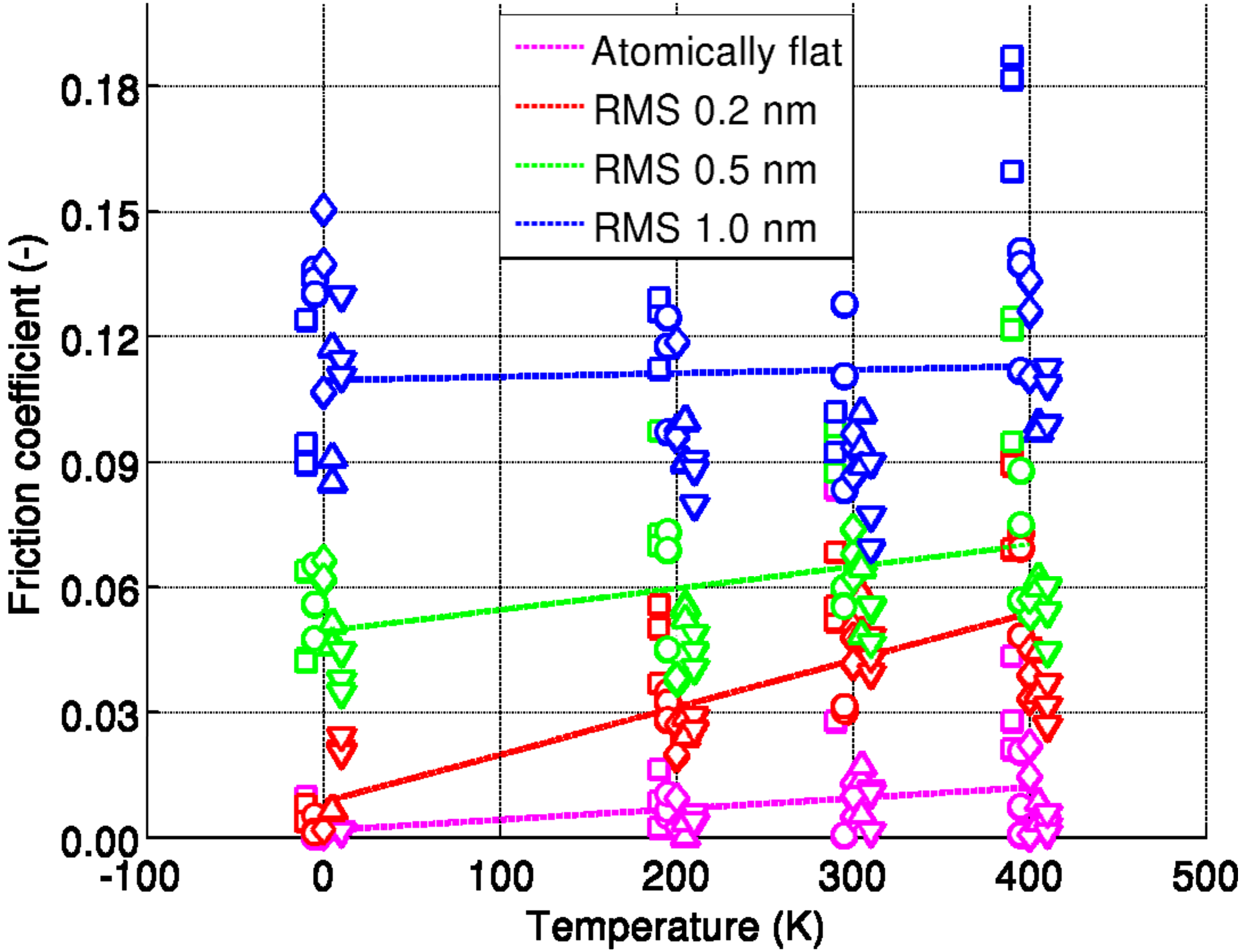
Influence of temperature

Change in roughness; 1 nm RMS roughness



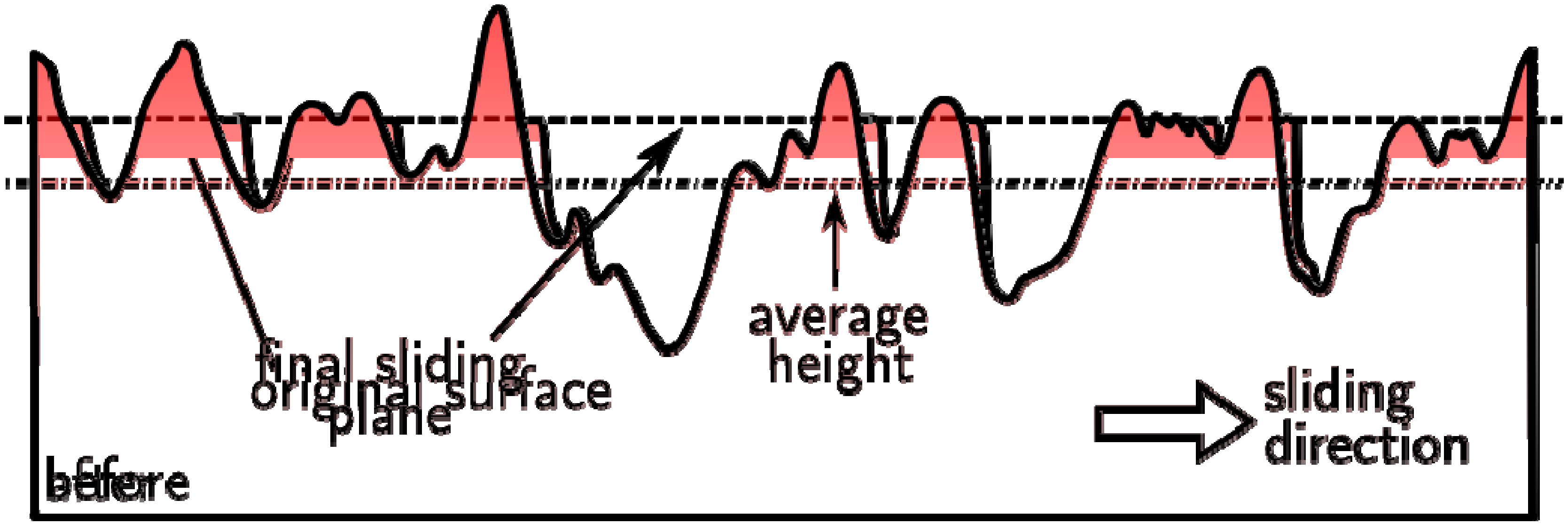
Simulation results

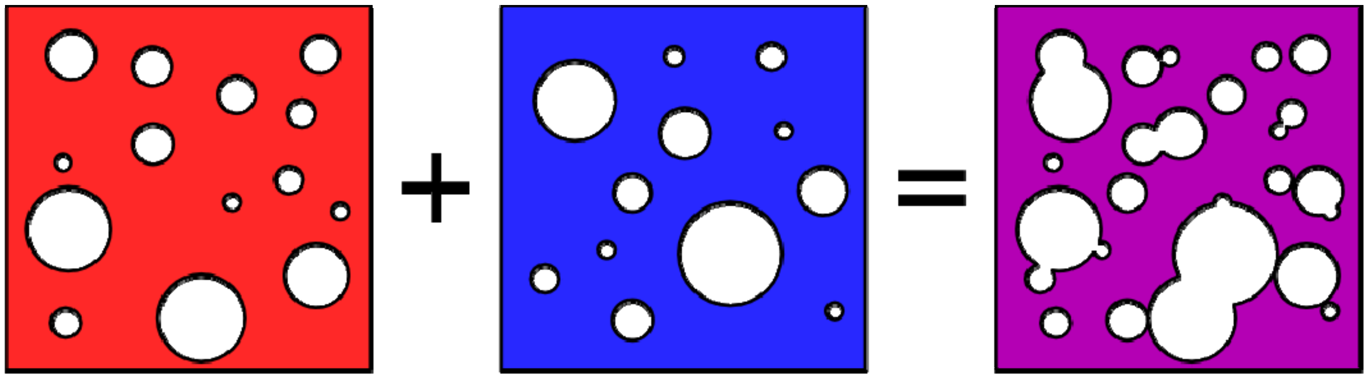
Thermal effect – Friction coefficient vs. temperature



Discussion

View on friction of rough surfaces





A 2D depiction of the sliding plane

Summary 1

- Rough deformable on rough deformable MD model
- Key role of roughness
  - Gives « *realistic* » friction coefficients
  - Geometric effect: friction proportional to number of atom direct collisions (scales with RMS roughness)

- But roughness decreases quickly (exp decay of friction with flatness)
- What is roughness at atomic scale?
  - Reserve of « fresh » (i.e. rough asperities)
  - Mechanisms for roughness creation? (ex: third bodies)

Publications:
Comput. Mech., DOI: 10.1007/s00466-011-0574-9 (2011)
Tribol. Lett., DOI: 10.1007/s11249-011-9846-y (2011)
Tribol. Int., submitted (2011)

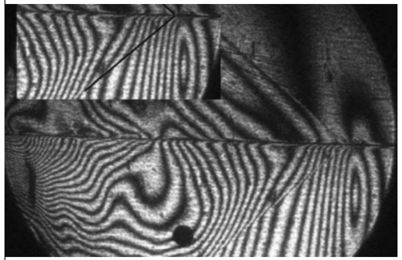
Large scale sliding

Mode II Fracture vs. Initiation of Dynamic Sliding

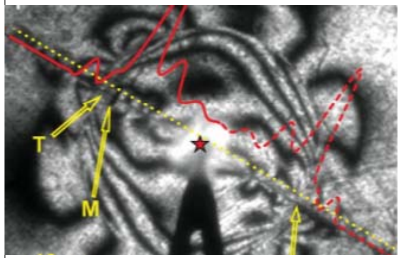
- Continuum scale
- Onset of sliding
- Friction or Fracture?

Lab earthquakes

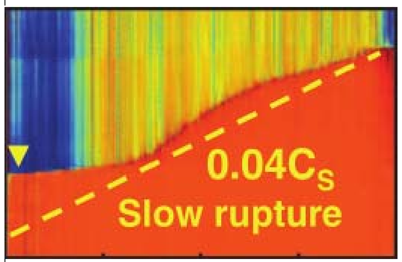
Experimental results for quasi-static shear loading



Coker, *Lapusta, Rosakis*
JMPS 2005

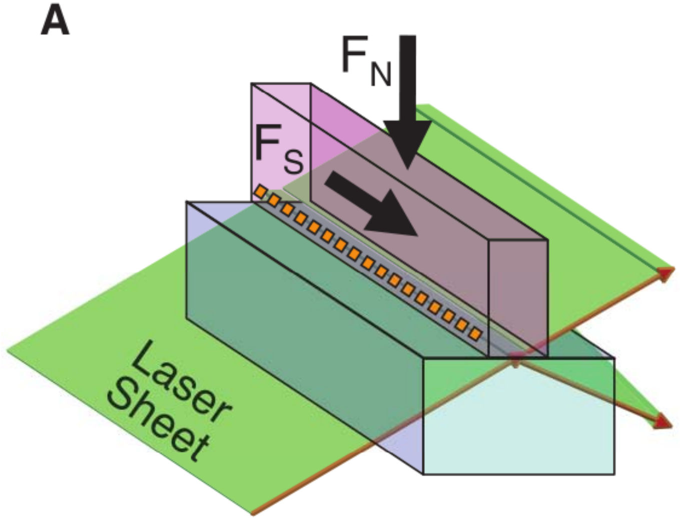


Lu *et al.*
PNAS 2007

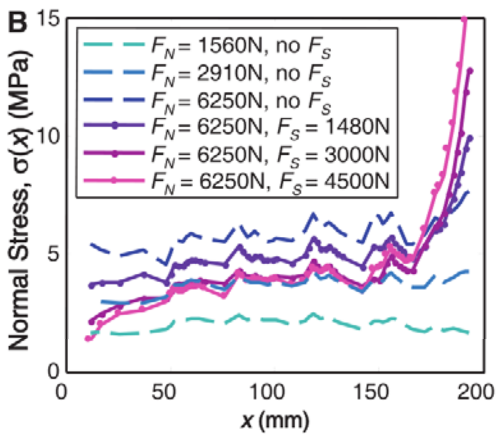


Ben-David, Cohen, Fineberg, Science 2010

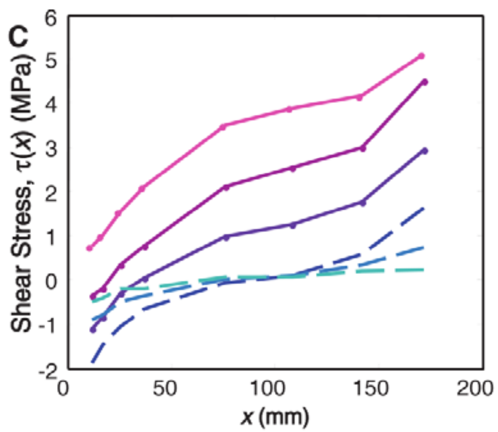
PMMA Interface under Quasi-static Shear Loading



Normal Stress Distribution



Shear Stress Distribution



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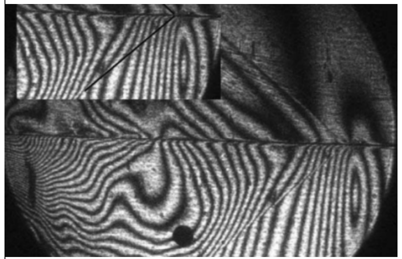
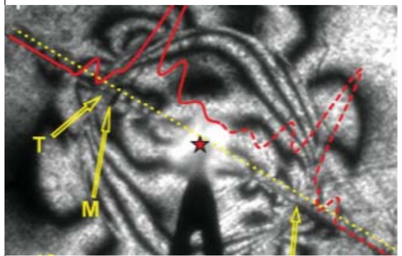
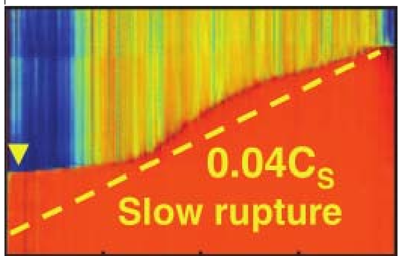


Coker *et al.*
JMPS 2005



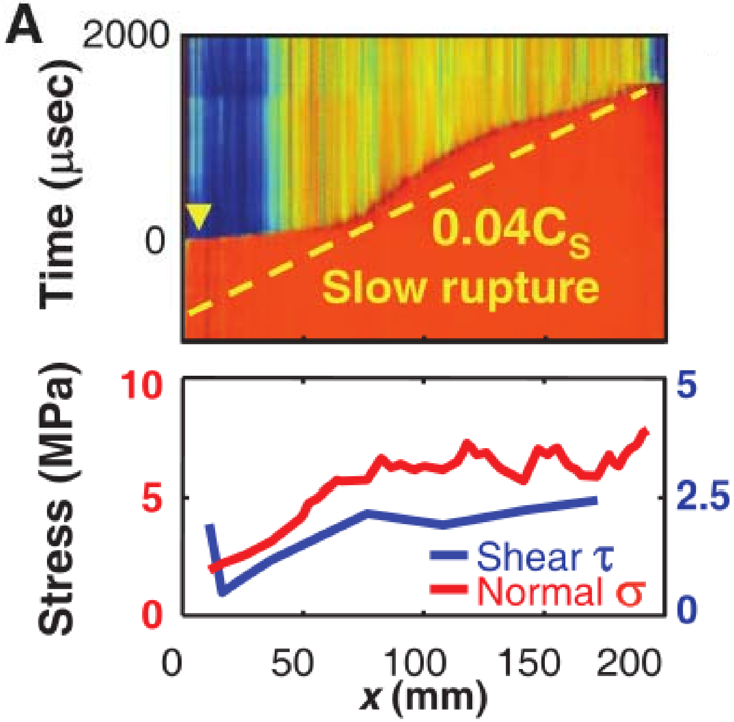
Lu *et al.*
PNAS 2007



Ben-David *et al.*
Science 2010

Real Contact Area
Indicates
Interface Rupture Propagation

Stress Distributions



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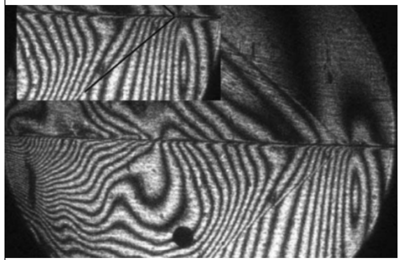
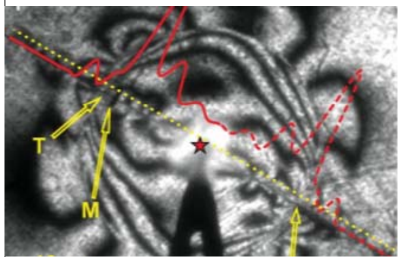
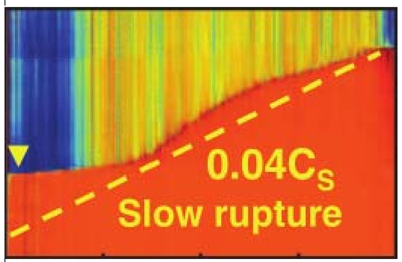


Coker *et al.*
JMPS 2005



Lu *et al.*
PNAS 2007



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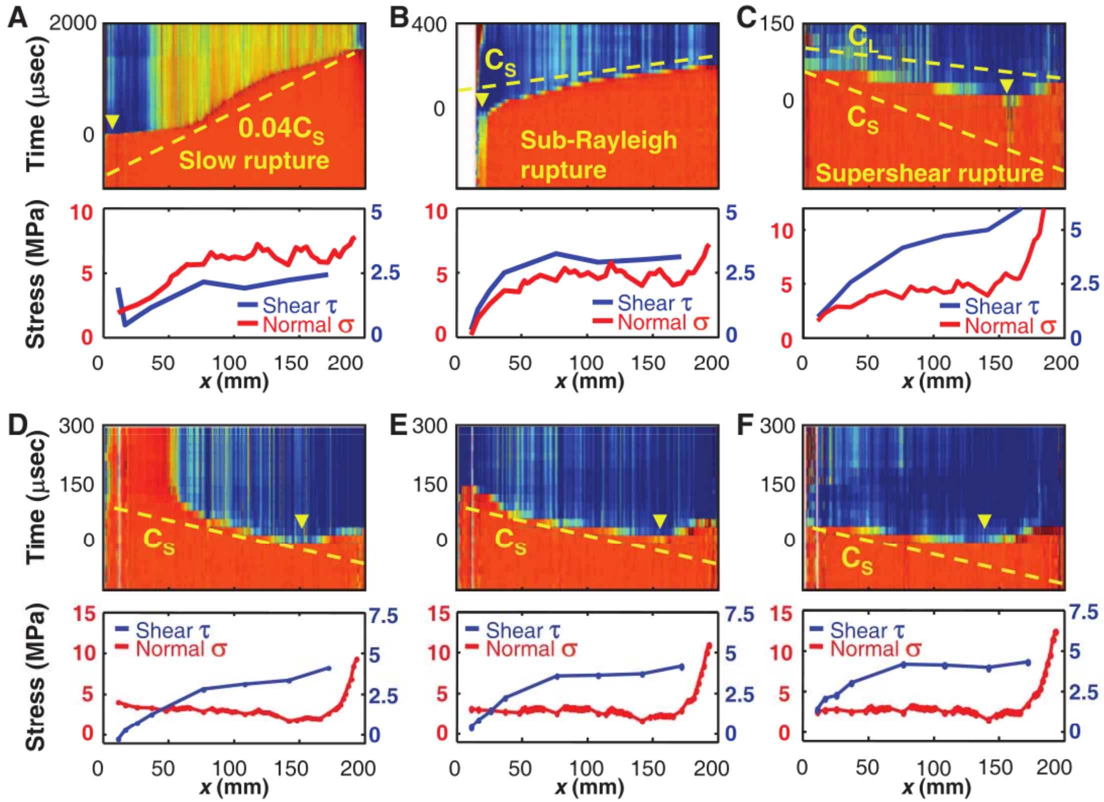

Experimental results

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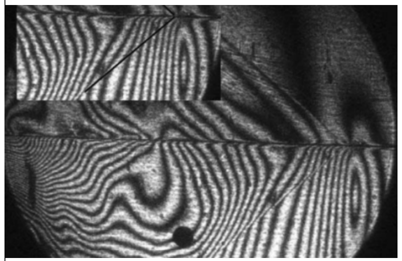

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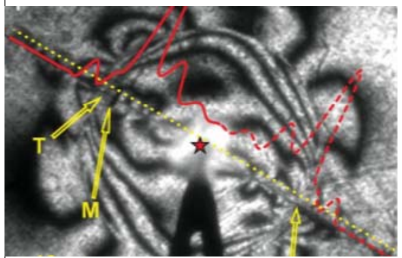

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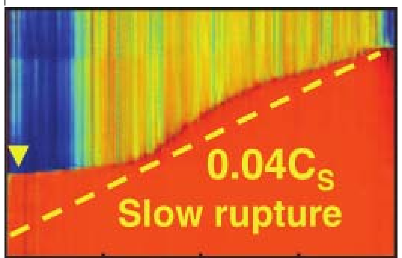

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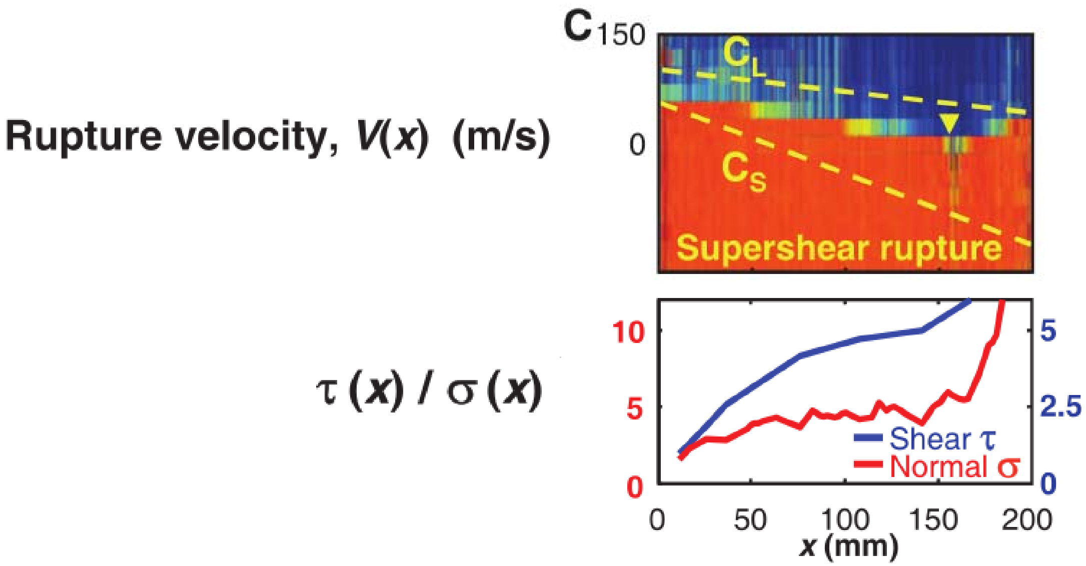
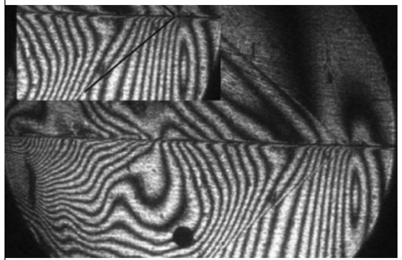
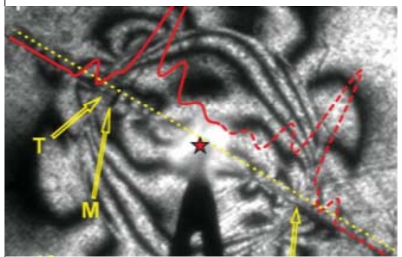


Experimental results

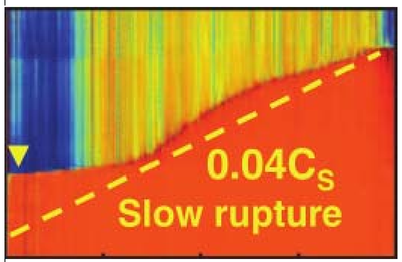
Experimental results for quasi-static shear loading



Coker *et al.*
JMPS 2005



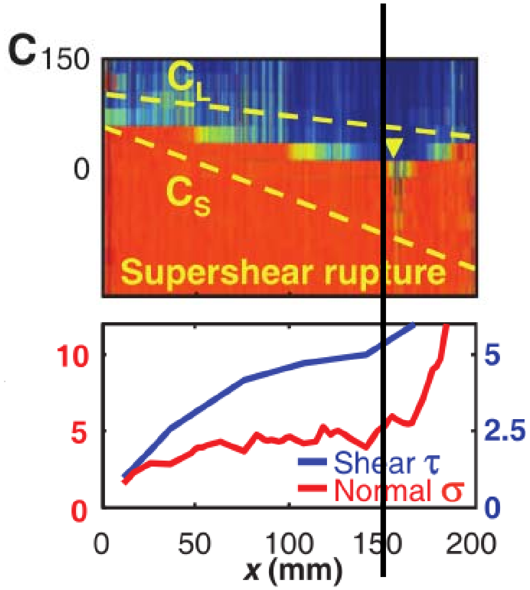
Lu *et al.*
PNAS 2007



Ben-David *et al.*
Science 2010

Rupture velocity, *V*(*x*) (m/s)

τ (*x*) / σ (*x*)



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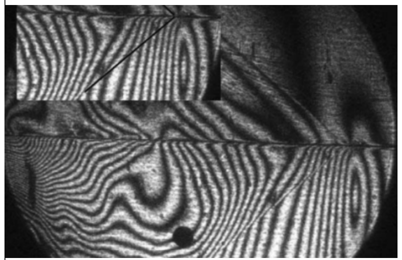

Coker *et al.*
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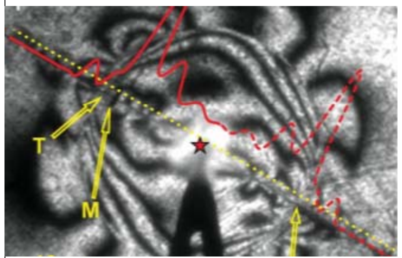
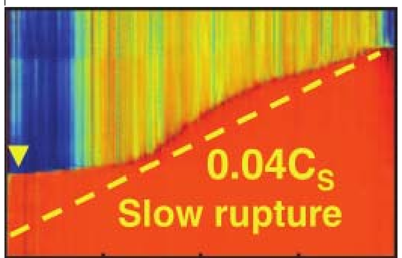
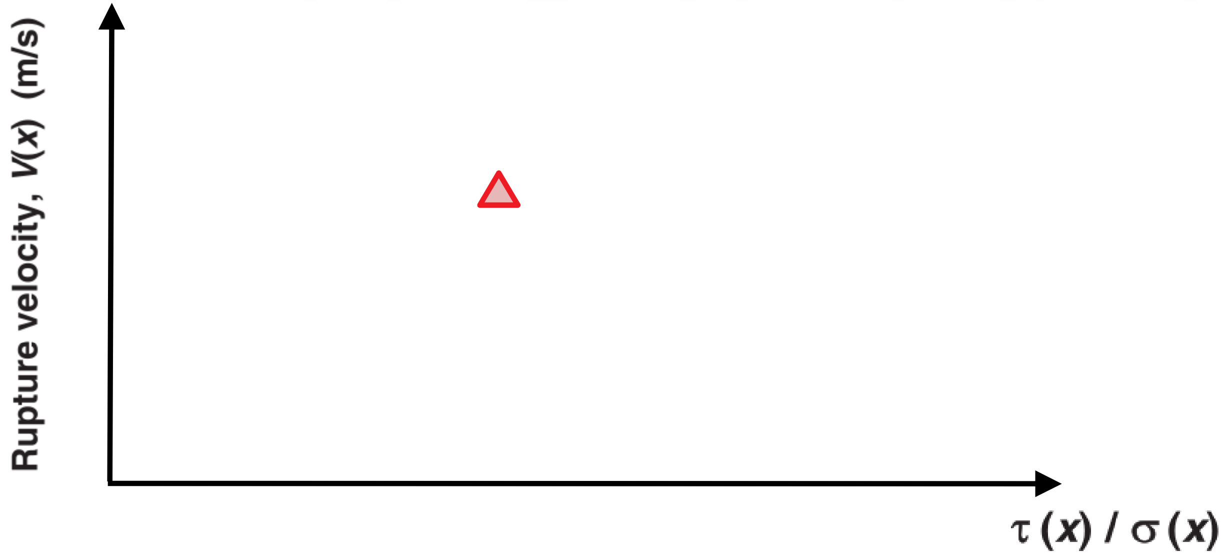


Lu *et al.*
PNAS 2007

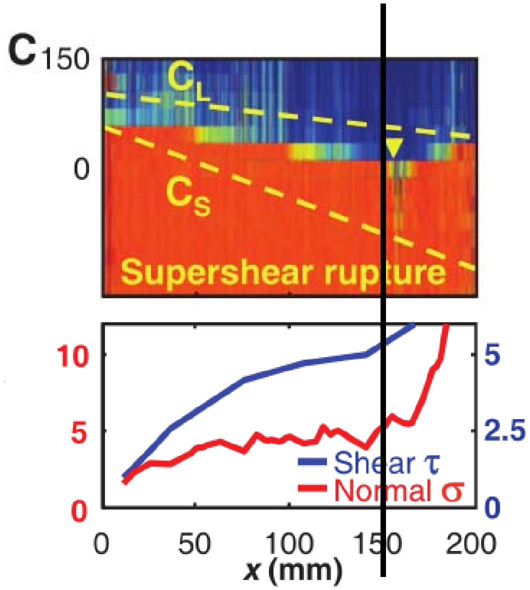


Ben-David *et al.*
Science 2010



Rupture velocity, $V(x)$ (m/s)

$\tau(x) / \sigma(x)$



Experimental results

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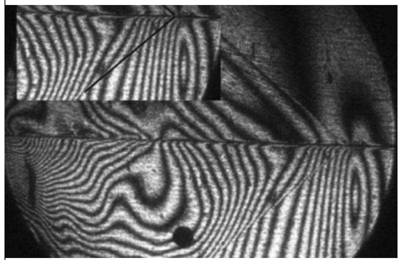

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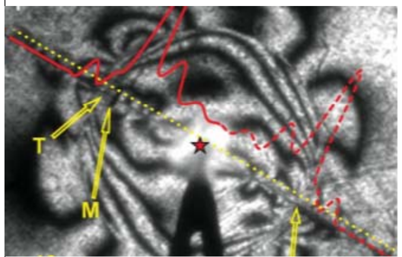
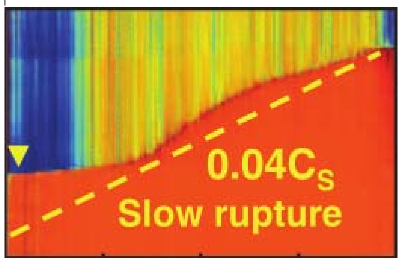
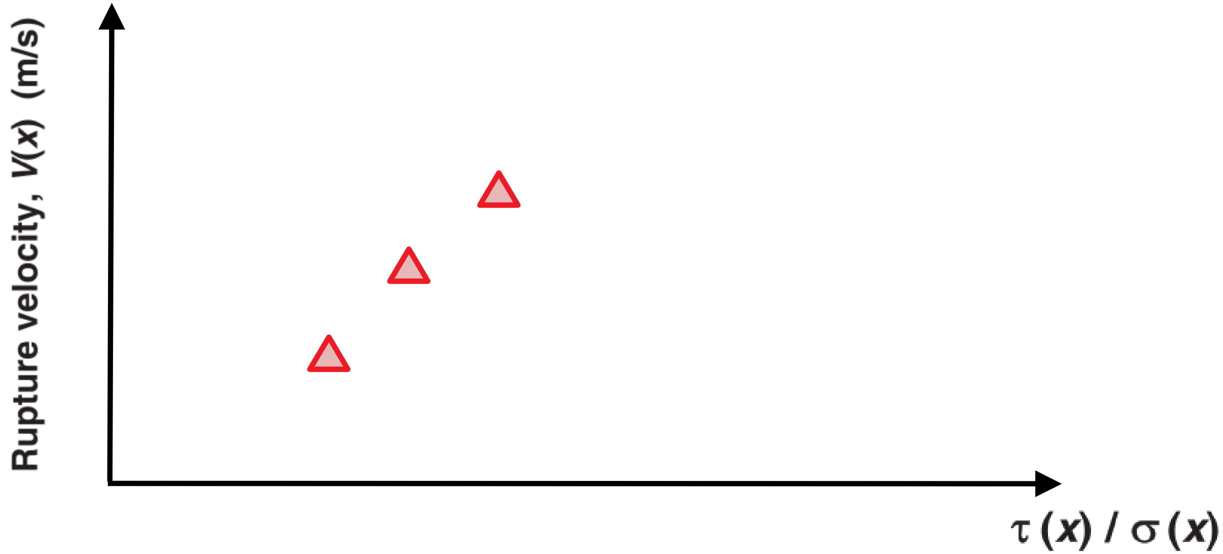


Lu *et al.*
PNAS 2007

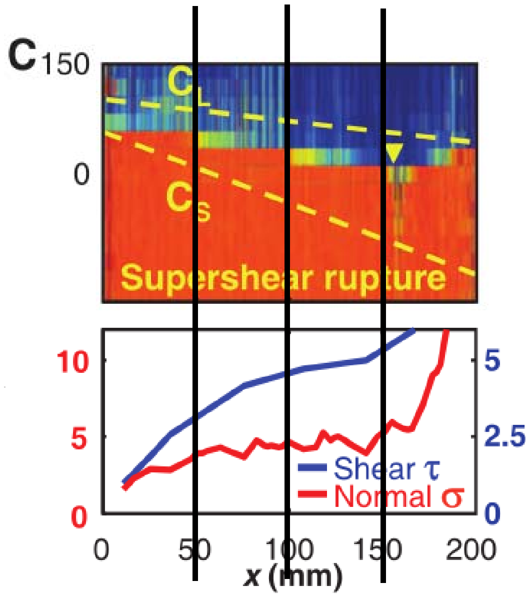


Ben-David *et al.*
Science 2010



Rupture velocity, *V*(*x*) (m/s)

$\tau\,(x)\,/\,\sigma\,(x)$



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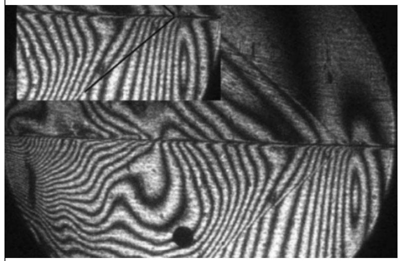
Experimental results for quasi-static shear loading



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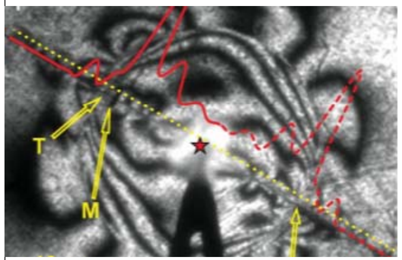
JMPS 2005



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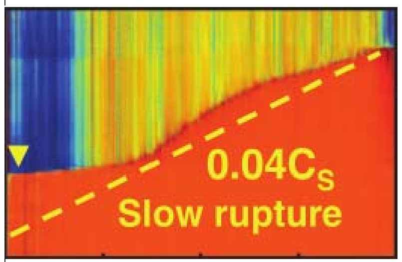
PNAS 2007



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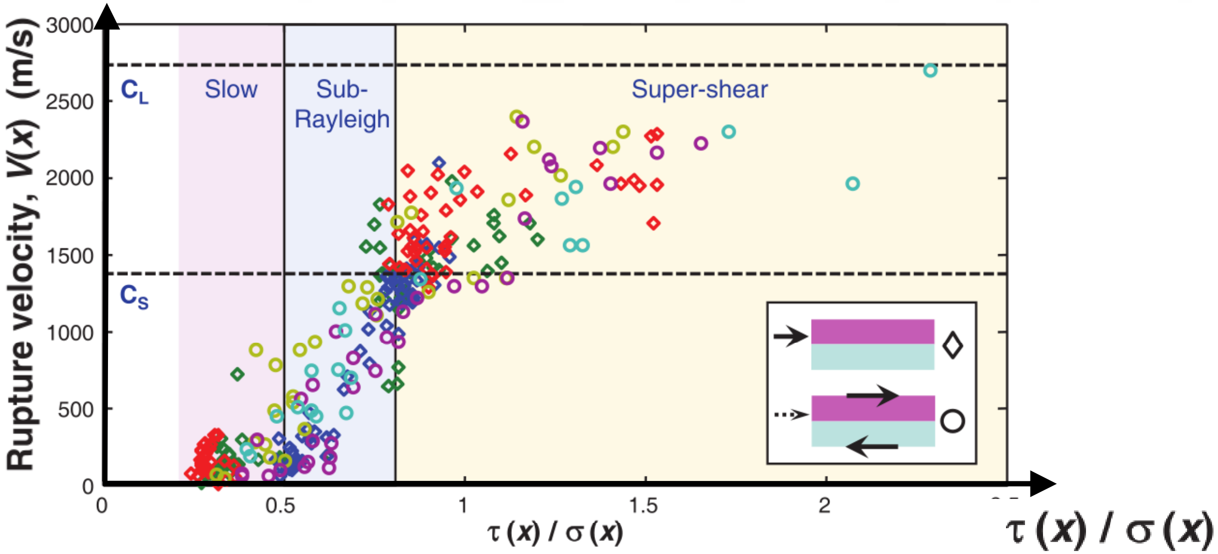

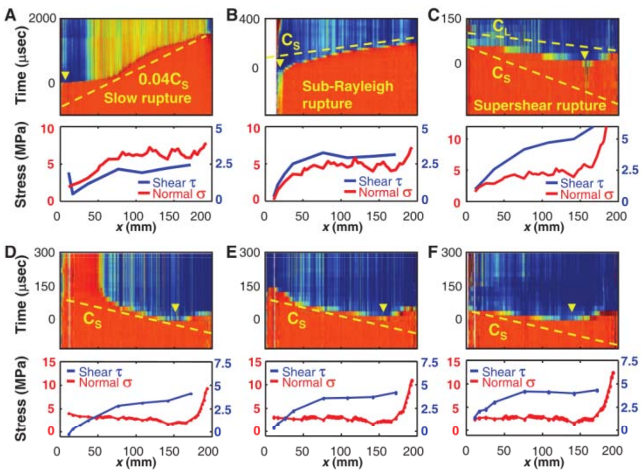

Experimental results

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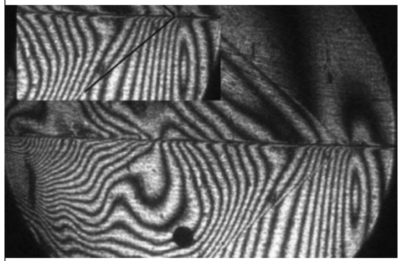

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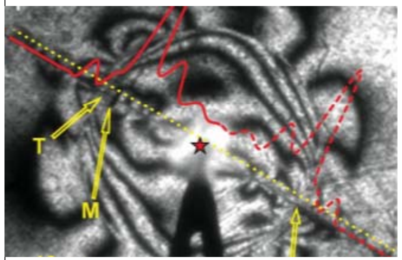

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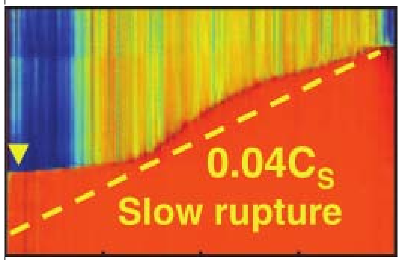

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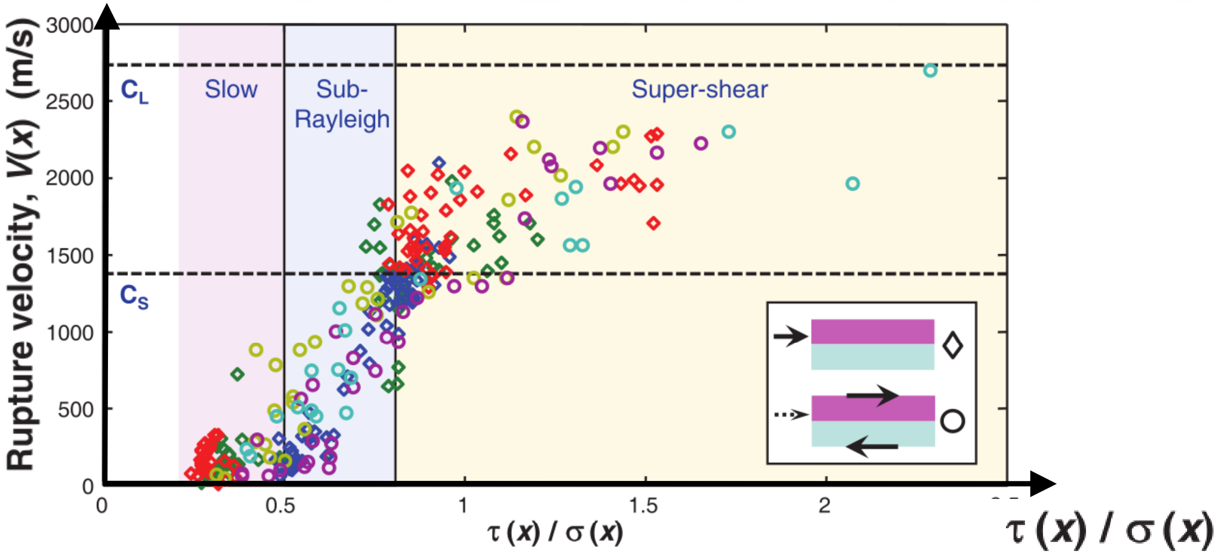
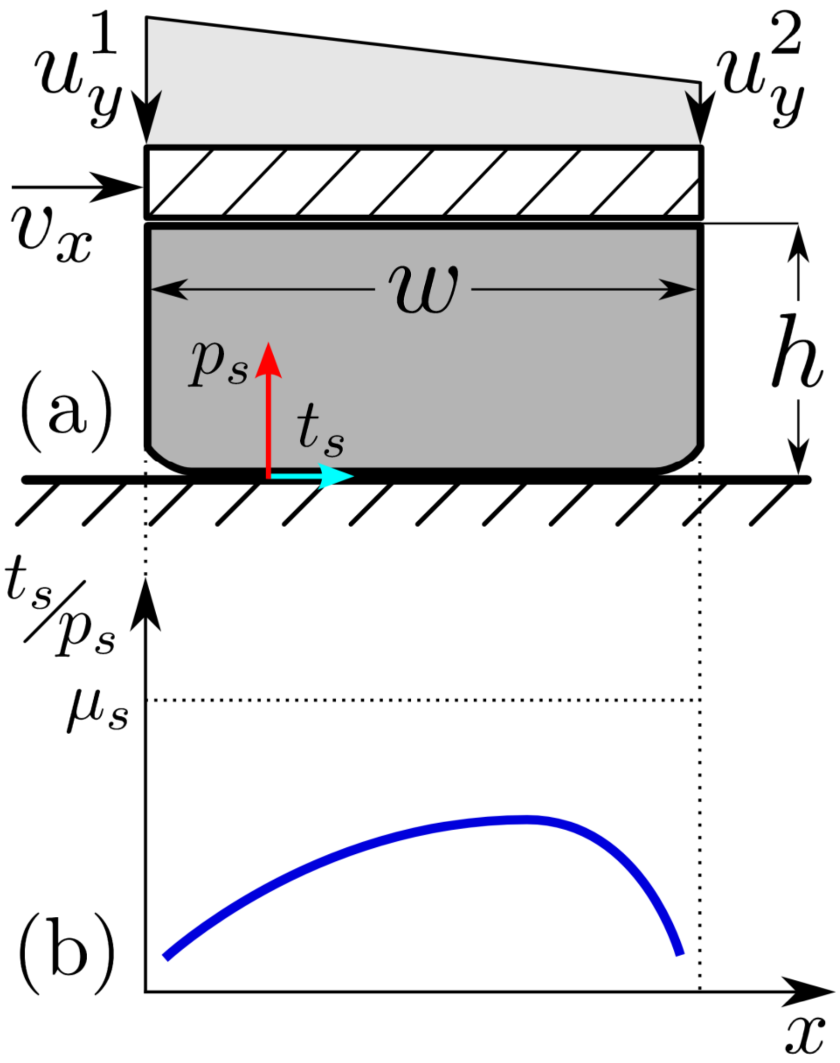


Features:
All modes of rupture velocity reproduced
Local friction can be much higher than macroscopic value
Key role of heterogeneities

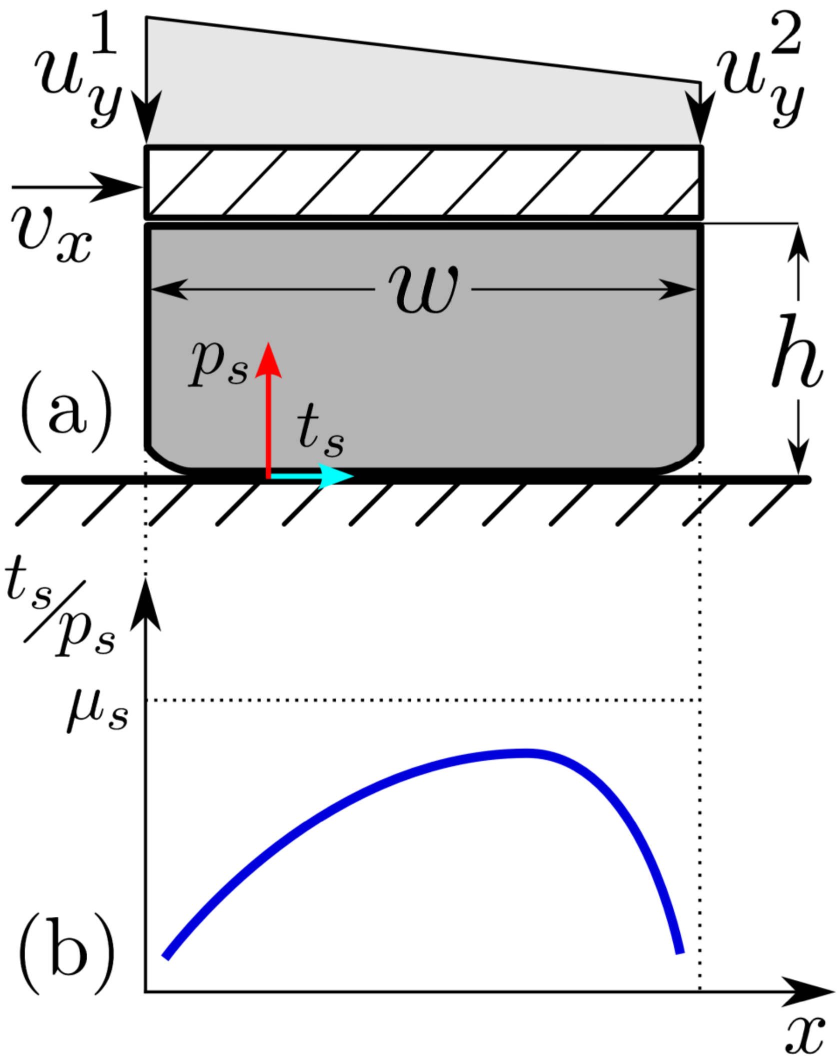
Fracture energy analogy:
More energy needed to break interface
→higher local interface strength
→ more real contact area
→ more local normal stress

Numerical model

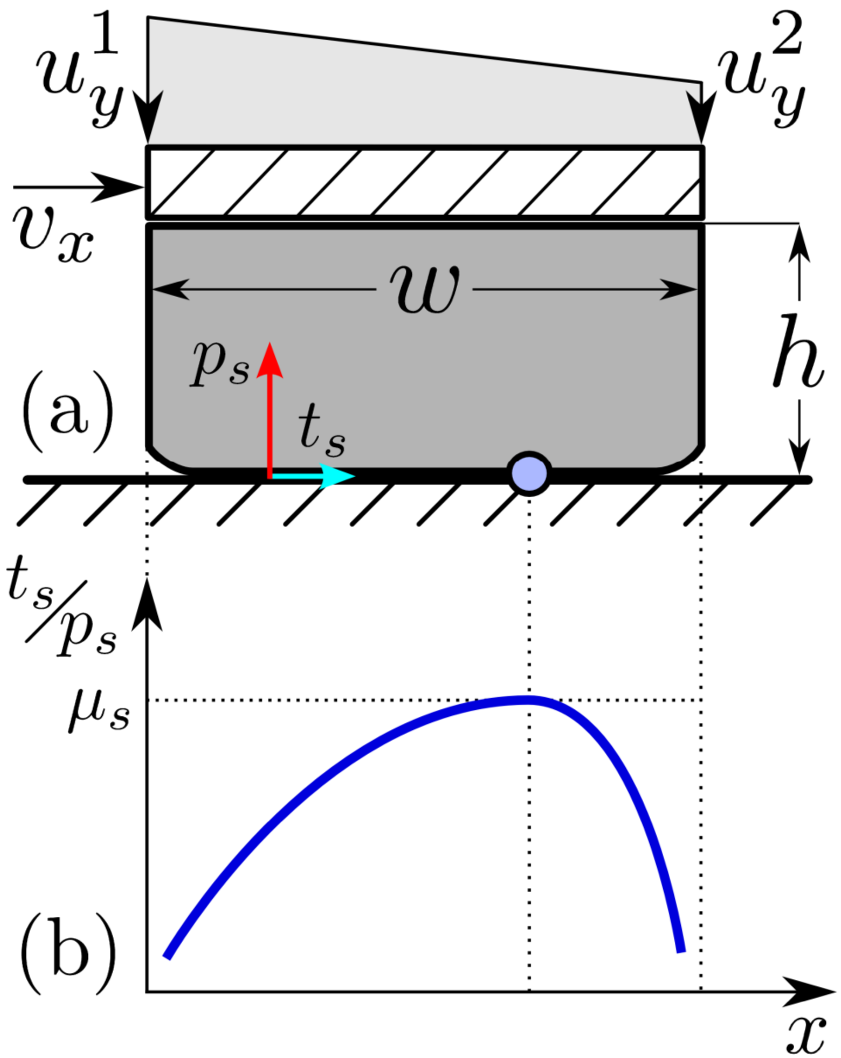
Explicit FE; energy-conserving contact



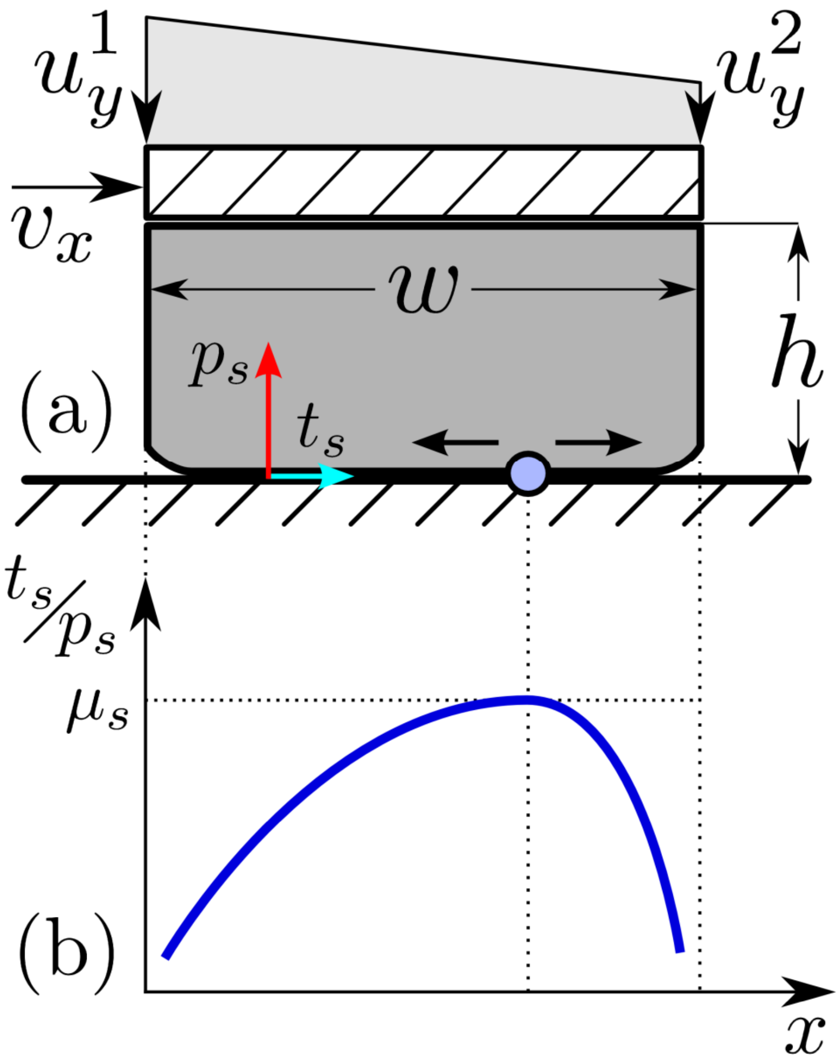
Problem setup



Problem setup

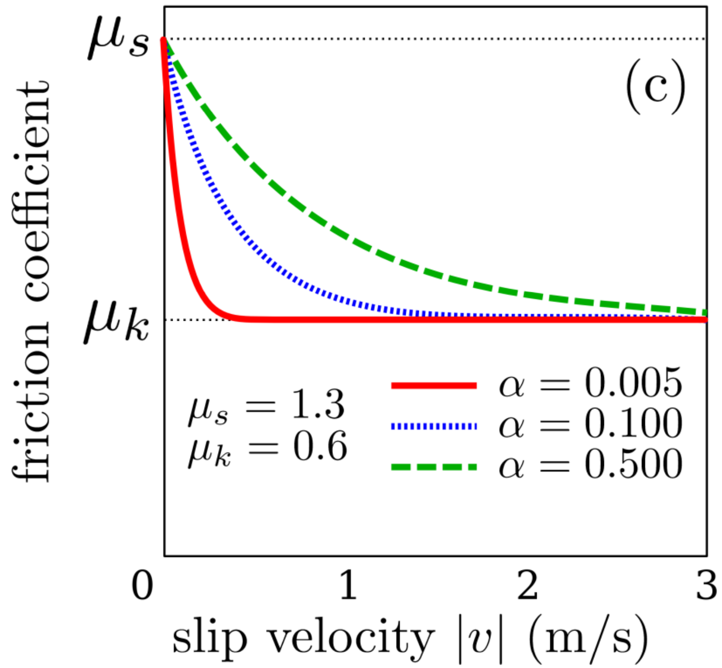


Problem setup



Velocity weakening friction law

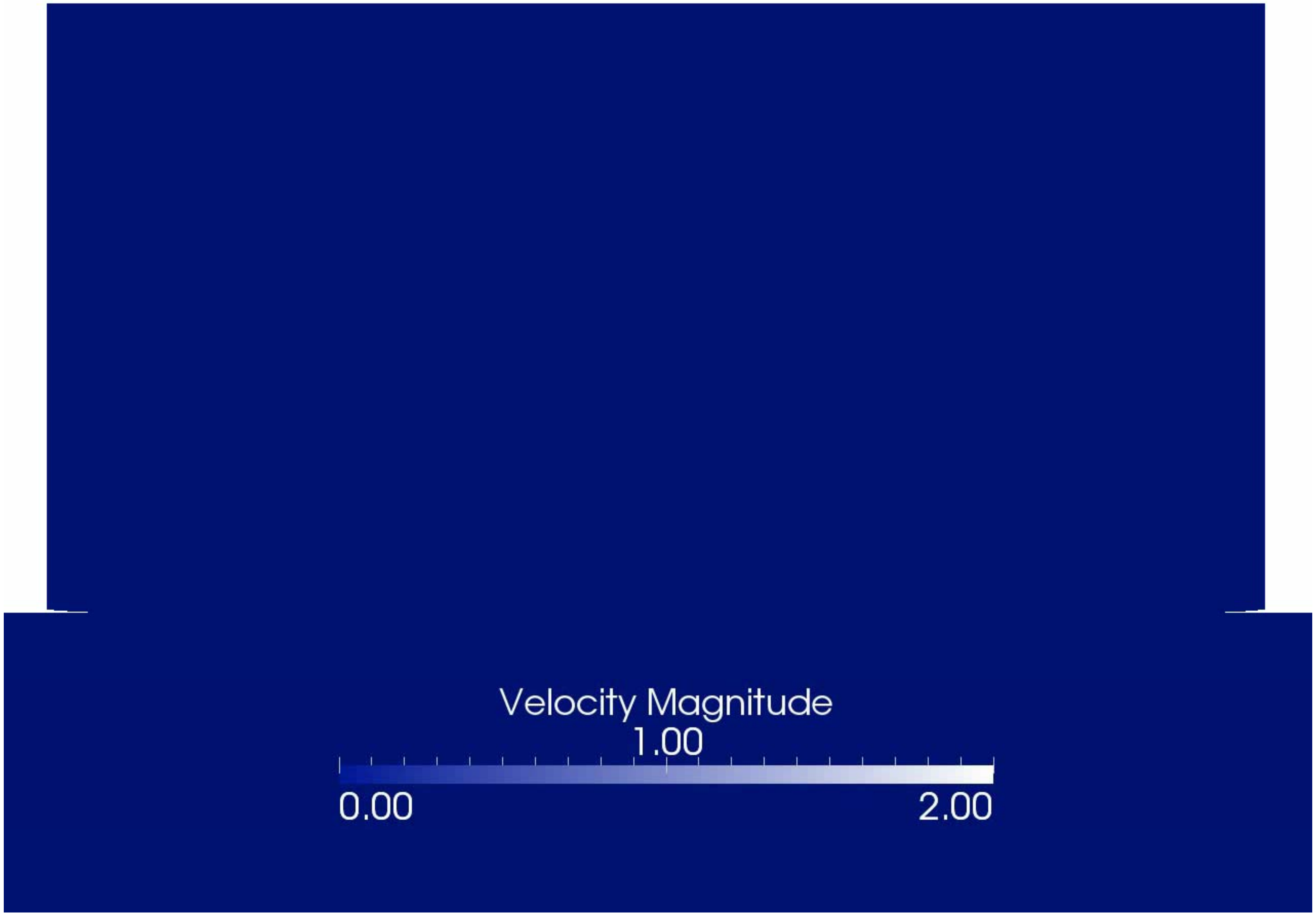
Tangential resistance is proportional to the contact pressure



$$\mu = \mu_s + (\mu_k - \mu_s)(1 - \exp(-|v|\sqrt{(\mu_s - \mu_k)/\alpha})),$$

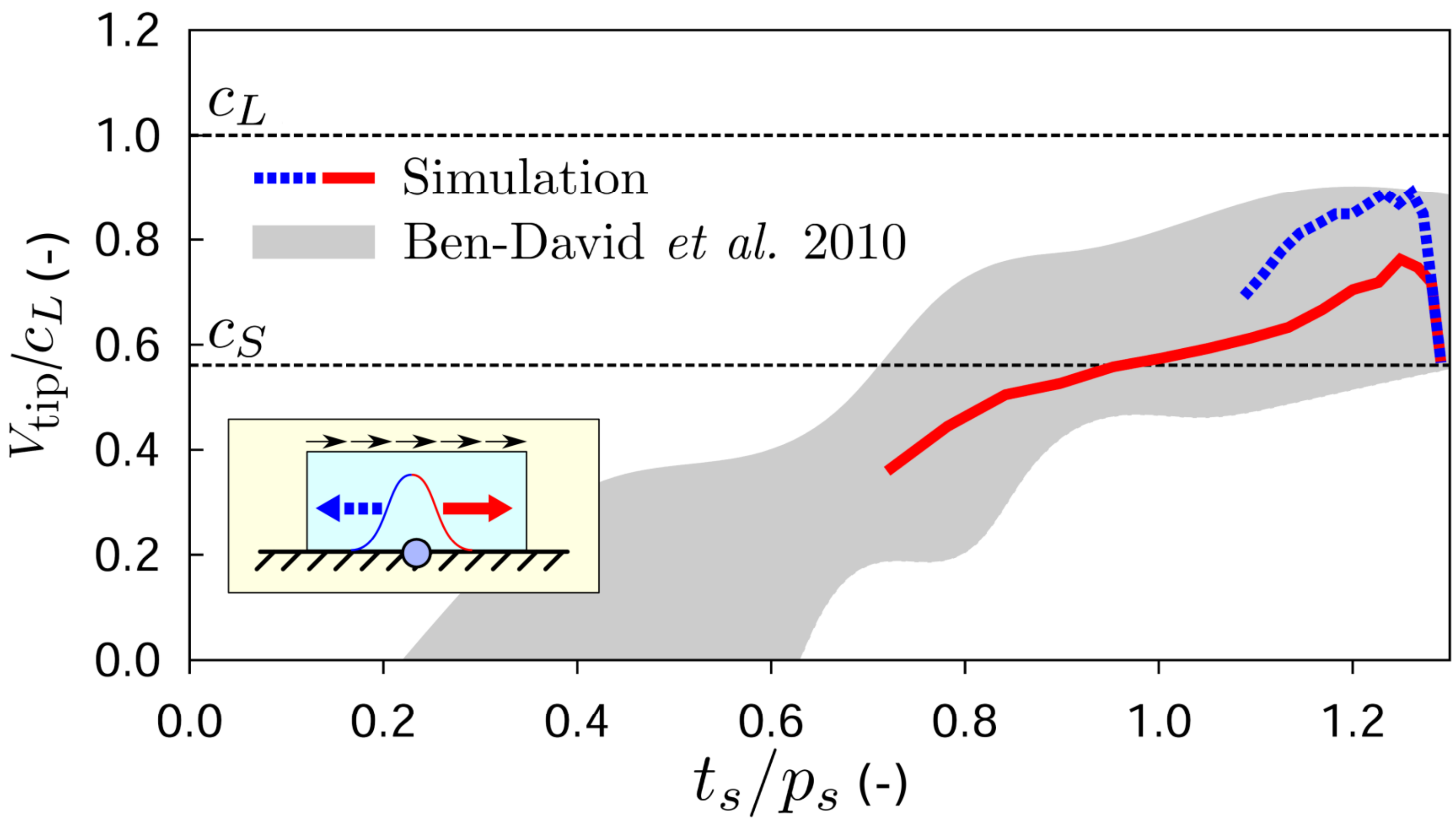
v is the material slip velocity, μ_s, μ_k are the static and the kinetic friction coefficients, α is the transition parameter

Animation



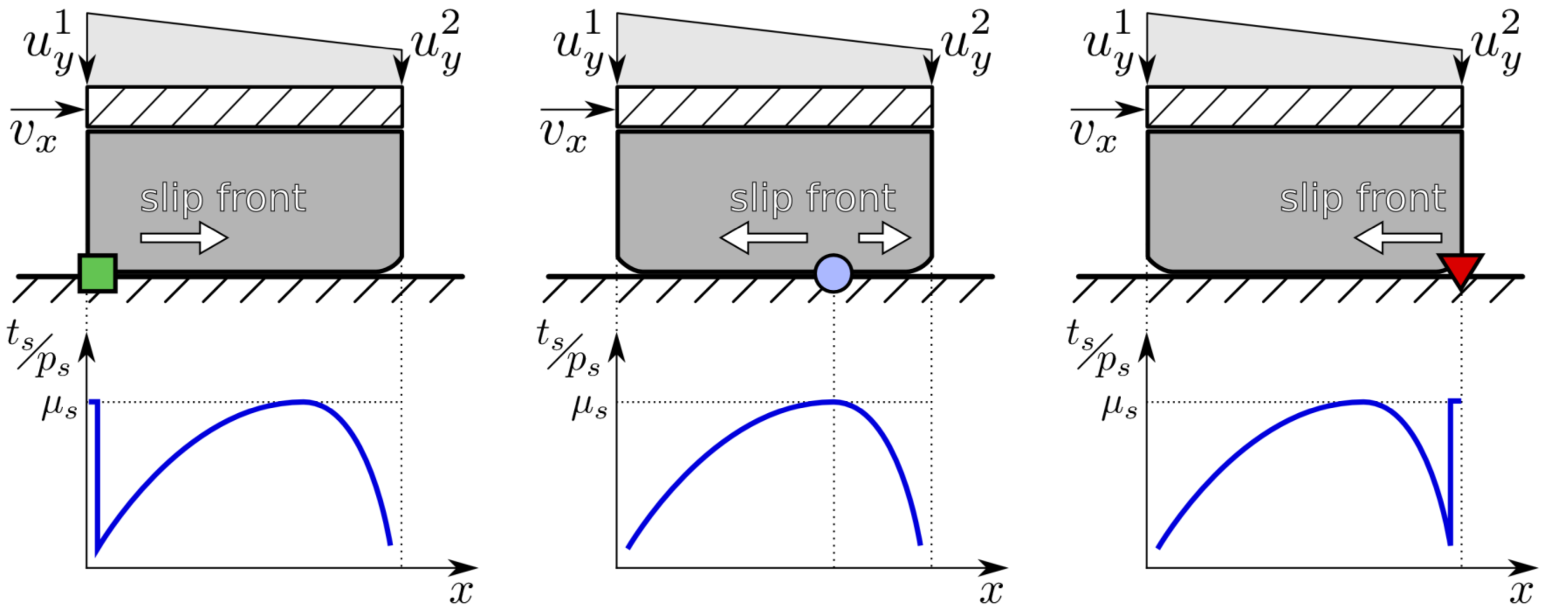
Comparison with experiments

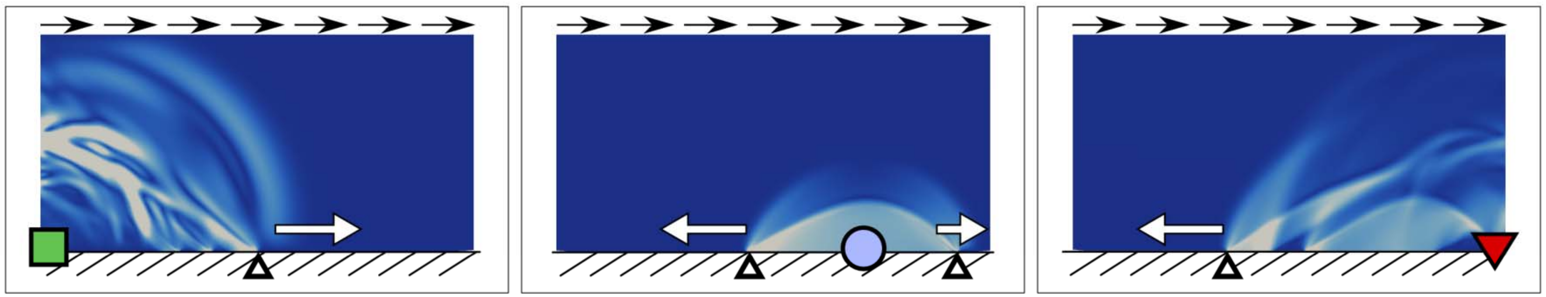
Matches but… non uniqueness of Vtip



Spontaneous and triggered slip initiations

Directionality effect?





Spontaneous and triggered slip initiations

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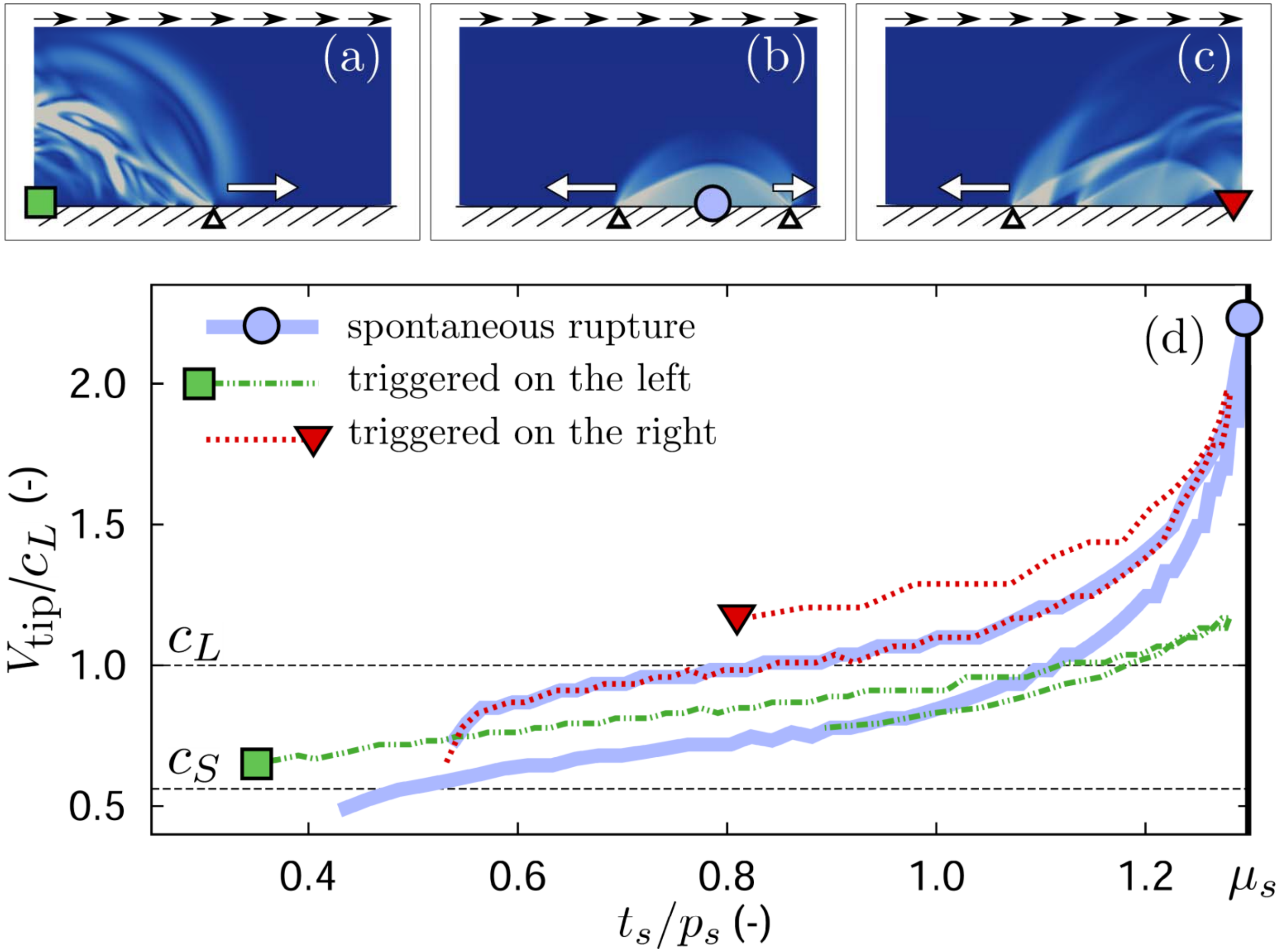
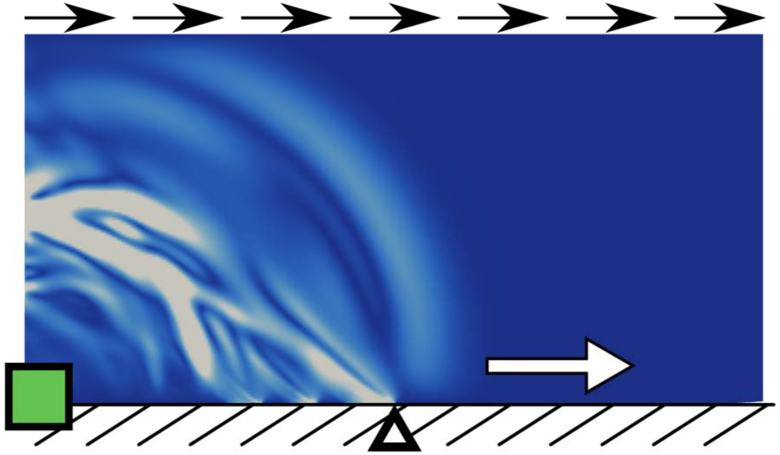
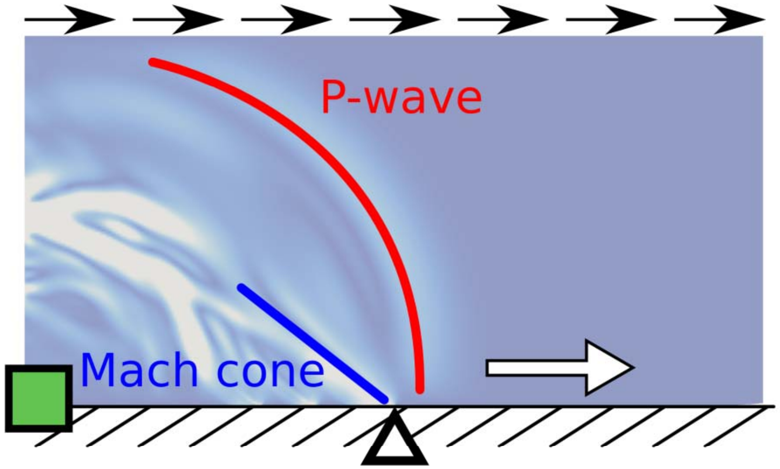
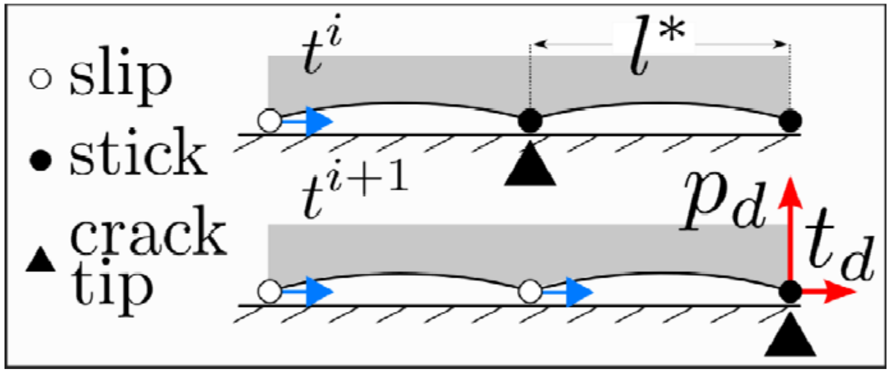


In front of the slip front

Things change …

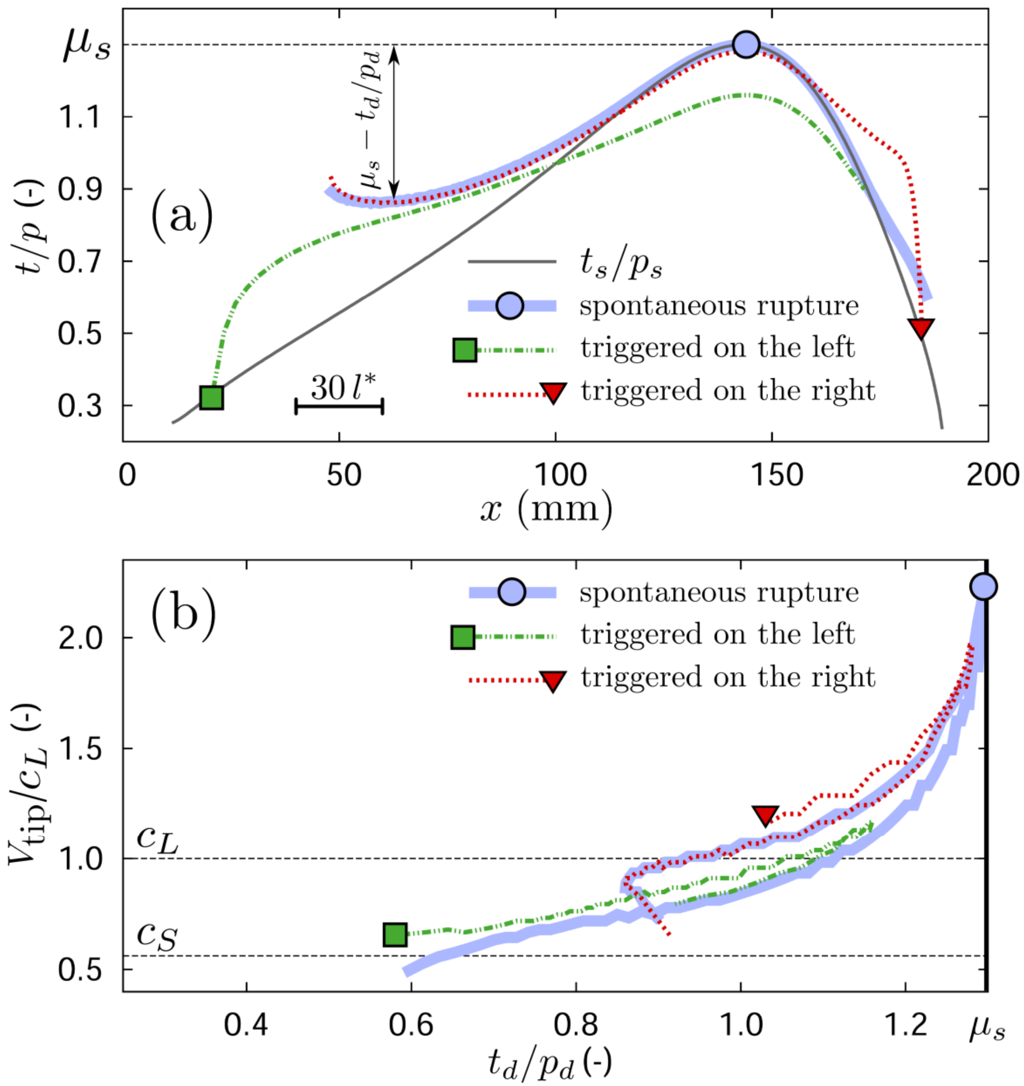






In front of the slip front

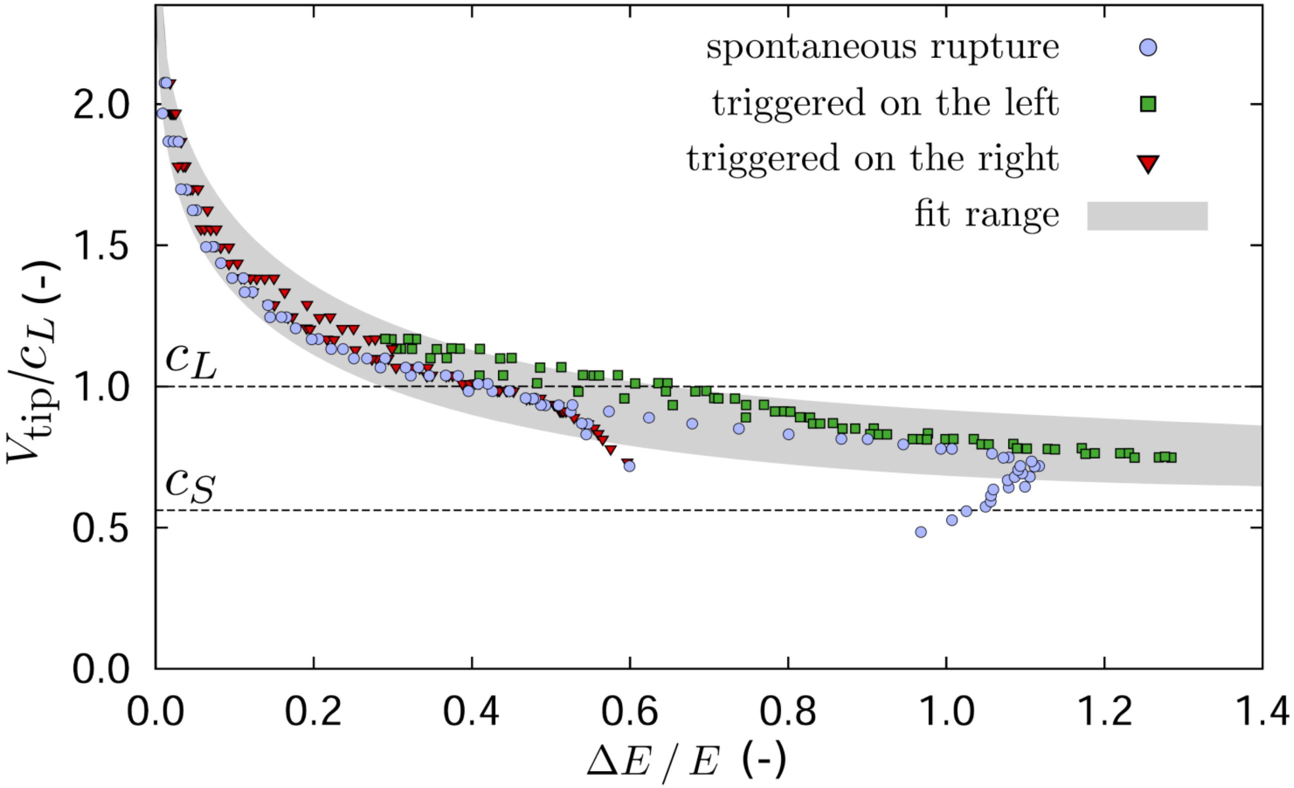
Dynamic effects help



Slip velocity as a function of local energy

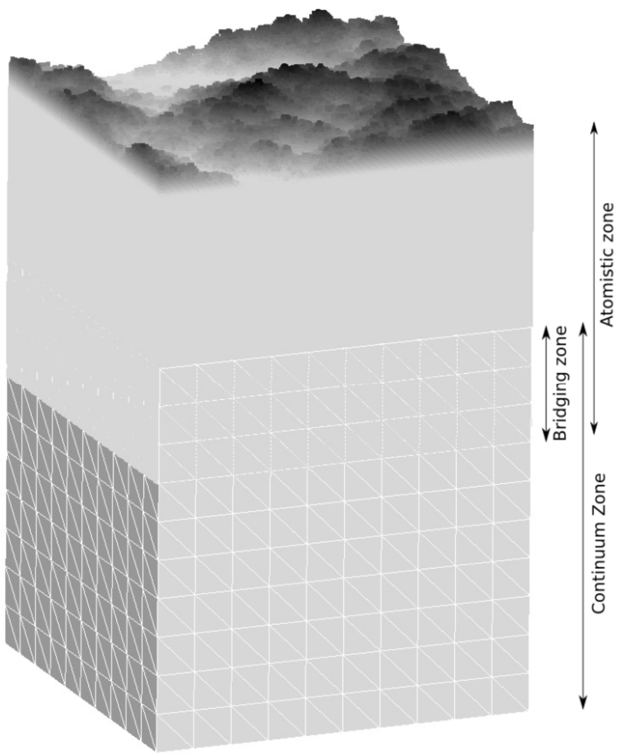
Back to fracture mechanics analogy

$$\Delta E / E = \frac{E_{\text{needed}} - E_{\text{stored}}}{E_{\text{stored}}}$$



Conclusions

- Simple model gives consistent observations (with Ben-David et.al 2010 Science paper)
  - Tau-Sigma ratio exceeds global friction coefficient
  - **Rupture velocity depends on local tau-sigma ratio**
- Additional observations
  - Different rupture modes
  - Non uniqueness of Vtip
  - Explained by energy flux (dynamics)
- Perspectives
  - More sophisticated friction law
  - Deformable-deformable contact
  - Interface heterogeneity
  - Access dynamic fields experimentally
- Adding roughness would be nice
  - At what scale roughness breaks down?
  - Challenge for multiscale modeling



3.2 Millions atoms (+2.4M in FE)

lsms.epfl.ch