**Multiscale Modeling of Friction**
International School on Complexity, Erice, June 20-25, 2009
Collaborators: S. Hyun, L. Pei, J. F. Molinari, N. Bernstein, J. Harrison, B. Luan, G. He, M. H. Müser, L. Wenning
K. M. Salerno, A. Libal
Rough Surface Contact  Atomic Effects  Friction

Supported by the National Science Foundation

**Precursors to My Talk and to Steady Sliding**

Measure contact area by transmission
Precursors to sliding:
• drop in the shear force $F_S$
• slip over part of the interface revealed through a drop in contact area

S. M. Rubinstein, G. Cohen, J. Fineberg
Hebrew University of Jerusalem

**Molecular Dynamics Simulation**

- 2D simulation of a block sliding on a surface
- Bottom roughened – multiple flat asperities
- Surfaces initially commensurate
- Lennard-Jones interactions: $4\varepsilon(\sigma/r)^{12} - 2\varepsilon(\sigma/r)^6$
- Normal force $F_N$ from uniform pressure
- Push block with constant low velocity at height $h$
- Measure pushing shear force $F_S$ and interfacial forces and dynamics

**Precursors → Drop in Pushing Force**

- Series of sharp drops in force as trailing edge moves forward
- At each, crack propagates part way along interface
- Propagation distance increases with time
- Final friction independent of pushing height
- Spacing between precursors proportional to pushing height

**Initial Precursors**

Different colors – black, red, blue, green, yellow, successive times

Lateral force on bottom atoms

Shear strain at height 10 $\sigma$

Friction to load ratio during initial precursors

Colors represent successive times black, red, blue, green, yellow, cyan
- Shear force peaks at end of previous “cracks”
- Precursors initiate at local shear force peaks
- Variation in peak force scales with normal force, which varies along surface
- Friction / Load approximately constant
- Load variations increase as precursors advance, …
After many precursors, before sliding

![Graph showing Fx and Fy forces vs. position](image)

**Force ratio before slip**

![Graph showing F/Fy ratio vs. position](image)

- Shear force to normal load ratio remains consistent along the entire contact area
- Shear force to normal load ratio consistent across pushing heights
- All regions near coefficient of static friction

**Typical measurement of friction**

- **Static friction** $F_s$ → minimum force needed to initiate sliding.
- **Kinetic friction** $F_k(v)$ → force to keep sliding at velocity $v$.
- Typically, $F_k(v)$ varies only as $\log(v)$ and $F_s \geq F_k(v)$ at low $v$.

**Amontons' Laws (1699):**
- Friction $\propto$ load $\rightarrow$ constant $\mu = F/\text{Load}$.
- Friction force independent of apparent contact area $A_{app}$.

**But:** Amontons coated all surfaces with pork fat

- $F \propto A_{app}$ for soft, flat solids
- $\mu$ often changes with load
- Find friction at zero and negative loads
- Friction depends on history

**Why Friction $\propto$ Load, Independent of Apparent Area?**

**Geometric explanation (Amontons, Parents, Euler, Coulomb):**

- Surfaces are rough
- Friction $= force$ to lift up ramp formed by bottom surface
- $F = N \tan \theta \Rightarrow \mu = \tan \theta$

**Problems:**
- Most surfaces can’t mesh, $A/A_0$ small
  (Müser, Wenning, Robbins, PRL 86, 1295 (2001))
- Roughening can reduce $\mu$ (hard disks)
- Once over peak, load favors sliding $\Rightarrow$ kinetic friction=0

**Static friction** $\Rightarrow$ Force to escape metastable state

- How can two surfaces always lock together?
- Kinetic friction $\Rightarrow$ Energy dissipation as slide

- Why is this correlated to static friction? Why does $T$ matter?

**Contact area $\propto$ Load (Dieterich & Kilgore)**

- Applied normal stress = Load/A

**Height variation $\delta h$ over length $\ell$ → $\delta h/\ell \propto H \leq 1$

**Average slope $\delta h/\ell$ → goes to zero as $\ell$ increases**

**Finer element calculation**

- Rough surface on rigid flat (maps to 2 rough)
- Elastic or $J^2$ isotropic plastic constitutive law
- Periodic boundary conditions, $L=512$ nodes per edge
- Full range of $H$ and roughness amplitudes

Constant mean pressure in contact \( \langle p \rangle = N/A \) at low \( N \).

Controlled by rms local slope, \( \Delta \), not total roughness.

Elastic: \( \langle p \rangle/E' = \Delta/\kappa \)

\[ E' = E/(1-v^2) \]

\( \Delta = \sqrt{\langle \kappa^2 \rangle} \)

= rms surface slope

\( \kappa(H,v) \) from 1.8 to 2.2.

Analytic predictions:

Bush et al., \( \kappa = (2\pi)^{1/2} \approx 2.5 \)

Persson \( \kappa = (8/\pi)^{1/2} \approx 1.6 \)

Plastic: \( \langle p \rangle \neq 3\sigma_y \)

3\( \sigma_y \)= single-asperity hardness

\[ \sigma_y = \text{single-asperity hardness} \]

Area \( \propto N \) for nonadhesive contact

Very different surface roughness profiles give same \( \kappa \).

Results here are for different synthetic and experimental surfaces at \( A/A_0 \approx 0.1 \).

Elastic: \( \langle p \rangle/E' \approx \Delta/\kappa \)

\[ \Delta < \sigma_y/E' \quad \kappa < 2 \] smooth!

Bowden and Tabor:

\( \langle p \rangle \approx 3\sigma_y \)

For small \( \sigma_y/E' \), \( \langle p \rangle \) is about twice this value. (Gao & Bower)

Power law regime \( \langle p \rangle \propto \sigma_y^x \),

\( x = 2/3 \) for typical \( \sigma_y/E' \).

High strength steel 6\times10^{-3}

Titanium 9\times10^{-3}

Bone 7\times10^{-3}, Silicon 3\times10^{-2}

Amorphous metal 2-5\times10^{-2}

Complex morphology varies with constitutive law

Power law distribution of connected areas \( a_c \): \( P(a_c) \propto a_c^{-\tau} \)

Connected regions are fractal \( a_c \propto r^{D_f} \)

Inconsistent with bearing area model

\[ \text{Ideal Elastic} \quad D_f = 1.6 \]

\[ \text{Perfectly Plastic} \quad D_f = 1.8 \]

\[ \text{Bearing Area Model} \quad D_f = 2 \]

Spread evenly

\( \tau < 2 \)

Near highest peak

\( \tau = (2-H)/2 \)

All results for same surface, 0.015% in contact.

Contact and Stress Correlation Functions

\[ C_c(r,r') = \langle c(r)c(r') \rangle_r \]

where \( c(r) = 1 \) in contacts, 0 otherwise.

Overlap & Greenwood-Williamson \( C(q) \sim q^{-2(1+H)} \)

Numerical and Persson \( C(q) \sim q^{-(1+H)} \)

Probability Distribution of Cluster Areas $a_c$

Power law distribution $P(a_c) \sim a_c^{-\tau}$: $\tau$ depends on $H$ if elastic, not if plastic. Cluster areas fractal.

Elastic $\tau > 2$
Plastic $\tau \approx 2$

Bearing area $a_c = 2 - H/2$

Mean area $<a_c>$ depends on $\tau$
$\tau > 2$, $<a_c> \sim 1$
$\tau = 2$, $<a_c> \sim \log(L)$
$\tau < 2$, $<a_c> \sim L^{2-\tau}$

Conclusions of Continuum Studies of Non-Adhesive Contact

- Area proportional to load $\rightarrow <p> = \text{constant}$
- Elastic: $<p>/E' = \Delta/\kappa$ with $\kappa \sim 2$
- Plastic: $<p> \propto \sigma_{y}^{2/3}$
- Expect plasticity when $\Delta > \sigma/E' \rightarrow$ most surfaces
- Ignoring interactions between asperities gives qualitatively wrong spatial distribution of contacts and distribution of contact sizes
- Most contacts at smallest scale $\rightarrow$ results dominated by small scale cutoff - $\Lambda$, $a_c$
  $\rightarrow$ continuum mechanics may fail even though total area is very large
  $\rightarrow$ reason $kT$ remains important at macroscale?

What are limits of Continuum Theory?

Continuum theories: Hertz, Johnson-Kendall-Roberts (JKR), Derjaguin-Muller-Toporov (DMT), Maugis-Dugdale
Assume: 1) continuous displacements, bulk elastic const.
2) smooth surface (often spherical) at small scales
Only tested for atomically flat mica bent into cylinders and elastomers with liquid behavior on small scales
Find (1) valid down to a few atomic diameters, but atomic scale roughness causes failure of continuum theories.
Important for small contacts between rough surfaces and ideal single asperities: scanning probe or nanoindenter

Atomic tip structure $\rightarrow$ Close as possible to curve
- Substrate- atomically flat 100 or 111 fcc surface
- Cylindrical or spherical tip constructed by:
  a) Bending crystalline solid
  b) Cutting amorphous solid
  c) Cutting crystalline solid

Pressure distribution for sphere on flat

Atomic scale roughness qualitatively changes pressure, yield Bent crystal agrees with Hertz/JKR, more realistic tips do not

Continuum vs. MD for Sphere or Cylinder on Flat

Rigid cylinder or sphere, elastic flat (dimensions $W, \tau \gg a$ so $\sim$irrelevant)
Substrate ideal elasticity $E'$
(111) surface of fcc crystal
Tip: $R = 100-1000\sigma$
$\sim 30-300\text{nm}$
$\sigma =$ mol. diameter
Units: length $\sigma \sim 0.3\text{nm}$
binding energy $\epsilon_{b}$, force $\epsilon_{b}/\sigma \sim 5\text{pN}$
Vary atomic scale roughness of tip amount of adhesion $V_{int} = 4\epsilon_{b}[(\sigma/\tau)^{12} - (\sigma/\tau)^{6}] r < r_{cut}$
Examine normal displacement $\delta$, radius $a$, friction $F$, lateral stiffness $k$ & pressure distribution $P(x) \text{ vs. load } N$
Comparison to Hertz Theory for Sphere on Flat

Fits of δ to Hertz give good E* and R (10%)
Contact radius a is shifted several σ away from Hertz, leading to 100% error for small contact radius.
Friction varies by factor of 200
Commens.: F ∝ N, μ = 0.7
Incomm.: F ∝ A, and small lateral stiffness varies 10 fold due to atomic scale lateral motion at interface.
Agrees with Hertz if don’t allow sliding at interface.

Effect of Adding Adhesion

Maugis-Dugdale (M-D) Model:
Constant adhesion force σ₀ for separations < h₀
Interpolates between DMT (long, rigid, λ<0.1) and JKR (short, pliant, λ>5) limits by varying λσ₀(9R/2πwE*)²/³
with w = σ₀h₀ = surface energy.
Typically 0.1 < λ < 1 for AFM
Dimensionless pulloff force N₀ always between DMT and JKR |N₀/πwR| between 1.5 and 2
Compare to inner repulsion rₐ radius at minimum rᵢ, close to JKR and outer radius rₐ.
Deviations similar to nonadhesive

Atomic Scale Roughness Changes Adhesion

Reduces adhesion energy up to factor of five as go from bent commensurate to amorphous
Pulloff force N₀ may be outside JKR/DMT bounds
|N₀/πwR| = 1.5 for JKR, 2.0 for DMT
Maugis-Dugdale |N₀/πwR| = 1.74 for w = 0.46 σ²
Commensurate: |N₀/πwR| = 1.77
Incommensurate: |N₀/πwR| = 1.79
Amorphous: |N₀/πwR| = 2.26
Stepped: |N₀/πwR| = 0.72 - less than half JKR

Experiments can’t measure contact area A.
Conclude continuum theory gives A by assuming F = τA and showing can fit F
Simulations show fits do not imply success of continuum theory
Do not fit for stepped tip can fit to Schwartz approx to M-D theory but not with right microscopic values

Fits of Friction to Continuum With F = τA_M-D

Use real area A ∝ r² from MD simulation
No adhesion → F ∝ r² for all i
Adhesion → F ∝ rᵢ for all i
Repulsive region counts
Shear stress τ changes by orders of magnitude with tip geometry

Stiffness k vs. r for Bent Crystal & Amorphous Tips

Use real radii from MD
No adhesion → k ∝ rᵢ for all i
Intercept → zero for ra
Repulsive region counts
Slope smaller than continuum by up to 1 order of magnitude
Elastic deformation at interface adds in series with substrate and dominates
Does Ratio $F/k^2$ Give Shear Stress?

Continuum: $F = \tau_{\text{eff}} \pi r^2$, $k = 8Gr$

$\tau_{\text{eff}} = (F/k^2) \left( \frac{64G^2}{\pi} \right)$

Find $\tau_{\text{eff}}$ relatively constant, but 10-100 times true $\tau$!

and $\tau$ not constant for stepped Similar curves in experiments, including rise at small loads

→ Not reliable way of estimating shear stress under general conditions. Main difficulty is that $k$ is dominated by interface which is not included in continuum expression.

Why is friction often proportional to load?

• Not just $A_{\text{real}} \approx$ Load and $F \propto A_{\text{real}}$ since $A_{\text{real}}$ varies with parameters like $A$ that have weaker effect on $\mu$.

• Static friction often vanishes between clean surfaces very sensitive to local structure, surface orientation, …, but measured $\mu$ is not

• How can one get less sensitive friction force in contacting regions that explains Amontons’ laws and exceptions to them?

Single Asperity Conclusions

• Bulk elastic modulus describes stress/strain to $\sim 3\sigma$

Atomic roughness $\rightarrow$ deviations from continuum theory

• Molecular scale geometry has little effect on normal displacement vs. force curves

$\rightarrow$ Elastic moduli from continuum fits are accurate

• Contact areas, morphologies and pressures are changed

$\rightarrow$ Yield stress, contact area, pulloff force off by factor $\sim 2$

$\rightarrow$ Pulloff force not between JKR & DMT limits

• Lateral stiffness and friction vary by more than order of magnitude with atomic geometry

$\rightarrow$ Contact stiffness dominated by interfacial stiffness

$\rightarrow$ Friction $\propto$ load or contact area

$\rightarrow$ Shear stresses from continuum fits too high


Amorphous Antimony Islands on Graphite


Experiments use AFM tip to move nanoscale islands.

Some islands move with nearly zero force while others require constant kinetic friction.

Antimony islands will lock to graphite structure during growth and this can lead to finite friction. Once start moving, orientation may become random, leading to zero friction.

Surface contamination inhibits observation of low friction state.

Friction Mechanisms in Contacts

Geometrical Interlocking: $F = N \tan \theta$

Unlikely to mesh, $F$ goes up as smooth Kinetic friction vanishes

Elastic Metastability: Intersurface interaction too weak

Mixing or Cold-Welding Hard to observe in sims. even with clean, unpassivated surfaces in vacuum

Plastic Deformation (plowing) Load and roughness dependent $\Rightarrow$ High loads, sharp tips

Mobile third bodies $\rightarrow$ “glassy state” hydrocarbons, wear debris, gouge, …

Glass seen in Surface Force Apparatus, Robust friction mech. on many scales

Quartz Crystal Microbalance – Krim et al.

Fluid or incommensurate layers on substrate $\rightarrow$ no static friction

$F = -v M t$ $\rightarrow$ velocity relative to substrate

Increase coverage $\rightarrow$ film solidifies $t$, increases $\rightarrow$ friction goes down!

Misaligned mica, MoS$_2$, graphite also show no static friction

(Hirano et al. PRL 67, 2042 (1991); Martin et al., Dienwiebel et al. PRL 2004)

Kr on Au: Cieplak, Smith, Robbins, Science 265, 1209 (1994)

Xe on Ag: Tomassone, Sokoloff, Widom, Krim, PRL 79, 4798 (1997)

Amorphous Antimony Islands on Graphite


Amorphous Antimony Islands on Graphite


Amorphous Antimony Islands on Graphite

**Why is friction often proportional to load?**

• Not just \( A_{\text{real}} \propto \text{Load} \) and \( F \propto A_{\text{real}} \) since \( A_{\text{real}} \) varies with \( \mu \) parameters like surface slope that have weaker effect on \( \mu \).

• Friction between clean surfaces very sensitive to local structure, surface orientation, … but measured \( \mu \) is not.

\[ \Rightarrow \text{Assume friction from yield stress } \tau_y \text{ of molecular contacts} \]

\[ \text{Glassy systems: } \tau_y \text{ rises linearly with pressure } p \]

If: \( F = A_{\text{real}} \tau_y(p) \) with \( \tau_y = \tau_0 + \epsilon p \) (Briscoe)

Then: \( \mu = F_y / \text{Load} = \alpha + \tau_0 / p \)

\[ \Rightarrow \text{Constant } \mu \text{ if } p = \text{Load} / A_{\text{real}} = \text{const.} \]

or \( \tau_0 << p \) (Independent of distribution of pressure)

\[ \Rightarrow \text{Friction at zero or negative load with adhesion, as observed} \]

\[ \Rightarrow \text{Adsorbed layers give } \tau_y = \tau_0 + \epsilon p \text{ with small } \tau_0 \text{ and } \epsilon \text{ nearly independent of factors not controlled in experiment} \]

---

**Model**

- N chains of \( n \) monomers \( \rightarrow \) bead-spring model.

- Lennard-Jones interaction between monomers:
  \[ V_{\text{LJ}} = 4\epsilon \left[ \frac{\sigma}{r} \right]^{12} - \frac{1}{2} K o \left[ \frac{1}{1 - r^2} \right] \quad \text{for } r < r_c \]

- Neighbors on chain:
  \[ V_{\text{ch}} = \frac{1}{2} K o \left[ \frac{R^2}{1 - r^2} - \frac{R^2}{R_o^2} \right] \]

- Wall atoms held to sites by springs (111) surface of fcc crystal here

- Interact with monomers with \( V_{\text{LJ}} \) but with \( \epsilon_w \) and \( \sigma_w \).

- Increase force on top wall till slides to find \( \tau_s \) (static).

- Study diffusion of top wall to test if \( \tau_s > 0 \)

- Move wall at constant velocity \( v \) to find \( \tau_k \) (kinetic).

- Vary \( \rightarrow \) Pressure \( P \)
  - Relative orientation and lattice constants \( d \) of walls
  - Direction and velocity of sliding
  - Surface density (coverage) of monomers
  - Chain length \( n \)
  - Strength \( \epsilon_w \), length \( \sigma_w \), and range \( r_c \) of potential.

---

**Wall Geometries**

- a) 0º
- b) 8.2º
- c) 90º
- d) \( d_{\text{wall}}/d_{\text{monolayer}} = 13/12 \)

\[ \alpha \text{ independent of coverage} = \frac{\# \text{monomers}}{\# \text{atoms on both walls}} \]

Small variation in \( \tau_0 \) with coverage

\[ \theta = 90º \]

---

**Find:** \( \tau_s > 0 \) for incommensurate walls with adsorbed film

- All incommensurate walls (b-d) give same \( \tau_s \)
- \( \tau_s \) independent of sliding direction: \( x, y, \) etc.

\[ \tau_s = \tau_0 + \alpha P \text{ up to } P > 1 \text{GPa} \quad (\epsilon \sigma^{-3} \approx 40 \text{MPa}) \]

---

**Effect of Potential**

\( \alpha \) indep. of coverage, chain length (\( n \leq 6 \)), \( \epsilon_w \) or \( r_c \)

\( \alpha \) increases with \( d/\sigma \) \( \rightarrow \) “routher” surface
**Geometric Explanation**

If pressure high enough → hard sphere limit

Repulsive force balances pressure

\[ F \sim \frac{P}{c} \sim 48 \left( \frac{\sigma_w}{\sigma_w} \right)^{13} \] where \( c \) = coverage

\[ \Rightarrow r \sim \frac{\sigma_w}{\frac{P}{\sigma_w}} \left( \frac{\sigma_w}{\sigma_w} \right)^{13} \]

Effective hard-sphere radius: insensitive to \( c, \sigma_w \), \( P \)

almost linear in \( \sigma_w \)

Surface of closest approach depends on \( d / \sigma_w \)

\[ \alpha \] maximum slope as in geometric model

→ larger \( d / \sigma_w \), steeper slope, bigger \( \alpha \)

Analytic theory: Müser, Wenning, Robbins PRL 86, 1295, '01

**Adsorbed layers explain many experiments**

- Lock surfaces together (even when diffusing)

  \[ \tau_s = \tau_0 + \alpha P \]

  for \( P \) up to \( \sim 1 \) GPa

  \( \tau_s \) independent of uncontrolled experimental parameters

- \( \alpha \) primarily depends on relative atomic sizes in our model

- Kinetic friction also linear:

  \[ \tau_k = \tau_0 + \alpha P \]

- \( \tau_0, \tau_k \) follow same trends as for \( \tau_s \)

  \( \alpha \) shows \( k_B T \log v \) dependence seen in experiment

  Most molecules stable at any time, resist sliding just as

  for static friction, each pops and dissipates separately

  Biggest contribution to friction from those close to popping

  \( \Rightarrow \) As \( v \) decreases, more thermal excitation, \( F \propto \log v \)

He, Müser & Robbins, Science 284, 1650 (1999)


**Complex Dynamics of Kinetic Friction**

Rate-state models (Dieterich, Ruina, Rice,...)

\[ \mu = \mu_0 + A \ln(v/v_0) + B \ln(\theta / \theta_0) - \frac{\partial \theta}{\partial t} = 1 - \theta / \theta_c \]

- \( A \) → change in shear stress with \( v \)

- \( B \) → change in area of contact with time

Dieterich & Kilgore

**Images of Real Area of Contact**

Dieterich & Kilgore - \( \ln(\theta / \theta_0) \) ⇒ Real area

\( A_{real} \) small fraction of total area

\( A_{real} \) goes up with log contact time, down with log \( v \)

What causes change in shear stress with \( v \)?

Dieterich & Kilgore
Connection to “Rate-State” Models

For rocks, wood, metals, ... (Dieterich, Ruina, Rice, ...)

\[ \mu = \mu_0 + A \ln(v/v_0) + B \ln(\Theta/\Theta_0) \]

\[ \dot{\varepsilon} = \frac{1 - \varepsilon}{D_c} \]

A represents change in shear stress with \( v \)

B change in area of contact with time

Our model has fixed area \( \rightarrow \) only see A

Find: \( A \approx 0.001 \) vs. 0.005 to 0.015 for rocks,

\( A/\mu_0 \approx 0.05 \) vs. 0.008 to 0.025 for rocks

\( A \propto T \) as in experiments

\( \mu \propto T \ln v \) follows from simple activation model

\( \rightarrow \) most molecules stable at any time

\( \rightarrow \) resist sliding just as for static friction

\( \rightarrow \) thermal activation over barrier reduces \( F \)

\( \Rightarrow \) lower \( v \), more thermal excitation \( \Rightarrow F \propto \log v \)

Rate-State Model of Yield in Bulk Glasses

Conventional Description:

I) Elastic response: \( \sigma = Y \varepsilon \)

II) Plastic deformation

III) Yield point, yield stress \( \tau_y \)

IV) Strain softening, followed by strain hardening

Yield stress depends on temperature, age and strain rate


Aging in glasses

• Below \( T_g \), glasses are not stationary, but continue to evolve configurational degrees of freedom (aging)

• Time-translation invariance broken, quantities depend on \( t \) and \( t_w \)

• Glass compactifies \( \logarithmically \) in absence of deformation when maintaining zero hydrostatic pressure

• Strongly temperature dependent, no change at \( T=0.01 \) \( u_0/k_B \)

\( \rightarrow \) aging suppressed as \( T \) decreases

\( T_g = 0.3 \) \( u_0/k_B \)

Effect of aging on shear yield stress: \( T=0.2 \) \( u_0/k_B \)

\[ \tau \propto \ln(t_w/t_L) \]

\( \rightarrow \) yield stress increases \( \logarithmically \) with waiting time

Effect too large to be attributed to density change

(see also Varnik, Bocquet & Barrat, J. Chem. Phys. (2004))

• Slope independent of shear rate at long times, \( \rightarrow \) flat at short times

• Qualitatively consistent with \( S(oft) \) \( G(lasy) \) \( R(heology) \) model

Combined rate/age effects at \( T=0.2 \) \( u_0/k_B \)

• \( t_w=750 \) \( \tau_{LJ} \): weak logarithmic behavior at smaller rates

• Stresses and rate sensitivity strongly increase with age

• Ideal logarithmic behavior at \( t_w=750,000 \) \( \tau_{LJ} \)

Temperature and Aging at Shear Rate \( 10^{-4} \tau_{LJ} \)

• Logarithmic behavior at all \( T \)

• Slope \( s_0 \) rises linearly with \( T \)

• Importance of thermodynamic temperature for aging

A phenomenological model

- Assume response depends on state variable 0(t) as in friction models
  \( \tau' = \tau_0 + s_0 \ln(\dot{\theta}) + s_1 \ln(\dot{\varepsilon}) \)
- Specify evolution of effective age 0(t), equilibrium \( \dot{\theta} = 1 \) under strain \( \dot{\varepsilon} \).
  Integrate to yield strain to find
  \( \tau' = \tau_0 + s_0 \ln(\dot{\theta}) + s_1 \ln(\dot{\varepsilon}) \)

  - if \( f \) independent of strain: \( \alpha = \varepsilon_y \) (strain at yield)
  - if rejuvenation before yield: \( \alpha < \varepsilon_y \)
  - if strain accelerates aging: \( \alpha > \varepsilon_y \)

  Predicts "universal" plot in
  \( \tau' + (s_1 - s_0) \ln(1/\dot{\varepsilon}) = \tau_0 + s_0 \ln(\dot{\theta} + \alpha) + (s_1 - s_0) \ln(\dot{\theta}) \)

  \( \tau_0 \alpha \rightarrow \) equilibrium processes; \( s_1 \rightarrow \) non-equilibrium, Eyring fails

  Note: description does not invoke simple relations between "relaxation time" and waiting time.

Microscopic Stress Dynamics

- \( \Delta \tau_{\text{dev}} \) change in local stress tensor over 7.5\( \tau_{LJ} \) in small volume elements containing 7-8 particles
- close to \( T_{\text{g}} \), \( P(\Delta \tau_{\text{dev}}) \) independent of shear strain
- low \( T \), tail grows with increasing strain
- tail can be fitted to exponential, similar slope near peak stress as for steady shear – dark lines

Universal behavior

- data collapses onto single curve when rate is rescaled with \( \tau_0 \) and shifted by waiting time dependent constant
- regime I: \( \tau_0 \) irrelevant, only aging during straining, \( \tau' \propto (s_1 - s_0) \ln(\dot{\theta}) \)
- regime II: no intrinsic dynamics before yielding, \( \tau' \propto s_1 \ln(\dot{\theta}) \)
- crossover when \( \tau_0 = \alpha / \dot{\varepsilon} \)

Stick-Slip Friction From Structural Change

Adsorbed layers also lead to stick-slip in simulation & experiment
Stick-slip does not reflect velocity weakening
Instead kinetic less than static friction because of structural change

Evolution in Stick-Slip Traces With Velocity


Linking Atomistic and Continuum Regions

Three overlap regions where solve both continuum and MD
Outermost \( \rightarrow \) Continuum solution gives MD boundary condition
Innermost \( \rightarrow \) MD gives continuum boundary condition
Middle \( \rightarrow \) Two solutions equilibrate independently
Fluids: Apply boundary conditions to velocities
Solids: Apply boundary conditions to displacements

For ALL temperatures!

(b and M. O. Robbins, Phys. Rev. Lett. 95, 225504 (2005))
Hybrid model for 2d self-affine surfaces
Easily treat volumes with \( \sim 10^8 \) atoms

At edge of overlap region MD and FEM displacements provide BC’s for each other

Continuum Treatment of Solid
- Linear finite elements
- Explicit dynamics for nodes
- Newmark method \( \Delta t_{FE} \sim 10 \Delta t_{MD} \), Langevin thermostat
- Staggered time grid as for fluids
- Constitutive law – quadratic in strain
  - accurate to 2% in each strain component

Atomistic Treatment of Solid
- Two dimensional triangular lattice
- Lennard-Jones interactions between neighbors
- Velocity Verlet, Langevin thermostat

Show low T results to minimize noise, but works at high T

Scaling of Contact Width \( a \) with Load

Excellent agreement of hybrid with MD
Deviate from continuum due to anelastic response and atomic discreteness

Multiscale simulation of dynamic friction
- Full MD
- Hybrid

Flat on flat geometry
Flat on self-affine rough surface
**Friction vs. Load for Rough Surface**

Friction for incommensurate \( \mu = 0.094 \)

**Smoother surfaces, \( \Delta = 0.26 \), little plasticity**

\( \Delta \) = rms surface slope

\( L = \) # atoms on side

\( N = \) Load

Results nearly converged for \( L = 4096 \) atoms \(-1\) \( \mu \)m

Find \( A \propto N \), but ratio 3-5 times continuum results

**Plastic results for \( \Delta = 0.78 \) show size effects**

- Still have \( A \propto \) Load, but \( L \) dependent
- Surface flattening before dislocations important

**Friction Between Two Rough Surfaces**

Friction for incommensurate: \( \mu = 0.094 \)

Key Results From Hybrid Method

- Large values of local slope on any surface cut from a crystal lead to large increase in \( k = E' \Delta / <p> = E' \Delta A / N \)
- Find \( k \approx 15 \) not 2
- Scale dependent mechanisms of plasticity lead to size dependent \( k \) for small systems
- Friction between two rough surfaces larger than that between flat and rough even when gap between surfaces is identical.
  For incommensurate case \( \mu = 0.094 \) vs. 0.03 to 0.05
  Coulomb slope like contribution to friction
- When both surfaces are rough, friction is less sensitive to atomic structure – commensurate vs. incommensurate

Deformation in Disordered Solids: Correlations in Displacement Derivatives and Avalanche Distributions
M. O. Robbins & K. M. Salerno, Johns Hopkins University
C. Maloney, Carnegie Mellon University

How do microscopic displacements accommodate total global strain?
How are “earthquakes” distributed in energy, location and time?
What is geometry of fault and nature of sliding on rough faults?

Method
Usually 2D Molecular Dynamics:
• Binary Lennard-Jones
  Mean diameter \( \sigma \)
• Quenched at pressure \( p=0 \)
• Relative velocity damping (Kelvin/DPD)
• Periodic boundaries
• Axial, fixed area strain or simple shear
• Quasi-static limit, Controlled by \( \Delta t \) not \( \Delta \)
• Make system brittle by making all initial bonds 4 times stronger

Prescribed \( L_y(t), L_x(t) \) to conserve area

Nonaffine Particle Displacements
Non-affine displacement \( u = \text{deviation from mean motion} \)
Integrate affine displacement along trajectory rather than using value for initial position.
For each particle at each time step find distance moved relative to affine displacement at instantaneous position.
Eliminates terms analogous to Taylor diffusion in simple shear

Local rotation, \( \omega = \nabla \times u \)
Find Delaunay triangulation for initial particle centers
For each triangle:
\[
\frac{\partial u_i}{\partial x_j} = F_{ij}
\]
\[
e_k = \frac{F_{xx} - F_{yy}}{2}
\]
\[
e_s = \frac{F_{xx} + F_{yy}}{2}
\]
Invariants:
\[
\epsilon = \sqrt{e_s^2 + e_t^2}
\]
\[
\omega = F_{wy} - F_{wy}
\]
“Right Strain” “Left Strain”

Mechanism for brittleness
Brittle model: 2.4. New bonds 4 times weaker.
Ductile model: 2.1. No “broken” bonds.

Left Strain
Uniaxial compression

<table>
<thead>
<tr>
<th>Stress</th>
<th>0.5%</th>
<th>1.0%</th>
<th>2.0%</th>
<th>4.0%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brit.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Duc.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

140 particles

Uniaxial compression...
Pressure Induced Ductility

Low pressure more brittle

High pressure more ductile

“Earthquakes” in Large Brittle Systems

Total Shear Strain

Incremental shear

Shift to Study of Ductile Systems

Steady state strain accommodation

Displacement and \( \omega \) in steady state

Most analysis looks at magnitude \( \Delta r = |\vec{u}| \) smallest in plastic band

Curl sharply localized in plastic zone, \(+\sigma\) regions correlate along \(+45^\circ\)

Strain accumulates to \( a - \sigma \) in plastic bands through many avalanches

Displacement \( a - \sigma \) allows all regions to find new metastable state

Strain over intervals \( \Delta \gamma > -\sigma / L \) occurs in uncorrelated locations

Spatial Variation of Nonaffine Displacement \( u \)

Components of \( u \) during 0.2\% strain

\(+\sigma\) white, \(-\sigma\) black

Strain localizes in plastic bands \( \rightarrow \) step in total displacement

Largest projection of \( u \) along bands \( \pm 45^\circ \)

Sign \( \rightarrow \) rotation sense

Length up to system

Typical \( a - \sigma \)

Displacements Diffusive with \( D \propto L \)

Plastic band formed in each strain \( -a / L \) gives \( |\Delta r| = a / 2 \), add incoherently

\( \Delta r^2 = \Delta \gamma \Delta r (a / L)^2 / 12 - D \Delta \gamma \rightarrow D = L a / 12 \)

Consistent with observed \( D \approx 57 \sigma^2 \) for \( a = 0.7 \sigma \) and for \( L \) down to 40

For \( \omega \), no \( L \) dependence
Distribution of Vorticity $\omega$

Sharp elastic peak at small $\omega$
Exponential tails at large $\omega$
Weight in tails grows ~linearly with strain

Characteristic $\omega^*$ for decay ~0.1
Since $\omega$ ~ twice strain, $\omega^* \rightarrow$ 5% strain
~ yield strain
Plastic bands have ~10 sharper localized bands

Vorticity Correlation Function $S(\theta) = \int \omega(\mathbf{r}) \omega(\mathbf{r} + \mathbf{q}) d\mathbf{r}$

Mean of log $S$ scales as power of wave vector.

Prefactor linear in $\Delta \gamma$
~Incoherent addition of successive intervals
BUT scaling highly anisotropic

Angle Dependence of Structure Factor, $\Delta \gamma = 0.1\%$

$\alpha = a + b \cos(4\theta)$
$A = c + d \cos(2\theta)$

$S(q; \theta) = A(\theta) q^{-\alpha(\theta)}$

A: broken shear symmetry
bigger for planes with low normal load
as predicted by Mohr-Coulomb

Mohr-Coulomb predicts shift to $\pi/8$

Avalanche Distribution

Deformation through series of avalanches
Find energy dissipated = change in potential energy - work done by system.
Drops have wide distribution, 0.03 to 20 here
Identify by sharp rises in dissipation rate.
Dissipation rate/Kinetic energy drops to constant as energy moves to longest wavelengths.
Ratio measures wavelength where have kinetic energy

$P(E) = \text{Number of Events per Unit Strain per E}$

Reduce strain rate so quasi-static, only affects small events.
Find power law $P(E) \sim 1/E$ over 5 decades.
$P(E)$ and maximum $E$ increase with system size
**EP(E) ~ Constant**

Find \( P(E) \sim E^{-1} \) rather than \( P(E) \sim E^{-5/3} \) for earthquakes.

Maximum event size grows more rapidly than length \( L \).

- \( E \) vs. \( P(E) \)
- \( L^{\beta} \)
- \( N(E/E_{\text{max}}) \)
- \( \beta = 1.1 \)

**Scaling Collapse of N(E) and E**

Scale \( E \) by \( E_{\text{max}} \sim L^\beta \).

Find \( \beta \sim 1.1 \).

\( N(E/E_{\text{max}}) \) must scale as \( L^{1-\beta} \) to maintain energy balance.

- \( E \) vs. \( N(E/L^{100}) \)
- \( 100x100 \)
- \( 200x200 \)
- \( 400x400 \)

**Comparison to Scaling of P(E) in Other Models**

Same system but with energy minimization, not dynamics.

Exponent \( \approx 0.5 \) for largest systems.

Largest size \( \sim 3 \).

3D amorphous metal \( N(E) \sim \exp[-E/L_x] \), \( x = 1.4 \).


Overdamped 2D Discrete dislocation model \( N(E) \sim E^{-\tau} \).


Why is power law different than Gutenberg-Richter?

**Power Law Independent of Potential, Geometry and Thermostat**

\( \log_{10}(\text{probability}) \) vs. \( \log_{10}(\text{energy drop}) \) for 3D amorphous metal.

\( N(E) \sim E^{-\tau} \).

- \( \tau = 1.8 \)


**Relation Between Duration and Energy**

Duration \( \sim \) square root of energy.

Consistent with area-energy and duration \( \sim \) length \( \sim \) area\(^{0.5}\).

\( \log_{10}(\text{duration}) \) vs. \( \log_{10}(\text{energy}) \)

Find moment \( \sim \) energy for large events.

Large dispersion for small events.

**Relation Between Stress Drop and Energy**

Mean stress over whole volume \( \times \) volume \( \sim \) moment.

Find moment \( \sim \) energy for large events.

Large dispersion for small events.
Our Quakes Include Fore and After Shocks

**How Does this Affect Statistics?**

**Integrated Density of Quakes Based on Kinetic Energy**

Large events are broken up. Find integrated density $\sim 1/E^{0.4}$

---

**Fractured Conclusions**

- Strain localizes in plastic bands that extend across system
  Typical slip distance along band $\sim$ particle diameter
  Typical thickness $h$ scales with system size $\sim L/20$
  Several sharper features in $h$ with strain $\sim 5 - 10$

- Non-affine displacement $\Delta r^2 \sim \Delta r/L \Delta a/12 \sim D \Delta a$, $D \sim La/12$

- Strain over short intervals has anisotropic power law correlations
  $S(|q|,\theta) \sim A(\theta)|q|^{-\alpha(\theta)}$ where $\alpha = a+b \cos(4\theta)$, $A = c+d \cos(2\theta)$
  Breaking of symmetry for $A \rightarrow$ Mohr-Coulomb

- Inertial motion seems to lead to qualitative changes in deformation statistics.

- Earthquake probability $P(E) \sim 1/E$ over $\sim 5$ decades
  Exponent independent of geometry, interactions
  May depend on how events are broken up