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# The TRIBOLOGY LETTERS Contact Mechanics Challenge

**Martin Müser**

Dept. of Materials Science and Engineering

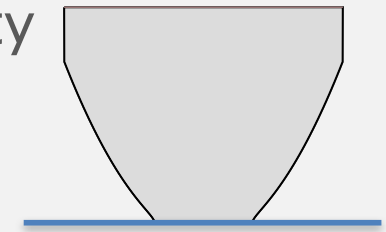
**Saarland University**

ICTP-COST-MODPHYSFRICT Conference: **Trends in Nanotribology**

# Contact Mechanics

deformation of solids that touch each other

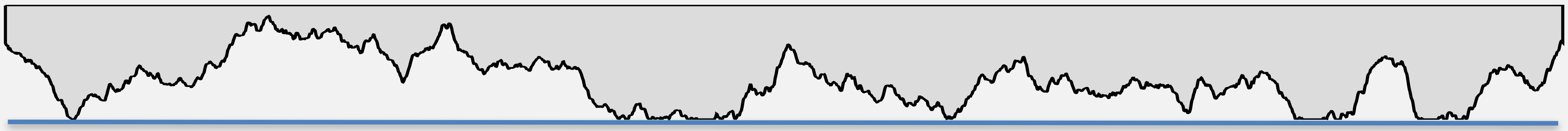
single-asperity contacts



quantities of primary interest:

- area of load or pressure
- displacement of load or *p*

**nominally rough surfaces**



quantities of secondary interest:

- distribution functions of gap, contact patch size, stress

# Why posing a contact-mechanics challenge?

GW model
50+ years

new theories
keep arising

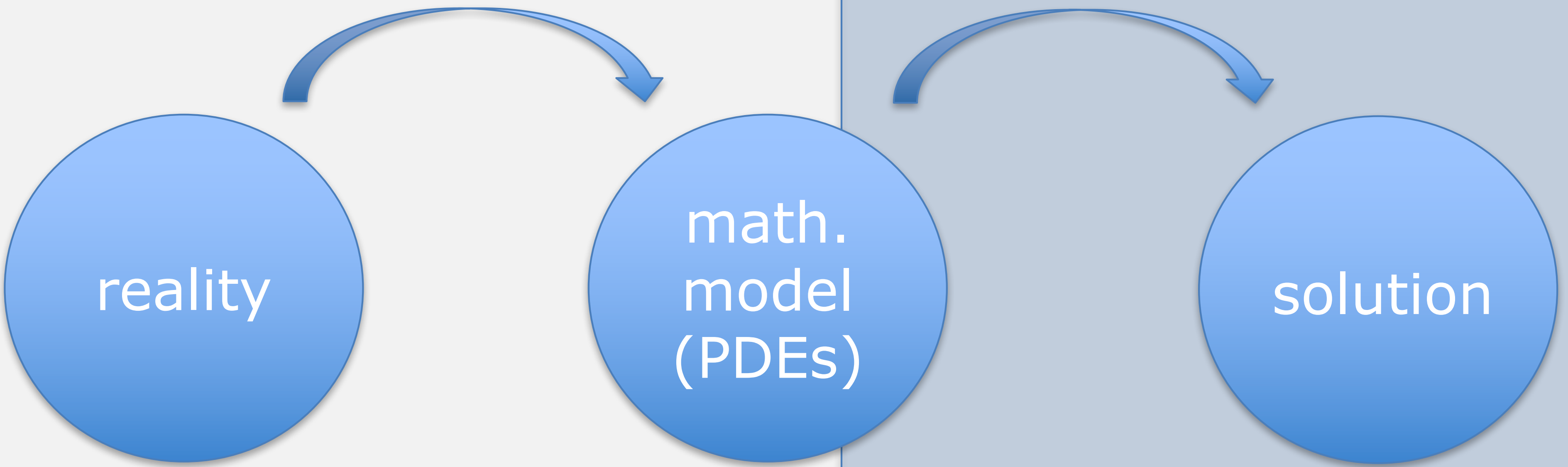
simulations are
becoming competitive

| | 2012 | 2013 | 2014 | 2015 | 2016 May | Total | Average Citations per Year |
|---|---|---|---|---|---|---|---|
| **CONTACT OF NOMINALLY FLAT SURFACES**<br>By: GREENWOO.JA; WILLIAMS.JB<br>PROCEEDINGS OF THE ROYAL SOCIETY OF LONDON SERIES A-MATHEMATICAL AND PHYSICAL SCIENCES Volume: 295 Issue: 1442 Pages: 300-& Published: 1966 | 162 | 174 | 167 | 183 | 60 | 2981 | 58.45 |
| **Theory of rubber friction and contact mechanics**<br>By: Persson, BNJ<br>JOURNAL OF CHEMICAL PHYSICS Volume: 115 Issue: 8 Pages: 3840-3861 Published: AUG 22 2001 | 36 | 48 | 53 | 57 | 16 | 424 | 26.50 |
| **ELASTIC CONTACT OF A ROUGH SURFACE**<br>By: BUSH, AW; GIBSON, RD; THOMAS, TR<br>WEAR Volume: 35 Issue: 1 Pages: 87-111 Published: 1975 | 18 | 15 | 21 | 20 | 5 | 320 | 7.62 |
| **A numerical method for solving rough contact problems based on the multi-level multi-summation and conjugate gradient techniques**<br>By: Polonsky, IA; Keer, LM<br>WEAR Volume: 231 Issue: 2 Pages: 206-219 Published: JUL 1999 | 20 | 14 | 17 | 23 | 7 | 192 | 10.67 |
| **Finite-element analysis of contact between elastic self-affine surfaces**<br>By: Hyun, S; Pei, L; Molinari, JF; et al.<br>PHYSICAL REVIEW E Volume: 70 Issue: 2 Article Number: 026117 Part: 2 Published: AUG 2004 | 17 | 12 | 6 | 20 | 5 | 141 | 10.85 |

# Contact mechanics: Course of action

make (reasonable) approximations

make (reasonable) approximations

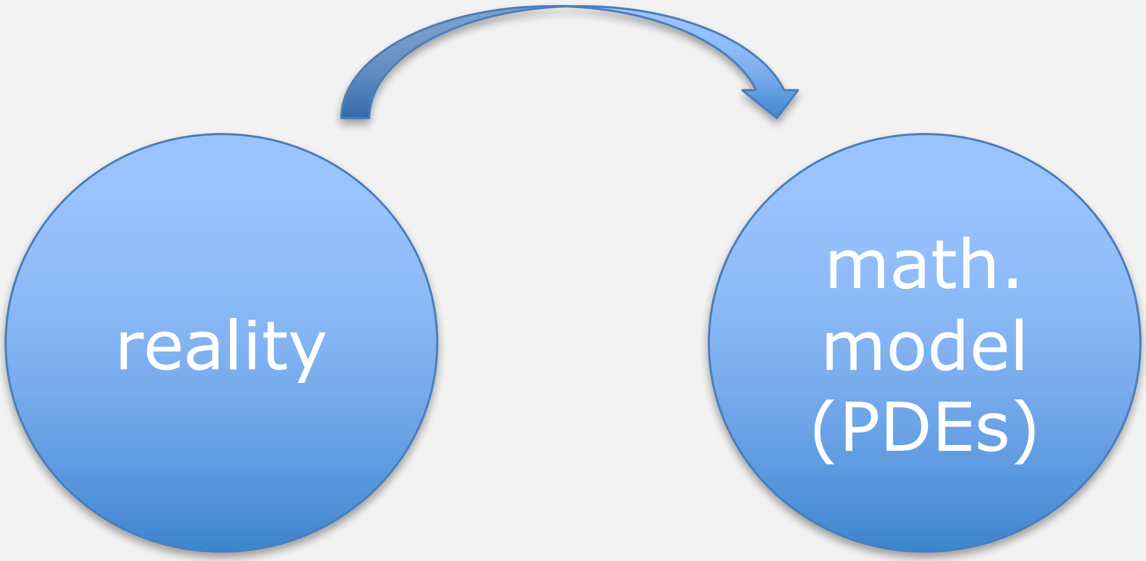



- small-slope approximation
- linear elasticity, no overlap
- randomly-rough surfaces
- short-range adhesion, …

brute-force computing
- controllable approximations

mapping onto simpler equations
- uncontrolled approximations

# Building the model




adhesion law

$$\sigma_{\text{local}} = \sigma_0 \exp(-gap/\rho)$$

details don't matter as long as $\rho$ is "small"

- small-slope approximation
- linear elasticity, no overlap
- randomly-rough surfaces
- short-range adhesion, …
- periodic boundary conditions, hard-wall constraint

$$\frac{A_{\text{true}}}{A_{\text{apparent}}} \approx 2 \frac{p}{E^* \bar{g}}$$

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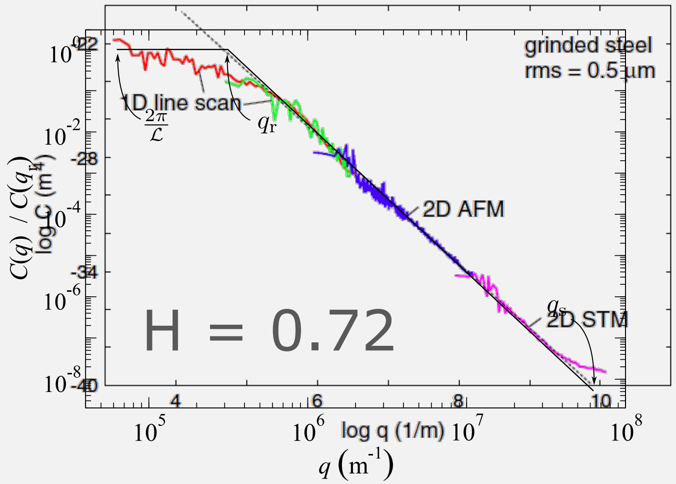
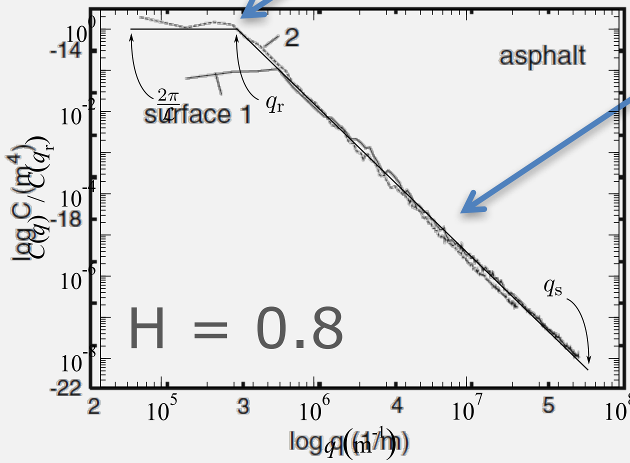
# Surface height spectra

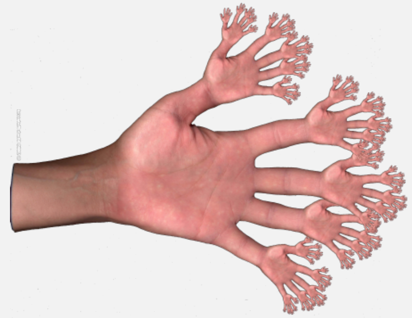
roll-off region

self-affine region

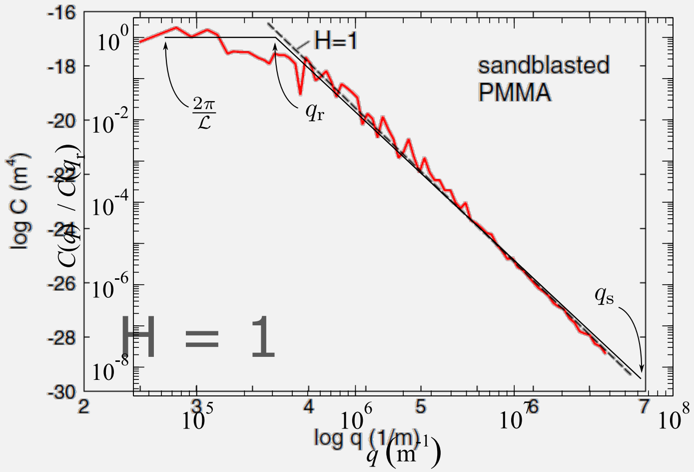
$$C(q) \sim q^{-2(1+H)}$$

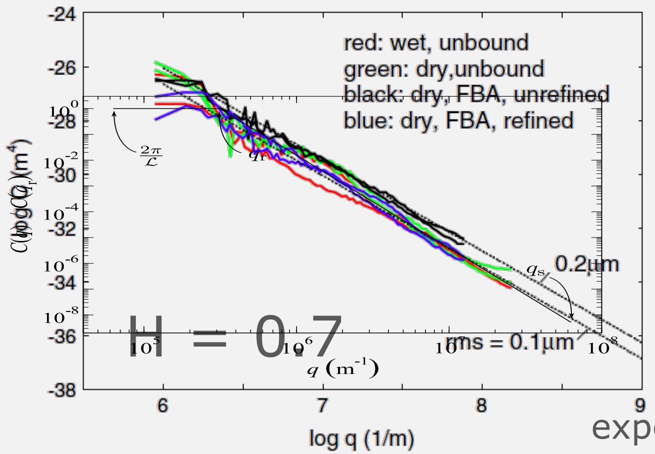


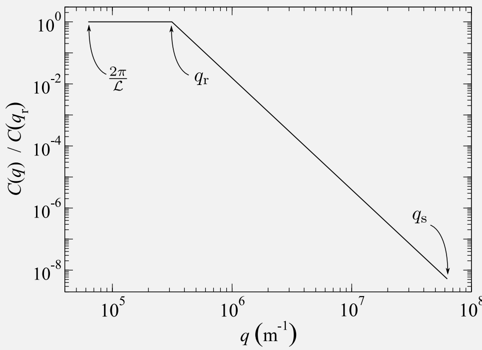



used spectrum




experimental data compiled in:
Persson, Tribol. Lett. (2014)

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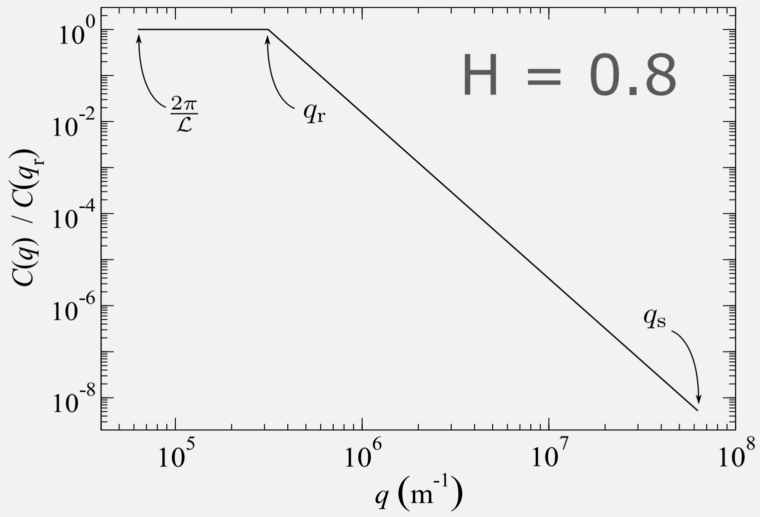
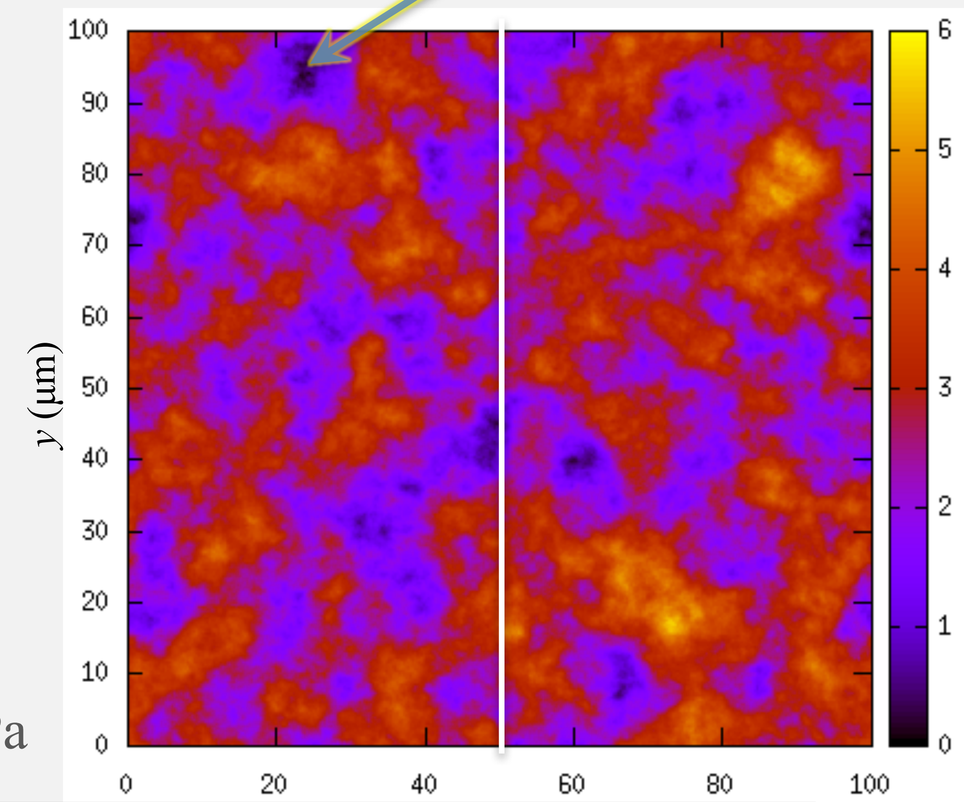
# Surface height in real space

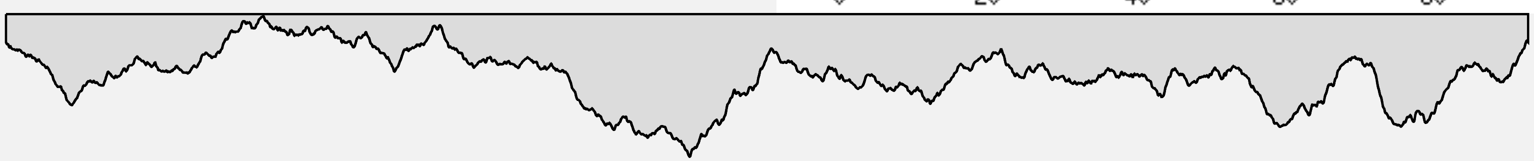
dark areas touch first




$L_{sys}$ = 0.1 mm ; rms-$h$ = 0.7 µm

$\rho$ = 2 nm ; $\gamma$ = 50 mJ/m$^2$ ; $E^*$ = 25MPa



# The tasks:

Compute any measurable and well-defined “observable”
(a function or functional of displacement field)

Spatially resolved observables (at a reference load ):
- gap and stress along the reference line

Histograms (at a reference load → 3% contact):
- gap, stress, and contact patch size

Mean values as function of load:
- relative contact area and mean gap

Omitted: Stress spectrum (too few submissions)

# The contestants:

| | | |
|---|---|---|
| Austria | AC2T research | G Vorlaufer, A Vernes |
| France | INSA Lyon | R Bugnicourt, P Sainsot … TA Lubrecht |
| Germany | FZ-Jülich | BNJ Persson |
| | Saarland Univ. | MH Müser, WB Dapp |
| Italy | Polytech Bari | G Carbons, F Bottiglione, L Afferante |
| Iran | Isfahan Univ. | HA Esfahani, M Kadkhodai, S Akbarzadeh |
| NL | Univ. of Groningen | S Solhjoo, AI Vakis |
| Taiwan | Chang Gung | J-J Wu |
| UK | Imperial College | D Dini, S Medina |
| USA | Johns Hopkins | J Monti, L Pastewka, MO Robbins |
| | Univ Florida | K Harris, A Bennett … WG Sawyer |
| | Auburn Univ. | KJ Streator, A Rostami |
| | Georgia Tech. | RL Jackson, Y Xu |

# The methods:

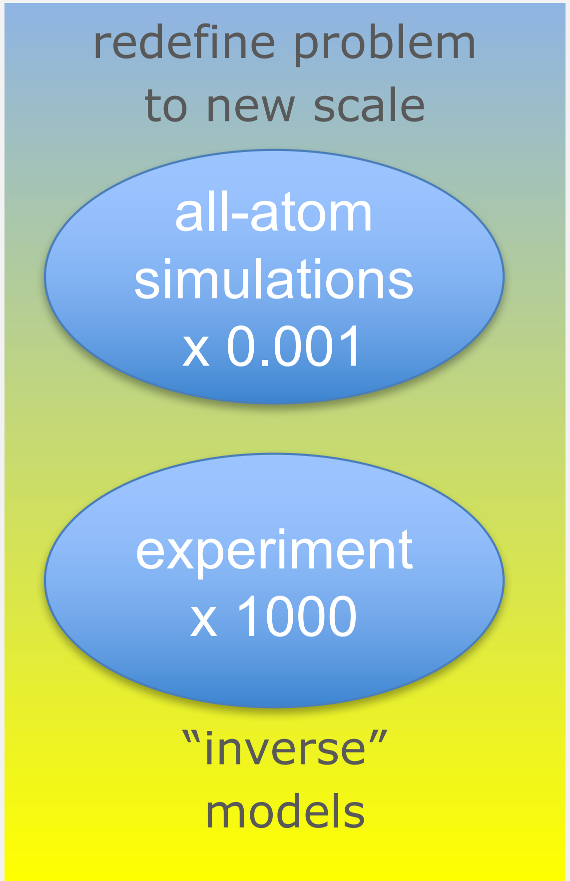

exact (boundary-value) methods (5 times)
- only controlled approximations

finite-element method (no showing)

Persson theory (1 time)
- renormalization group approach

dimensionality reduction (no showing)

Bearing models (5 times)
- local constitutive relations
- no interaction between contact patches



# exact boundary-value methods

effectively all minimize total energy or zero forces

- elastic energy in Fourier space, constraint & adhesion in real space
- all employ fast Fourier transform (FFT) $\tilde{\sigma}(\vec{q}) \approx \frac{qE^*}{2}\tilde{u}(\vec{q}) + \tilde{\sigma}_{\text{ext}}(\vec{q}) + \tilde{\sigma}_{\text{adh}}(\vec{q}) + \dots$

  elastic stress of a semi-infinite solid in q-space →
- alter displacements until energy minimized / stress disappears

| | | |
|---|---|---|
| **FFT-BVM** | + conjugate gradient | Bugnicourt, Sainsot, Lubrecht |
| **BICGSTAB** | finite-range repulsion | Wu |
| **BEM+B** | splining at small scales | Vorlaufer, Varnas |
| **FFT-IA** | elastic stress field is varied | Dini, Medina |
| **GFMD** | Green's function molecular dynamics | Müser, Dapp, Pastewka, Robbins |

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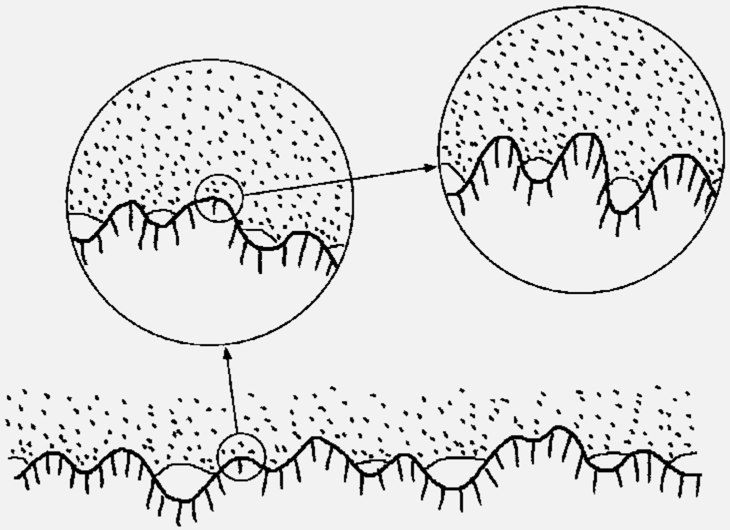
# Persson theory

maps contact mechanics problem onto diffusion process

magnification → time, stress → position
stress = 0: absorbing boundary
roughness at magnification q → diffusion constant

starting assumption: $\Pr(\sigma) = \delta(\sigma)$
broaden $\Pr(\sigma)$ with each
newly resolved $h(\mathbf{q})$

J Chem. Phys. (2001)



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# Bearing-area models

base models (such as Greenwood-Williamson):

- assume local model for asperity interactions, e.g., Hertz, JKR, or simple springs (Winkler)
- assume a distribution of asperity heights and curvatures
- ignore elastic deformation between asperities

| | | |
|---|---|---|
| **Winkler** | simple springs | Angelini, Sawyer |
| **SR-GW** | spatially resolved GW | Esfahani, Kadkhodaei, Akbarzad |
| **Archard** | fly-on-a-fly-on-a-fly… | Jackson, Xu, Streator, Rostami |
| **SC-GW** | slightly-corrected | Bottiglione, Carbone |
| **ICHA** | interacting & coalescing Hertz asp's | Afferante, Carbone |

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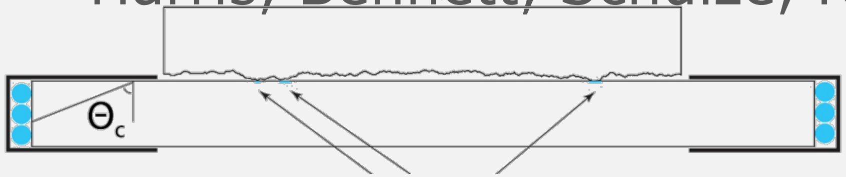
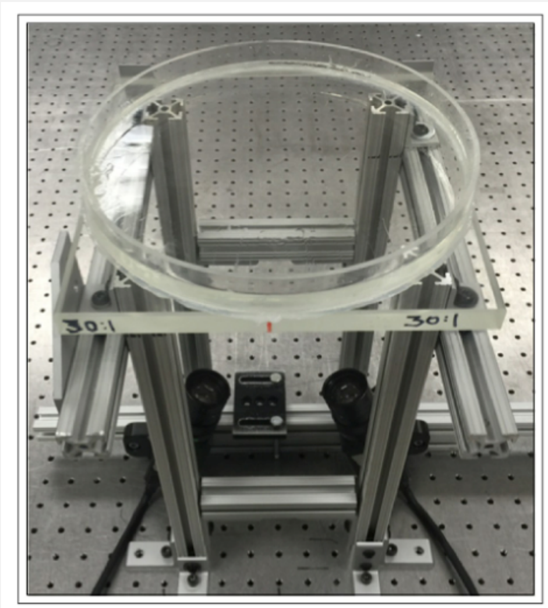
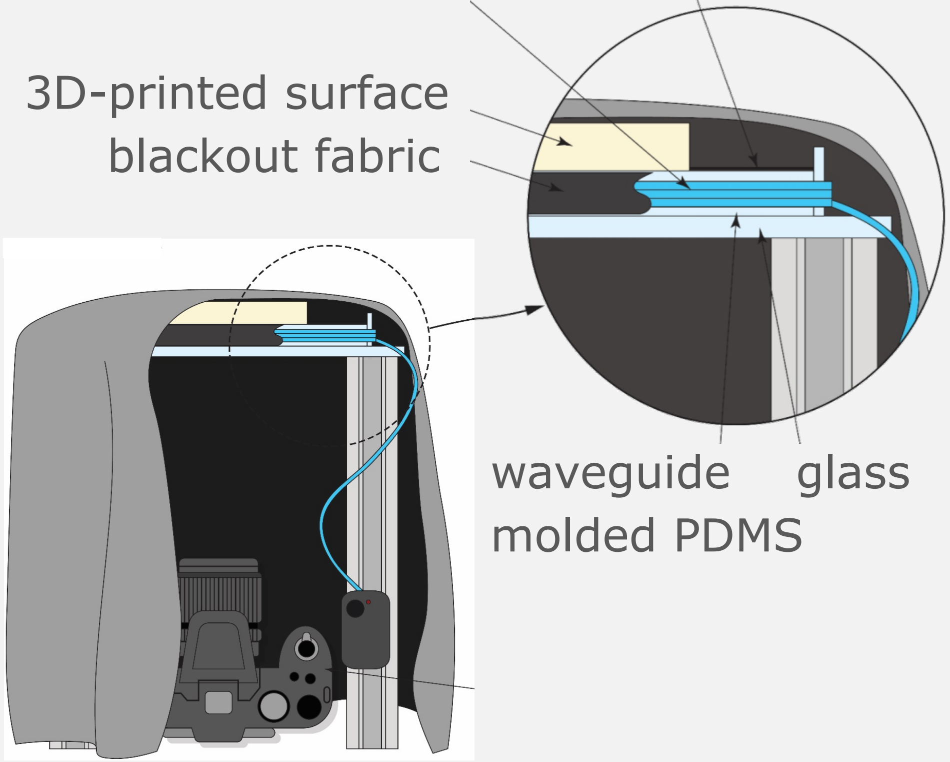
# **Experiments** 3D print surface topography

Harris, Bennett, Schulze, Rohde, Ifju, Sawyer



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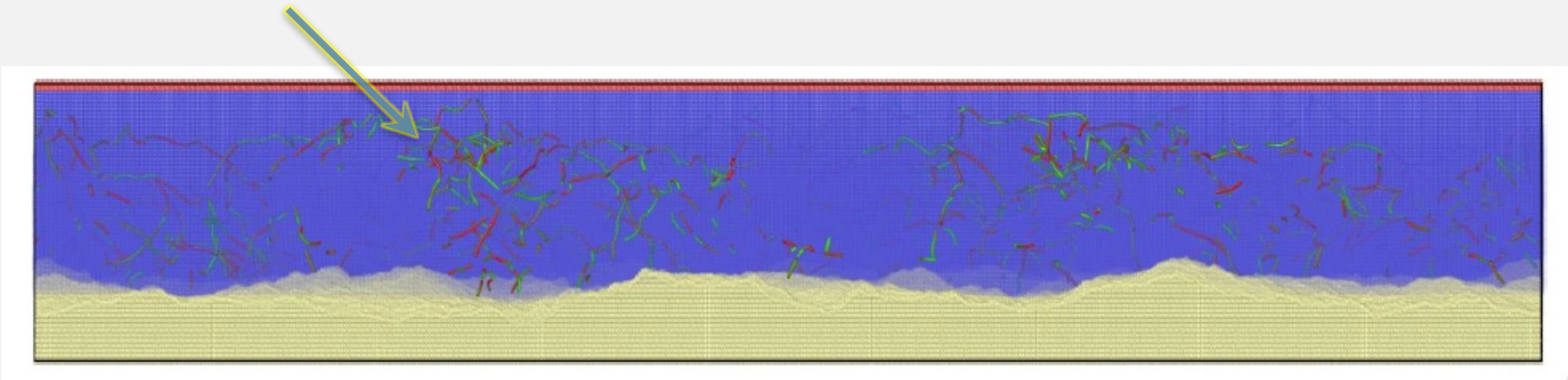
# **All-atom MD** scale problem to atomic scale

Solhjoo, Vakis

all-atom simulations: EAM potential for calcium

$E^{*} = 30$ GPa → $p = 0.3$ GPa; $p_c = 10$ GPa

dislocations



rigid substrate with given height profile

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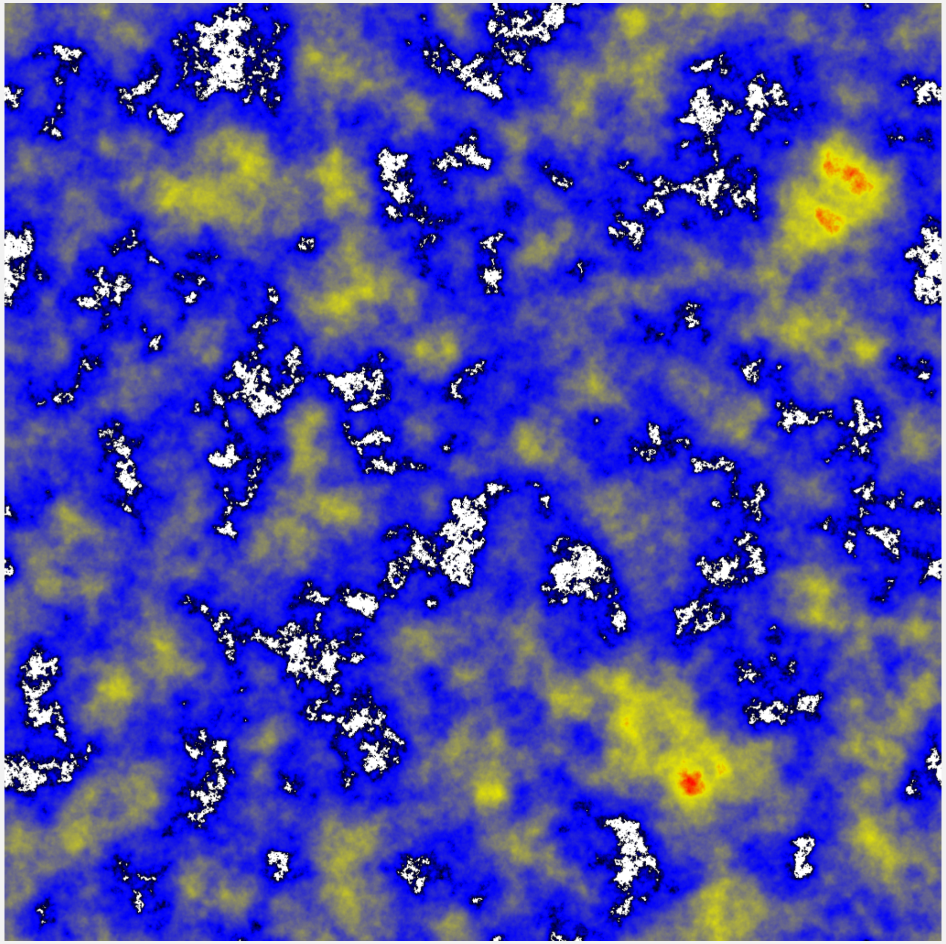
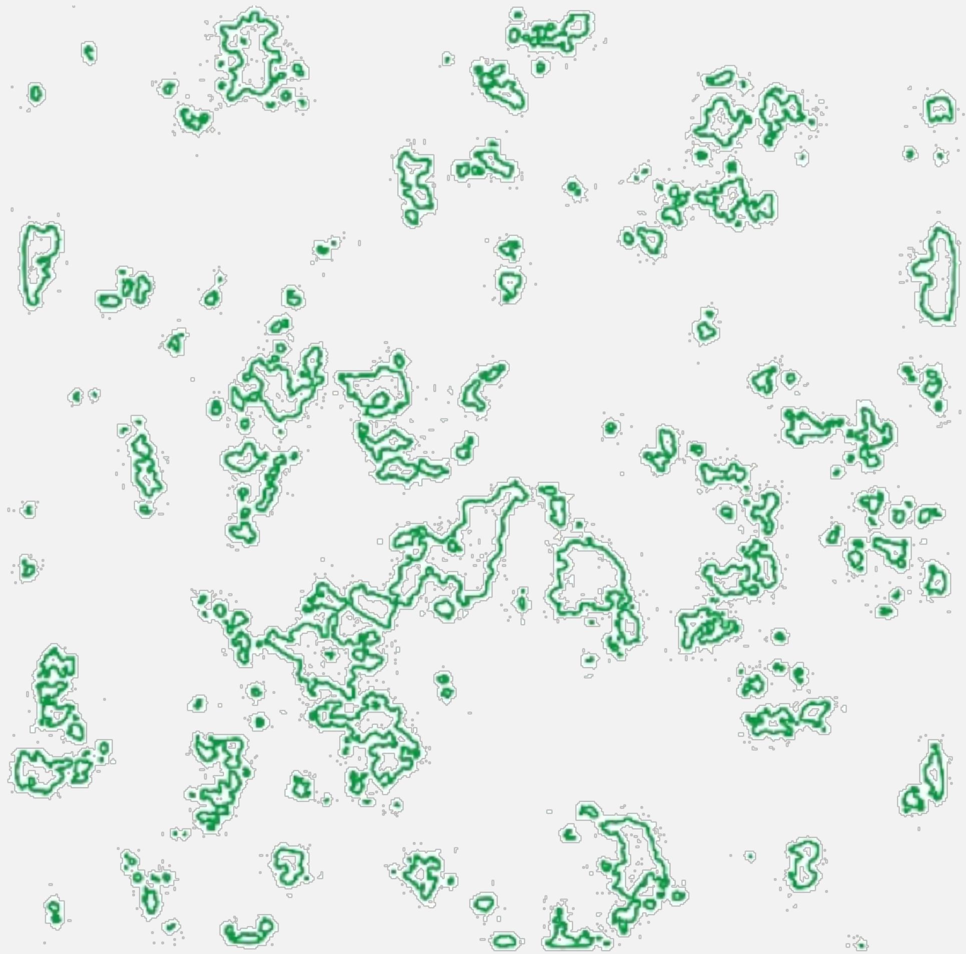
# Contact visualization

**experiment**





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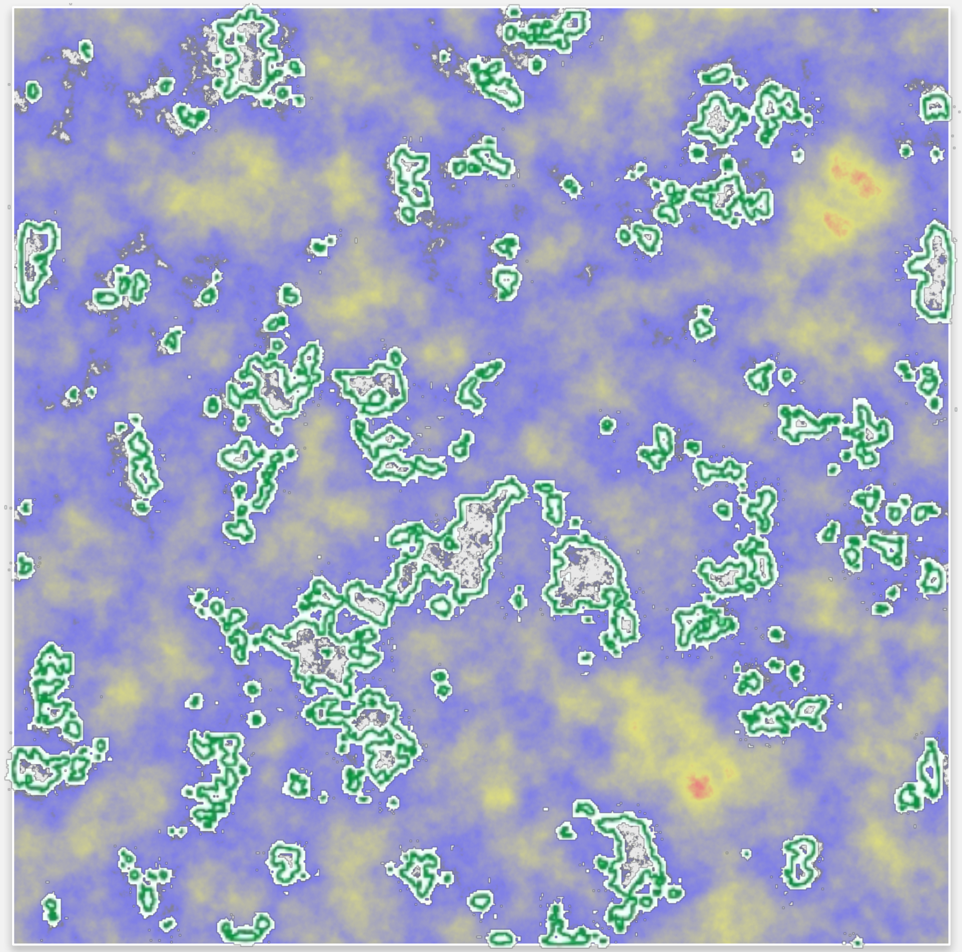
# Contact visualization



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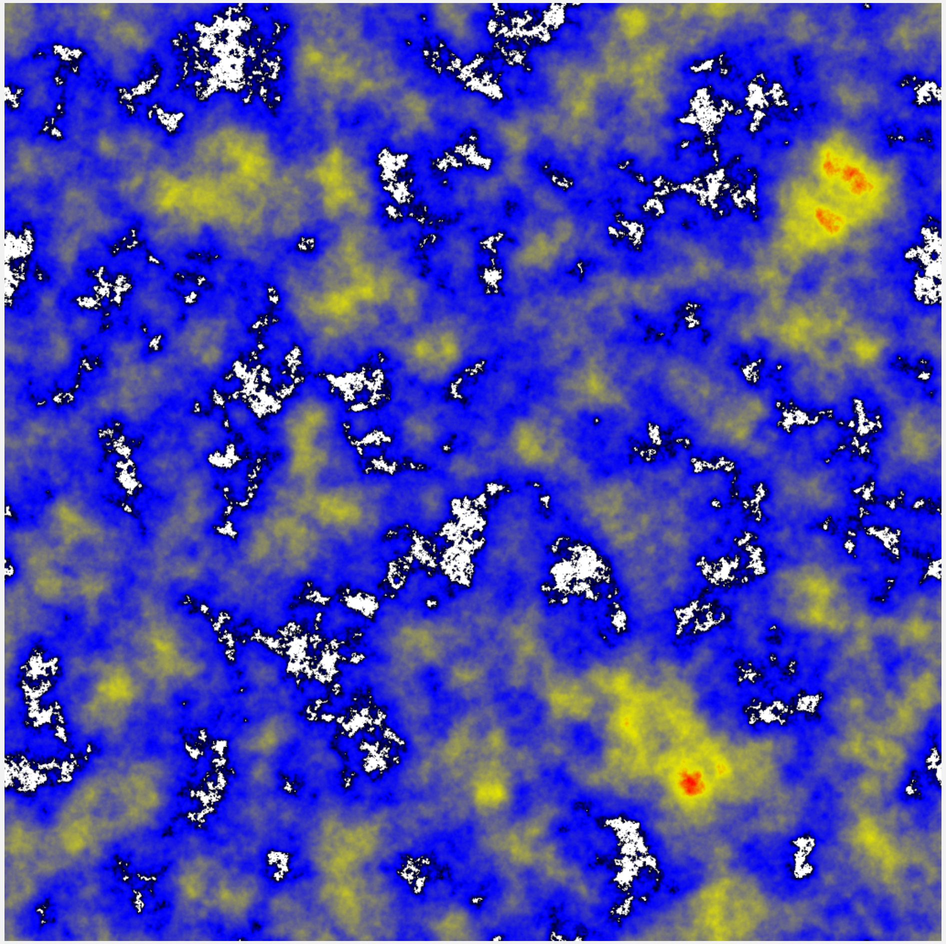
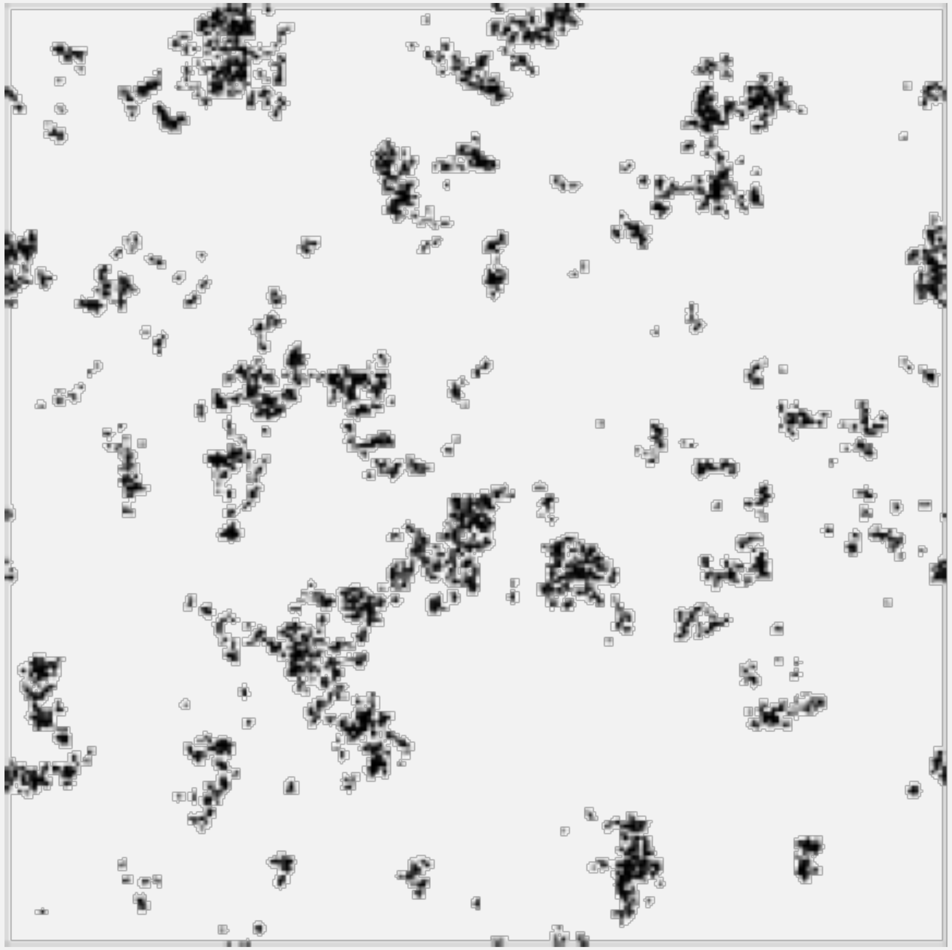
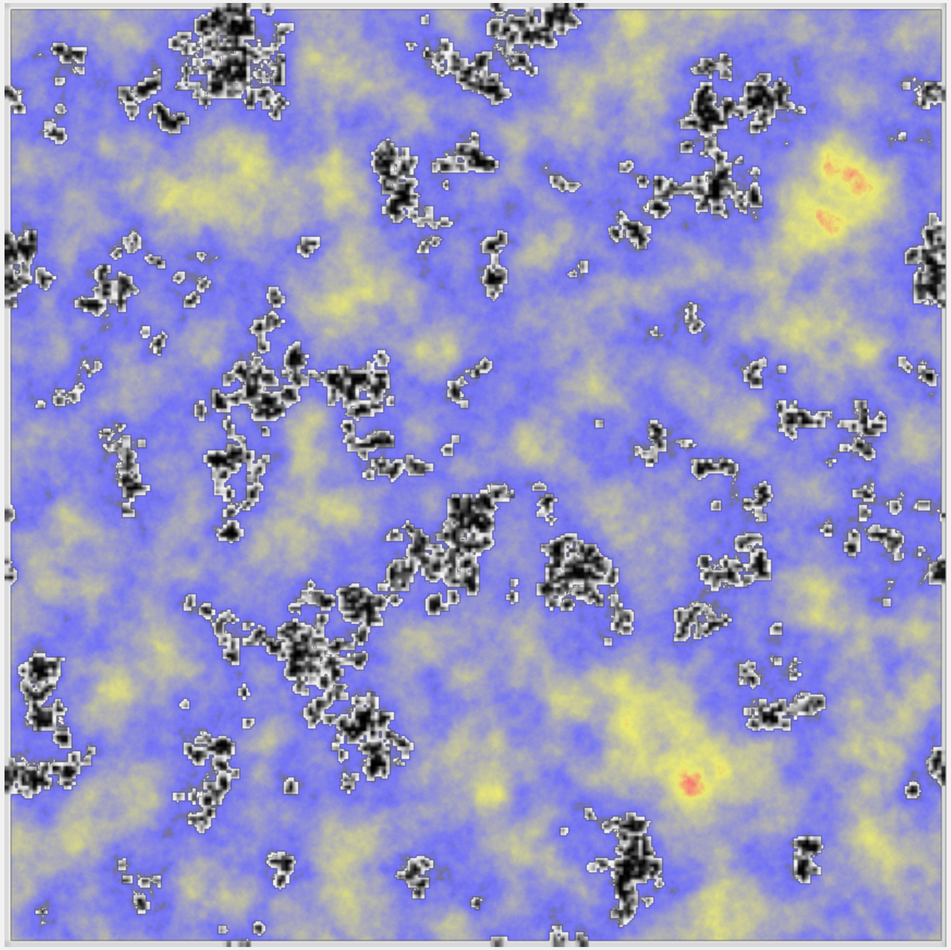
# Contact visualization

**all-atom MD**

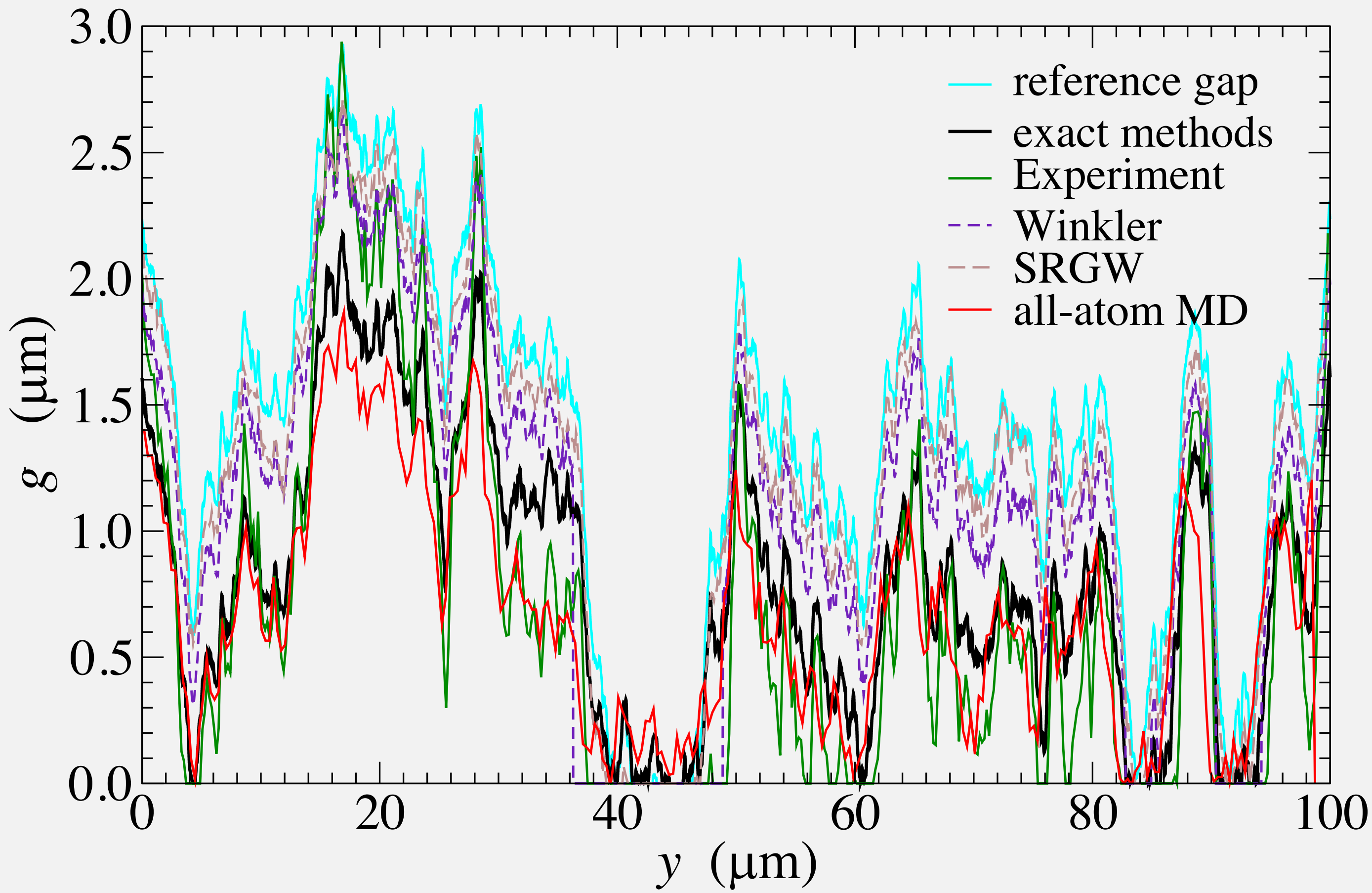




# Contact visualization



# Results: Spatially resolved quantities
## Gap across reference line (appr. methods)



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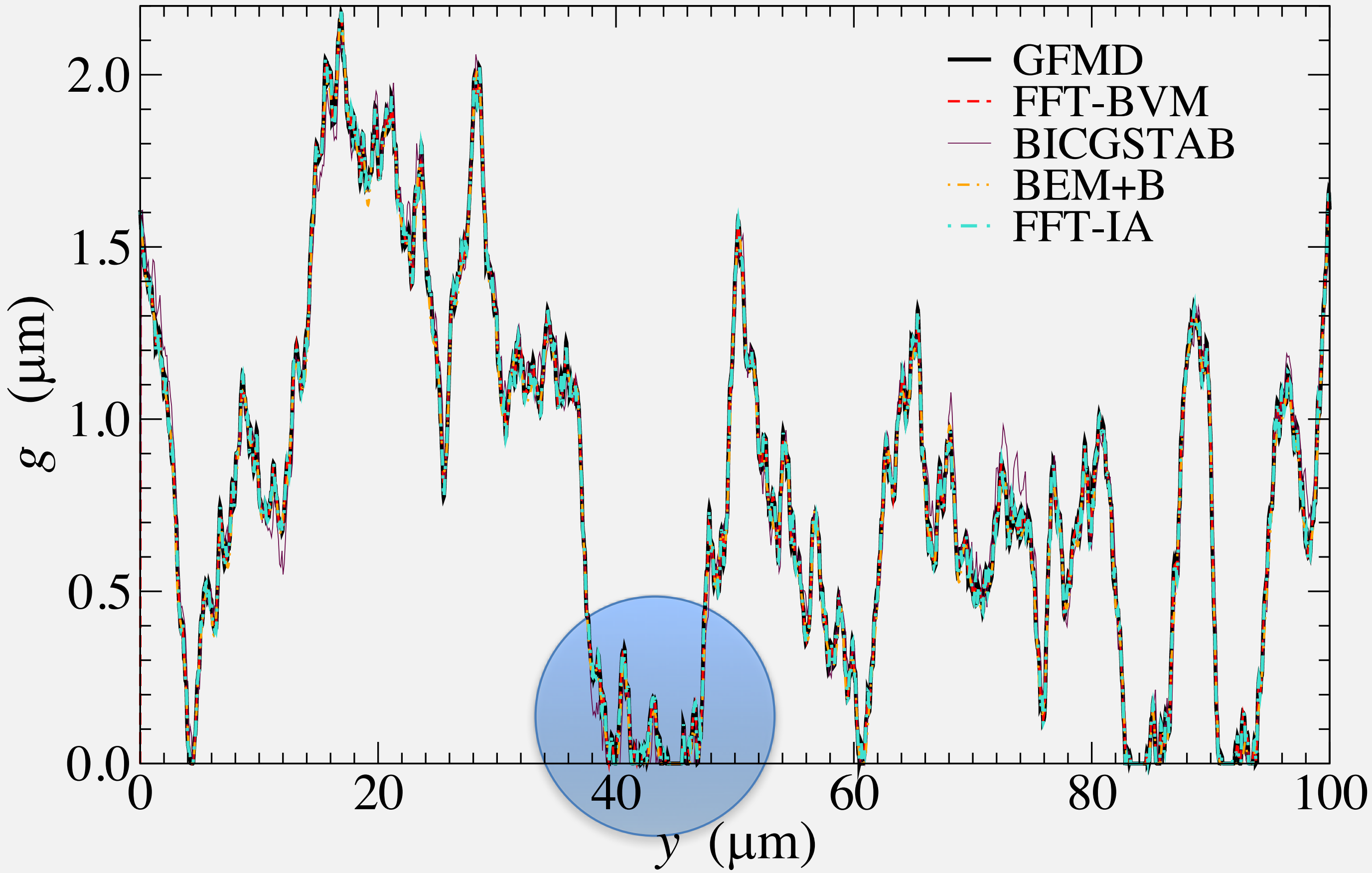
# Results: Spatially resolved quantities
## Gap across reference line (exact methods)



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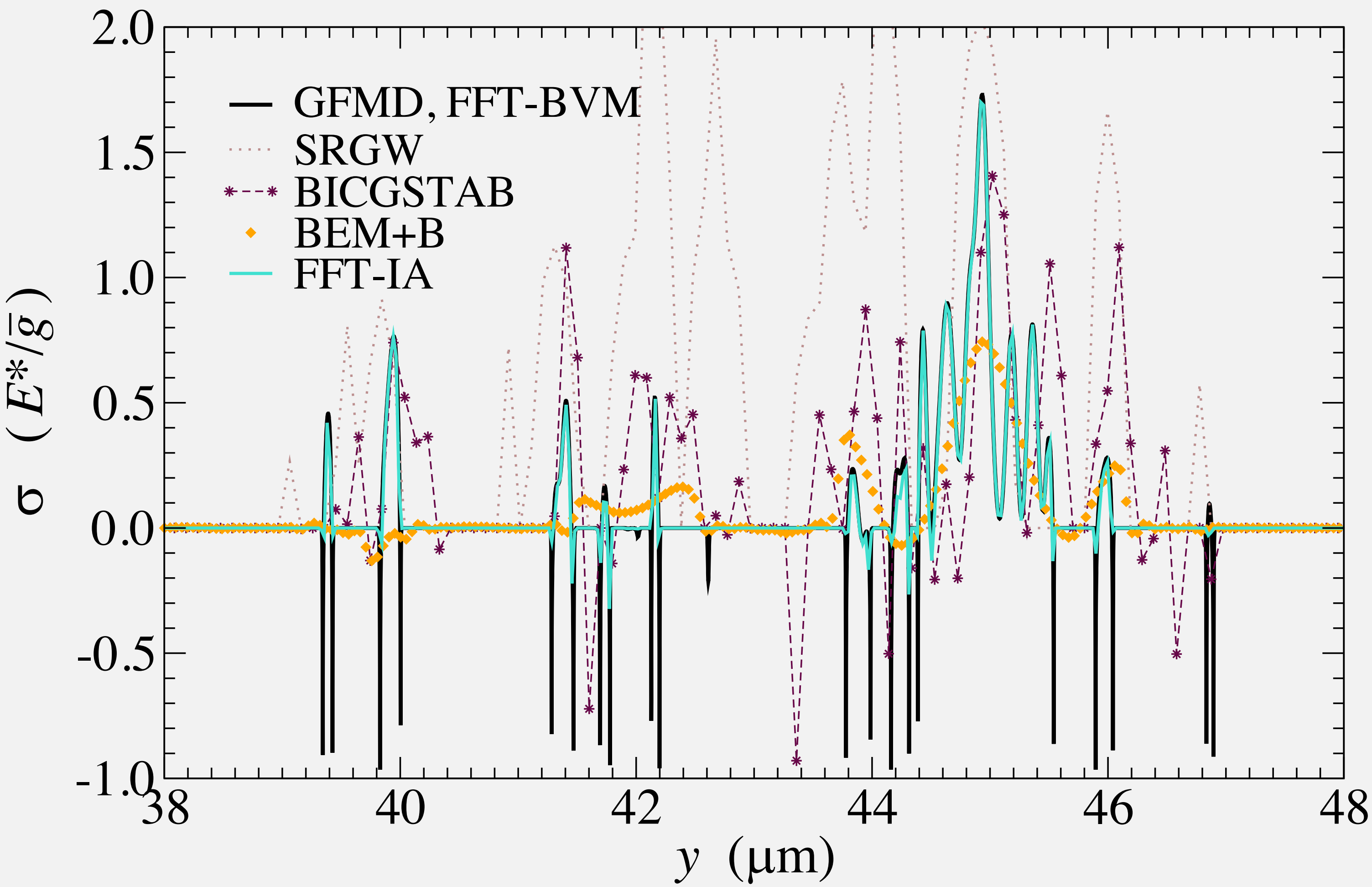
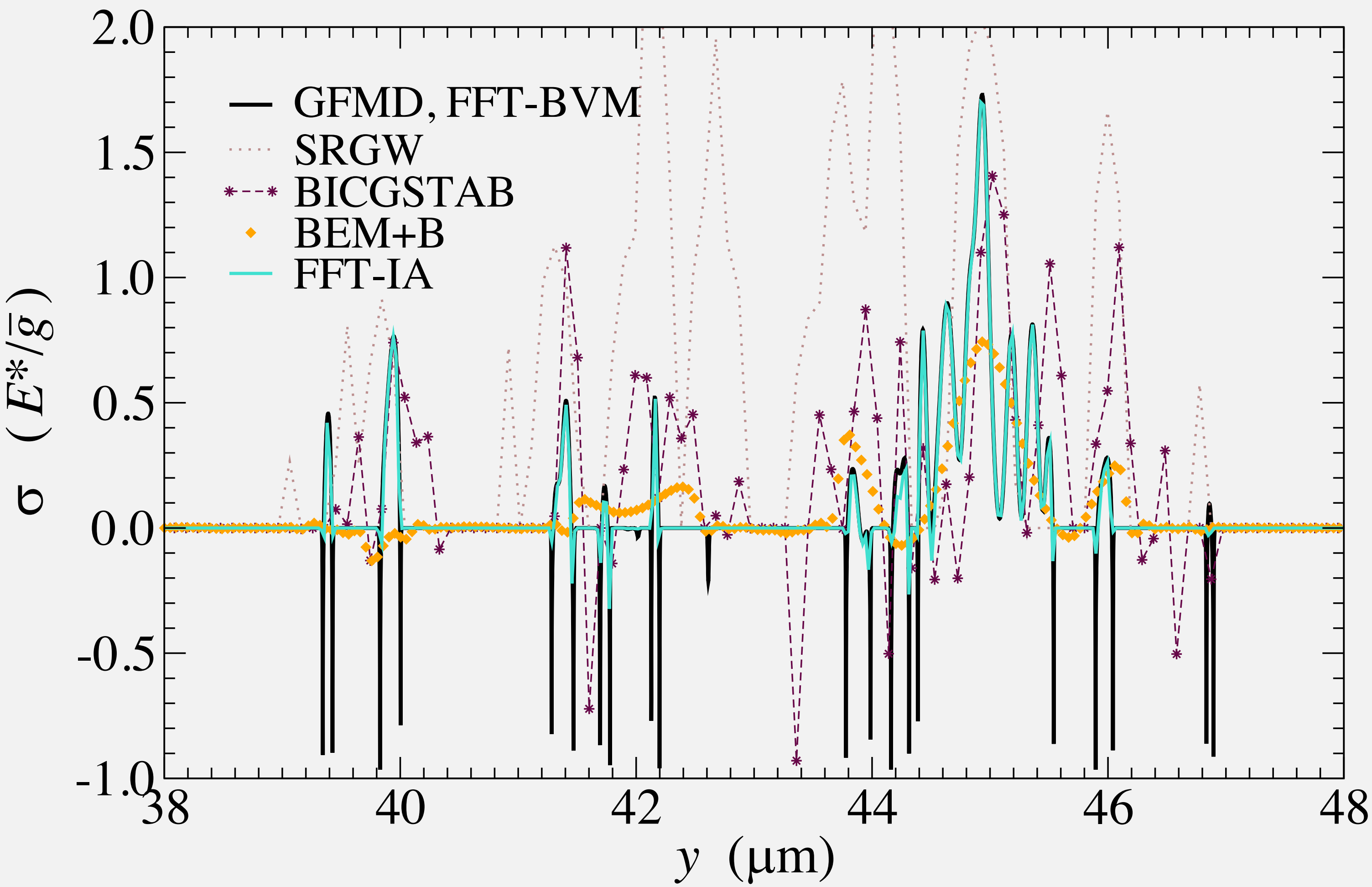
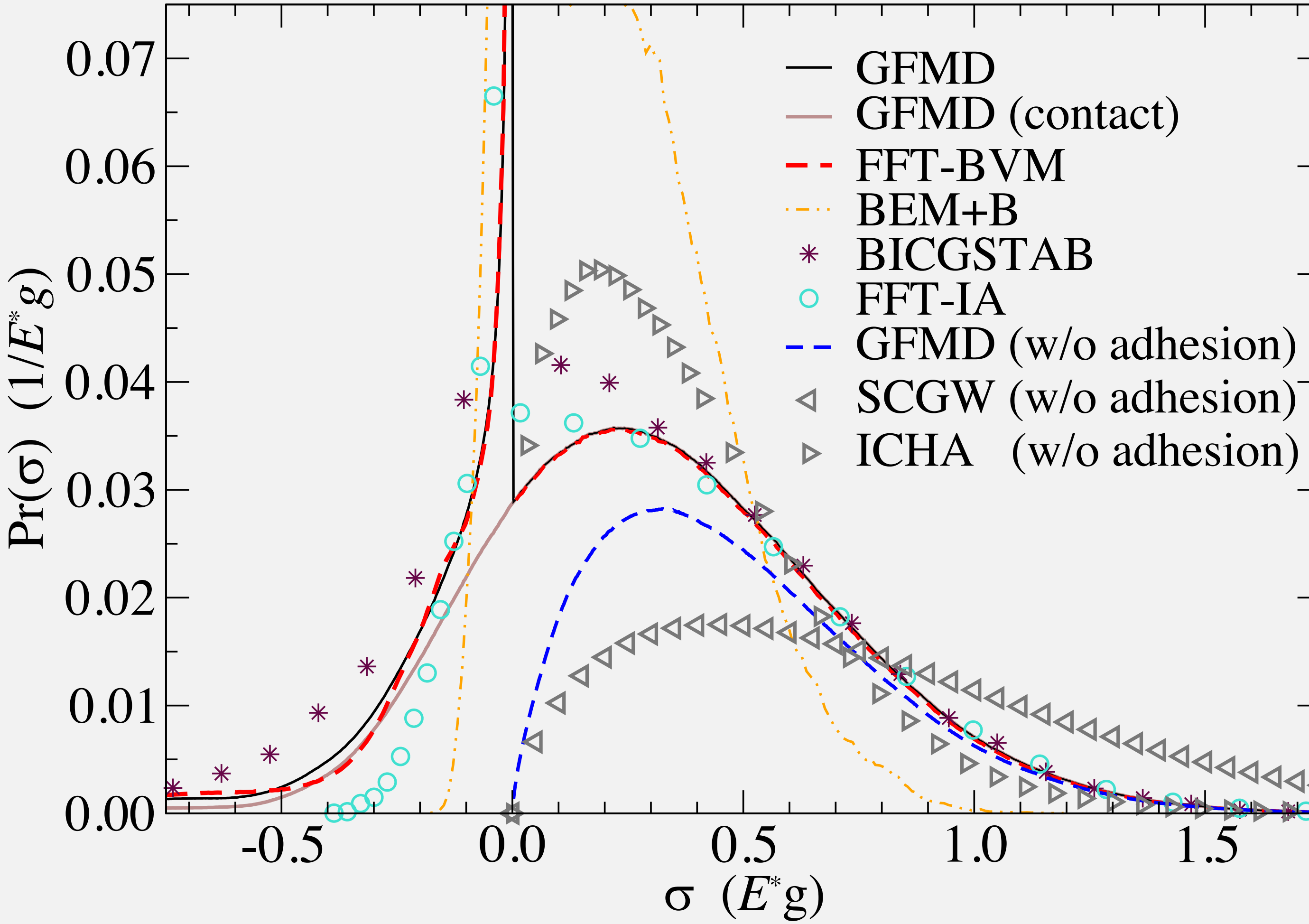
# **Results:** Stress across reference line (local zoom-in)



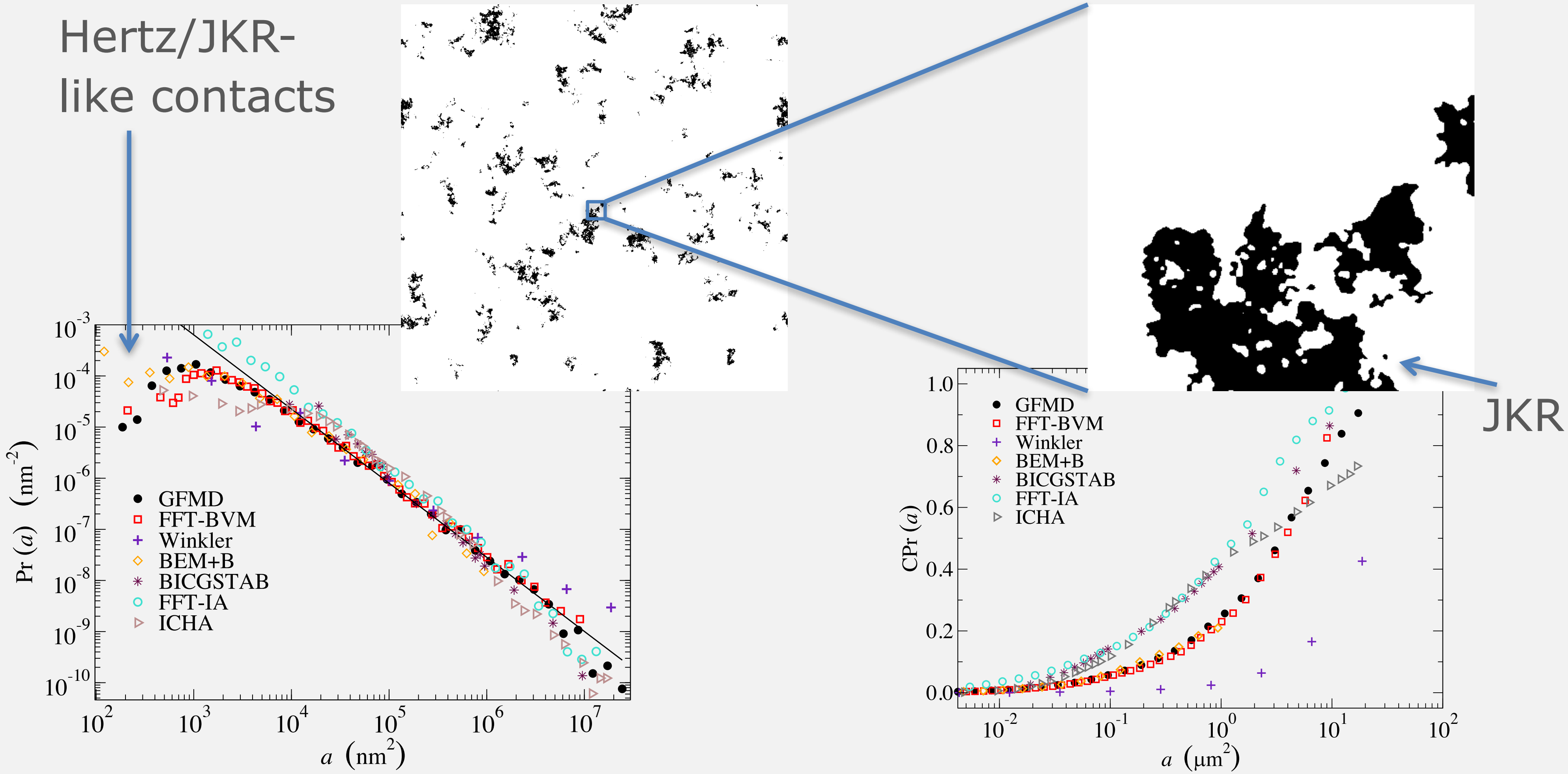
# **Results:** Stress across reference line (local zoom-in)



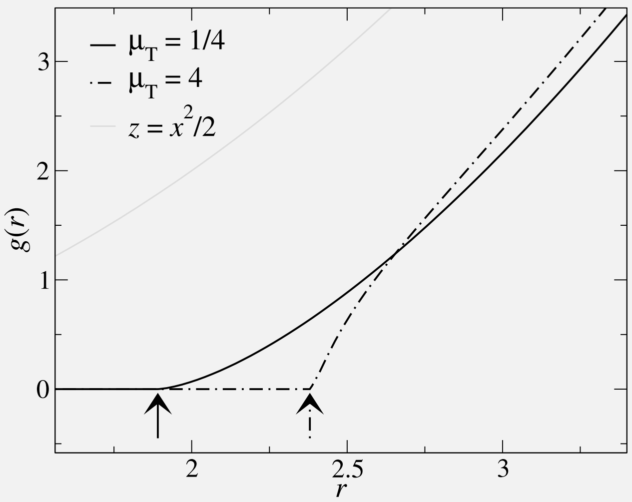
# Results: Stress distribution



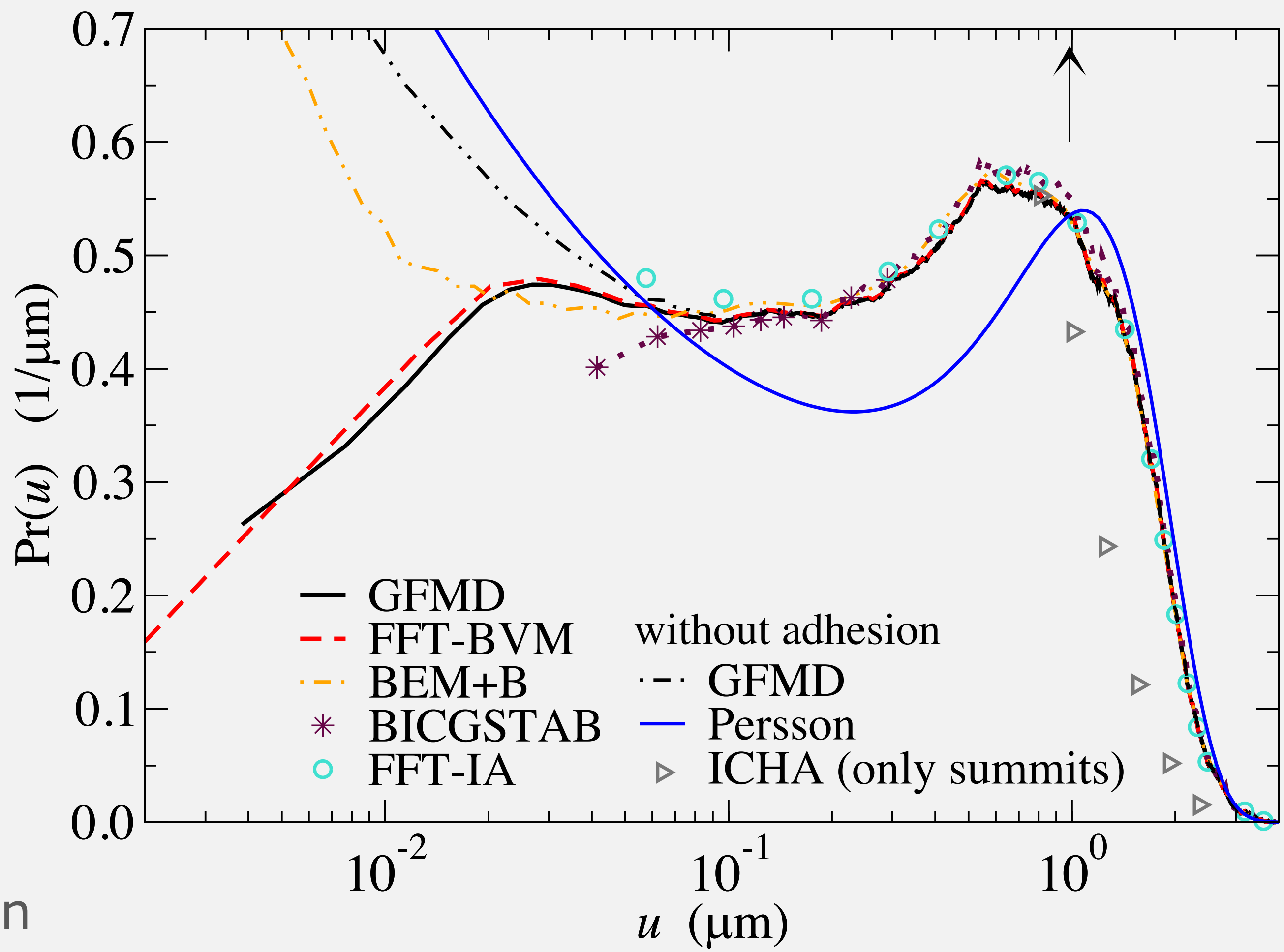
# **Results:** Patch-size distribution



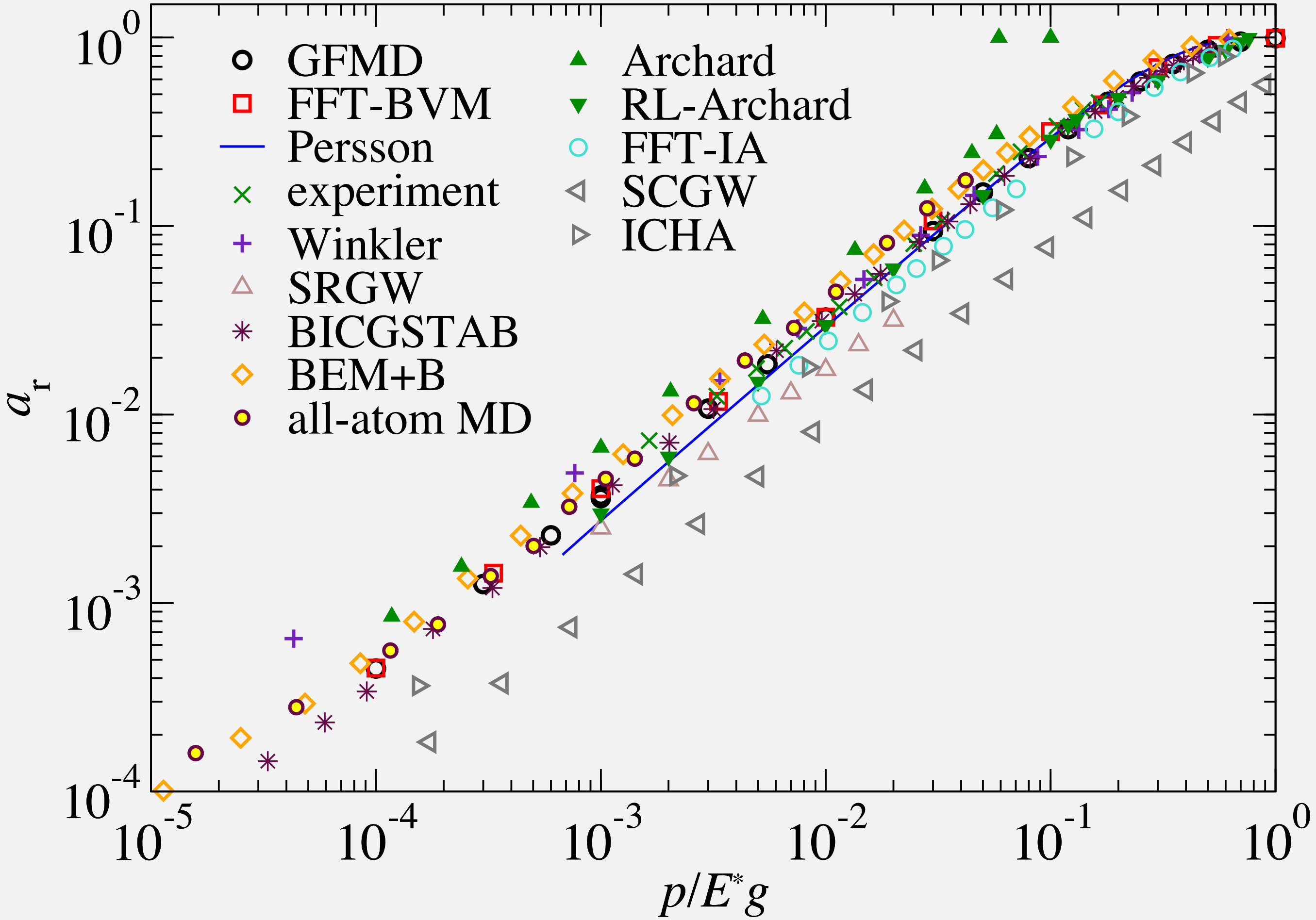
# **Results:** Gap distribution



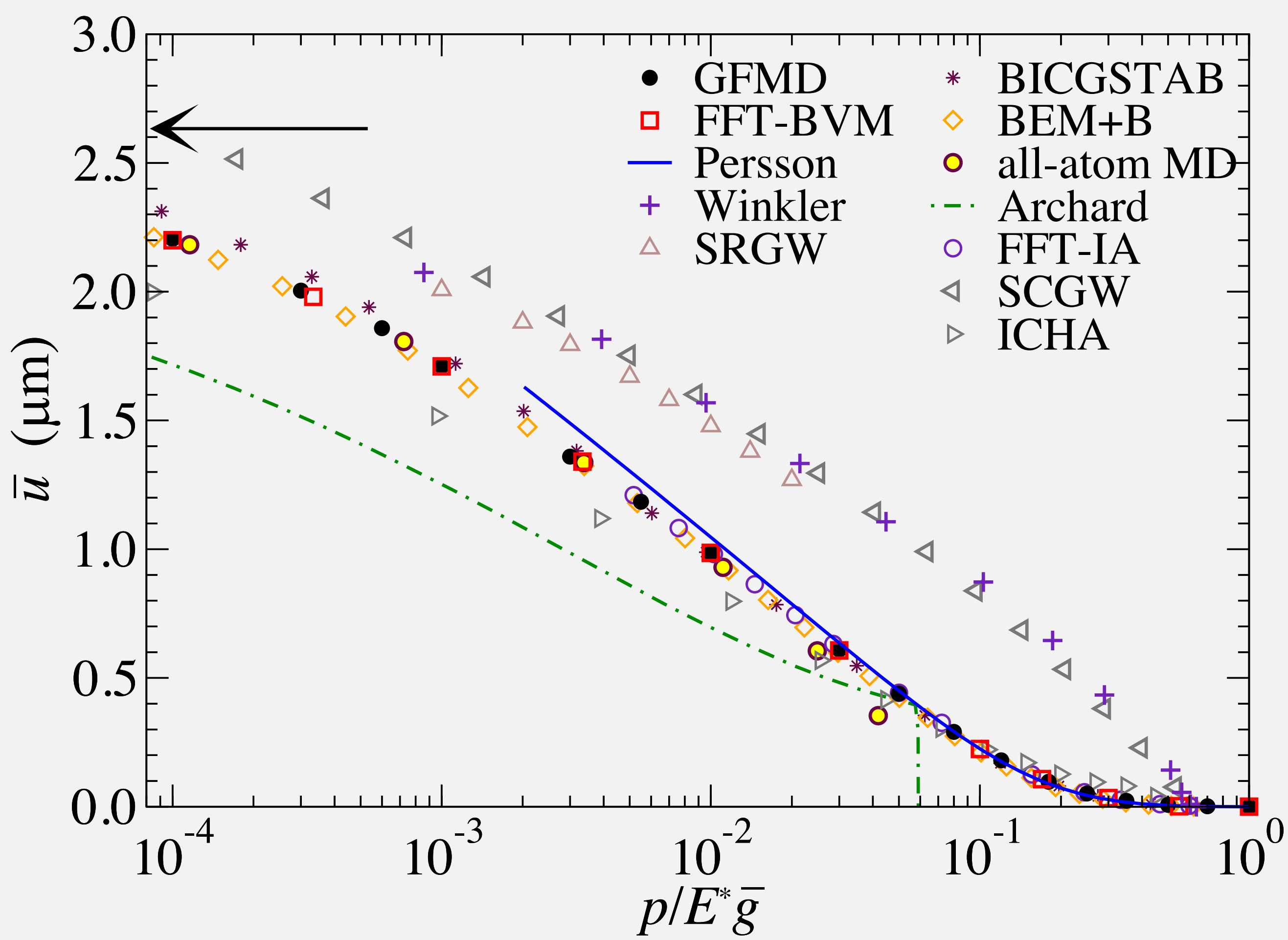

local gap for long-range and short-range adhesion



# **Results:** Average quantities $a_r(p)$



# Results: mean gap as a function of load



# Conclusions I

- **close agreement between all systematic approaches**

  differences in quantities that need high resolution

  GFMD (128k x 128k) and FFT-BVM (32k x 32k) match

- FFT-BVM (INSA-Lyon) stands out in that

  results obtained on a single core (with added RAM) for 32k x 32k

  and on standard workstation for 4k x 4k (1 hour)

  → rigorous treatment of measured profiles feasible

# Conclusions II

- **good agreement between all systematic approaches and inverse models (experiment & all-atom)**

  reverse conclusion: approximations that are commonly made in contact mechanics might be less problematic than believed
- reasonable agreement with Persson theory

  on all reported properties

  Pr(gap,stress) for small gap but with adhesion missing ☹
- bearing models reproduce $a_{rel}(p)$ relation

  but otherwise do not predict correct trends