Linking Discrete Dislocations and Molecular Dynamics in 3D: a Start

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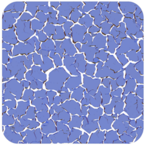
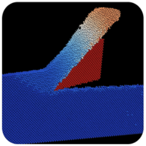

Laboratoire de Simulation en Mécanique des Solides
Computational Solid Mechanics Laboratory

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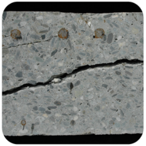
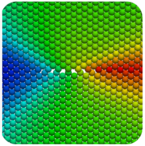




Outline

Outline

MD modelling of friction
- Advances through atomic force microscopy
- MD scratching - simplest case
- MD size restrictions

CADD

Test case

MD modelling of friction

Motivation

Friction is complex and poorly understood

Heat Q

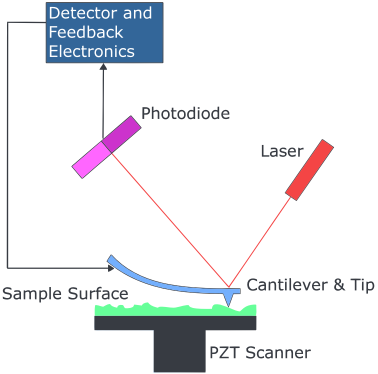
Plastic work W_{pl}

Questions

- Role of plasticity in friction?
- Proportion of W ending up as W_{pl}?

MD modelling of friction

Advances through atomic force microscopy



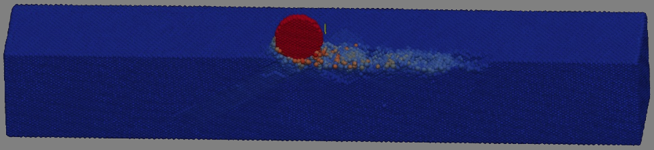
Atomic scale measurements

Source: Wikipedia

MD modelling of friction

MD scratching - simplest case

Molecular Dynamics Scratching Simulation at $\sim 0\,\mathrm{K}$



Advantages

- very few a priori assumptions
- deep understanding because of complete knowledge of each atom in the simulation box
- Dislocation nucleation and motion handled accurately

MD modelling of friction

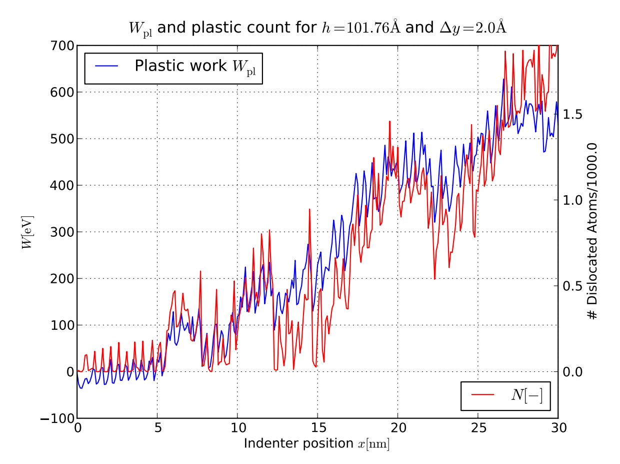
MD scratching - Computation of plastic work W_{pl}

Using molecular statics (MS)

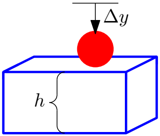
MD simulation	•	•	•	t
	$\{r_0, \dot{r}_0\}$	$\{r_1, \dot{r}_1\}$	$\{r_n, \dot{r}_n\}$	
MS quenching	↓	↓	↓	
	$\{r_0^{\mathrm{min}}, 0\}$	$\{r_1^{\mathrm{min}}, 0\}$	$\{r_n^{\mathrm{min}}, 0\}$	
Potential Energy	E_0^{min}	E_1^{min}	E_n^{min}	
Plastic work W_{pl}	$E_0^{\mathrm{min}} - E_0^{\mathrm{min}}$	$E_1^{\mathrm{min}} - E_0^{\mathrm{min}}$	$E_n^{\mathrm{min}} - E_0^{\mathrm{min}}$	

MD modelling of friction

MD size restrictions - small indentation, simulation size sufficient

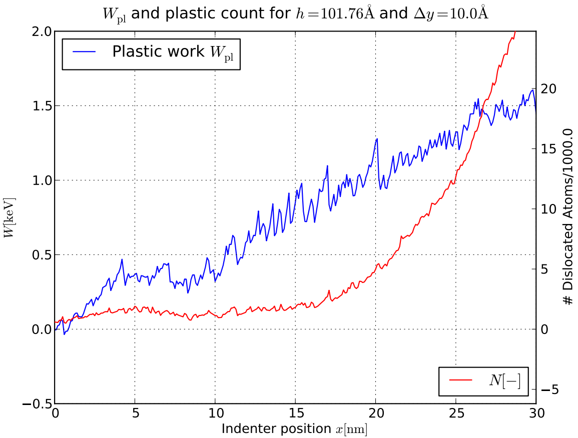


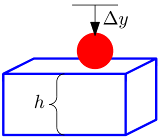
Plastic event count and W_{pl} **coincide**



MD modelling of friction

MD size restrictions - deeper indentation, too small simulation box



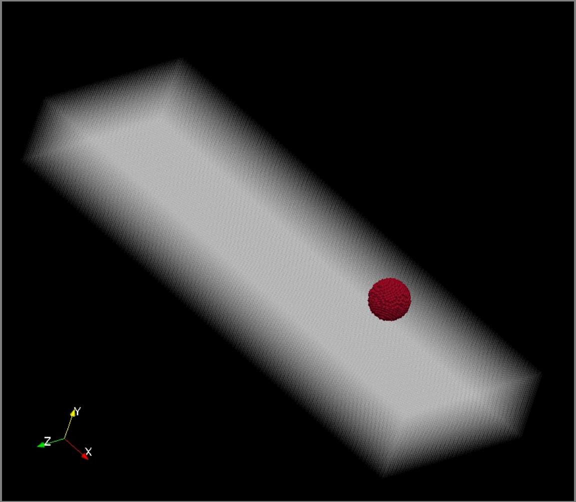


Plastic event count and W_{pl} **deviate**

MD modelling of friction

MD size restrictions

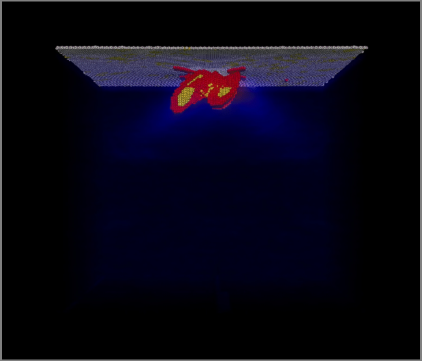
Visual inspection



MD modelling of friction

What to do?

Molecular dynamics simulations



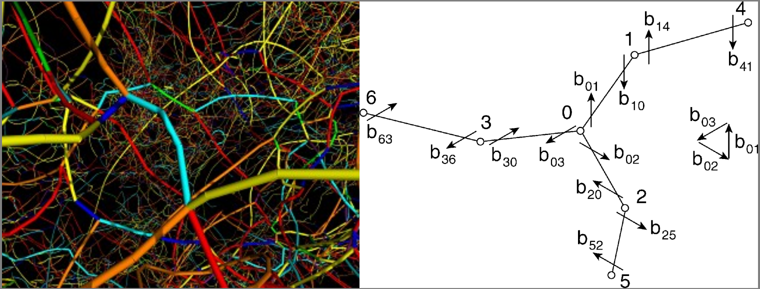
Source: Ziegenhain et al. / J. Mech. Phys. Solids 57 (2009)

Accurate dislocation nucleation, but too small scale

MD modelling of friction

What to do?

Discrete dislocation dynamics simulations



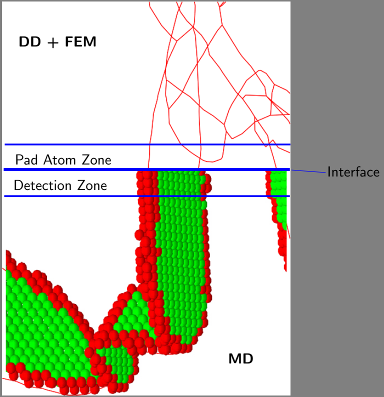
Source: ParaDiS (paradis.stanford.edu)

Larger scale, but problematic dislocation nucleation

MD modelling of friction

A combined approach

Coupled atomistics and discrete dislocations (CADD)



Pioneered by Shilkrot, Curtin / J. Mech. Phys. Solids 50 (2002) (in 2D)

Outline

MD modelling of friction

CADD

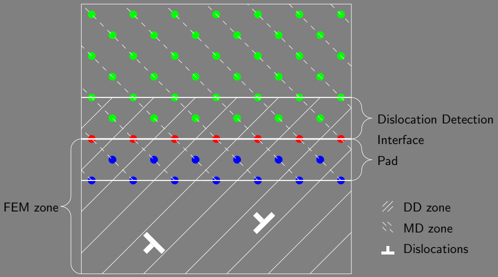
- Overview
- Coupling Scheme
- 3D Difficulties

Test case

CADD

Overview

2D representation



Shilkrot, Curtin / J. Mech. Phys. Solids 50 (2002)

1. Interface atoms (red) are **FEM boundary conditions**
2. Pad atoms (blue) are **MD boundary conditions**
3. DD are driven by **FEM stress** in continuum and by **detection** in atomistics

CADD

Coupling Scheme

MD

1. move atoms

DD

1. move dislocations

FEM

1. move elements

CADD

Coupling Scheme

MD

1. move atoms
2. detect disls $\rightarrow$ DD

DD

1. move dislocations
2. adjust pad atoms $\rightarrow$ MD

FEM

1. move elements
2. adjust pad atoms $\rightarrow$ MD

MD

1. move atoms
2. detect disls $\rightarrow$ DD
3. set interface $\rightarrow$ FEM

DD

1. move dislocations
2. adjust pad atoms $\rightarrow$ MD
3. set image forces $\rightarrow$ FEM

FEM

1. move elements
2. adjust pad atoms $\rightarrow$ MD
3. set stresses $\rightarrow$ DD

MD

1. move atoms
2. detect disls → DD
3. set interface → FEM
4. return to 1

DD

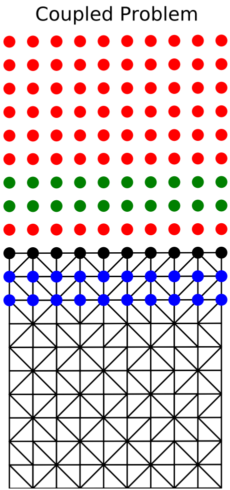
1. move dislocations
2. adjust pad atoms → MD
3. set image forces → FEM
4. return to 1

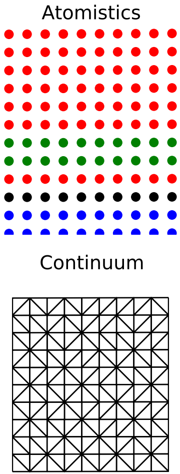
FEM

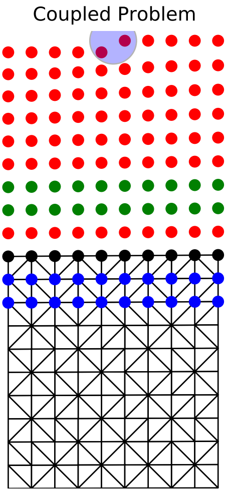
1. move elements
2. adjust pad atoms → MD
3. set stresses → DD
4. return to 1

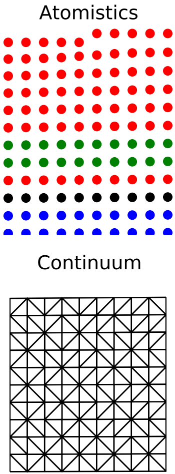
CADD

CADD in 2D



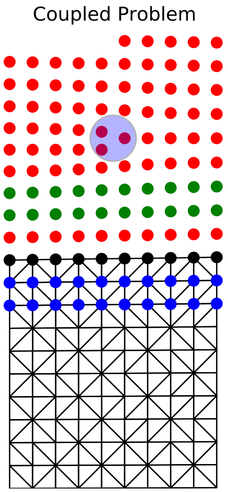


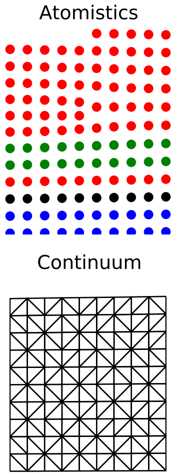

Coupled Problem


Atomistics
Continuum

CADD

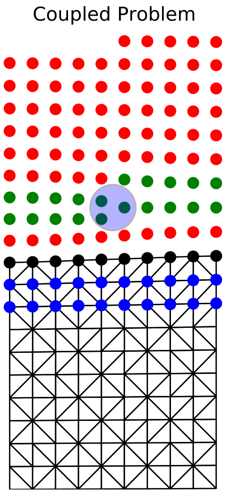
CADD in 2D

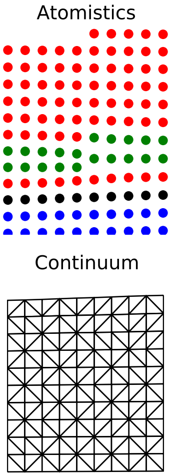


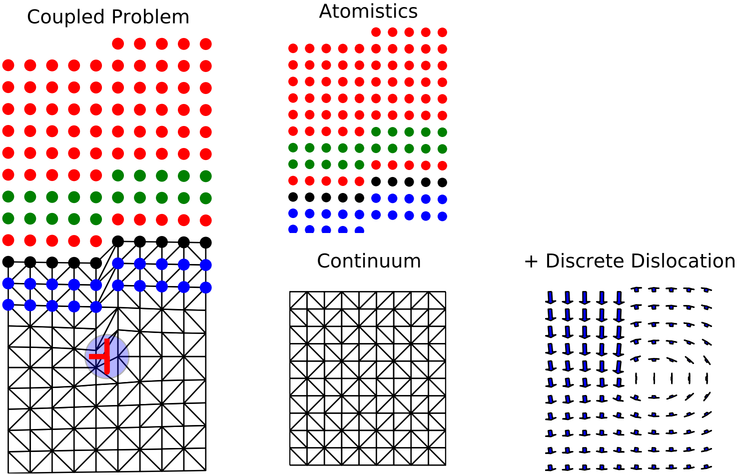


CADD

CADD in 2D







Coupled Problem
Atomistics
Continuum
+ Discrete Dislocation

CADD Simplifications obsolete in 3D

- **2D Dislocations are point entities**
  Dislocations always in **either** the MD **or** the FEM+DD zone

- **2D Dislocations never touch the interface**
  High energy (and **non-linear**) cores **don't interfere** with interface

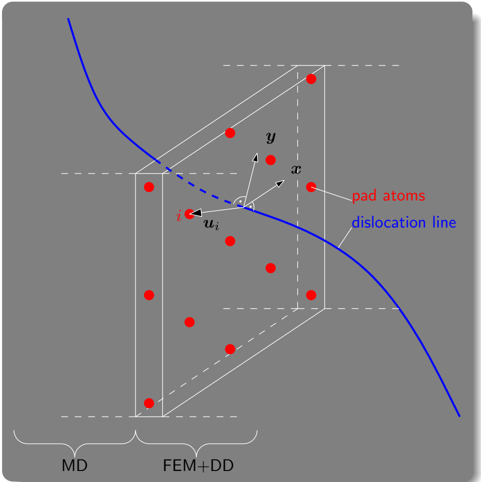
CADD Simplifications obsolete in 3D

- **2D Dislocations are point entities**
  Dislocations always in **either** the MD **or** the FEM+DD zone
- !! **3D Dislocations are loops**
  Dislocation may be partly in the MD **and** the FEM+DD zone

- **2D Dislocations never touch the interface**
  High energy (and **non-linear**) cores **don't interfere** with interface
- !! **3D Dislocations can cross the interface**

For each Dislocation line

Apply displacement
$\boldsymbol{u}_i = \boldsymbol{u}(x - x_{\text{core}}, y - y_{\text{core}})$
to each pad atom i



Outline

MD modelling of friction

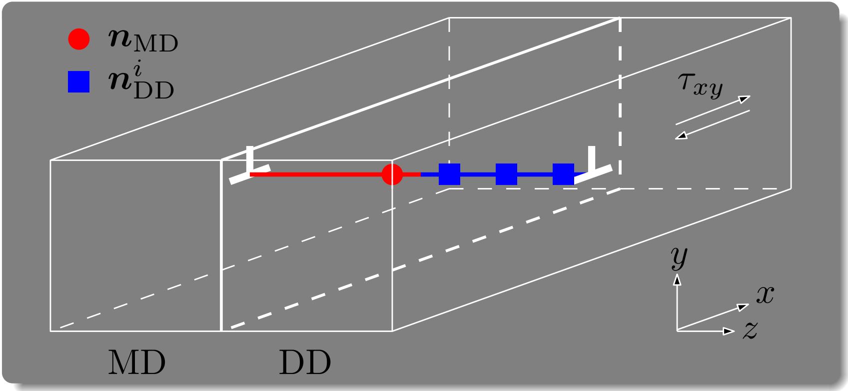
CADD

Test case

- Simplest case: no FEM required
- Simplest template
- Preliminary results

Test case

Simplest case: no FEM required



Simplification

No out-of-plane displacement $\Rightarrow$ **no need for solving elasticity**

Test case

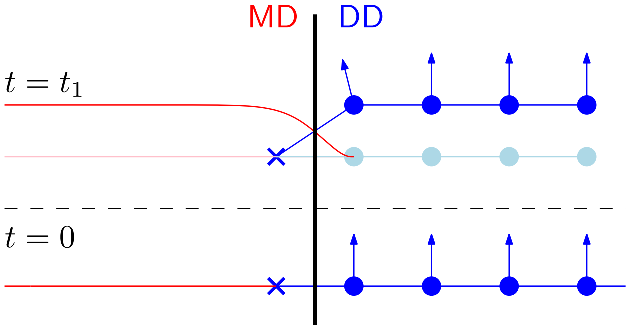
Revisit coupling scheme

MD

1. move atoms

DD

1. move dislocations



Test case

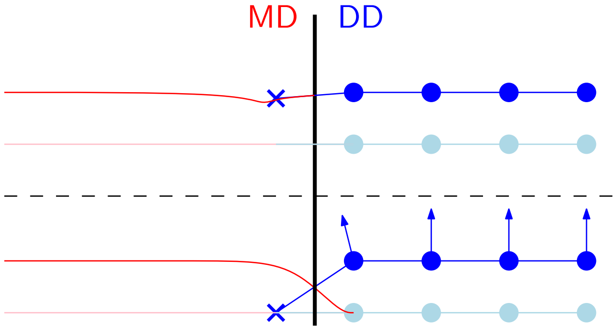
Revisit coupling scheme

MD

1. move atoms
2. detect dislocations → DD

DD

1. move dislocations
2. adjust pad atoms → MD



Test case

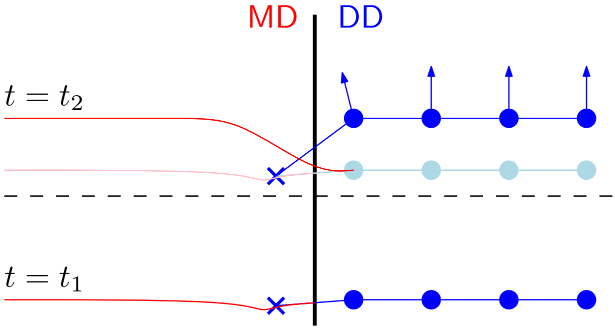
Revisit coupling scheme

MD

1. move atoms
2. detect dislocations → DD
3. return to 1

DD

1. move dislocations
2. adjust pad atoms → MD
3. return to 1

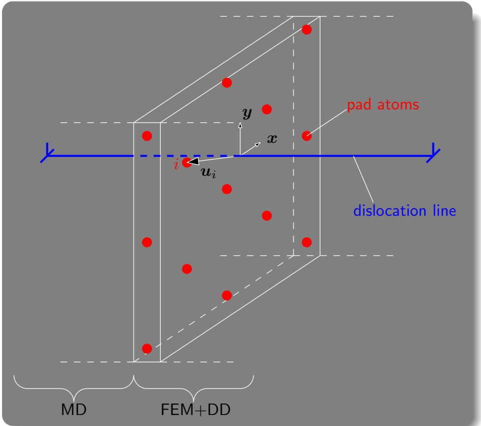


Test case

Simplest case: simple template

$\boldsymbol{u}_z = 0$

Straight edge dislocation
$\perp$ interface
The template is a **2D Problem**



Test case

Simplest template

isotropic linear elastic displacement field

$$u_x(\bar{x},\bar{y}) = \frac{b}{2\pi}\left(\arctan\frac{\bar{x}}{\bar{y}} + \frac{\bar{x}\bar{y}}{2(1-\nu)(\bar{x}^2+\bar{y}^2)}\right),$$

$$u_y(\bar{x},\bar{y}) = -\frac{b}{2\pi}\left(\frac{1-2\nu}{1(1-\nu)}\ln(\bar{x}^2+\bar{y}^2) + \frac{\bar{x}^2-\bar{y}^2}{4(1-\nu)(\bar{x}^2+\bar{y}^2)}\right),$$

where $\bar{x} = \frac{x}{b}, \quad \bar{y} = \frac{y}{b}$

Trivial core tracking

The slip plane of the dislocation is known!

1. discretise the detection zone in bins
2. compute for each bin $\Delta u_x = \max(u_x) - \min(u_x)$
3. check for which bin Δu_x is closest to $b/2$

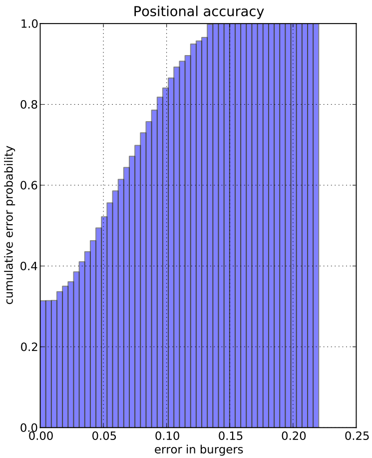
Test case

Accuracy of the template

Material sytem

- Magnesium (hcp, MEAM [1])
- Prismatic edge dislocation
- Very compact core
- Good accuracy of linear elastic approximation

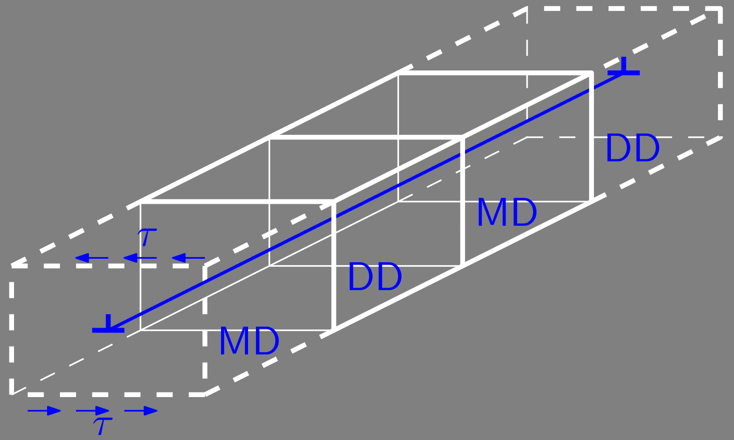
[1] M.I. Mendelev, M. Asta, M.J. Rahman and J.J. Hoyt, Phil. Mag. 89, 3269-3285 (2009)



Test case

Preliminary results- setup

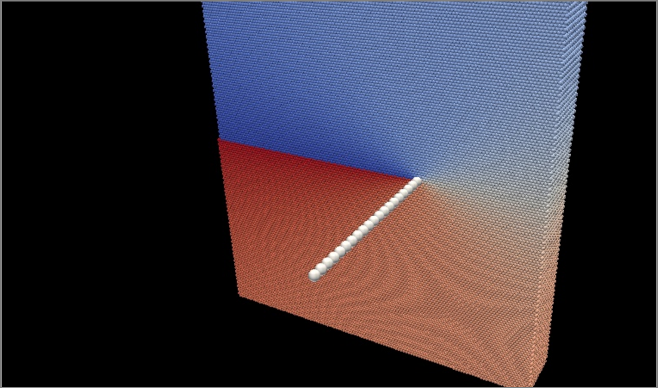
Periodic boundaries



Test case

Preliminary results

A sample movie



Observations

- **Detection and pad work**
  The dislocation information is accurately communicated between the domains
- **Dislocation line stays straight**
  Same dislocation velocity in MD and DD
- **No apparent artificial pinning**
  The elastic solution is a good enough template for this case

Conclusion and Outlook

Outlook - FEM coupling

FEM $\Leftarrow$ MD

Interface atoms serve as FEM displacement boundary condition

FEM $\Rightarrow$ MD

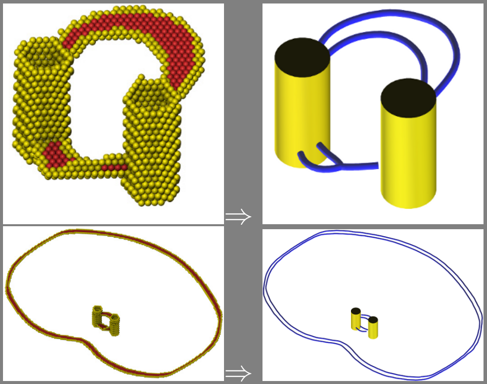
FEM computes **elastic** contribution to pad atom displacement

FEM $\Leftarrow$ DD

Image forces serve as FEM traction boundary condition

FEM $\Rightarrow$ DD

FEM computes stresses on DD node positions



Stukowski Modelling Simul. Mater. Sci. Eng. 18 (2010)

Stukowski 2010

Method based on burgers circuits,
parallel, on the fly implementation.

Conclusion and Outlook

Conclusions

1.

MD **insufficient** to treat friction problems of meaningful size

Conclusion and Outlook

Conclusions

1.

MD **insufficient** to treat friction problems of meaningful size

2.

The 3D CADD method **is functional**

Conclusion and Outlook

Conclusions

1\.

MD **insufficient** to treat friction problems of meaningful size

2\.

The 3D CADD method **is functional**

3\.

The 3D CADD method is a promising candidate to work out the size problem in atomic scale contact.

Conclusion and Outlook

Conclusions

1. MD **insufficient** to treat friction problems of meaningful size

2. The 3D CADD method **is functional**

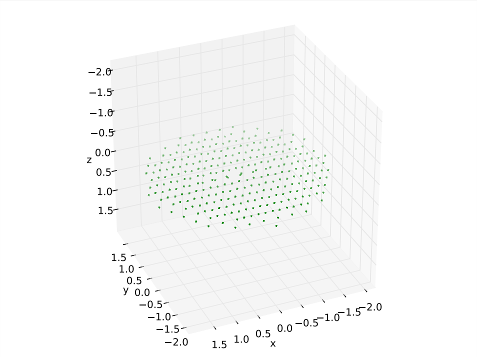
3. The 3D CADD method is a promising candidate to work out the size problem in atomic scale contact.

4. CADD also applicable to many **other problems** such as
   - Fracture, crack propagation
   - Dislocation interaction with grain boundaries

Appendix – Core templates

Using real core data

Core extraction

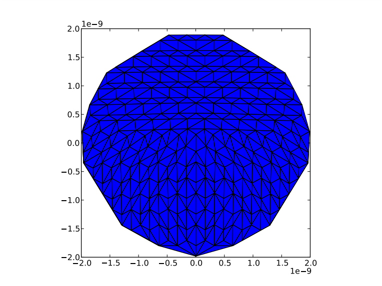


- generate a dislocation core (MS)
- filter out low energy atoms

Appendix – Core templates

Using real core data

Generating a core mesh



- Triangulate core using projected atoms as nodes
- compute displacement and interpolation shape functions S_u and S_x for each element:

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{S}_u \; S_x^{-1} \; \boldsymbol{x}$$