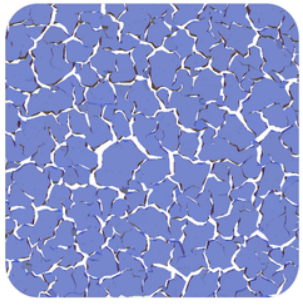
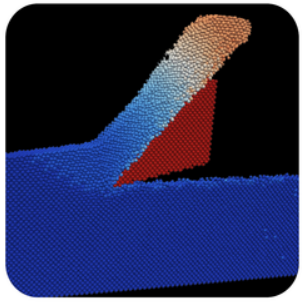
Investigation of the size of plastic zones in nano indentation and nano scratching

Till Junge J.-F. Molinari W. Curtin J. Song

LSMS
Laboratoire de Simulation en Mécanique des Solides
Computational Solid Mechanics Laboratory

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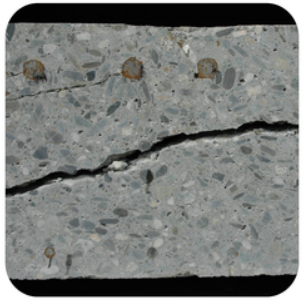
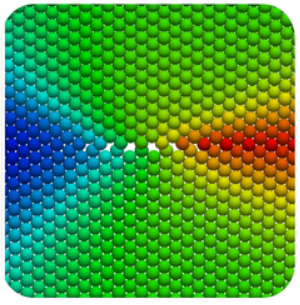


Outline

- Motivation
  - Description
  - Why look at plasticity in friction?
- Molecular Dynamics/Statics Approach
  - Virtual Experimental Setup
  - Method
  - Preliminary Results
- Extension to larger Systems
  - CADD
  - Requirements for CADD 3D

Outline

Motivation

Description

Friction converts mechanical Work W in

Heat Q

Plastic work W_{pl}

Questions

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

Motivation

Why look at plasticity in friction?

Situation

Plastic effects are an important factor in friction, but

- they are **poorly understood**
- they are **rarely investigated**
- they are **hard to quantify**

Motivation

Why look at plasticity in friction?

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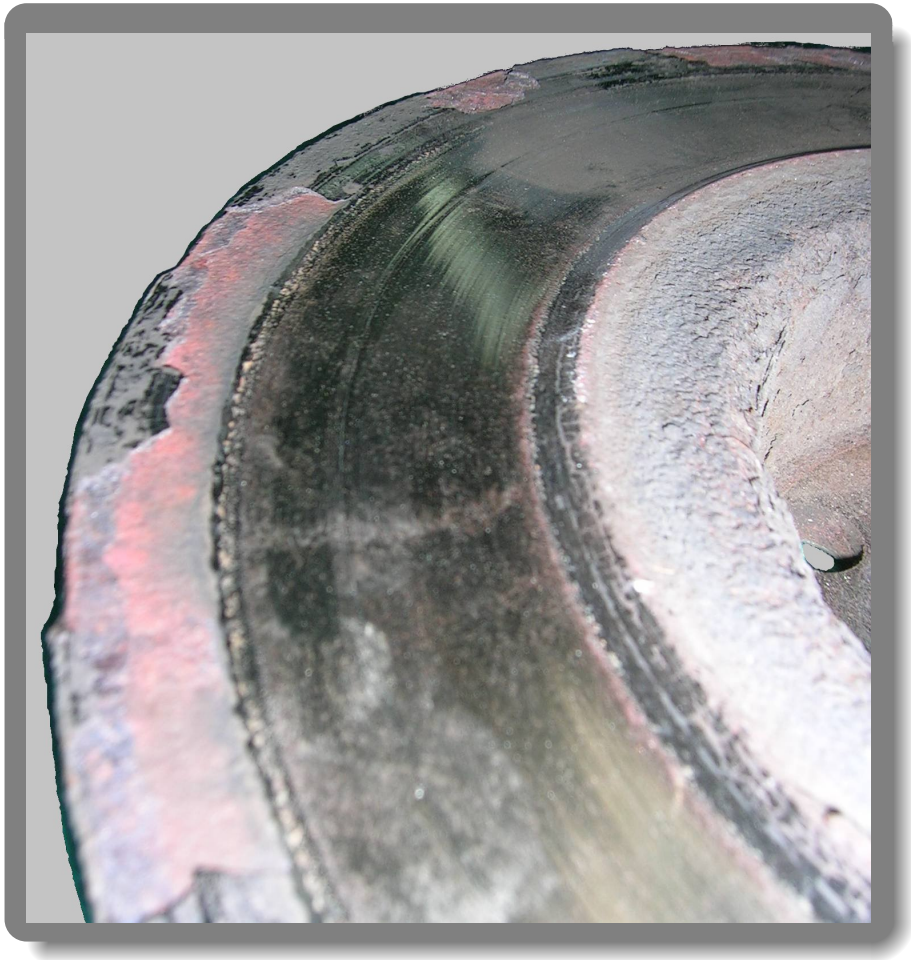
Interest

Plasticity in friction is the **source of wear and tear**

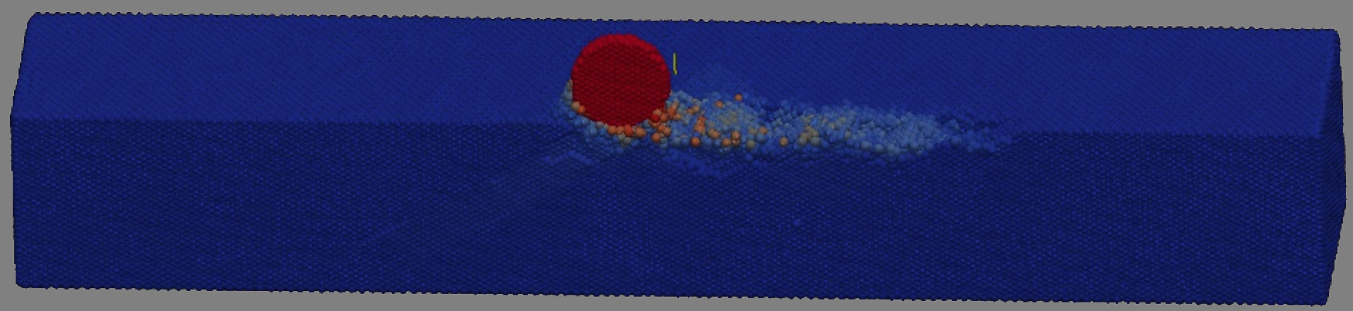


Outline

Molecular Dynamics/Statics Approach

Virtual Experimental Setup

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

Molecular Dynamics/Statics Approach

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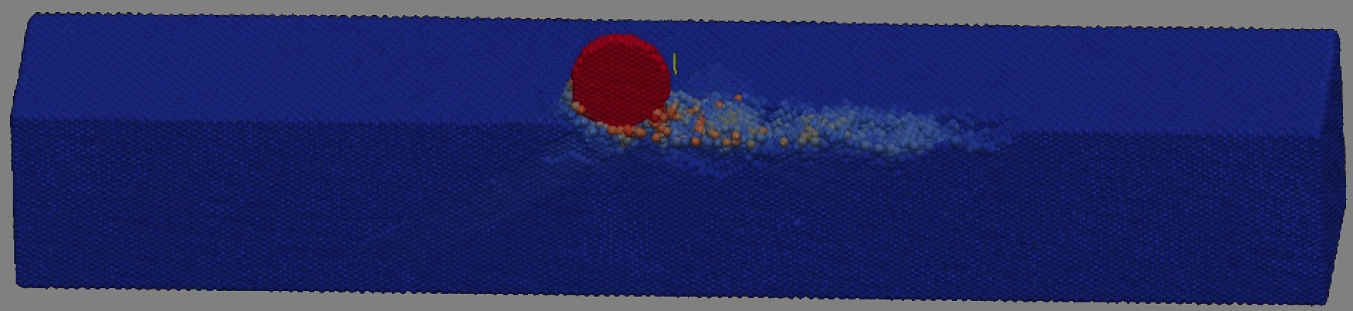


Advantages

- very few a priori assumptions
- deep understanding because of complete knowledge of each atom in the simulation box

Main Drawback

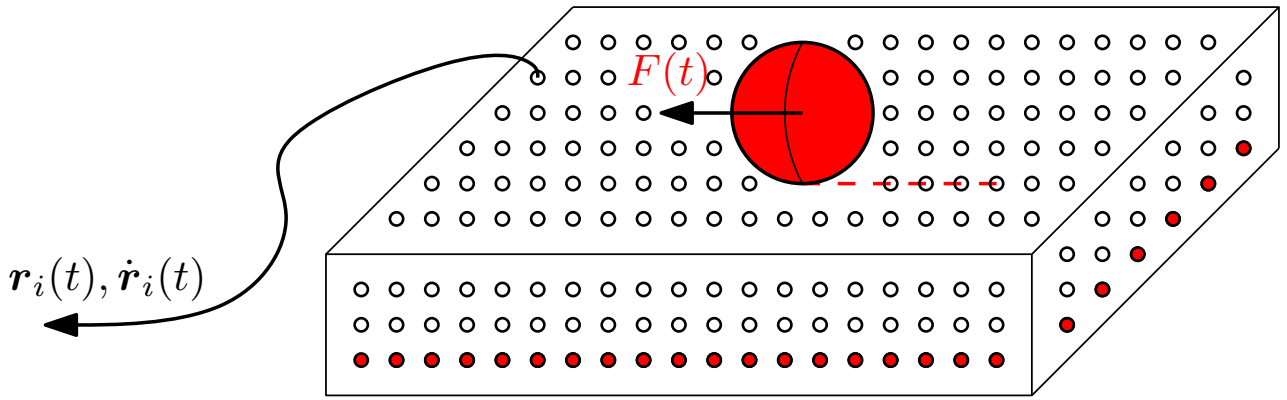
Very limited simulation box size and simulation time

Molecular Dynamics/Statics Approach

Method — Part I: the MD simulation

Setup

- fixed boundary conditions for bottom atoms
- prescribed indenter path $x(t)$



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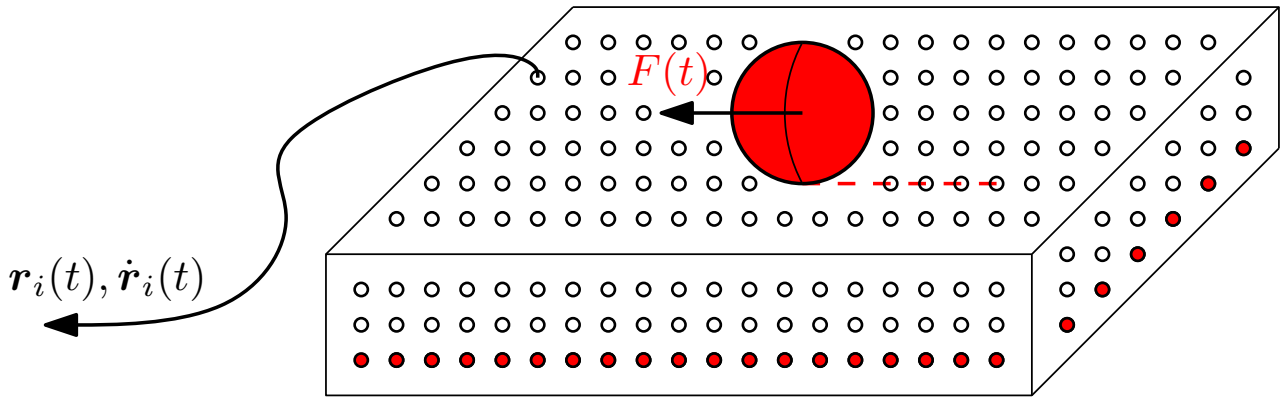
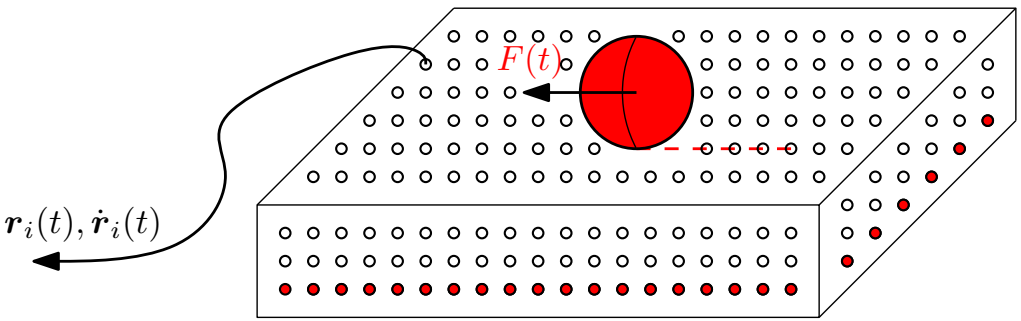


At different time steps t

- Evaluate Force $F(t)$ acting on the indenter,
- Save positions $\boldsymbol{r}_i(t)$ and velocities $\dot{\boldsymbol{r}}_i(t)$

Molecular Dynamics/Statics Approach

Method — Part II: the energy balance



Energy influx

$$E_{\text{in}}(t) = \int_0^t F(t)\mathrm{d}l$$

Molecular Dynamics/Statics Approach

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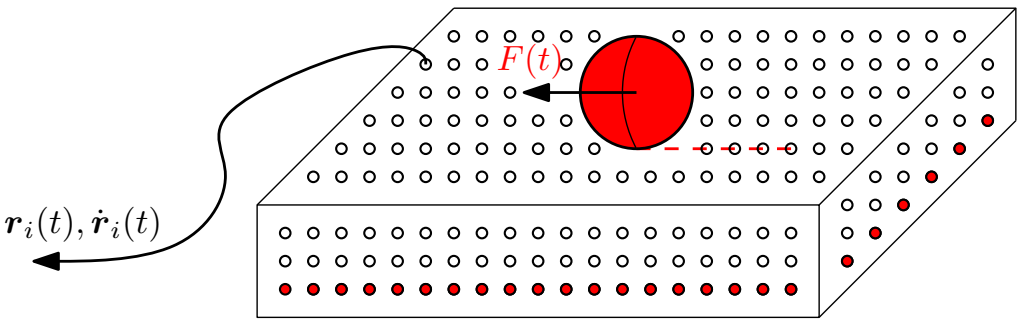

Energy influx

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Stored as

$$\begin{aligned} E(t) &= E\left[\boldsymbol{r}_1(t), \ldots, \boldsymbol{r}_N(t), \dot{\boldsymbol{r}}_1(t), \ldots, \dot{\boldsymbol{r}}_N(t)\right] \\ &= \sum_{i,j,k,\ldots} E_{\text{pot}}(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k, \ldots) + \sum_i E_{\text{kin}}(\dot{\boldsymbol{r}}_i) \end{aligned}$$

Molecular Dynamics/Statics Approach

Method — Part II: the energy balance

Stored Energy

$$E = \sum_{i,j,k,\ldots} E_{\mathrm{pot}}(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{r}_k, \ldots) + \sum_i E_{\mathrm{kin}}(\dot{\boldsymbol{r}}_i)$$

Potential Energy

- empirical interatomic potential function
- here EAM potential for Cu:

$$E_{\mathrm{pot}_i} = F_\alpha\left(\sum_{i\neq j} \rho_\alpha(r_{ij})\right) + \frac{1}{2}\sum_{i\neq j} \phi_{\alpha\beta}(r_{ij})$$

Kinetic Energy

- Classic mechanics:

$$E_{\mathrm{kin}i} = \frac{1}{2} m_i \dot{\boldsymbol{r}}_i^2$$

- summed over all atoms

Molecular Dynamics/Statics Approach

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- ~~summed over all atoms~~

But we won't use this!

Molecular Dynamics/Statics Approach

Method — Part III: Minimizing the potential energy

Main Idea

Monitor variation of potential energy at $0\,\mathrm{K}$: $\Delta E_{\mathrm{pot}}(0\,\mathrm{K}) = W_{\mathrm{pl}}$

Problem

MD Snapshots $\{\boldsymbol{r}_i, \dot{\boldsymbol{r}}_i\}(t)$ are **close** to Static Equilibrium ($\sim 0\,\mathrm{K}$)

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Molecular Statics:

$$E_{\mathrm{pot}}^{\mathrm{min}}(t) = \min_{\boldsymbol{R}=(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)} E_{\mathrm{pot}}(\boldsymbol{R}(t))$$

$$W_{\mathrm{pl}}(t) = E_{\mathrm{pot}}^{\mathrm{min}}(t) - E_{\mathrm{pot}}^{\mathrm{min}}(0)$$

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Advertisement

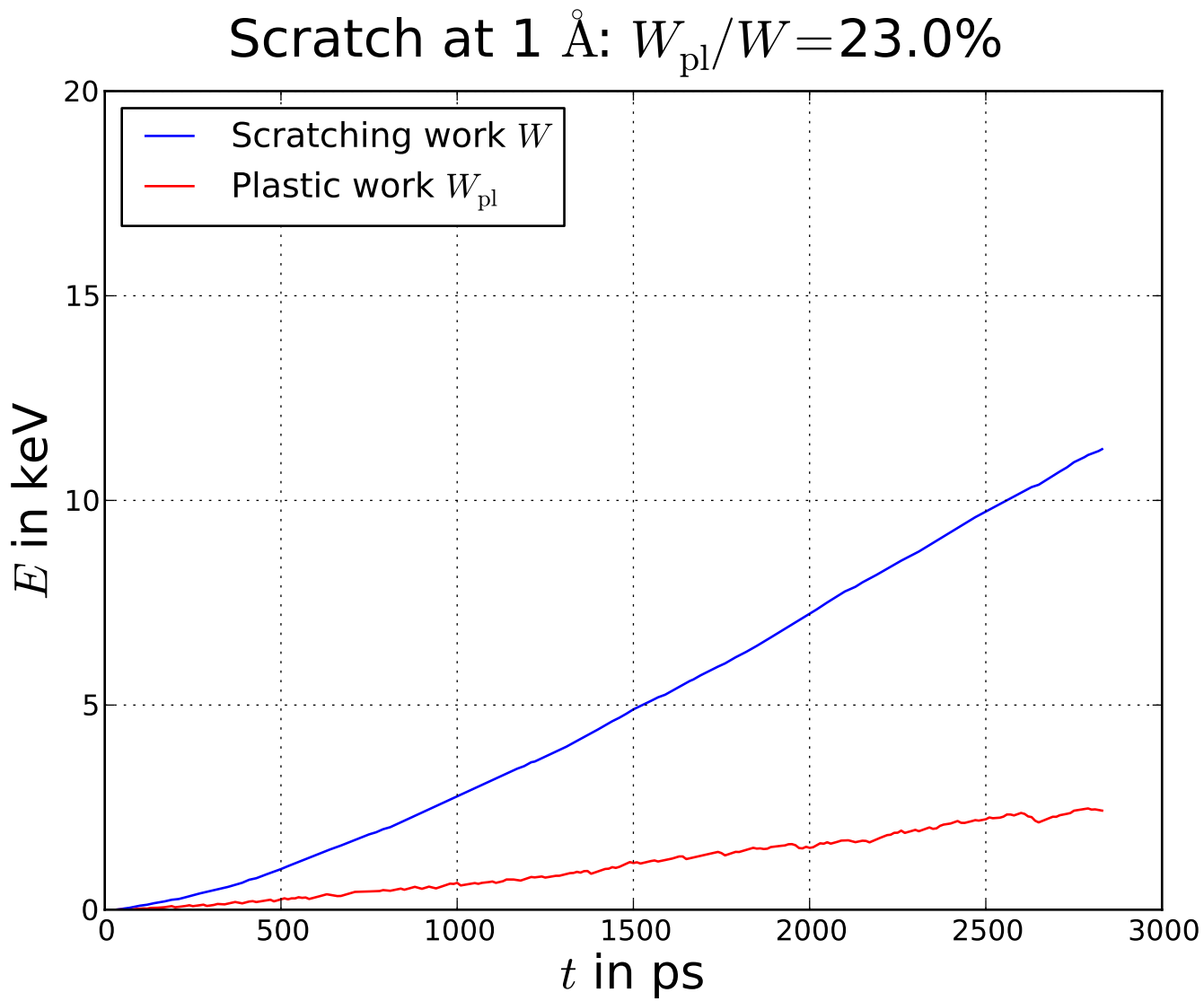
All molecular simulations: modified LAMMPS (**L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator):

Libmultiscale

`lsms.epfl.ch`

Molecular Dynamics/Statics Approach

Preliminary Results — Plastic Energy



Molecular Dynamics/Statics Approach

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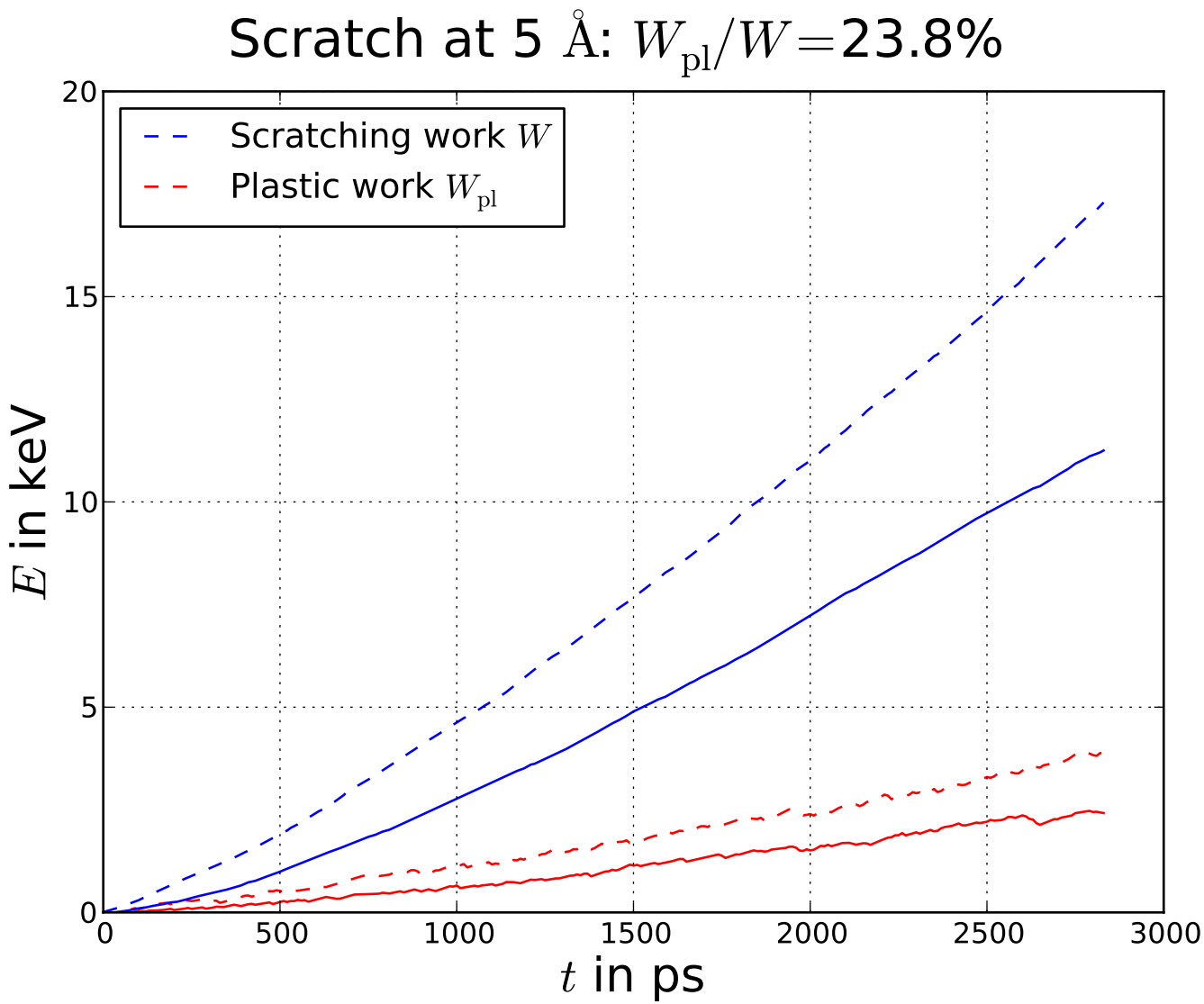
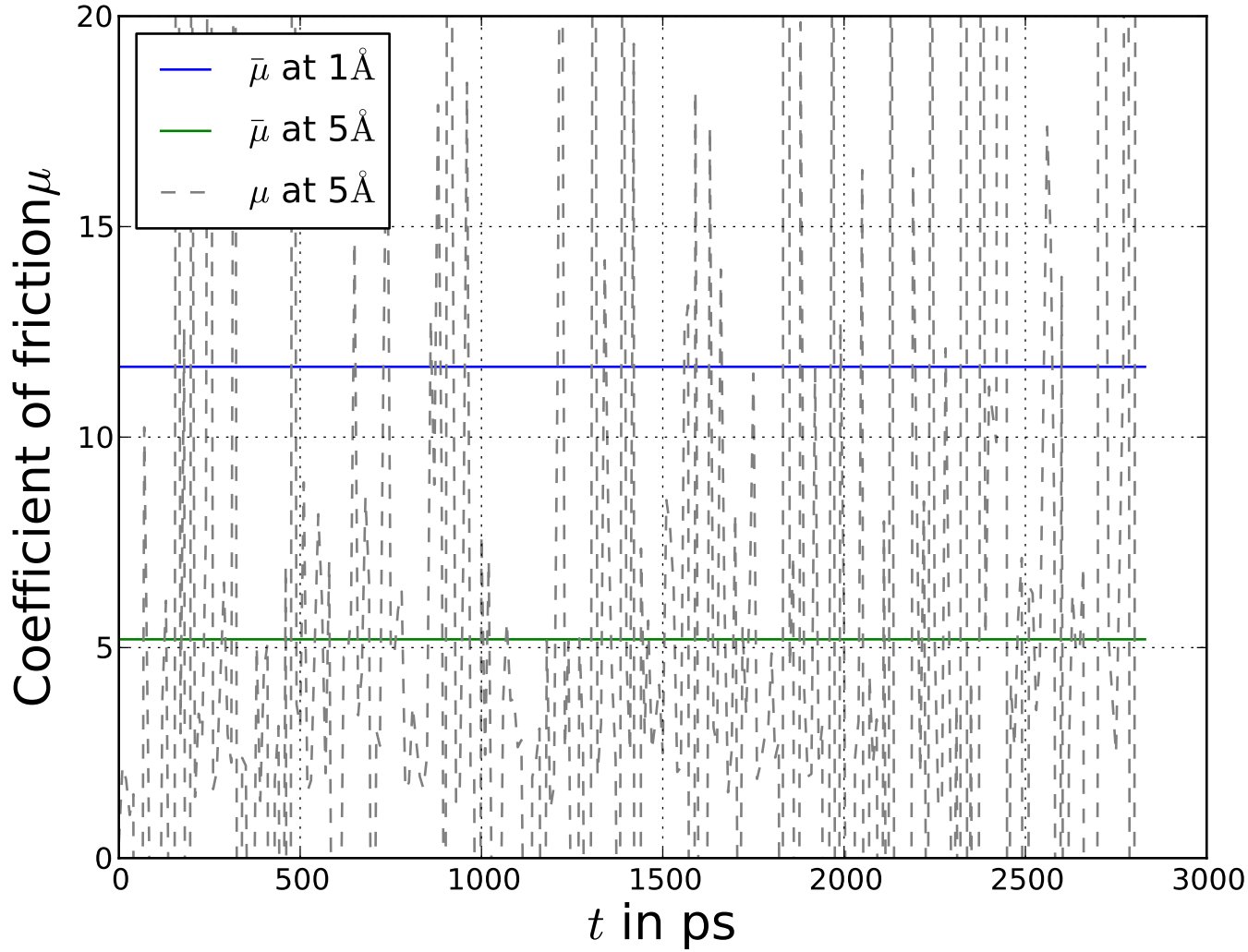


Molecular Dynamics/Statics Approach

Preliminary Results — Friction Coefficient

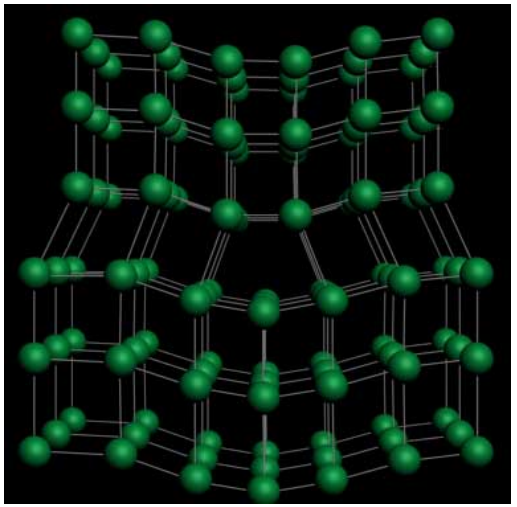


Molecular Dynamics/Statics Approach

Interlude - Preliminary Results — Dislocations

Dislocation: the "unit" of crystal plasticity

Luan and Robbins [Tribology Letters, 2009]:
$W_{\mathrm{pl}} \sim$ Count plastic events

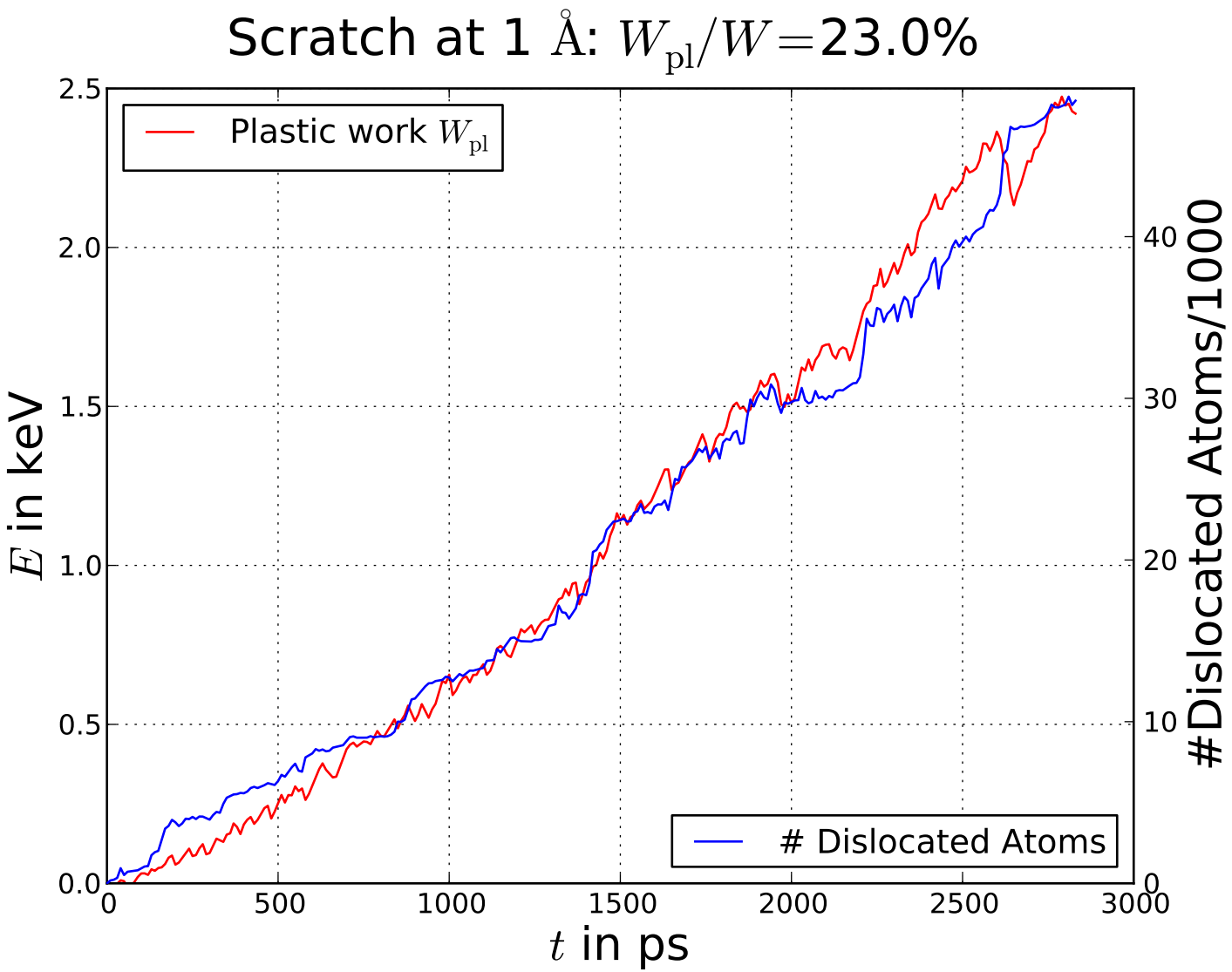


Test

1. Count #atoms N which changed nearest neighbours
2. Plot $N(t)$ over $W_{\mathrm{pl}}(t)$

Molecular Dynamics/Statics Approach

Preliminary Results



Molecular Dynamics/Statics Approach

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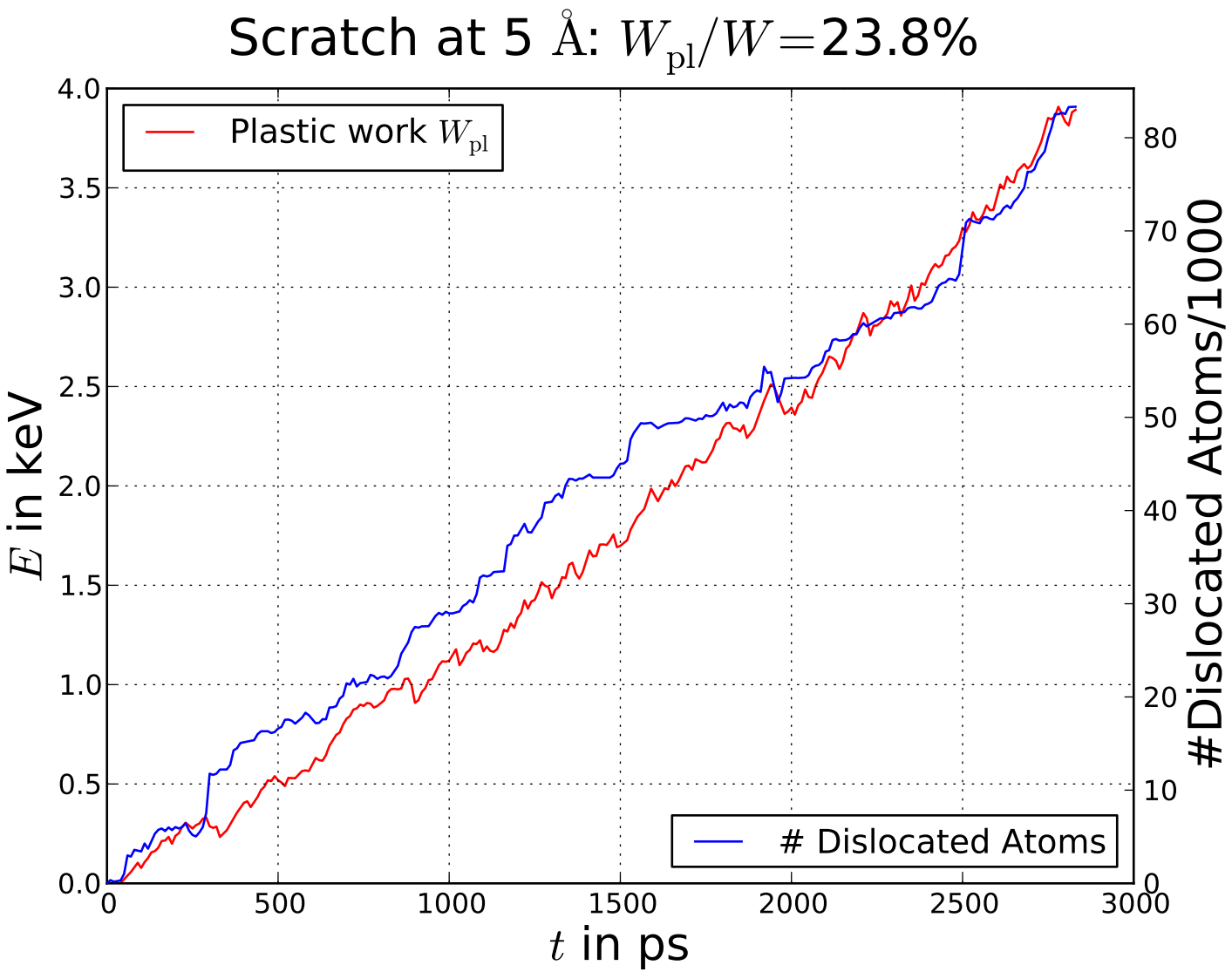

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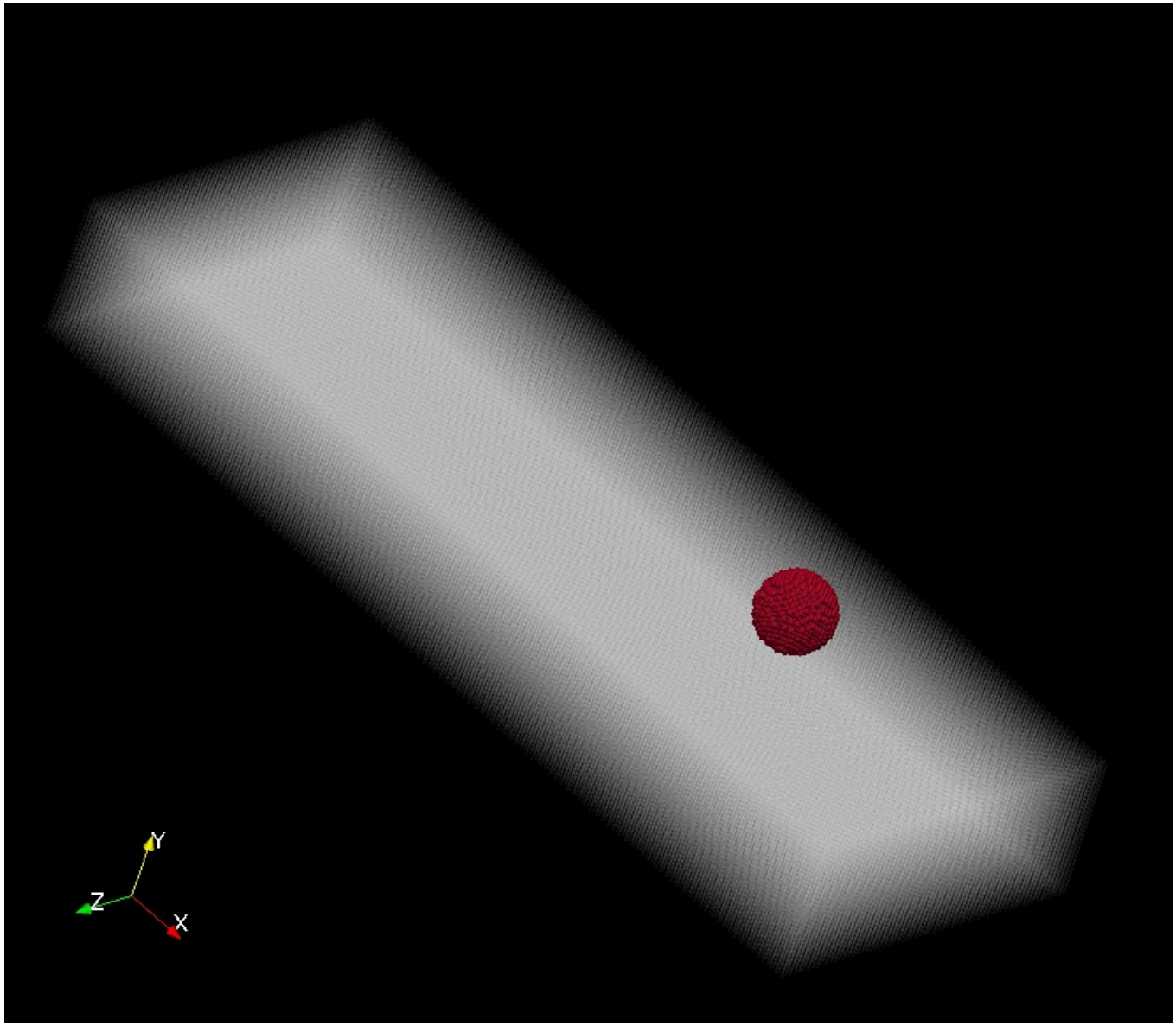
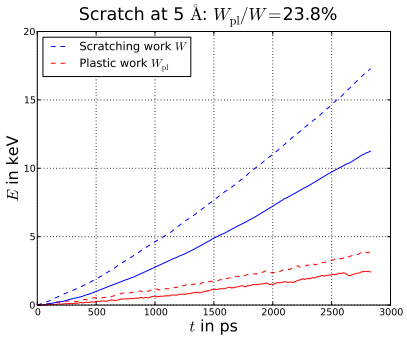


Molecular Dynamics/Statics Approach

PAUSE

- **Method**
  Allows to **quantify** W_{pl} for a special case



Molecular Dynamics/Statics Approach

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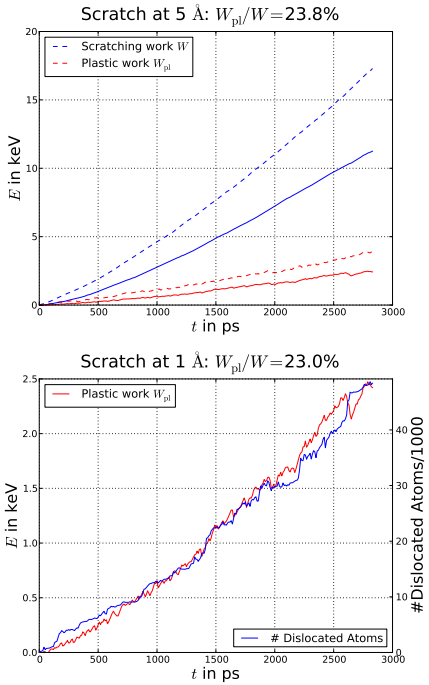
- **Results**
  Physically **intuitive**



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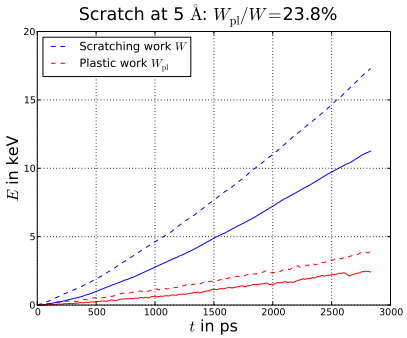
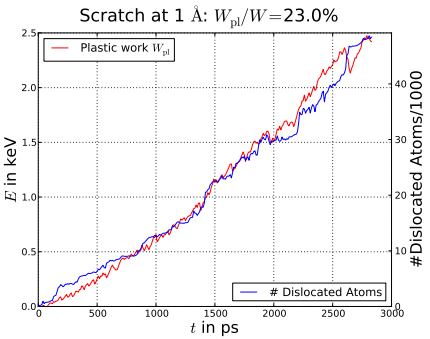
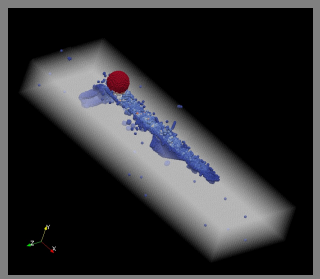






- **But**
  Simulations are too small!

Conclusions

- **The method is functional**
  It allows a clean separation between plastic and kinetic energy.

- **Dislocations get trapped at the sim box boundary**
  Inherent problem of Molecular Simulations

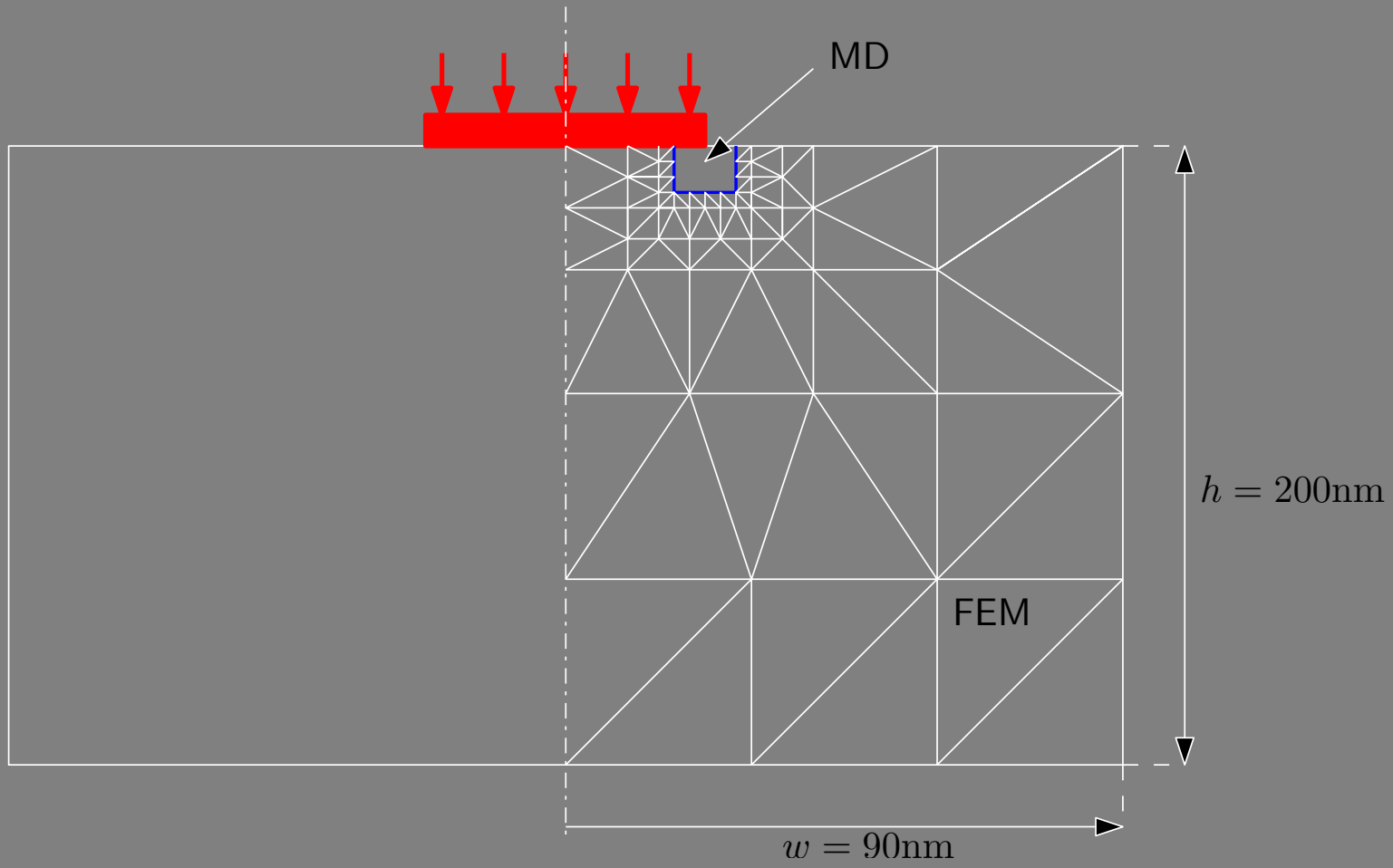
- **Limited to $\sim 0\,\mathrm{K}$ simulations**
  Thermal expansion prohibits mixed use of Molecular Dynamics **and** Statics

Outline

Extension to larger Systems

CADD

Coupled Atomistics and Discrete Dislocations



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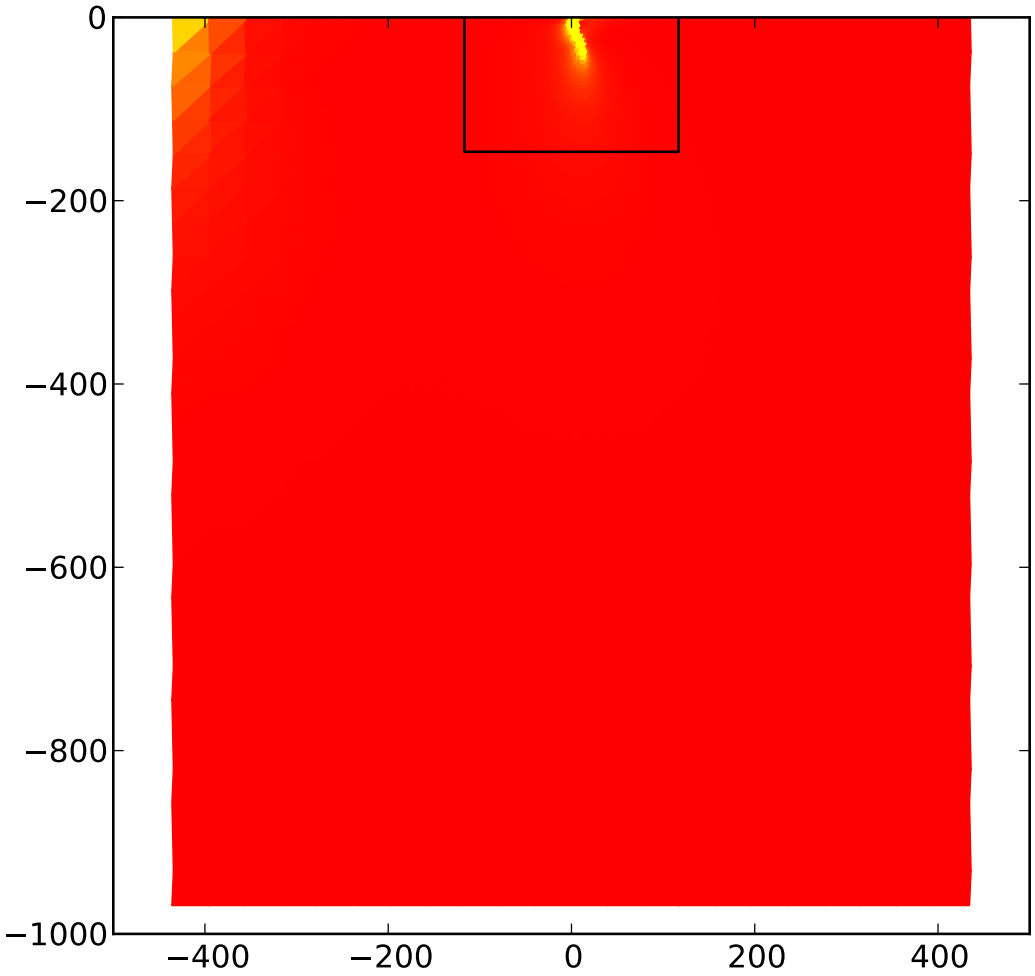

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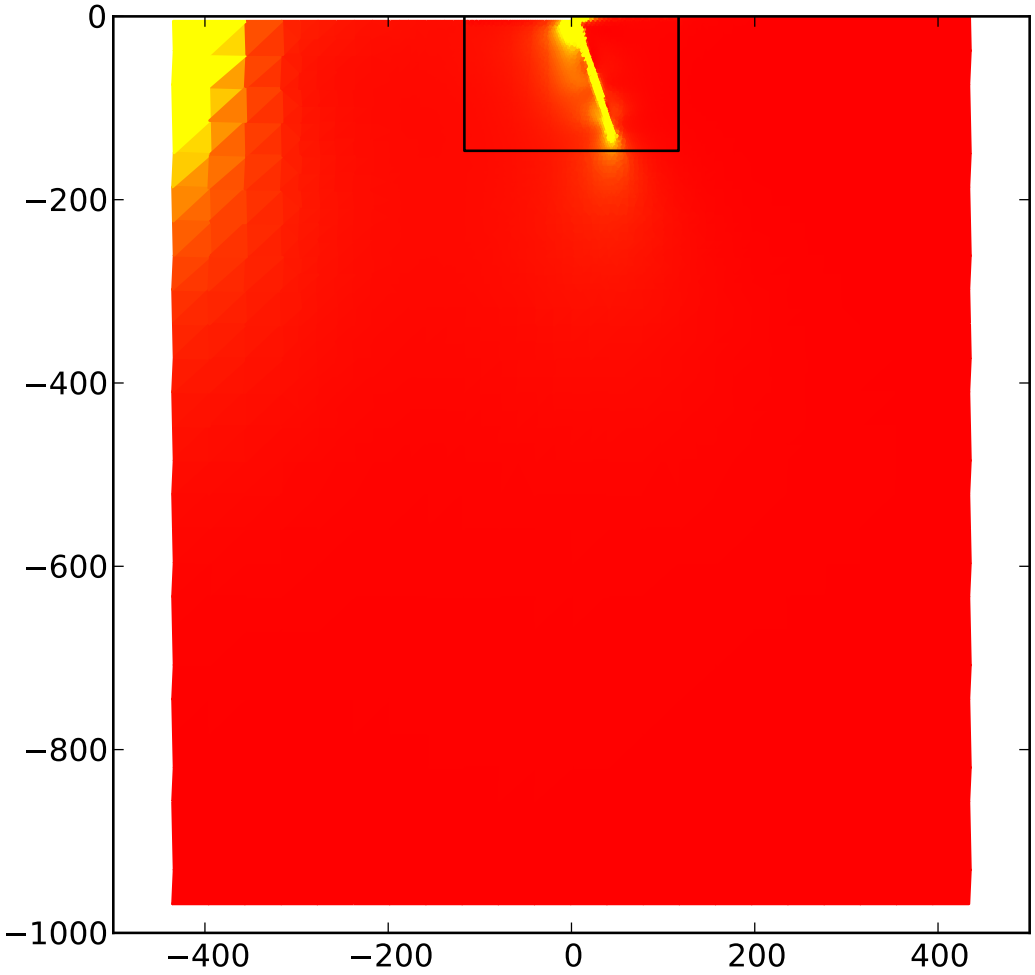

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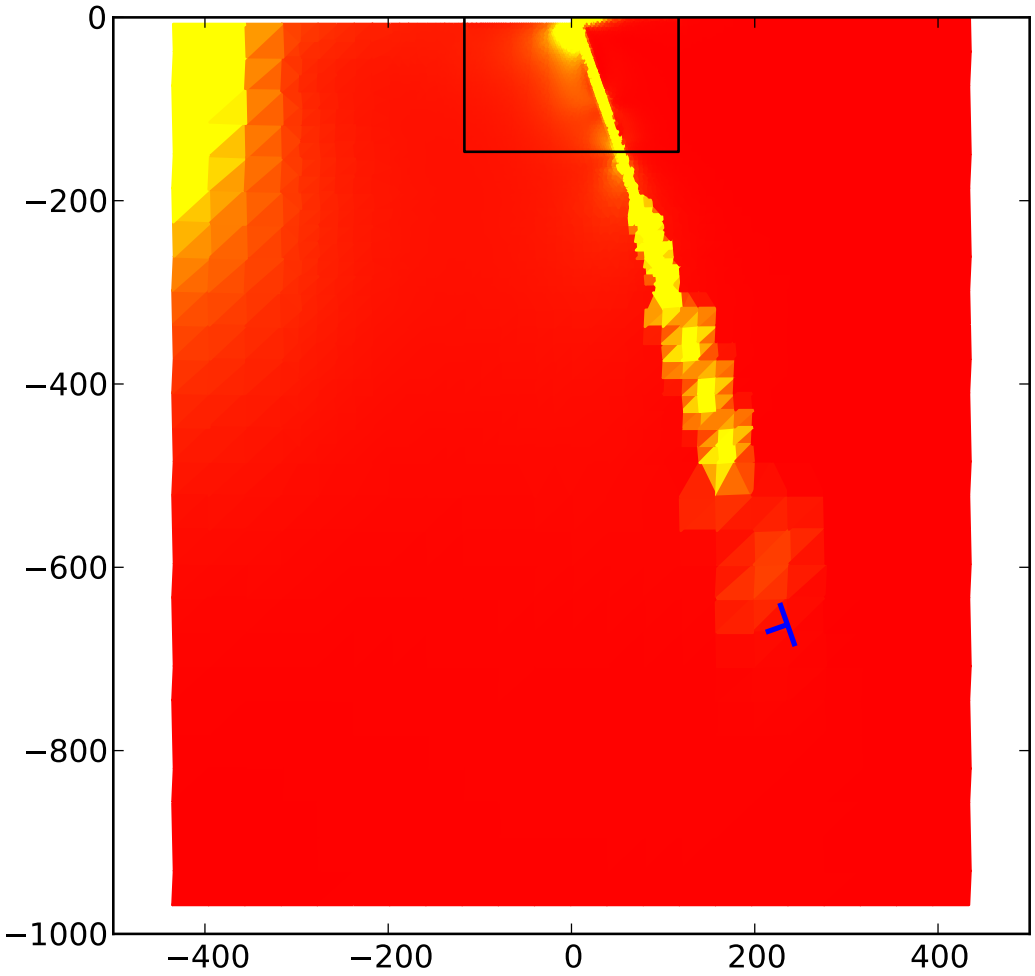
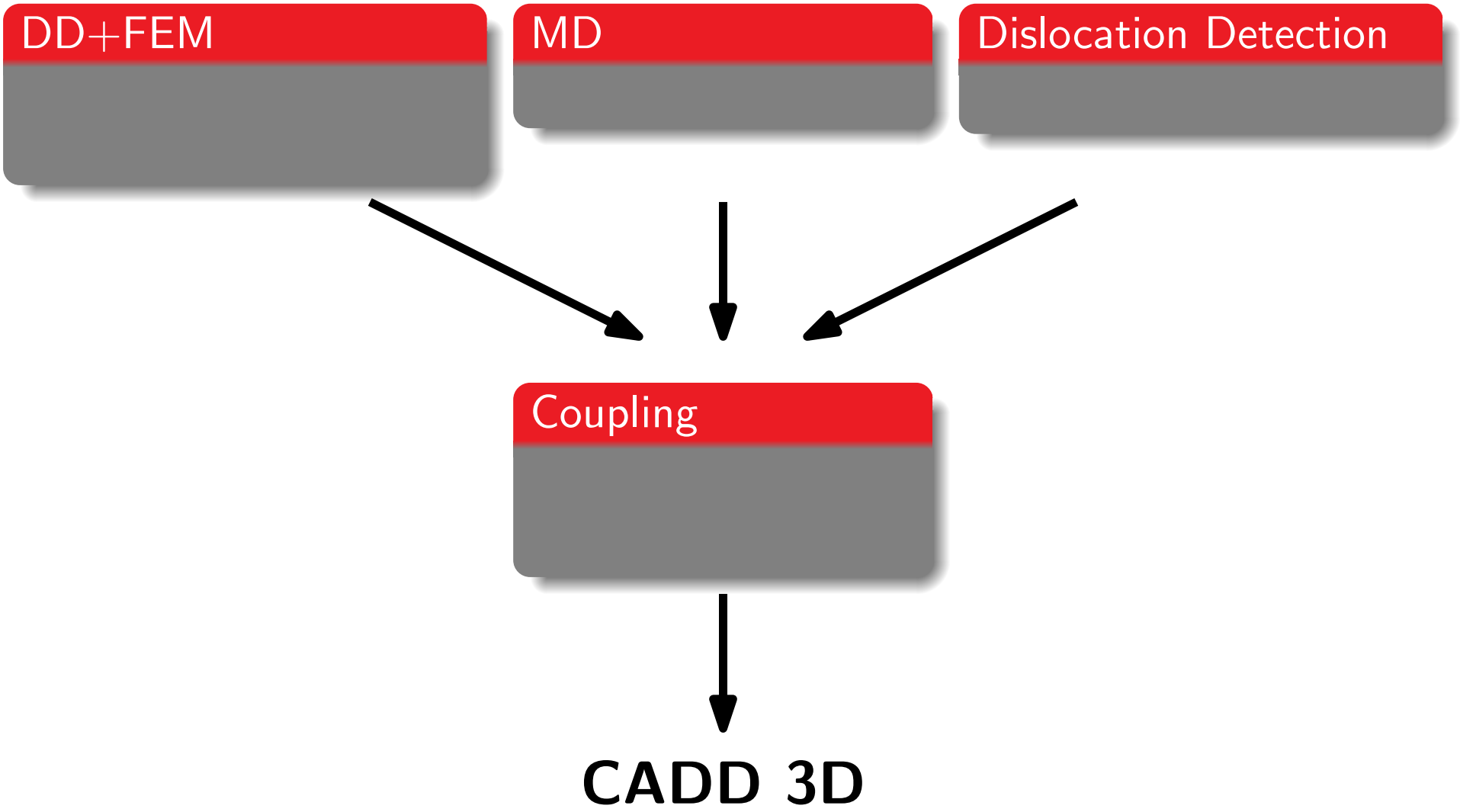


Extension to larger Systems

Requirements for CADD 3D



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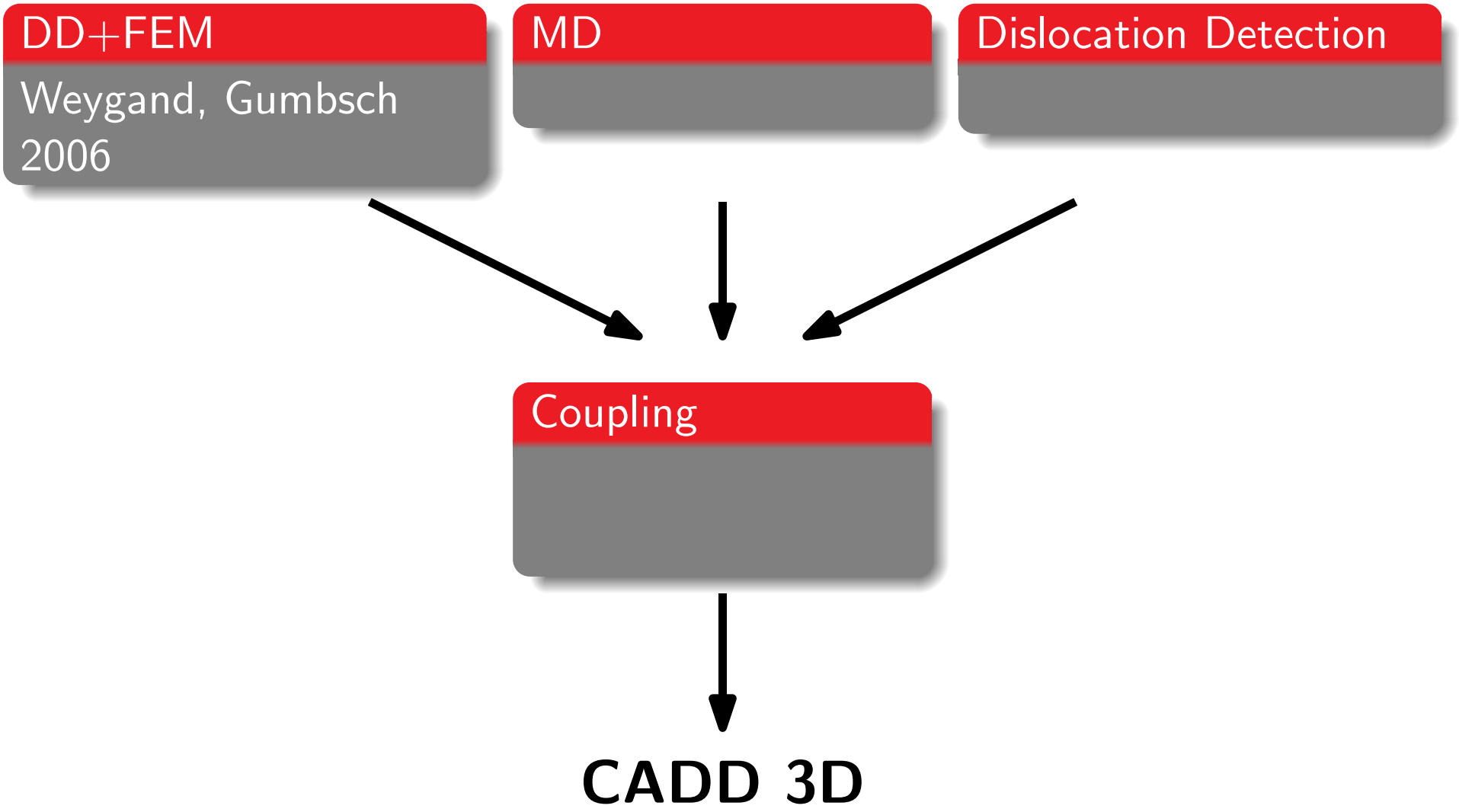

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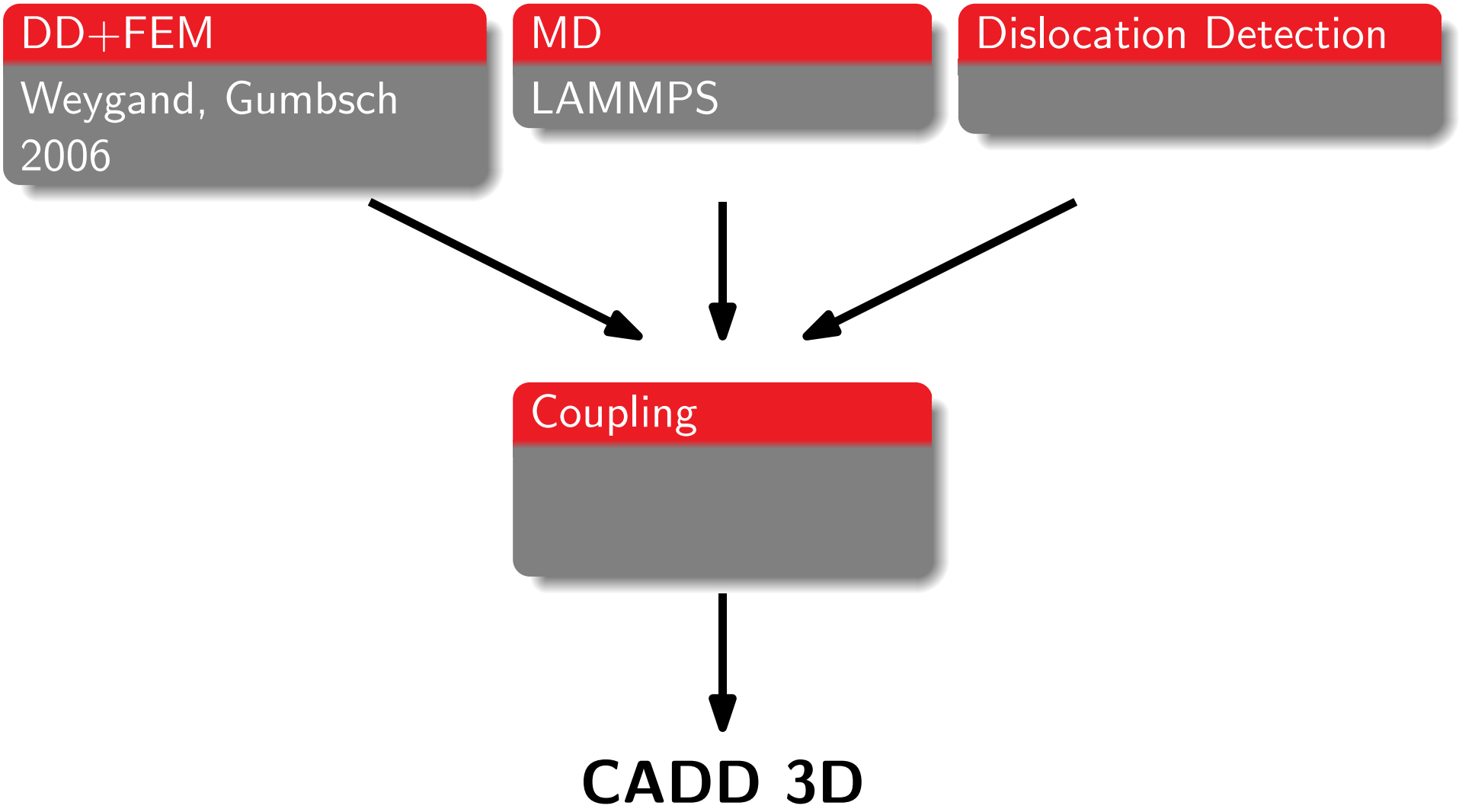

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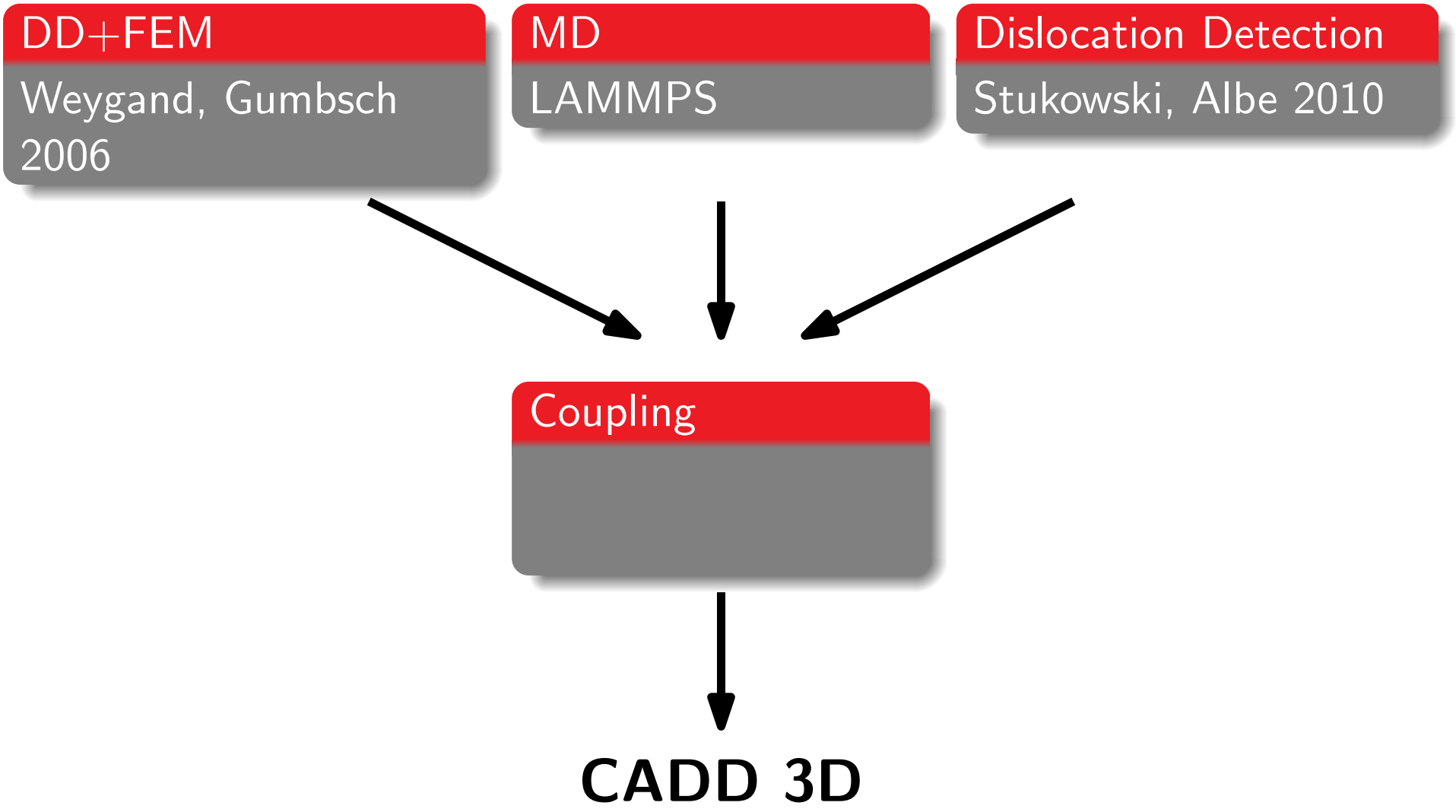

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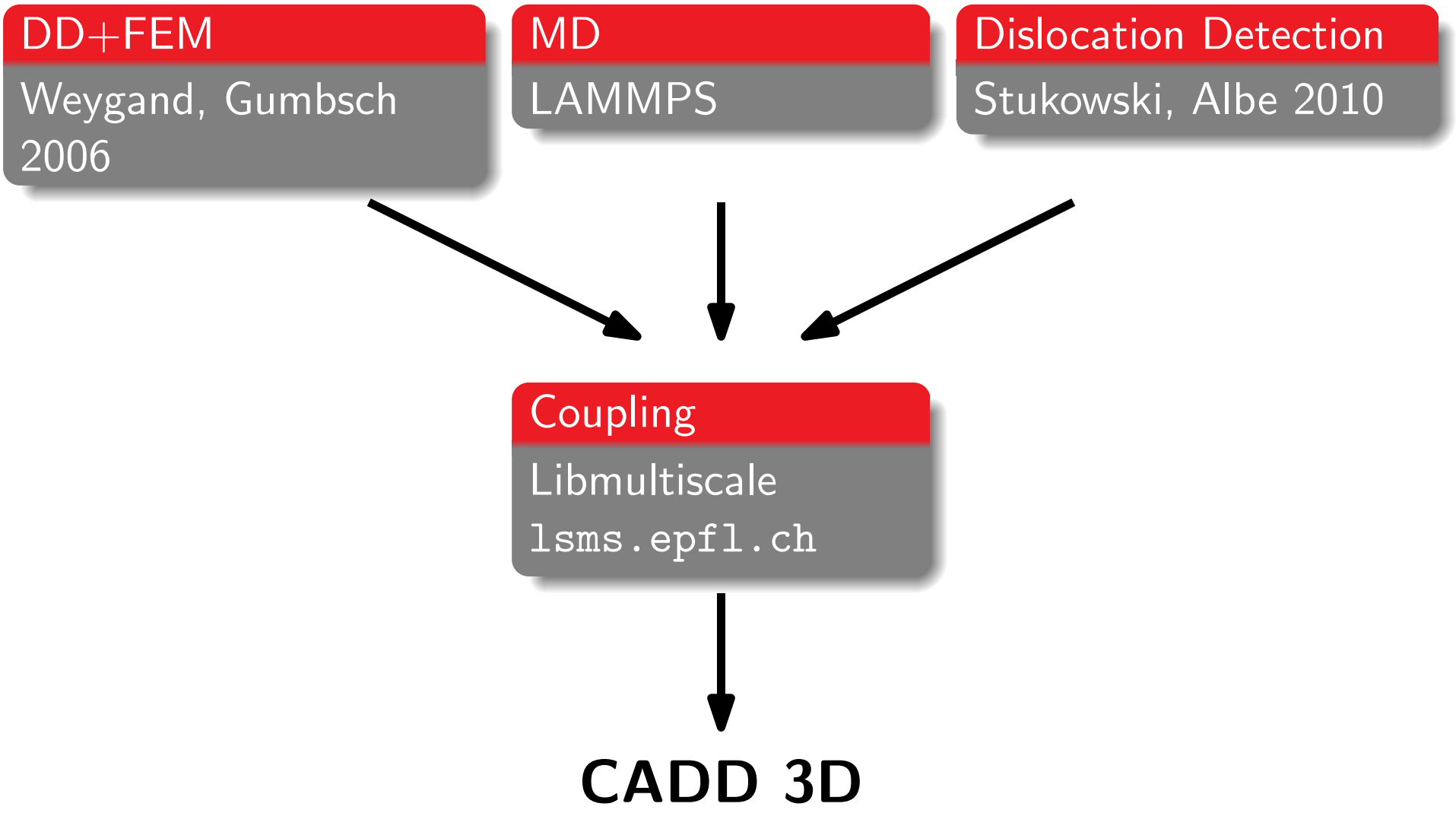
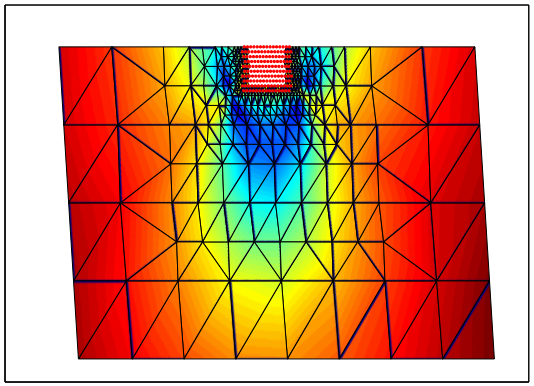


Extension to larger Systems

Outlook

- **Couple MD to FEM/DD to avoid dislocation trapping**
  Requires 3D CADD [Curtin et al. JMPS 2008]



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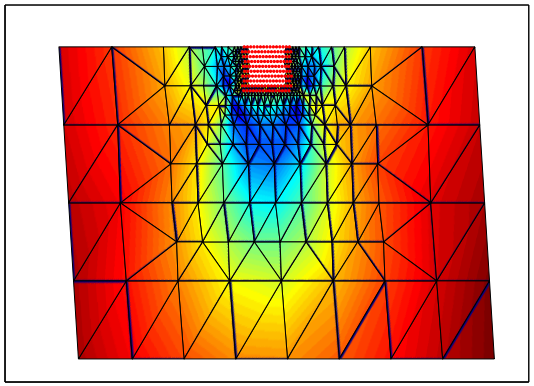
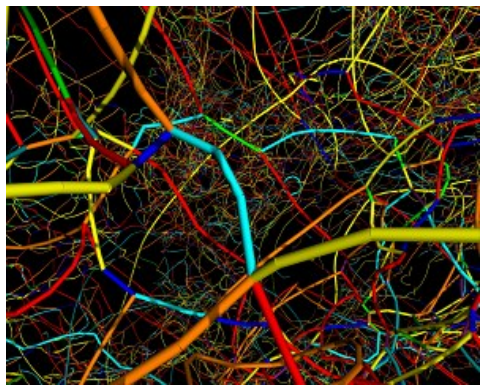


- **Extension to finite T by computing dislocation self-energy**
  Requires finding dislocation loops



Source: ParaDiS