Multiscale modelling

PGP internal seminar · 17 October 2006

Håkon Enger

Multiscale modelling

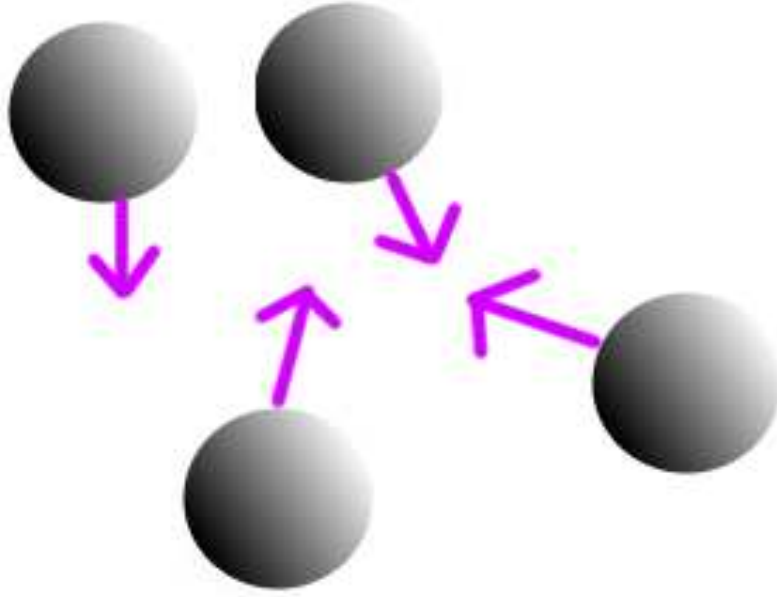
Outline

- What is multiscale modelling?
- Why multiscale modelling?
- Challenges
- Different approaches
- Our approach

What is multiscale modelling?

- Coupling of computer models for different (length) scales
- In our case: Coupling of *molecular dynamics* (particle modelling) with *continuum* (finite difference/element/volume) model

Molecular dynamics



Molecular dynamics

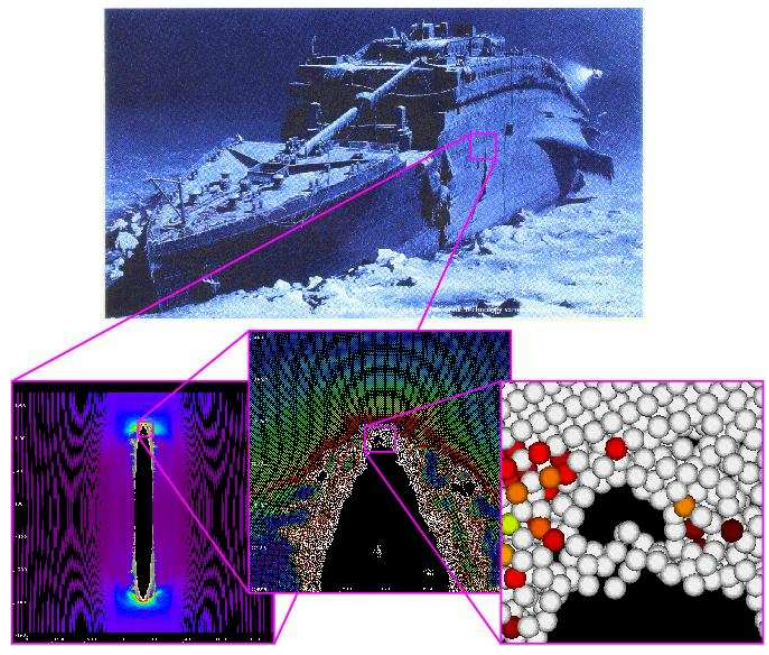
(Andrea Delapaz, Gelb Research Group at Washington University in St. Louis

http://www.chemistry.wustl.edu/∼gelb/gchem/materials/lve/

Why multiscale modelling?

Many phenomena are dependent on microscopic structure, e.g.,

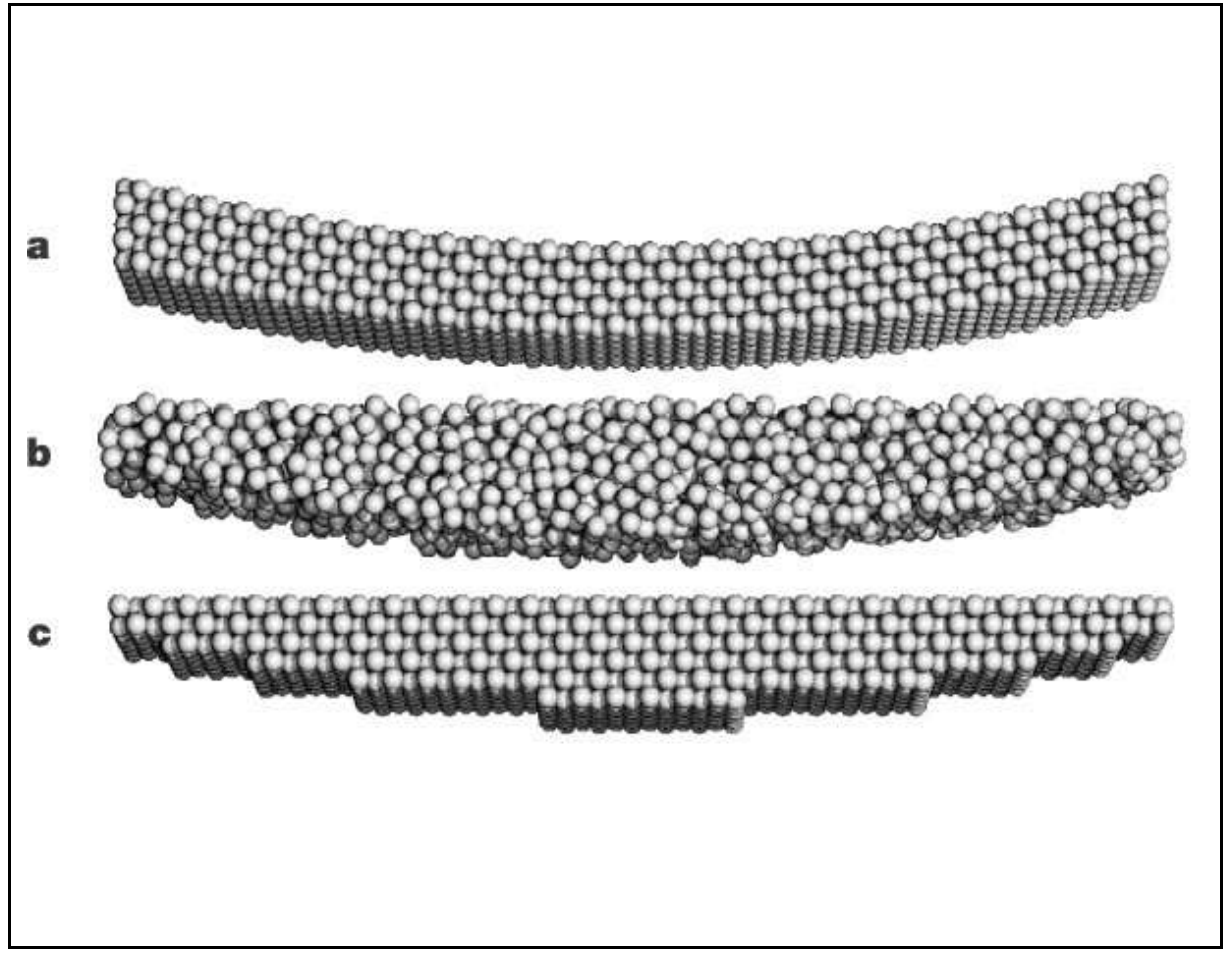
- Friction
- Adhesion
- Fluid flow
- Fractures



Ellad B. Tadmor

http://tx.technion.ac.il/∼tadmor/MMM/

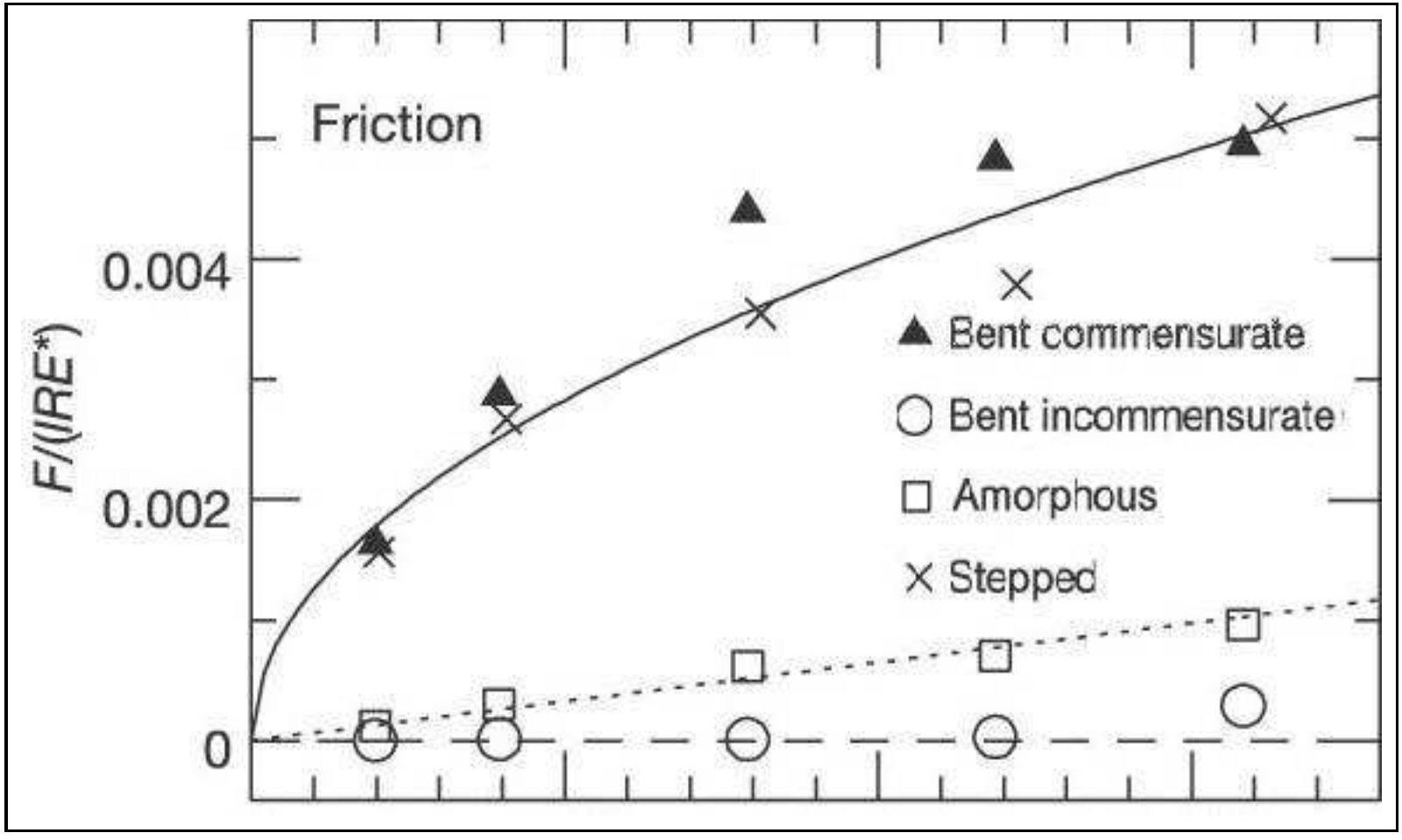
Friction and adhesion



Luan and Robbins: Nature **435** (2005), 929

- Friction and adhesion depends on atomic structure

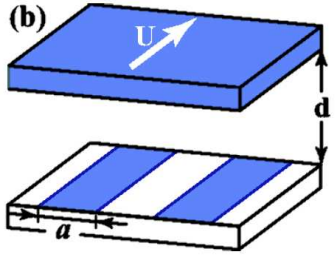
Friction and adhesion

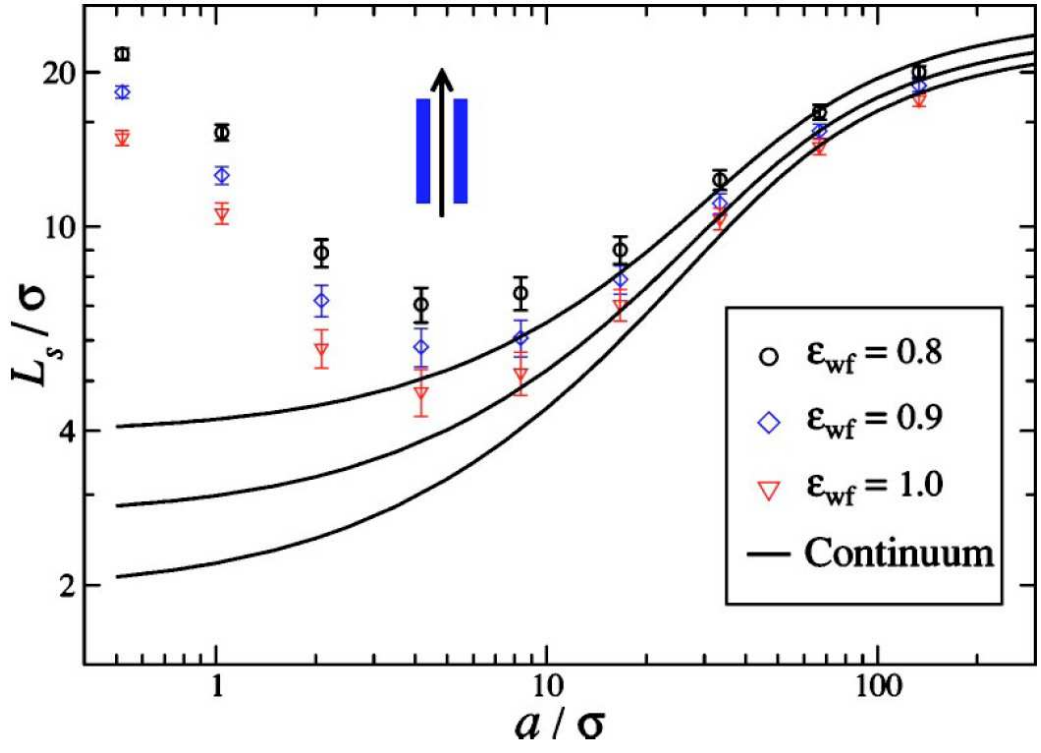


Luan and Robbins: Nature **435** (2005), 929

- Friction and adhesion depends on atomic structure

Fluid Flow





Priezjev et al: Phys. Rev. E **71** (2005), 041608

- Effective slip length not predicted by continuum model

Fractures

L. Hua, H. Rafii-Tabar and M. Cross, Phil. Mag. Lett. **75** (1997), 237

(University of Greenwich Nano-Science Research group, http://www.gre.ac.uk/∼rh01/)

- Continuum models do not correctly model speed of fracturing and roughness of crack

Why not microscale only?

Large molecular dynamics simulation:
1 billion particles

- Current computers not fast enough for sensible size and timescale of simulated systems
- . . . and will not become fast enough for the forseeable future

Image from Technology@Intel Magazine
http://www.intel.com/technology/magazine/computing/HPC-cluster-1205.htm

Challenges

- Different view

• Density • Average velocity • Temperature	• Particle positions • Particle velocities • Forces

- Fluctuations
  - To go from **P** to **C**, we can average
  - But, from **C** to **P** we must *introduce* fluctuations
  - Must be done in “physically correct” way
- Continuity – seamless coupling
  - Molecular dynamics equations must give the continuum equations when averaging
  - Must find correct constitutive equations

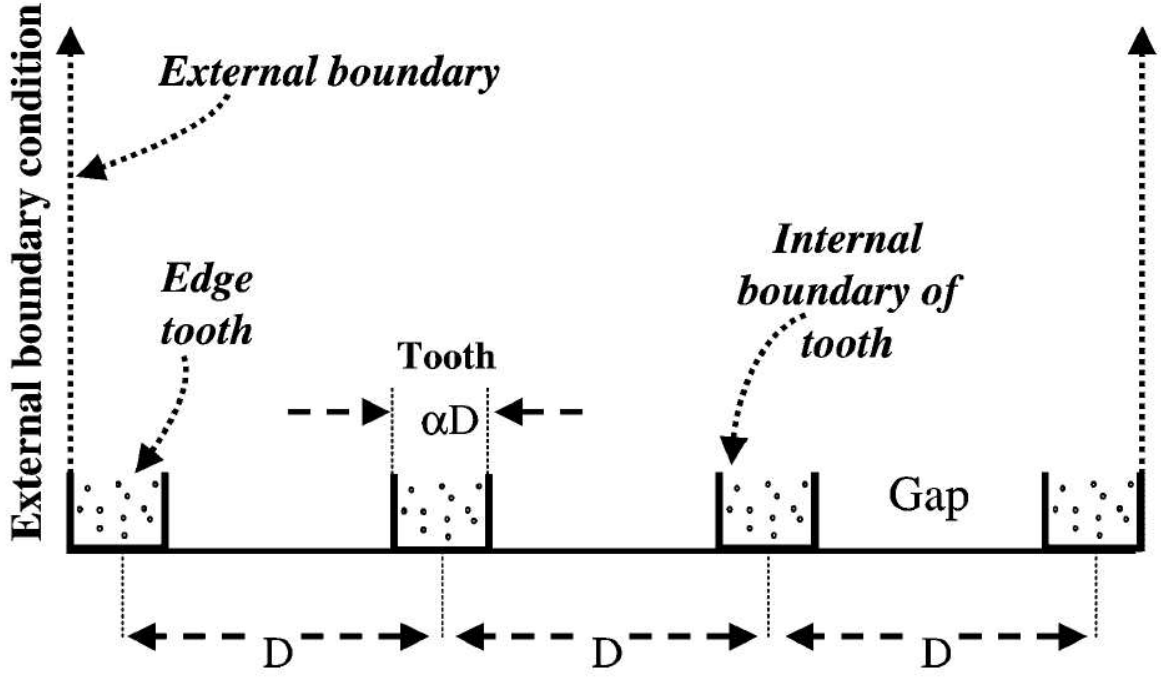
Different approaches

- W. E, B. Engquist (Princeton)
  - Using molecular model to find constitutive equations

  - Main model: Continuum
    1. Stop continuum model
    2. Use molecular model to find viscosity, etc.
    3. Restart continuum model

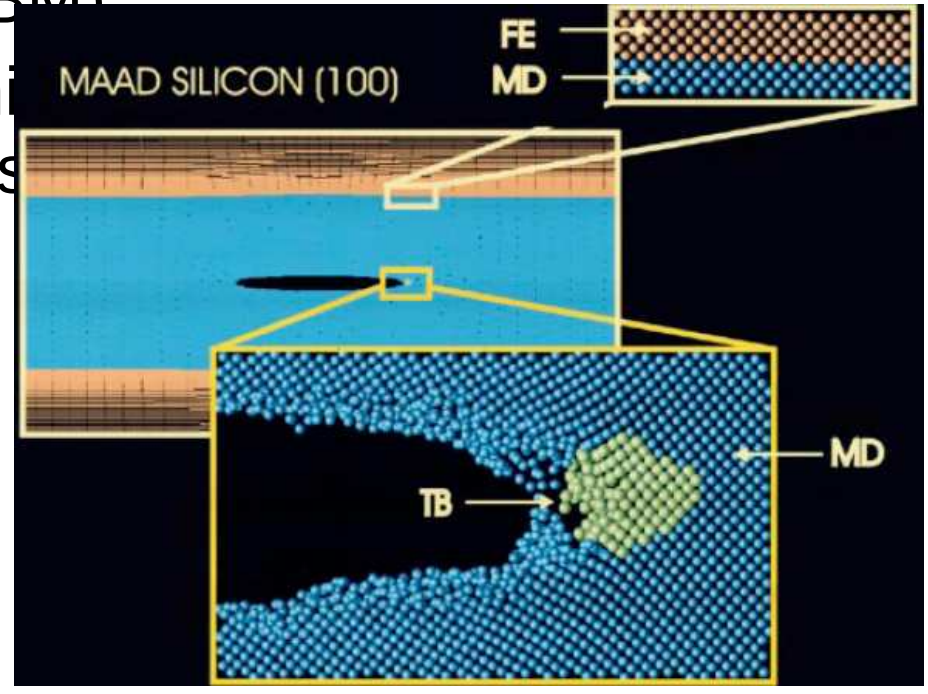
Different approaches

- W. E, B. Engquist (Princeton)
  - Using molecular model to find constitutive equations
- I. G. Kevrekidis et. al. (Princeton) - “gap-tooth”
  - “Equation-free” coupling of “teeth” with microscopic model



Different approaches

- W. E, B. Engquist (Princeton)
  - Using molecular model to find constitutive equations
- I. G. Kevrekidis et. al. (Princeton) - “gap-tooth”
  - “Equation-free” coupling of “teeth” with microscopic model
- F. F. Abraham et. al. (IBM)
  - MAAD: Macro Atomi
    - Solids (silicon crys

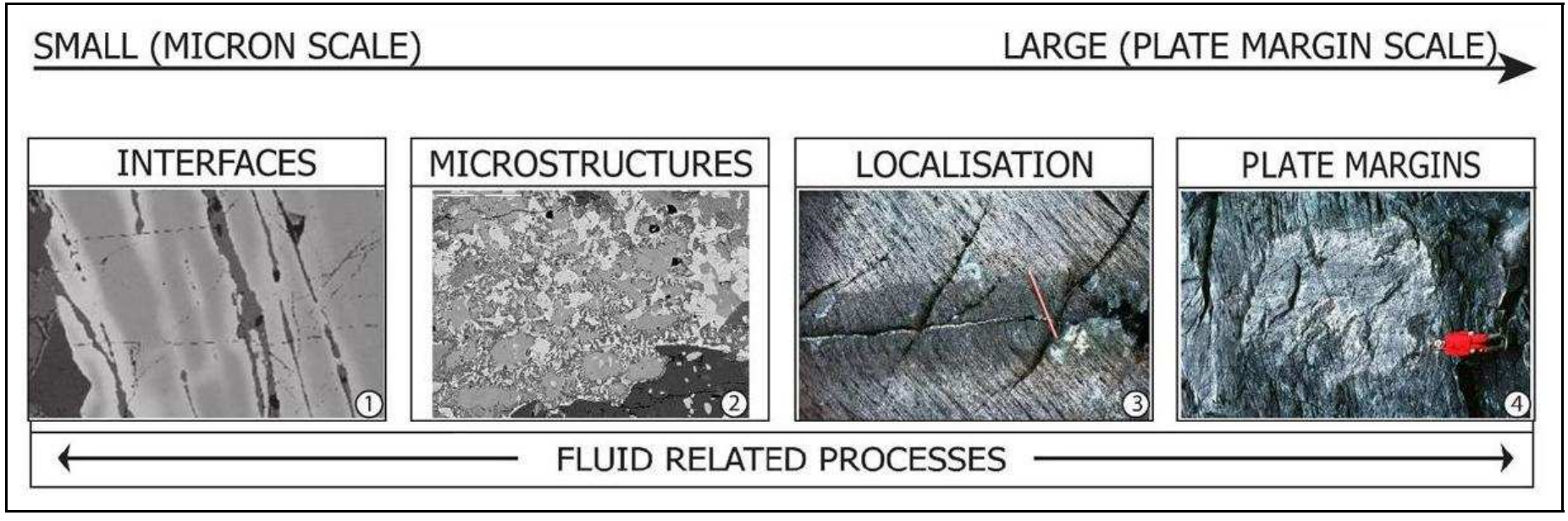


Different approaches

- W. E, B. Engquist (Princeton)
  - Using molecular model to find constitutive equations
- I. G. Kevrekidis et. al. (Princeton) - “gap-tooth”
  - “Equation-free” coupling of “teeth” with microscopic model
- F. F. Abraham et. al. (IBM)
  - MAAD: Macro Atomistic Ad initio Dynamics
    - Solids (silicon crystal) – fractures
- Flekkøy, Feder, et. al. (UiO)
  - Flux-based (i.e., conservative) coupling

Our approach

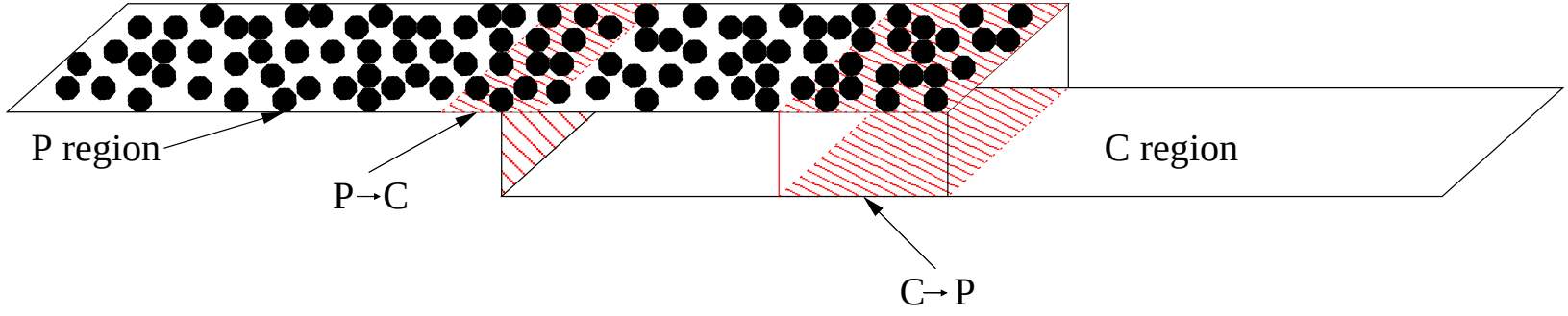
- Coupling must be physically correct
- Coupling must be conservative, flux-based
- Long term goal: General algorithm
- Short term goal: Focus on applications



Progress so far

To test various schemes for coupling, we decided to write from scratch a simple molecular dynamics code and finite difference (Navier-Stokes and solid) solvers.
In the future, we plan to use the best coupling scheme with publicly available MD and FD/FE solvers.

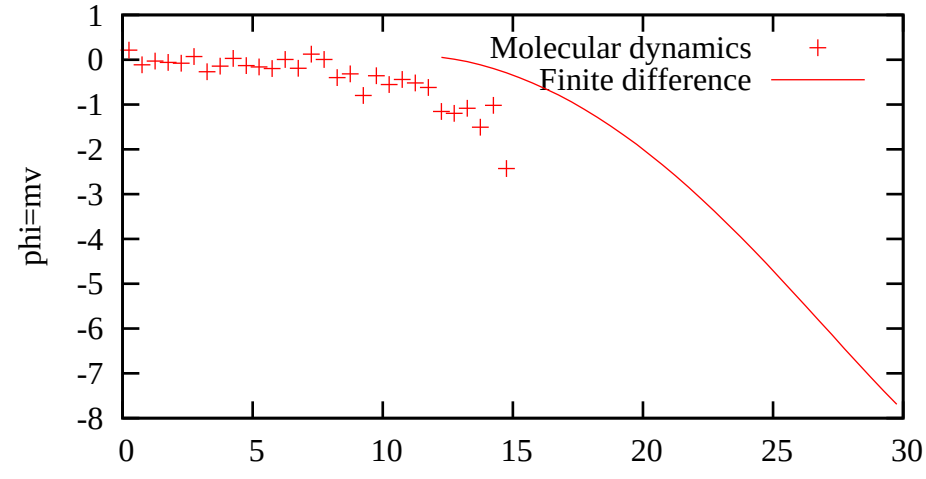
- Molecular dynamics code: Done
- Fluid coupling: In progress

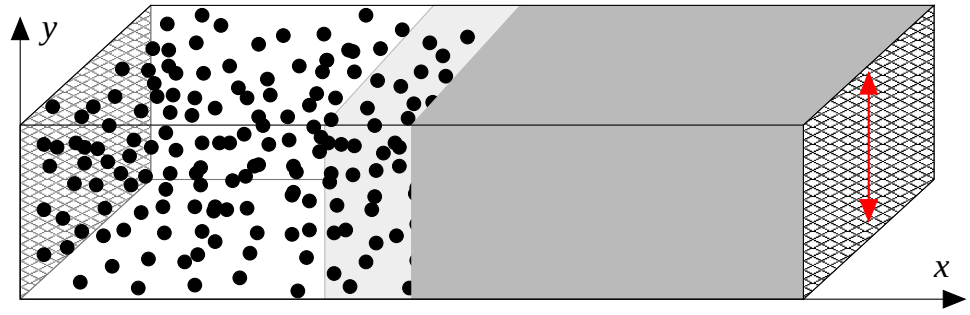


- Solid coupling: Just started

Problems so far

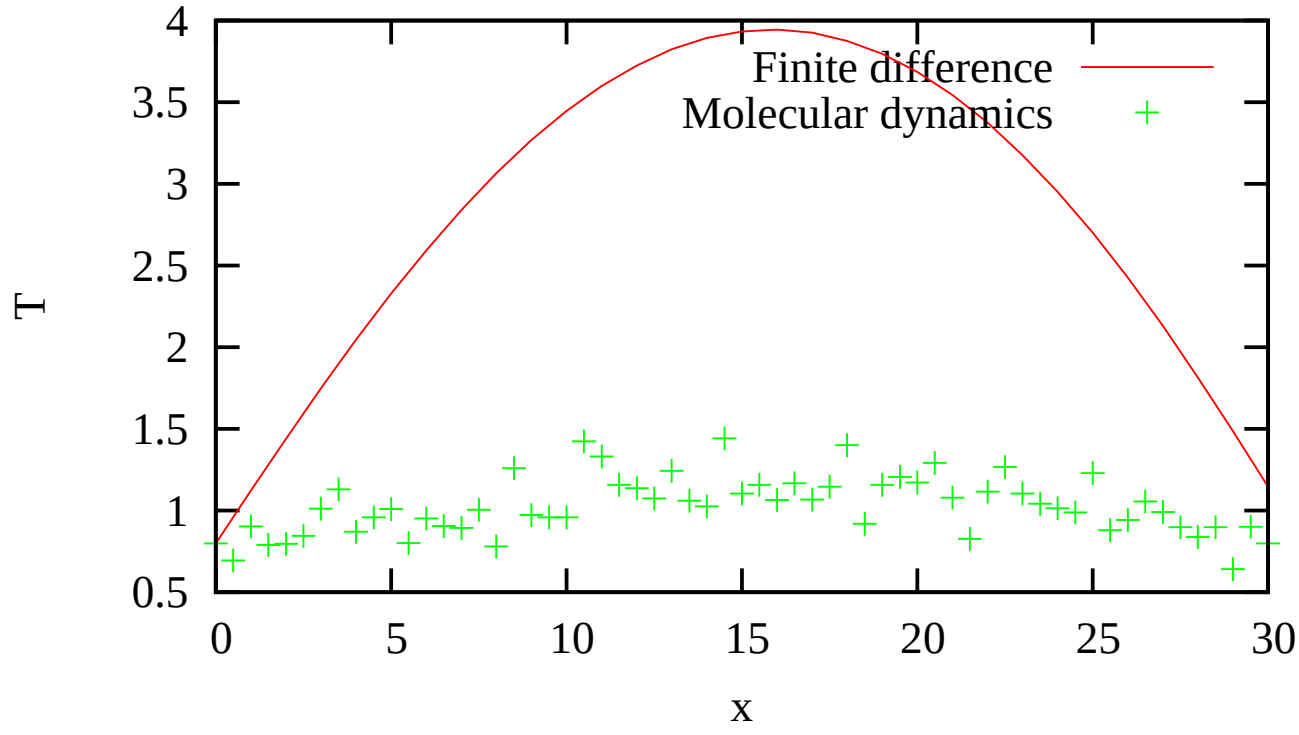
- Flux-based coupling gives non-continous fields on interface





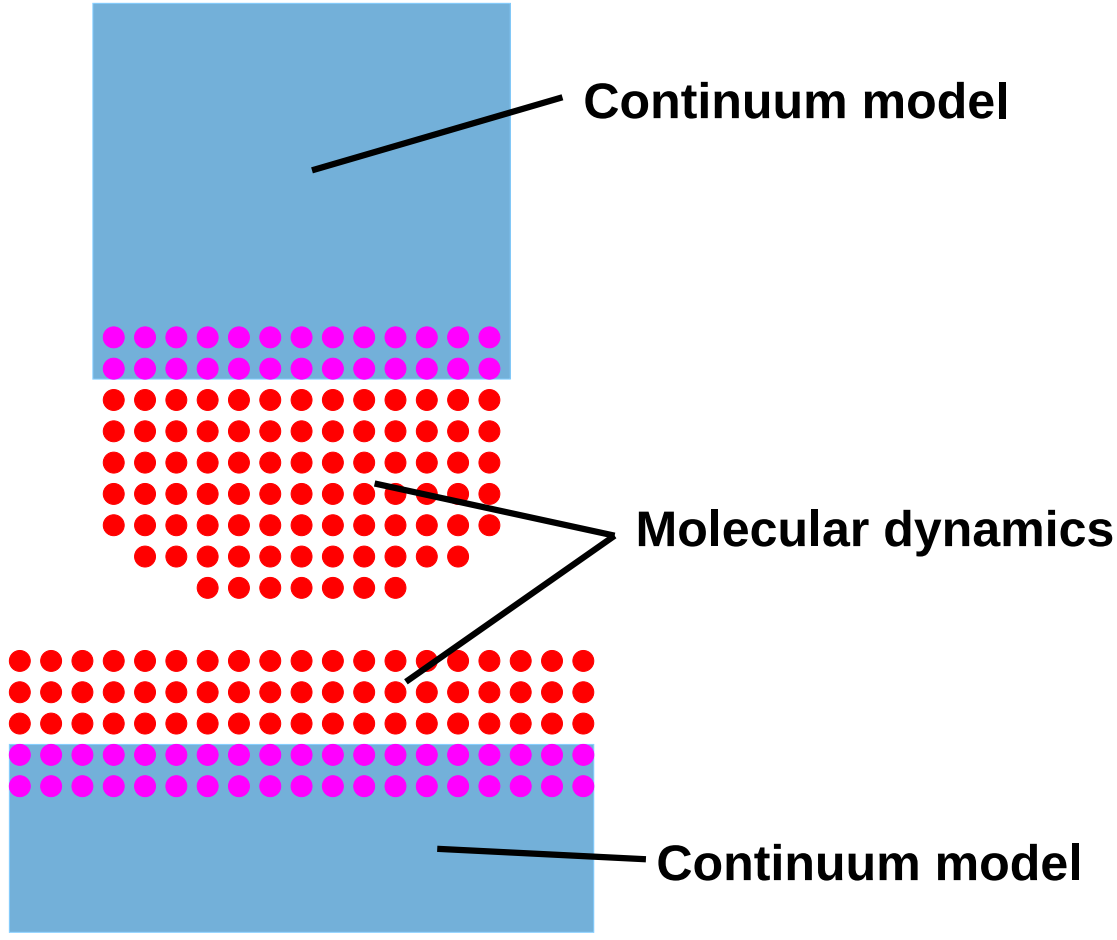
Problems so far

- Constitutive equations must match molecular dynamics



Plan

- Focus on easier case of adhesion first



Summary

- Multiscale modelling: An active field of research
- Important tool to study phenomena like
  - Friction
  - Adhesion
  - Fluid flow
  - Fractures
- Important to get coupling “physically correct”
- Our goal is a general coupling algorithm
- Short-term plan is to focus on adhesion