

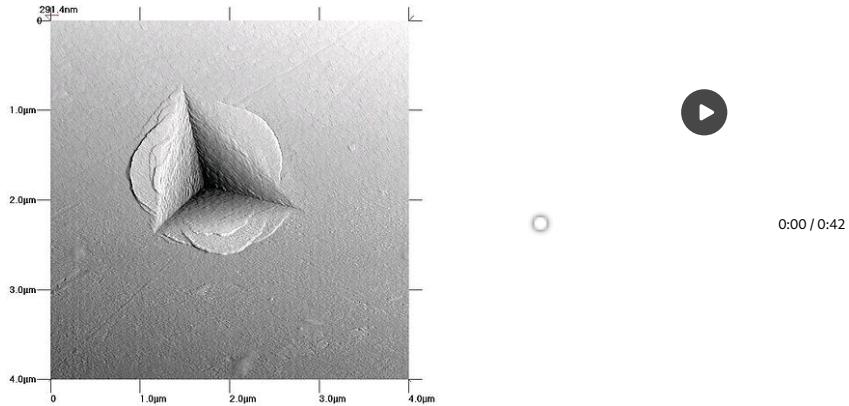
# **Multiscale simulation of solids by coupling finite elements with discrete models**

**Guillaume Anciaux**

**EPFL**

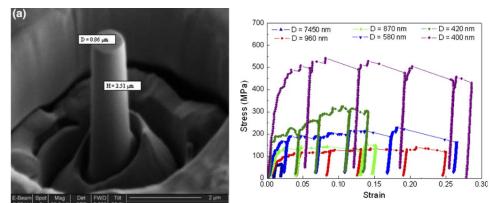
# Motivation

## Nano indentation



## Nano pillars

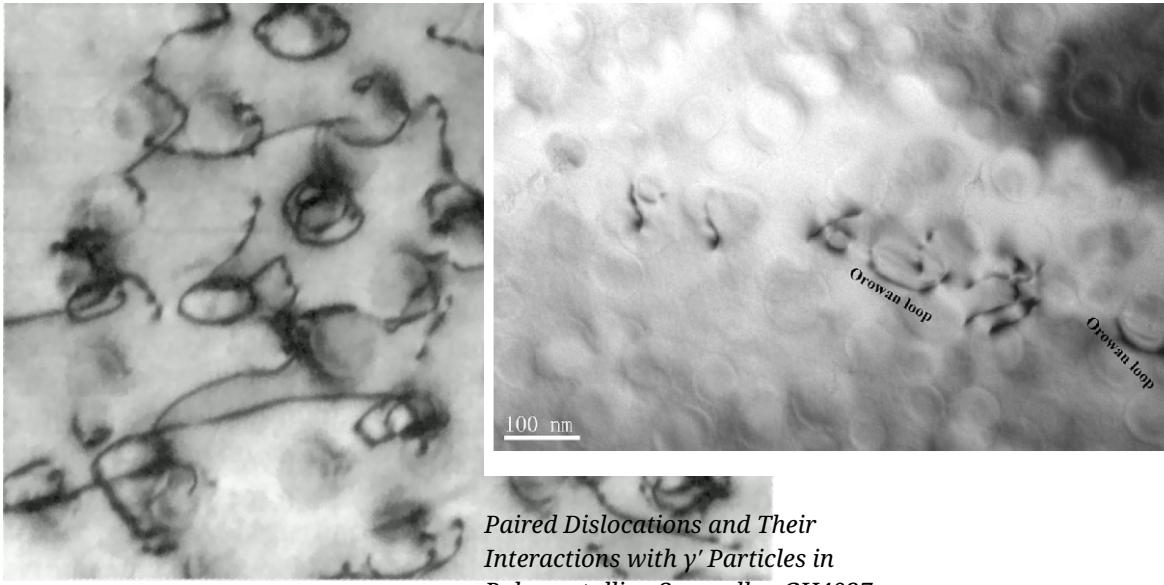
### Plasticity study



Jang et. al. Scripta Materialia (2011)

## Precipitation hardening

### Alloys engineering

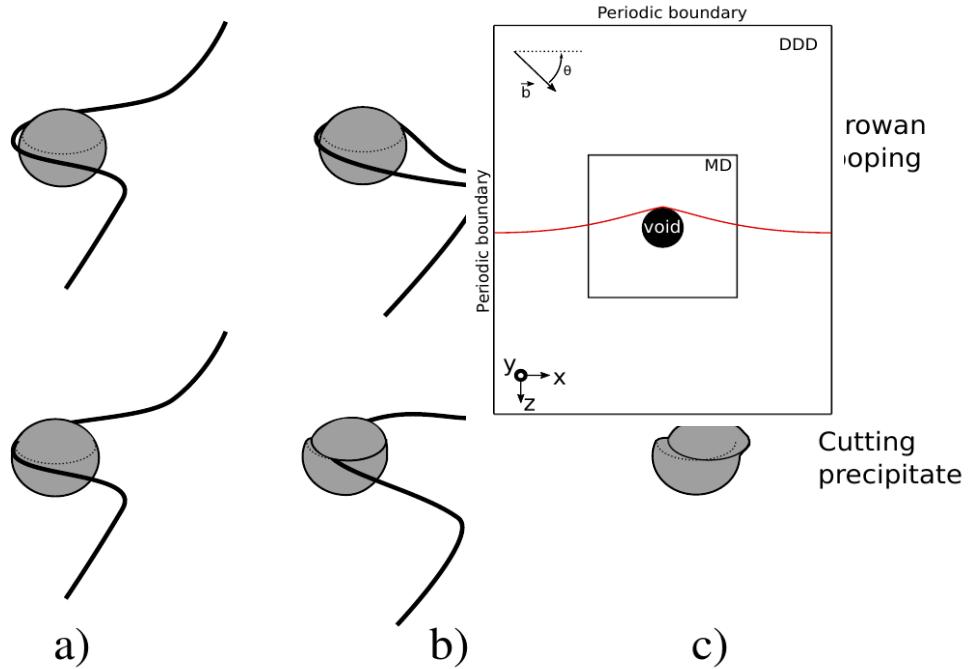


*Dislocation rings upon bow-out of Ni<sub>3</sub>Si particles in NiSi alloy*

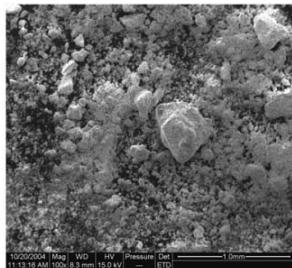
*Paired Dislocations and Their Interactions with γ' Particles in Polycrystalline Superalloy GH4037*

Xianzi Lv et al.

[https://www.giessereilexikon.com  
/en/foundry-lexicon/](https://www.giessereilexikon.com/en/foundry-lexicon/)

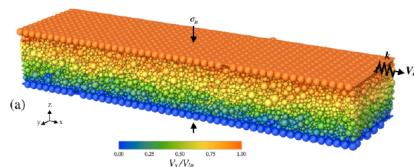


## Multiscale methods: classical approaches



*Disaggregated fault gouge used in friction experiments.*

[T. Numelin et al., Tectonics. (2007).]



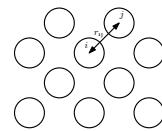
*Numerical representation of gouge using LAMMPS.*

[B. Ferdousi and A. M. Rubin, J. Geophys. Res. Solid Earth. (2020).]

Microscopic approach (molecular dynamics)

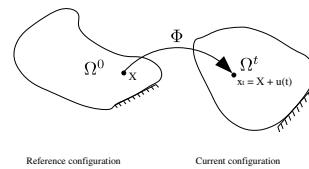
$$M \frac{d^2 q(t)}{dt^2} = -\nabla V(q(t)) + f^{ext}$$

$V$ : atomic potential (Lennard-Jones, EAM)



Macroscopic approach (continuum mechanics)

$$\rho \frac{d^2 u(t)}{dt^2} = \operatorname{div} \sigma + f^{ext}$$



## Pros and cons

### Advantages and limitations of molecular dynamics (MD)

- (+) Good description of all structural microscopic mechanisms (dislocations, irreversible phenomena)
- (-) Spatial scale:  $1\mu m^3$  silicone crystal owns about  $10^{11}$  atoms
- (-) Gigantic volumes of data  $\sim 6.5$  Tera-octets by step for  $10^{11}$  simulated atoms.
- (-) Time scale: timestep = femtosecond ( $10^{-15}$  s.)

### Advantages and limitations of finite elements (FE)

- (+) Allow to model macroscopic objects
- (-) Discontinuities (free surfaces), singularities (crack tip), empirical constitutive laws
- (-) Need for a fine mesh to capture pertinent information.

# Coupling Methods

Idea : use the benefits of both models

## Continuum model

Allow to deal with big domains.

## Atomic model

Good description of microscopic mechanisms.

## Concurrent Partitioned-Domain Multiscale Methods



## Principles

- Split domain
- Atomistics only where nonlinear behaviour expected ( $\Omega_A$ )
- Cheap continuum methods elsewhere ( $\Omega_C$ )

## Various governing Formulation

### Energy-Based

- Energy of system well defined
- Energy-conserving
- Ghost forces!

### Examples

- QC
- BDM

### Displacement Coupling

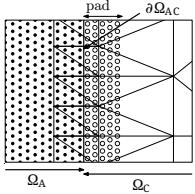
- Mutual Dirichlet boundary conditions
- Ghost force-free
- (Generally unstable!)

### Examples

- FEAT, CADD
- HSM

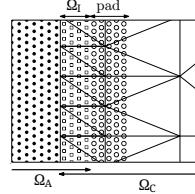
# Various coupling Interface

**Sharp**



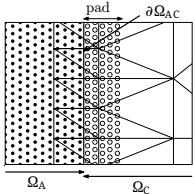
*Most methods*

**Handshake region**



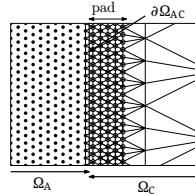
*E.g., BDM*

**Coarse; Weak Compatibility**



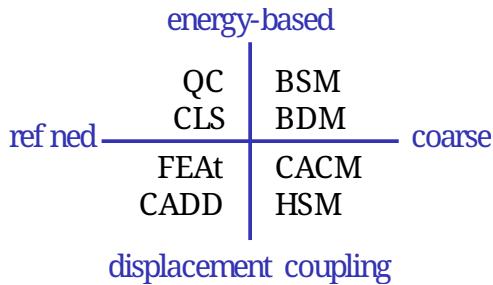
*HSM, BDM, BSM, ...*

**Refined; Strong Compatibility**



*FEAt, CADD, QC, ...*

## Selecting a Method



A UNIFIED FRAMEWORK AND PERFORMANCE  
BENCHMARK OF FOURTEEN MULTISCALE  
ATOMISTIC/CONTINUUM COUPLING METHODS\*

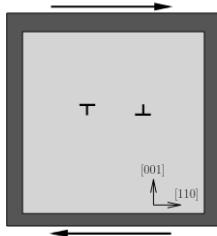
Ronald E. Miller<sup>1</sup> and E. B. Tadmor<sup>2</sup>

Method	Acronym	Key References	Continuum Model	Handshake	Coupling Boundary Condition	Governing Formulation
Quasicontinuum	QC	[53, 45] section 4.1	Cauchy-Born	None	Strong Compatibility	Energy-Based
Coupling of Length Scales	CLS	[44] section 4.2	Linear Elasticity	None	Strong Compatibility	Energy-Based
Bridging Domain	BD	[60] section 4.3	Cauchy-Born	Linear mixing of energy	Weak Compatibility (penalty)	Energy-Based
Bridging Scale Method	BSM	[59, 39] section 4.4	Cauchy-Born	None	Weak/Stong Mix (least-squares fit)	Energy-Based
Composite Grid Atomistic Continuum Method	CACM	[10] section 4.5	Linear Elasticity	None	Weak Compatibility (average atomic positions)	Iterative Energy-Based (two energy functionals)
Cluster-Energy Quasicontinuum	CQC(m)-E	[15] section 4.6	Averaging of atomic clusters	None	Strong Compatibility	Energy-Based
Ghost-force corrected Quasicontinuum	QC-GFC	[46] section 4.7.1	Cauchy-Born	None	Strong Compatibility	Energy-Based with dead load GFC
Ghost-force corrected Cluster-Energy QC	CQC(m)-GFC	[15] section 4.7.2	Averaging of atomic clusters	None	Strong Compatibility	Energy-Based with dead load GFC
Finite-Element/Atomistics Method	FEAt	[25] section 6.1	non-linear, nonlocal elasticity	None	Strong Compatibility	Force-Based
Coupled Atomistics and Discrete Dislocations	CADD	[47, 48] section 6.1	Linear Elasticity	None	Strong Compatibility	Force-Based
Hybrid Simulation Method	HSM	[28] section 6.2	Non-Linear Elasticity	atomic averaging for nodal B.C.	Weak Compatibility (average atomic positions)	Force-Based
Concurrent AtC Coupling	AtC	[19, 4, 5, 35] section 6.3	Linear Elasticity	Linear mixing of stress and atomic force	Strong Compatibility	Force-Based
Ghost-force Corrected Concurrent AtC Coupling	AtC-GFC	unpublished section 6.3.1	Linear Elasticity	Linear mixing of stress and atomic force	Strong Compatibility	Force-Based
Cluster-Force Quasicontinuum	CQC(m)-F	[24] section 6.4	Averaging of atomic clusters	None	Strong Compatibility	Force-Based

Table 1: Summary of the methods discussed in this presentation.

## Coupling errors

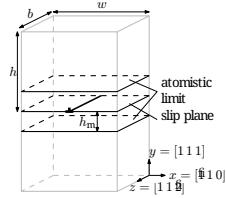
Method	Model-10	Model-20	Mode
CADD/FEAt	11.42 %	5.13 %	3.93
QC-GFC	12.42 %	5.72 %	4.05
AtC-GFC	14.59 %	8.28 %	5.04
BD	14.63 %	9.09 %	6.44
QC/CLS	14.66 %	9.54 %	8.50
BSM	17.59 %	12.07 %	10.1
HSM	22.03 %	15.44 %	12.2
CQC(13)-E	22.59 %	16.62 %	16.55 %
CQC(1)-GFC	40.06 %	20.10 %	20.19 %
CQC(1)-E	86.75 %	43.61 %	38.48 %
CACM	42.59 %	40.13 %	39.92 %
CQC(13)-F	70.84 %	60.75 %	46.42 %
AtC	55.11 %	70.17 %	83.65 %



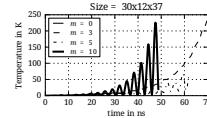
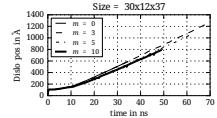
## Dynamical stability of Displacement Coupling Methods

Dynamic stability of displacement-based atomistic/continuum coupling methods

Till Junge <sup>a</sup>, Guillaume Anciaux <sup>a</sup>, Jean-François Molinari <sup>a,b,\*</sup>



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**Instability: method or bug?  $\Rightarrow$  Simplify problem**

**JMPS**

## Instability study on a simple 3d problem

**An atomic-continuum coupled bar**

**Instability is**

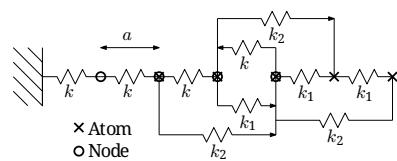
- $\Delta t$ -independent
- $T$ -dependent

**Instability is not**

- due to thermostat
- due to external work
- due to integrator

**Method or bug?  $\Rightarrow$  Simplify problem**

## One-Dimensional Problem



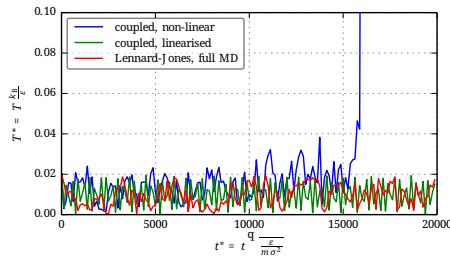
## Simple One-Dimensional Case

- Some springs directional
- $k_1, k_2$  nonlinear (Lennard-Jones)

## Linear Stability Analysis

- Continuous-time system: **stable**
- Discretised-time system: **stable**

# One-Dimensional Instability



Instability due to nonlinear effects in coupling scheme  $\Rightarrow$  **Not a bug**

## Origin of the problem: Traction-Compression Asymmetry



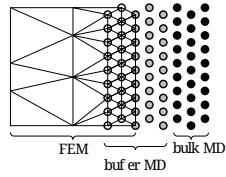
*Linear Stability Analysis*

**But: Unstable**

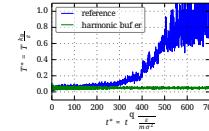
## Implications of instability

- Traction-compression asymmetry present in *all* local/non-local displacement coupling methods
- Similar to well known contact mechanics instabilities

# Solution: Harmonic Buffer Layer



Harmonic Buffer



- Harmonic potential for buffer atoms
- Bulk  $\leftrightarrow$  buffer-interaction with bulk potential

- Solves instability
- Preserves dynamics
- No ghost forces
- Requires precomputation of harmonic potentials

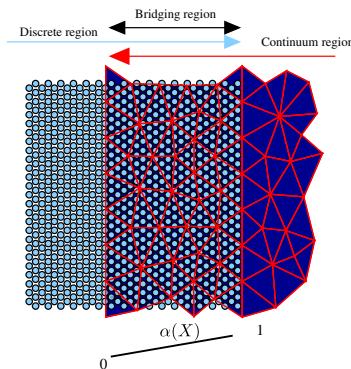
## Stability conclusions

- Refined displacement coupling is dynamically unstable.
- Traction-compression asymmetry in MD potentials are the source of instability.
- Solution:
  - adding a harmonic buffer layer
  - using a bridging domain (because of ... **dissipation**)

## A handshake approach

## Bridging domain formulation

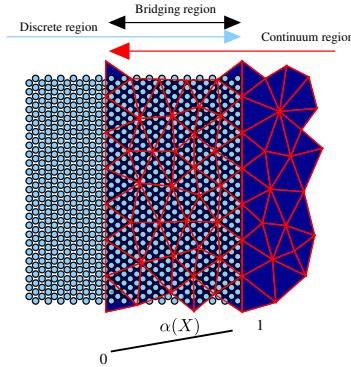
- Energy weighting:
  - $H = \int_{\Omega} \alpha(X) E^C(X) + (1 - \alpha(X)) E^A(X) dX$
- Lagrange constraint:
 
$$\vec{g} = N^T \vec{u} - \vec{d} = \vec{0}$$
- Lagrange problem:
  - $H_L = H + \vec{\lambda}^T \vec{g}$
- Verlet time integration Kinematic constraint:



### Numerical difficulties:

- Correct account of energy in coupling zone
- Different time/space scales
- Wave reflexions

Principle of the energy-based **Bridging Method** [S. Xiao], which is based on the **Arlequin method** [H. Ben Dhia]:



### Idea:

- Hamiltonian formulation
- Velocity Verlet
- Weighting of energy  $\Rightarrow$  smooth the transition
- Constrain displacements with *Lagrange multipliers*

$$\circ \dot{\vec{g}} = \vec{A} \vec{\lambda}$$

- Correct velocities using  $\lambda$

$E^C$ : energy in the continuum region

$E^A$ : energy in the atomic/discrete region

$\vec{\lambda}$ : Lagrange multipliers

$\vec{A}$ : constraint matrix

### Which constraint formulation

#### 1. Strong coupling

[S. P. Xiao and T. Belytscko, *Comput Methods Appl Mech Eng.* (2003).]

$$g = N^T u - d = 0$$

Constraint on particles

#### 2. Weak coupling

$$g = N(N^T u - d) = 0$$

Constraints on nodes

$g$ : Lagrange constraint

$N$ : shape functions

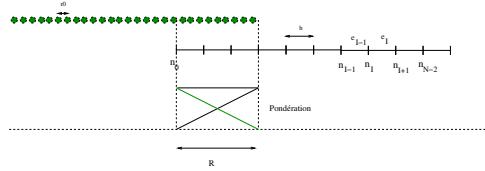
$u$ : nodes displacement

$d$ : particles displacement

# Ghost Forces

Force appears at rest

**Example: 1D monoatomic chain coupled with a homogeneous mesh**



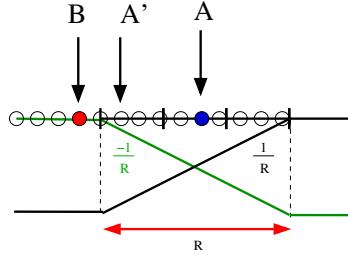
**Forces modified by energy weighting:**

$$\tilde{\mathbf{F}}_I = \int_{\Omega} \alpha(\mathbf{X}) \frac{\partial E^C(\mathbf{u}, \vec{X})}{\partial \mathbf{u}_I} d\mathbf{X}$$

$$\tilde{\mathbf{f}}_i = \sum_{\mathbf{q}_k} \left[ 1 - \frac{\alpha(\mathbf{X}_i) + \alpha(\mathbf{X}_k)}{2} \right] \frac{\partial E^A(\mathbf{q}_i, \mathbf{q}_k)}{\partial \mathbf{q}_i}.$$

Without deformation:

- Atom A: equilibrium
- Atom A': contribution from atom B perturbs equilibrium
- Do not appear for **first neighbor interaction**



## Approximation: neglect the non local term

- Continuum:

$$\tilde{\mathbf{F}}_I = \int_{\Omega^R} \alpha(\mathbf{X}) \frac{\partial E^C(\mathbf{u}_{\Omega^R})}{\partial \mathbf{u}_I} d\mathbf{X}$$

$$\simeq \alpha(\mathbf{X}_I) \int_{\Omega^R} \frac{\partial E^C(\mathbf{u}_{\Omega^R})}{\partial \mathbf{u}_I} d\mathbf{X}$$

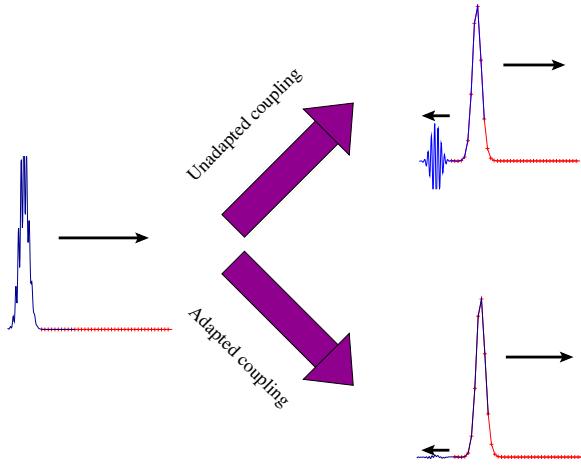
- Discrete:

$$\begin{aligned} \tilde{\mathbf{f}}_i &= \sum_{\mathbf{q}_k \in \Omega^A} \left[ 1 - \frac{\alpha(\mathbf{X}_i) + \alpha(\mathbf{X}_k)}{2} \right] \\ &\quad \left. \frac{\partial E^A(\mathbf{q}_i, \mathbf{q}_k)}{\partial \mathbf{q}_i} \right] \\ &\simeq (1 - \alpha(X_i)) \sum_{\mathbf{q}_k \in \Omega^A} \frac{\partial E^A(\mathbf{q}_i, \mathbf{q}_k)}{\partial \mathbf{q}_i} \end{aligned}$$

**Leads to the simplest force formulation**

- Continuum and discrete forces weighted locally
- No equilibrium ghost forces
- Easier implementation
- Error scales with the inverse of the bridging region size

# Dynamics wave transmission



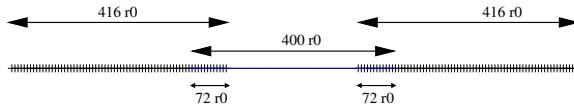
The coupling quality depends on:

- The lumping of coupling matrix  $A$
- Size of the bridging zone
- Size of finite elements
- Weight associated to the first element

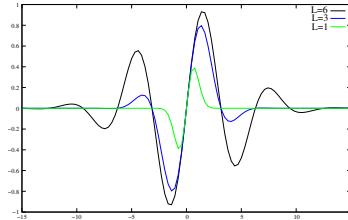
⇒ study of the transfer function

## Wave reflection rates and dissipation

- 1D coupling model: monoatomic chain and homogeneous mesh

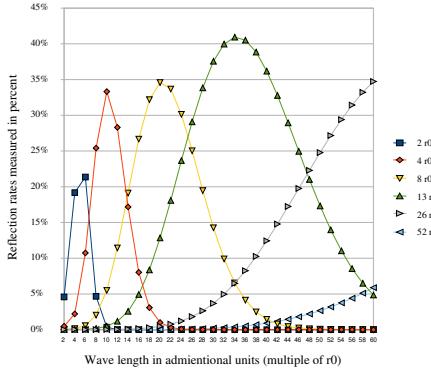


- Stimulation with an impulse
  - controlled frequency
- Measure kinetic energy in discrete region
- Compare with single scale model



Why is there a peak of wave reflections ?

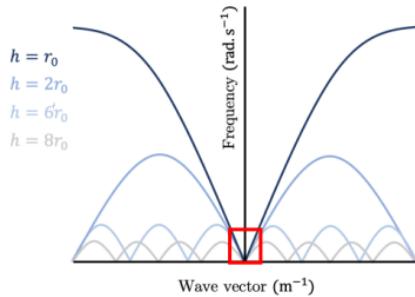
## Dispersion relation



- Large wavelength are transmitted
  - Small wave lengths are absorbed
- ⇒ Energy dissipation

Due to lumping  
Stabilization effect

Wave speed depend on frequencies in discrete medium



Dispersion relation for a 1D domains

## Linearized governing equation - eigen value/vector problem

Eigen modes study by linearization of

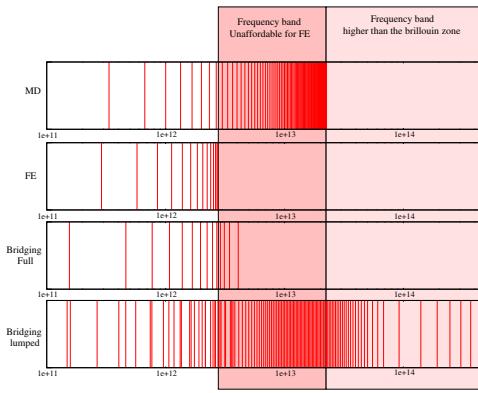
single scale forces

coupling constraint forces.

$$\begin{pmatrix} m & 0 \\ 0 & M \end{pmatrix} \begin{pmatrix} \ddot{d} \\ \ddot{u} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \begin{pmatrix} d \\ u \end{pmatrix}$$

## Spectral study ( $R = 13h, = 8r_0$ )

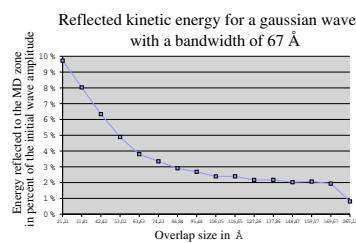
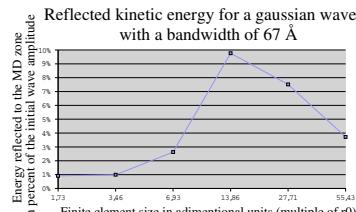
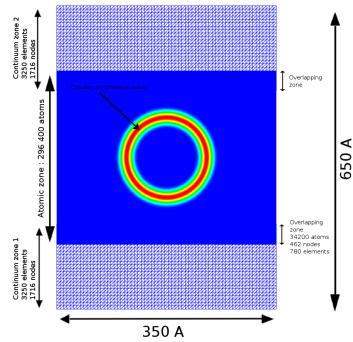
1D coupling model



## Wave propagation in 2D

- Argon crystal coupled to structured mesh
- Periodic boundary conditions ( $X$  axis)
- Initial condition: gaussian displacements

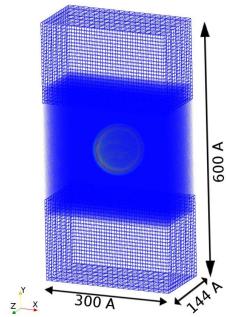
**Confirms the eigen mode conclusions**



## Wave propagation in 3D

- Copper crystal at zero Kelvin (EAM Potential, 1 024 000 atoms).
- Structured mesh (2× 9 216 elements, 10 625 nodes), P1, Cauchy-Born.
- Periodic boundary conditions along  $X$  and  $Z$  axis.
- Initial condition by gaussian displacements

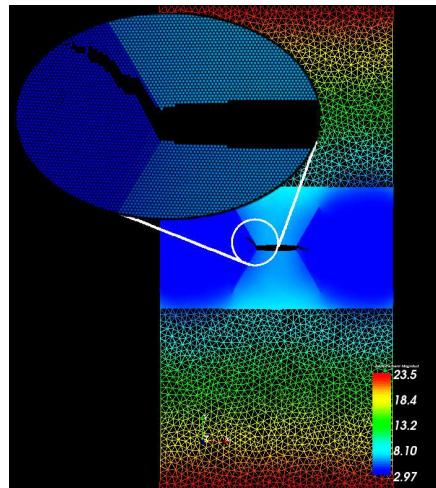
## Crack propagation in an argon crystal (2D)



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### Box of $600 \text{ \AA} \times 800 \text{ \AA}$

- 91 556 atoms(Lennard Jones)
- 1 129 nodes, 2 082 elements.
- Periodic boundary conditions along  $X$  axis.
- *penny shaped crack*: occlusion created by removal of atoms (ellipsoid  $50\text{\AA} \times 2.5\text{\AA}$ ).
- Perturbation of dynamics by mirror waves due to periodic boundary conditions.



0:00 / 0:50

# Indentation in a copper crystal (3D)

- Copper crystal at zero Kelvins, EAM potential (379 149 atoms).
- Unstructured mesh, P1, Linear CL. (327 982 elements and 60517 nodes)
- Cauldron coupling zone to avoid periodic boundary conditions
- Quasi-static simulation
- Spherical indenter
- Run on two processors



0:00 / 0:39

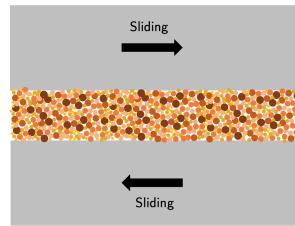
## Conclusion on BDM

- Necessary approximation on weighted forces
- Control of the **ghost forces**
- Wave reflections results from
  - discrete - continuum/mesh characteristic sizes
  - distinct admissible frequencies
- *LibMultiscale* implementation for 1D/2D/3D problems

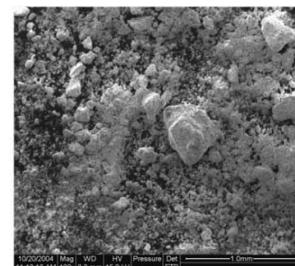
## Amorphous granular to continuum

# What is a gouge ?

- Two first bodies sliding on top of each other
- Accumulation of wear third body/gouge
- Complex medium:
  - Amorphous – disordered
  - Evolution of particles with time
  - Physical and chemical interactions



*Schematic of gouge/first body.*

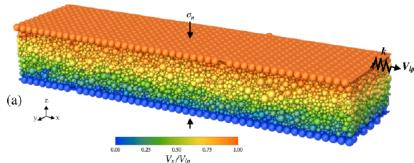


*Disaggregated fault gouge used in friction experiments.*

[T. Numelin et al., *Tectonics*. (2007).]

- Numerical simulations ?

## Numerical studies of gouge (DEM)



*Numerical representation of gouge using LAMMPS.*

[B. Ferdowsi and A. M. Rubin, *J. Geophys. Res. Solid Earth*. (2020).]

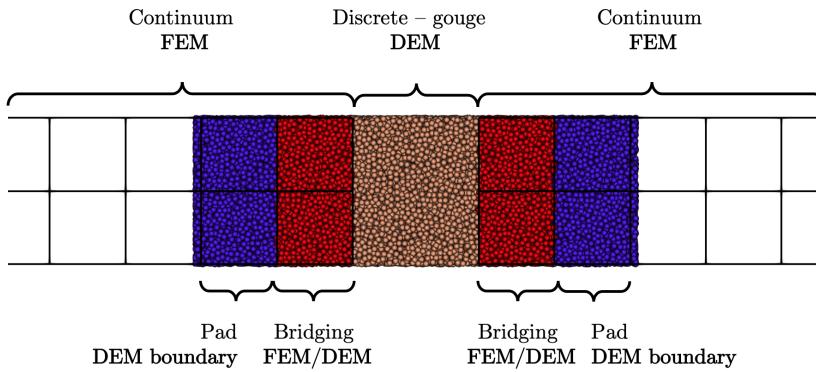
- Challenges

- Grain scale mechanisms in the gouge/third body (DEM)
- Model the right boundary conditions/first bodies (FEM)
- Access gouge properties
- Study interaction first/third bodies

- Drawback:

- Only represents the gouge not the first body
- 3D box of 20cm by side, with a particle diameter of 3mm > 1.5 million DOF
- Computationally expensive

# FEM/DEM coupling

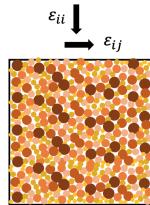
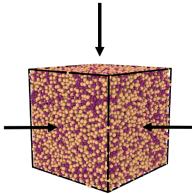


- Bridging coupling method
- Need same material properties in FEM and DEM (small deformation)
  - To validate coupling

## Elastic properties of DEM samples

At which sample size a granular material can be described as elastic ?

- DEM sample properties: [LAMMPS]
  - 9 different box sizes
  - 20 realizations per box sizes
  - 2 size of particles: = 3 mm
  - Glass bead elastic properties
  - Hertz contact
  - Hydrostatic confining pressure: 5 MPa

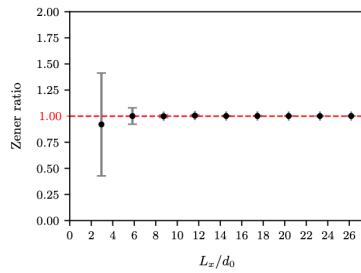


- 12 tests are conducted:

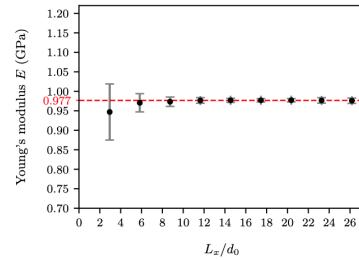
- $\pm \epsilon_{xx}, \pm \epsilon_{yy}, \pm \epsilon_{xy}, \pm \epsilon_{xz}, \pm \epsilon_{yz}$
- 36  $C_{ij}$  are determined  
 $(\sigma_i = C_{ij}\epsilon_j)$
- Elastic tensor

- At which sample size a granular material can be described as isotropic and elastic ?
- Zener ratio

Does the Bridging method applies in the case of amorphous structure ?



*Zener ratio in terms of number of particles by box length*

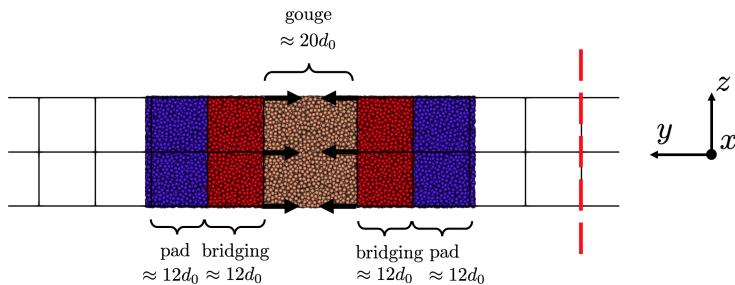


*Young's modulus in terms of number of particles by box length*

## Constant elastic properties

# Elastic properties of DEM samples

- Constant elastic properties for box size
- Determine the minimum mesh size at the interface to match elastic properties
- Determine material properties of the FEM
  - Correspond to the properties of the DEM box of size



1. Strong coupling

$$g = N^T u - d = 0$$

Constrain particles

2. Weak coupling

$$g = N(N^T u - d) = 0$$

Constraints on nodes

### Definitions

$g$ : Lagrange constraint

$N$ : shape functions

$u$ : nodes displacement

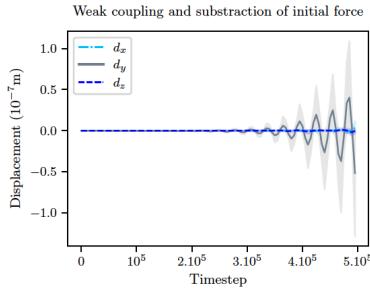
$d$ : particles displacement

3. Subtraction of the initial force at the FEM/DEM interface Ghost forces

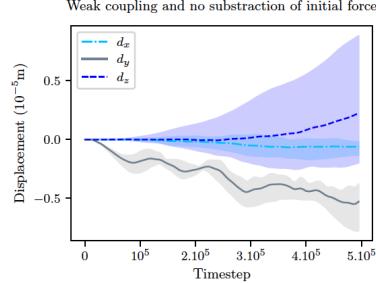
[V. B. Schenoy et al., J. Mech. Phys. Solids. (1999).]

# Coupling comparison - No external excitation

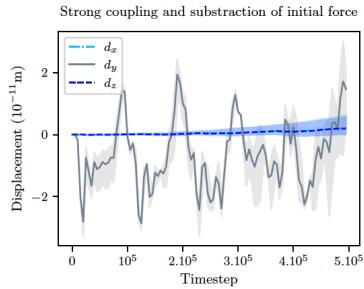
Subtraction initial force (weak coupling)



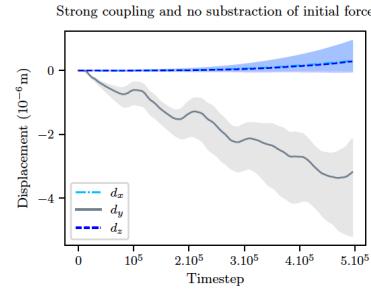
No subtraction initial force (weak coupling)



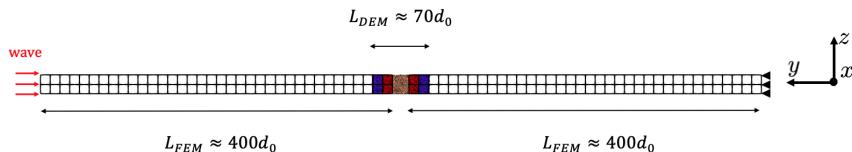
Subtraction initial force (strong coupling)



No subtraction initial force (strong coupling)



## Wave propagation



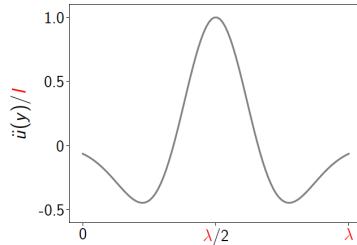
- Seismograph can be decomposed as Ricker wavelet:

[N. Ricker, Geophysics. (1940).]

$$u_y(t) = I \exp \left( -\frac{1}{2} \left( \frac{2\pi c(t - t_0)}{\lambda} \right)^2 \right)$$

- How to select  $I$  and  $\lambda$  ?

- Continuum remains linear



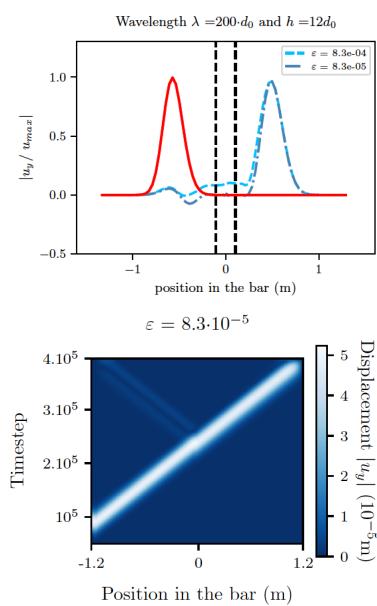
Acceleration of the generated wave.

elastic if:

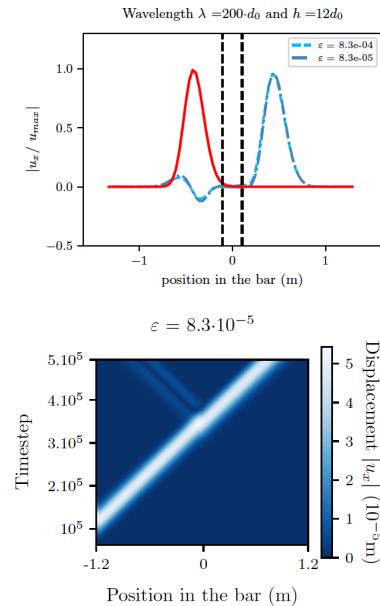
$$\varepsilon \sim \frac{\partial u}{\partial y} \sim \frac{I}{\lambda} \ll 1$$

## Wave propagation - Matching elastic properties

*Compressive wave*



*Shear wave*



- Origin ?

$h$ : mesh size in the bridging

$d_0$ : mean diameter

## Reflected wave

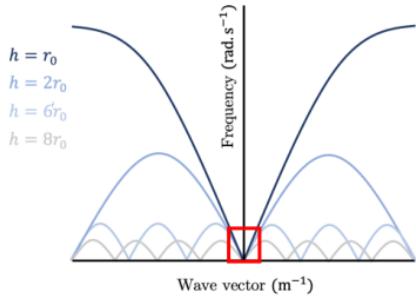
Is the reflected wave due to dispersion ?

Analogy MD/FEM

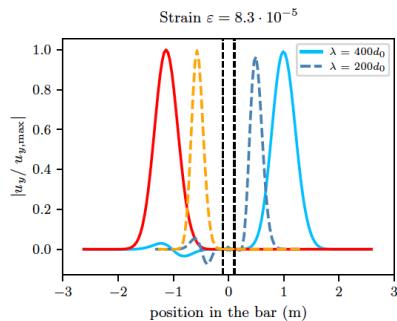
- Increase wavelength  $\Rightarrow$  decrease of reflected waves

## Conclusion

- Compare two coupling formulations:
  - Strong and weak coupling
- Study the impact of the subtraction of the initial forces at the interface
  - Ghost forces



*Dispersion relation for a domain discretized using FEM.*



*Reflected wave Dispersion*

### Strong coupling with substraction of the initial force

- Good propagation of compressive/shear waves
- Future work:
  - Adaptive coupling (strain based)

## Open source

LibMultiscale  
[\[https://gitlab.com  
/libmultiscale/libmultiscale\]](https://gitlab.com/libmultiscale/libmultiscale)

Akantu [https://akantu.ch] FEM  
Lammps [https://www.lammps.org]  
DEM

