# Coupled 3d dislocation dynamics at nano- and micro-scales

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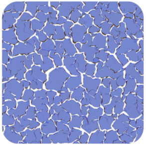
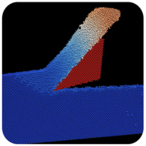
Ben Szajewski  Jean-François Molinari  William A. Curtin

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Computational Solid Mechanics Laboratory

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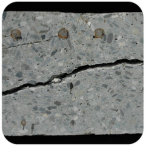
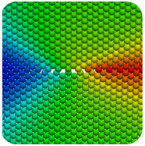

Fonds National Suisse
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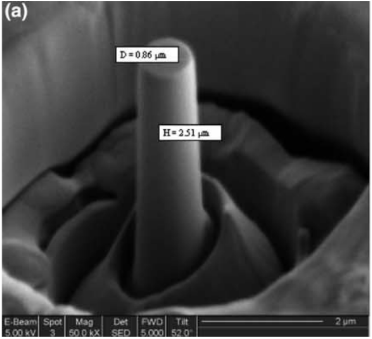
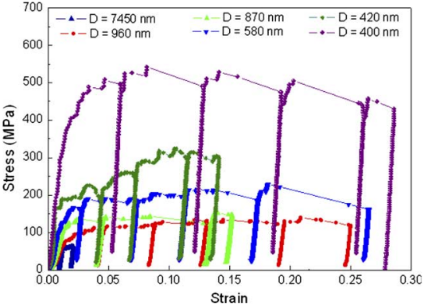
# Size effects in plasticity deformations

## Compression of a micro-pillar

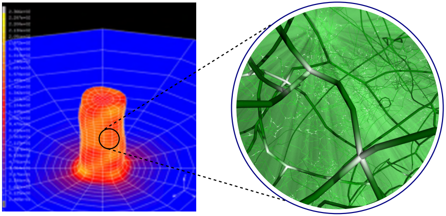



Sun et. al. Scripta Materialia 65 (2011)

# Computational tools for dislocation dynamics

## Multiscale problem



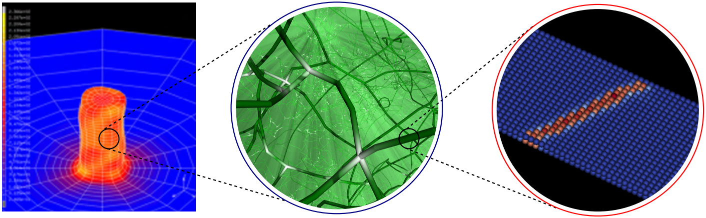
Raabe & Roters 2007    ParaDiS, LLNL

### Discrete Dislocation Dynamics

- Simple representations
- Large domain sizes
- Comparable to experiments
- Long-range elastic field
- (-) Adhoc approach for nucleation

# Computational tools for dislocation dynamics

## Multiscale problem



Raabe & Roters 2007　　ParaDiS, LLNL

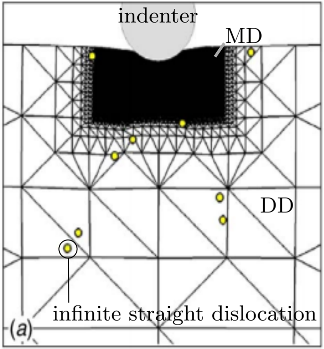
| Discrete Dislocation Dynamics | Molecular Dynamics |
|---|---|
| Simple representations | Explicit representation |
| Large domain sizes | Nonlinear atomistic fields |
| Comparable to experiments | Inherited nucleation |
| Long-range elastic field | (-) Small domain sizes |
| (-) Adhoc approach for nucleation | (-) Periodic BCs |

# CADD3d

Coupled **A**tomistic/**D**iscrete **D**islocations method in **3d**

## From 2D to 3D

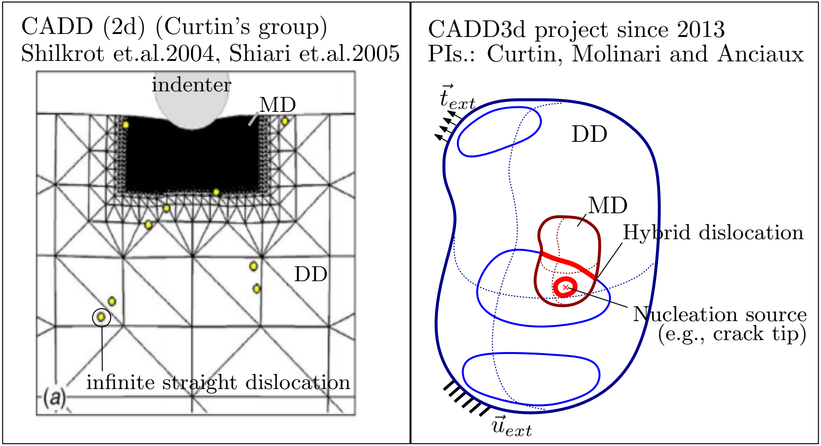
CADD (2d) (Curtin's group)
Shilkrot et.al.2004, Shiari et.al.2005



# CADD3d

## Coupled Atomistic/Discrete Dislocations method in 3d

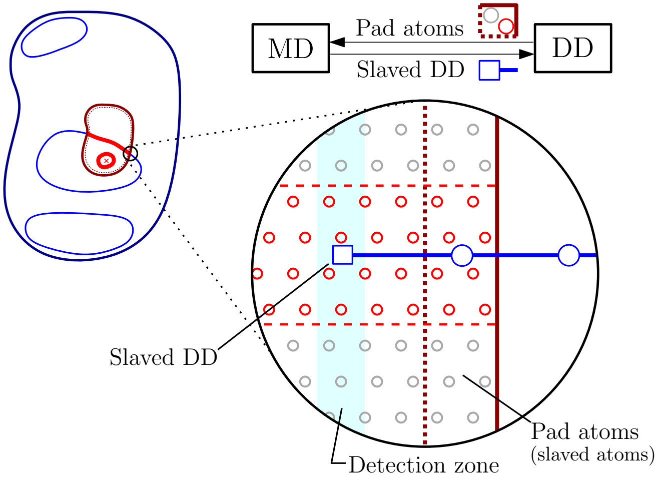
### From 2D to 3D




Hybrid dislocation should behave as one single dislocation structure → Reciprocal boundary conditions

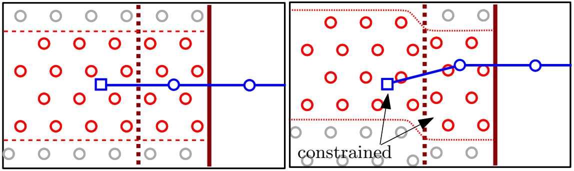
# Reciprocal boundary condition

## Communications between MD and DD



# Application of the BC during dynamics

## Periodic synchronization of the BCs



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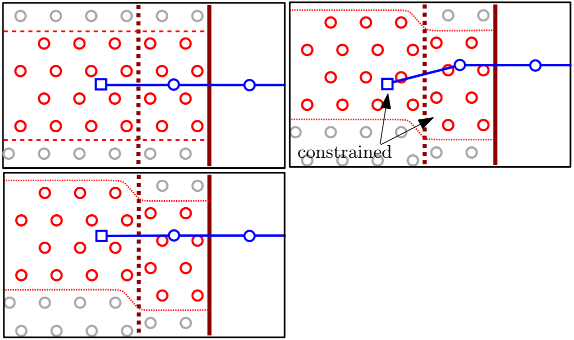

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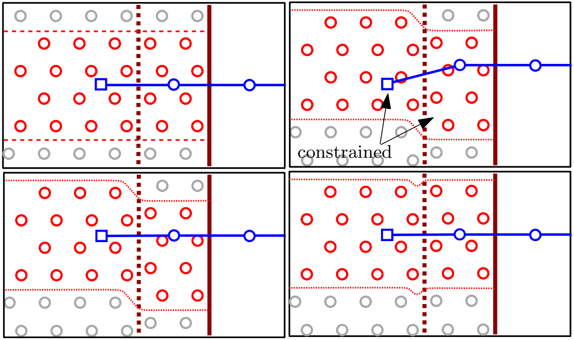
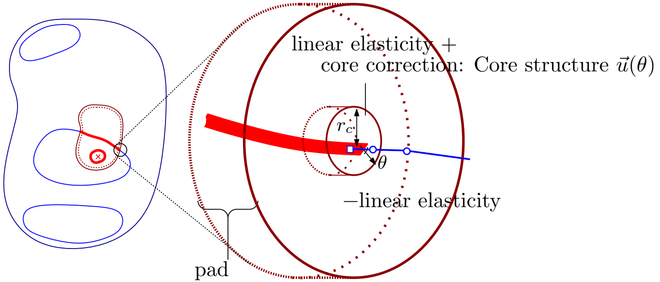



- Detection: DXA (Stukowski et.al.2012) & Centro-symmetry
- Update pad atoms: Linear elasticity & core corrections
- Exact mobility law compared to MD dislocations $M(\theta, T)$

# Update pad atoms

## Pad domain decomposition

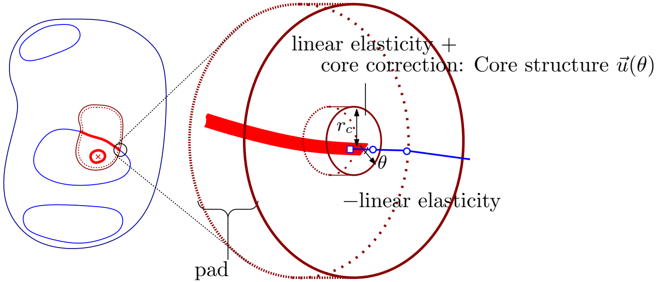
### Correction of core structure



# Update pad atoms

## Pad domain decomposition

### Correction of core structure

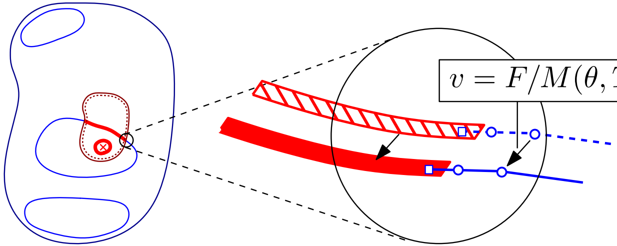



### J.Cho, T.Junge, J-.F.Molinari, G.Anciaux, AMSES 2016

- Total 8 character angles $\theta$ were considered ($0^\circ \leq \theta \leq 90^\circ$).
- The obtained MS core structures are validated by the analytic model (Peiers-Nabarro method).
- The displacement meshes are stored in template forms.

# Mobility law

## Mobility law as functions of characters angle and temperature



# Mobility law

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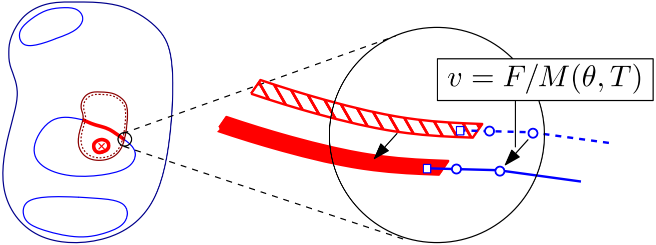
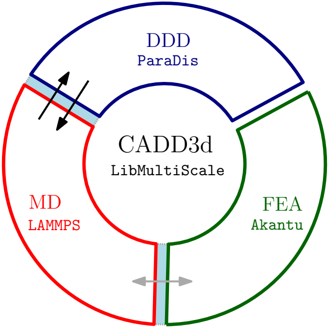



## J.Cho, J-.F.Molinari, G.Anciaux, (Submitted on August 2016)

- The various character angles $\theta$ and temperatures (1,100,200 and 300K) are considered.
- The mobility law (acceleration and gliding) is constructed.
- It is implemented in the DDD engine (`ParaDiS`).

# Simulation engines

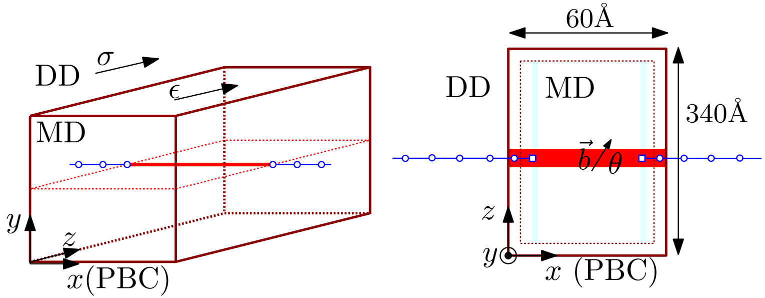
## The third-party software components




- The three (open-source) codes communicate with each other through (open-source) `LibMultiScale` developed by Dr. G. Anciaux and co-workers.
- The (presented) MD$\leftrightarrow$DDD scheme is parallelized with MPI.

# Test1: Hybrid straight dislocations

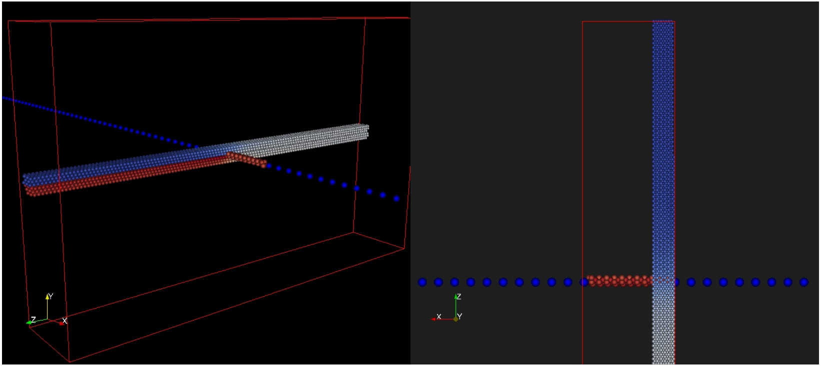
## Perspective view and Top view




- The various character angles $\theta$ are considered.
- Several shear stresses 100MPa$\leq \sigma \leq$ 1000MPa are applied in Burgers vector $\vec{b}$ direction on DD domain.
- The corresponding strains $\epsilon$ are applied on MD atoms, and updated every coupling step.

# Simulation video

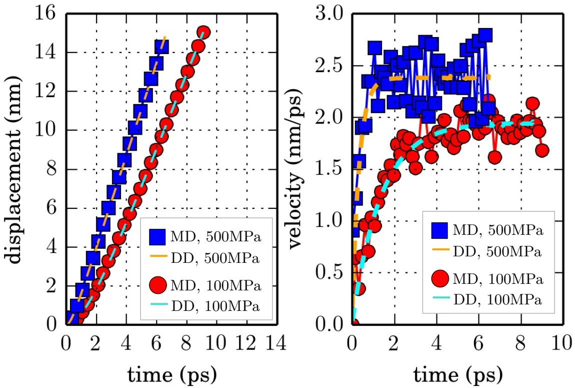
## Example: Mixed 30° dislocation, Shear stress 100MPa



# Simulation result

## Evolution of displacements and velocities

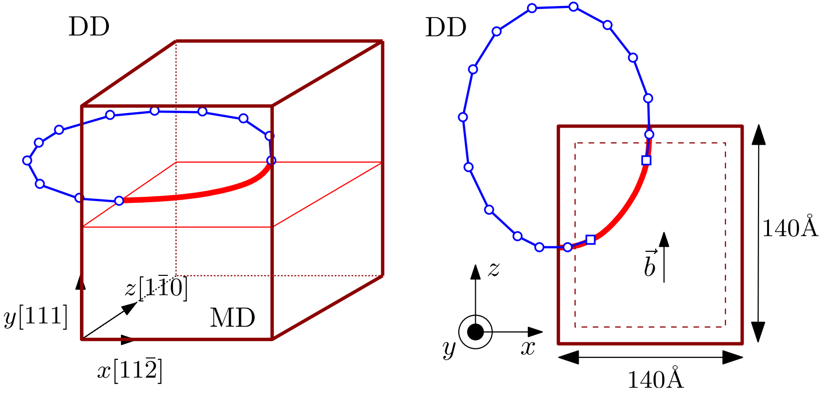
### Example: Mixed 30° dislocation with 100MPa and 500MPa




All the cases with the various character angles and shear loading are successfully tested.

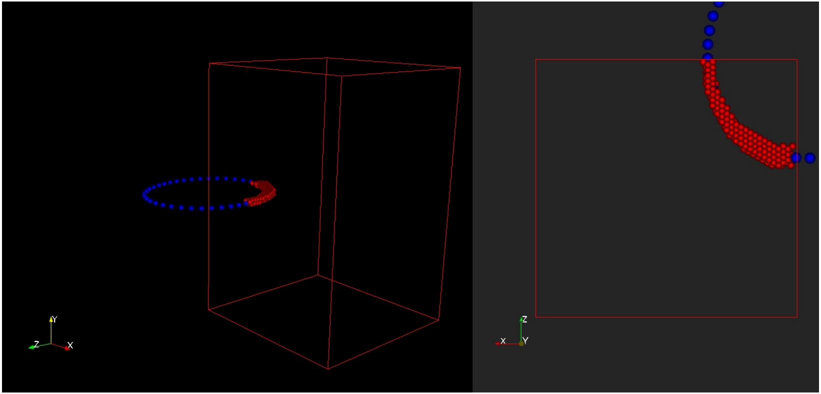
# Test2: Hybrid dislocation loop

## Perspective view and Top view

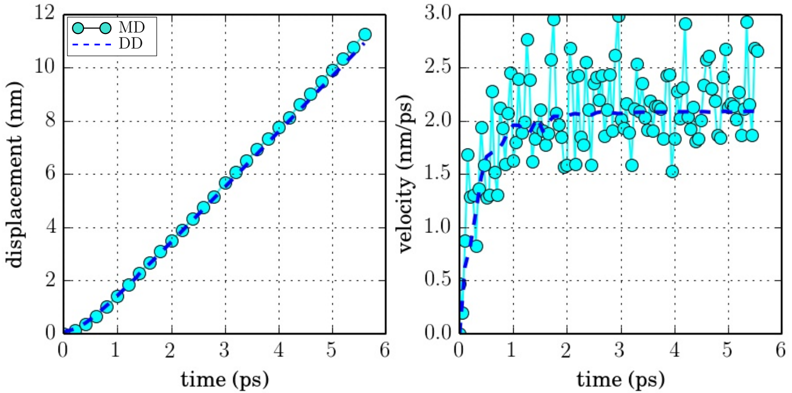


# Simulation video

## Example: shear stress 400MPa

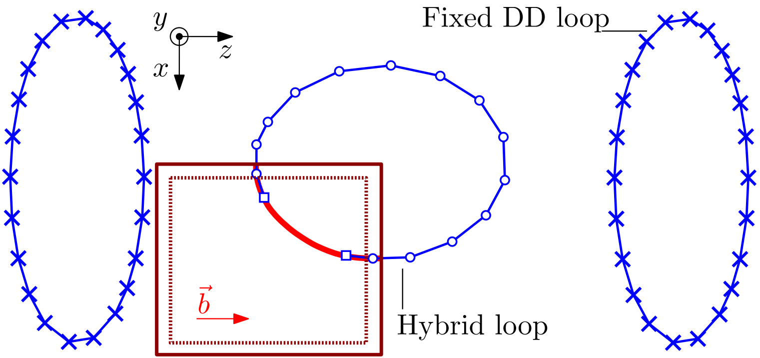


## Evolution of displacements and velocities along $x + z = 0$ axis



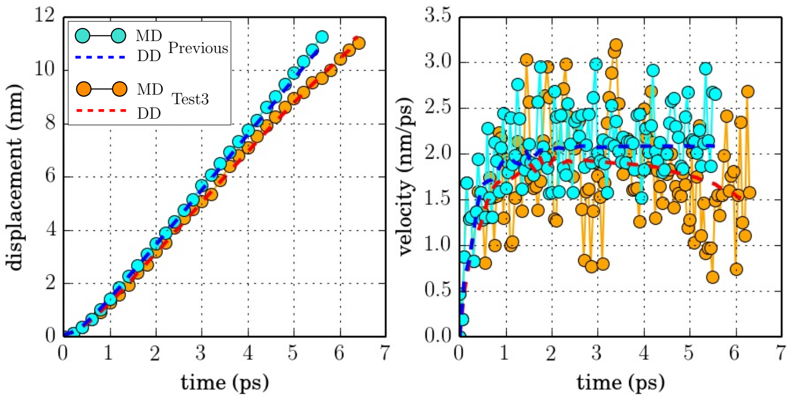
# Test3: Multiple dislocations

## Perspective view and Top view

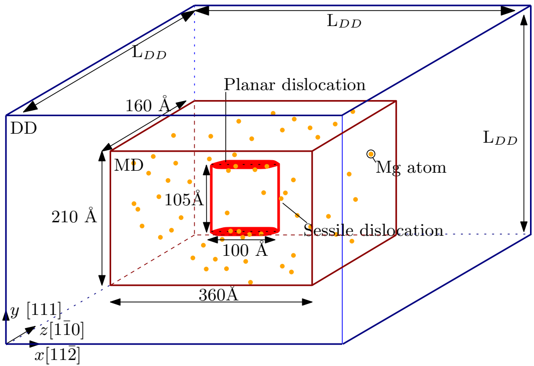


# Simulation results

## Evolution of displacements and velocities along $x + z = 0$ axis



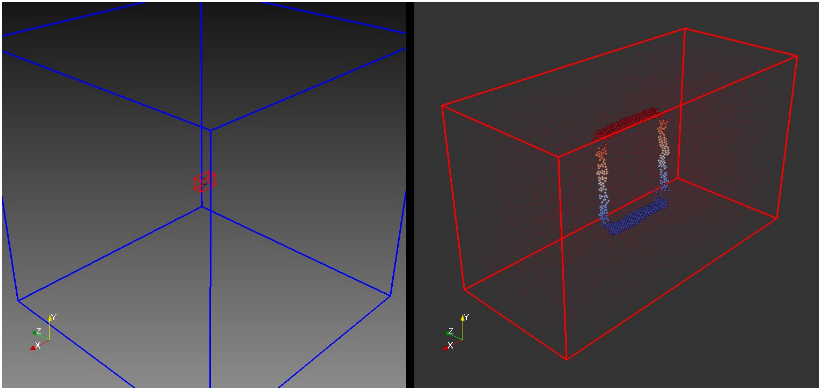
# Frank-Read source in Al-5%Mg alloy




- Nucleation source: a double Frank-Read source
- 5% magnesium substituents are randomly distributed in MD.

# Simulation video (on-going)

## Example: applied stress 1.0GPa and $L_{DD}$=0.5$\mu$m



# Conclusions

## Highlights of CADD3d

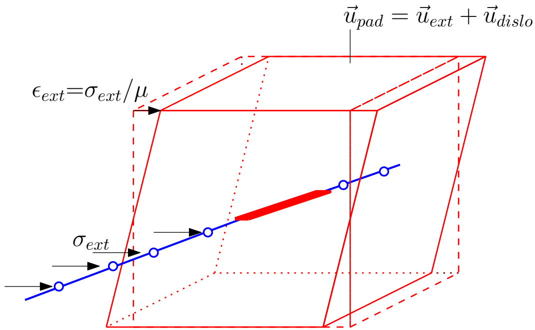
- Unique capability to handle dislocation dynamics coupled between MD and DD.
- Natural dislocation nucleation in DD.
- Enable infinite boundary condition in MD (no PBCs).

## Outlook

- Possible application: single-arm Frank-Read source
- Future development: coupling with FEM $\rightarrow$ Indentation

# Boundary conditions

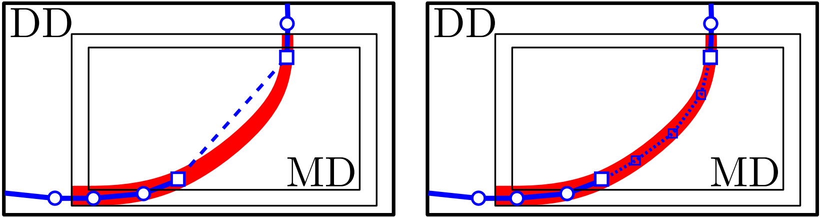
## Constant stress $\sigma_{ext}$



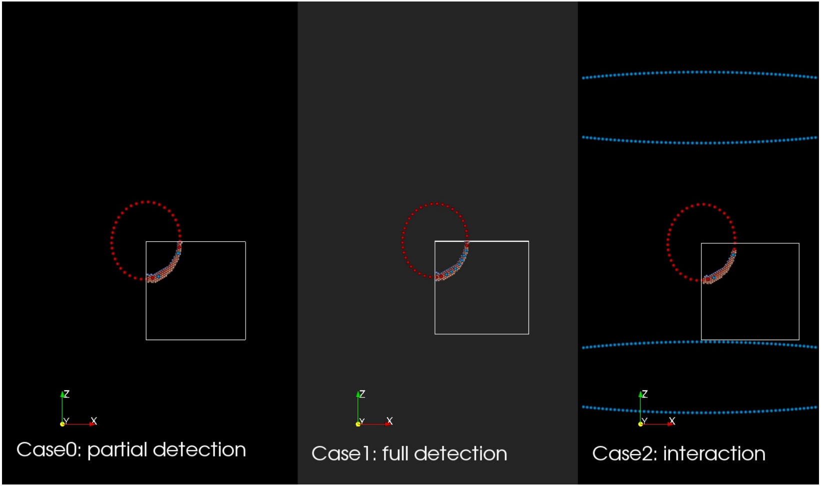

, where $\mu$ the shear modulus.

# Connection between two slave DD nodes

## Two strategies to close dislocation network



# Simulation videos (test2 and test3)



# Validation (on-going)

## Comparison between MD, DDD and CADD3d

### Example: Aluminum, Single FR source, 700MPa, and L=50nm