The Discrete-Continuum Model: An important breakthrough to simulate the mechanical properties of crystalline materials

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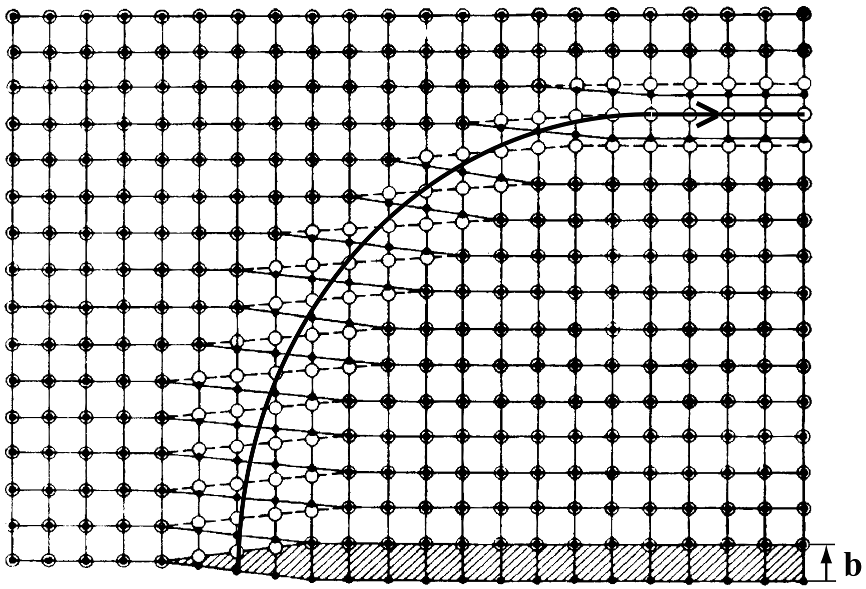
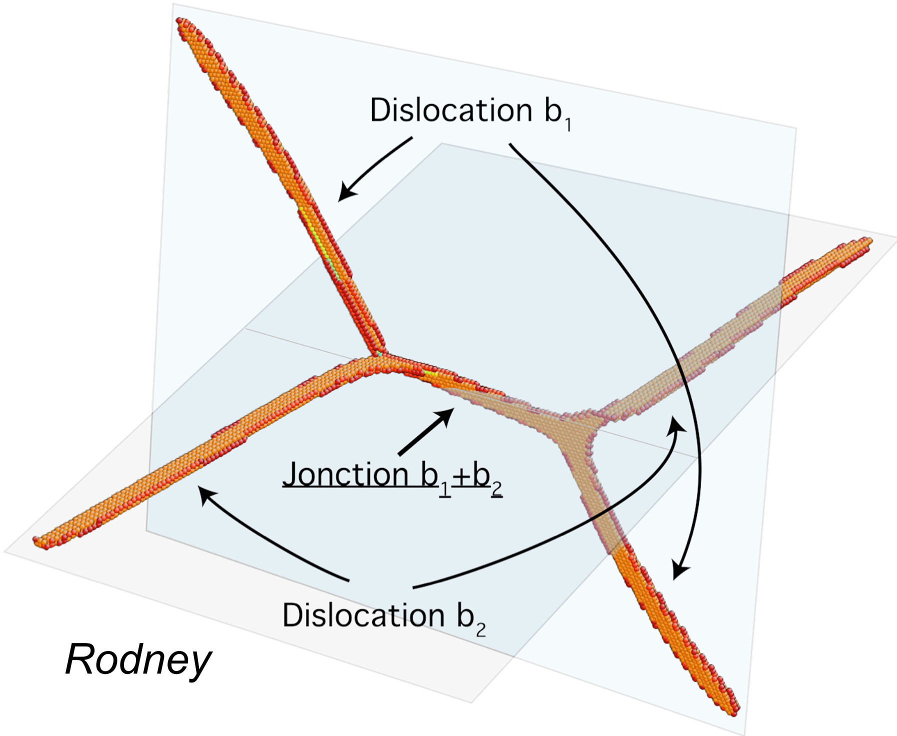
Dislocations



Read(1953)



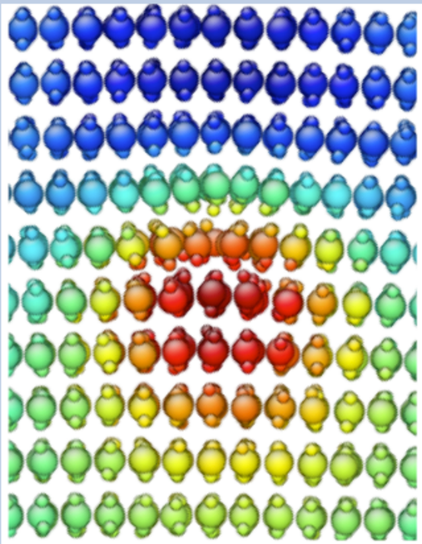
Rodney

- Linear crystalline defect
- Long range elastic field (singular at the line)
- Short range properties (core properties)
- A crystal contain a huge density of dislocations

Multiscale modeling of plasticity

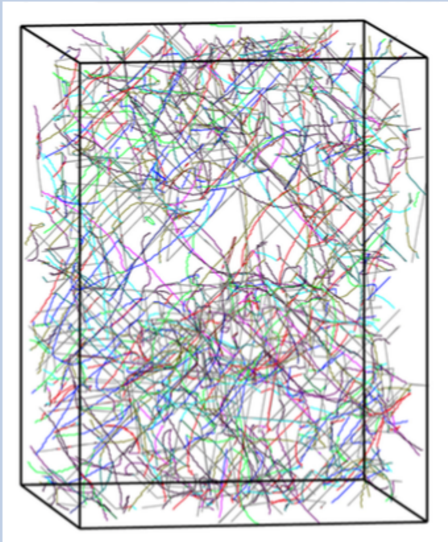
MD - MS - etc..

nm and 10^{-15} s



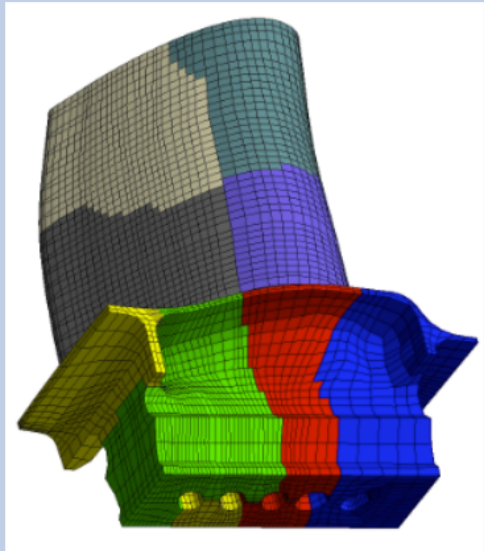
DD (DDD)

μm and $10^{-10} - 10^{-5}$ s



FEM - BEM - etc ...

mm - km and s - y



DD simulation is the Key element between discreet (ϕ) and continuous (M) modeling of crystal plasticity

Outplane

1. The Discrete-Continuous Model (DCM)

2. Performence analysis

3. Simulation exemples

4. Concluding remarcks

3D - Dislocation Dynamics Simulation

(microMegas (mM) a free GPL code)

Discretization

Time(10^{-6} - 10^{-15} s) & Space (1 - 100 b)

Line & Character

1 = Elastic Properties

Peach-Koehler force

Line tension

Junctions

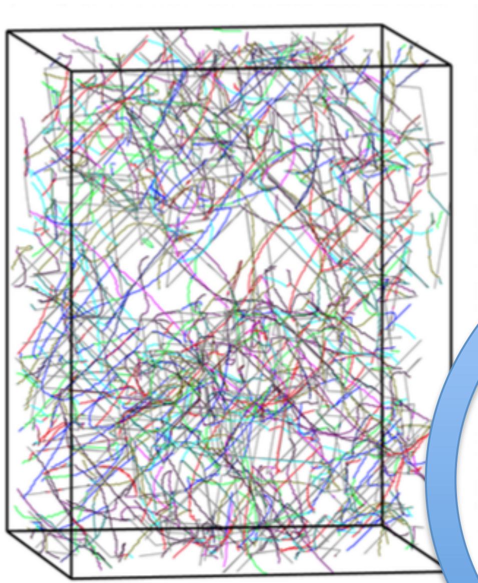
2 = Local rules

Velocity-stress

Cross-slip

Climb

Other crystal defects interac.
(Grain boundary,
precipitates…)



5 - 20 μm

FCC, BCC, HCP, DC, orthorhombic ...

3 = Initial conditions

Defects density

Loading conditions

4 = Boundary conditions (periodic or finite)

Dislocation flux

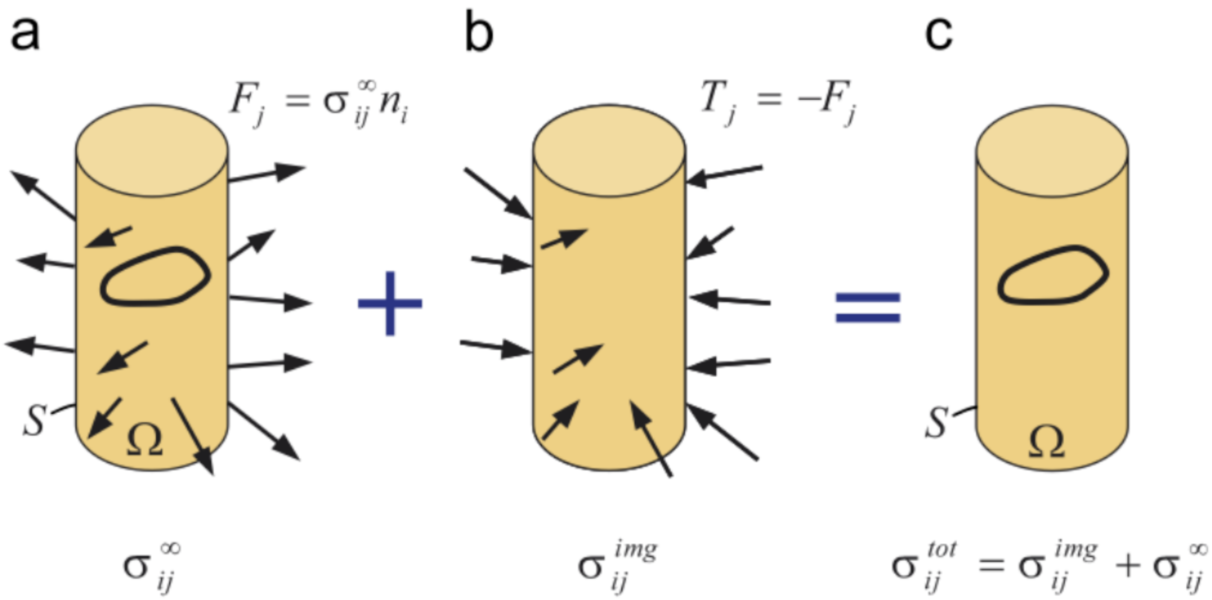
Crystal equilibrium

+

Surfaces & interfaces

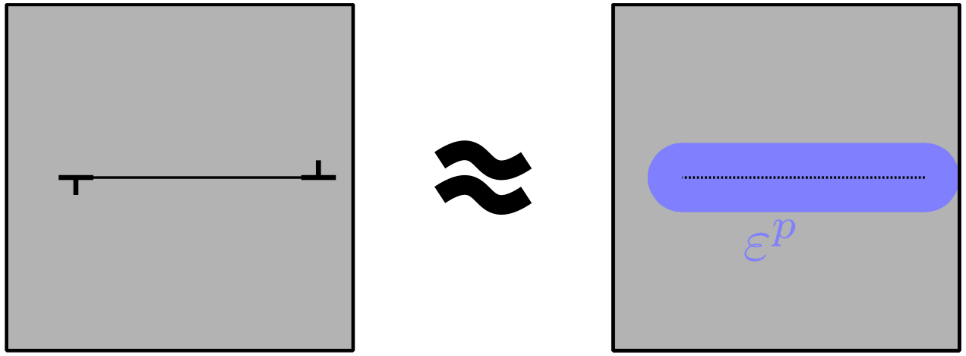
Superposition method

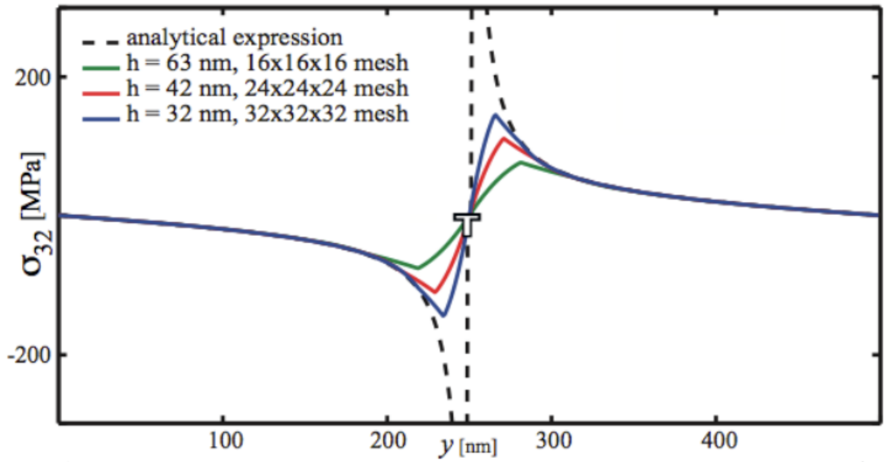
-> 2D, van der Giessen and Needleman (1995); …
-> 3D, Fivel; Weygand and van der Giessen, Weinerger and Cai; …



- Dislocation singular field is a problem at surfaces and interfaces
- Not adapted to simulate periodic systems

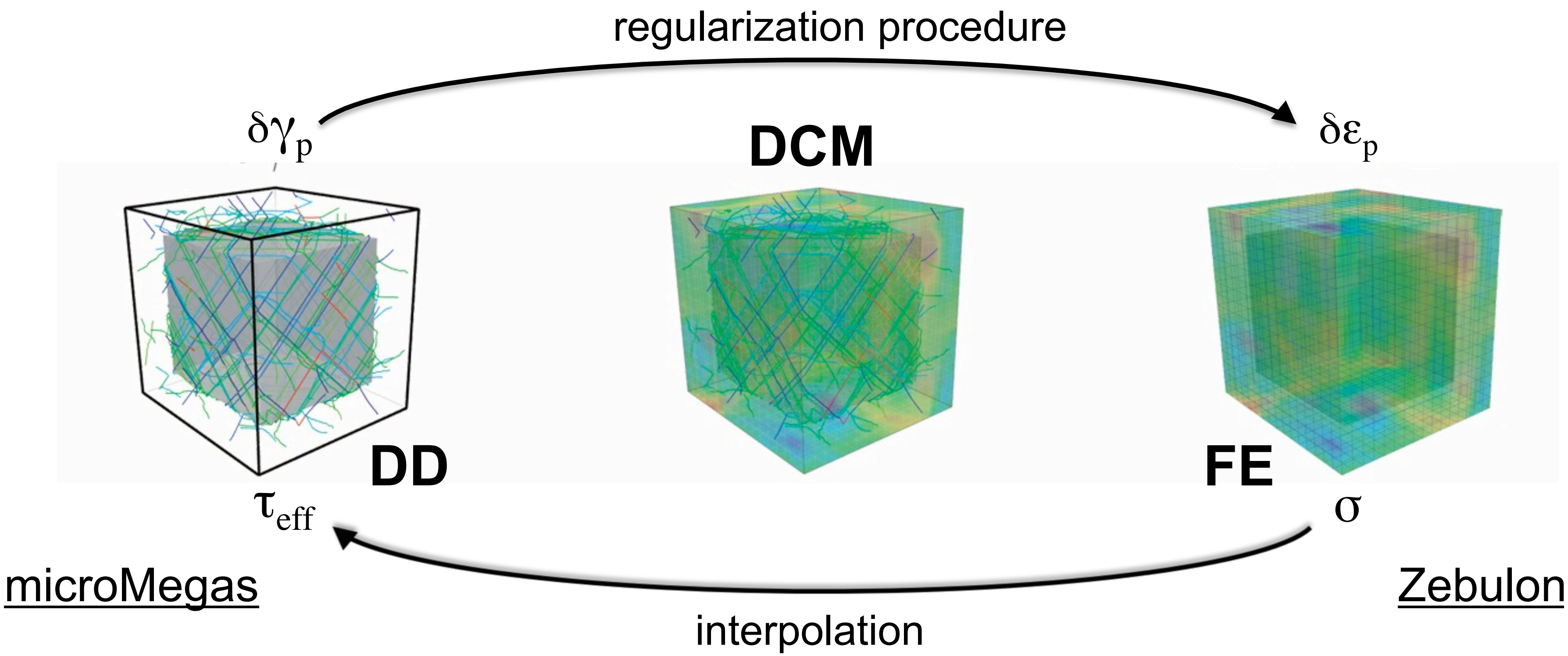
Mura theory: Dislocation ≈ Eigenstrain





Need for a local correction in the DD code to handle for dislocation-dislocation short range interaction.

The Discrete Continuum Model



- Short range interaction
- Dislocation microstructure

- Mechanical equilibrium
- boundary conditions
- Long range interaction

C. Lemarchand, J. L. Chaboche, B. Devincre, and L. P. Kubin. Multiscale modelling of plastic deformation. J. Phys. IV, 9:271, 1999.

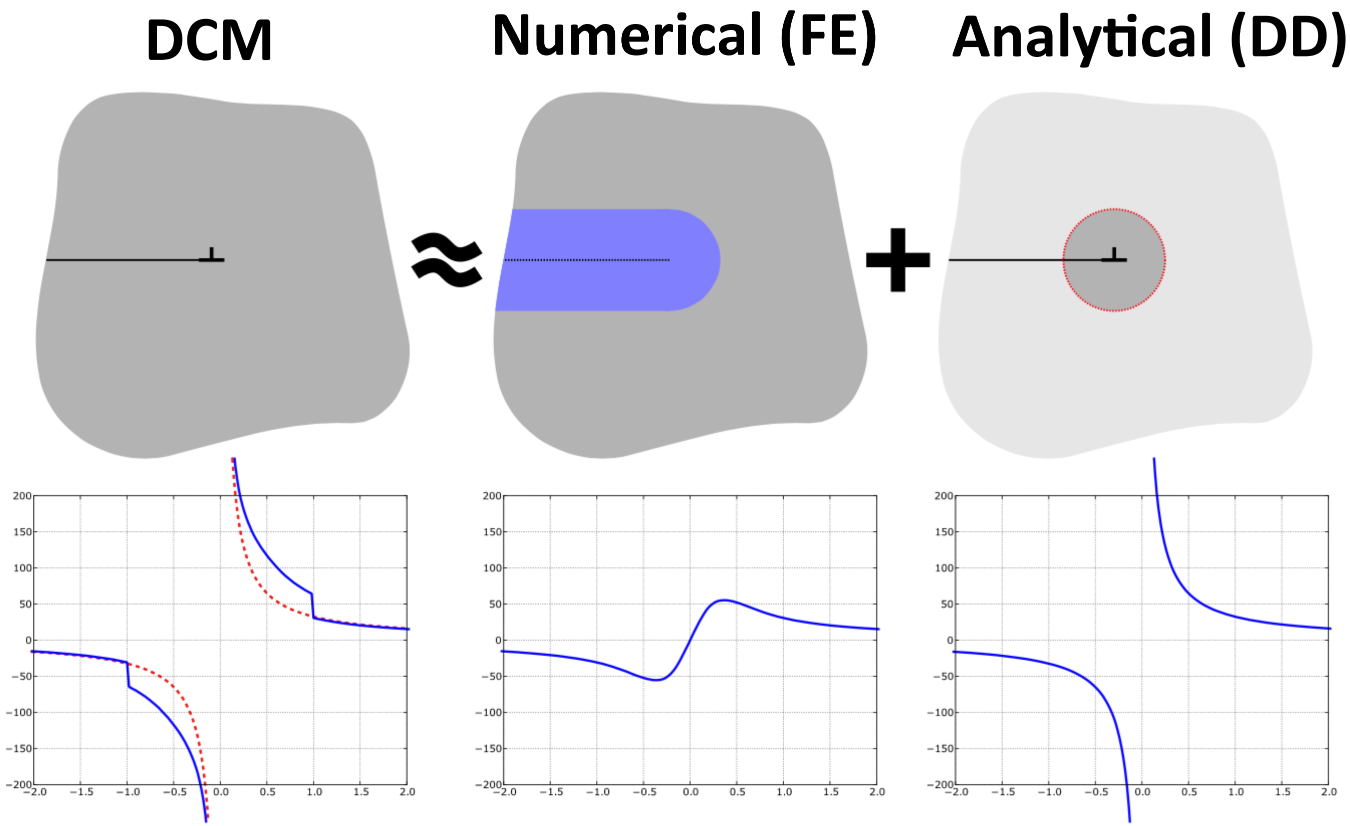
The Discrete Continuum Model (V.2)

The model was revised in the last 2 years:
(Post-Doc: O. Jamond)

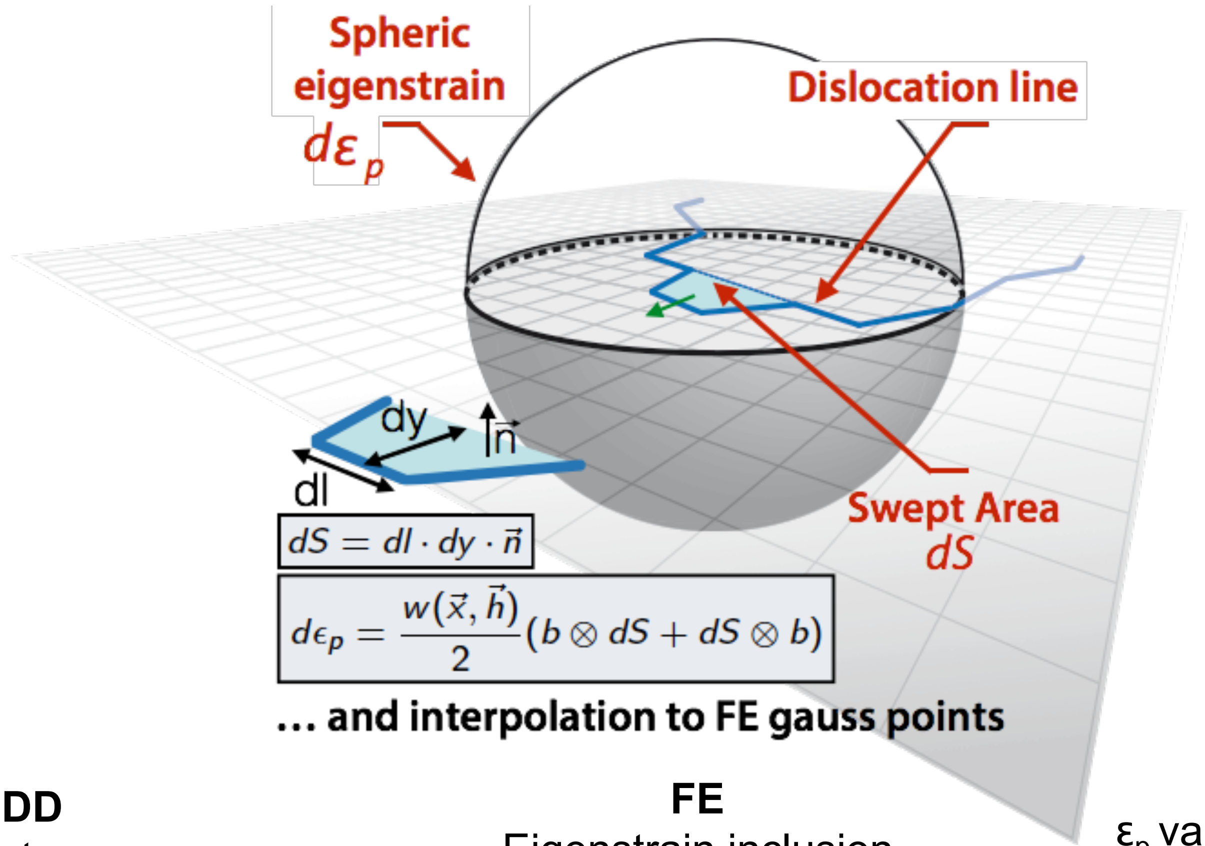
- New regularization procedure
- Unstructured meshes to run simulation in complex domains
- Performance and accuracy improvements
- New computation possibilities

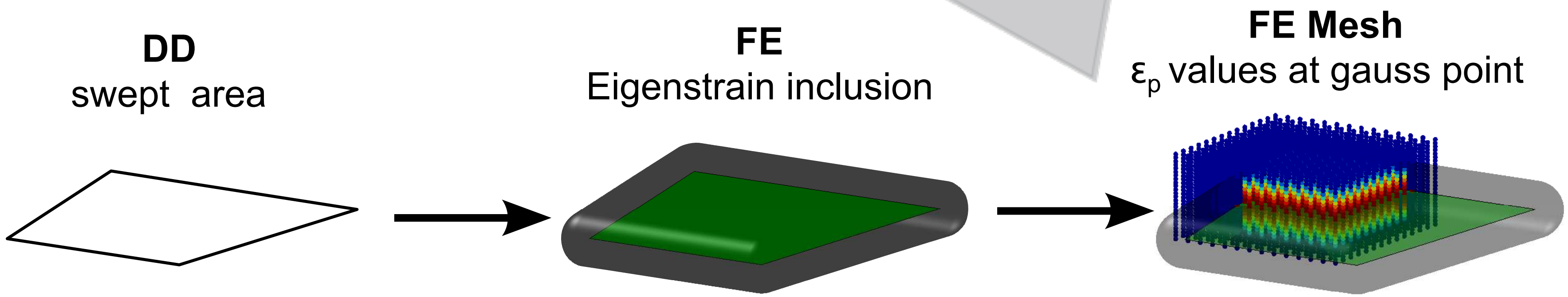
The DCM initial solution

Local analytical correction in the DD code to handle dislocation short distance interaction.



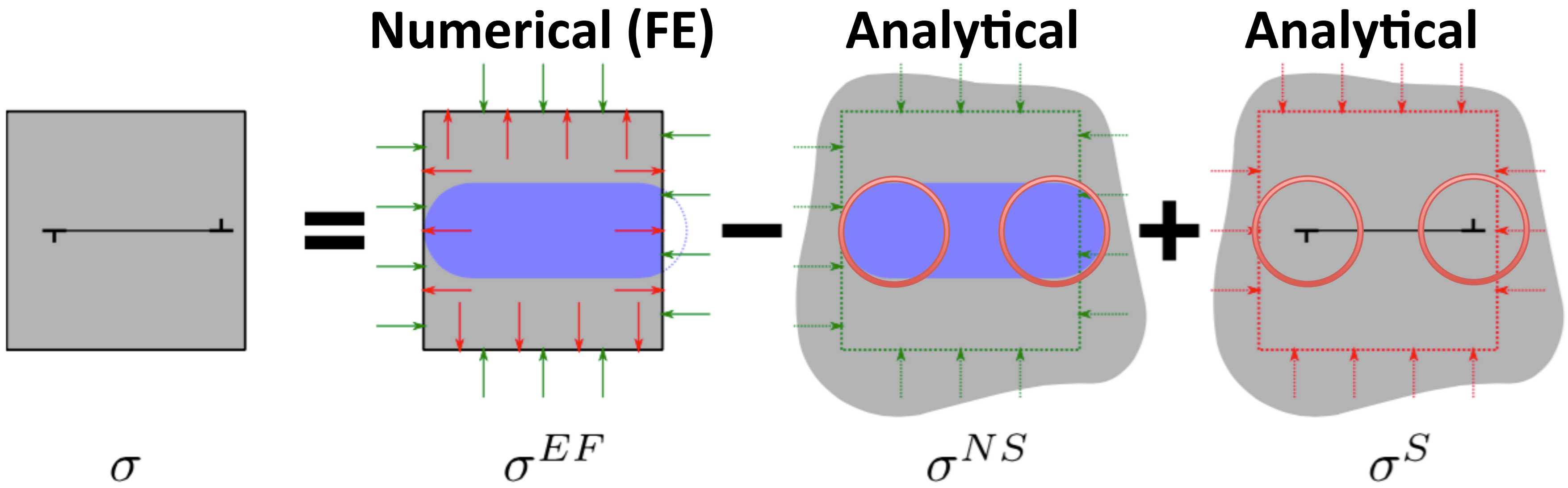
DCM: New regularization procedure

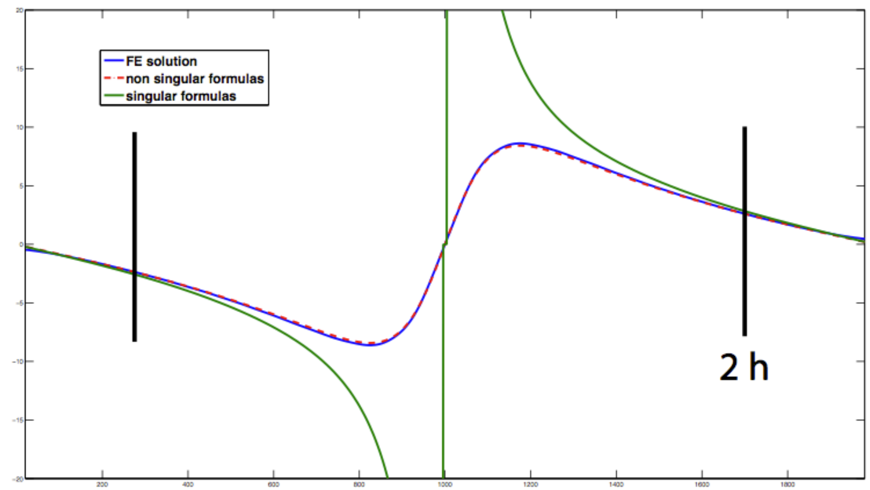




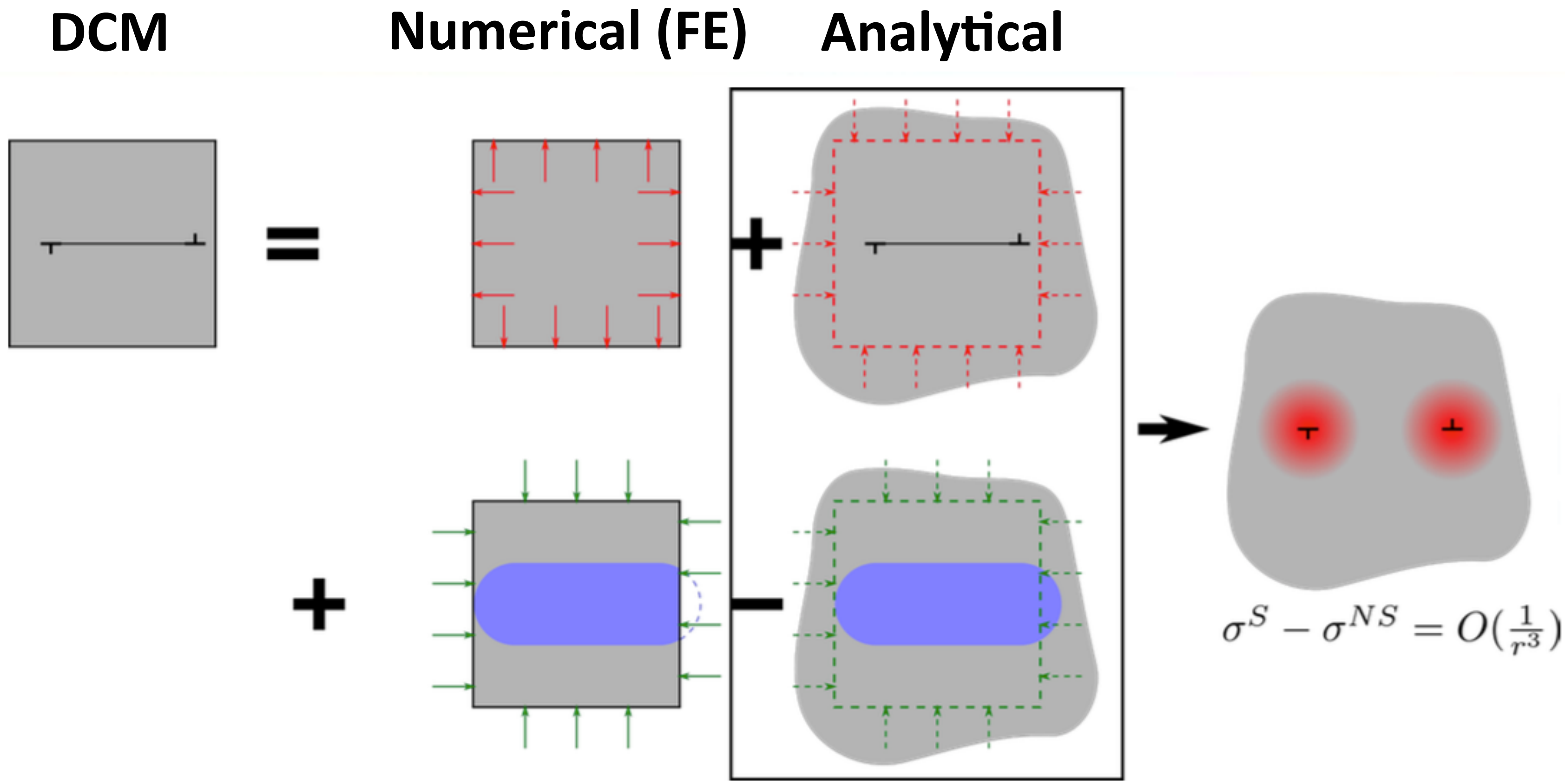
The DCM new solution

The mechanical problem of dislocated solids is now exactly solve





Main benefit of the new solution

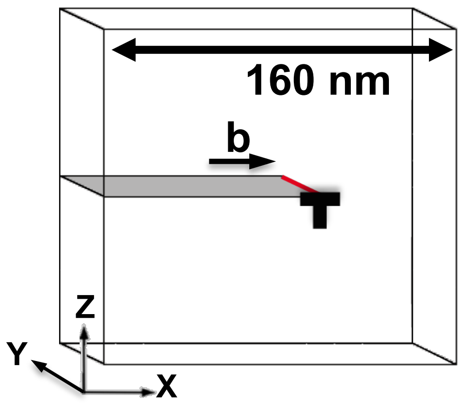


The difference between the two analytical fields is decreasing fast.
Hence, the FE mesh can handle many dislocations in one element!
The boundary value problem is more easily solved!

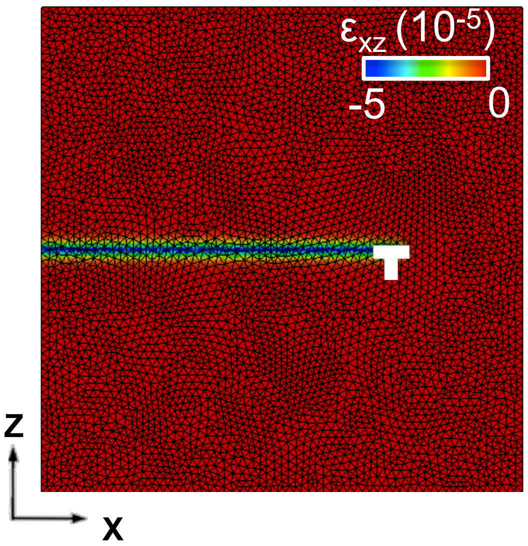
DCM: unstructured meshes

Example: Infinite edge dislocation interacting with 4 free surfaces

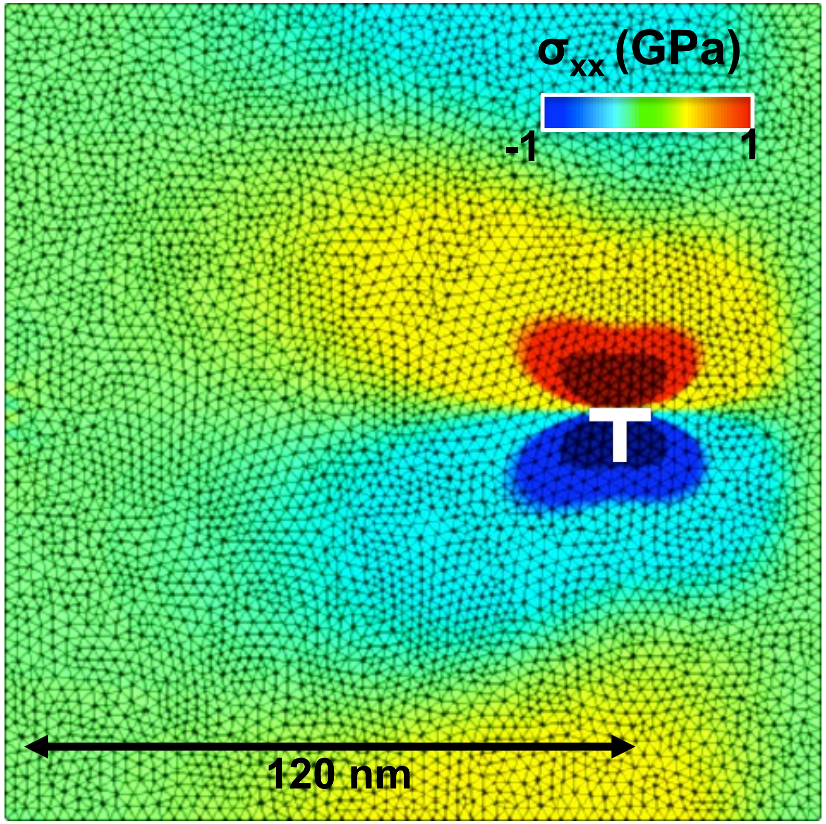
Simulation settings



Plastic eigenstrain



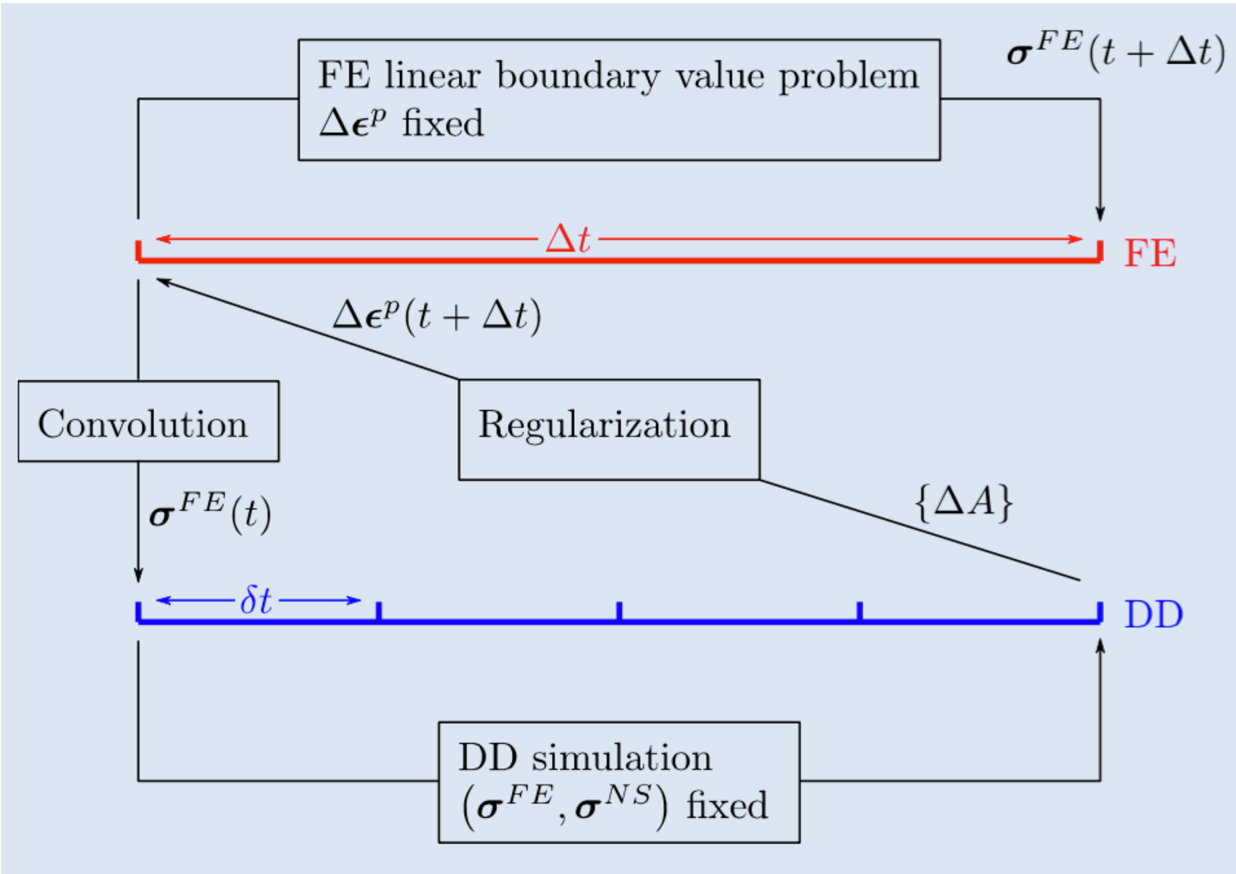
Stress field



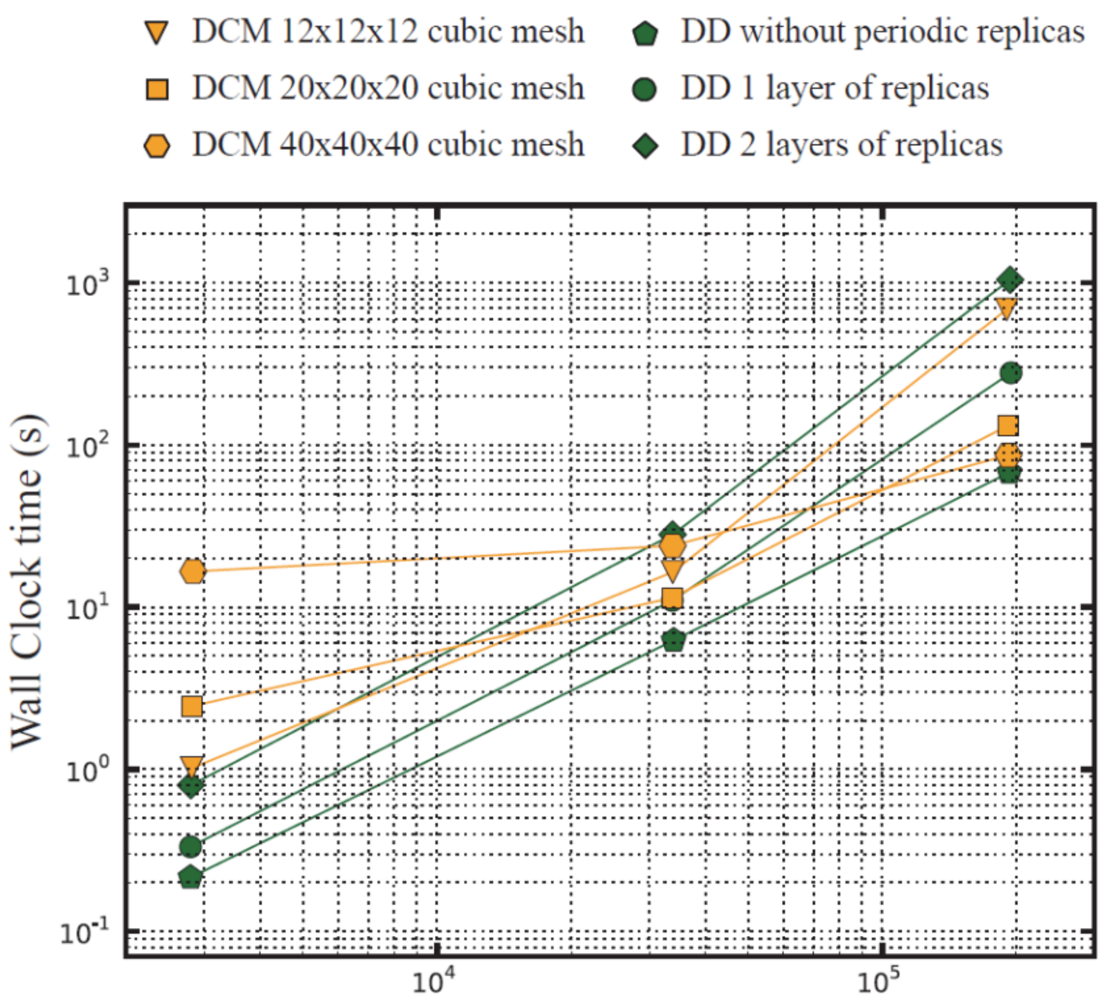
Complex domains

Time integration algorithm

- Linear elasticity problem
- Forward Euler (explicite)
- Two time steps



DCM performance



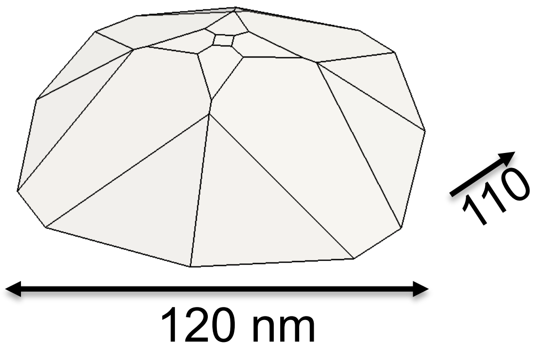
- Periodic system
- DD computations: FMM algorithm, 12 proc MPI
- DCMcomputations : 12 proc MPI, 12 Proc FEM multithread, time step ratio=1
- 24 x X5670 2.9 GHz Xeon CPU

At large number of segments and with a fine mesh, the DCM becomes faster that standard DD simulation codes with the FMM algorithm.

DCM simulation exemples

Plastic deformation in nano-objects

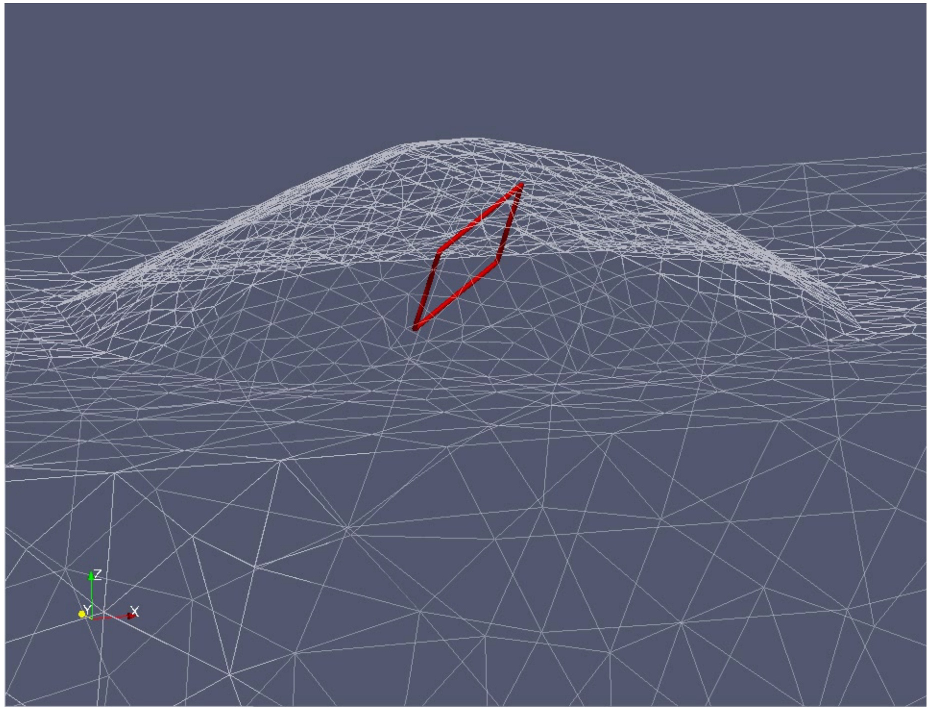
SiGe self-assembled island

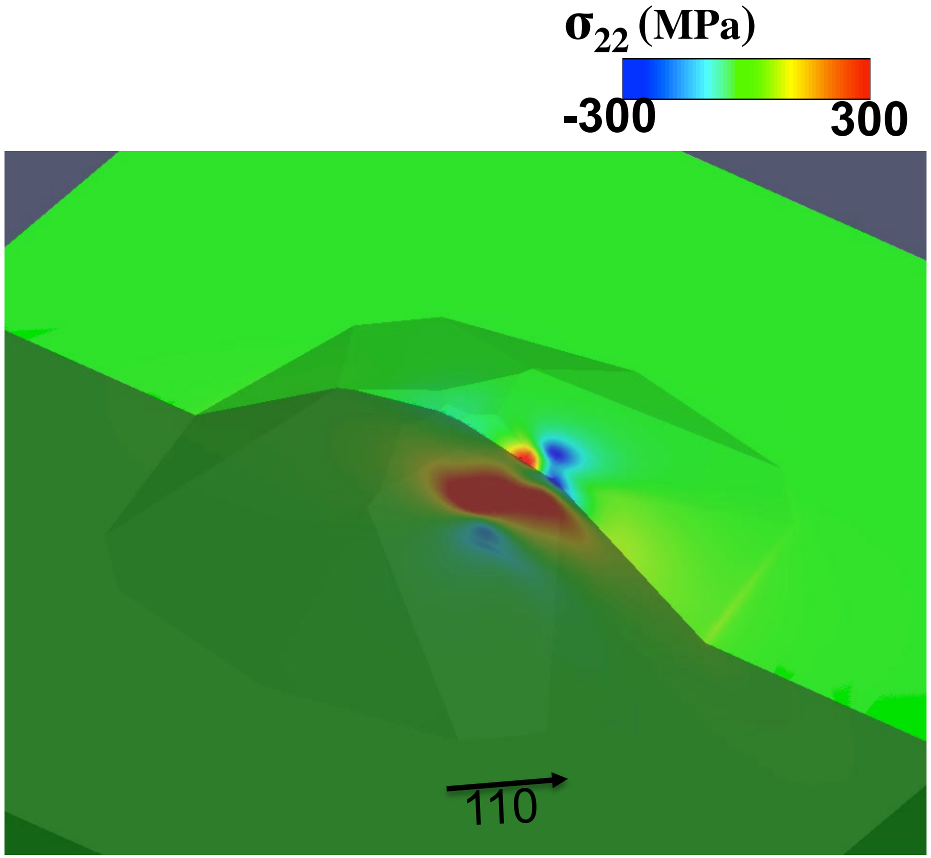


Ge content = 0.4

Anisotropic elastic constant

h= 5 nm





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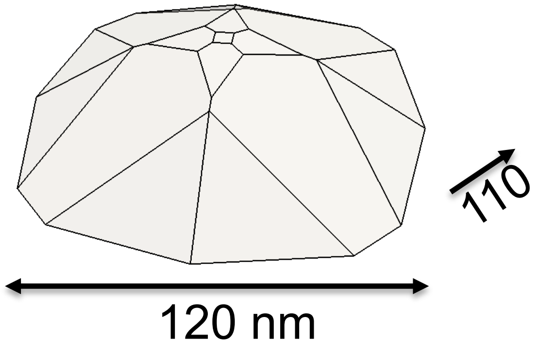

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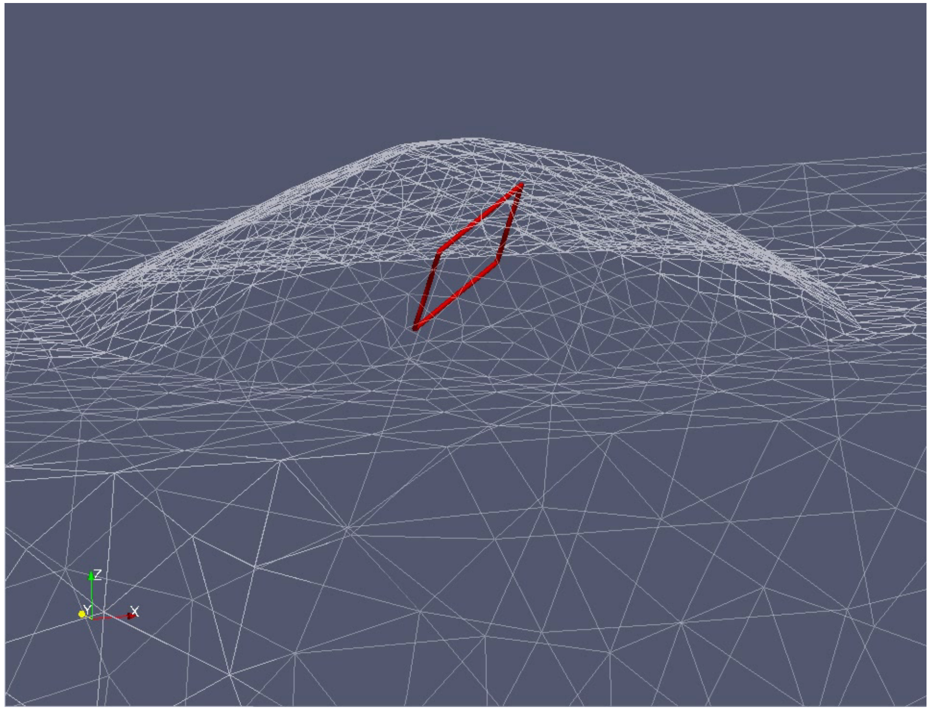

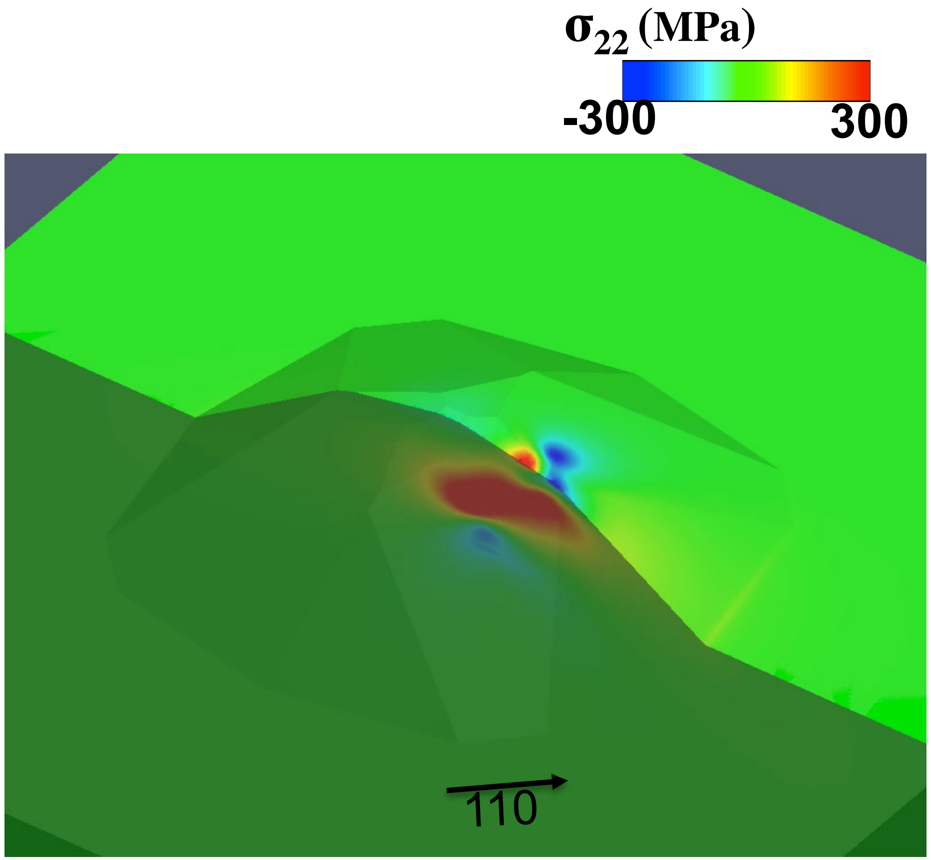

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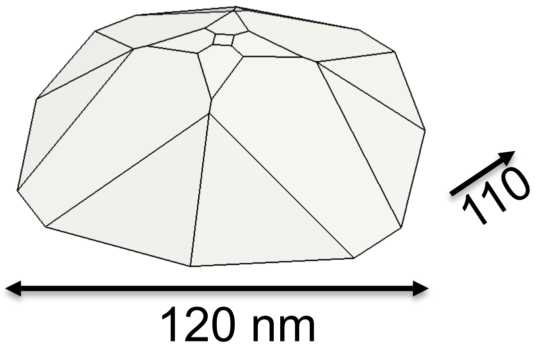

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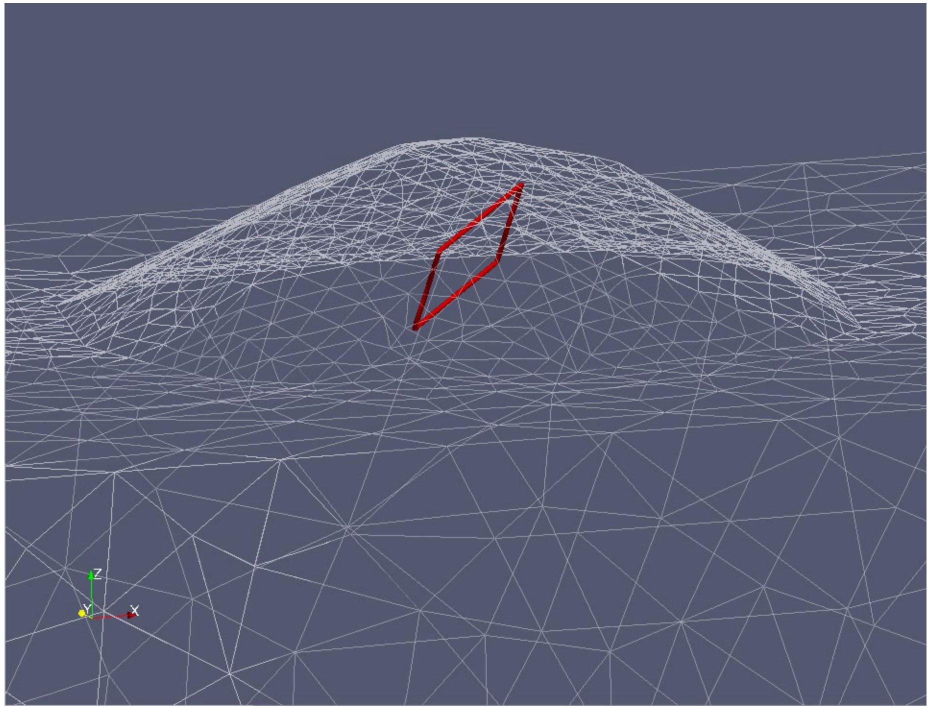
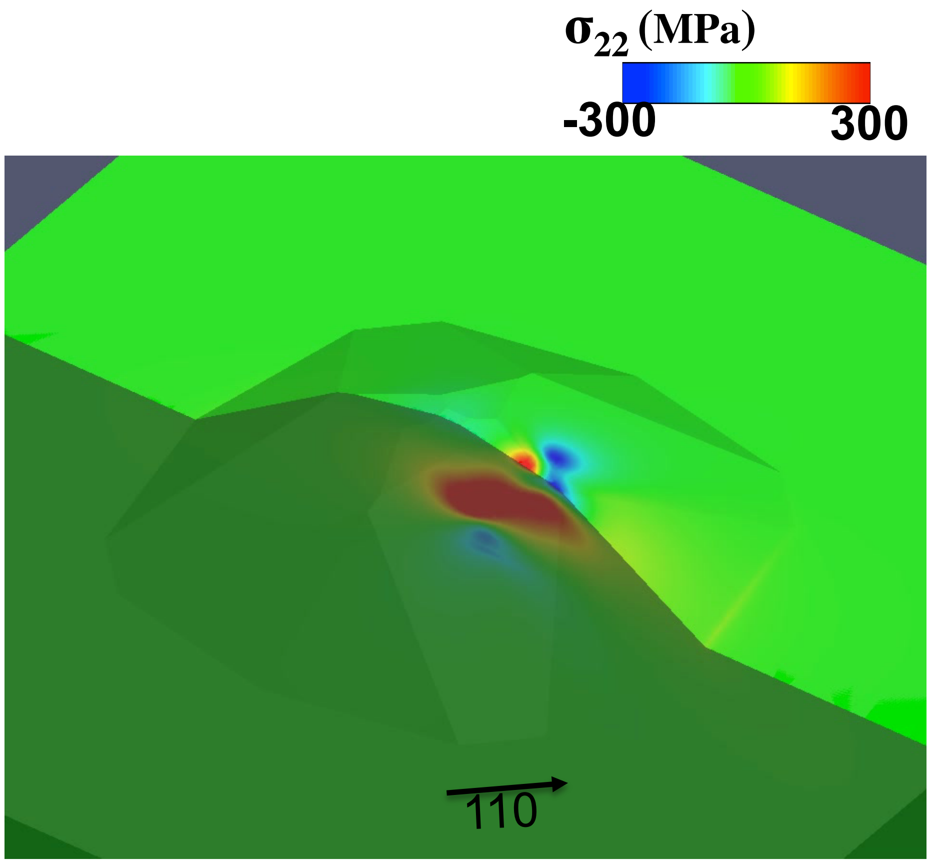
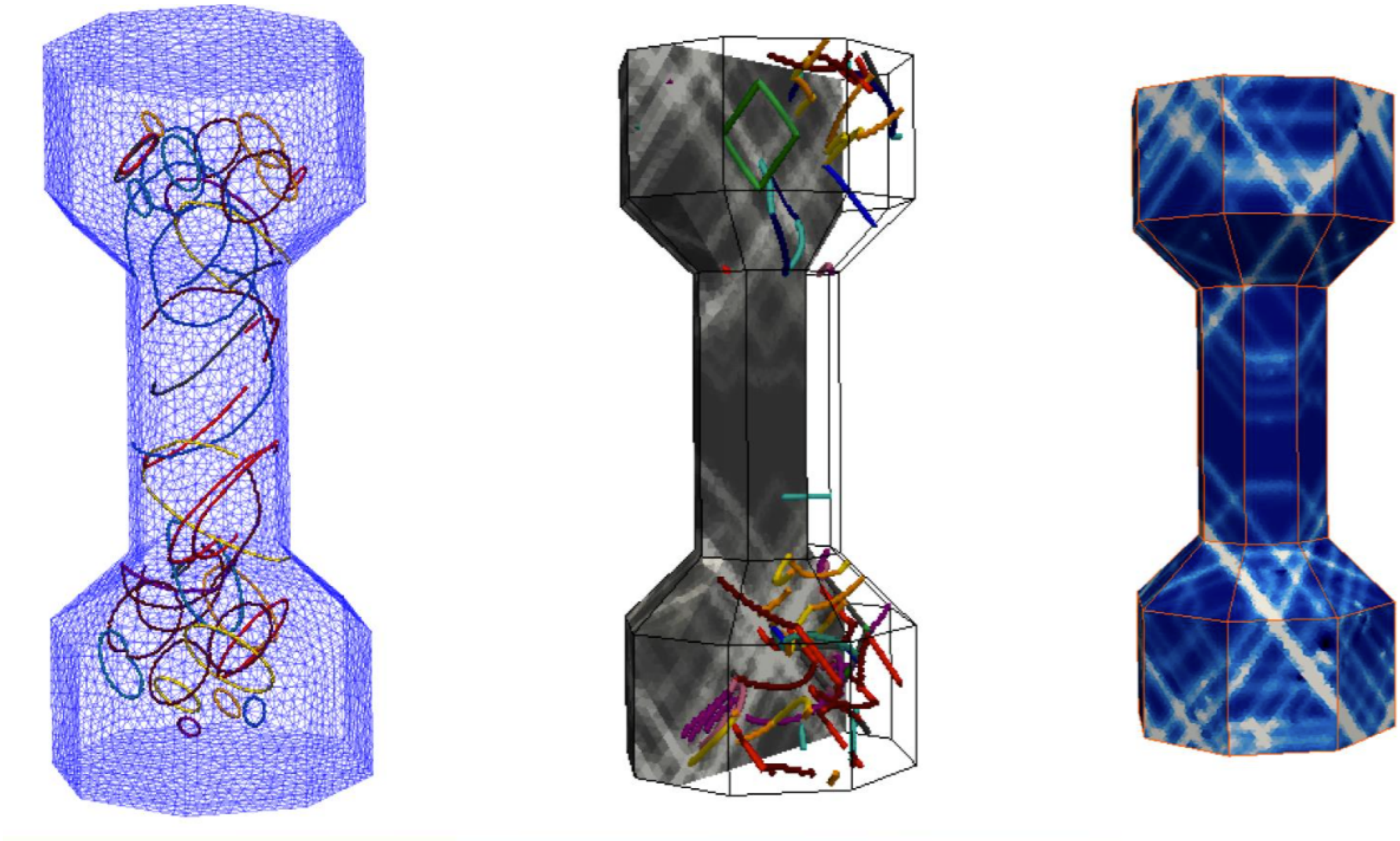




No local correction to study nano-objects (100 nm -500 nm)

Deformation test on a micro-sample

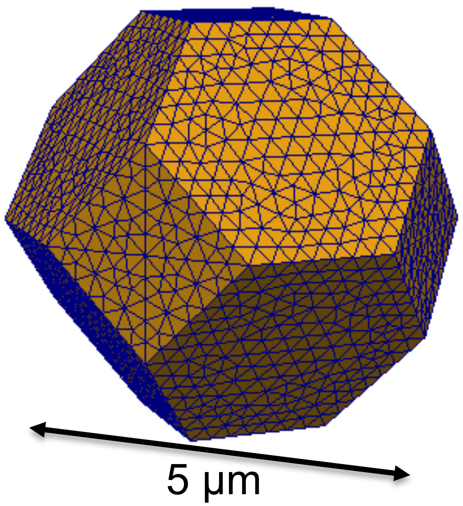
(D=0.5μm)



DD + Crystal Plasticity

Cu polycrystal plastic deformation

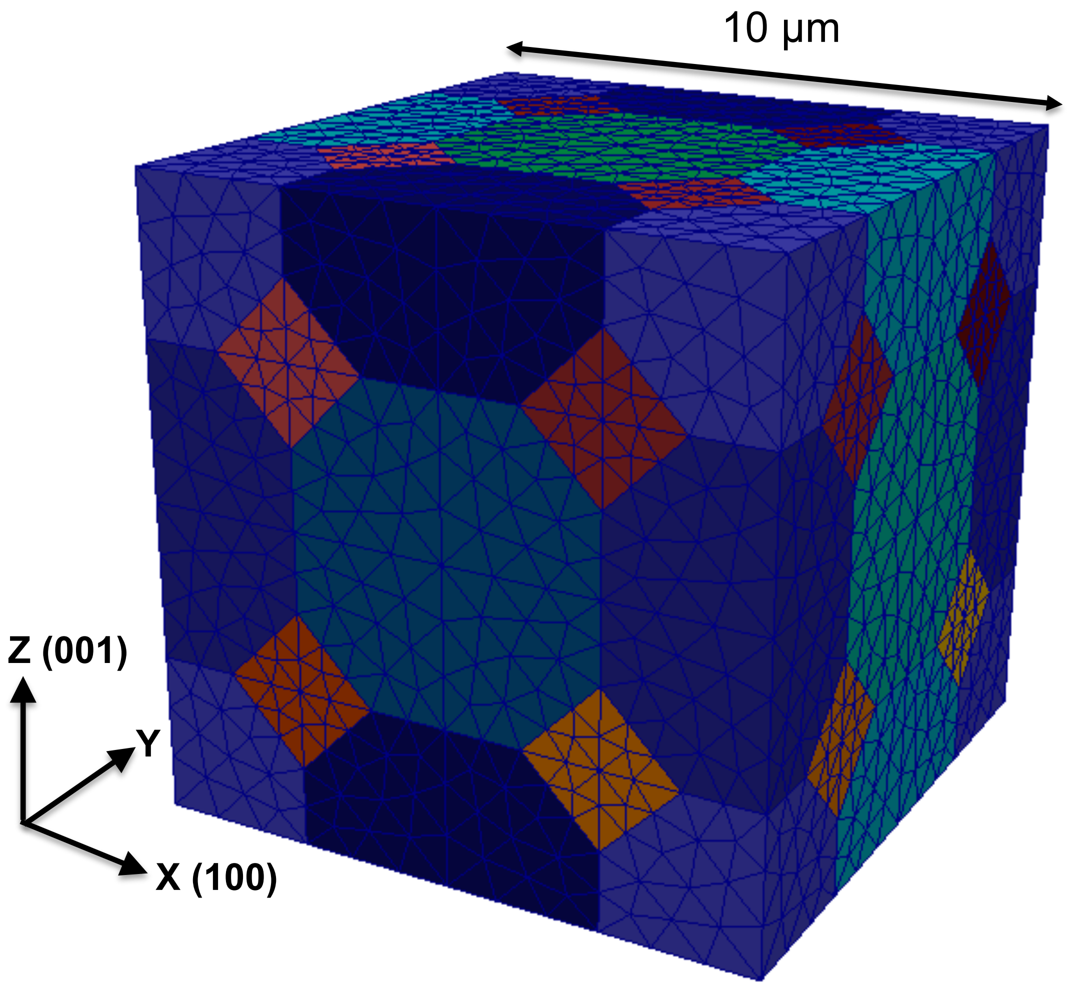
Grain shape



(111) and (001) boundaries

- 1 DCM grain oriented following x, y, z axis (central grain)
- 15 Crystal Plasticity grain randomly oriented

FE Mesh (16 grains)



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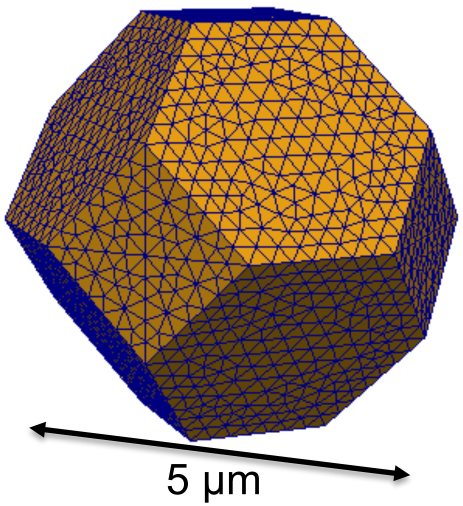
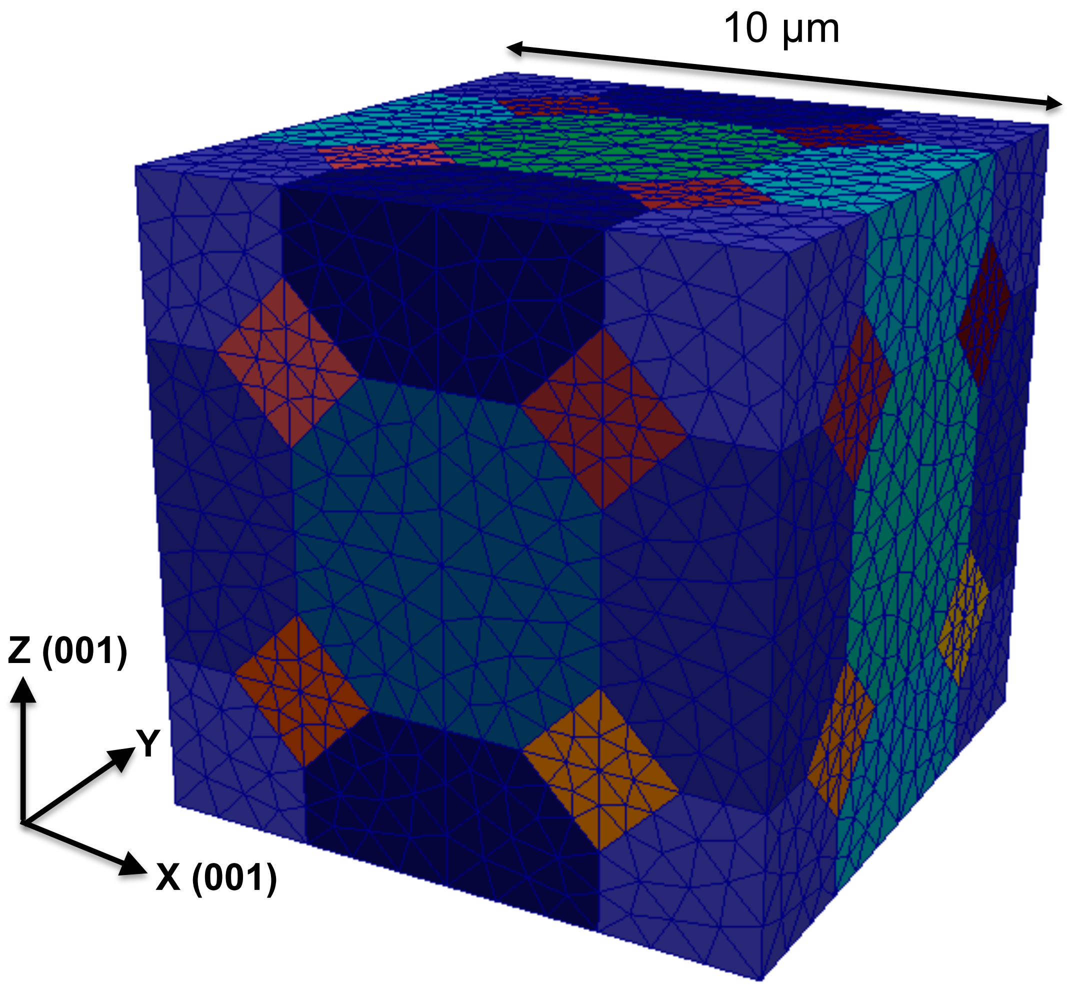


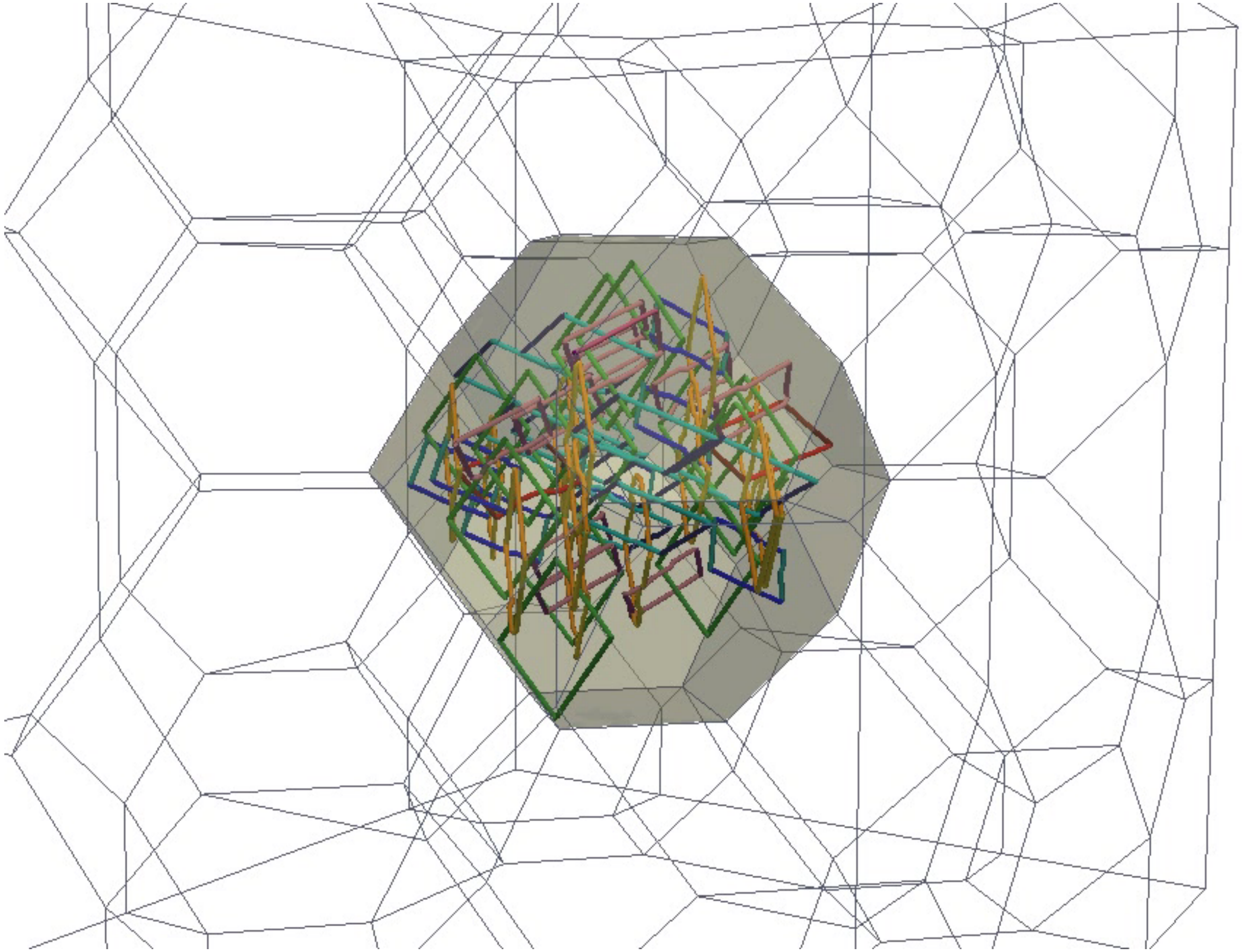
FE Mesh (16 grains)



- Periodic boundary condition in X, Y, Z direction
- uniaxial loading in Z direction
- Strain rate 10^2 s^{-1}
- dislocation density $3x10^{12}$ m^{-2}

DD + Crystal Plasticity

Cu polycrystal plastic deformation



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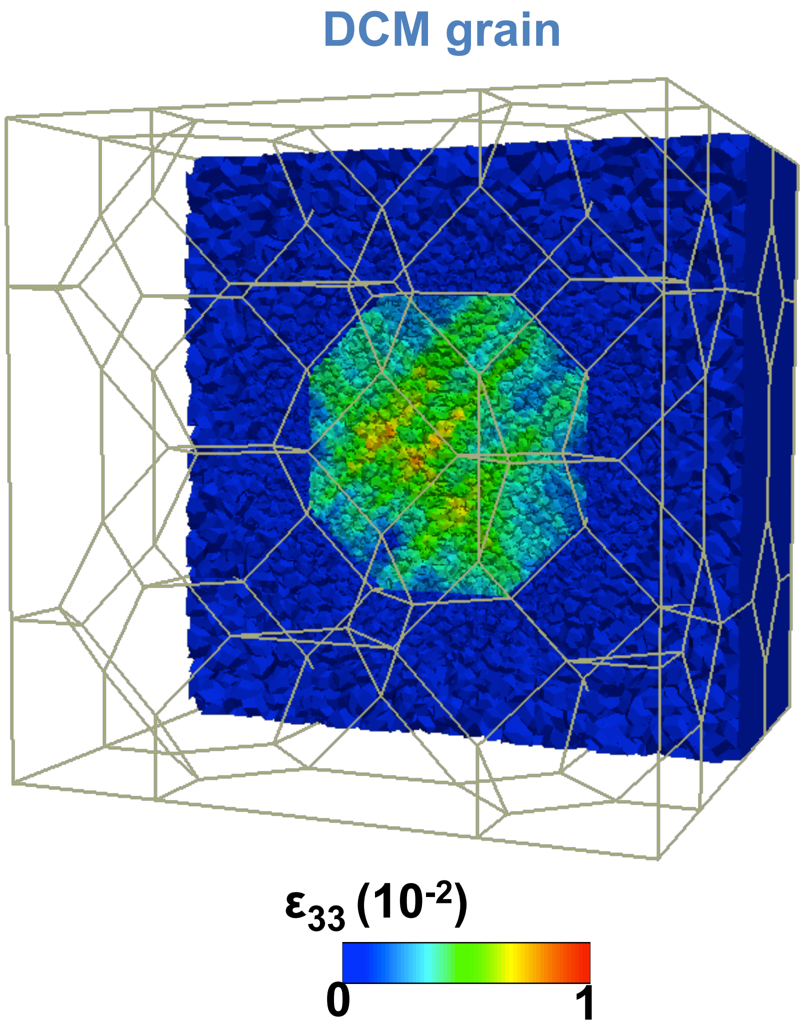

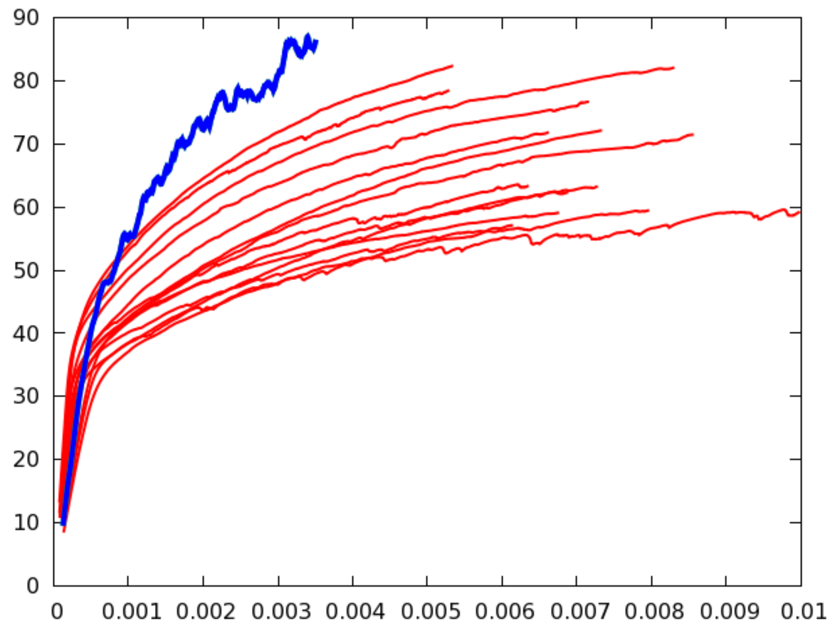

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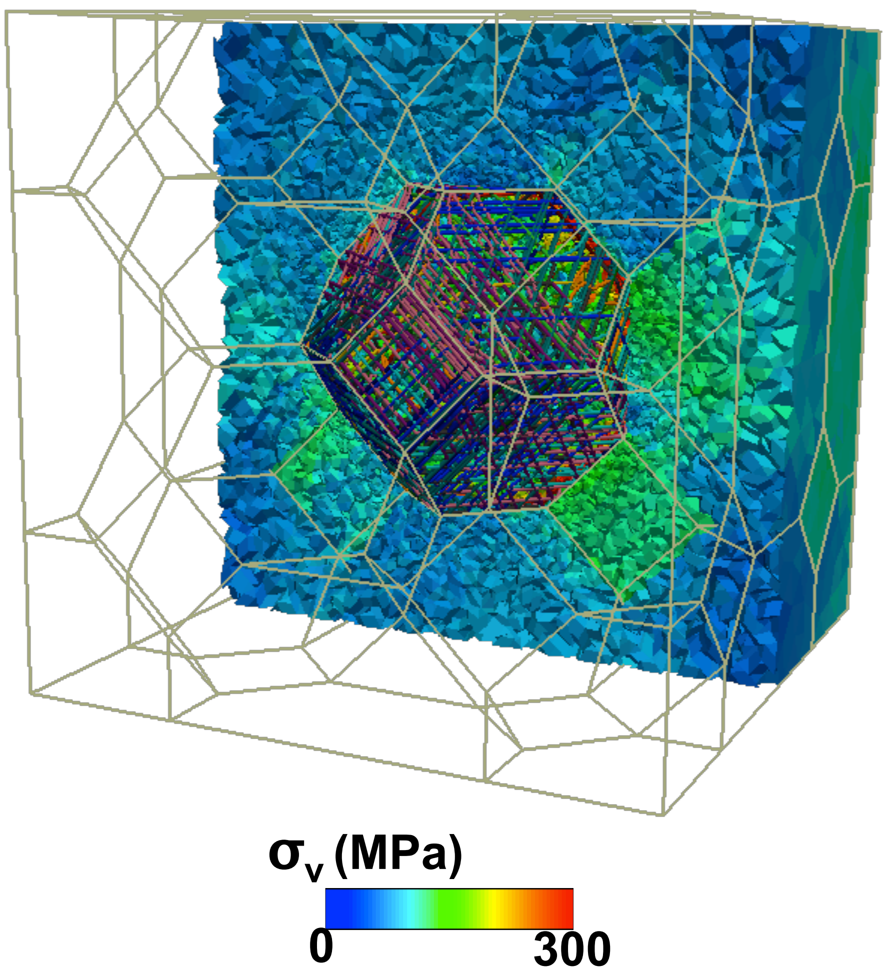
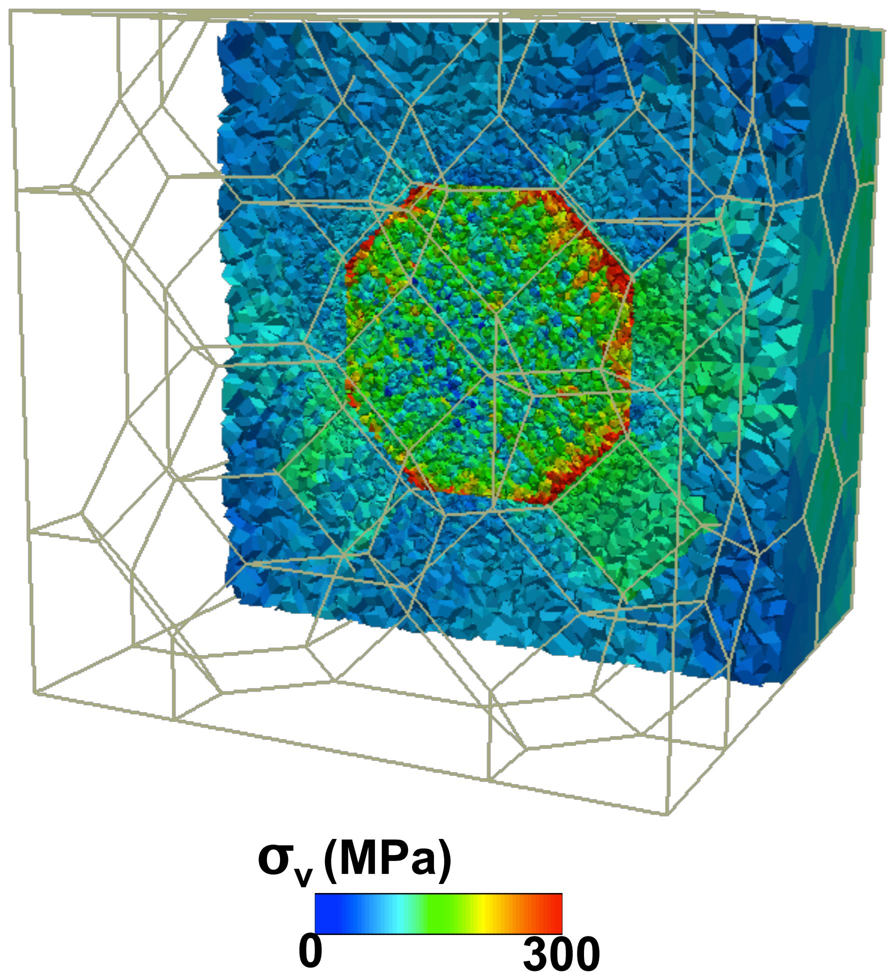
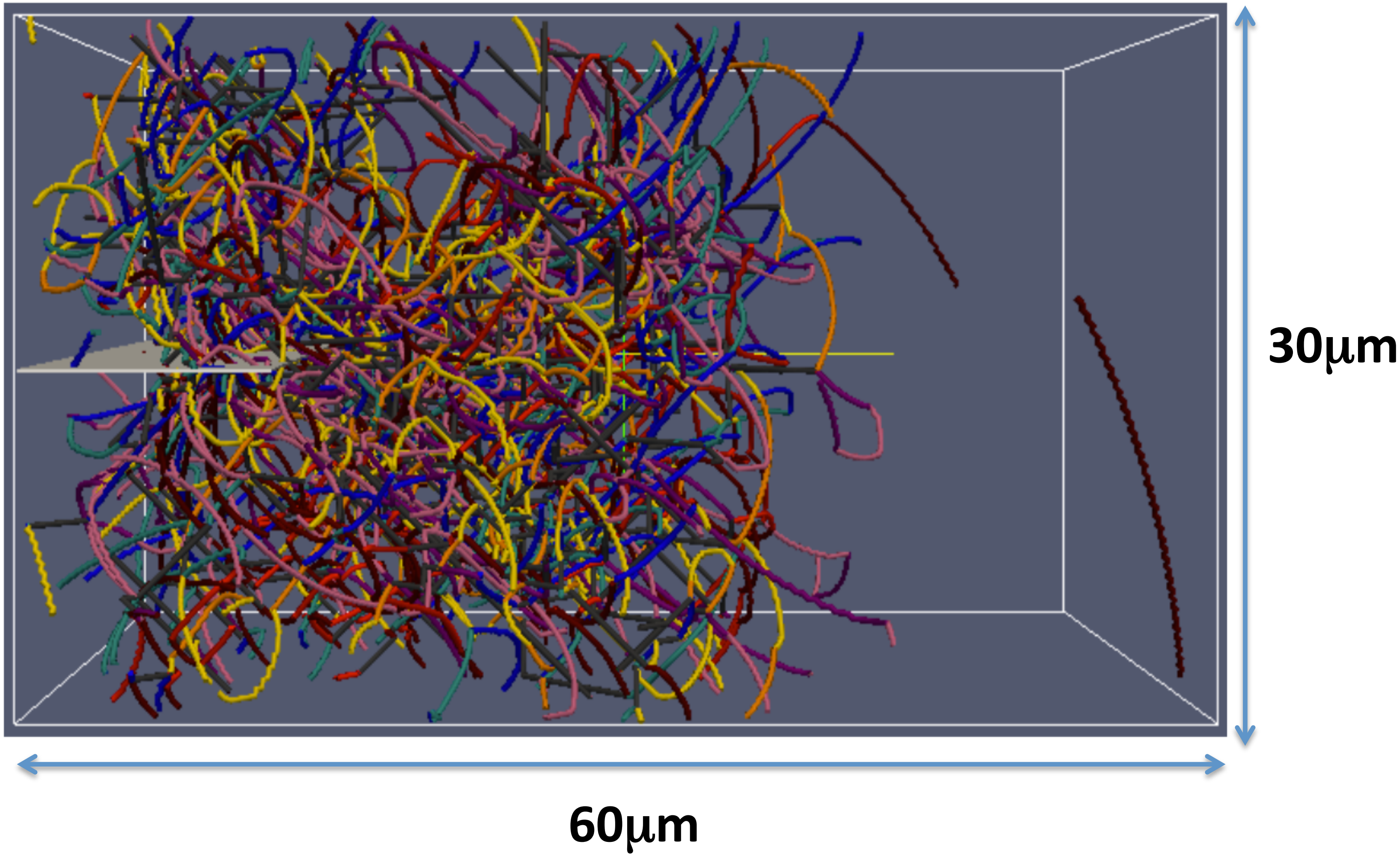


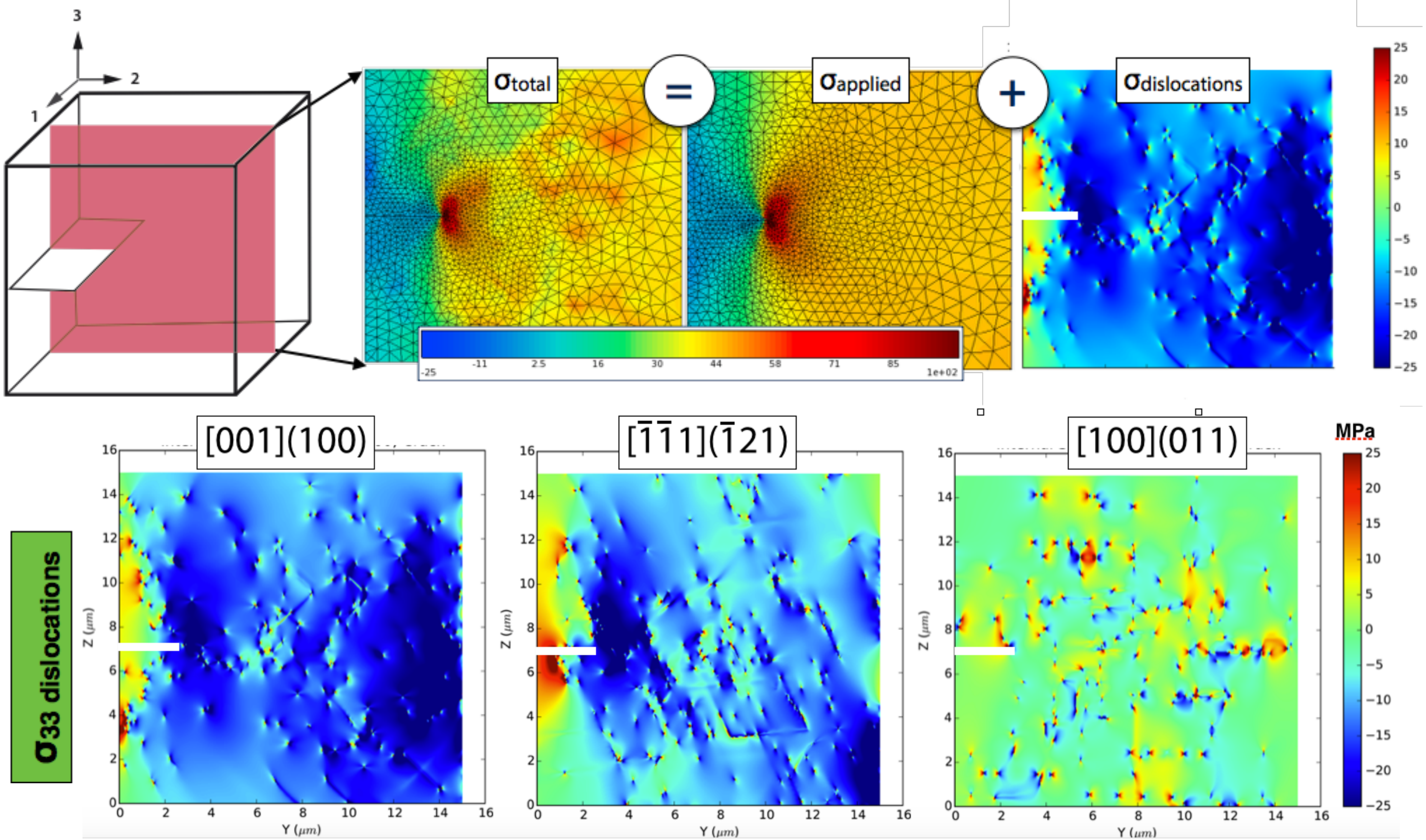


3D dislocation-crack interactions

PhD L. Korzeczek (2013-2016)



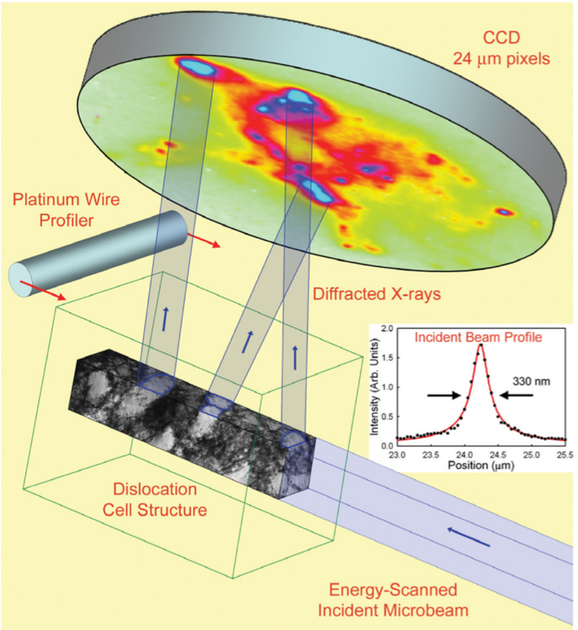
3D Crack Shielding and Blunding



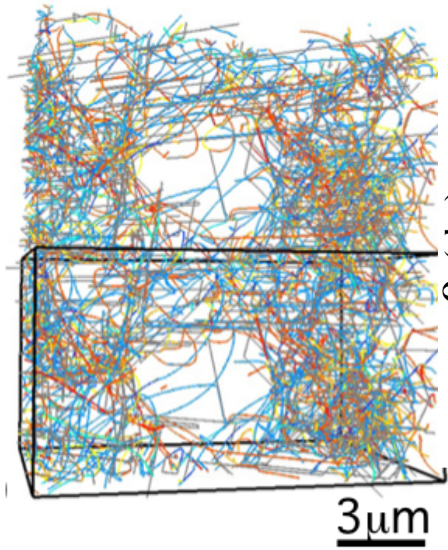
μ-XRD simulations

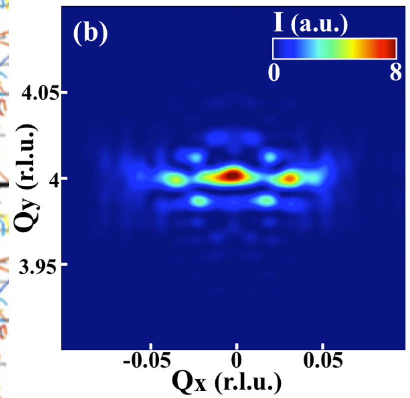
Synchrotron recent improvements

Coll. P. Geantil et M. Kassner (Univ Cal.)



XRD simulation with the DCM





Concluding remarcks

We revised The Discrete Continuum Model (DCM) :

- A new regularization procedure to improve the treatment of short range interaction between dislocations has been introduced

- The possibility of handling unstructured meshes was included in order to run simulation in complex domains

- Performances were improved

↓

> The DCM is a unique and powerful tool to investigate, in a physically justified manner, 3D micro-mechanics problems!

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