

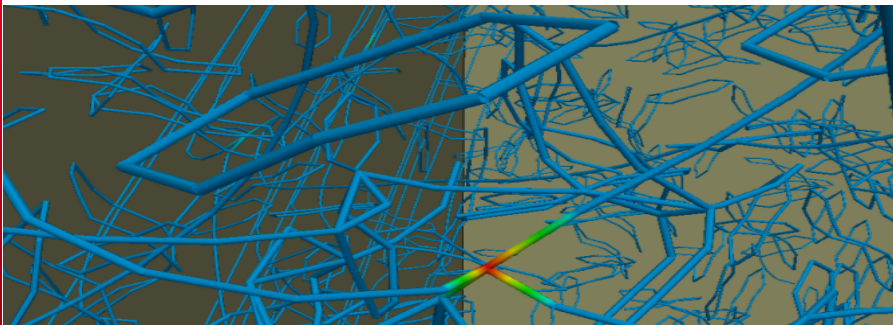
DE LA RECHERCHE À L'INDUSTRIE



Maison de la Simulation

# Dislocation Dynamics Simulation

## Large scale simulations with Numodis



**Arnaud Durocher**

DEN/DMN/SRMA/LC2M

**CEA**

Laurent DUPUY

DEN/DMN/SRMA/LC2M

**Inria**

Olivier COULAUD

HiePACS

| May 12, 2018

## Context

Introduction

Discrete Dislocation Dynamics Simulation

Step-by-Step Algorithm

## Contributions

Distributed datastructure for Dislocation Dynamics

Designing a datastructure for Dislocation Dynamics

Datastructure for distributed memory clusters

Collision algorithm for junction formation

Fast collision detection

Accurate collision handling

## Results

Accuracy

Validation of collision algorithm

Full simulation validation

Performance

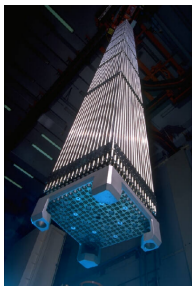
Large scale simulations

### Studied Effects

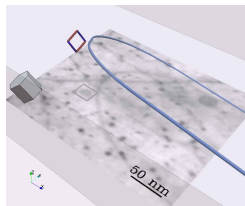
- ▶ Material ageing under irradiation
- ▶ Hardening, embrittlement, creep, ...



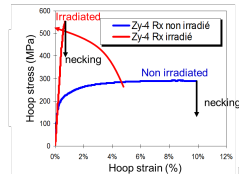
(a) Vessel (Steel)



(b) Fuel Assembly (Zirconium)



(a) Drouet et al. 2016

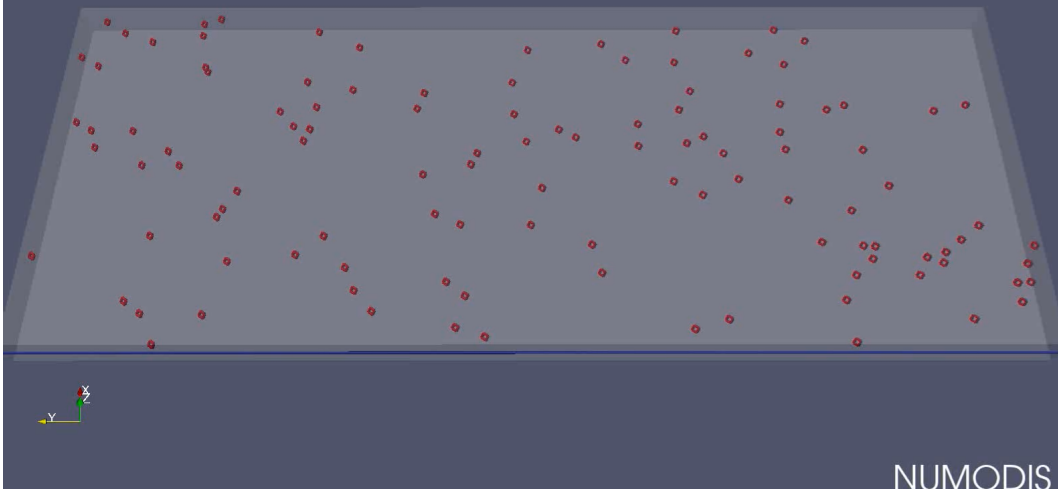


(b) Onimus et al.

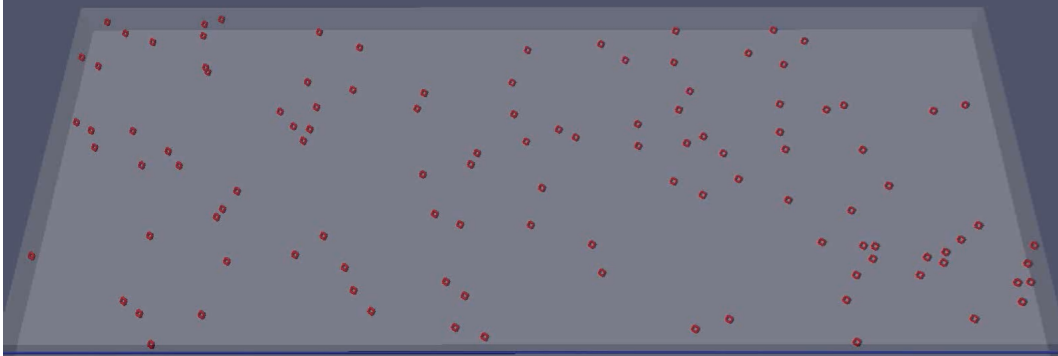
### Dislocations

- ▶ Linear defects in crystalline materials;
- ▶ Modeling plasticity in solids

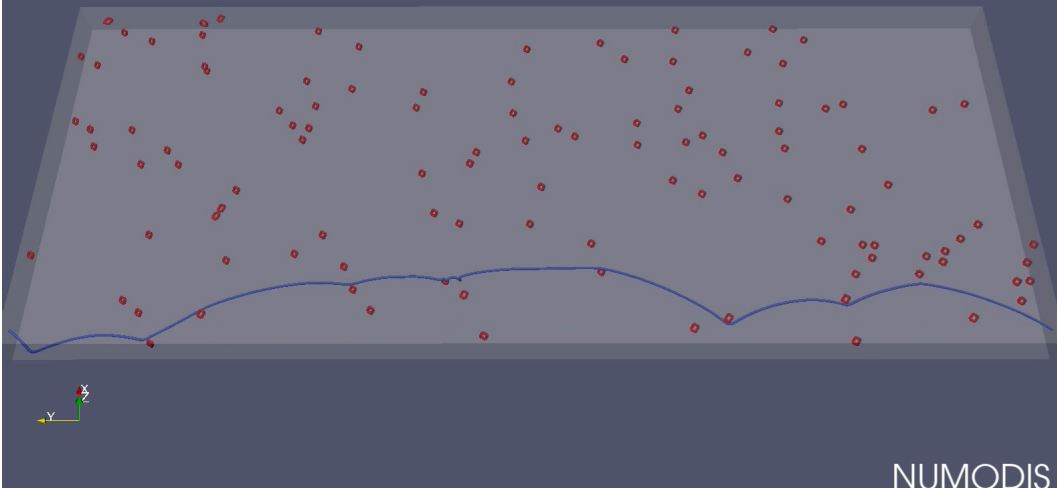
C5: size = 2.6 nm, density =  $4 \cdot 10^{22} \text{ m}^{-3}$



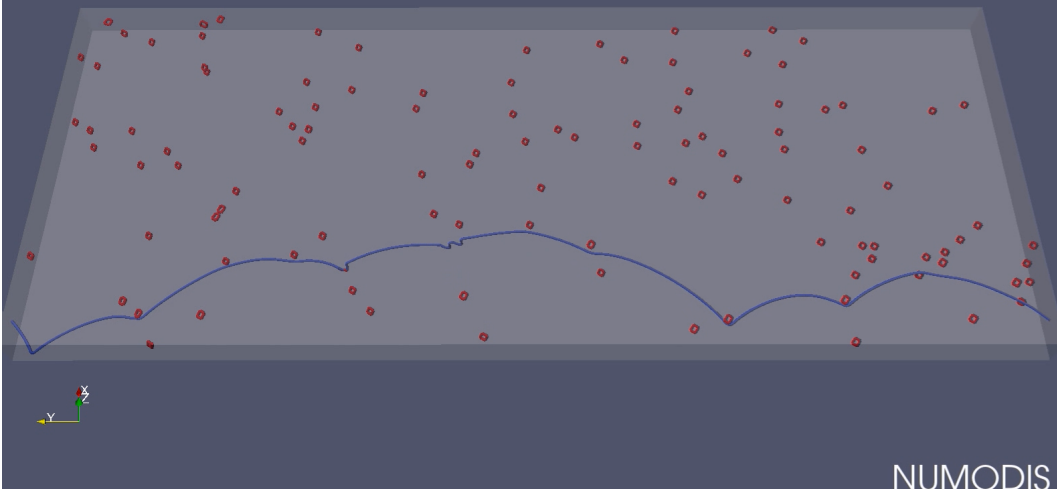
C5: size = 2.6 nm, density =  $4 \cdot 10^{22} \text{ m}^{-3}$



C5: size = 2.6 nm, density =  $4 \cdot 10^{22} \text{ m}^{-3}$

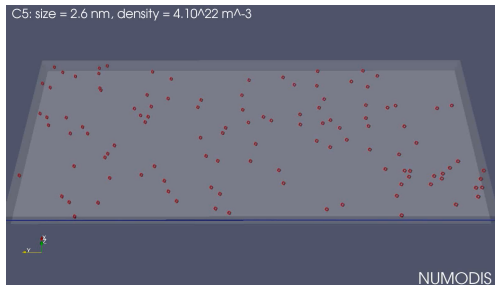


C5: size = 2.6 nm, density =  $4 \cdot 10^{22} \text{ m}^{-3}$



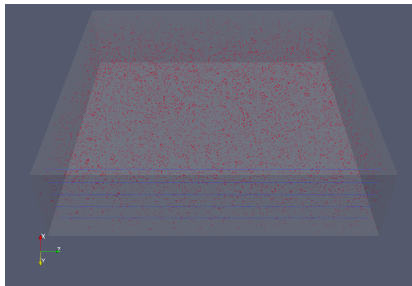
## Numodis

- ▶ Mono-CPU computations
- ▶ Up to 10 000 dislocations segments



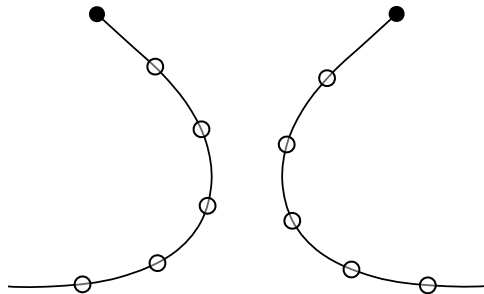
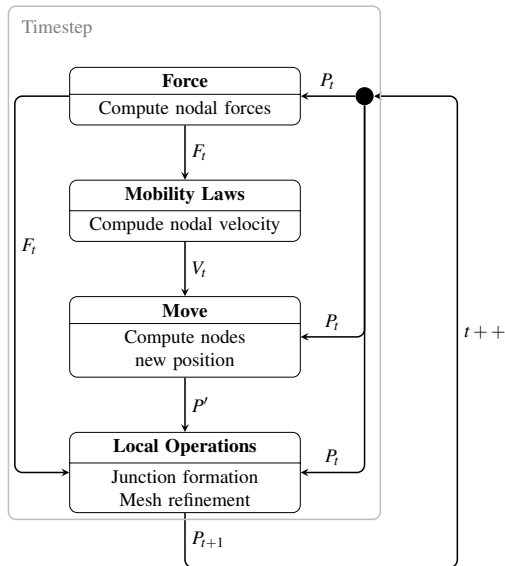
## Parallel Numodis

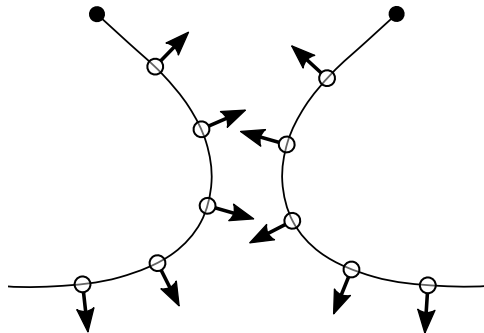
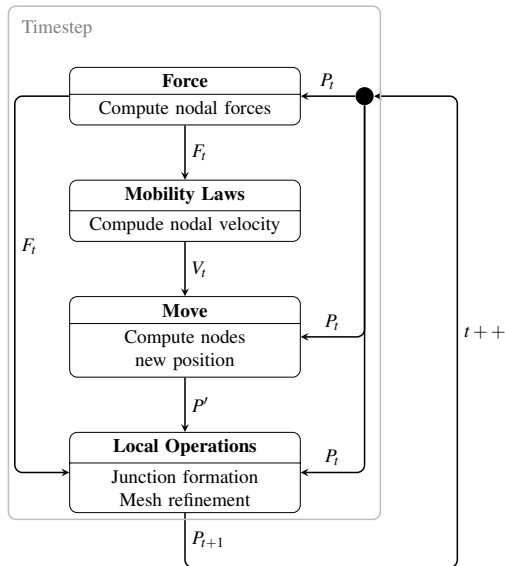
- ▶ Parallel and distributed architectures
- ▶ Up to 1 000 000 dislocations segments

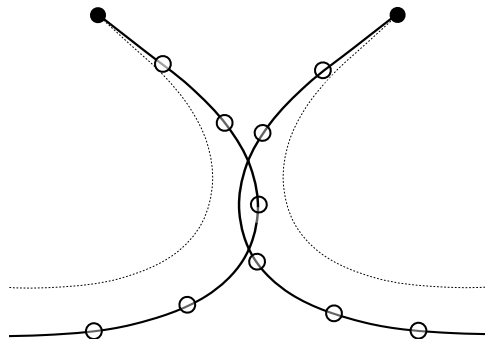
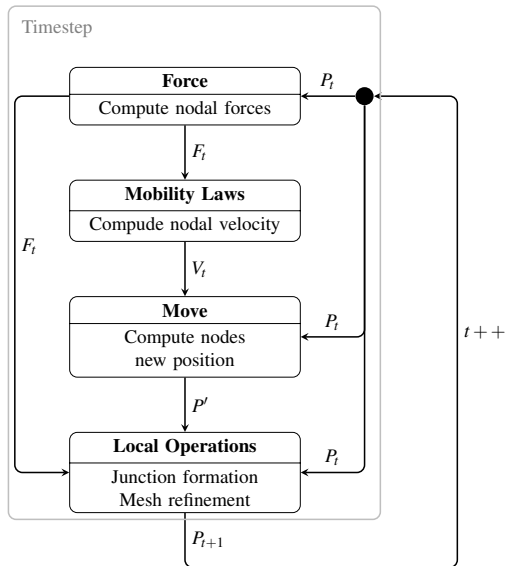


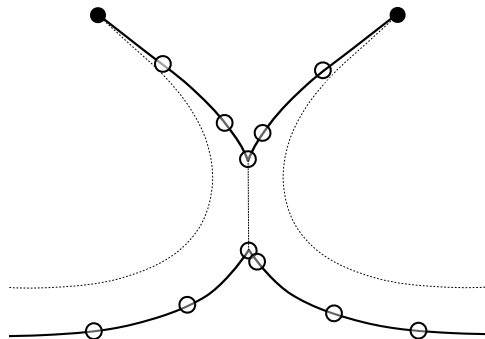
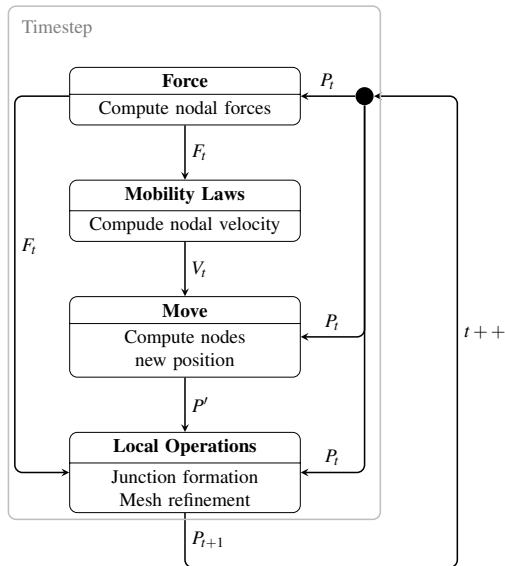
⇒ **Simulate a dislocation mesh dense enough to reliably modelise a grain.**

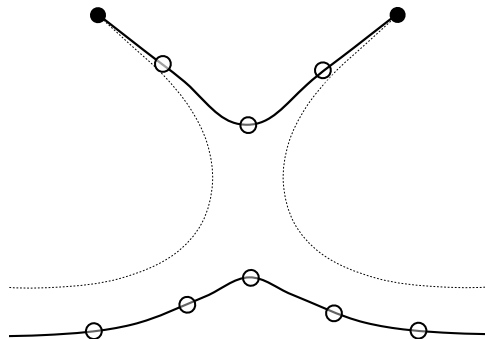
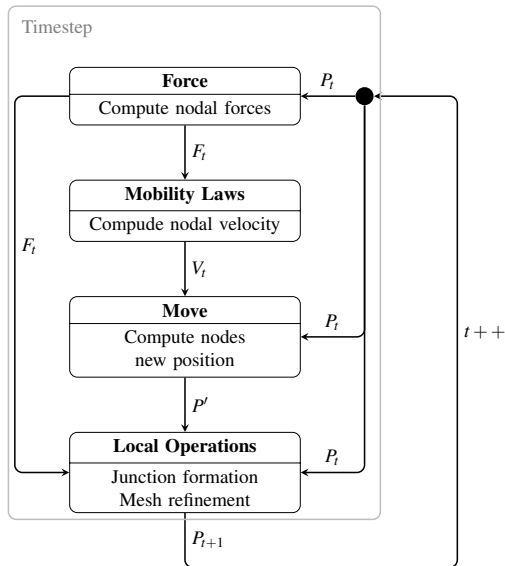


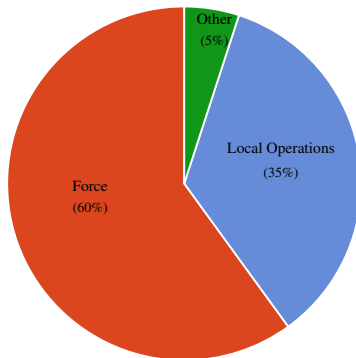
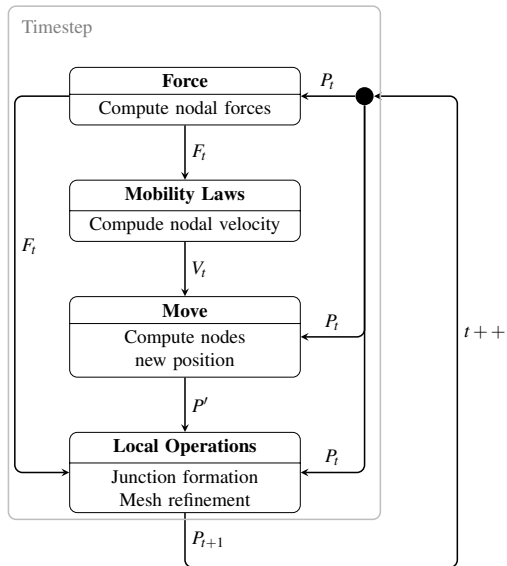




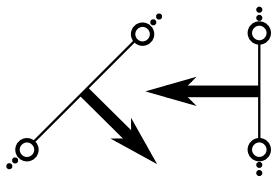








## Fast Multipole Method



Peach-Koehler Force between dislocation segments

### Segment Elastic Interaction

- ▶ Interact with each other

$N^2$  complexity

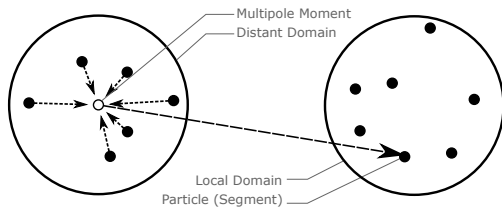
### Fast Multipole Method

- ▶ Far-field approximation
- ▶ Hierarchical Domain Decomposition
- ▶ ScalFMM (inria Hiepac)

$\sim N$  complexity

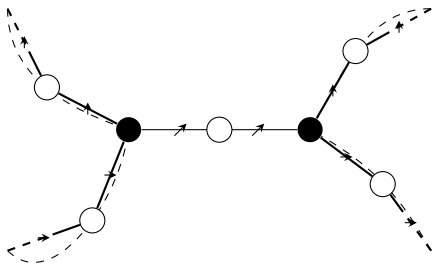
## SCALFMM

C++ Fast Multipole Method Library for HPC



# Contributions





## Node and segment data

Nodes :

- ▶ Position
- ▶ Velocity
- ▶ Force

Segments :

- ▶ End nodes forces
- ▶ Physical properties
  - ▶ Burgers vector
  - ▶ Glide plane

## Operations on data

Topological operations :

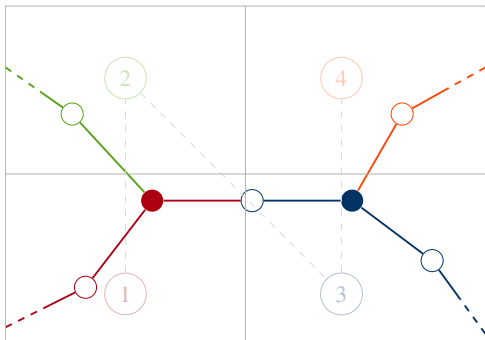
- ▶ Add/remove nodes
- ▶ Add/remove segments

→ *Dynamic mesh*

Iterate over nodes and segments:

- ▶ Nodes with connected segments
- ▶ Segments with connected nodes

→ *Irregular access*



## Distributed data (MPI)

- ▶ Too big to fit in 1 computer
- ▶ Distributed supercomputers

## Challenges

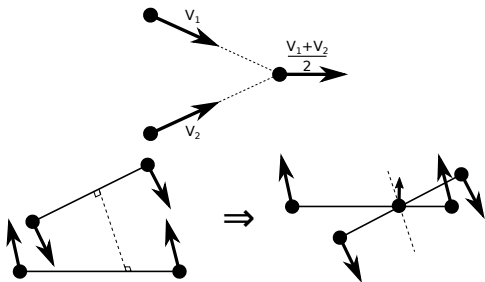
- ▶ Keep data coherency
- ▶ Access remote data

## ⇒ Distributed Abstract Datatype

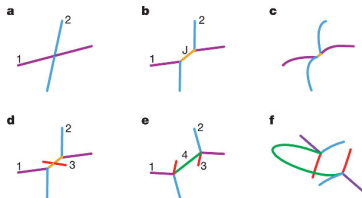
- ▶ Safe mesh modification
- ▶ Safe access to remote data
- ▶ Easier to use to write algorithms
- ▶ Easier to change implementation

## Dislocation Junctions

- ▶ Merging of dislocations at collision;
- ▶ Important role in material behavior (strain and radiation hardening)



Dislocation multi-junctions and strain hardening  
(Bulatov et al. - nature 2006)



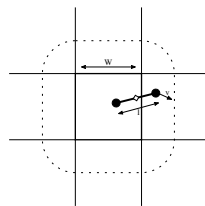
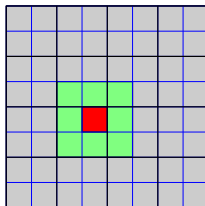
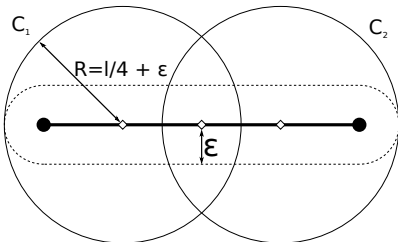
## Simulate junction formation

- ▶ **Collision detection** (N body)  
→  $N^2$  complexity
- ▶ Handle dislocation merging.

## Uniform grid space partitioning

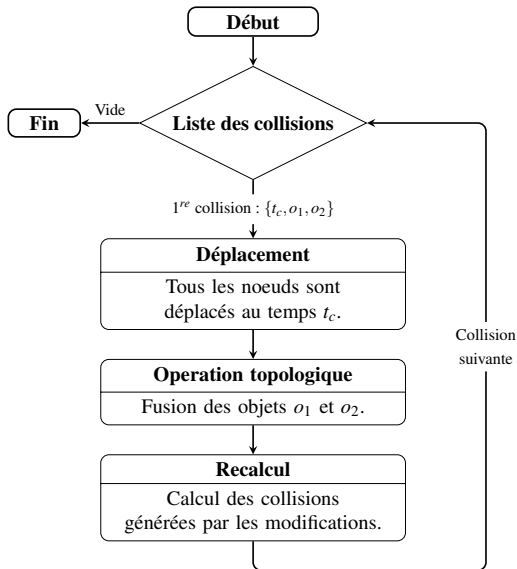
- ▶ Only test collision on nearby boxes;
- ▶ Determined the minimum box size  
*Depends on object size and velocity*

**Complexity  $N^2$  to  $\sim N$**



## Bounding spheres

- ▶ Segments simplified by 2 spheres;
- ▶ Sphere/Sphere collision faster to detect;
- ▶ Smaller objects = Smaller box size.



## New topological operations

- ▶ Nodes/segments fusion on collision
- ▶ Using new datastructure

## Collision recomputation

- ▶ Mesh modifications can generate more collisions
- ▶ One object can collide into multiple objects in one timestep

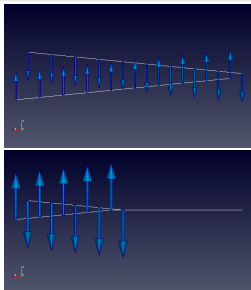
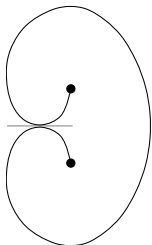
⇒ **More reliable collision handling**

# Results

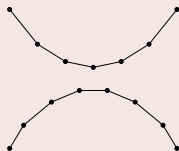
### More reliable collision handling

- ▶ Complex geometry;
- ▶ Multiple collisions.

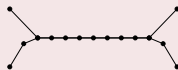
Detect collisions missed before



### Impact of collision recomputation



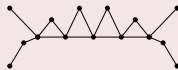
(a) Initial ( $t=0$ )



(b) Expected result



(c) Result with recomputation



(d) Result without recomputation

## Simulation is validated with known results from the litterature



Figure: The Frank-Read source



## Simulation is validated with known results from the litterature



Figure: The Frank-Read source

## Simulation is validated with known results from the litterature

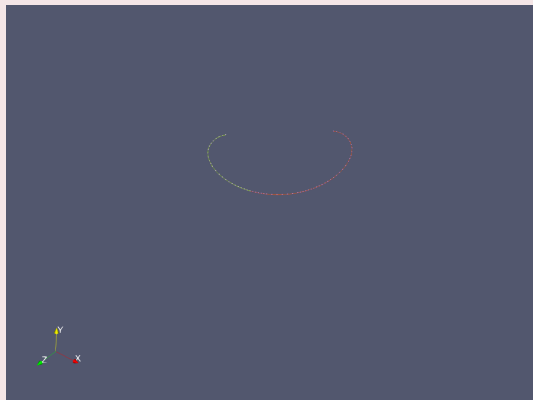


Figure: The Frank-Read source

## Simulation is validated with known results from the literature

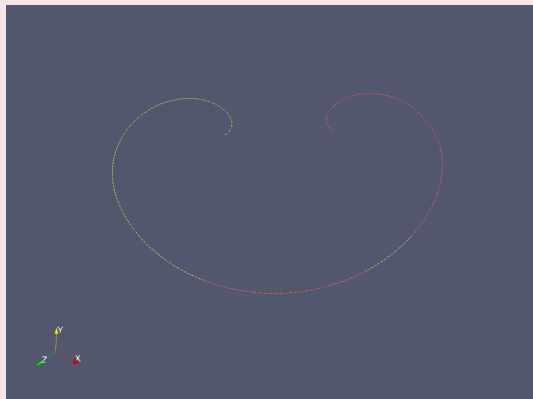


Figure: The Frank-Read source

## Simulation is validated with known results from the literature

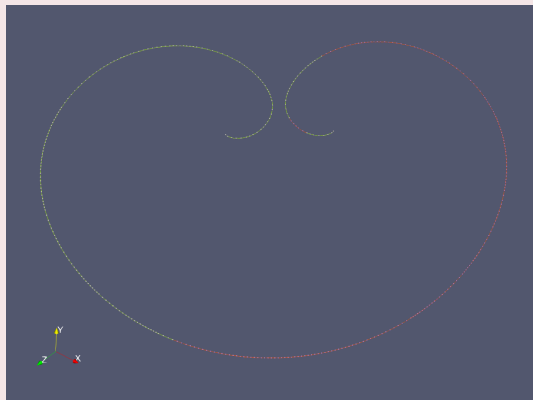
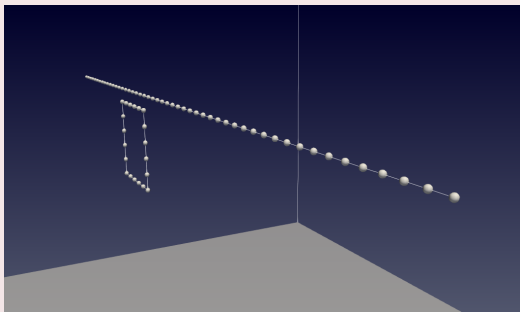
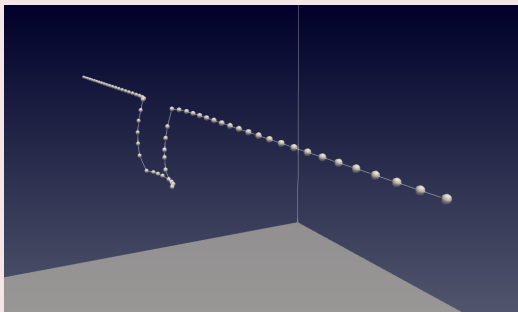


Figure: The Frank-Read source

## Simulation is validated with known results from the litterature



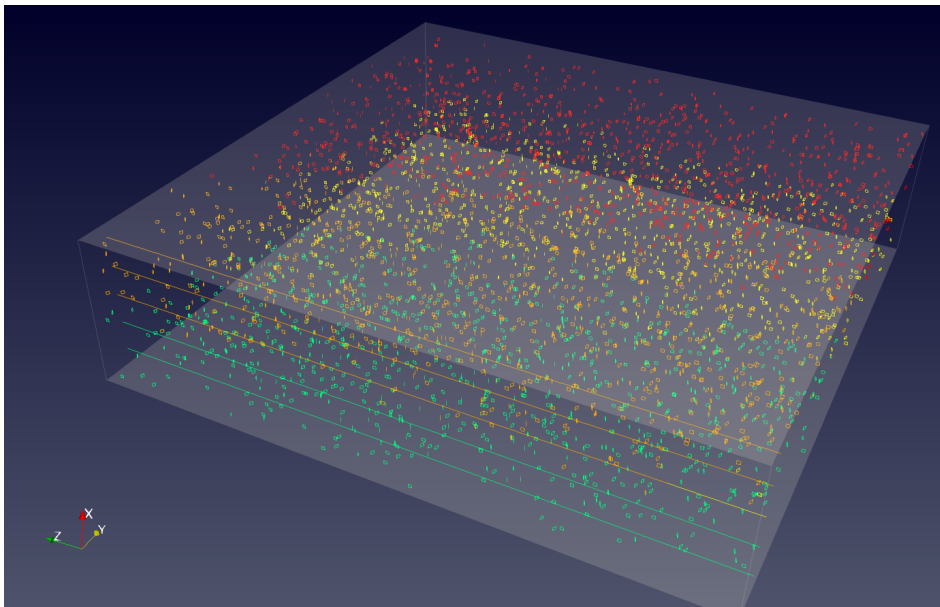
(a) Initial situation

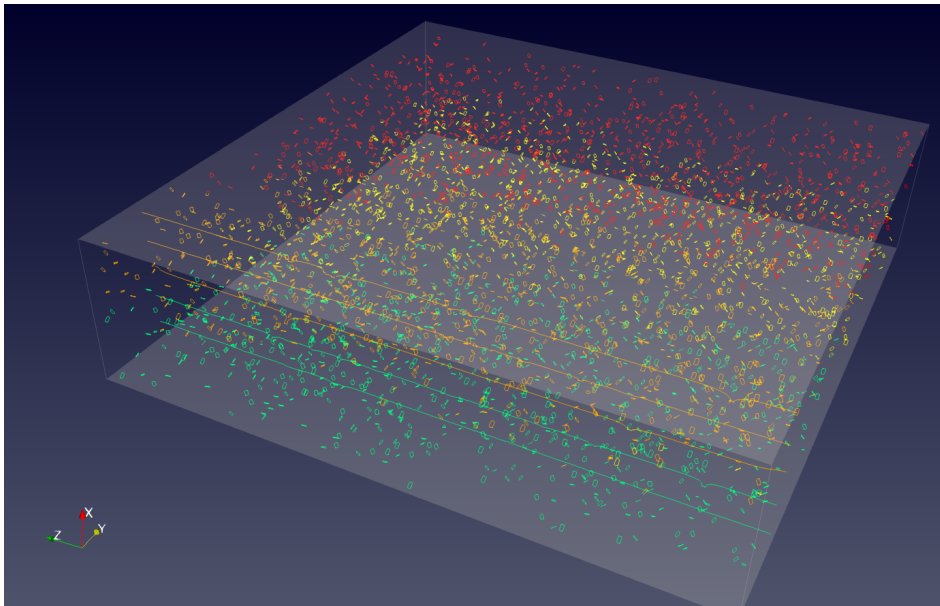


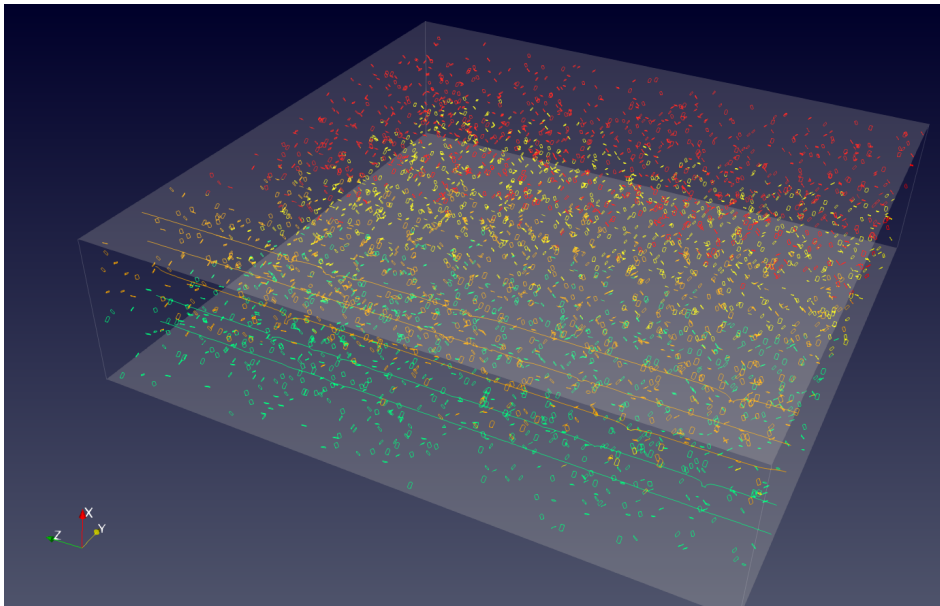
(b) Final situation

Comparison to known Molecular Dynamics simulations <sup>a</sup>

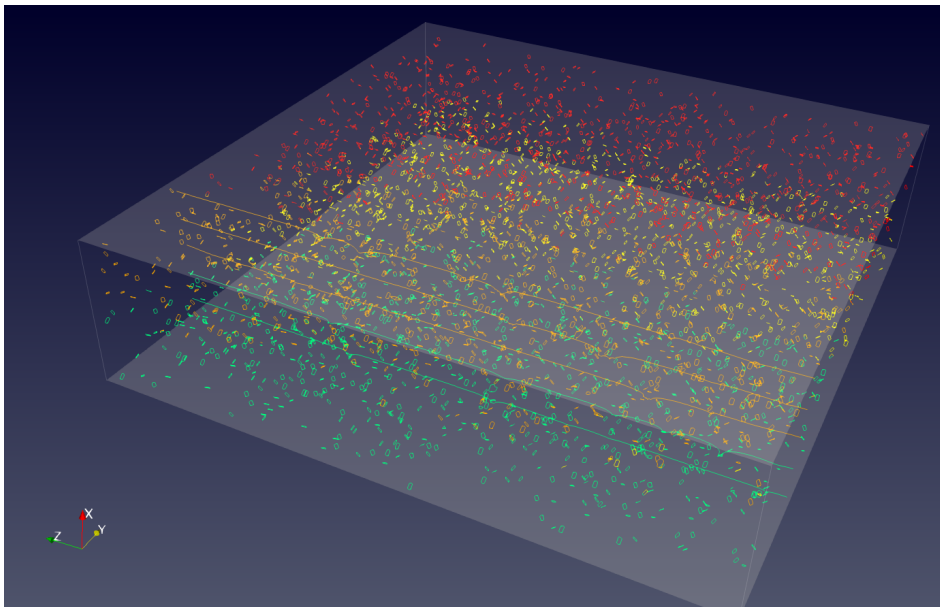
<sup>a</sup>Serra & Bacon - 2013 - "Atomic-level computer simulation of the interaction between  $\frac{1}{3}\langle 11\bar{2}0\rangle\{1\bar{1}00\}$  dislocations and  $\frac{1}{3}\langle 11\bar{2}0\rangle$  interstitial loops in  $\alpha$ -zirconium"

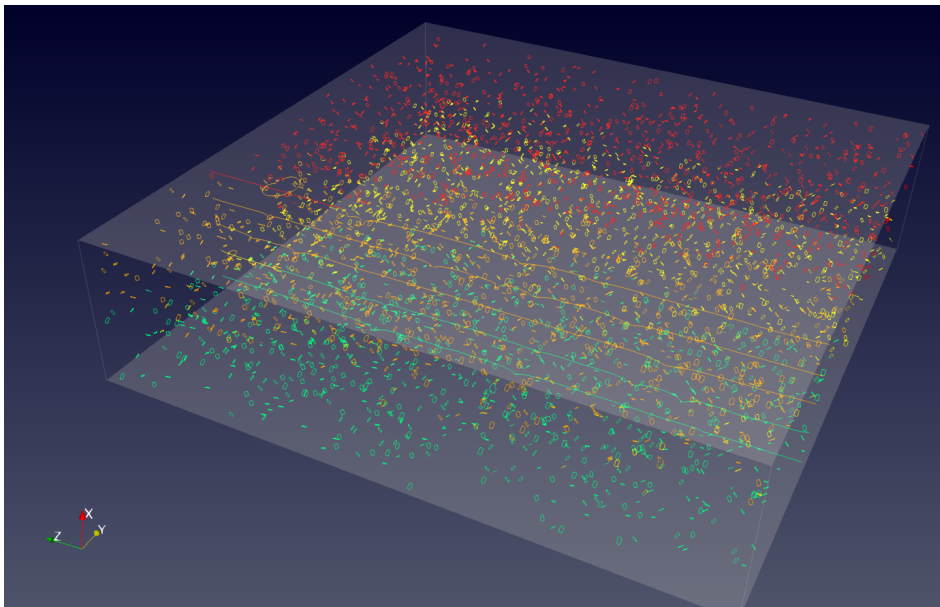












## Conclusion

### Improved Reliability

- ▶ New Abstract datastructure
- ▶ More Reliable algorithms (collisions)

### Parallel performance

- ▶ Using MPI + OpenMP parallelism
- ▶ Using Hierarchical algorithms

⇒ Simulating 100 000<sup>+</sup> dislocation segments sceneries overnight

## Ongoing work and perspectives

### Physical Validation

- ▶ Measure result accuracy
- ▶ Bigger simulations using more cluster nodes

### Performance improvement and validation

- ▶ Experiment with datastructure implementations
- ▶ Parallel scalability

# The end.

Thank you