NePeR : Un programme pour la generation de microstructures

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Applications a la plasticite cristalline

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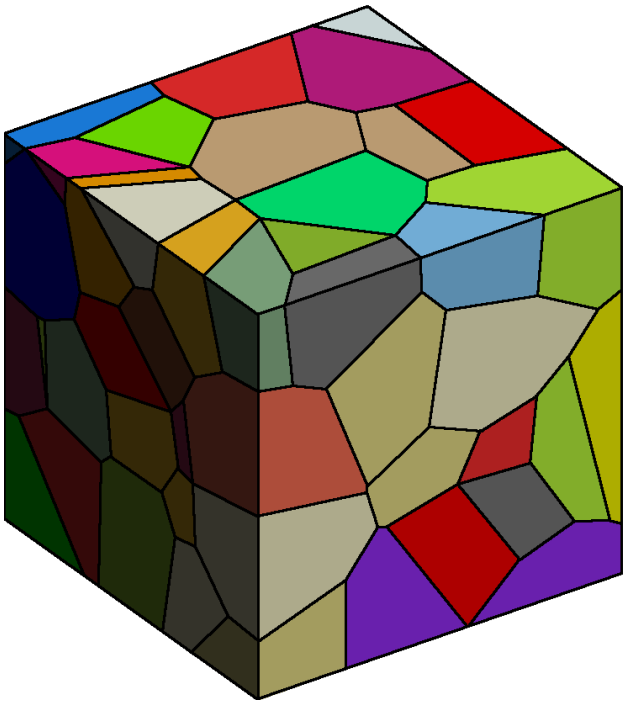
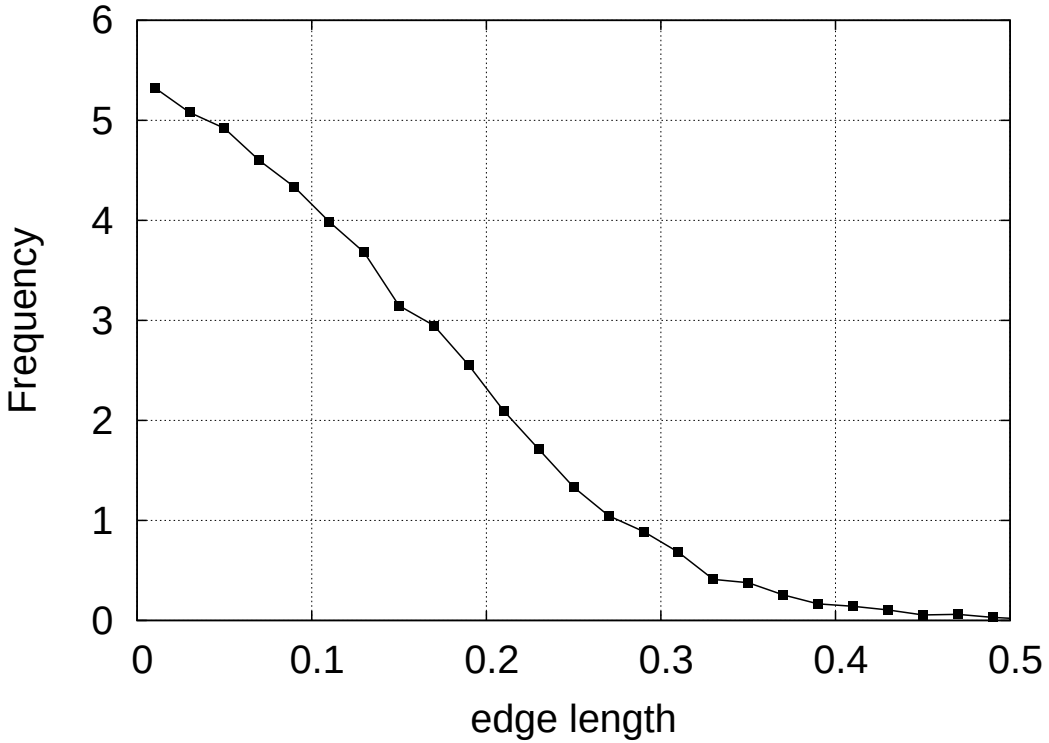
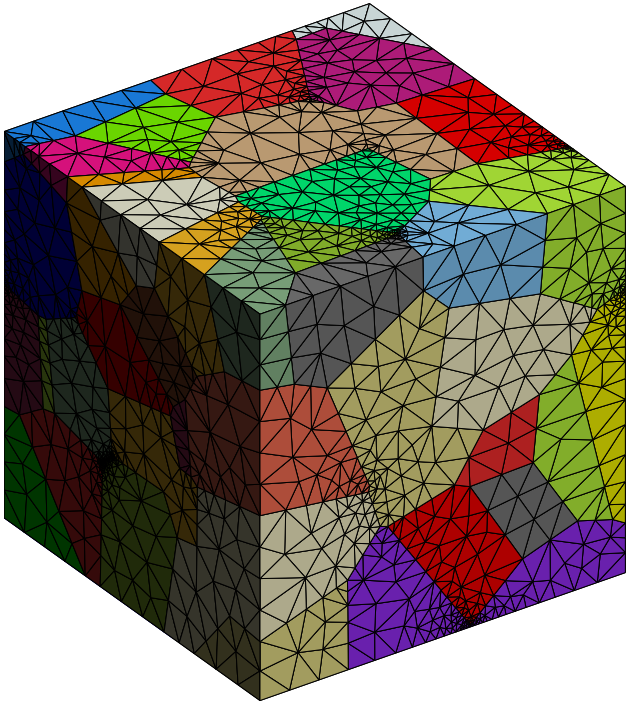
Focus on Voronoi tessellations





Voronoi tessellations contain *a lot* of small edges.

Focus on Voronoi tessellations



(free meshing: Gmsh internally used)

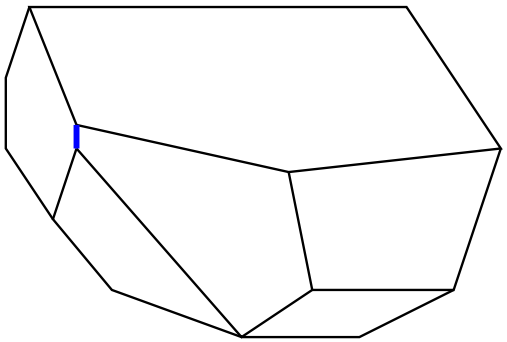
- the small tessellation edges *must* be taken into account: mesh refinement;
- the smaller the edge, the higher the number of elements;
- as many elements in the refined zone than in the non-refined zone

...

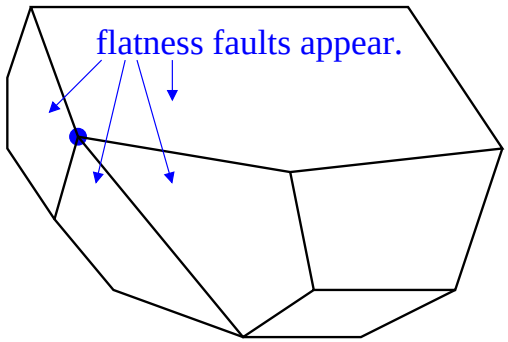
Why do not delete the *small edges* (that require refinement)?

Morphological modification and meshing

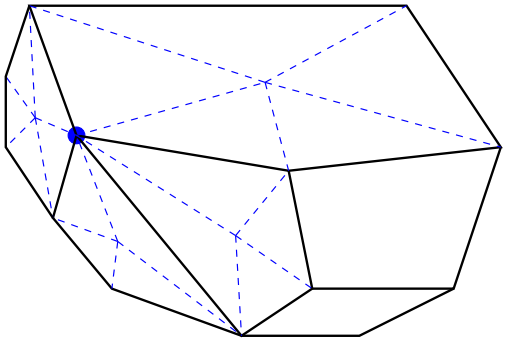
- Main principle:



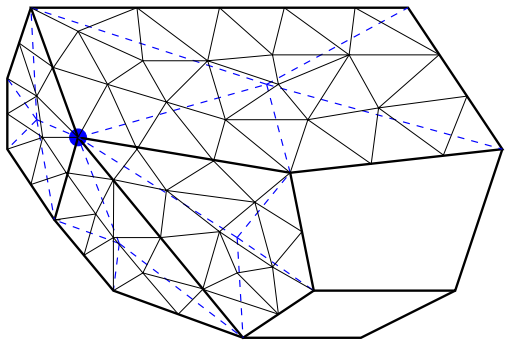
1. small edge to delete.



2. small edge $\leftarrow$ one vertex.



3. face interpolation (triangles)

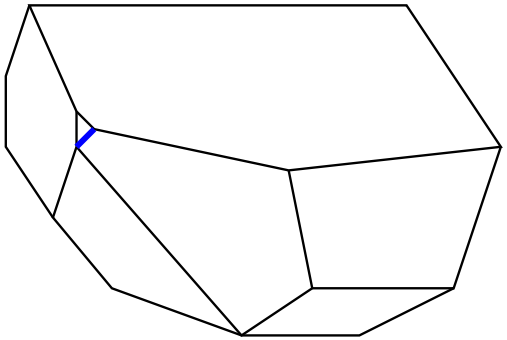


4. . . . will apply to the *mesh*.

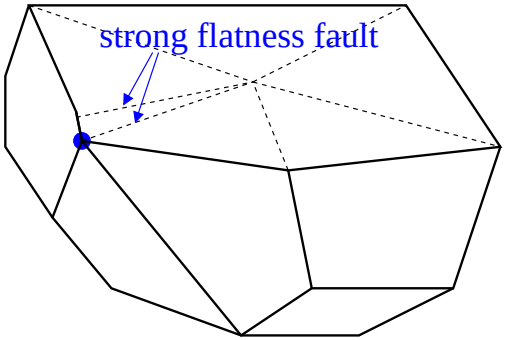
criterion: flatness fault (ff) $<$ maxff $\Longleftrightarrow$ edge deletion

Morphological modification and meshing

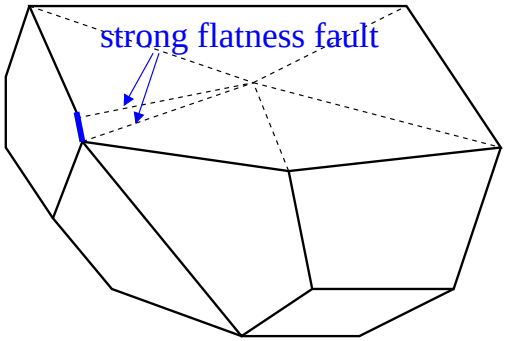
- A frequent configuration:



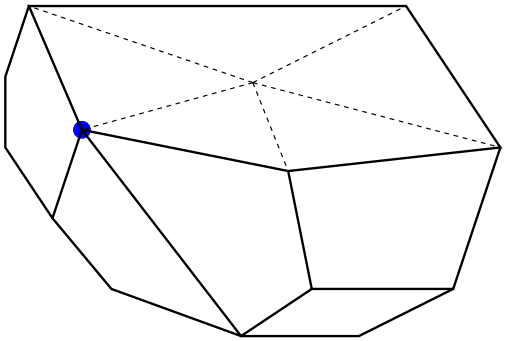
1. small edge to delete.



2. strong flatness fault.



3. deleting another edge.

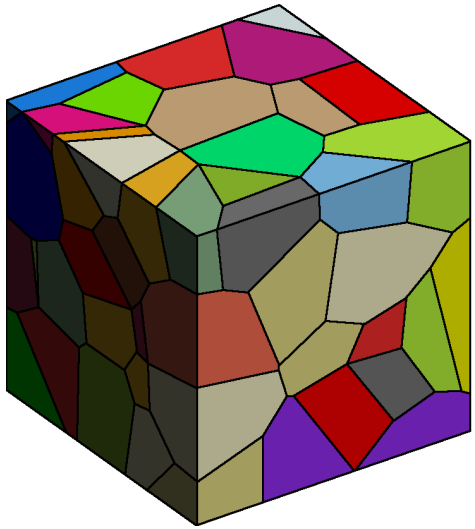


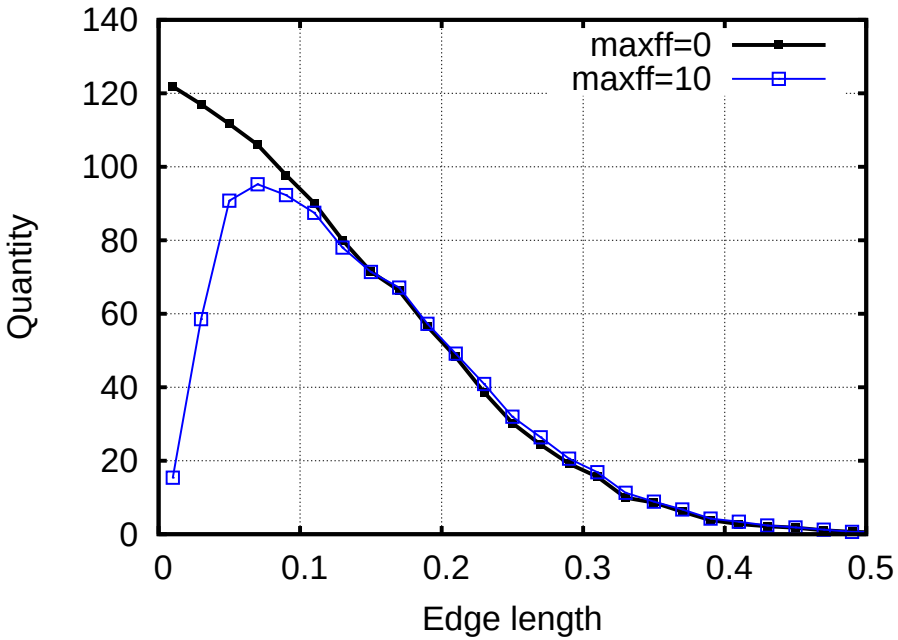
4. smaller flatness fault.

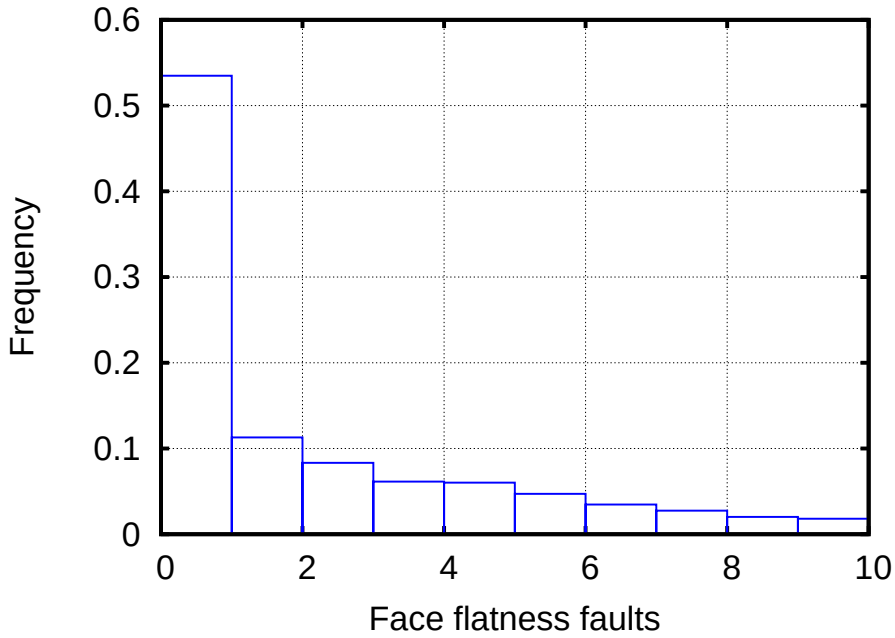
(ff $>$ maxff) $\rightarrow$ del. a new edge $\rightarrow$ (ff $<$ maxff $\Leftrightarrow$ edge deletions)

Results: morphology modification

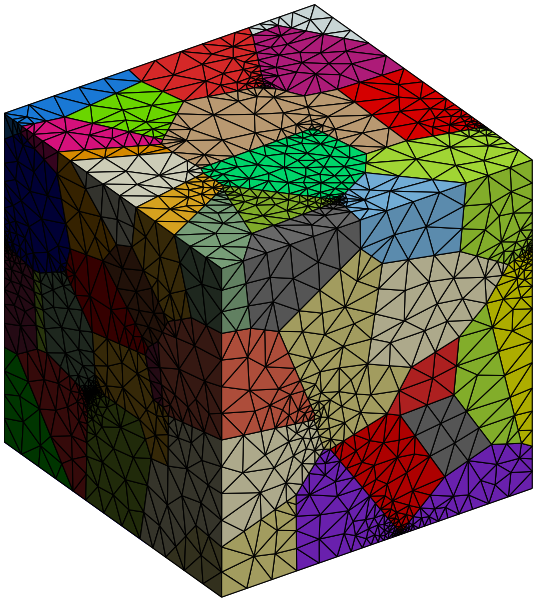
- The global morphology does not really change;
- new edge length distribution;
- flatness fault distribution ...

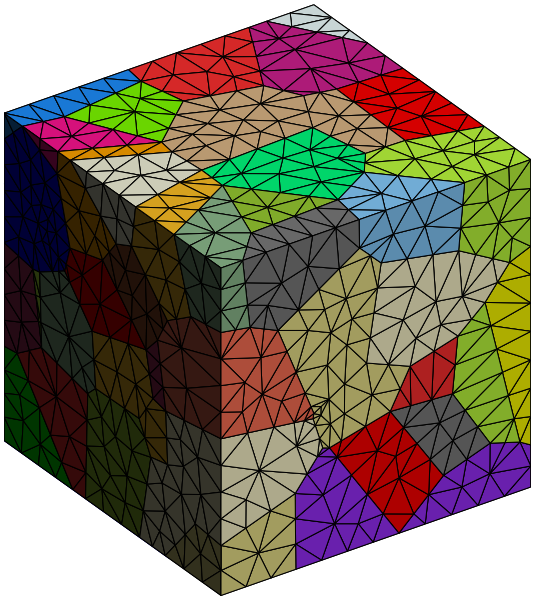


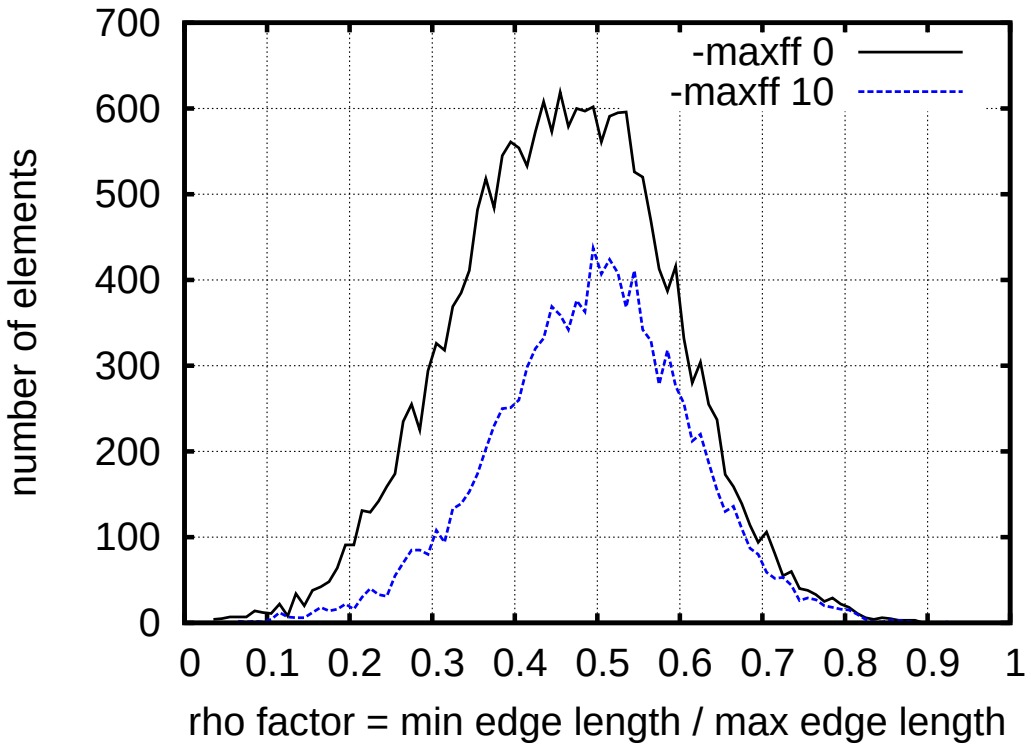




Results: mesh modification







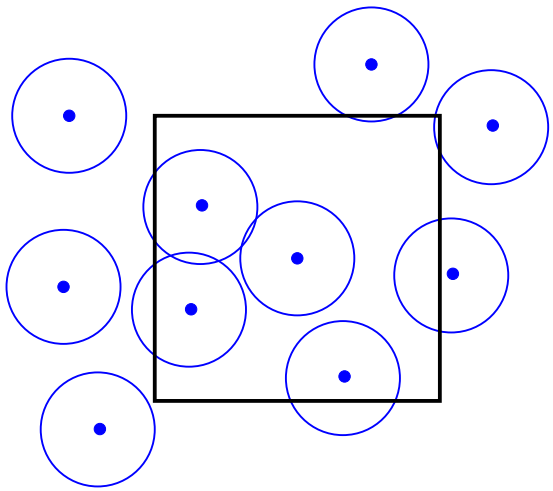
- maxff=10 $\rightarrow$ half-size mesh;
- some bad quality elements (geometry acute angles) ...

Type of transformations

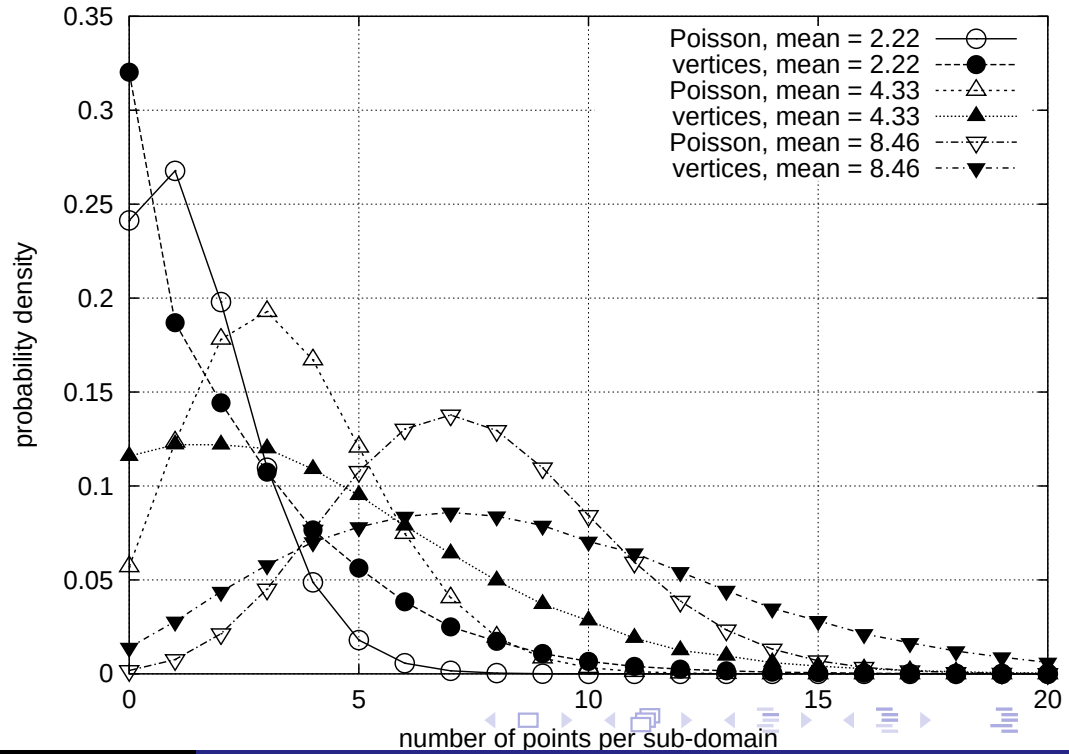
Motivation: study of TRIP (diffusive case)

Previous transformation models: (Barbe et al., 06) (Hoang et al., 06)

- homogeneous parent and product phases;
- randomly positionned nuclei;
- nucleation at $t = 0$, or through time.
- growth at $v = cste$

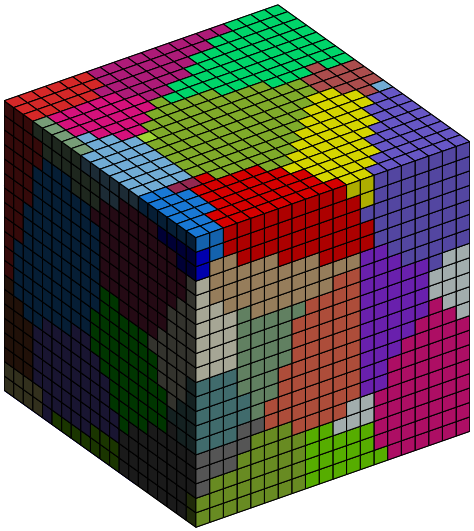


(Barbe et al., 06)



Type of transformations

NePeR: simulation of *diffusive* transformations that occur by *nucleation* and *growth*



Parent medium = tessellation like picked up in a MV (Voronoi cell seeds inside and outside the domain)

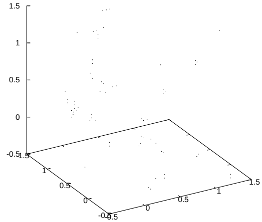
Transformation

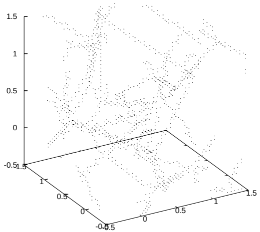
We need to define:

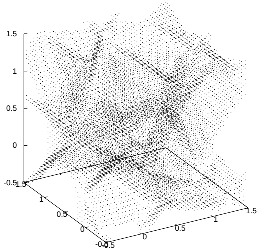
1. nucleation sites (inside and outside the domain)
2. nucleation laws
3. growth laws

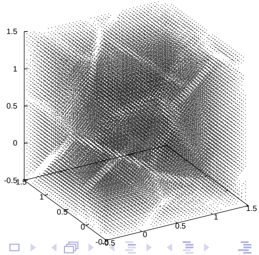
Nucleation sites

- type 4: quadruple points
- type 3: triple lines
- type 2: grain boundaries
- type 1: grain interior









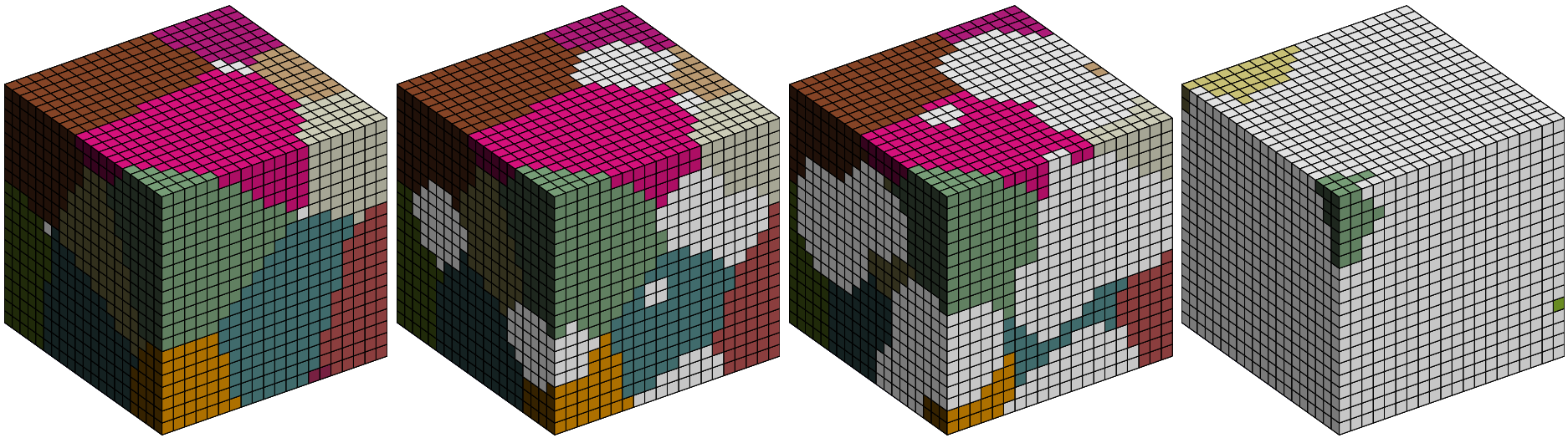
Kinetics laws

Kinetics laws apply to the MV. Any *analytical* law can be prescribed:

- Nucleation: one law for *every* type of site: $N(t)$
  number of nuclei as a function of t (per unit vol. or per grain)
- Growth
  - $R(t)$: radius as a function of t (t: time since nucleation)
  - 2 types of morphology: cubic & spherical

Results: example

nucleation: $N_4(t) = t$; $N_{i\neq 4}(t) = 0$ (quadruple points only)
growth: $R(t) = 0.05 \times t$, spherical shape
provide microstructure every $1\,s$



step 2 step 5 step 7 step 11

What **NePeR** can do (at the moment):

- Polycrystals
  - morphology = (slightly) modified Voronoi tessellations
  - Mapped meshing and free meshing
  - Generation of crystallographic orientations
- Phase transformations: diffusive (nucleation & growth)
  - Parent phase includes crystallography, product phase is homogeneous
  - Nucleation on favorable sites
  - Any analytical kinetics laws

Things to do (non-exhaustive):

- Use for prediction of polycrystal effective properties & TRIP simulations
- generation of tessellations with seeds outside the domain (for the free meshing)
- improve the meshing process