The Neper/FEPX Project and its Application to Polycrystal Homogenization

`https://neper.info`, `https://fepx.info`

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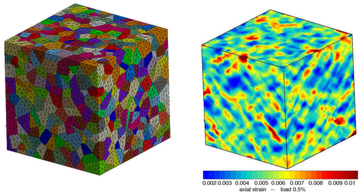
Context: Simulation of the (Large) Plastic Deformation of Polycrystals

Neper

Voronoi tessellations
meshing, regularization
2003–2005 — 2009

First release
Neper v1.8



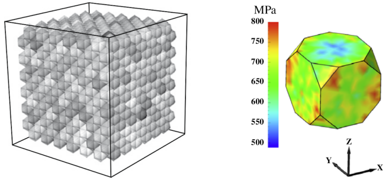
(Barbe, Quey, Musienko and Cailletaud, 2008)

FEPX

- - - -1995–1998 — 2009

Parallel implementation
Sheet forming applications

Application to finely
meshed polycrystals



(Wong and Dawson, 2009)

Context: Simulation of the (Large) Plastic Deformation of Polycrystals

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Neper v1.9

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meshing, regularization
2003–2005 — 2009 — 2009–2011

Robust meshing
and remeshing

FEPX

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Support for
remeshing

First convergence:
Large-scale random polycrystals to large strains

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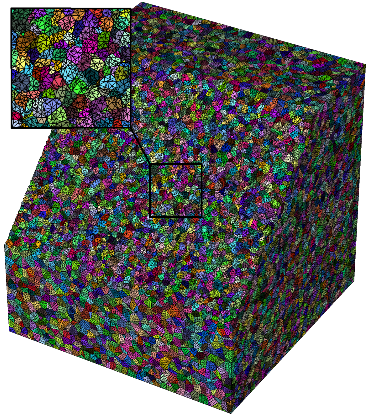
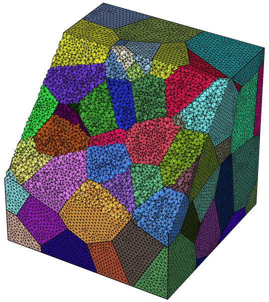
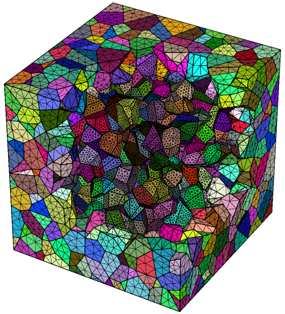
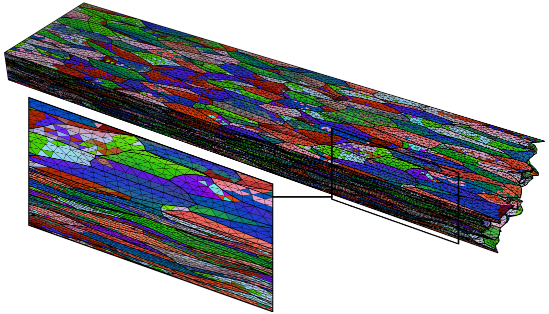
(Quey, Barbe and Dawson, 2011)



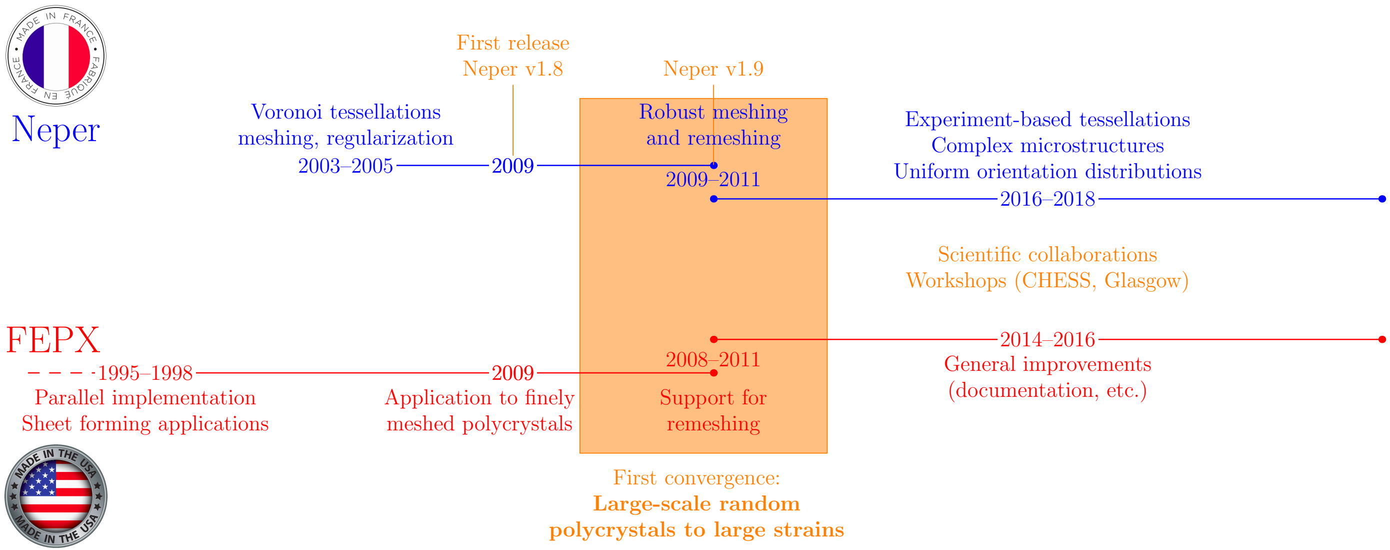






Neper/FEPX: Context and History

Context: Simulation of the (Large) Plastic Deformation of Polycrystals



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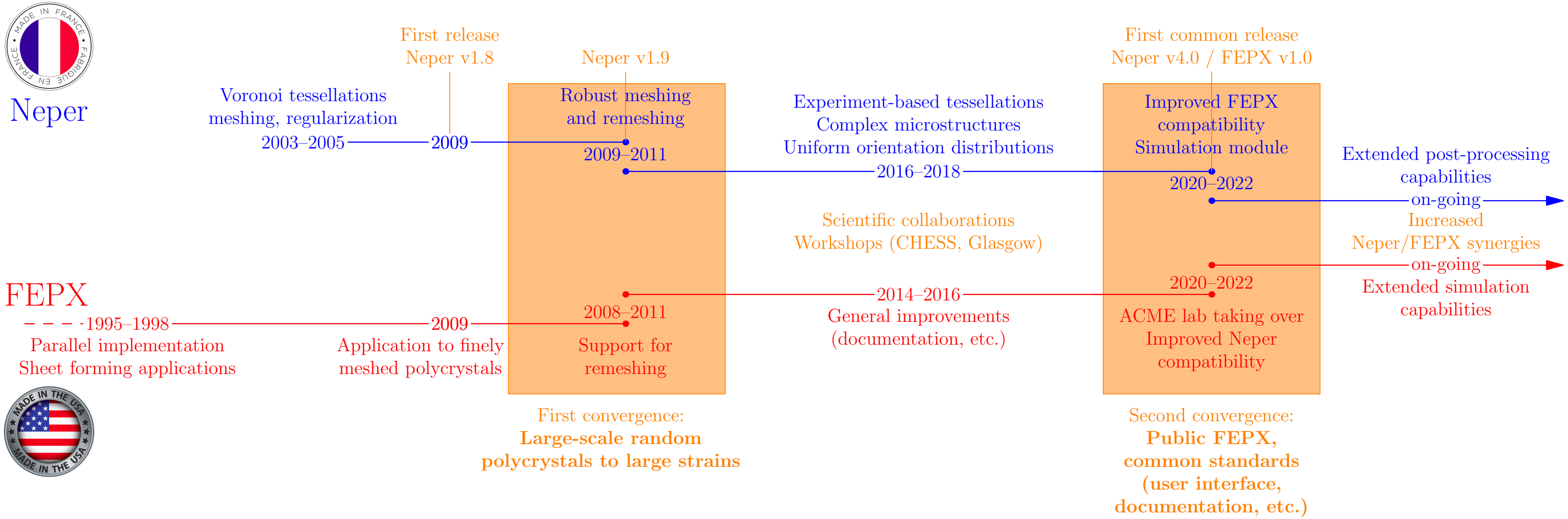

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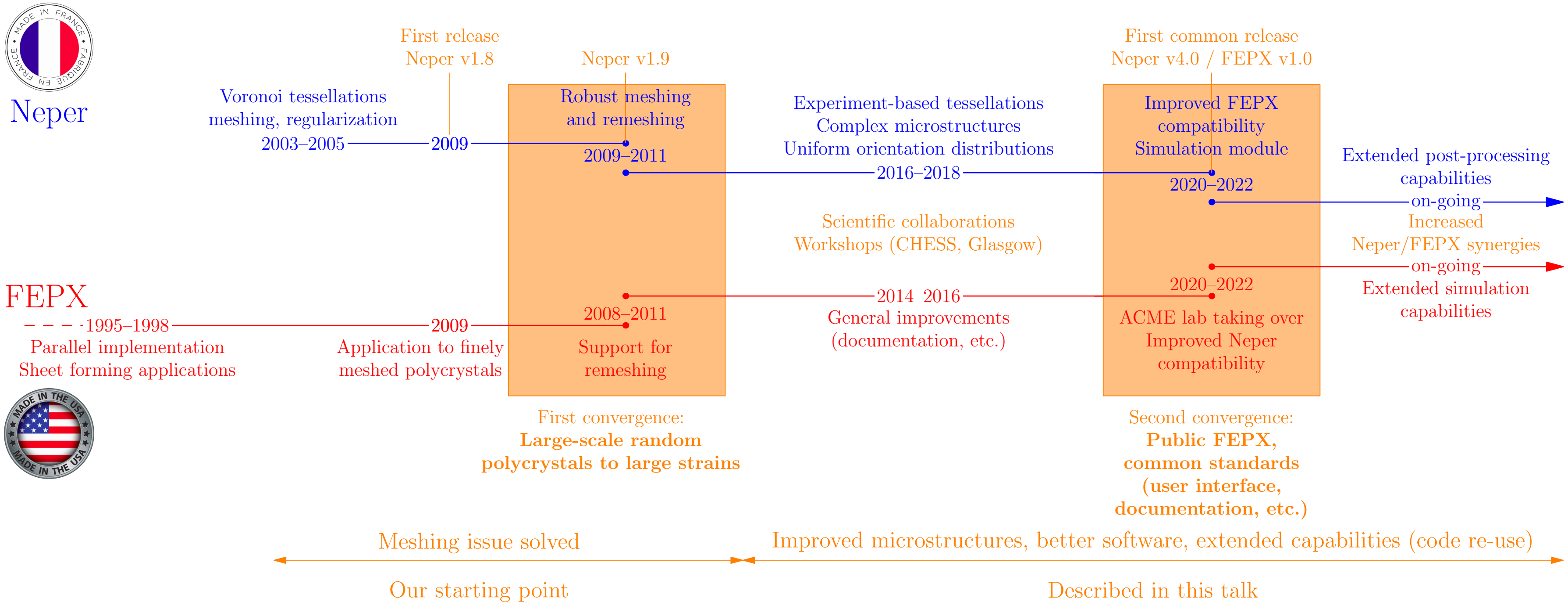
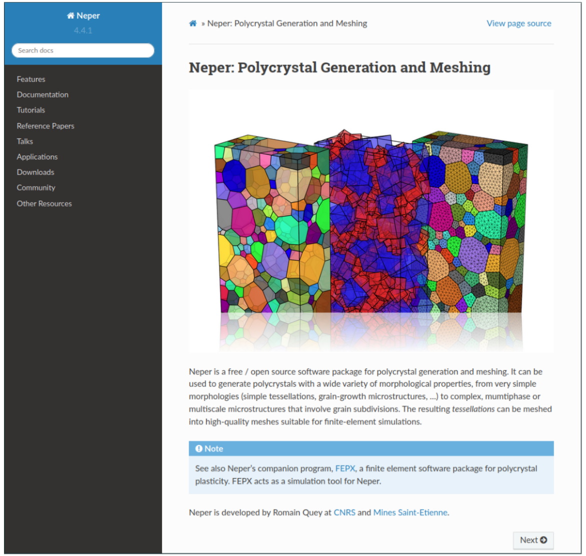
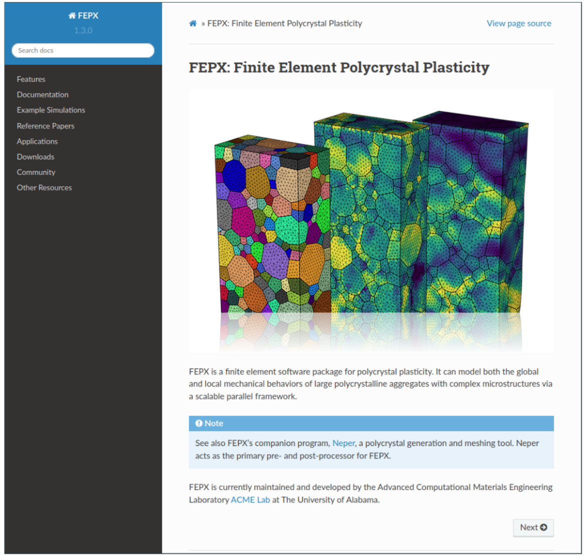


Lab-scale Free / Open-Source Software

https://neper.info



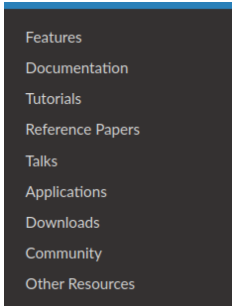
https://fepx.info



- Code distributed on the websites / GitHub
- Proper workflow (code versioning, testing, issue tracker, ...)

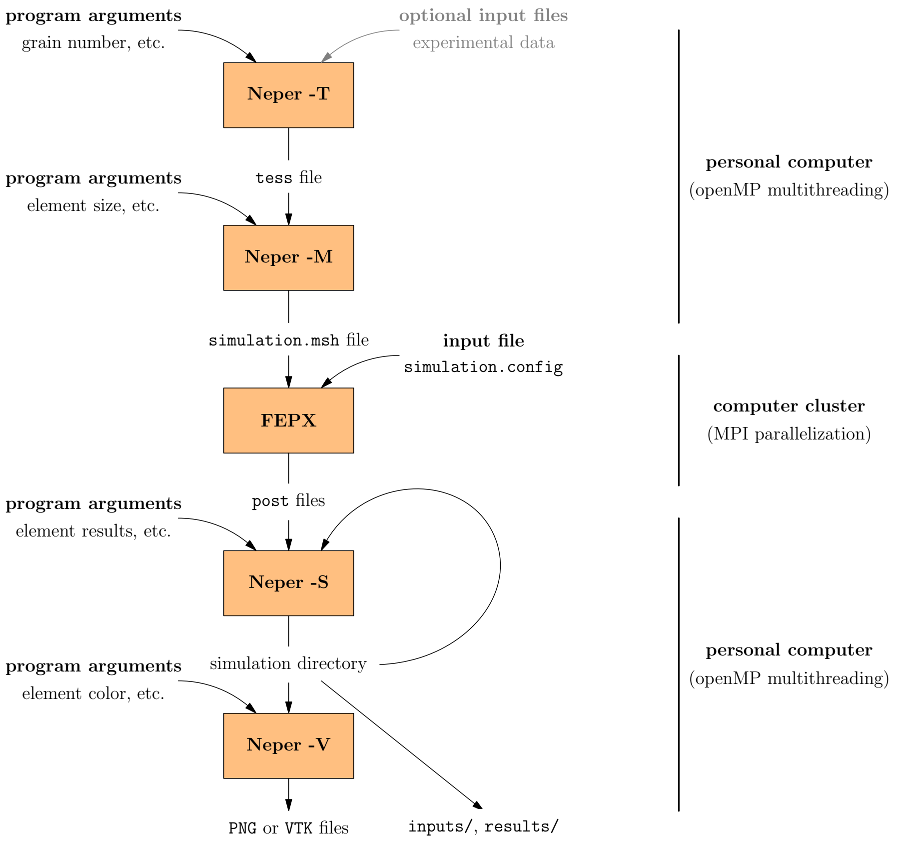
Boosted (not rewarded) by Ouvrir la science ! **Open Science Free Software Award**

- Expanding array of resources



- Active discussion forum and responsive user support

Neper/FEPX Now: Full Range of Features for Polycrystal Plasticity Studies



Neper -T: Tessellation Generation

- Single-Scale Tessellations — described next
- Multi-Scale Tessellations — described next
- Crystal Orientation Distributions — described in Part 2

Neper -M: Meshing

- Meshing
- Remeshing

FEPX: Crystal-plasticity FE simulations — described next

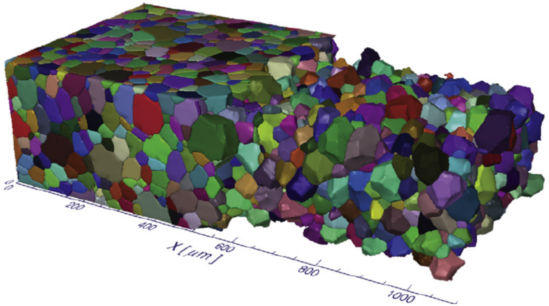
Neper -S: Simulation / Post-Processing

- Simulation Archiving — described next
- Post-processing — described next

Neper -V: Visualization

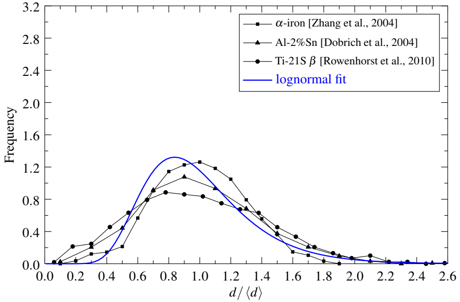
- Tessellation and mesh visualization — described next
- Results visualization — described next
- Pole figures — described next
- Orientation space — described next

Typical Polycrystal

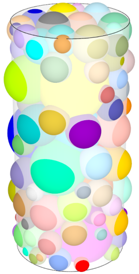


(Rowenhorst et al., 2010)

Typical Types of Microstructure Properties / Input

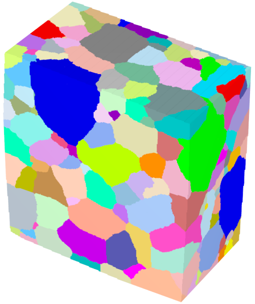


Statistical Data



Incomplete Grain Data (ff-3DXRD)

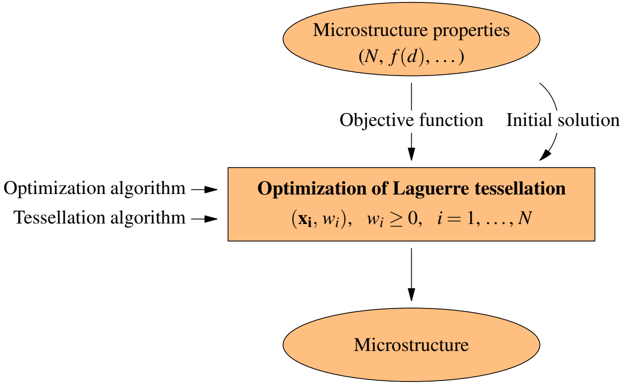
(courtesy H. Proudhon)



Grain Maps (DCT)

(courtesy A. Dimanov)

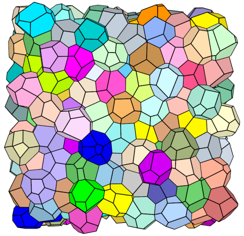
Generation of Optimal Convex-Cell Tessellations



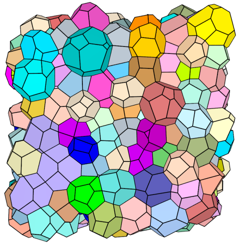
- Variables: for each seed, 3 coordinates + 1 weight ($4 \times N$)
- Objective function: application dependent (grain size distributions, grain centroids, ...)
- Non-linear, local, gradient-free, large-scale optimization problem (NLopt)

Any microstructure can be generated as long as *(i)* it can be represented using convex cells and *(ii)* an objective function can be defined

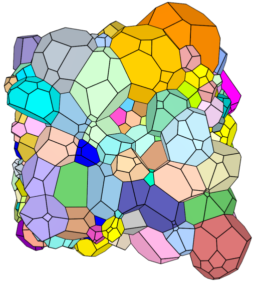
Polycrystals of Various Properties



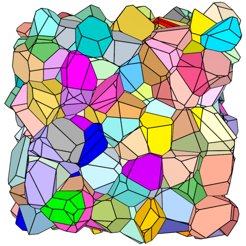
$\sigma_d = 0, s = 0.90$



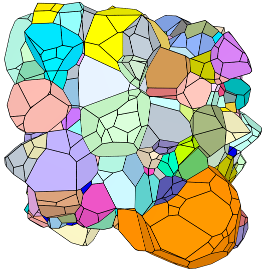
$\sigma_d = 0.15, s = 0.90$



$\sigma_d = 0.55, s = 0.90$



$\sigma_d = 0, s = 0.80$



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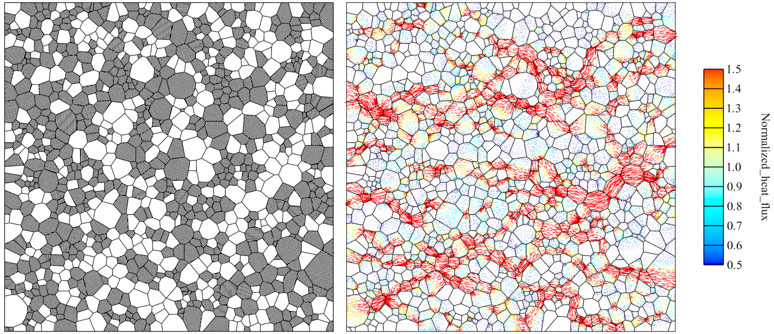
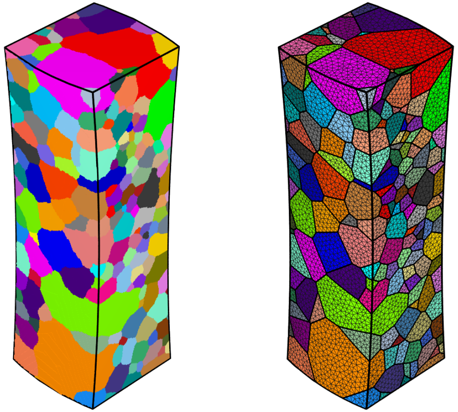
Grain size distributions in 2-phase or “textured” MoS_2 sheets

(Sledzinska et al, 2017)

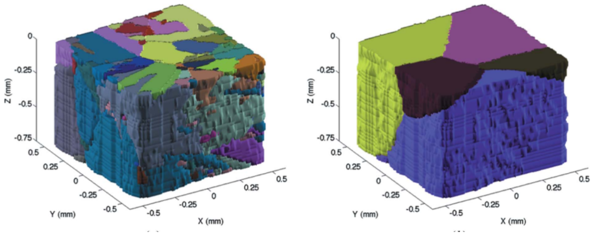


White grains: high conductivity; gray grains: low conductivity;
different grain boundary types: different conductances

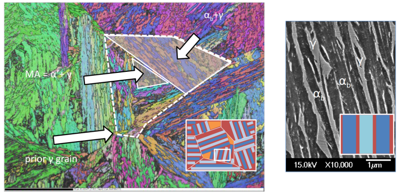
6D-DCT Polycrystal



Typically Microstructures (pearlitic / bainitic steels, lamellar Ti64, multilayer materials, ...)



Ti64 (Wielewski et al., 2015)

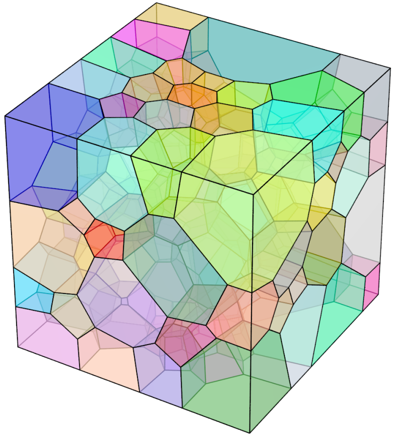


Carbide-free bainitic steel (Hell, 2011)

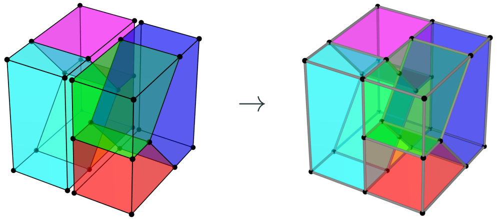
Characterized by grain subdivisions
→ "non-normal" tessellations

Principle: replicating material's processing (example of bainitic steel)

- Scale 1: grain-growth statistics, random orientations
- Scale 2, in each cell:
  - Morphology: seeds on GBs + Voronoi tessellation
  - Orientations: KS, NW relationships, ...
- Scale 3, in each cell: lamellae



Before Meshing: Flattening



Flattening of a 2-scale tessellation

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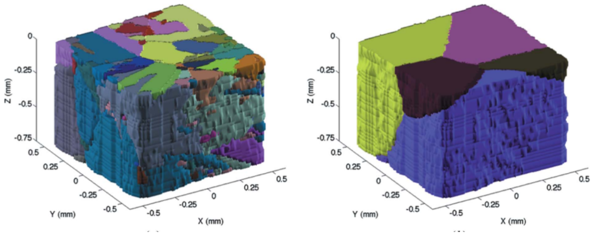

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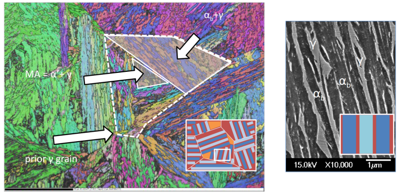

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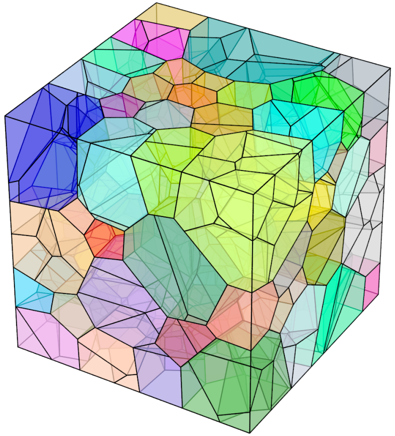

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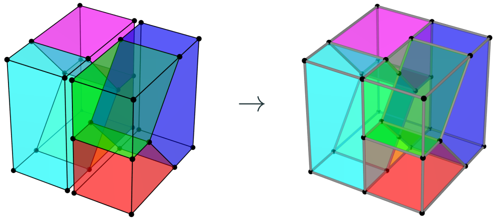

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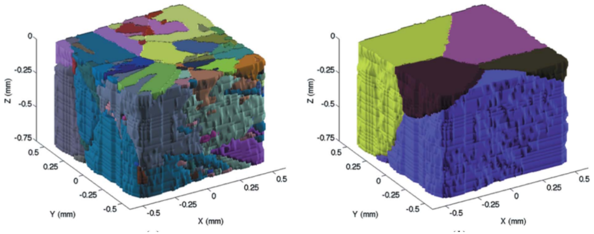

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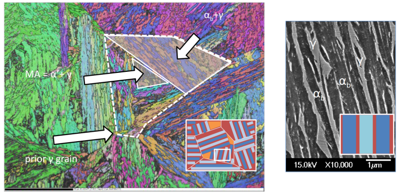

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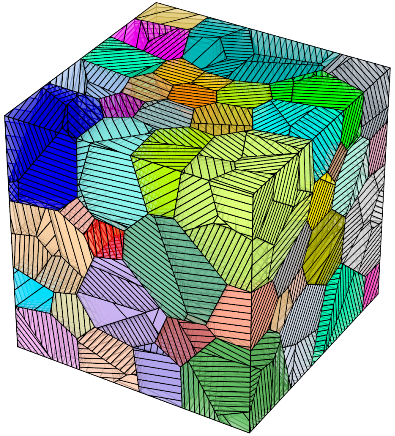

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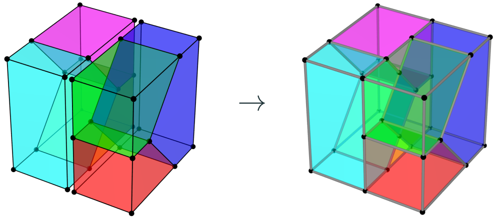

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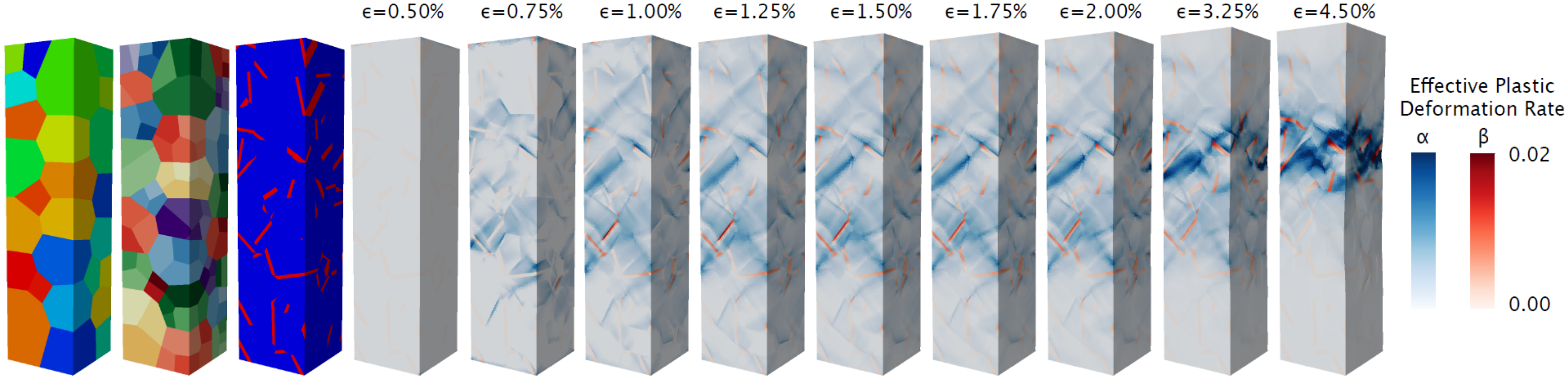
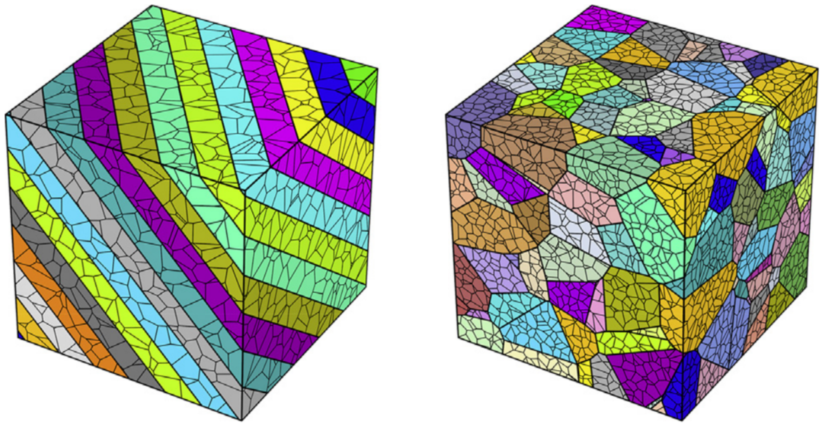
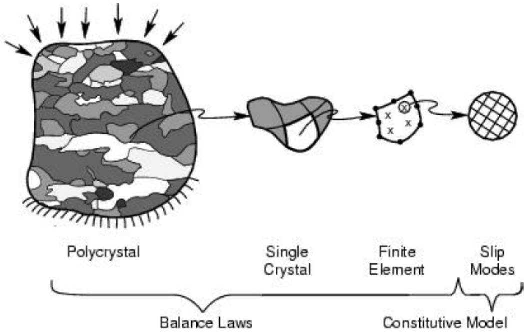


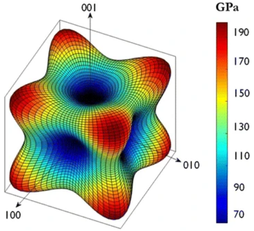
Deformation of Ti64 (Kasemer et al, 2017)



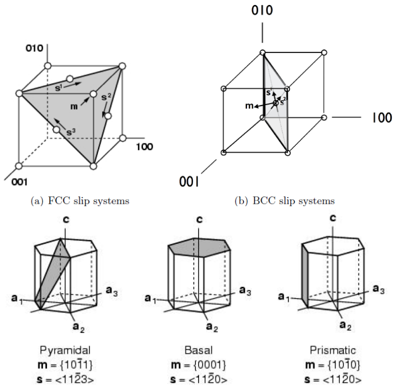
(Left) Sedimentary rocks, (right) intra-grain cracking path (Ghazvinian et al, 2014)

Principle





Crystal elasticity



Anisotropic plasticity

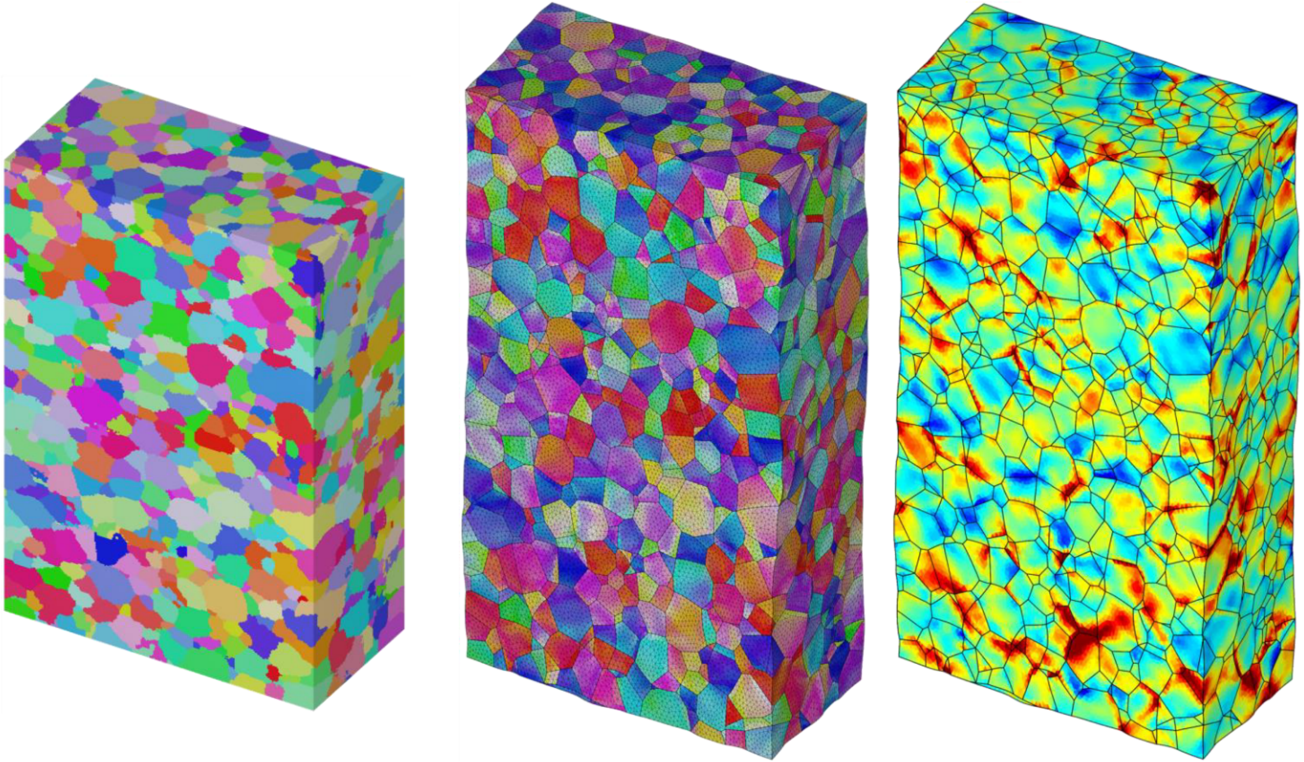
Specifics

- Finite strain formulation
- Elasto-viscoplastic behavior

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{|\tau^{\alpha}|}{g^{\alpha}} \right)^{1/m} \mathrm{sgn}(\tau^{\alpha})$$

- Different hardening models (isotropic, anisotropic, cyclic)
- Formulated in displacement velocities
- Multiphase (cubic, hexagonal, tetragonal)
- Simple boundary conditions (no friction or changing contact conditions)
- Parallelized with Open MPI, dependency-free

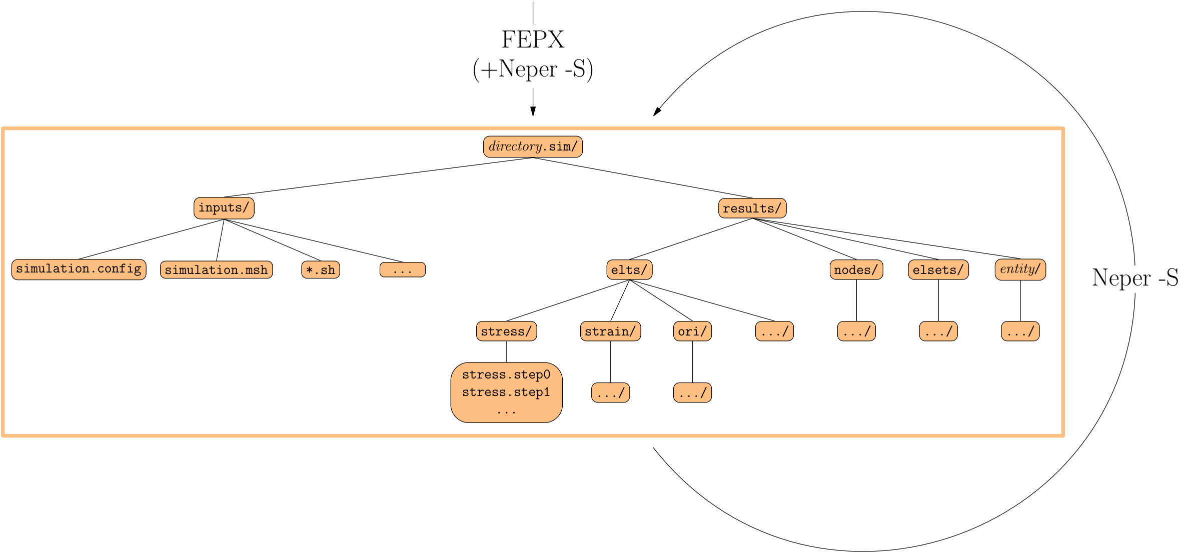
Can simulate deformation of polycrystals with 1000+ grains discretized 10^6 nodes/elements to small or large plastic strain routinely



Deformation of Al-4%Cu (postdoc Runguang Li, M4D ERC Project, DTU, Denmark)

Goal: define a structure to archive a simulation and facilitate postprocessing

Definition of a Simulation directory



Postprocessing Operations

- Computation of mesh results: `-reselset vol,x,y,z`
- Definition of new (simulation) results: `-reselt myvar:2*stress33`
- Grain averaging: `-reselset stress`
- Sample averaging: `-resmesh stress`
- Definition of ROIs or *entities*: `-entity top:z>0.5 -restop stress ...`
- Result management
- ...

Has a simple and browsable structure

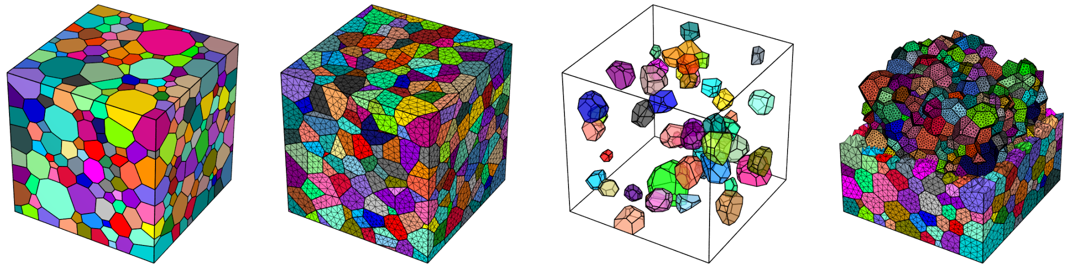
Can be loaded all at once in Neper -V for visualization

Can be used for experimental results

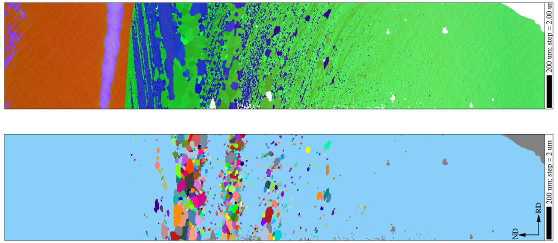
Top-quality Images or VTK for Interactive Visualization

3D images produced by ray-tracing (POV-Ray) with full control (camera, light, projection, etc.)

Advanced visualizations of tessellations and meshes

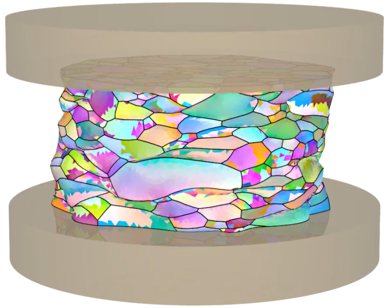


EBSD maps, etc.

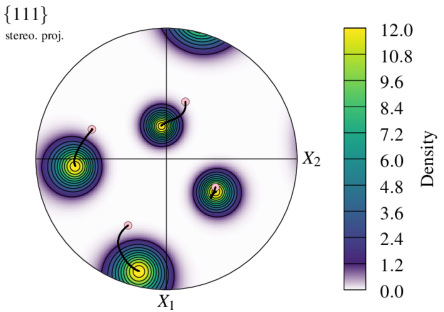


Orientation field and cell field (matrix / nuclei)

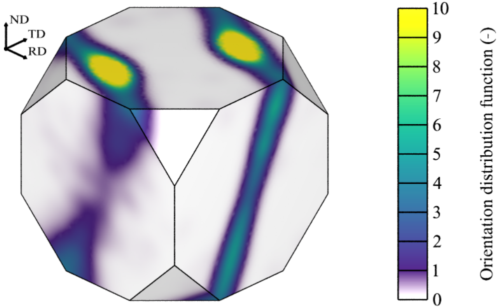
Simulation Results in Real Space...



Pole Figure Space...



and Orientation Space



Conclusions

Our Goals on the Neper/FEPX Project

- Continue to improve over the years...
- Provide a full range of features for polycrystal plasticity studies including post-processing and advanced visualization
- Provide more resources
- Build a community or users / active users / developers