The Neper/FEPX Project and its Application to 4D Experiment/Simulation Studies

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

Romain Quey[1] and Matthew Kasemer[2]

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Outline

The Neper/FEPX Project

Application to a 4D Experiment/Simulation Study

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Application to a 4D Experiment/Simulation Study

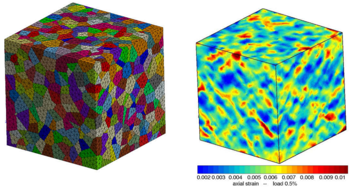
Neper/FEPX: Context and History

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

Neper

First release
Neper v1.8

Voronoi tessellations
meshing, regularization
2003–2005 —— 2009



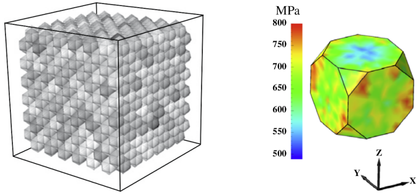
(Barbe, Quey, Musienko and Cailletaud, MRC, 2008)

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

Neper

First release
Neper v1.8

Neper v1.9

Voronoi tessellations
meshing, regularization

2003–2005 — 2009 — 2009–2011

Robust meshing
and remeshing

FEPX

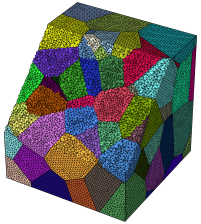
1995–1998 — 2009 — 2008–2011

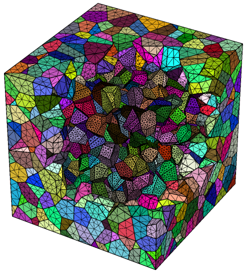
Parallel implementation
Sheet forming applications

Application to finely
meshed polycrystals

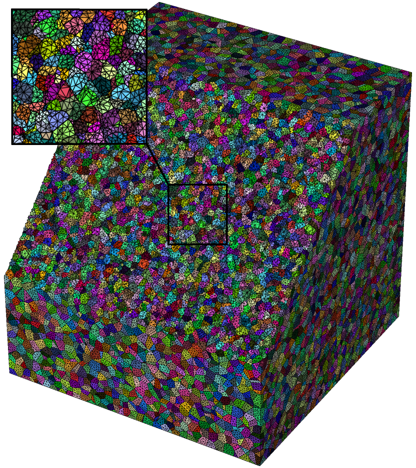
Support for
remeshing

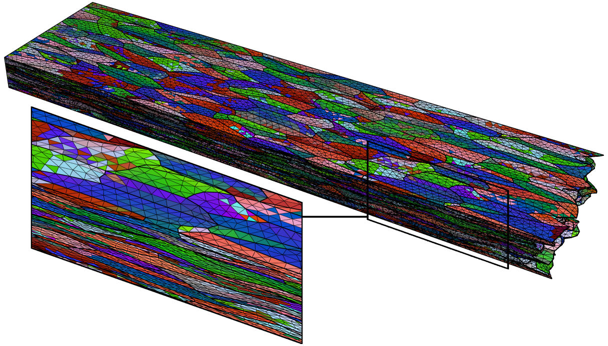
First convergence:
Large-scale random polycrystals to large strains





(Quey, Barbe and Dawson, 2011)





Neper/FEPX: Context and History

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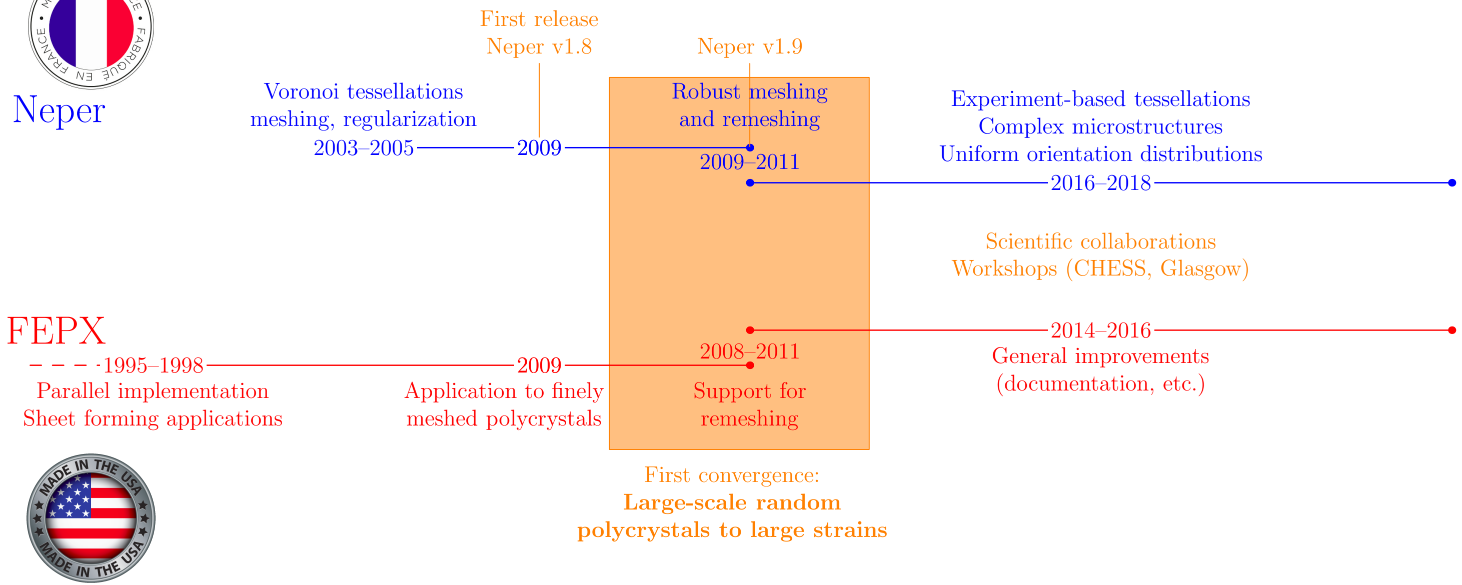

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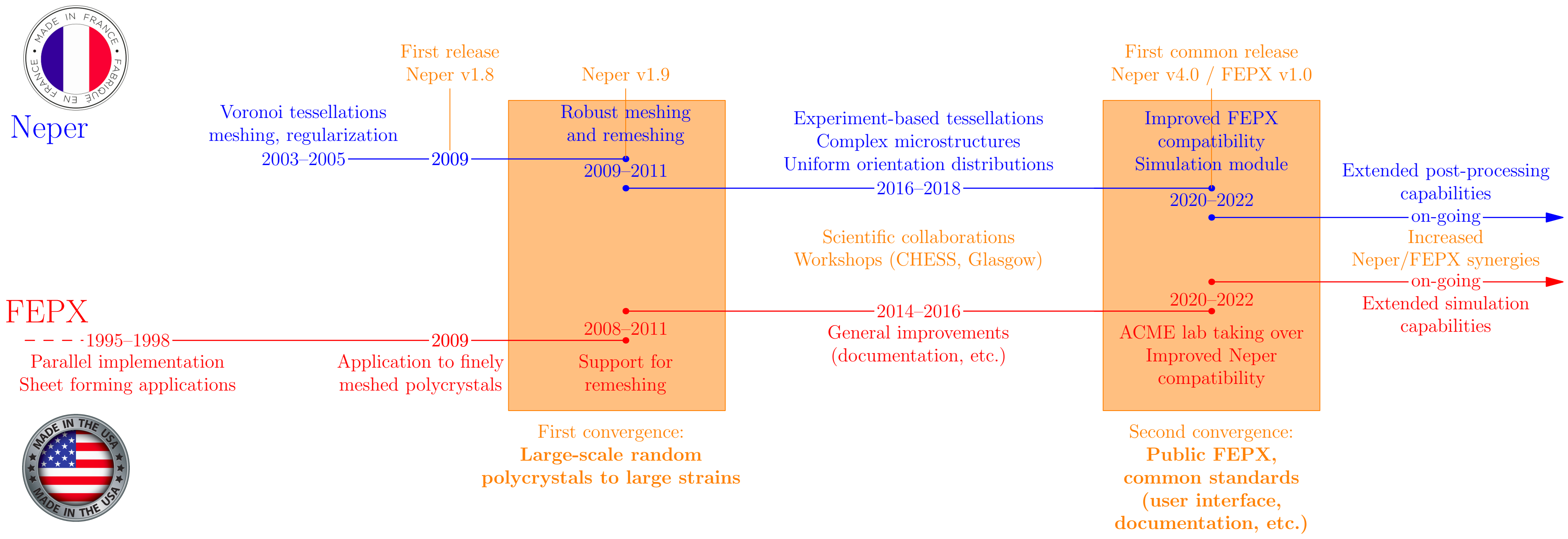
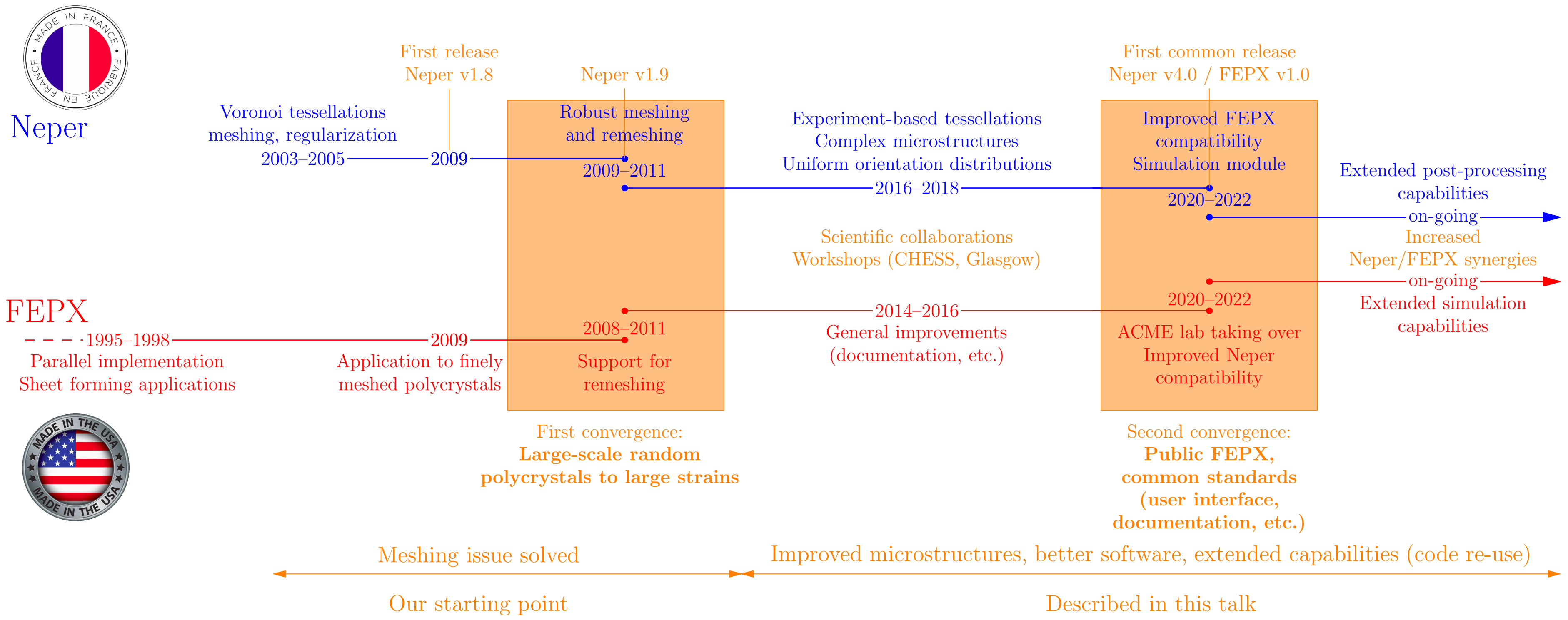


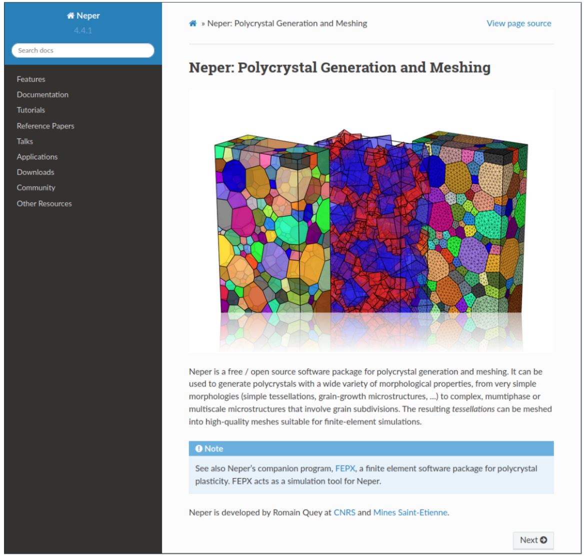
Context: Simulation of the (Large) Plastic Deformation of Polycrystals



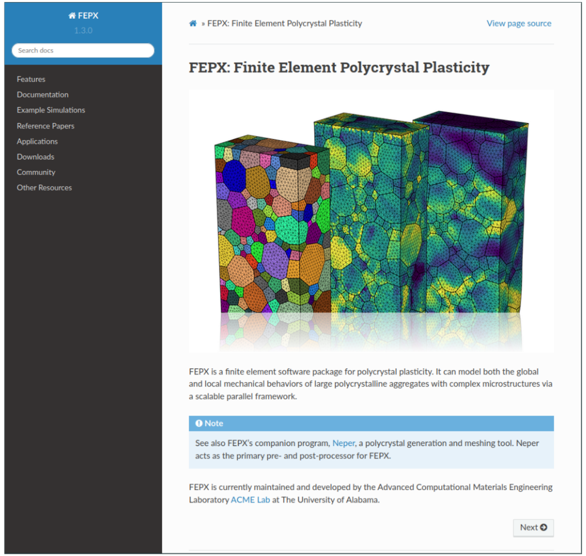
Established codes, products of 40 collective years or development and use, 400–500 papers

Lab-scale Free / Open-Source Software

https://neper.info



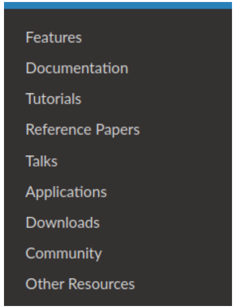
https://fepx.info



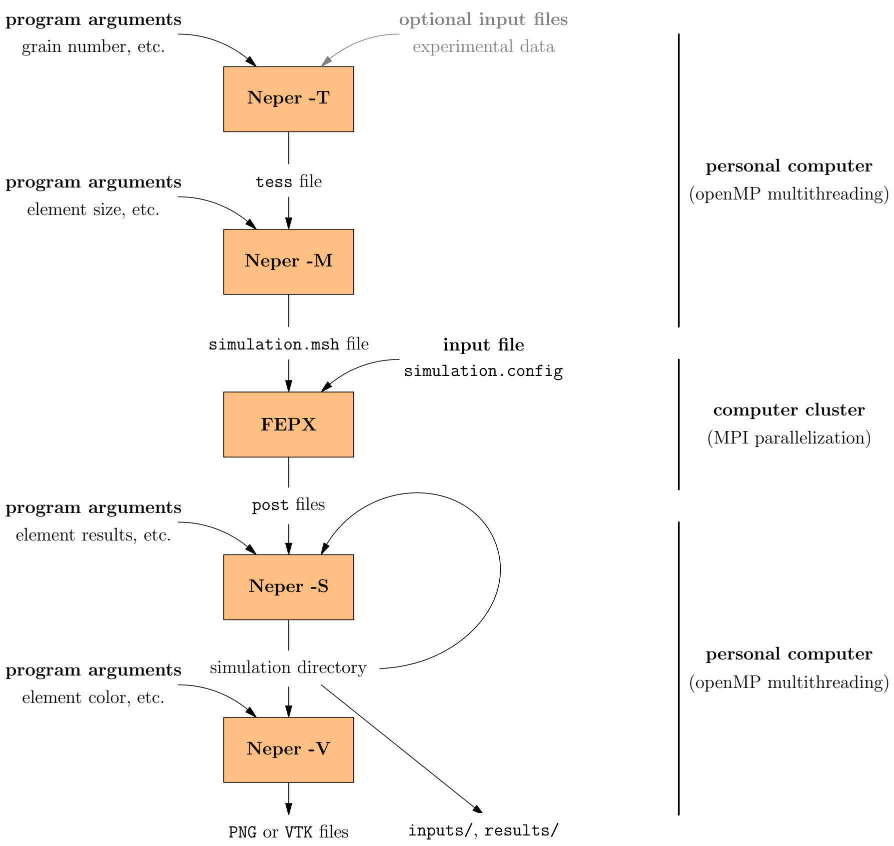
- Code distributed on the websites / GitHub
- Proper workflow (code versioning, testing, issue tracker, ...)

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

- Expanding array of resources



- Active discussion forum and responsive user support



Neper -T: Tessellation Generation

- Single-scale tessellations
- Multi-scale tessellations
- Crystal orientation distributions (random or uniform)

Neper -M: Meshing

- Meshing
- Remeshing

FEPX: Crystal-plasticity FE simulations

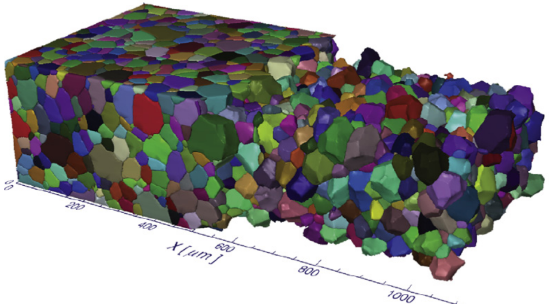
Neper -S: Simulation / Post-Processing

- Simulation archiving
- Post-processing

Neper -V: Visualization

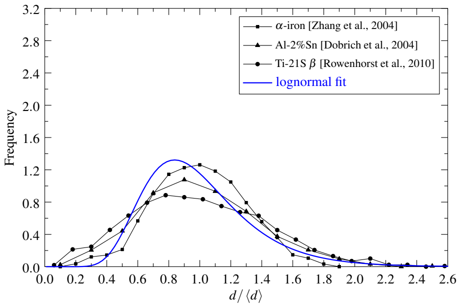
- Tessellation and mesh visualization
- Results visualization
- Pole figures
- Orientation space

Typical Polycrystal

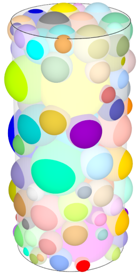


(Rowenhorst et al., 2010)

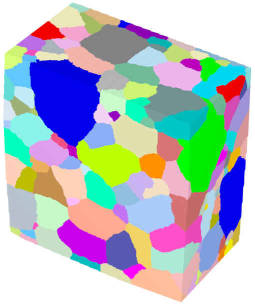
Typical Types of Microstructure Properties / Input



Statistical Data

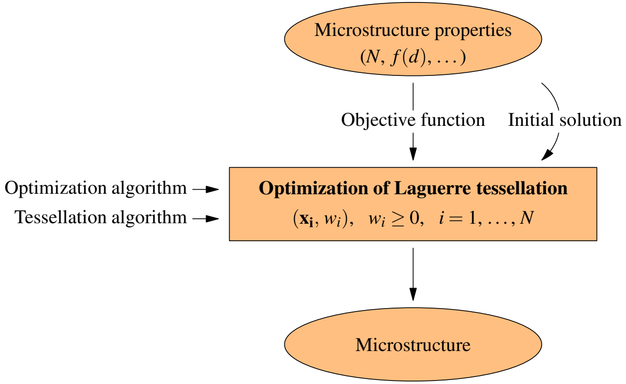


Incomplete Grain Data (ff-3DXRD)
(courtesy H. Proudhon)



Grain Maps (DCT)
(courtesy A. Dimanov)

Generation of Optimal Convex-Cell Tessellations



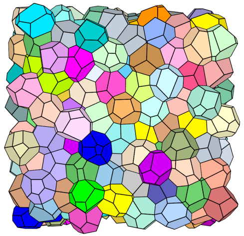
Optimization of (general) Laguerre tessellations:

- 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)

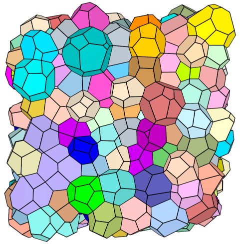
Any microstructure can be generated as long as *(i)* it can be represented using convex cells and *(ii)* an objective function can be defined

Generation of Single-Scale Polycrystals: Applications (Neper -T)

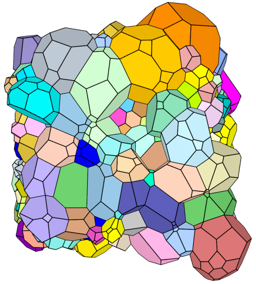
Polycrystals of Various Properties



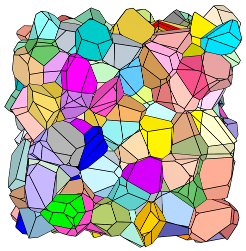
$\sigma_d = 0, s = 0.90$



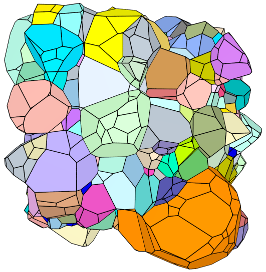
$\sigma_d = 0.15, s = 0.90$



$\sigma_d = 0.55, s = 0.90$



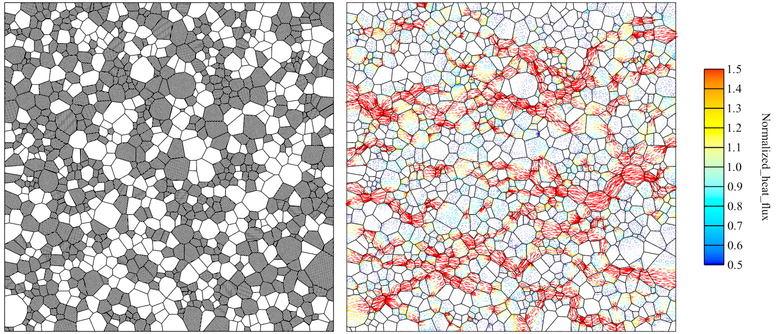
$\sigma_d = 0, s = 0.80$



$\sigma_d = 0.55, s = 0.80$

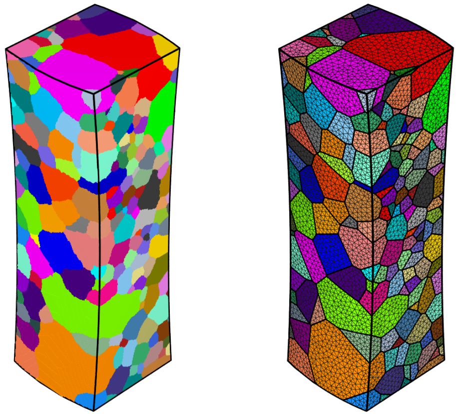
Grain size distributions in 2-phase or “textured” MoS_2 sheets

(Sledzinska et al, 2017)

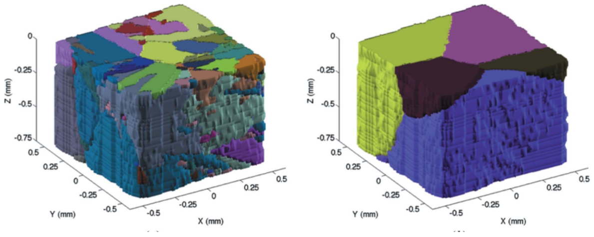


White grains: high conductivity; gray grains: low conductivity; different grain boundary types: different conductances

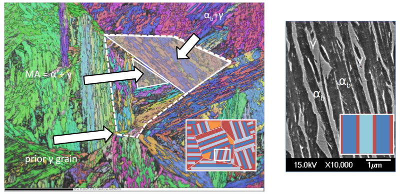
6D-DCT Polycrystal



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



Ti64 (Wielewski et al., 2015)

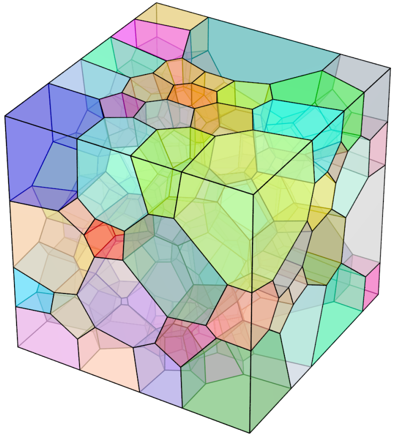


Carbide-free bainitic steel (Hell, 2011)

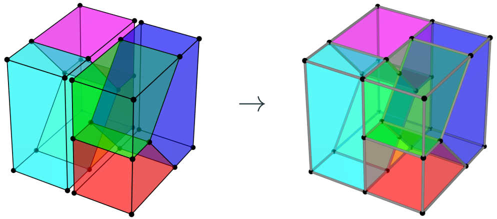
Characterized by grain subdivisions
→ “non-normal” tessellations

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



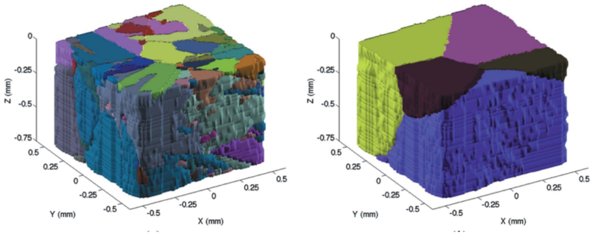
Before Meshing: Flattening



Flattening of a 2-scale tessellation

Generation of Multiscale Polycrystals: Principle (Neper -T)

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



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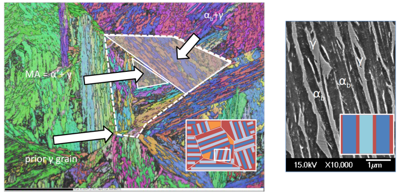

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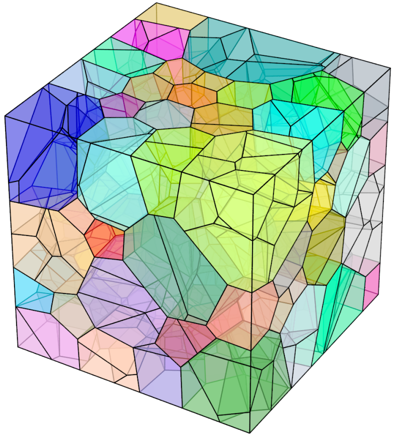

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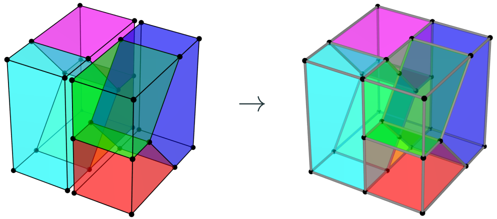

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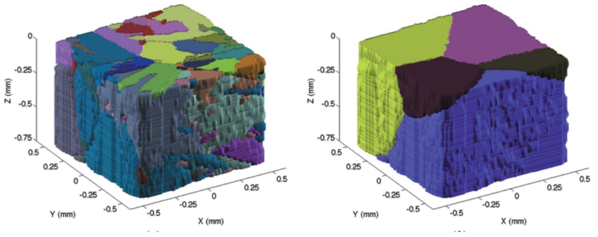

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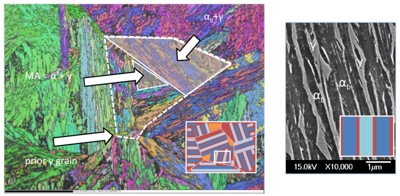

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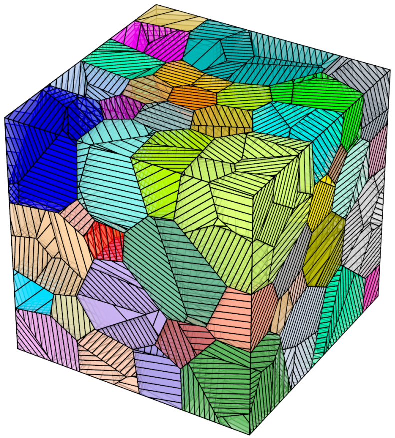

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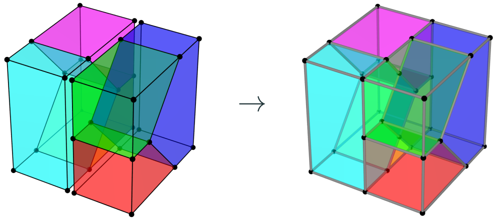

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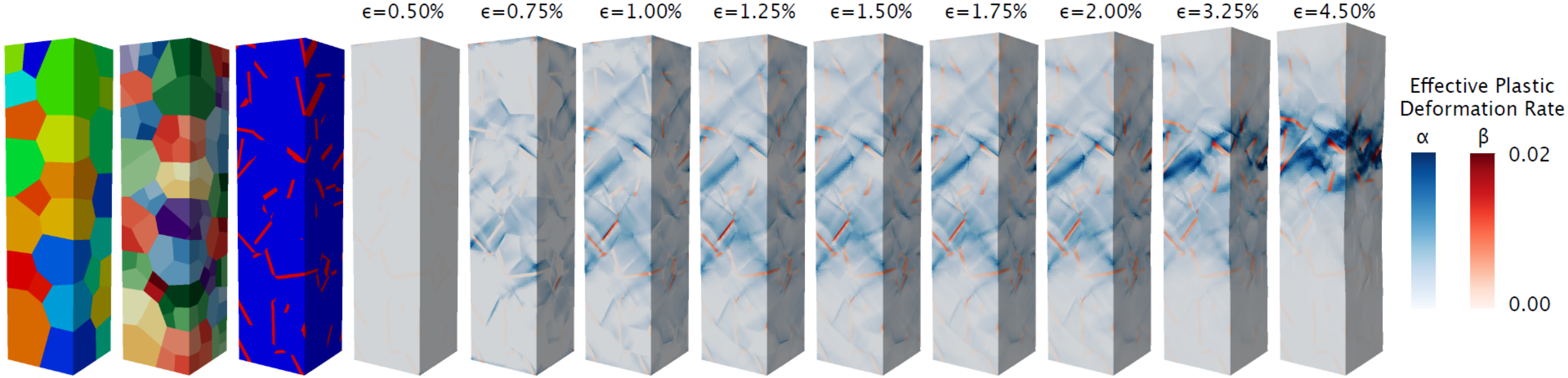
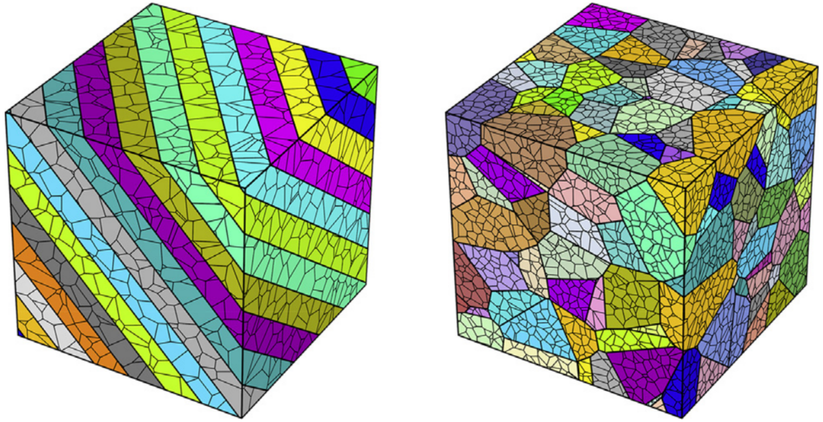


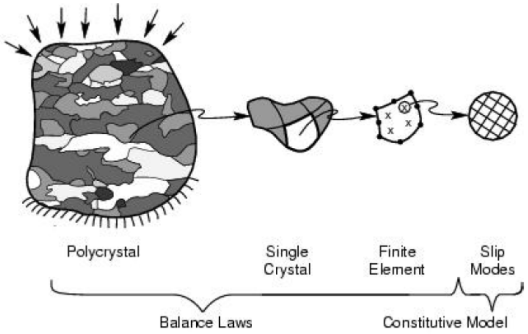
Deformation of Ti64 (Kasemer et al, 2017)

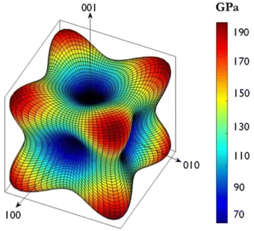


(Left) Sedimentary rocks, (right) intra-grain cracking path (Ghazvinian et al, 2014)

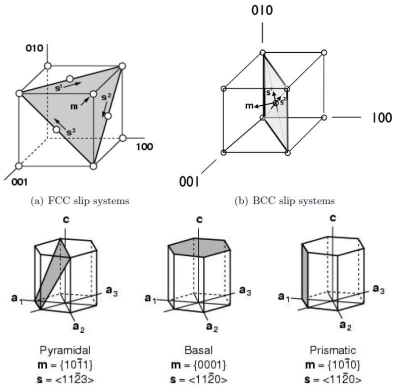
Finite-Element Simulation (FEPX)

Principle





Crystal elasticity



Anisotropic plasticity

Specifics

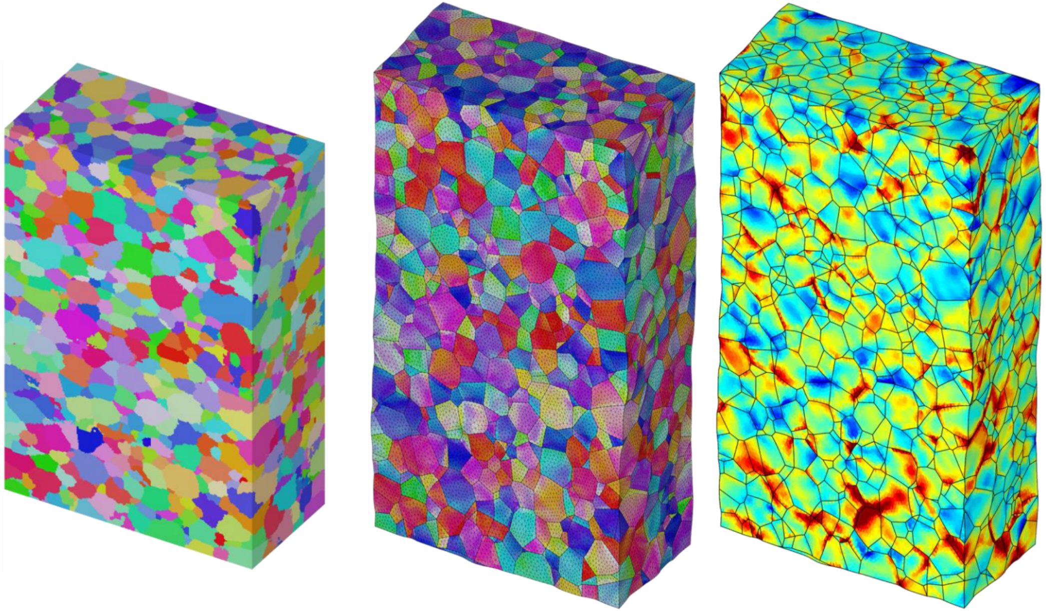
- Finite strain formulation
- Elasto-viscoplastic behavior

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

- 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

M4D erc
Metal Microstructures in 4D



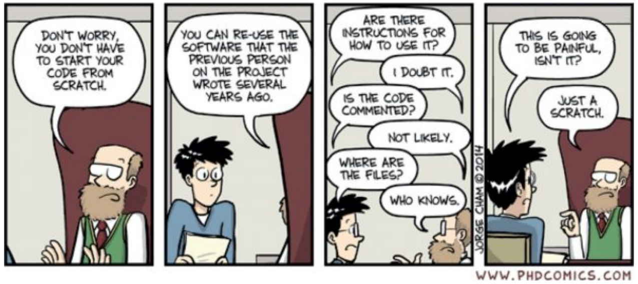
Deformation of Al-4%Cu (postdoc Runguang Li, M4D ERC Project, DTU, Denmark)

Next talk!

Deformation movie

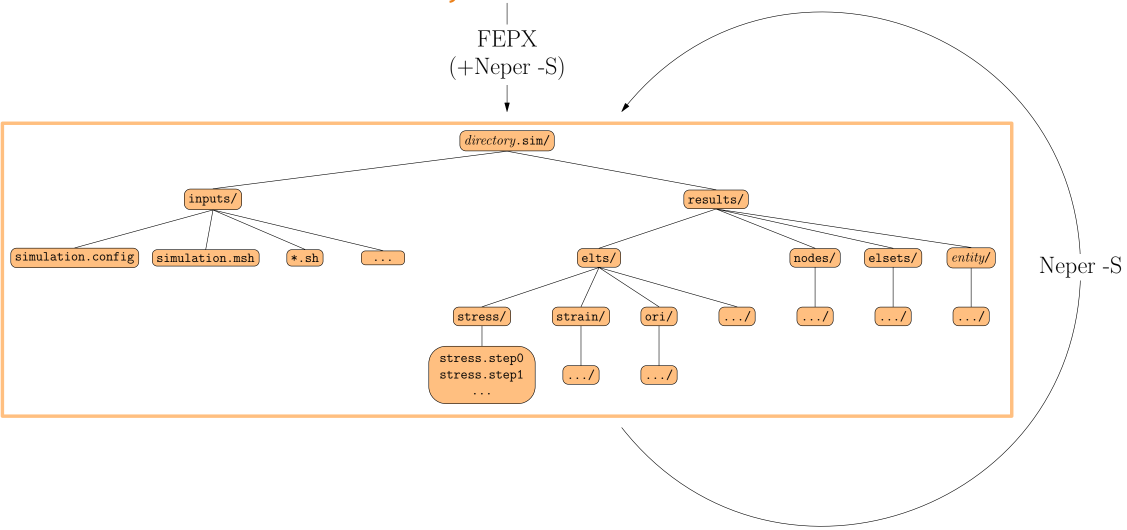
Simulation / Post-processing (Neper -S)

Doing post-processing...



Goal: facilitate / standardize data management and post-processing

Definition of a Simulation directory



Post-processing 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

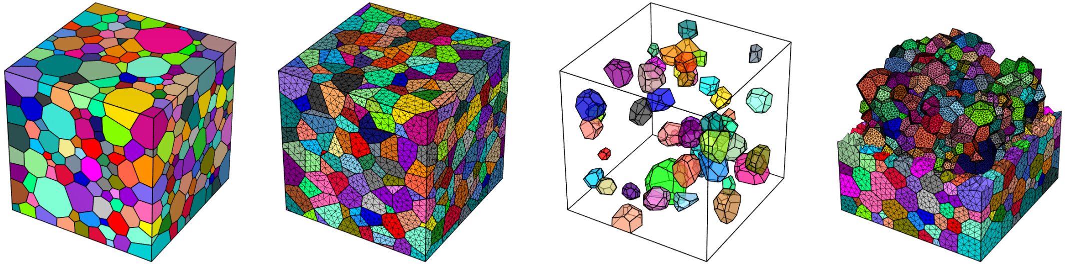
Can be used for experimental results

Visualization (Neper -V)

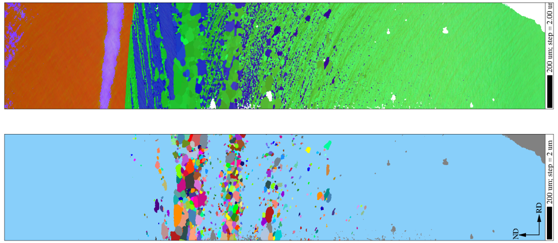
Top-quality Images or VTK for Interactive Visualization

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

Advanced visualizations of tessellations and meshes

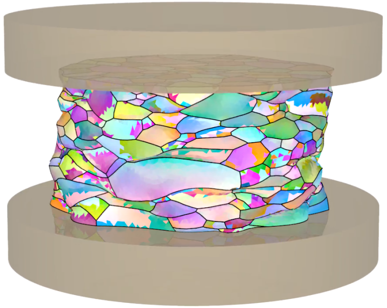


EBSD maps, etc.

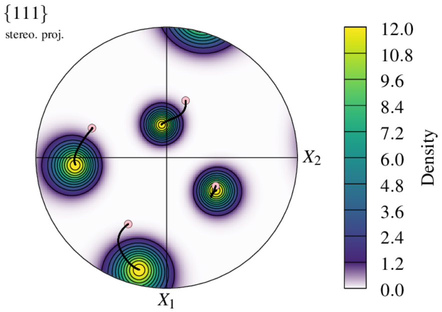


Orientation field and cell field (matrix / nuclei)

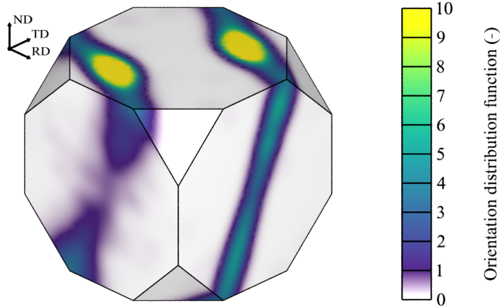
Simulation Results in Real Space...



Pole Figure Space...



Orientation Space...

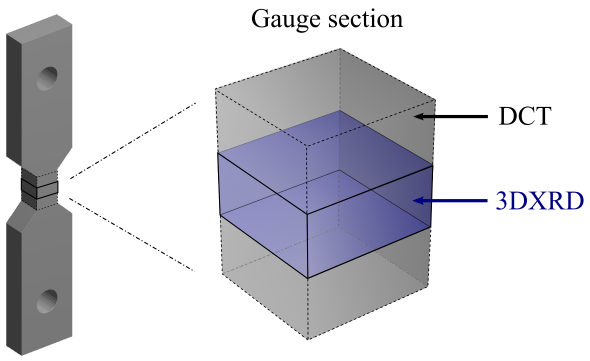


Outline

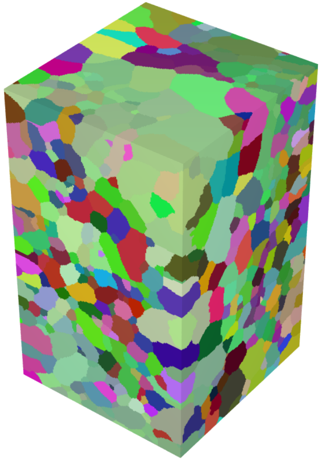
The Neper/FEPX Project

Application to a 4D Experiment/Simulation Study

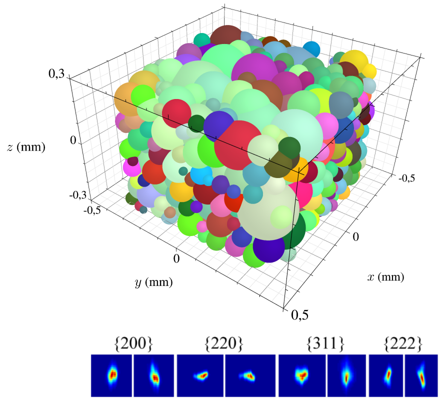
In situ analysis at ESRF / ID11 (Renversade and Quey, 40th Risø Symposium)



Al polycrystal, $\bar{d} = 200\ \mu m$



DCT



ff-3DXRD

Specimen and scanning regions

$\varepsilon = 0$

↓

Grain map
(`.dat` file + grain orientations)

$\varepsilon = 1.0, 1.5, 2.0, 2.5$ and 4.5%

↓

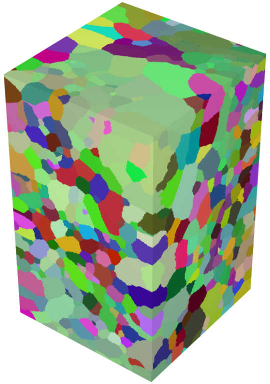
Grain-scale results:
average orientation, in-grain disorientation statistics, etc.

Writing the DCT Volume (`.dat`) at Neper's Format (`.tesr`)

`volume.tesr`:

```
***tesr
 **format
   2.1
 **general
   3
   600 600 1000
   0.0014 0.0014 0.0014
 **cell
   1987
  *crysym
   cubic
  *ori
   rodrigues:active
    0.021351228152     0.271788287376     0.157120856687
   [...]
 **data
   binary16
  *file volume.dat
***end
```

↓



```
$ neper -T -loadtesr volume.tesr \
           -transform "scale(0.25,0.25,0.25),autocrop,renumber"
```

↪ Generate a standalone `tesr` file

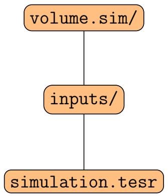
↪ Apply various transformations

```
$ neper -V volume.tesr -datacellcol ori -print img
```

Simple input file, various transformations, direct visualization

Initializing the Simulation Directory

```
$ neper -T -loadtesr volume.tesr -for sim
```



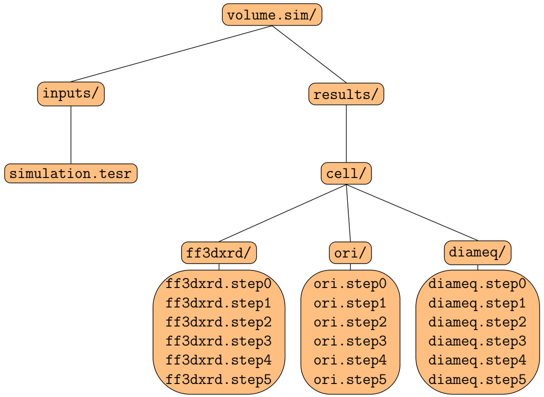
Computing Results

```
$ neper -S volume.sim -step 5 \
  -cellres "ff3dxrd:file(ff3dxrd),ori:file(ori),diameq"
```

ff3dxrd:

```
1
0
0
1
0
1
[...]
```

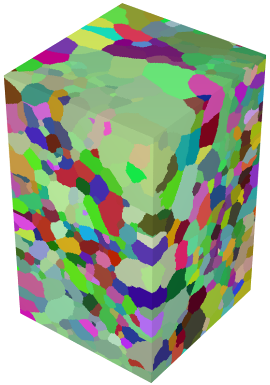
ori.step0, ori.step1, ...



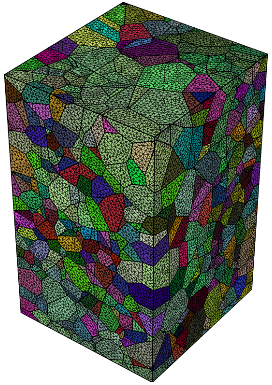
Simple *simulation directory*, custom or built-in results (morphological, topological or orientation-related), custom visualization

```
$ neper -T -morpho "tesr(volume.tesr)" \
           -domain "cube(0.8386,0.8092,1.3622)" -o volume

$ neper -M volume.tess -order 2 -rcl 0.5 -part 100
```



↓



Simulation file, `simulation.config`

```
## Material Parameters
    number_of_phases 1

    phase 1
    crystal_type FCC
    m 0.03
    gammadot_0 1.0
    h_0 47.0
    g_0 6.0
    g_s0 455.0
    m_prime 0.0
    gammadot_s0 1.e10
    n 2.6
    c11 107.3e3
    c12  60.9e3
    c44  28.3e3

## Deformation History
    def_control_by uniaxial_strain_target

    number_of_strain_steps 5
    target_strain 0.010  60 print_data
    target_strain 0.015  30 print_data
    target_strain 0.020  30 print_data
    target_strain 0.025  30 print_data
    target_strain 0.045 120 print_data

## Boundary Condition
    boundary_conditions uniaxial_minimal
    loading_direction Z
    loading_face Z_MAX
    strain_rate 1e-2

## Printing Results
    print coo
    print ori
    print slip
    print sliprate
    print crss
    print stress
```

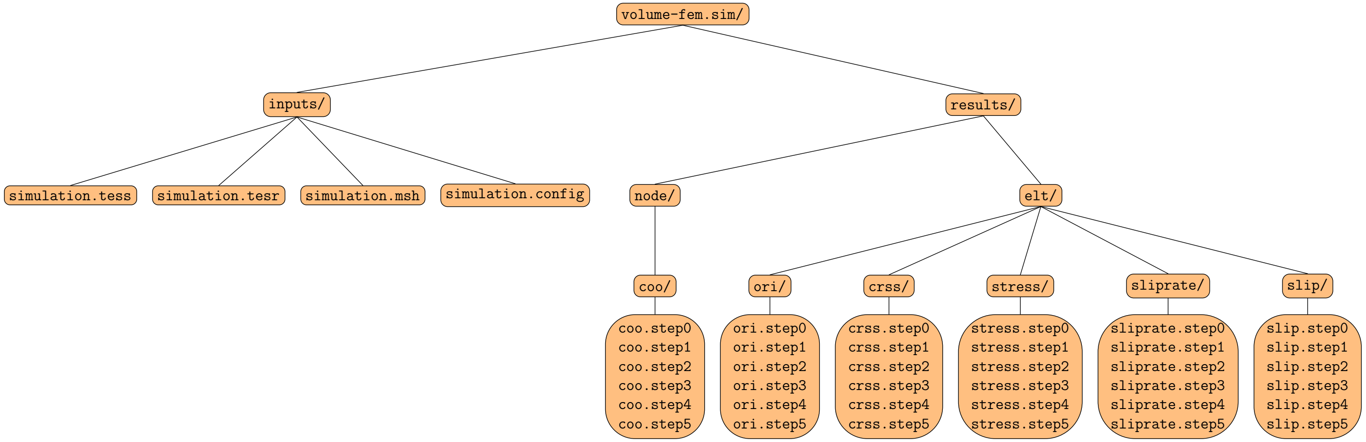
Running FEPX

$ mpirun -np 100 fepx (on a computer cluster, in a submission script)

↪ per-core files (`post.core#`)

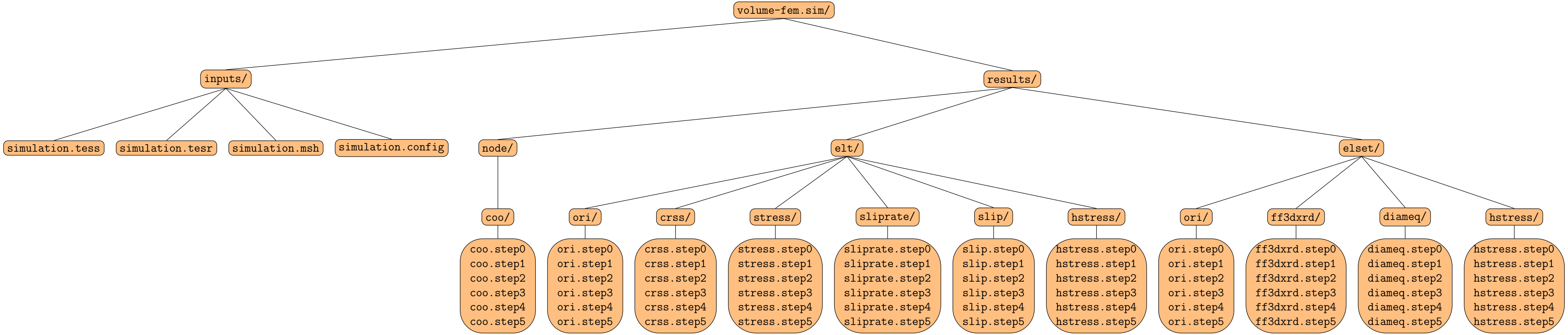
$ neper -S volume-fem/

↪ simulation directory, `volume-fem.sim`



Simulation Post-Processing: Grain Averaging, etc.

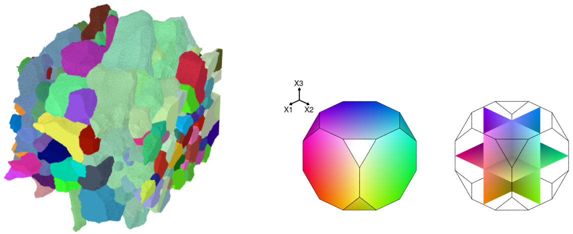
```
$ neper -S volume-fem.sim                                        \
           -reselt    "hstress:(stress11+stress22+stress33)/3"   \
           -reselset "ori,ff3dxrd:file(ff3dxrd),diameq,hstress"
```

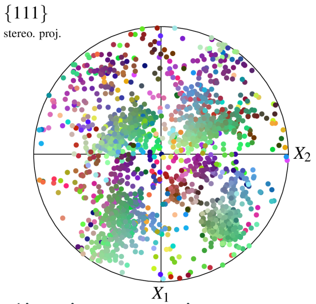


Visualization

Experiment

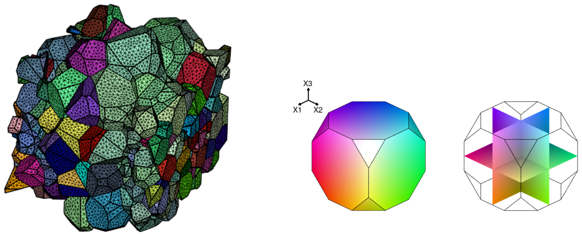
```
$ neper -V volume.sim       \
        -step 5             \
        -showcell "ff3dxrd" \
        -datacellcol ori    \
        -print exp          \
        -space pf           \
        -print exp-pf
```

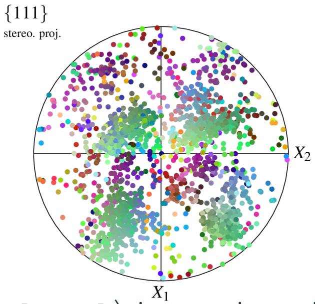




Simulation

```
$ neper -V volume-fem.sim    \
        -step 5              \
        -datanodecoo coo     \
        -showelset "ff3dxrd" \
        -dataelsetcol ori    \
        -print fem           \
        -space pf            \
        -print fem-pf
```





Custom visualization, consistent across possible inputs (experiment and simulation, 2D or 3D), interactive using VTK files

Conclusions

The Neper/FEPX Project

- Convergence of 2 established codes, product of 40 collective years of development and use
- Goal: Full range of features for polycrystal plasticity studies, especially in the experiment / simulation context
  - → Generation, meshing, simulation, ...
  - → ... post-processing, visualization, *data management* (+ Jupyter notebooks)
  - → *Many* features are implemented, others *can be* added
- Open-science approach: open-source code, open resources, ...
- Growing community of users (discussion forums)