Parent grain reconstruction in MTEX

Frank Niessen
Technical University of Denmark, Department of Mechanical Engineering, Kongens Lyngby, Denmark

Ralf Hielscher
Institute of Mathematics, TU Chemnitz,Germany

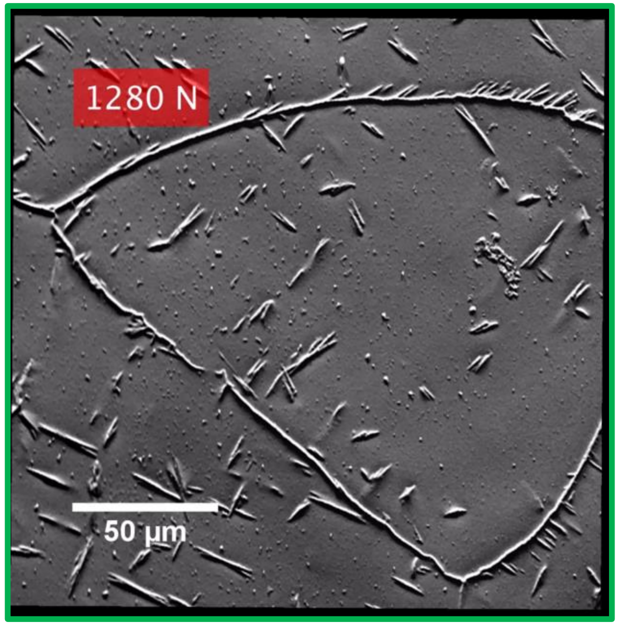
Parent grain reconstruction in MTEX

- Introduction
  - *to martensitic transformations*
  - *to parent grain reconstruction*
- MTEX implementation
  - *Example "$\gamma \rightarrow \alpha'$ transformation in steel"*
- Further application examples
- Conclusion

Introduction – Martensitic transformation

- The martensitic transformation is a technologically important **diffusionless transformation** from a metastable **parent** to a martensitic **child phase**
  - γ-to-ε and γ-to-α' transformations in steels -> *TRIP*
  - β-to-α' and β-to-α'' transformation in titanium alloys -> *TRIP & Shape Memory Effect*

[http://www.phase-trans.msm.cam.ac.uk/2002/martensite.html
Professor Toshihiko Koseki, Tokyo University]

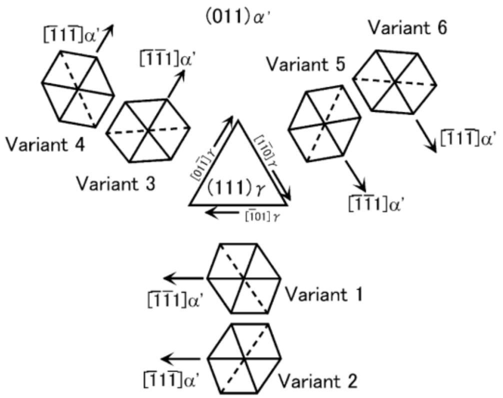


[F. Niessen, A.A. Gazder, D.R.G. Mitchell, E. V. Pereloma, Mater. Sci. Eng. A 802 (2021).

Introduction – Martensitic transformations

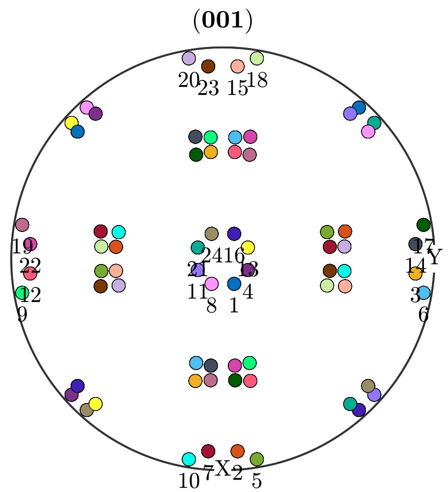
- The **orientation relationship** is defined by a set of **parallel planes** and **directions**
  - Kurdjumow-Sachs (K-S): $\{111\}_\gamma \,||\, \{110\}_{\alpha'},\ \langle 1\bar{1}0\rangle_\gamma \,||\, \langle 1\bar{1}1\rangle_{\alpha'}$
  - Nishiyama-Wasserman (N-W): $\{111\}_\gamma \,||\, \{110\}_{\alpha'},\ \langle 0\bar{1}1\rangle_\gamma \,||\, \langle 001\rangle_{\alpha'}$
  - …
  - Shoji-Nishiyama (S-N): $\{111\}_\gamma \,||\, \{0001\}_\varepsilon,\ \langle 1\bar{1}0\rangle_\gamma \,||\, \langle 11\bar{2}0\rangle_\varepsilon$
- Crystal symmetry leads to the formation of several orientation variants

Orientation relationship in steel



[S. Morito, H. Tanaka, R. Konishi, T. Furuhara, T. Maki, Acta Mater. 51 (2003) 1789–1799.]

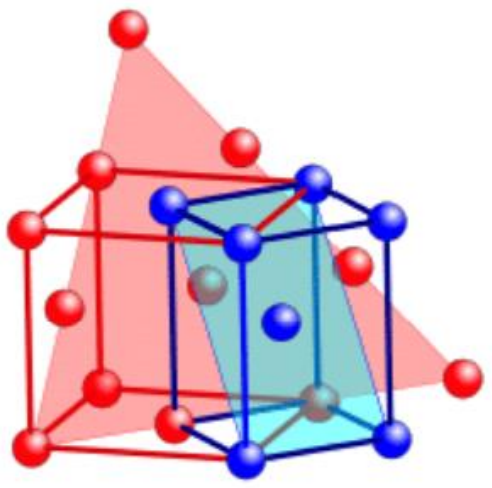
Orientation variants in steel



Introduction – Martensitic transformations

- The **experimentally observed OR** is generally close, but not identical to **rational** OR's
  - In lath martensite in steels it is about **halfway between K-S and N-W**
  - This seemingly marginal difference becomes **important in parent grain reconstruction**

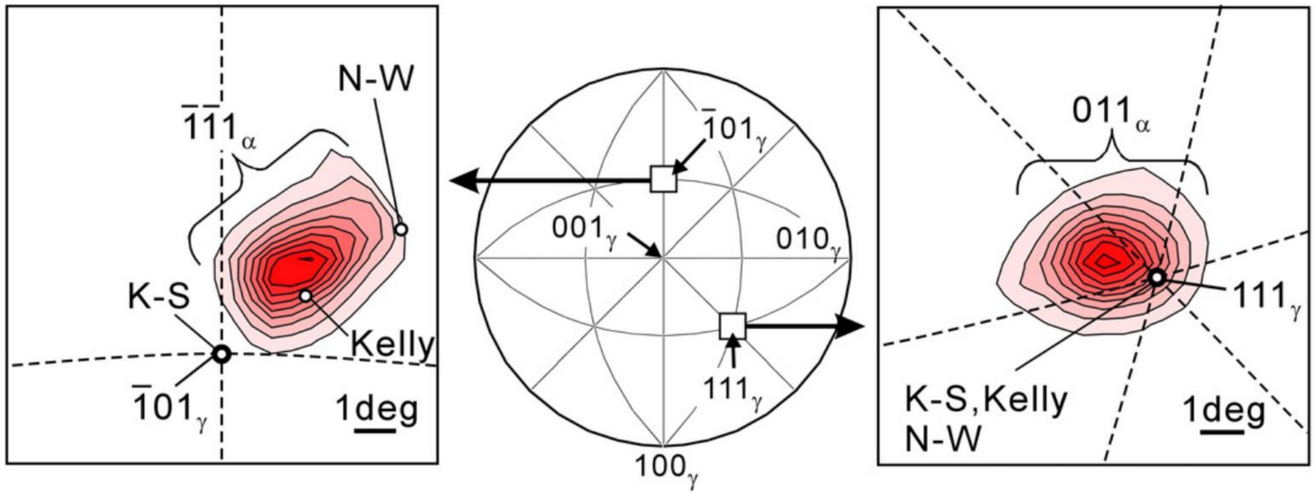
Rational OR



[G. Nolze, Zeitschrift Für Met. 95 (2004) 744–755.]

Experimentally observed OR

Parallel directions **Parallel planes**



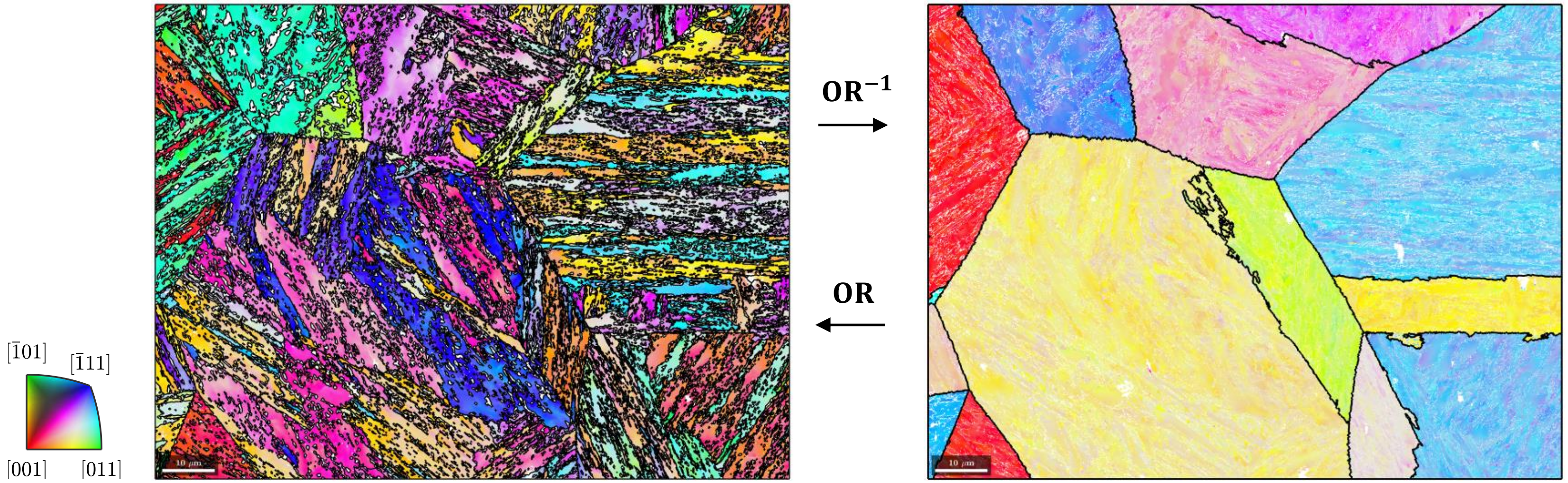
[G. Miyamoto, N. Iwata, N. Takayama, T. Furuhara, Acta Mater. 58 (2010) 6393–6403]

Introduction – Parent grain reconstruction

- **Parent grain reconstruction** aims at calculating the parent microstructure from the orientations of the child phase
- **One parent** orientation can form **several** child orientation **variants** (up to 24 in steel)
  – Therefore **one child** orientation can have **multiple** potential **parent orientations**
- Goal: Find **sufficient** distinct **child orientations** of the **same prior parent** grain to **calculate** the **parent orientation**

Martensitic microstructure

Parent phase microstructure



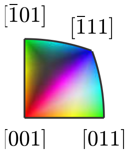
α' orientations

Reconstructed γ orientations

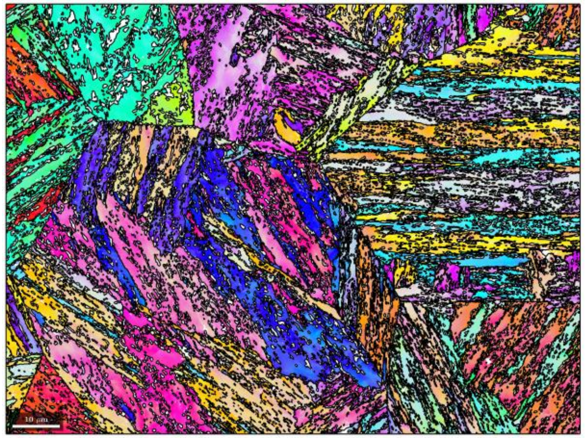
Introduction – Parent grain reconstruction

Why care?!?

- Parent grain reconstruction is **more than an academic exercise –** Two purposes:
  - **Optimizing high-temperature processing** (hot-rolling,forging)
  - **Detailed analysis of the hierarchy of martensitic microstructures**
    - Variant and mechanical analysis



Martensitic microstructure →



α' orientations

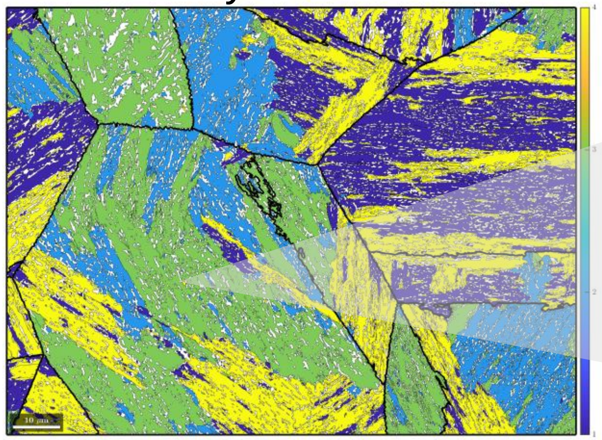
OR^{-1} →

← OR

Parent phase microstructure →

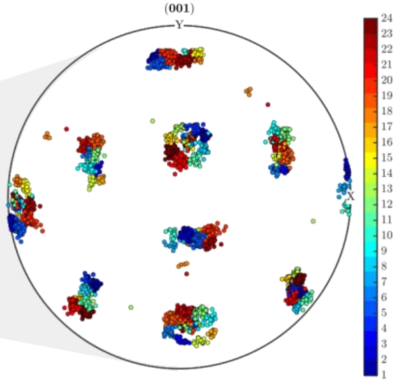
Reconstructed γ orientations

Variant analysis →



Packet map

Local analysis

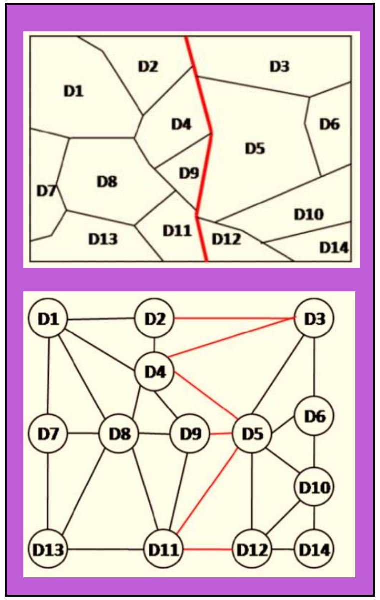


Variant polefigure

Introduction – Parent grain reconstruction

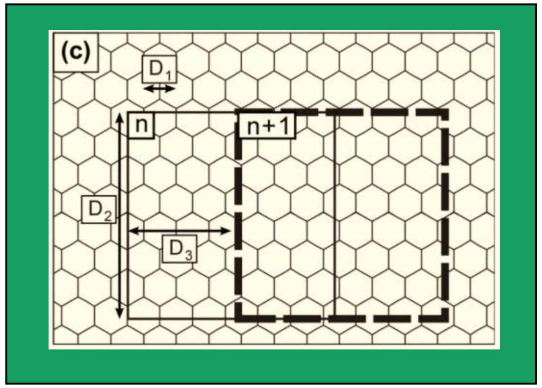
There are **two types of methods** for **parent grain reconstruction**:

- Operations on a **weighted graph** constructed from a **grain map** [1–7]
  - *Computationally efficient*
- Operations on **cropped sections** of the **orientation (EBSD) map** that has been segmented into a **square grid** [8–10]
  - *Claimed to be more accurate on ambiguous orientations (i.e. twins)*



Ref. [2]

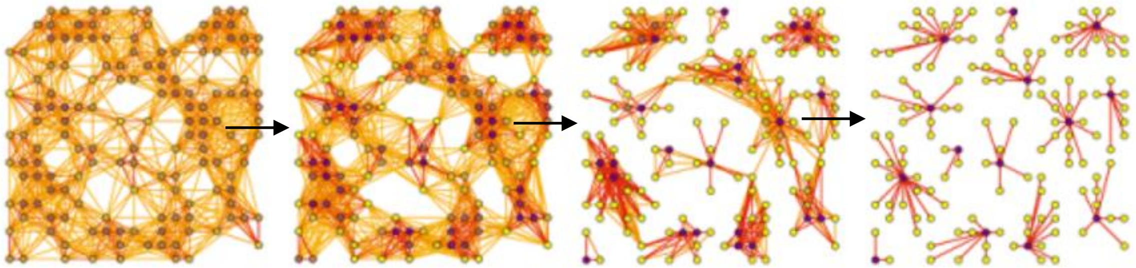
[1] C. Cayron, B. Artaud, L. Briottet, Mater. Charact. 57 (2006) 386–401.
[2] L. Germain, N. Gey, R. Mercier, P. Blaineau, M. Humbert, Acta Mater. 60 (2012) 4551–4562.
[3] E. Gomes, L.A.I. Kestens, in: 17th Int. Conf. Textures Mater. (ICOTOM 17), 2015.
[4] T. Nyyssönen, P. Peura, V.T. Kuokkala, Metall. Mater. Trans. A 49 (2018) 6426–6441.
[5] A.H. Pham, T. Ohba, S. Morito, T. Hayashi, Mater. Trans. 56 (2015) 1639–1647.
[6] C.Y. Huang, H.C. Ni, H.W. Yen, Materialia 9 (2020).
[7] S.K. Giri, A. Durgaprasad, K. V. Manikrishna, C.R. Anoop, S. Kundu, I. Samajdar, Philos. Mag. 99 (2019) 699–717.
[8] G. Miyamoto, N. Iwata, N. Takayama, T. Furuhara, Acta Mater. 58 (2010) 6393–6403.
[9] N. Bernier, L. Bracke, L. Malet, S. Godet, Mater. Charact. 89 (2014) 23–32.
[10] D. Wang, J. Jin, Q. Li, X. Wang, Crystals 9 (2019).



Ref. [8]

Introduction – Parent grain reconstruction

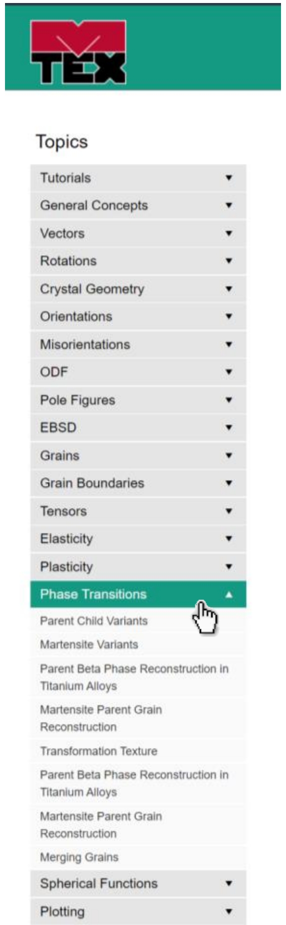
- Most **weighted graph** approaches
  - **first** calculate **all possible parent orientations** for all child orientations
  - **then group child grains** that have a common parent orientation
- Method by *Gomes et al.*[1] and *Nyssönnen et al.*[2]
  - Apply **Markov clustering** algorithm to
    - **first group child grains** and **then** calculate the **common parent orientation**
  - Markov clustering discovers natural groups in graphs by simulating a random walk



[1] *E. Gomes, L.A.I. Kestens, in: 17th Int. Conf. Textures Mater. (ICOTOM 17), 2015.*

[2] *T. Nyyssönen, P. Peura, V.T. Kuokkala, Metall. Mater. Trans. A 49 (2018) 6426–6441.*

MTEX implementation



- **Only open and freely available parent reconstruction method ->** released in **MTEX 5.6**
- Supports the analysis of **transitions** between **arbitrary parent** and **child** phases
- **Different reconstruction models** can be combined
  - **Boundary based** vs. **triple point based**
  - **Graph clustering** algorithms
  - **Nucleation based** algorithms
    - ➢ Child grain reversion by vote of neighboring child grains
  - **Growth based** algorithms
    - ➢ Growth of parent grains into child grains
- Straight forward **local reversion** of bad reconstructions
- **Iterative reconstruction** with increasing threshold

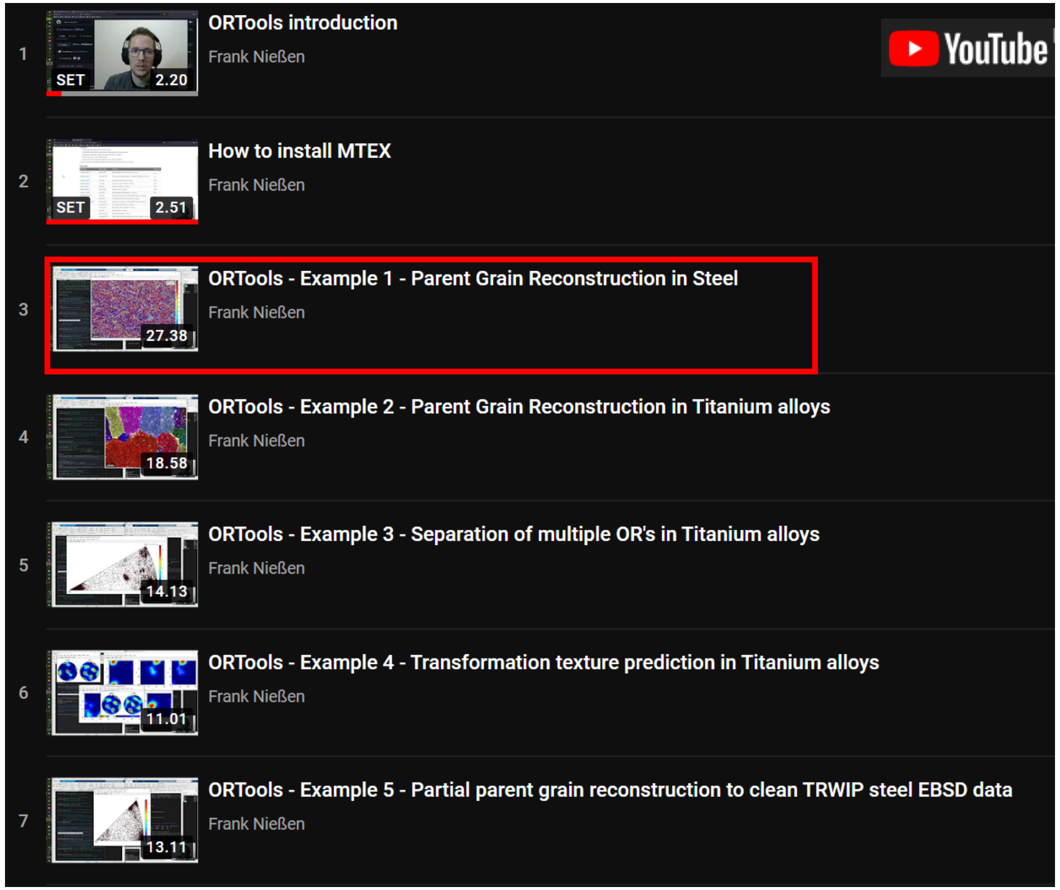
https://mtex-toolbox.github.io/

Commercial break!

OR Tools

https://github.com/frankNiessen/ORTools

- Add-on to MTEX focusing on phase transitions
- A function library for OR discovery, OR analysis and the plotting of publication-ready figures of martensitic transformations in MTEX
- The library contains
    - Several automated and preformatted plotting functions
    - Interactive exploration of several OR's in one EBSD map
    - Transformation texture prediction
    - Useful auxiliary functions
    - More to follow soon …



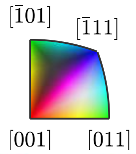
Dr. Azdiar Gazder, University of Wollongong

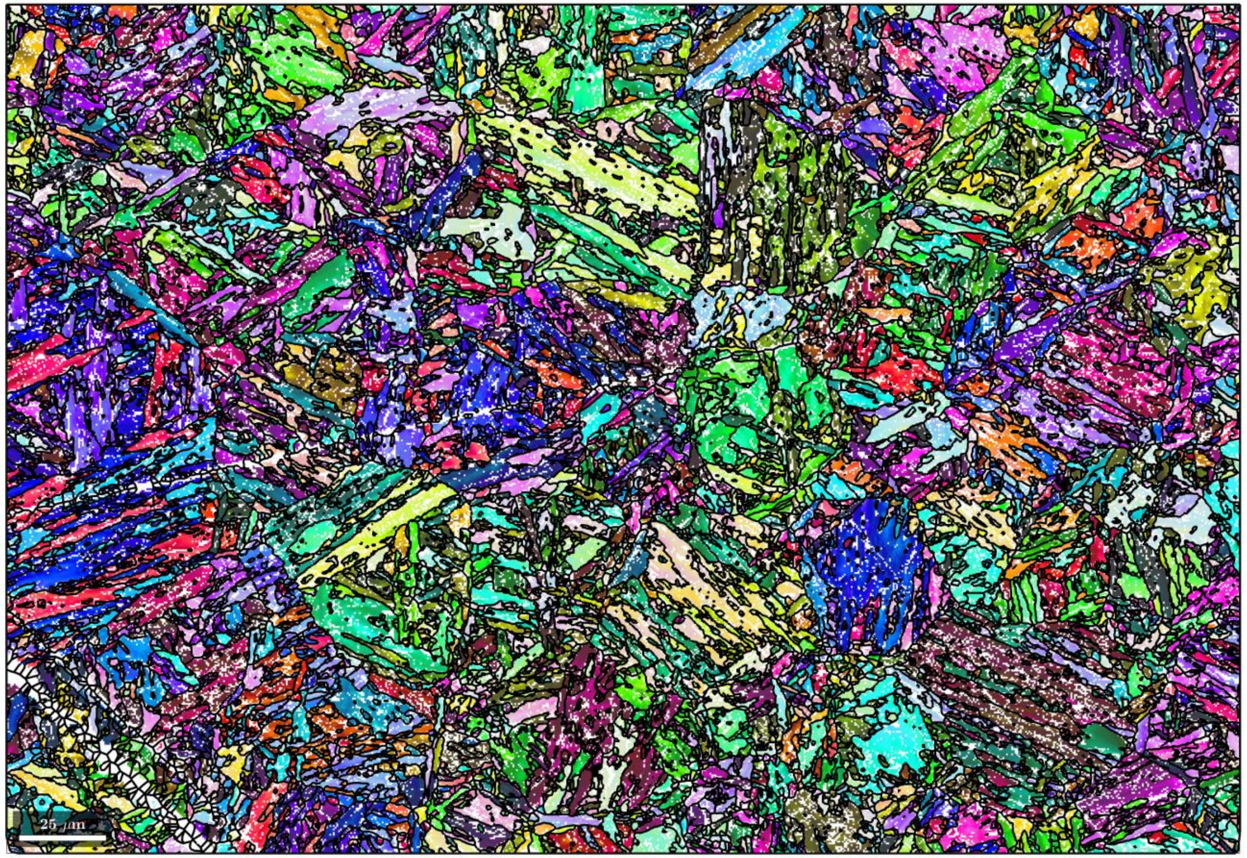
https://mtex-toolbox.github.io/MaParentGrainReconstruction.html

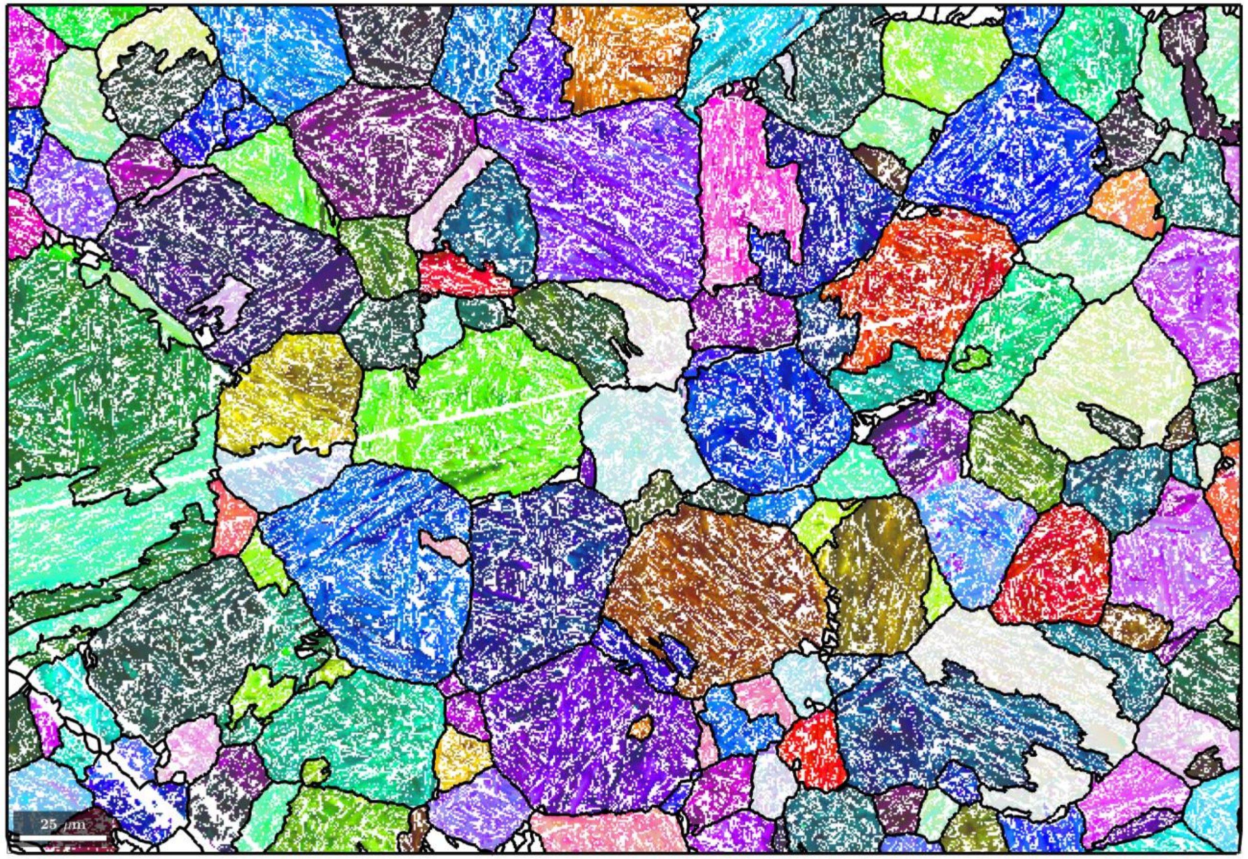
ORTools https://github.com/frankNiessen/ORTools/blob/develop/README.md#example-1

Example 1 – Lath martensite $\gamma \rightarrow \alpha'$

- We want to transfer the EBSD lath martensite microstructure on the left to an austenite microstructure on the right

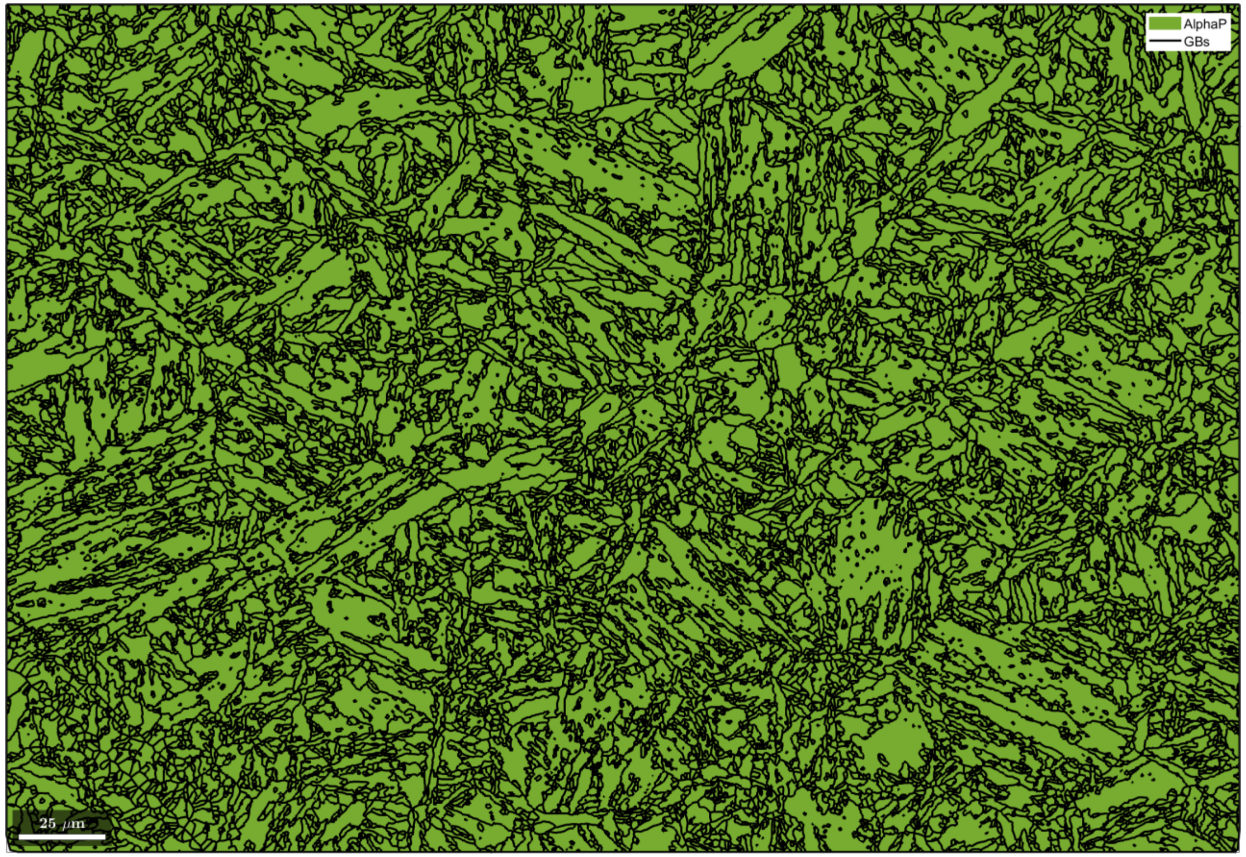






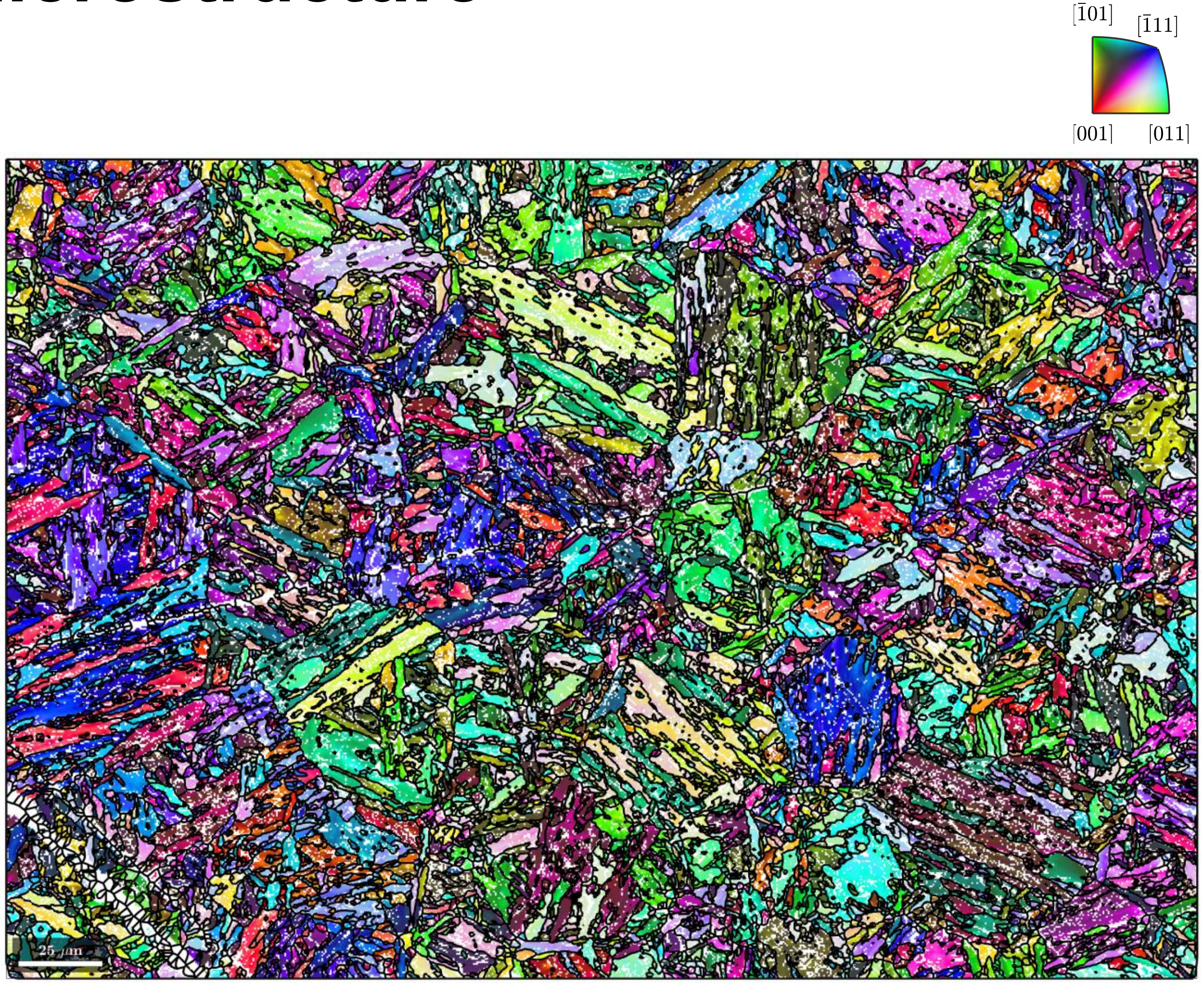
Example 1 – Initial microstructure

- We have only martensite



Example 1 – Initial microstructure

- The prior austenite grain boundaries are not obvious everywhere
- We have 29% unindexed points



Example 1 – OR determination

Define and refine orientation relationship

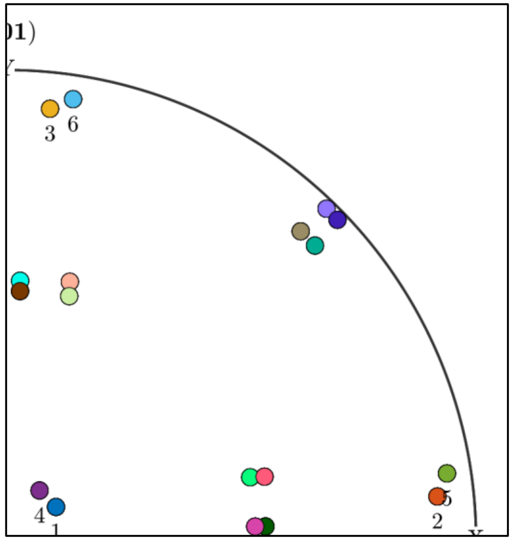
```
job = parentGrainReconstructor(ebsd,grains);
job.p2c = orientation.KurdjumovSachs;
job.calcParent2Child; %*
```

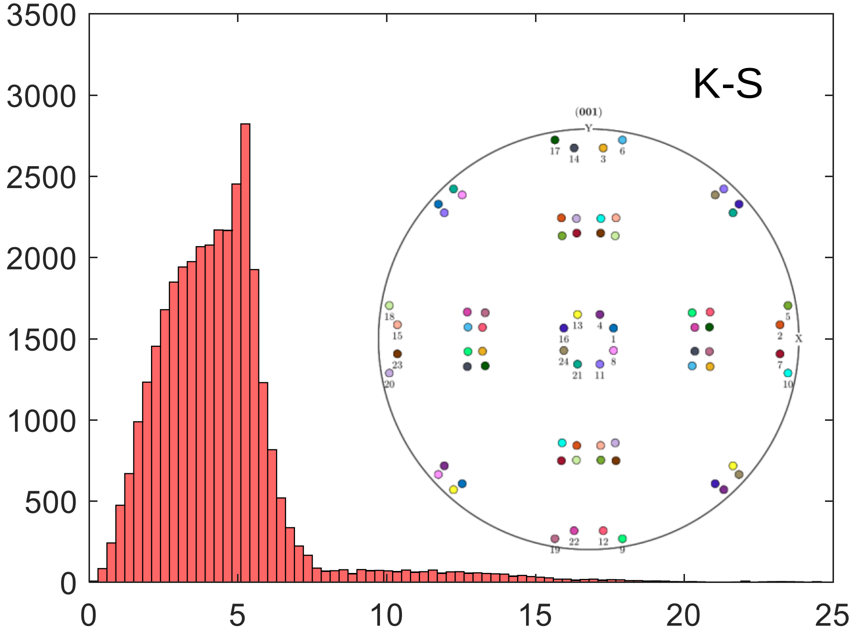
```
optimizing parent to child orientation relationship
 (335.8°  ,10.5°  ,65.8°  ) 3.7
 (345.4°  ,10.3°  ,60.1°  ) 2.7
 (356.4°  ,9.6°  ,50°  )    2.7
 ...
```

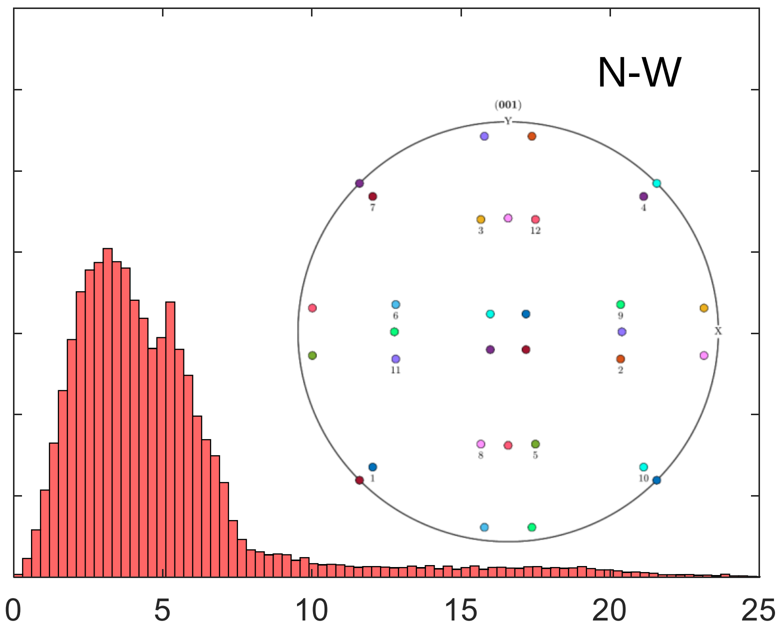
Automatic adaption of Morito convention

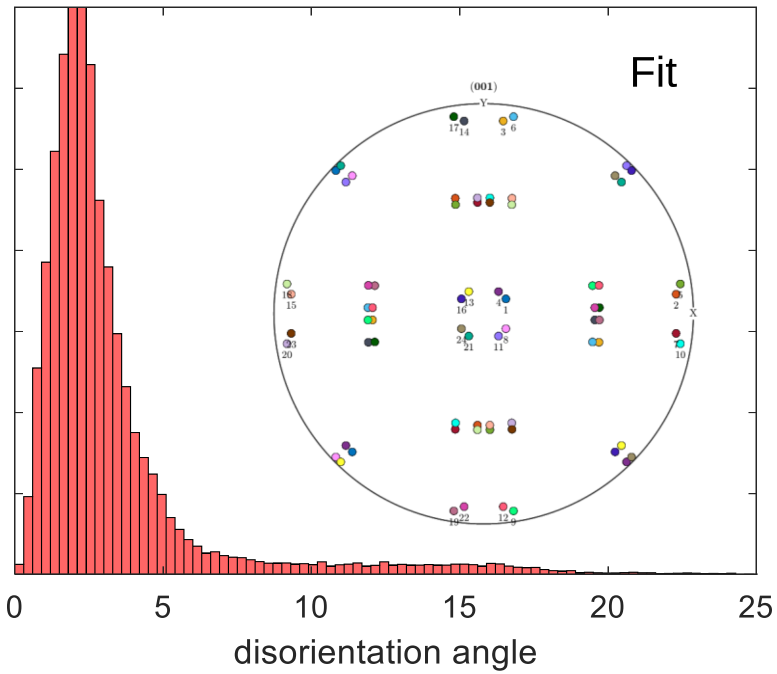
```
job.variantMap
```

```
=[1 3 5 21 23 19 11 7 9 16 14 18
  24 22 20 4 2 6 13 15 17 8 12 10]
```









*[T. Nyyssönen, M. Isakov, P. Peura, V.T. Kuokkala, Metall. Mater. Trans. A 47 (2016) 2587–2590.]

Example 1 – OR inspection

```
job.parent2ChildInfo
```

-> OR info:
- OR misorientation angle = 44.9863º

-> Parallel planes
- Closest parent plane = (1,-1,0)
- Closest child plane = (1,0,0)
- Ang. dev. from parallel plane relationship from OR = 2.4033º

-> Parallel directions
- Closest parent direction = [1,1,1]
- Closest child direction = [0,1,1]
- Ang. dev. from parallel directions relationship from OR = 0.61727º

-> OR misorientation rotation axes
- Parent rot. axis = [-0.0532,0.0363,0.2655]
- child rot. axis = [-0.0679,0.0463,0.3391]

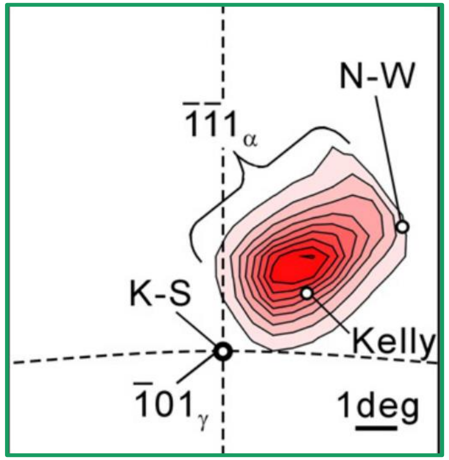
-> Angle & rot. axes of unique variants
- 1: 0.00º / [0.3489,-0.0000,-0.0000]
- 2: 60.01º / [-0.1690,0.1747,0.2503]

…

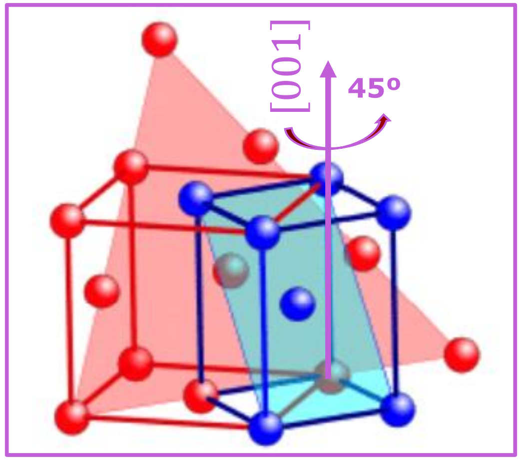
K-S: $\{111\}_\gamma || \{110\}_{\alpha'}$ $\langle 1\bar{1}0\rangle_\gamma$ $\langle 1\bar{1}1\rangle_{\alpha'}$

N-W: $\{111\}_\gamma || \{110\}_{\alpha'}$ $\langle 0\bar{1}1\rangle_\gamma$ $\langle 001\rangle_{\alpha'}$

Parallel directions



[G. Miyamoto, N. Iwata, N. Takayama, T. Furuhara, Acta Mater. 58 (2010) 6393–6403]



[G. Nolze, Zeitschrift Für Met. 95 (2004) 744–755.]

*[T. Nyyssönen, M. Isakov, P. Peura, V.T. Kuokkala, Metall. Mater. Trans. A 47 (2016) 2587–2590.]

Example 1 – OR inspection

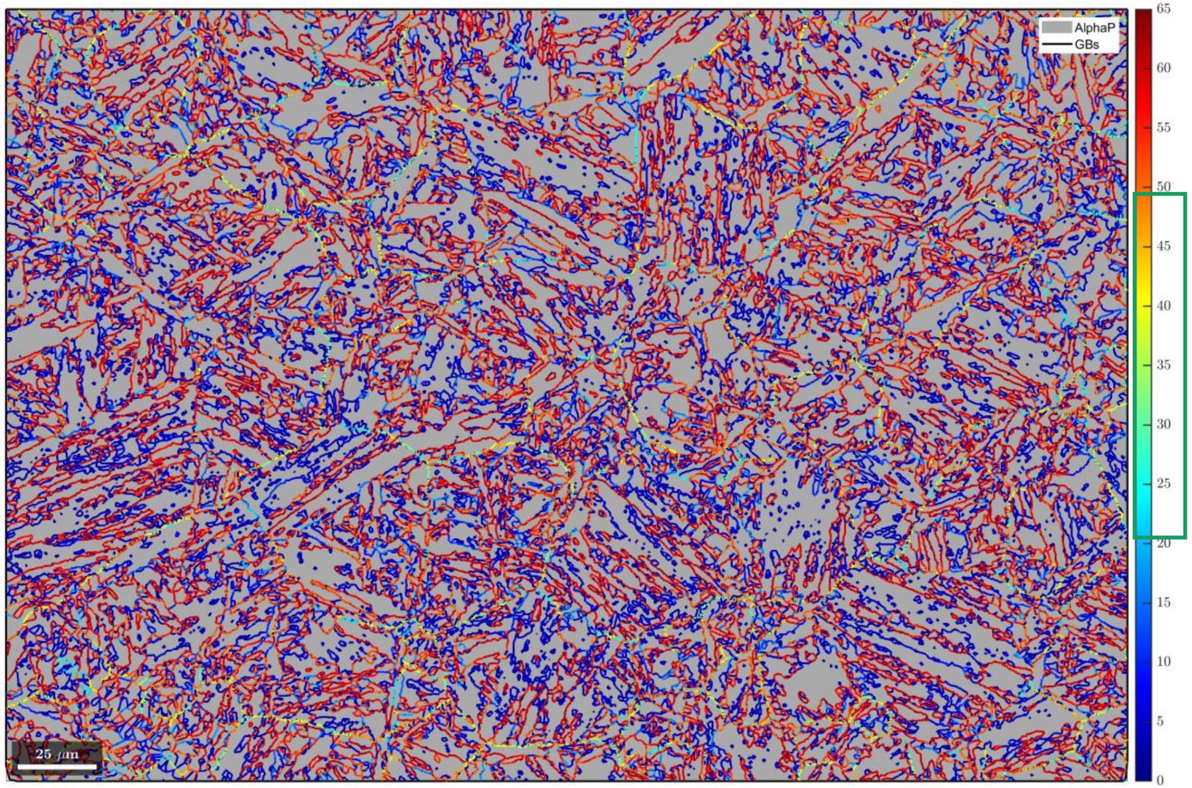
```
job.parent2ChildInfo
```

…

-> Angle & rot. axes of unique variants

- 1: 0.00º / [0.3489,-0.0000,-0.0000]
- 2: 60.01º / [-0.1690,0.1747,0.2503]
- 3: 60.01º / [-0.1747,0.1690,0.2503]
- 4: 20.38º / [-0.0332,-0.0000,0.3473]
- 5: 55.17º / [-0.2350,0.0818,0.2445]
- 6: 51.55º / [-0.0705,0.2303,0.2524]
- 7: 14.62º / [-0.1878,0.0223,0.2932]
- 8: 49.96º / [-0.2082,0.1871,0.2082]
- 9: 51.55º / [-0.2303,0.0705,0.2524]
- 10: 17.45º / [-0.2426,0.0633,0.2426]
- 11: 49.63º / [-0.1977,0.1668,0.2342]
- 12: 50.62º / [-0.0918,0.2312,0.2447]
- 13: 20.69º / [-0.0746,-0.0000,0.3408]
- 14: 50.62º / [-0.2312,0.0918,0.2447]
- 15: 56.21º / [-0.0631,0.2302,0.2545]
- 16: 4.81º / [-0.1940,-0.0000,0.2900]
- 17: 60.27º / [-0.1910,0.1810,0.2292]
- 18: 55.29º / [-0.2467,0.0015,0.2467]
- 19: 14.62º / [-0.0223,0.1878,0.2932]
- 20: 55.17º / [-0.0818,0.2350,0.2445]
- 21: 49.45º / [-0.2240,0.1463,0.2240]
- 22: 11.56º / [-0.2448,0.0437,0.2448]
- 23: 56.21º / [-0.2302,0.0631,0.2545]
- 24: 49.63º / [-0.1668,0.1977,0.2342]

No OR-misorientations between 21 and 49°

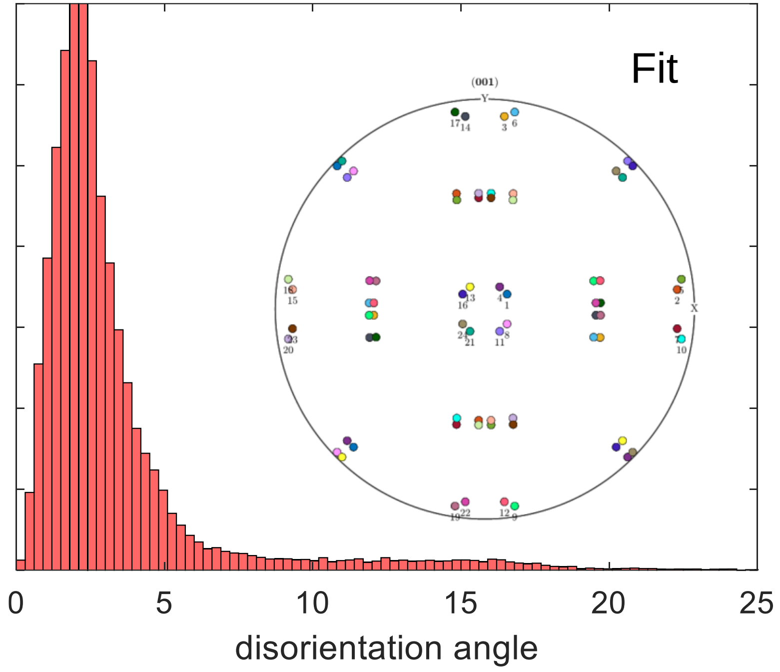


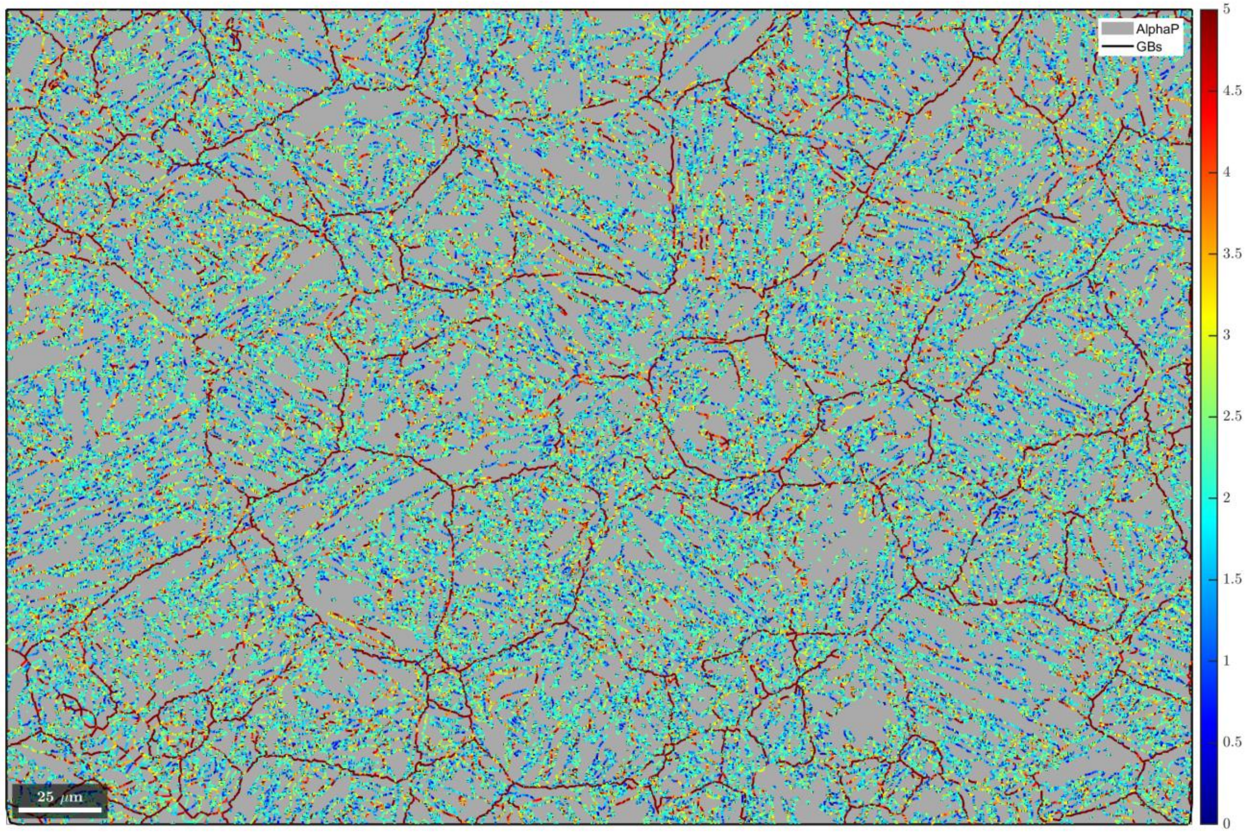
ORTools `plotMap_gB_c2c`

Example 1 – Disorientation

Plot disorientation on boundaries

```
[fit,c2cPairs] = job.calcGBFit;
[gB,pairId] = job.grains.boundary.selectByGrainId(c2cPairs);
plot(gB, fit);
```





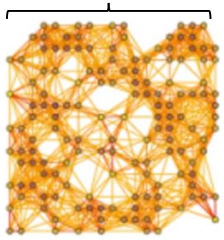
ORTools plotMap_gB_misfit

Example 1 – Graph of OR probability

Reconstruct parent orientations from graph

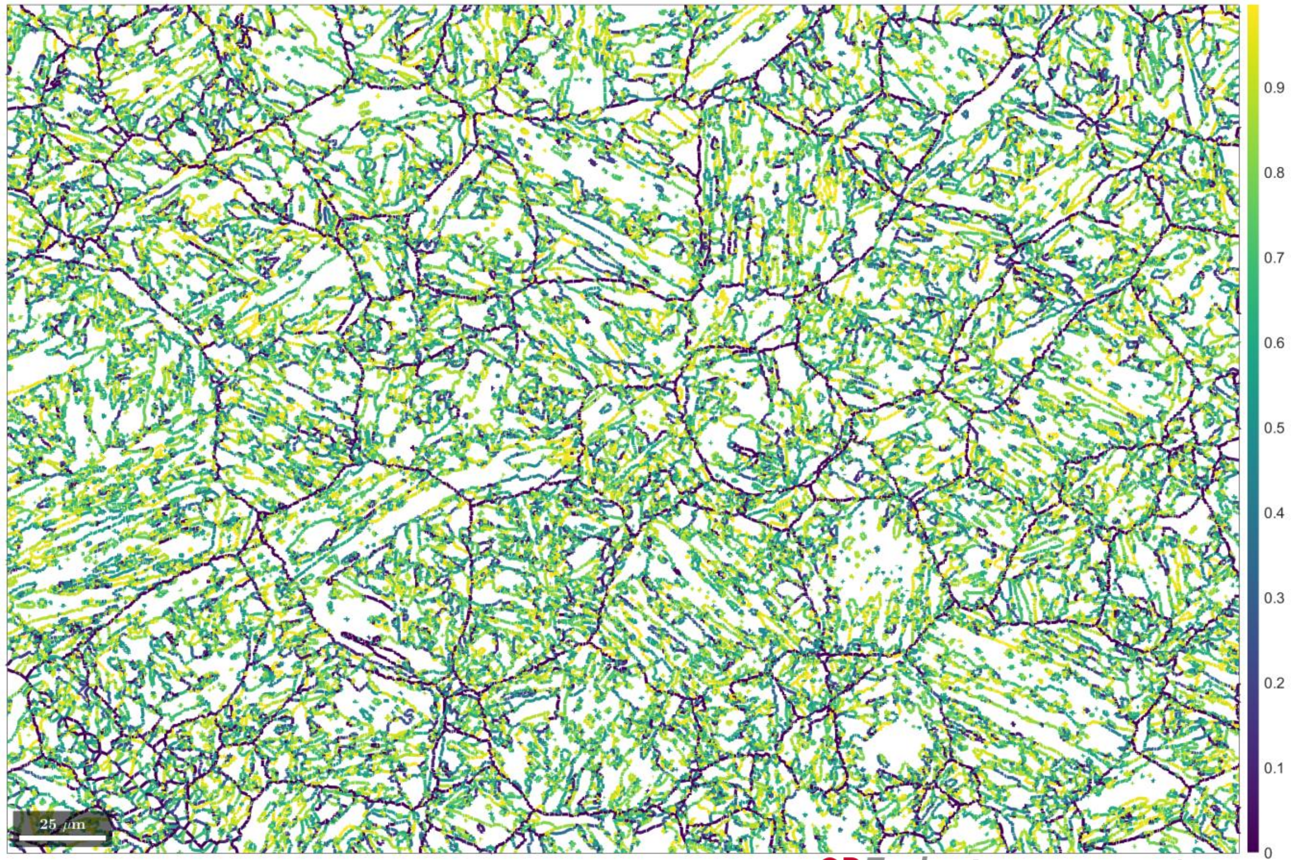
```
% compute parent orientations
1) job.calcGraph
```

1)



Markov Clustering - https://micans.org/mcl/

1) Probability that a boundary is an OR boundary (and the associated grains share the same parent grain)



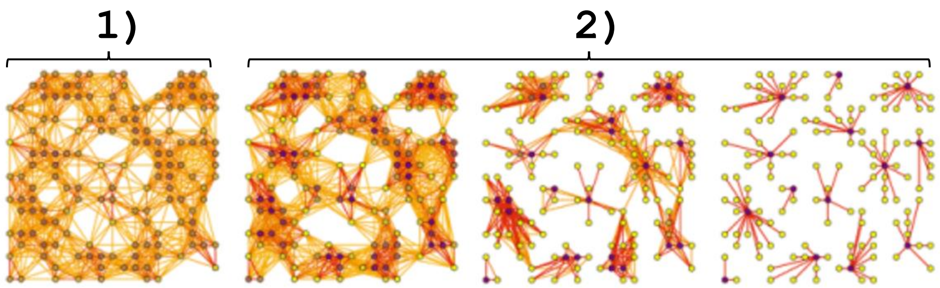
ORTools `plotMap_gB_prob`

Example 1 – Clustering of the graph

Reconstruct parent orientations from graph

```
% compute parent orientations
1) job.calcGraph
2) job.clusterGraph %*
```

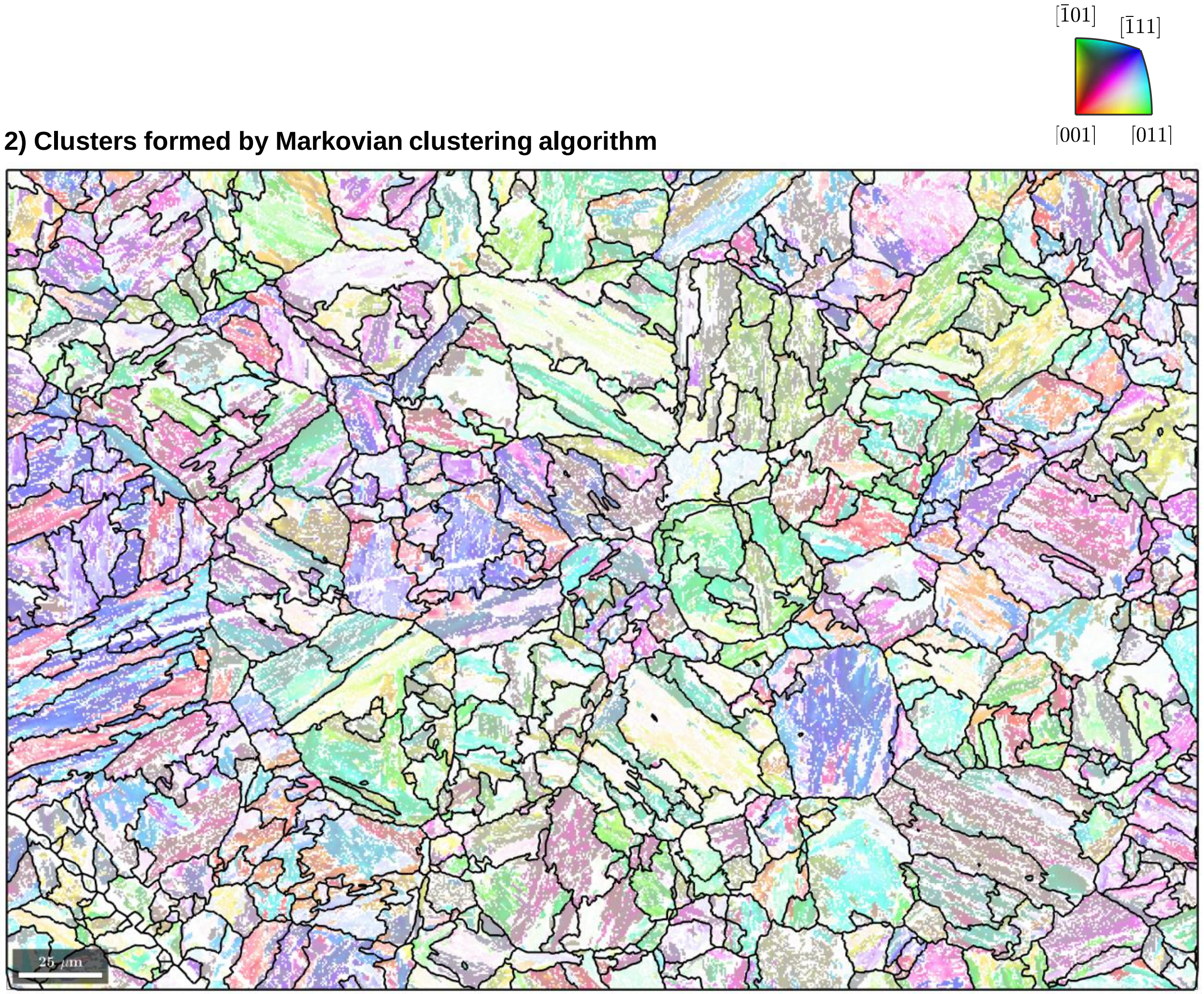
… graph: 19470 grains in 2615 clusters + 2127 single grain clusters



Markov Clustering - https://micans.org/mcl/

*[T. Nyyssönen, P. Peura, V.T. Kuokkala, Metall. Mater. Trans. A 49 (2018) 6426–6441.]

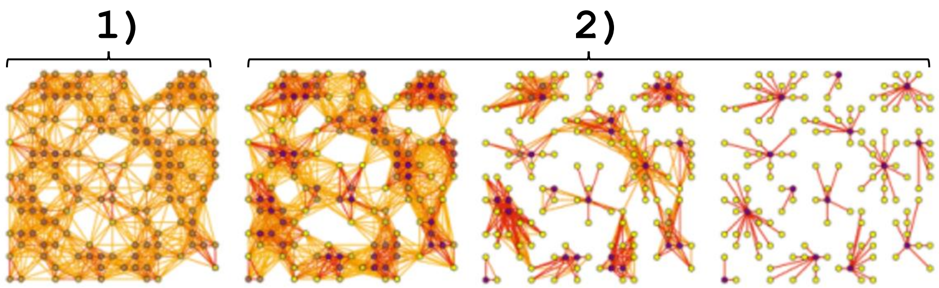
2) Clusters formed by Markovian clustering algorithm



Example 1 – Parent reconstruction from clusters

Reconstruct parent orientations from graph

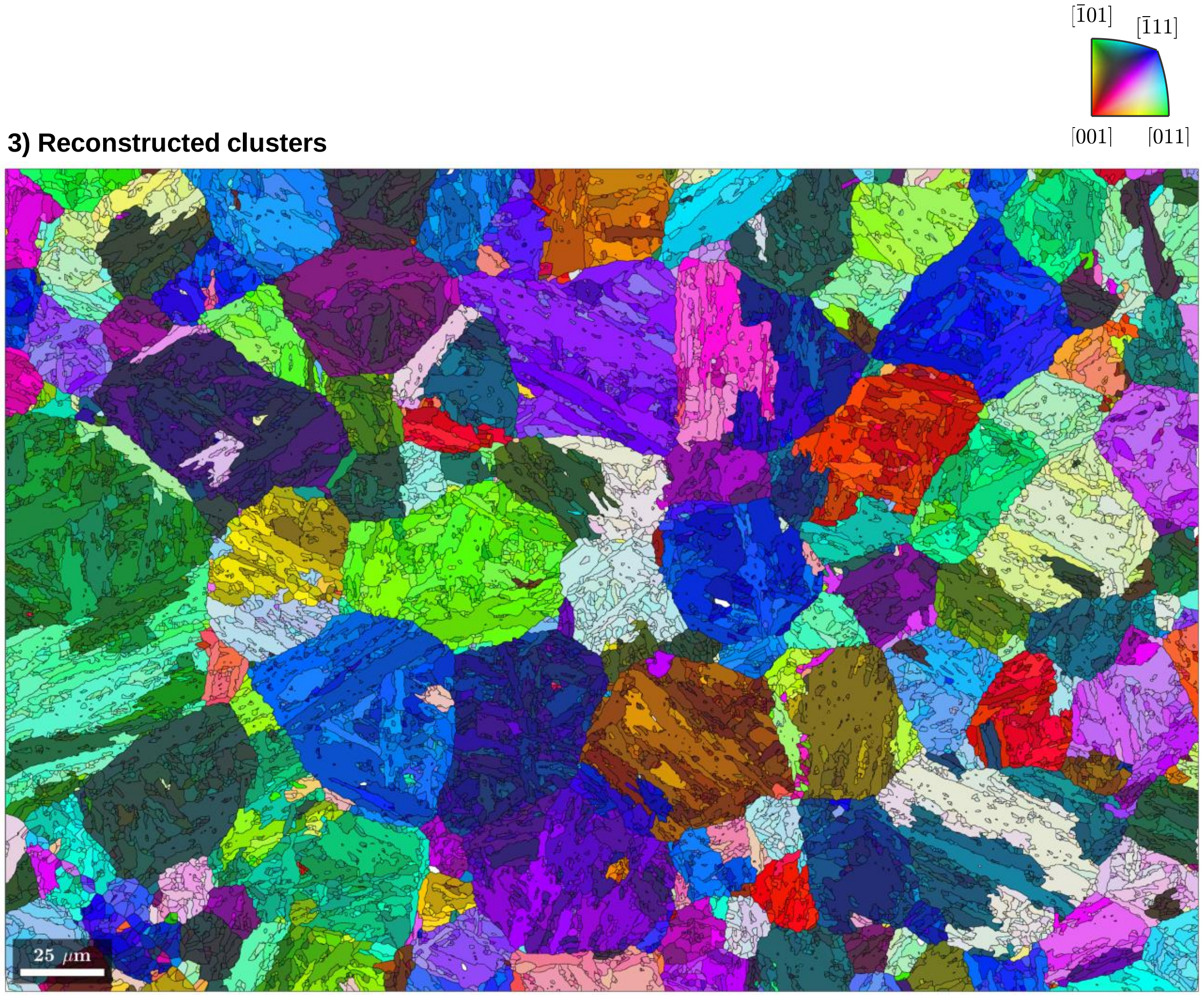
```
% compute parent orientations
1) job.calcGraph
2) job.clusterGraph %*
3) job.calcParentFromGraph
```



Markov Clustering - https://micans.org/mcl/

*[T. Nyyssönen, P. Peura, V.T. Kuokkala, Metall. Mater. Trans. A 49 (2018) 6426–6441.]

3) Reconstructed clusters

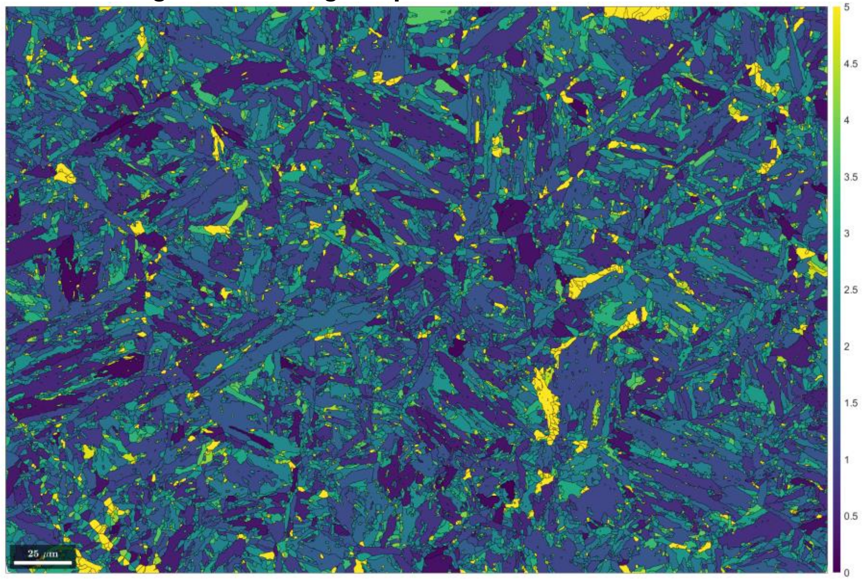


Example 1 – Reverting bad reconstructions

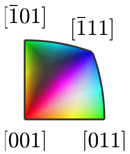
Reconstruct parent orientations from graph

```
% plot fit and revert bad fits
plot(job.grains,job.grains.fit./degree)
job.revert(job.grains.fit > 5)
job.revert(job.grains.clusterSize < 15)
job.calcParentFromGraph
```

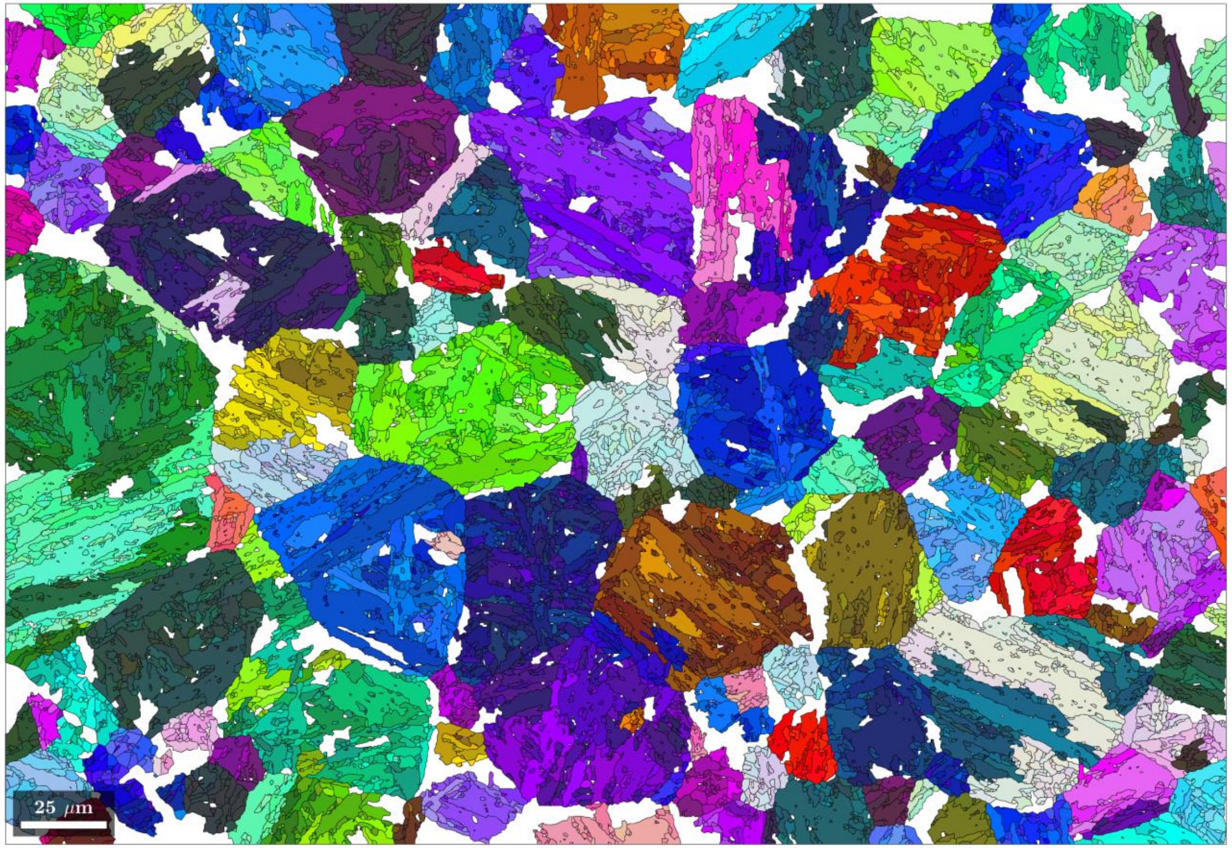
Fit of child grains to assigned parent orientation via the OR



`job.revert`



3) Reconstructed clusters after removal of bad fits



Example 1 – Growth-based reconstruction

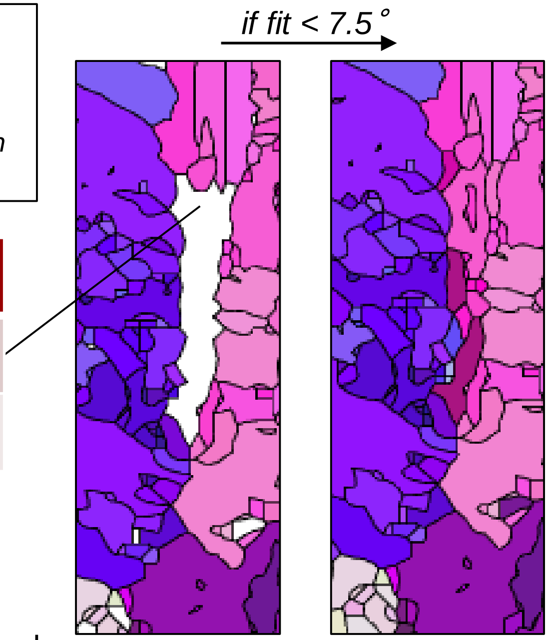
Fill in empty regions with *calcParentFromVote*

```
for k = 1:3 % do this three times
    job.calcGBVotes('noC2C');
    job.calcParentFromVote('minFit',7.5*degree)
end
```

job.calcGBVotes('noC2C')

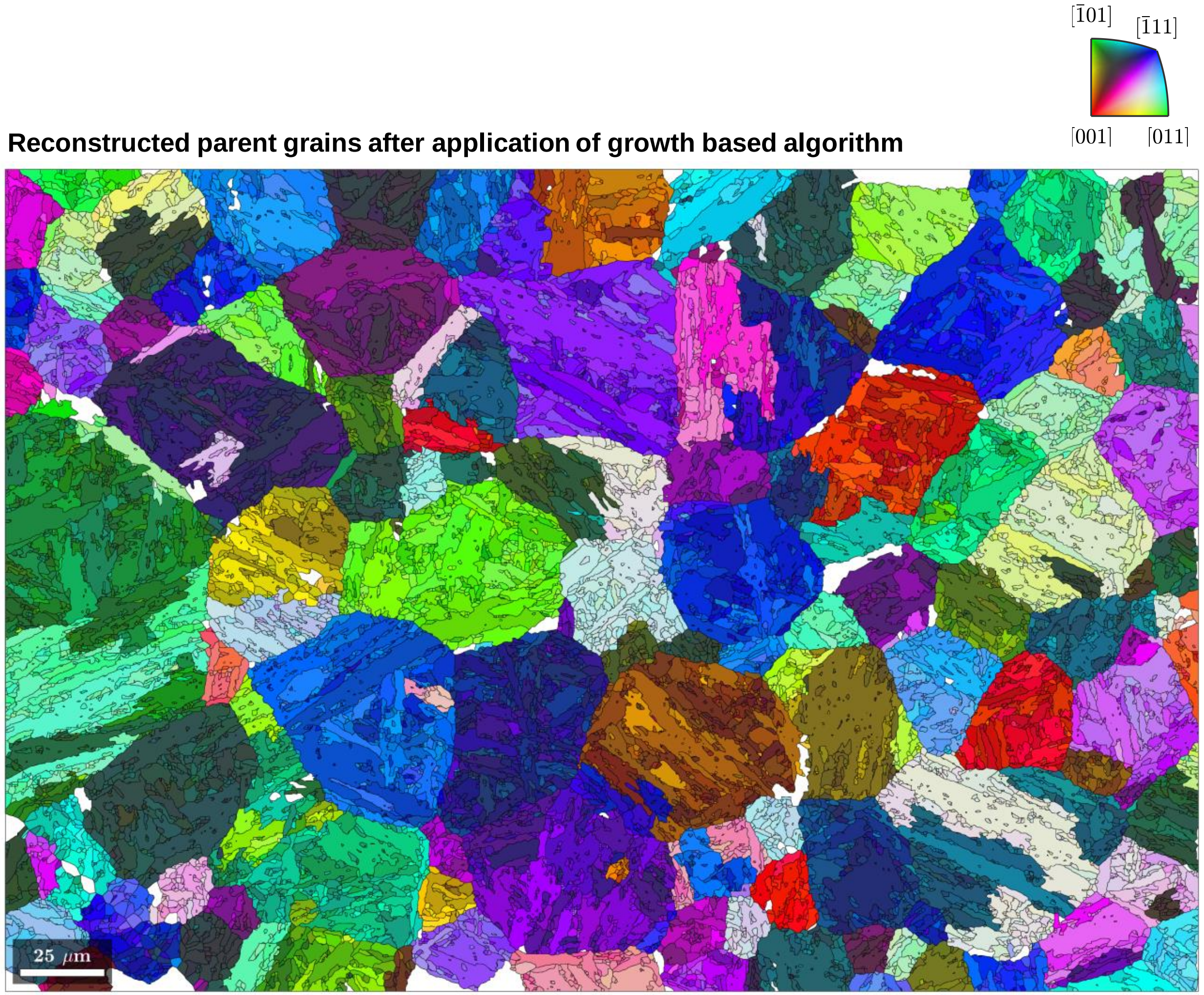
Calculate all parent orientations from a child orientation by applying the OR and find the best fitting parent orientation with the neighboring parent grains

Parent neighbors	Fit
(pink)	1.8°
(purple)	5.7°

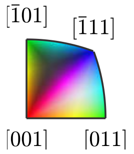


- By iteration (**`k = 1:3`**), the parent phase grows into the child phase
- This can also be applied in cases when a lot of parent phase is retained

Reconstructed parent grains after application of growth based algorithm

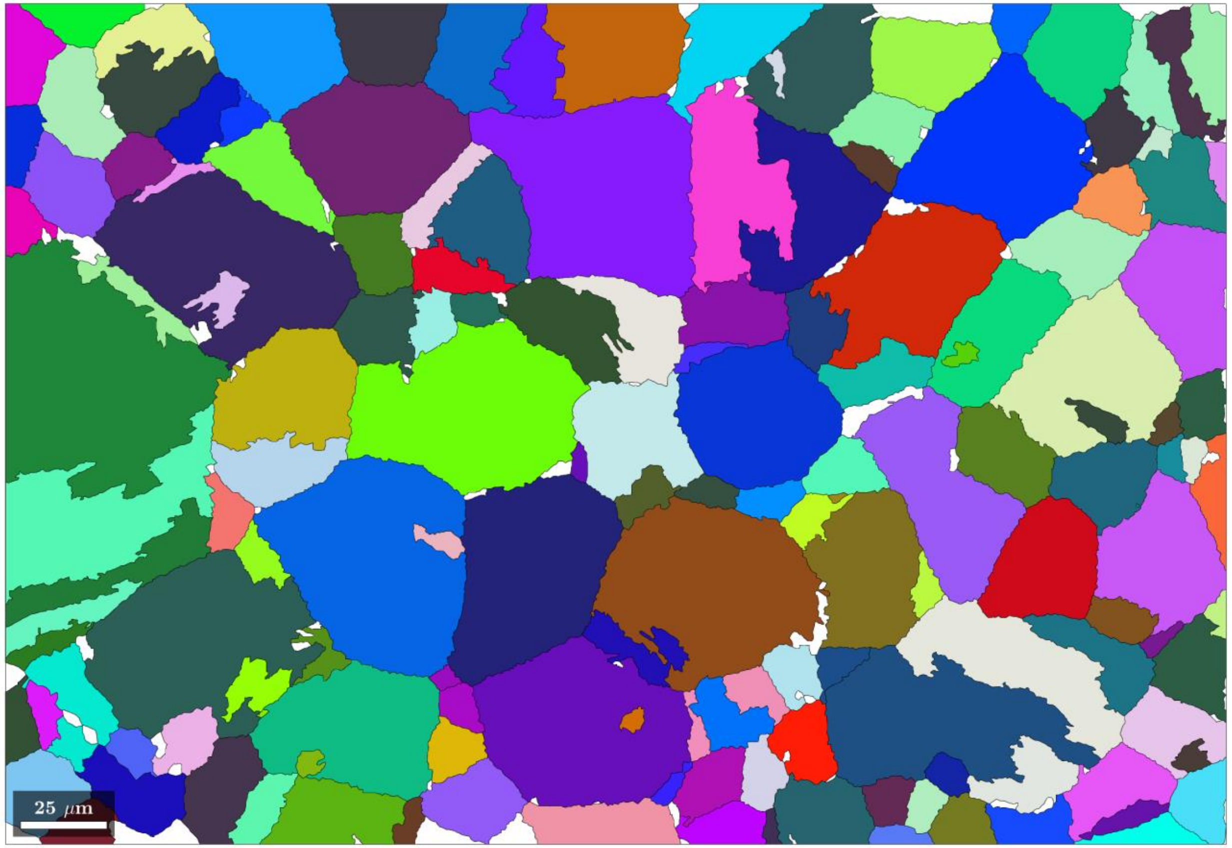


Example 1 – Cleaning of the microstructure



Clean up the map

```
% merge grains with similar orientation and absorb inclusions
job.mergeSimilar('threshold',7.5*degree);
job.mergeInclusions('maxSize',50);
```



Comment on computational performance

MTEX is written in MATLAB

- MATLAB is often said to be slow – not generally true!
  - Fortran and C++ are of course faster, but MATLAB uses external libraries
  - This is not true when code is properly vectorized (**MAT**rix**LAB**oratory)

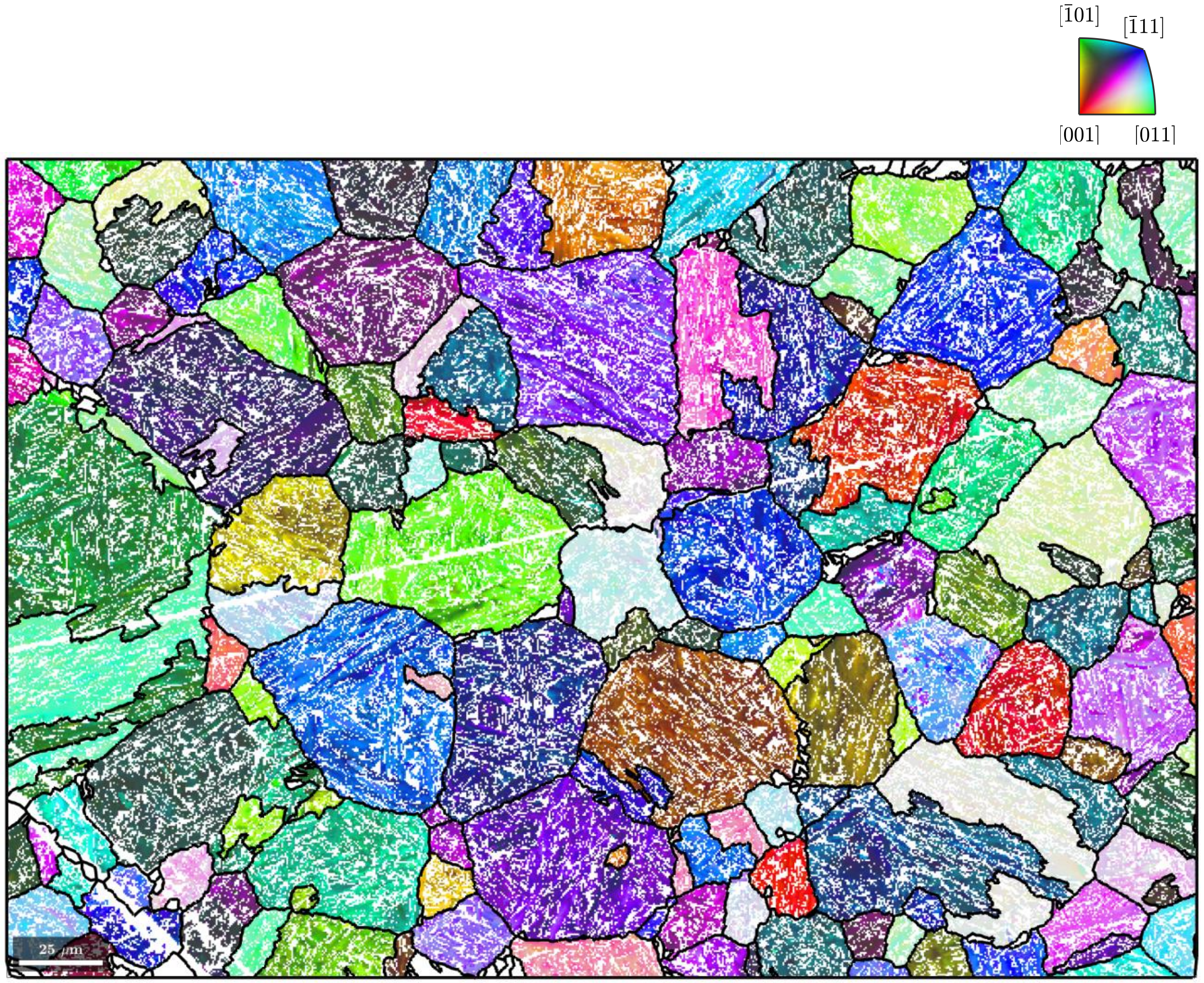
Lath martensite example: 486 x 707 EBSD map with 21,600 grains

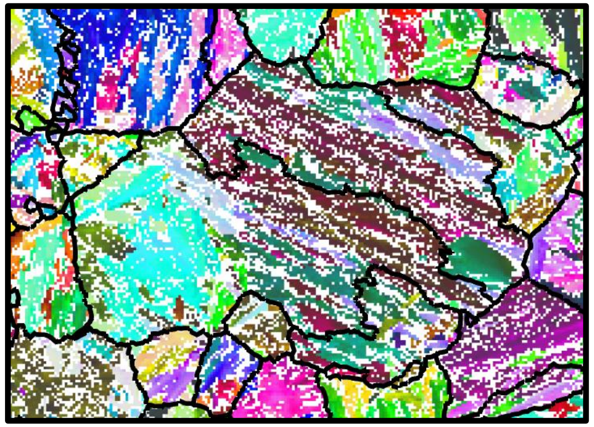
- Reconstruction of lath martensite in 2 stages: 1 min 16 s (conventional office laptop)
  - Graph construction, clustering, parent calculation, filtering, voting algorithm
- Entire script: 3 min 35 s (https://github.com/frankNiessen/ORTools#example-1)
  - Grain reconstruction, OR refinement, Parent grain reconstruction (2 stages), Microstructure cleaning, Variant and packet indexing, Plotting of 13 publication ready figures

Example 1 – Reconstructing the parent EBSD data

Reconstruct the parent EBSD data

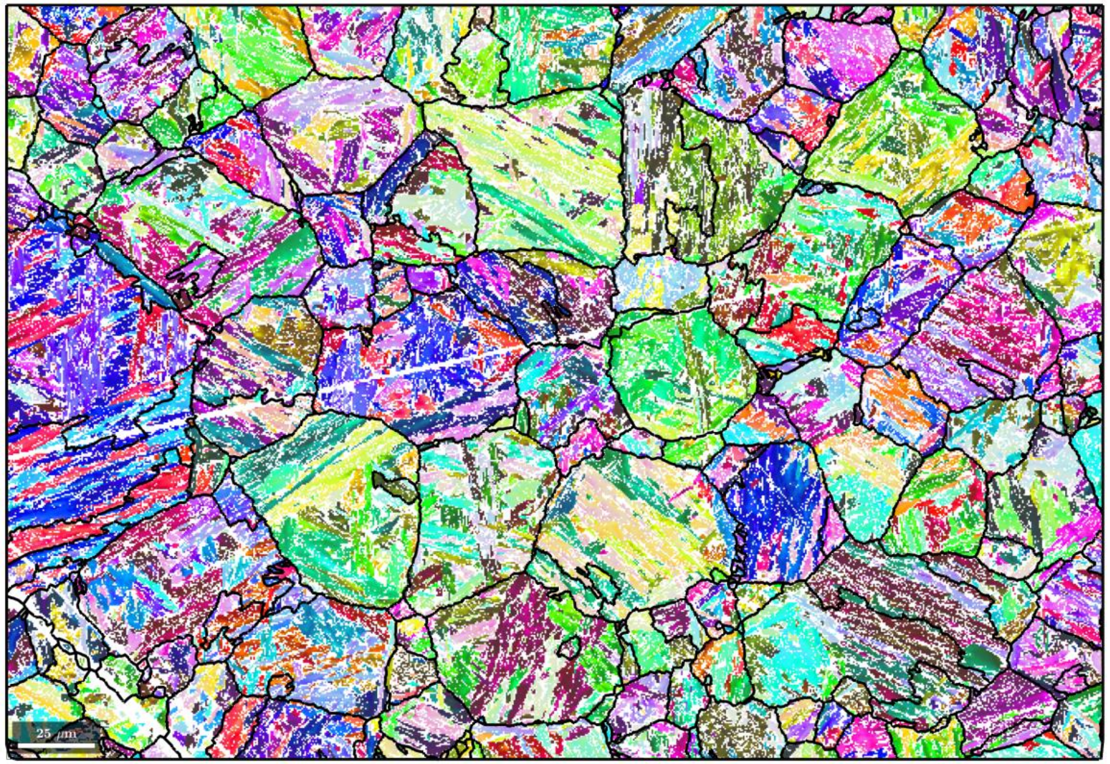
```
% we can now obtain the reconstructed EBSD data

job.calcParentEBSD
```

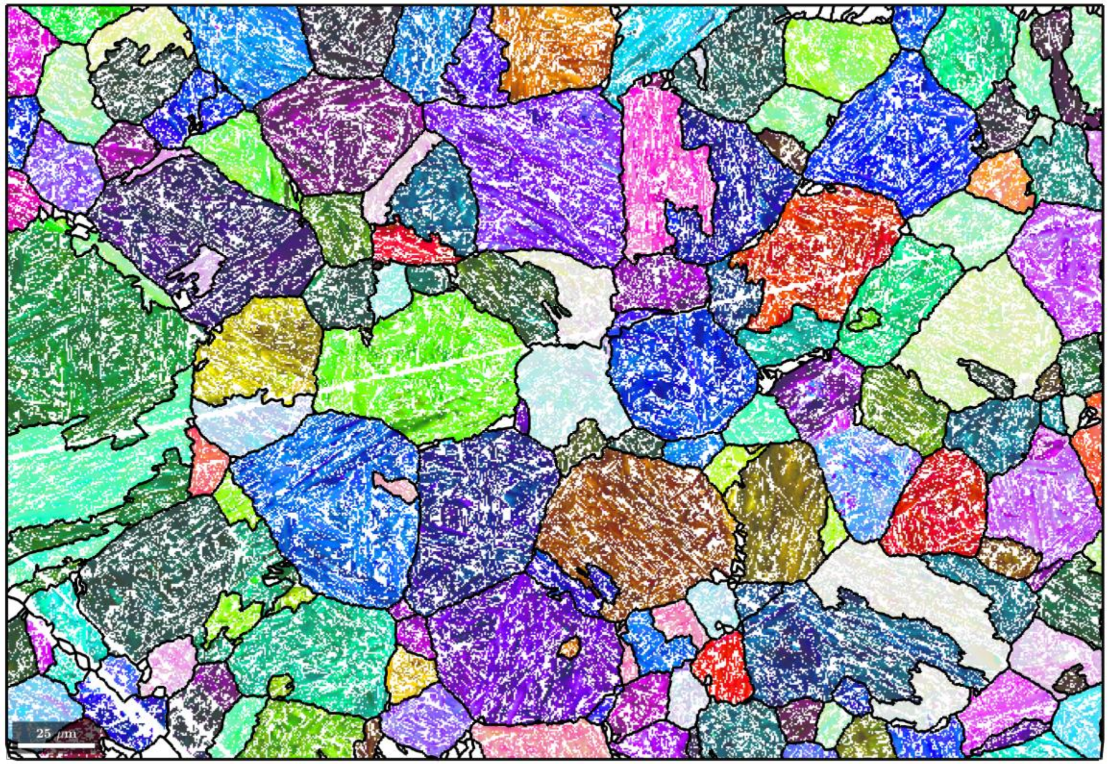


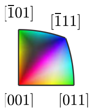


Example 1 – Evaluation

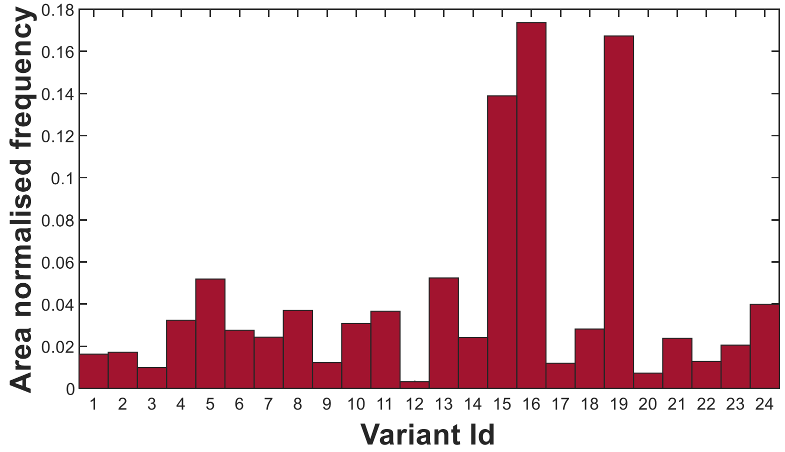
- Generally the agreement looks quite well
- Some grains look unnatural





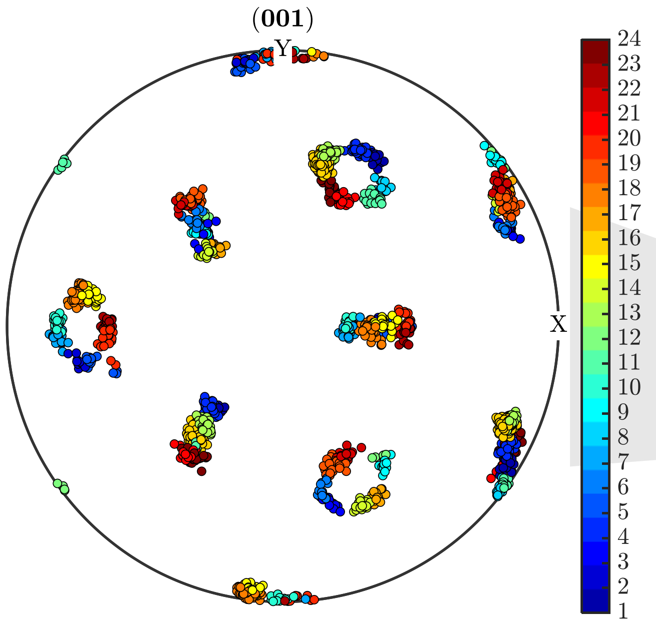


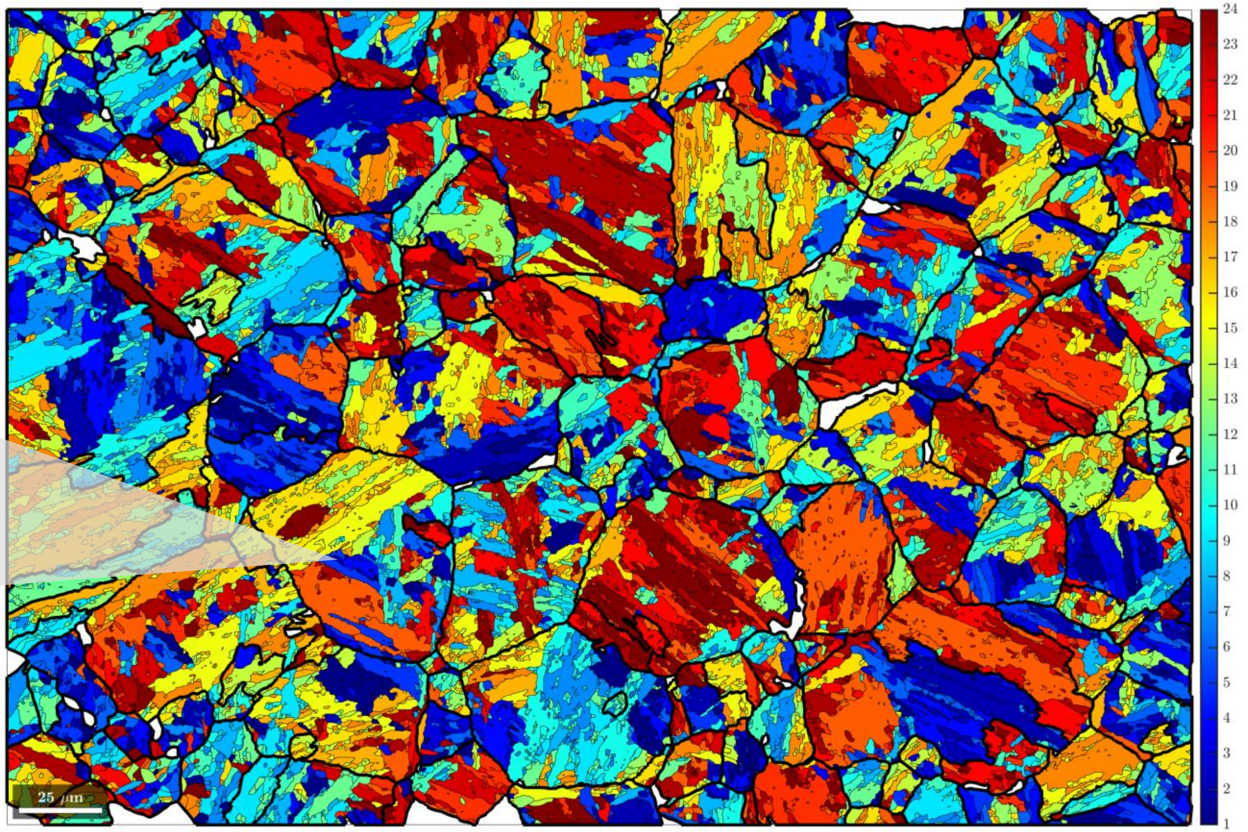
Example 1 – Variant analysis



Calculating orientation variant and packet Id's

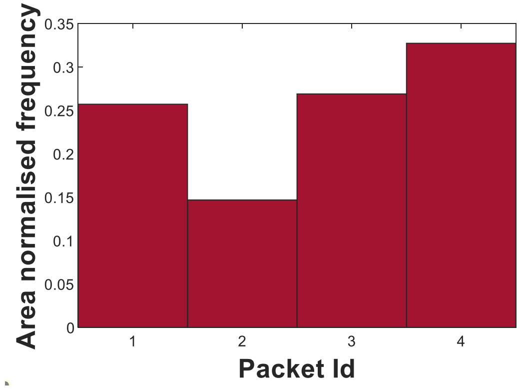
```
job.calcVariants;
plotMap_variants(job,'linewidth',3); %ORTools
```





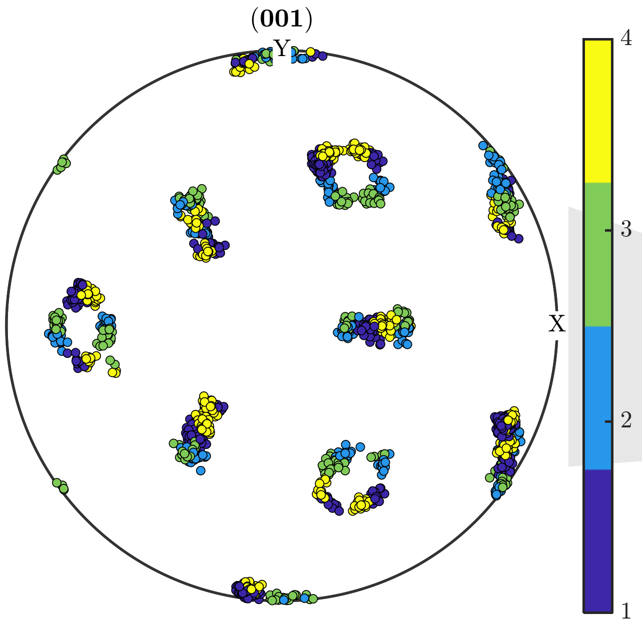
OR*Tools* `plotMap_variants`

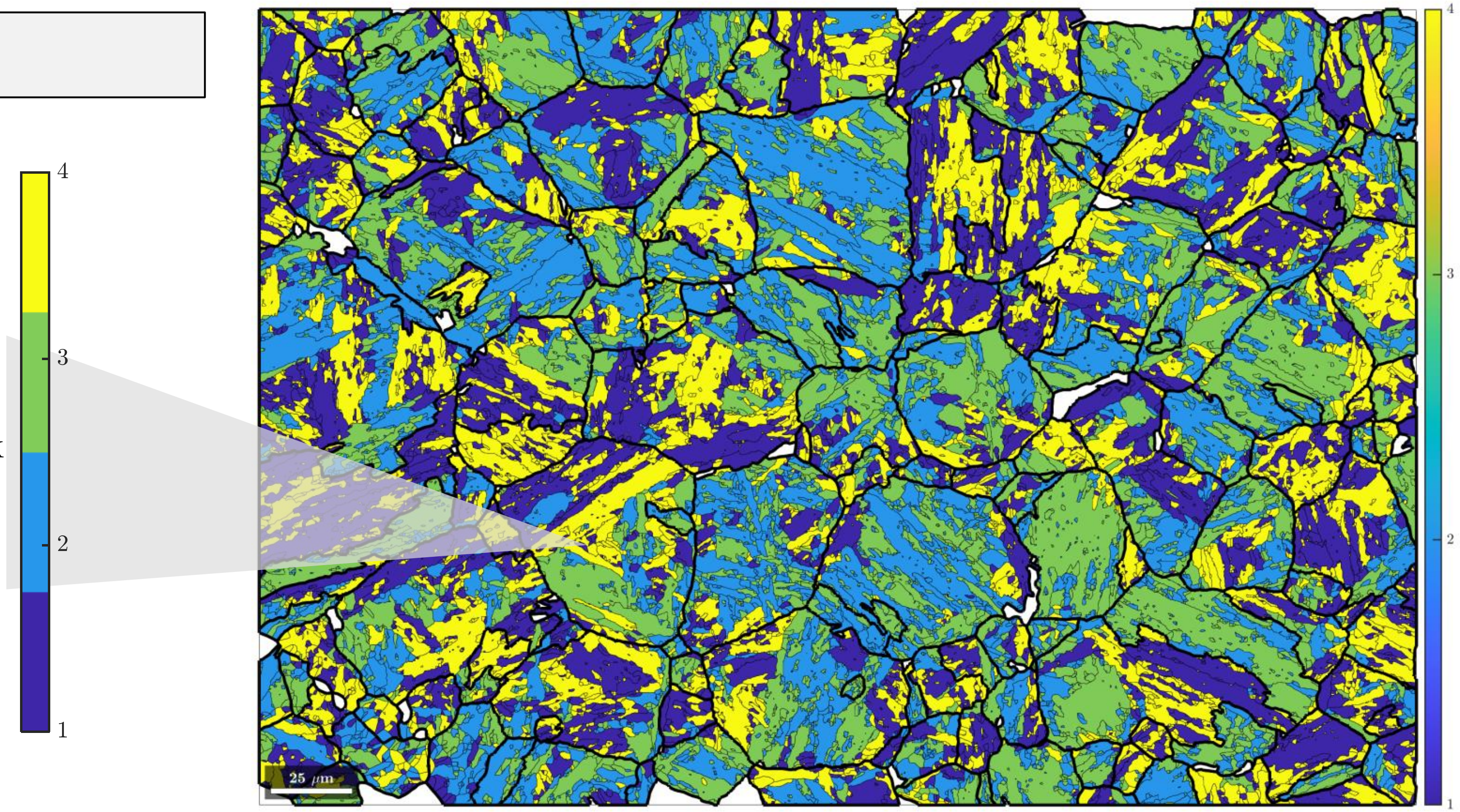
Example 1 – Variant analysis



Calculating orientation variant and packet Id's

```
job.calcVariants;
plotMap_packets(job,'linewidth',3); %ORTools
```



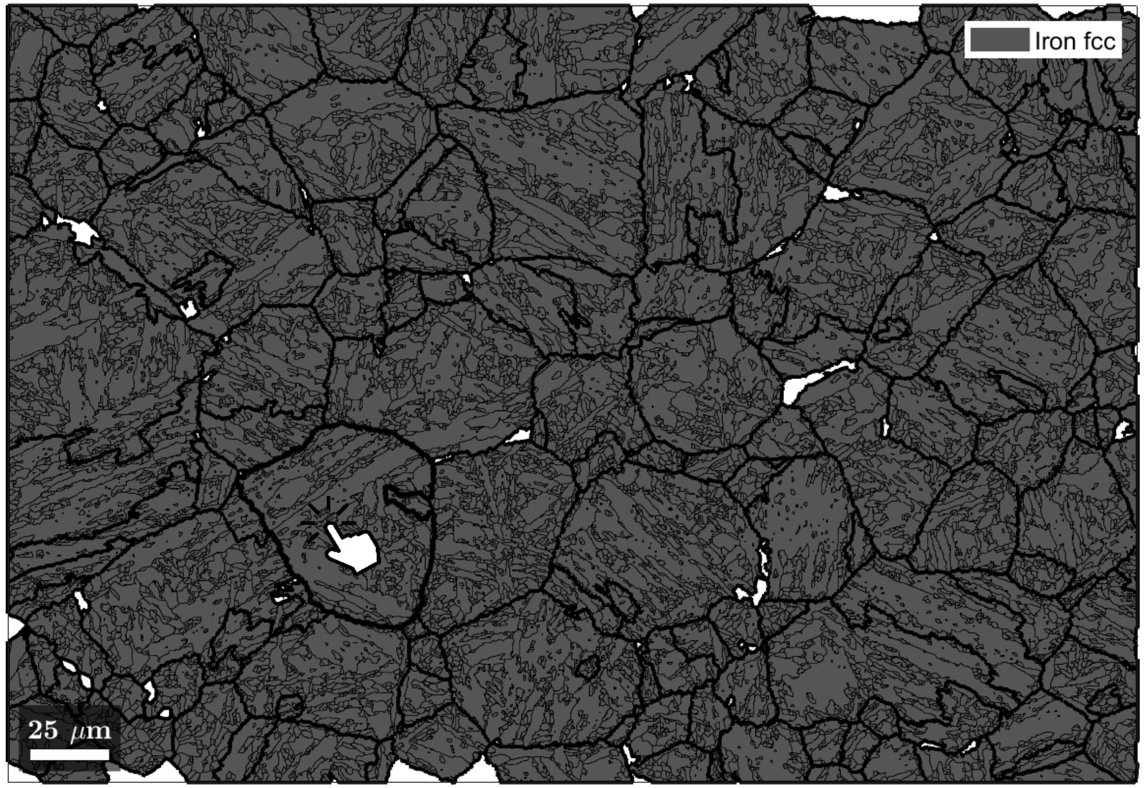


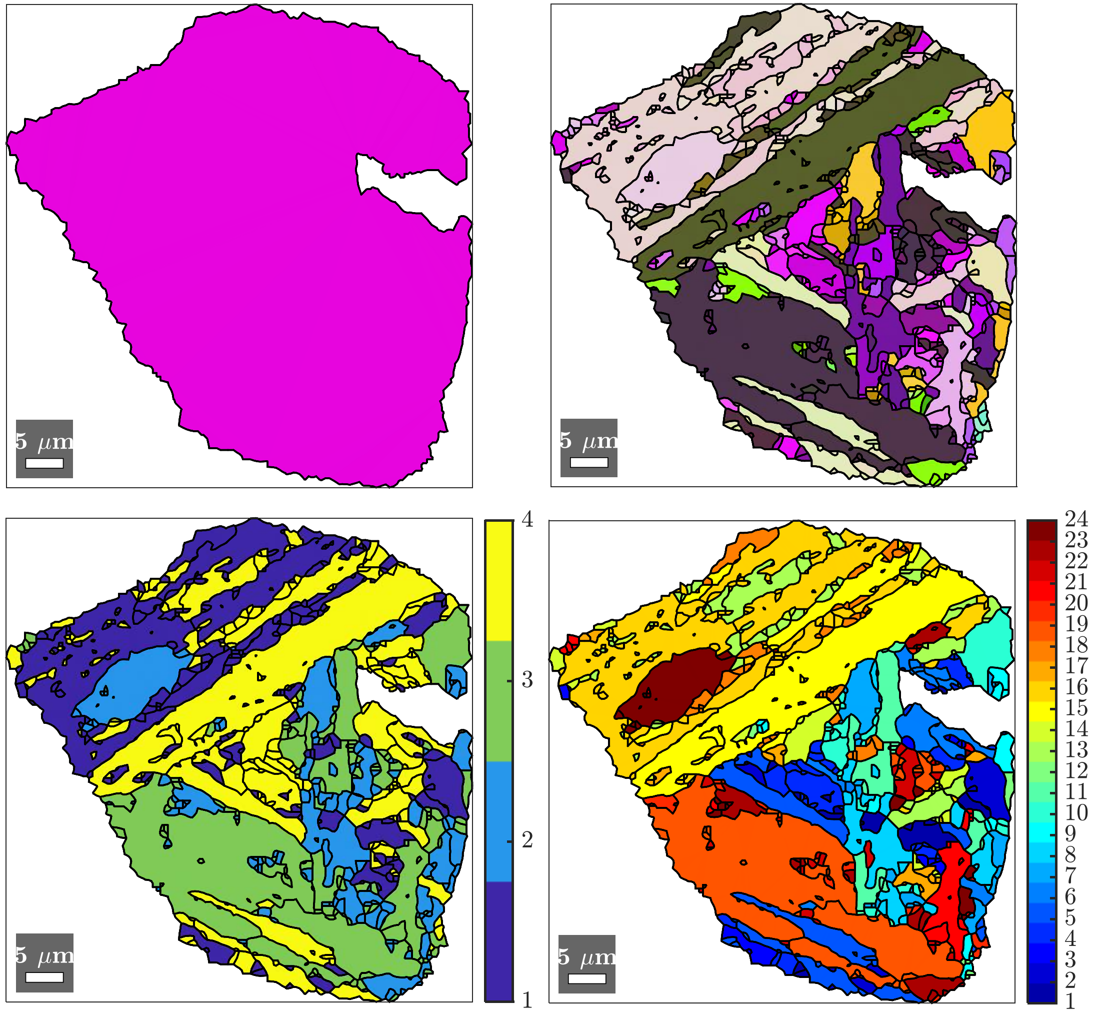
ORTools plotMap_packets

Example 1 – Interactive variant analysis

ORTools grainClick

- Interactive grain specific variant analysis

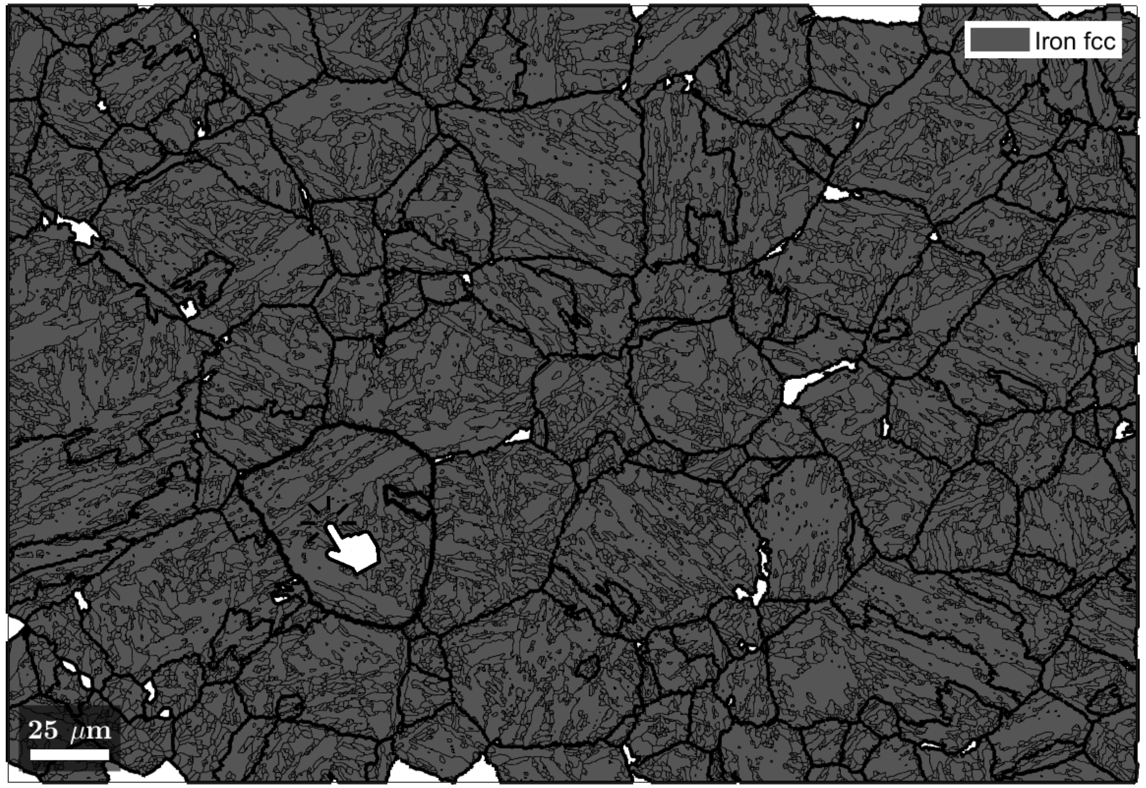


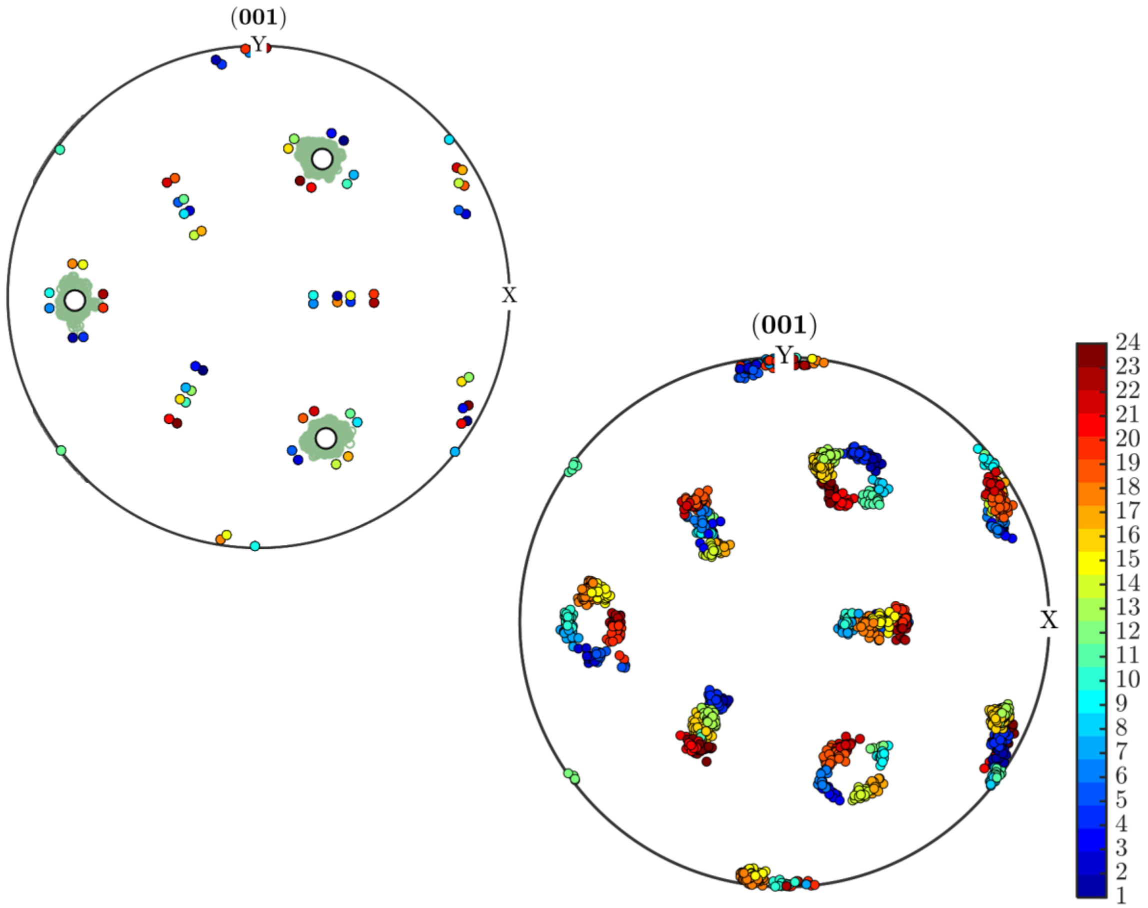


Example 1 – Interactive variant analysis

ORTools grainClick

- Interactive grain specific variant analysis

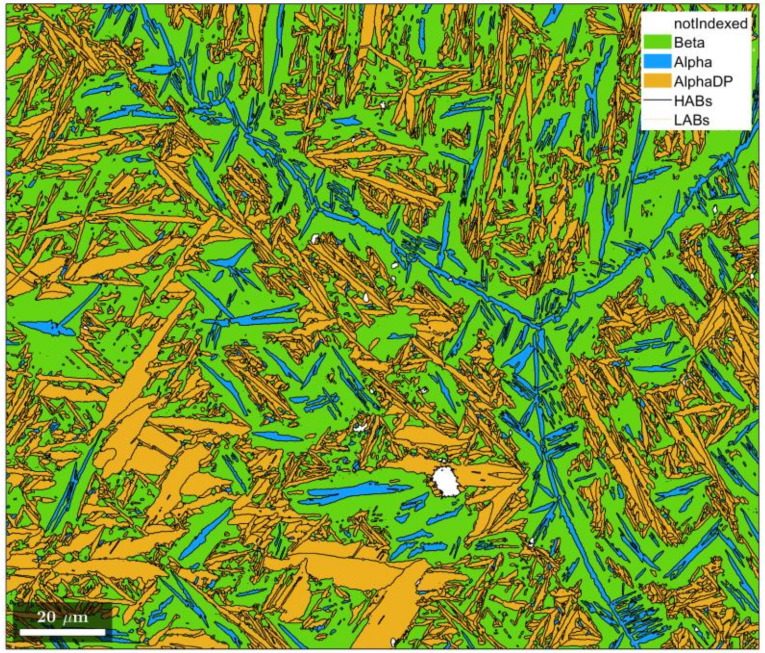




Example 2 – Annealed Ti-10V-2Al-3Fe – $\beta \rightarrow \alpha''$

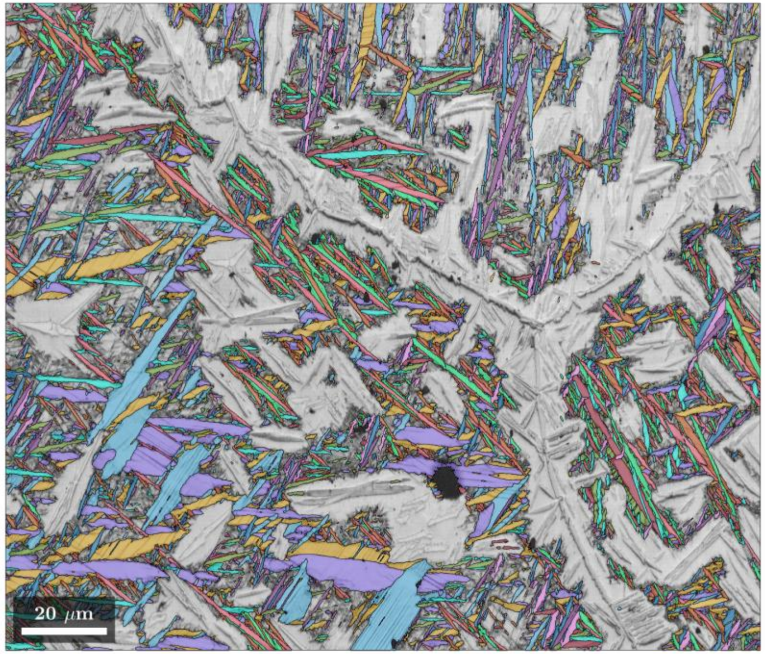
- $\boldsymbol{\alpha}$ (hcp) + $\boldsymbol{\beta}$ (bcc) **titanium** alloy with **athermal** $\boldsymbol{\alpha''}$ (orthorhombic) **martensite**
- The implemented parent grain reconstruction
  – generally **works with any** combination of **parent** and **child** phase
  – **ignores** presence of **additional phases** (here $\boldsymbol{\alpha}$)

Initial phase map: $\alpha + \beta + \alpha''$



Reconstructed: $\alpha + \beta$

Reconstructed: Individually colored α'' variants



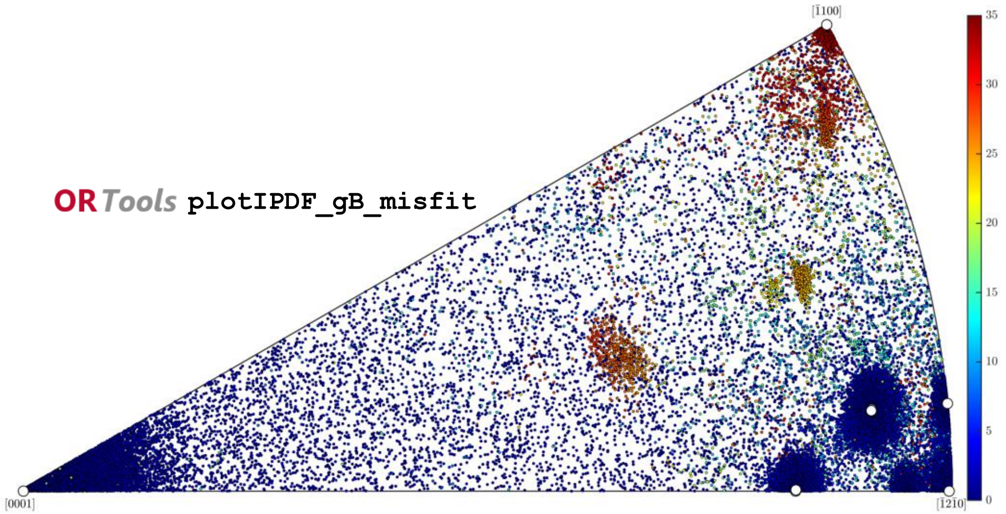
MTEX https://mtex-toolbox.github.io/TiBetaReconstruction.html

ORTools https://github.com/frankNiessen/ORTools/blob/develop/README.md#example-2

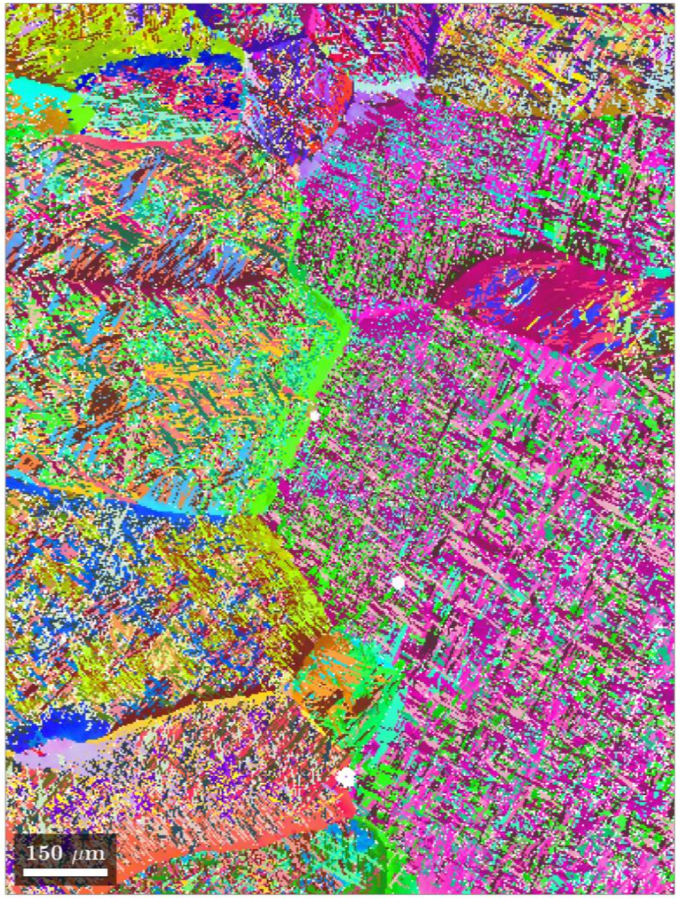
Example 3 – $\beta \rightarrow \alpha$ phase transition in Ti-alloys

- Low symmetry of α leads to distinct misorientation axes between α grains
- Therefore triple points between α grains can be used for reconstruction of β
- Remaining regions are reconstructed by the growth-based algorithm

ORTools `plotIPDF_gB_misfit`



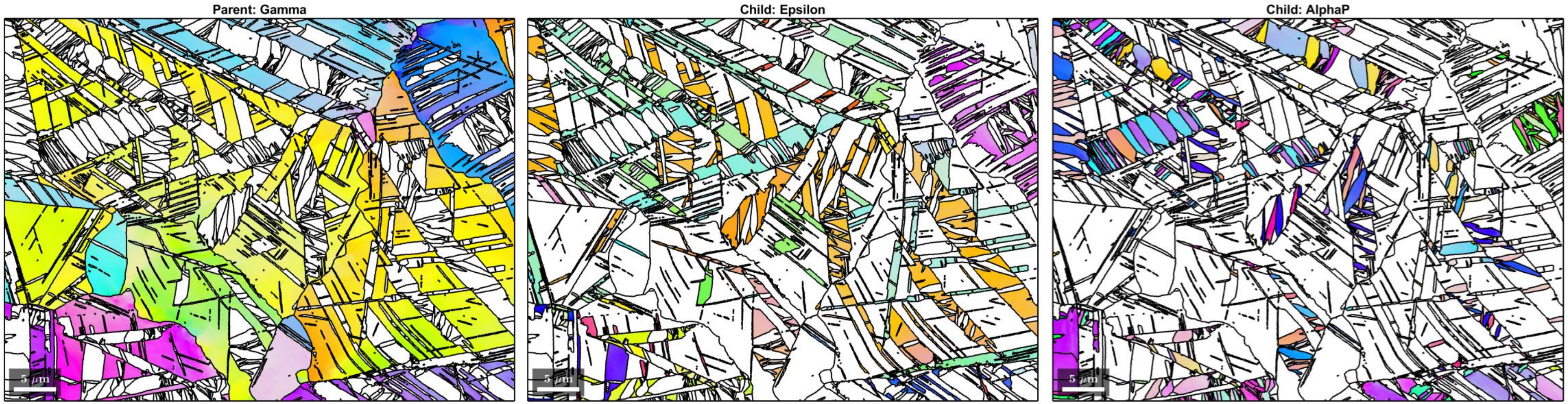
Initial phase map: 99.7% α



Reconstructed β phase

Example 4 – Cold rolled High-Mn steel – $\gamma \rightarrow \varepsilon \rightarrow \alpha'$

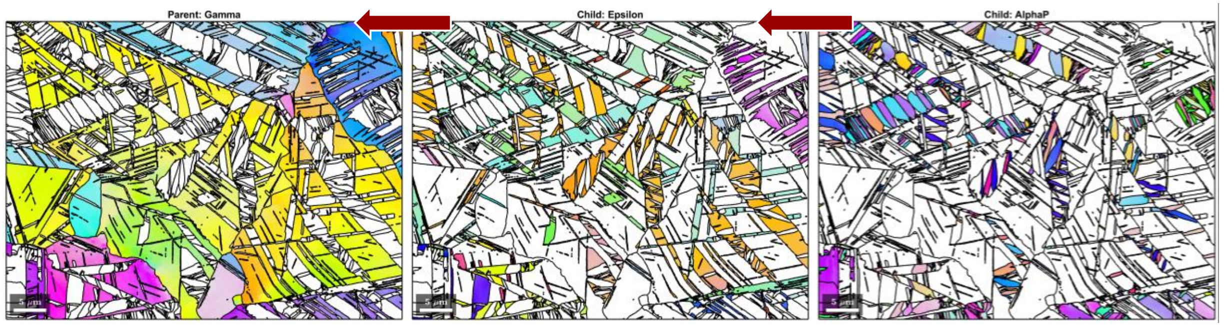
- In 10% cold rolled high Mn steel two martensitic transformations are observed
  - $\gamma \rightarrow \varepsilon$ (fcc → hcp): Partially athermal and partially strain-induced
  - $\varepsilon \rightarrow \alpha'$ (hcp → bct): Entirely strain-induced

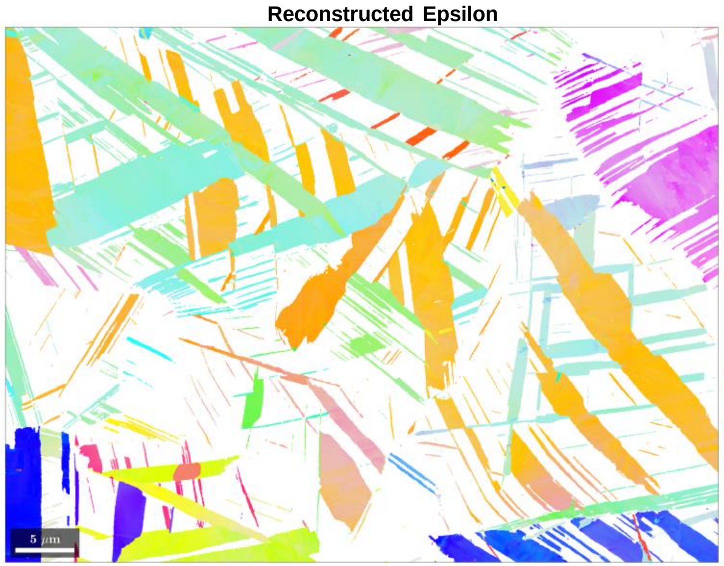


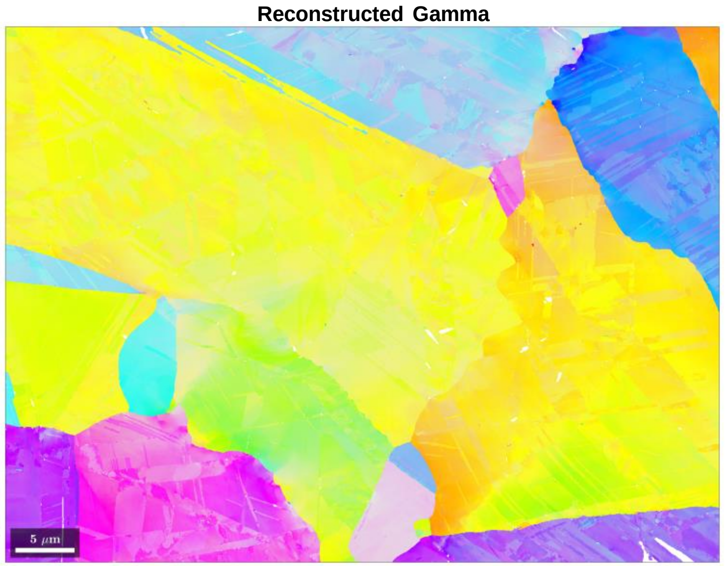
With courtesy to [S. Pramanik, A.A. Gazder, A.A. Saleh, E. V. Pereloma, Mater. Sci. Eng. A 731 (2018) 506–519.]

Example 4 – Cold rolled High-Mn steel – $\gamma \rightarrow \varepsilon \rightarrow \alpha'$

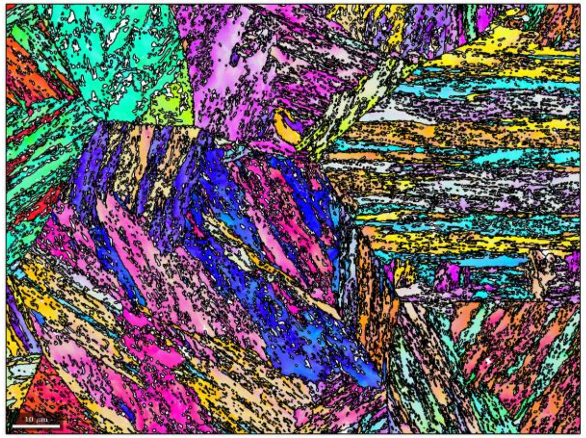
- The implemented algorithm can deal with multiple orders of transformation





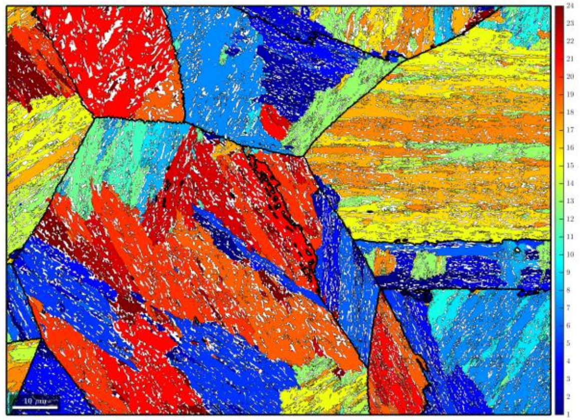


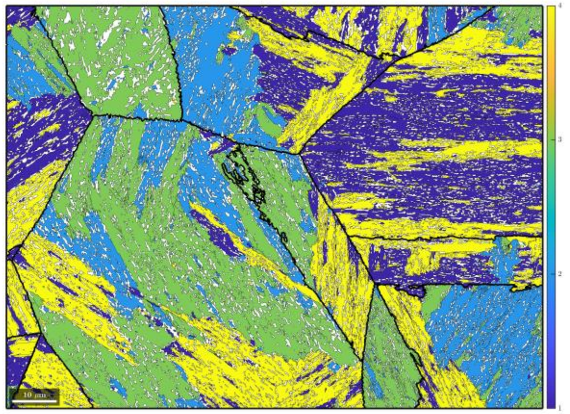
Example 5 –
Intercritically annealed martensitic stainless steel



- Growth-based reconstruction from reverted austenite


```
for k = 1:3 % do this three times
    job.calcGBVotes('noC2C');
    job.calcParentFromVote('minFit',7.5*degree)
end
```





Conclusion

- A versatile framework for analysing phase transitions has been implemented into MTEX 5.6
- The implementation is implemented in a class with modular methods and properties
- Depending on the microstructure, different reconstruction strategies can be chosen
- The reconstruction is automated as much as possible, while maintaining full user control over the reconstruction process
- ORTools is an add-on to MTEX with some additional capabilities for analysis of martensitic microstructures

To-do

- Improving reconstruction accuracy for martensitic microstructures in steel
  - Considering local grain boundary misorientation
  - Experimenting with different clustering algorithms
- Implementation of transformation texture prediction
  - Available work and variant selection analysis
- What do you think needs to be done?