A Toolbox for Geometric Grain Boundary Characterization

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Introduction

❑ Recently, progress in 3D microstructure imaging techniques has been made

❑ Resulting data sets are large enough for carrying out statistical studies

❑ Our goal is to get quantitative information about grain boundary networks based on all five macroscopic parameters

❑ For this purpose, dedicated software tools are needed
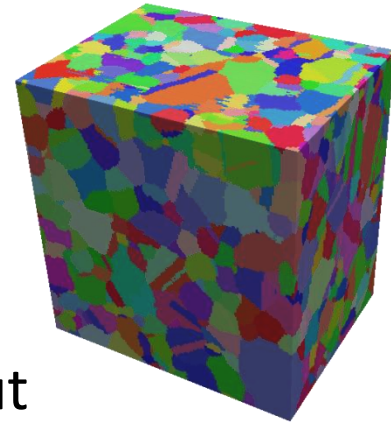
Software toolbox for geometric grain boundary characterization
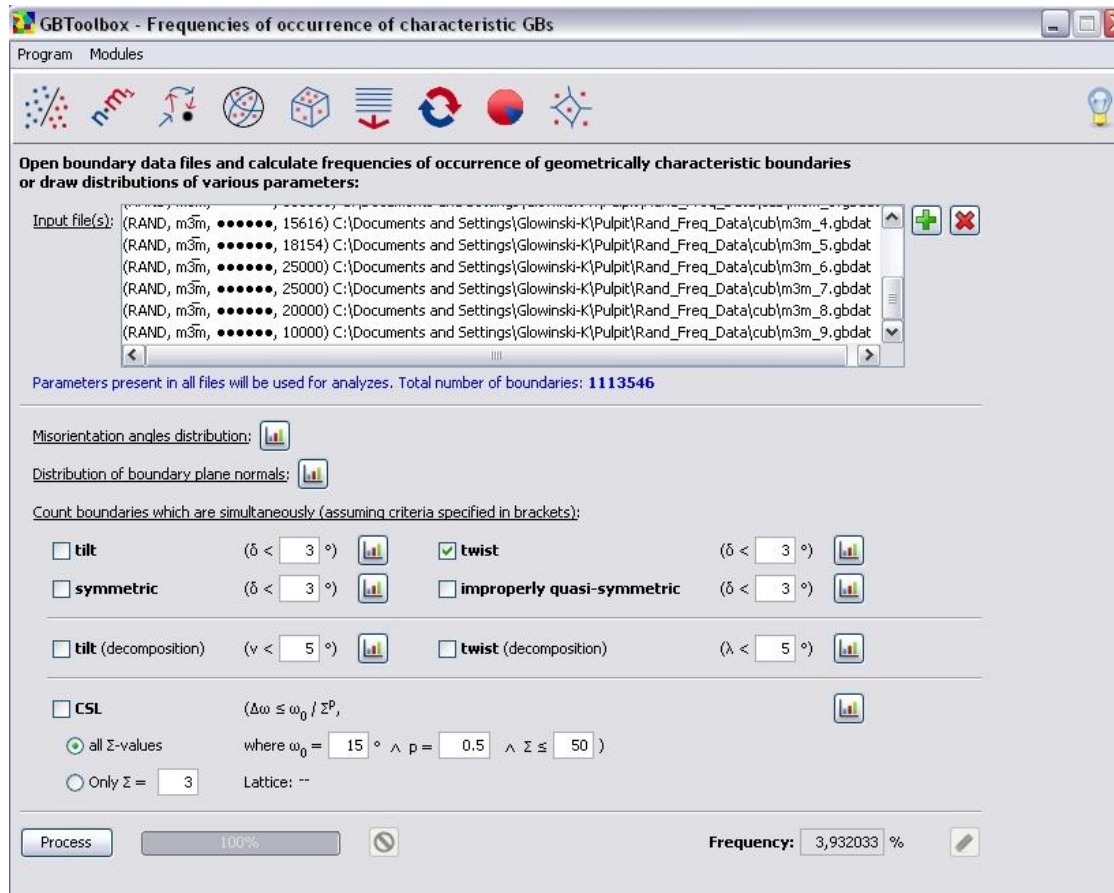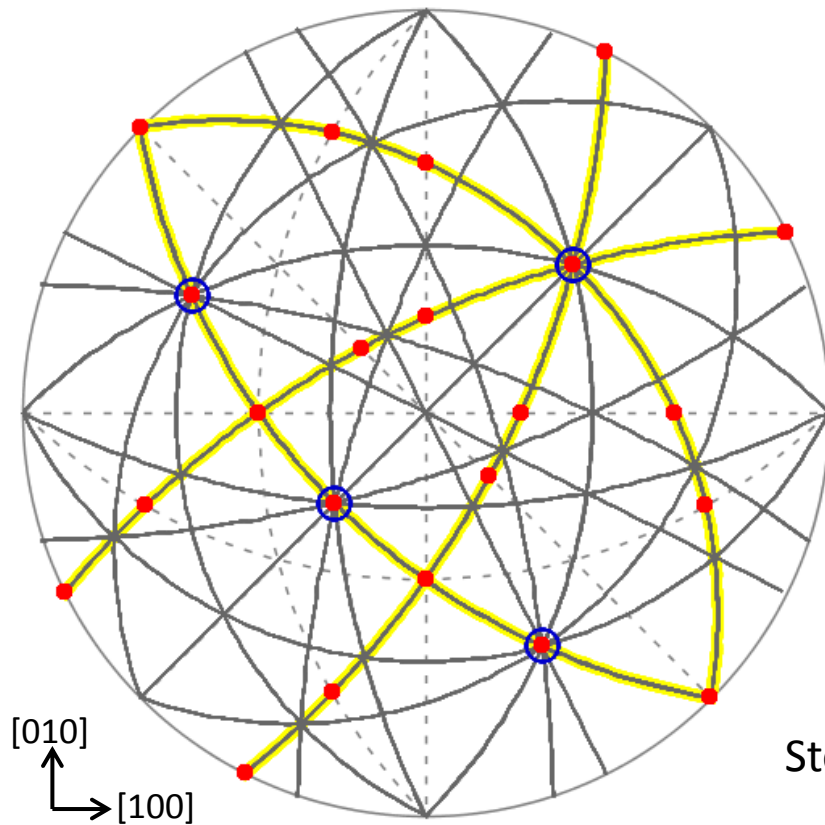

❑ We have developed pieces of computer software essential for quantitative analysis of grain boundaries

❑ The results and figures on the following slides have been obtained mainly using our program

Screenshot of one of the modules included in the package

All characteristic GBs for a given fixed misorientation

- ❑ Exact locations of characteristic GBs are calculated analytically

- ❑ Crystal symmetry is taken into account

- ❑ The catalogs can be directly linked to experimentally measured boundary distributions

○ symmetric   ▬ improperly quasi-symmetric

● twist   — tilt

Stereographic projections of boundary plane normals of various characteristic boundaries for the Σ3 misorientation (cubic symmetry)

Experimental errors. Classification as tilt, twist, etc.

What do the catalogs look like if we introduce experimental errors?

a) ● twist ● tilt

b) ● twist ● tilt

[010]
[100]

[010]
[100]
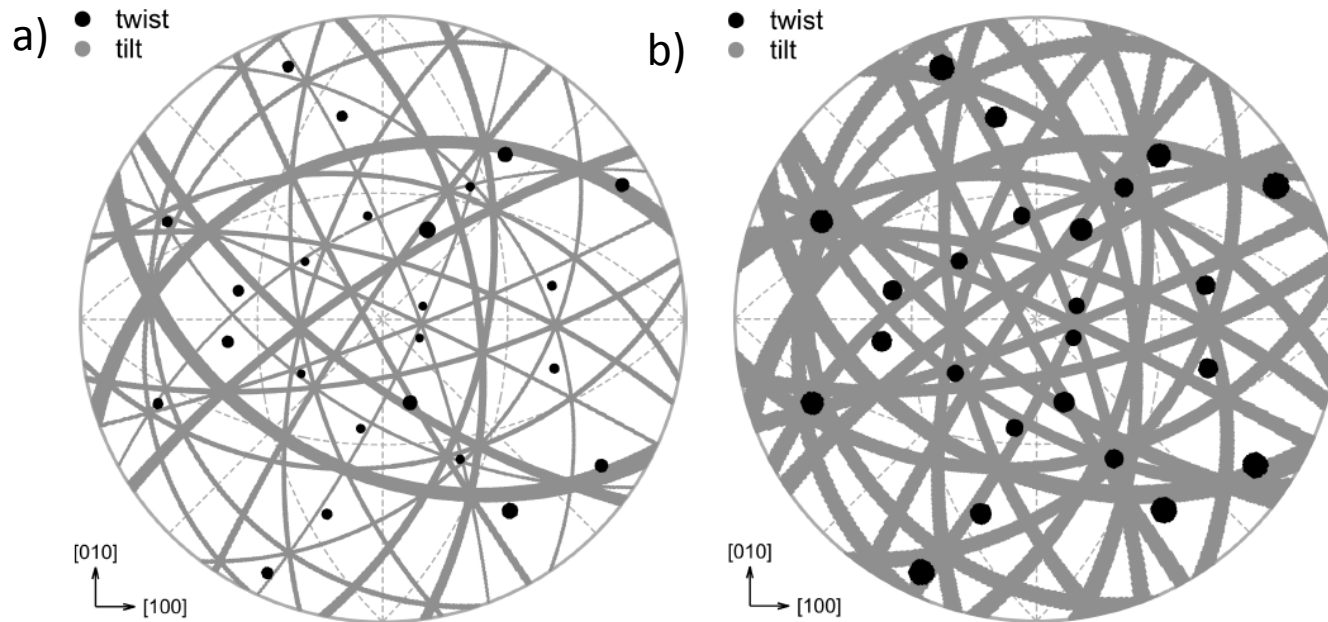
❑ The decomposition (a) and minimization (b) methods have been compared
❑ The decomposition technique appears to be more dependent
  on particular geometric configuration
❑ Moreover, the distance minimization method can be easily extended
  to search for symmetric, quasi-symmetric boundaries

Frequencies of occurrence of geometrically characteristic boundaries among random grain boundaries

The frequencies have been calculated for various types
of boundaries and different crystal symmetries

Cubic symmetry

Tol.	Tilt*	Twist*	Symmetric	Improp. quasi-sym.
1°	39.2	0.4	0.002	0.3
2°	66.4	1.7	0.02	1.3
3°	84.0	3.9	0.07	2.9
5°	98.5	10.7	0.33	8.0

Hexagonal symmetry

Tol.	Tilt*	Twist*	Symmetric	Improp. quasi-sym.
1°	21.2	0.2	0.002	0.28
2°	39.2	0.9	0.01	0.7
3°	54.3	2.0	0.03	1.5
5°	76.8	5.4	0,16	4.0

Probability density functions for the distances to the nearest characteristic boundaries and for the angles of components
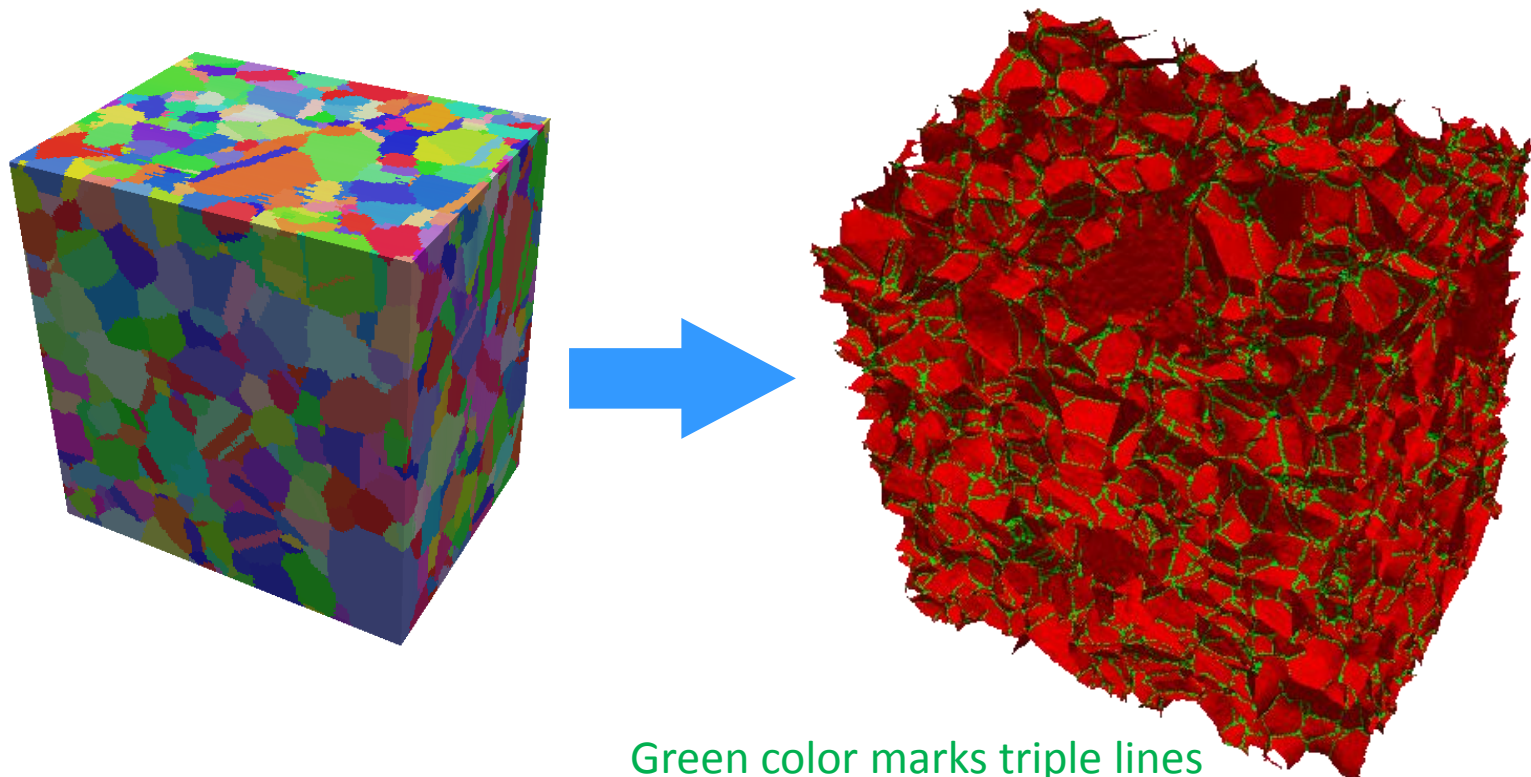
Some examples for cubic symmetry
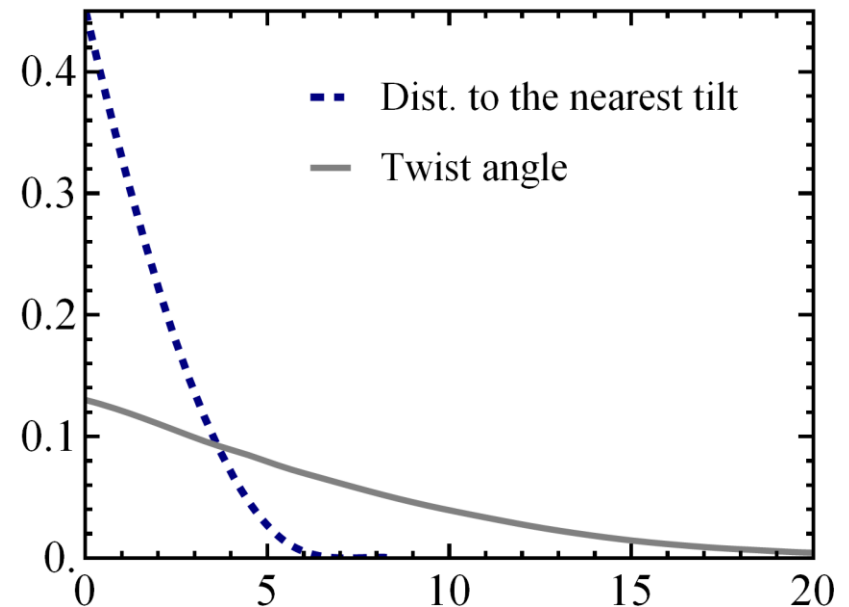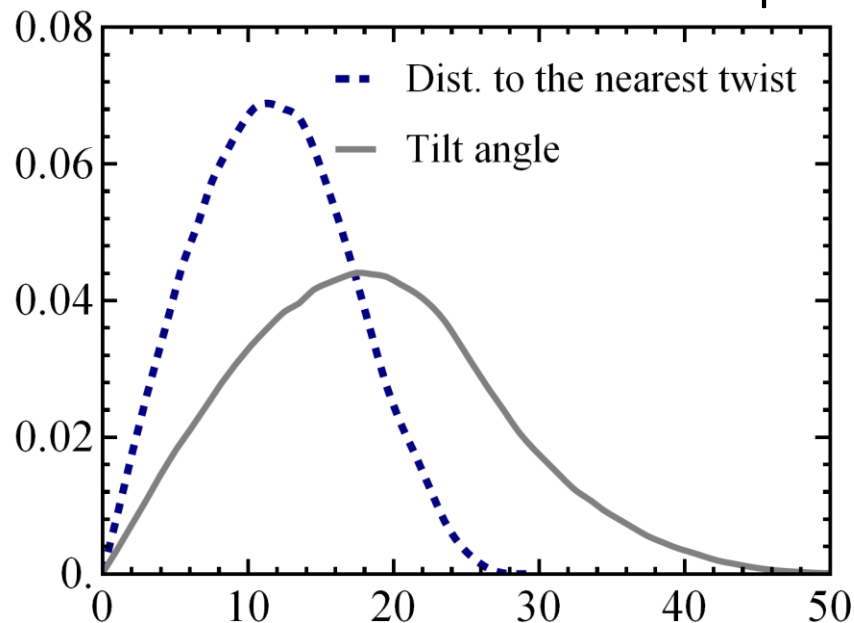
Analogous plots have been obtained also for hexagonal, tetragonal and orthorombic symmetries, and for distances to other types of characteristic boundaries.
Moreover, corresponding cumulative distribution functions have been calculated.

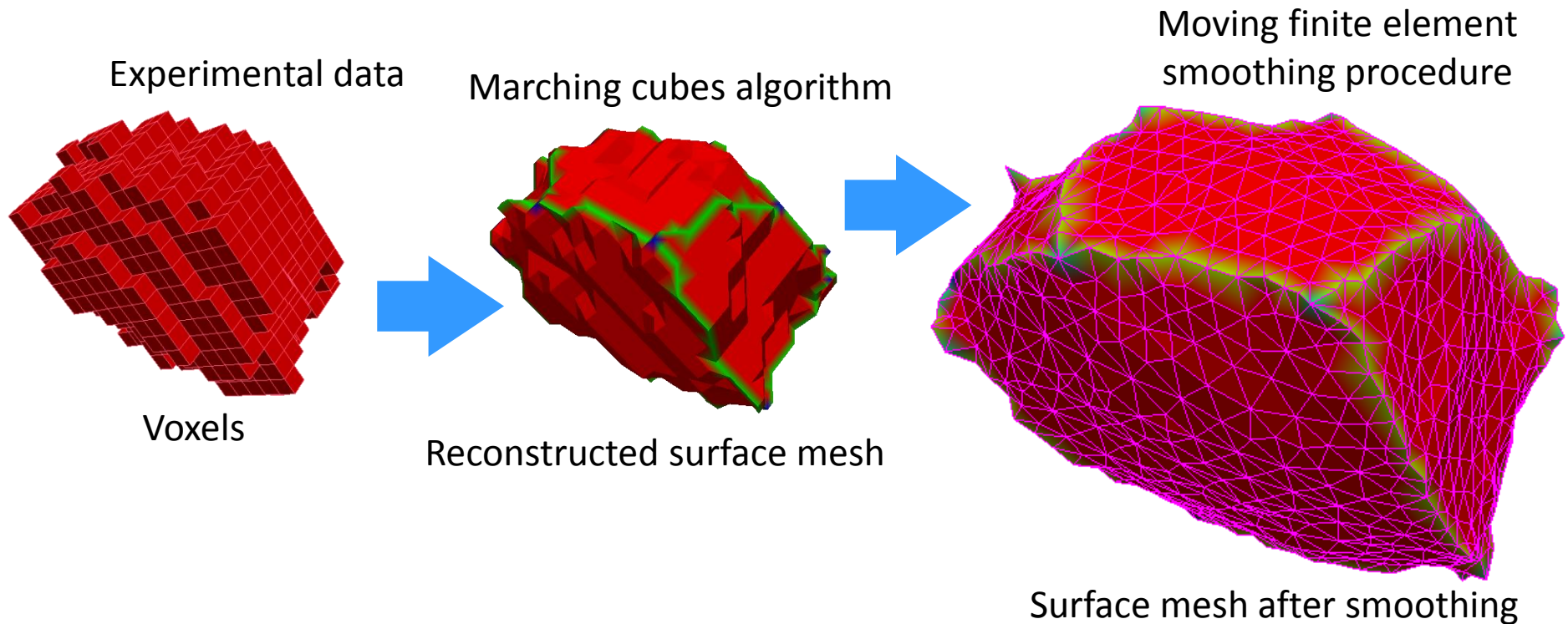# Reconstruction of grain boundary surfaces from experimental data

Our software tools have been tested on randomly generated boundaries. The next step is to apply our algorithms to experimental data.

Green color marks triple lines

Boundary segments reconstruction

Experimental data

Marching cubes algorithm

Moving finite element smoothing procedure

Voxels

Reconstructed surface mesh

Surface mesh after smoothing

❑ Reconstruction is done using DREAM.3D computer program
❑ The output from DREAM.3D can be easily read
❑ These data are then processed by our software (in progress)

Summary

❑ The first version of our program is ready

❑ Using the package, one can generate catalogs of characteristic boundaries for a fixed misorientation, it is also possible to calculate the frequencies of occurrence of characteristic GBs

❑ Tools for analysis of experimental data are being developed