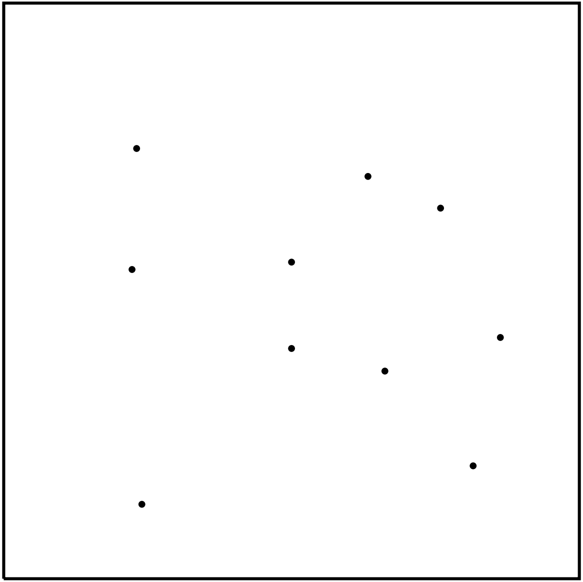
Modeling grains

Input: Spatially indexed individual orientations given as list of tuples $(\mathbf{x}_\ell, p_\ell, q_\ell)$, $\ell = 1, \ldots, n$ with

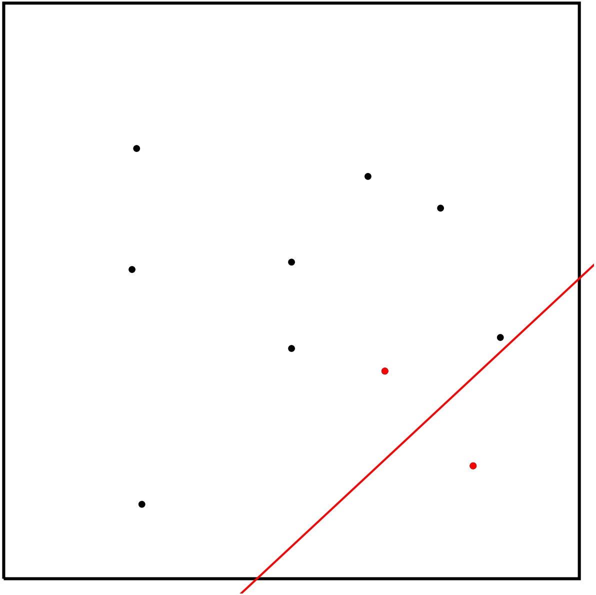
- locations $\mathbf{x}_\ell \in \mathfrak{D}$ bounded to some area $\mathfrak{D} \subset \mathbb{R}^d$,
- phase information $p_\ell \in \mathbb{N}^+$ (includes crystal symmetry),
- orientations $q_\ell \in \mathrm{SO}(3)$.

Output: A graph based data model representing grains and grain boundaries.

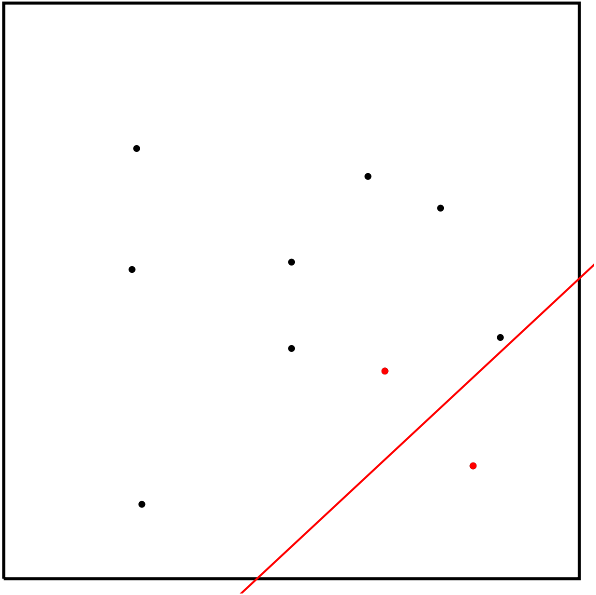
Modeling grains



Modeling grains



Modeling grains



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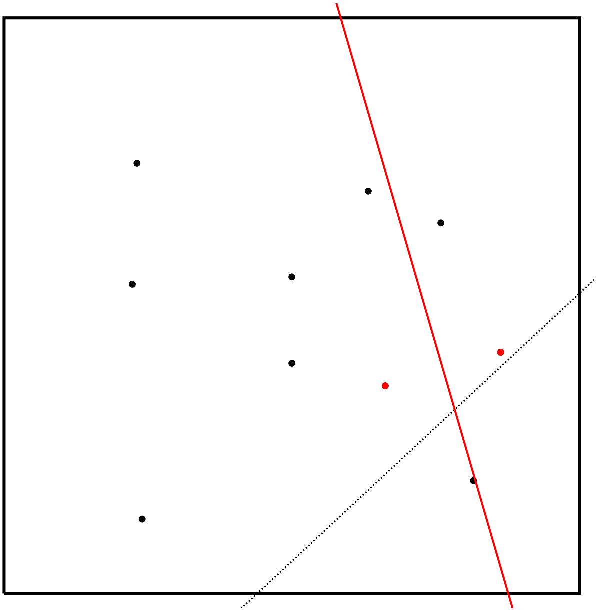

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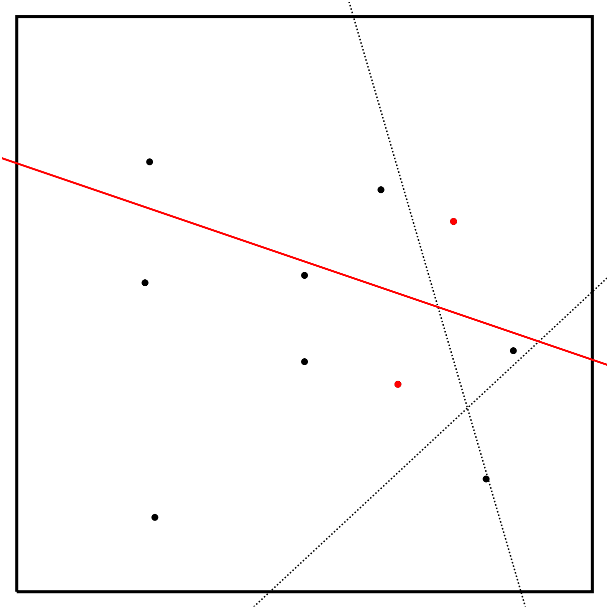
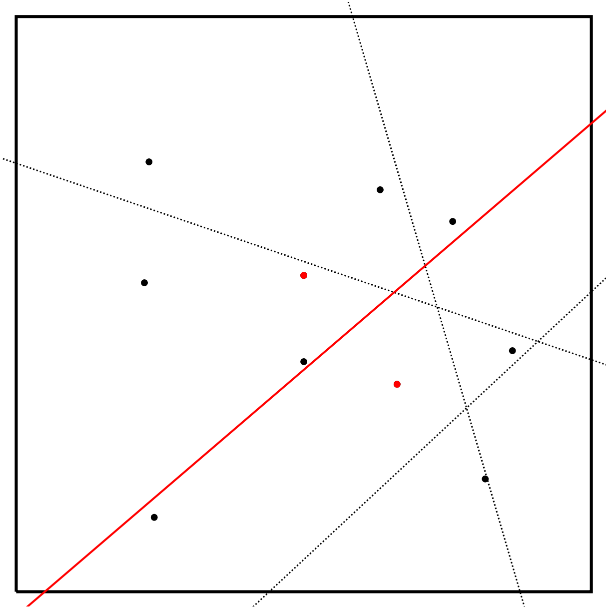
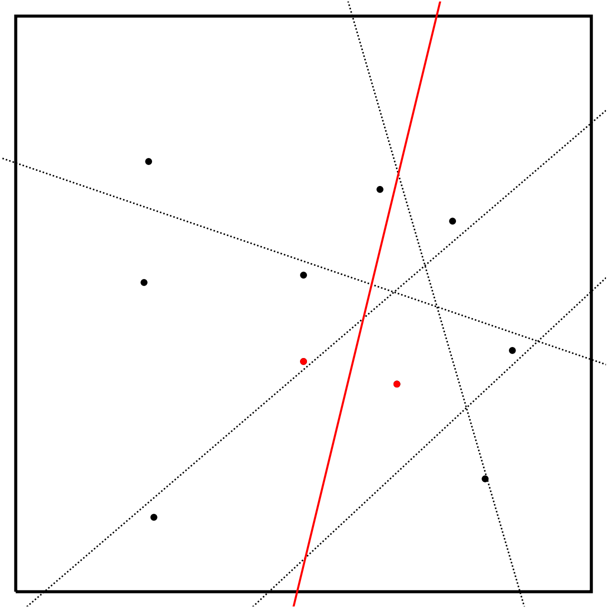


Modeling grains



Modeling grains



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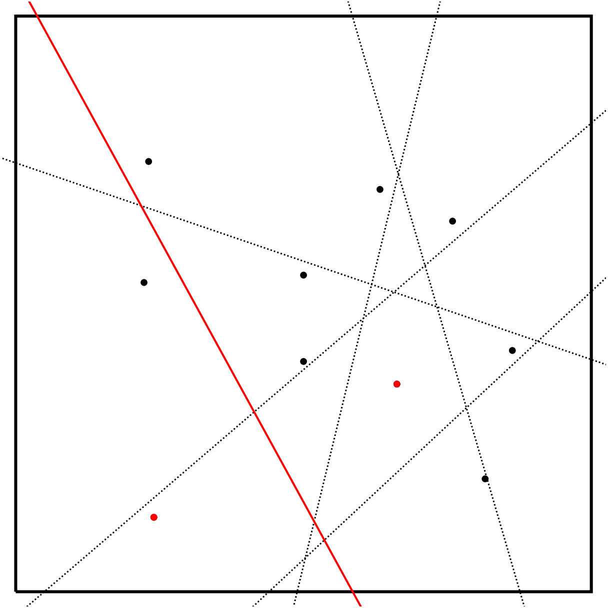

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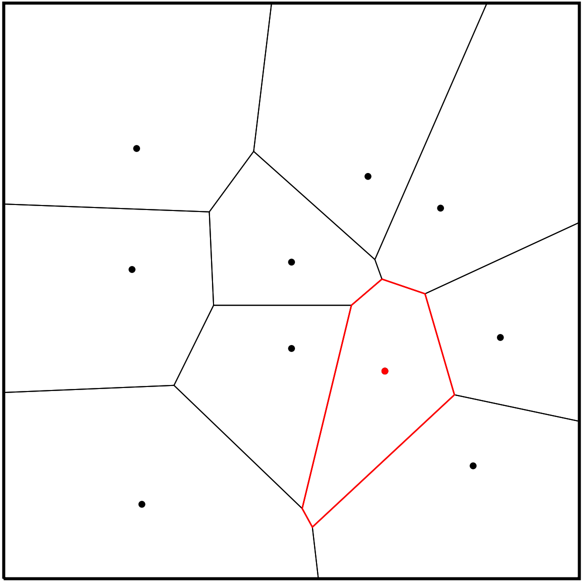

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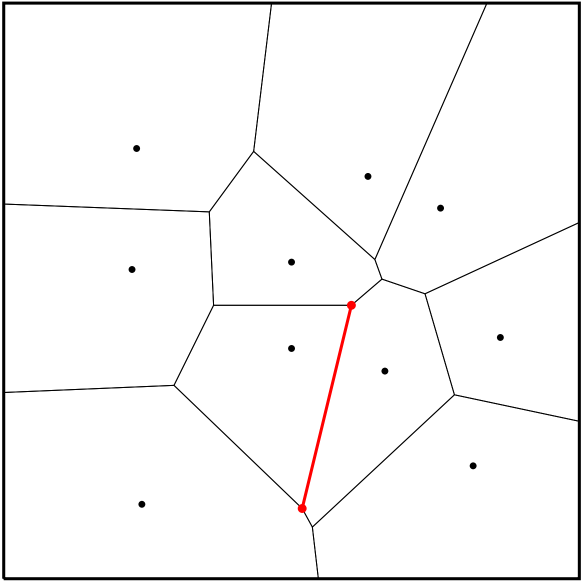

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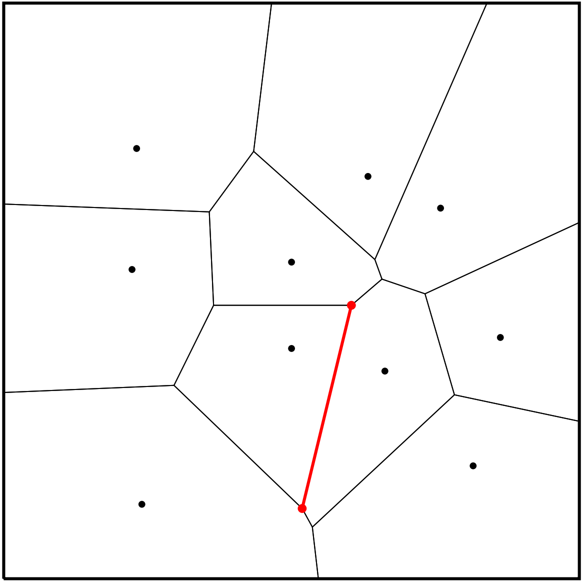

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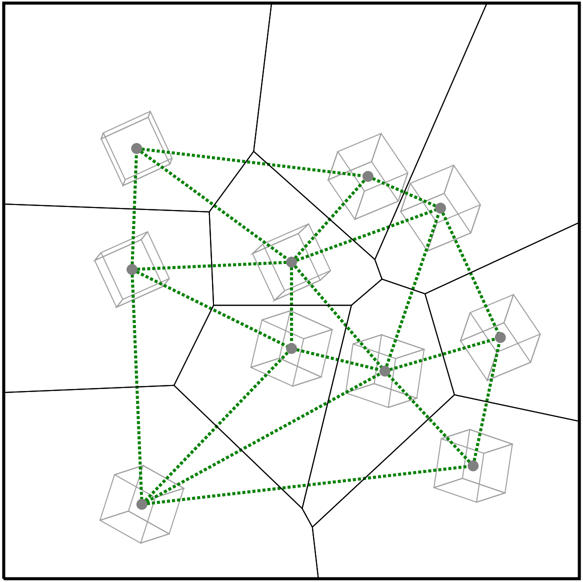

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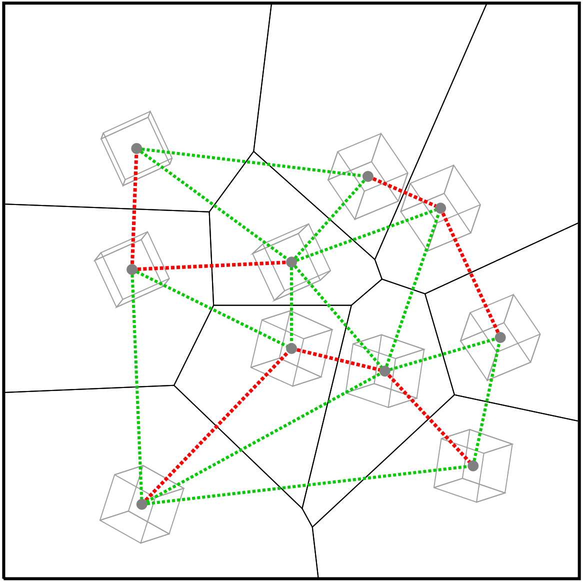

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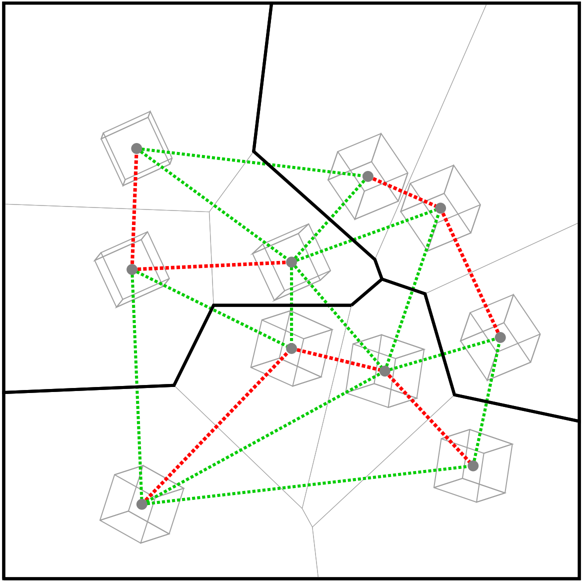

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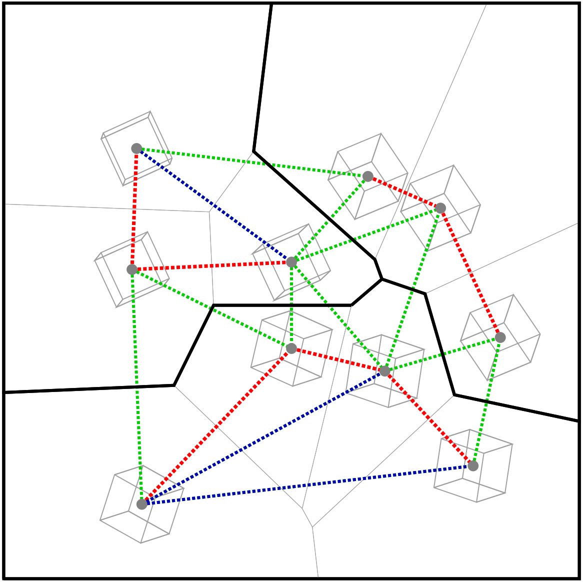

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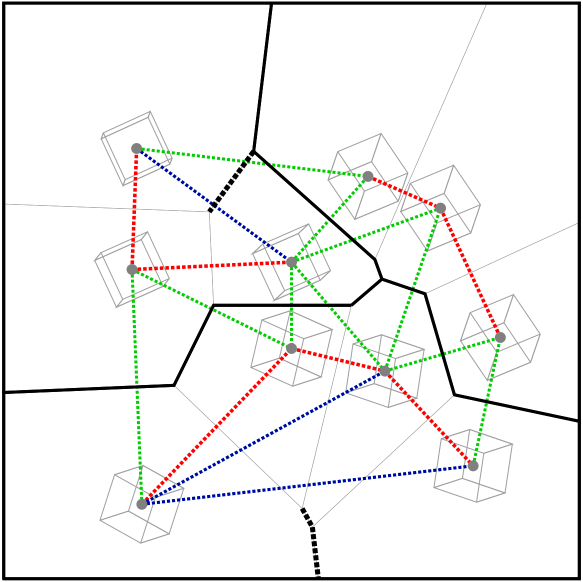

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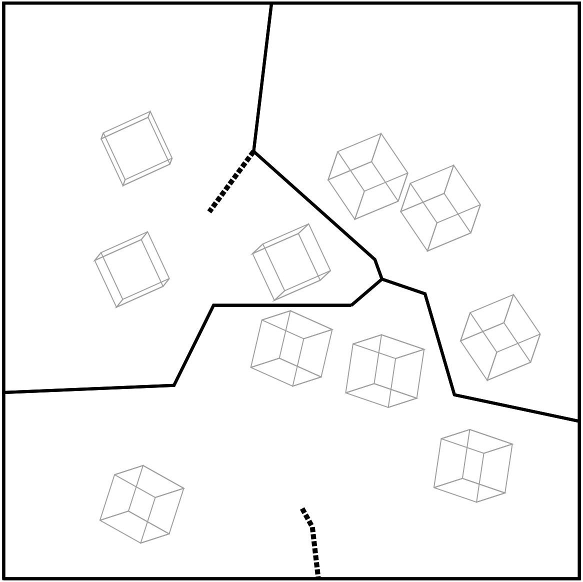

Modeling grains: algorithm

1. Voronoi-decomposition resulting in incidence matrix $\mathbf{I}_{VE}$, $\mathbf{I}_{ED}$ and adjacency matrix $\mathbf{A}_D$.
2. Decompose adjacencies $\mathbf{A}_D = \mathbf{A}_D^{\circ} + \mathbf{A}_D^{\partial}$
3. Search components of $\mathbf{A}_D^{\circ}$ via depth-first search and determine incidence matrix $\mathbf{I}_{DG} \subseteq D \times G$
4. Represent adjacencies of grains in a matrix $\mathbf{A}_G \subseteq G \times G$
5. Decompose adjacencies $\mathbf{A}_D^{\partial} = \mathbf{A}_D^{\partial_{\mathrm{sub}}} + \mathbf{A}_D^{\partial_{\mathrm{ext}}}$
6. Compute incidence matrix $\mathbf{I}_{EG} = \mathbf{I}_{ED}\mathbf{I}_{DG}$ and decompose $\mathbf{I}_{EG} = \mathbf{I}_{EG}^{\circ} + \mathbf{I}_{EG}^{\partial}$, with $\mathbf{I}_{EG}^{\partial} = \mathbf{I}_{EG}^{\partial_{\mathrm{sub}}} + \mathbf{I}_{EG}^{\partial_{\mathrm{ext}}}$.

Modeling grains: algorithm

1. Voronoi-decomposition resulting in incidence matrix $\mathbf{I}_{VE}$, $\mathbf{I}_{ED}$ and adjacency matrix $\mathbf{A}_D$

$$\left[\mathbf{I}_{VE}\right]^{i,j} = \begin{cases} 1, & \text{if vertex } v_i \text{ incident to edge } e_j, \\ 0, & \text{otherwise.} \end{cases}$$

2. Decompose adjacencies $\mathbf{A}_D = \mathbf{A}_D^{\circ} + \mathbf{A}_D^{\partial}$.
3. Search components of $\mathbf{A}_D^{\circ}$ via depth-first search and determine incidence matrix $\mathbf{I}_{DG} \subseteq D \times G$
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Modeling grains: algorithm

1. Voronoi-decomposition resulting in incidence matrix $\mathbf{I}_{VE}$, $\mathbf{I}_{ED}$ and adjacency matrix $\mathbf{A}_D$.

$$\left[\mathbf{I}_{ED}\right]^{j,\ell} = \begin{cases} 1, & \text{if edge } e_j \text{ incident to Voronoi-cell } D(\mathbf{x}_\ell), \\ 0, & \text{otherwise.} \end{cases}$$

2. Decompose adjacencies $\mathbf{A}_D = \mathbf{A}_D^\circ + \mathbf{A}_D^\partial$
3. Search components of $\mathbf{A}_D^\circ$ via depth-first search and determine incidence matrix $\mathbf{I}_{DG} \subseteq D \times G$
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Modeling grains: algorithm

1. Voronoi-decomposition resulting in incidence matrix $\mathbf{I}_{VE}$, $\mathbf{I}_{ED}$ and adjacency matrix $\boxed{\mathbf{A}_D}$.

$$\left[\boxed{\mathbf{A}_D}\right]^{\ell,\ell'} = \begin{cases} 1, & \text{if Voronoi-cell } D(\mathbf{x}_\ell) \text{ adjacent to Voronoi-cell } D(\mathbf{x}_{\ell'}), \\ 0, & \text{otherwise.} \end{cases}$$

2. Decompose adjacencies $\mathbf{A}_D = \mathbf{A}_D^{\circ} + \mathbf{A}_D^{\partial}$
3. Search components of $\mathbf{A}_D^{\circ}$ via depth-first search and determine incidence matrix $\mathbf{I}_{DG} \subseteq D \times G$
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2. Decompose adjacencies $\mathbf{A}_D = \boxed{\mathbf{A}_D^{\circ}} + \mathbf{A}_D^{\partial}$,

$$\left[\boxed{\mathbf{A}_D^{\circ}}\right]^{\ell,\ell'} = \begin{cases} 1, & \text{if } D(\mathbf{x}_\ell) \text{ and } D(\mathbf{x}_{\ell'}) \text{ adjacent and no grain boundary}, \\ 0, & \text{otherwise.} \end{cases}$$

3. Search components of $\mathbf{A}_D^{\circ}$ via depth-first search and determine incidence matrix $\mathbf{I}_{DG} \subseteq D \times G$
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3. Search components of $\mathbf{A}_D^{\circ}$ via depth-first search and determine incidence matrix $\boxed{\mathbf{I}_{DG}} \subseteq D \times G$,

$$\left[\boxed{\mathbf{I}_{DG}}\right]^{\ell,m} = \begin{cases} 1, & \text{if } D(\mathbf{x}_\ell) \text{ is part of grain } g_m, \\ 0, & \text{otherwise.} \end{cases}$$

4. Represent adjacencies of grains in a matrix $\mathbf{A}_G \subseteq G \times G$
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4. Represent adjacencies of grains in a matrix $\boxed{\mathbf{A}_G} \subseteq G \times G$,

$$\left[\boxed{\mathbf{A}_G}\right]^{m,m'} = \begin{cases} 1, & \text{if grain } g_m \text{ and } g_{m'} \text{ have a common grain boundary,} \\ 0, & \text{otherwise.} \end{cases}$$

5. Decompose adjacencies $\mathbf{A}_D^{\partial} = \mathbf{A}_D^{\partial\mathrm{sub}} + \mathbf{A}_D^{\partial\mathrm{ext}}$
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4. Represent adjacencies of grains in a matrix $\mathbf{A}_G \subseteq G \times G$,

$$[\mathbf{A}_G]^{m,m'} = \begin{cases} 1, & \text{if } \left[\mathbf{I}_{DG}^\top \mathbf{A}_D^\partial \mathbf{I}_{DG}\right]^{m,m'} > 0, \\ 0, & \text{otherwise.} \end{cases}$$

5. Decompose adjacencies $\mathbf{A}_D^\partial = \mathbf{A}_D^{\partial \mathrm{sub}} + \mathbf{A}_D^{\partial \mathrm{ext}}$
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5. Decompose adjacencies $\mathbf{A}_D^{\partial} = \boxed{\mathbf{A}_D^{\partial_{\mathrm{sub}}}} + \mathbf{A}_D^{\partial_{\mathrm{ext}}}$.,

$$\left[\boxed{\mathbf{A}_D^{\partial_{\mathrm{sub}}}}\right]^{\ell,\ell'} = \begin{cases} 1, & \text{if } D(\mathbf{x}_\ell) \text{ and } D(\mathbf{x}_{\ell'}) \text{ adjacent and sub grain boundary}, \\ 0, & \text{otherwise.} \end{cases}$$

6. Compute incidence matrix $\mathbf{I}_{EG} = \mathbf{I}_{ED}\mathbf{I}_{DG}$ and decompose $\mathbf{I}_{EG} = \mathbf{I}_{EG}^{\circ} + \mathbf{I}_{EG}^{\partial}$, with $\mathbf{I}_{EG}^{\partial} = \mathbf{I}_{EG}^{\partial_{\mathrm{sub}}} + \mathbf{I}_{EG}^{\partial_{\mathrm{ext}}}$.

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5. Decompose adjacencies $\mathbf{A}_D^{\partial} = \mathbf{A}_D^{\partial\mathrm{sub}} + \boxed{\mathbf{A}_D^{\partial\mathrm{ext}}}$,

$$\left[\boxed{\mathbf{A}_D^{\partial\mathrm{ext}}}\right]^{\ell,\ell'} = \begin{cases} 1, & \text{if } D(\mathbf{x}_\ell) \text{ and } D(\mathbf{x}_{\ell'}) \text{ adjacent and grain boundary}, \\ 0, & \text{otherwise.} \end{cases}$$

6. Compute incidence matrix $\mathbf{I}_{EG} = \mathbf{I}_{ED}\mathbf{I}_{DG}$ and decompose $\mathbf{I}_{EG} = \mathbf{I}_{EG}^{\circ} + \mathbf{I}_{EG}^{\partial}$, with $\mathbf{I}_{EG}^{\partial} = \mathbf{I}_{EG}^{\partial\mathrm{sub}} + \mathbf{I}_{EG}^{\partial\mathrm{ext}}$.

Modeling grains: algorithm

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Output:
$\mathbf{A}_D^{\circ}, \mathbf{A}_D^{\partial_{\mathrm{sub}}}, \mathbf{A}_D^{\partial_{\mathrm{ext}}}, \mathbf{A}_G,$
$\mathbf{I}_{DG}, \mathbf{I}_{ED}^{\partial_{\mathrm{sub}}}, \mathbf{I}_{ED}^{\partial_{\mathrm{ext}}},$

Modeling grains: algorithm

Benefits ...

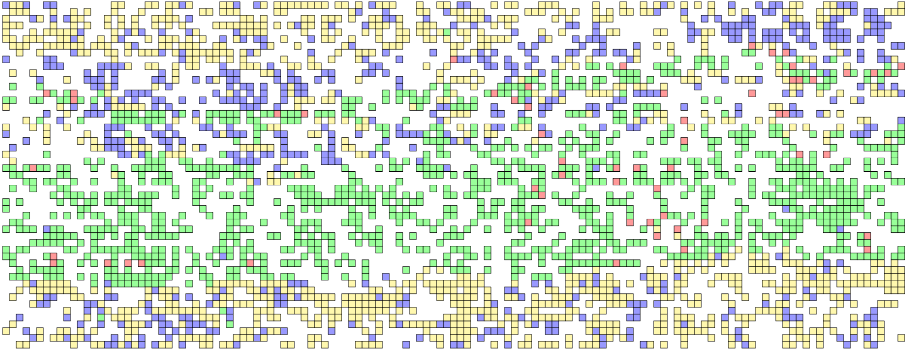
- Works in 2d and 3d
- Voronoi-decomposition flexible against not indexed data
- No interpolation of orientation
- Explicit data model ensures fast access to adjacencies and incidences.
- Almost every spatial relationship of EBSD data and its grains can be represented.

... Disadvantages

- Voronoi-decomposition is expensive.
- Large memory costs to store all adjacencies and incidences.

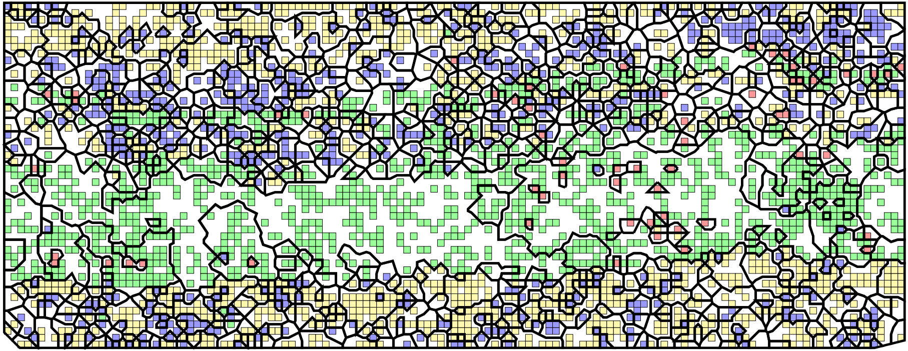
Modeling grains

```
mtexdata mylonite
plot(ebsd,'property','phase');
```



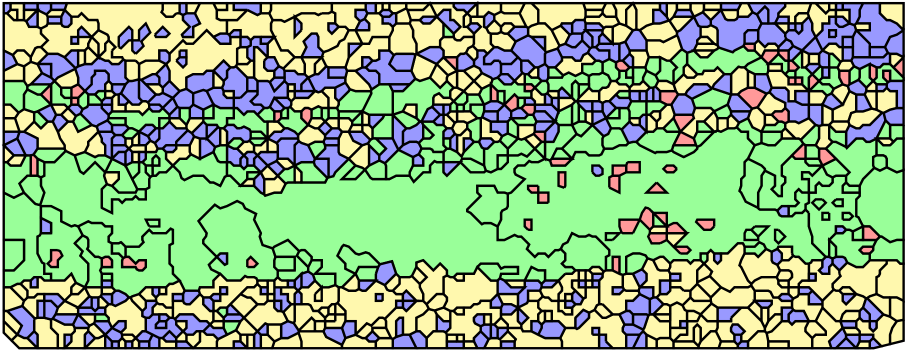
Modeling grains

```
grains = calcGrains(ebsd,'angle',5*degree);
hold on, plotBoundary(grains);
```



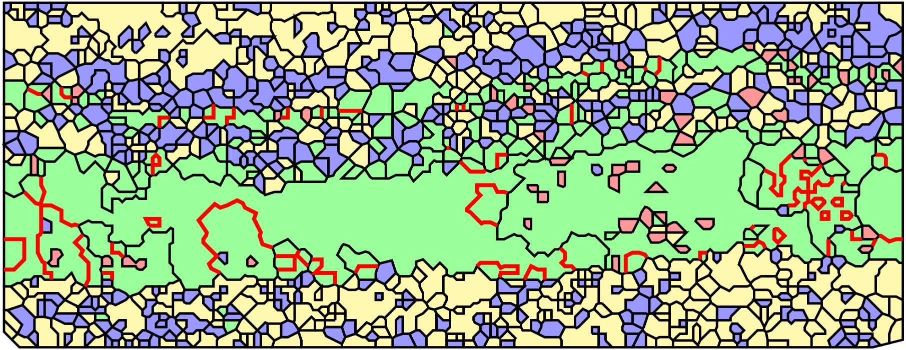
Modeling grains

```
plot(grains,'property','phase')
```



Modeling grains

```
hold on, plotBoundary(grains,'property',...
   orientation(...));
```



Properties of grains

Incidencies and Adjacencies

```
get(grains,'I_VF')
get(grains,'I_DG')
get(grains,'I_FG')
get(grains,'I_FDext')
get(grains,'I_FDint')
get(grains,'A_D')
get(grains,'A_G')
```

Properties

```
get(grains,'EBSD')
get(grains,'orientation')
get(grains,'orientations')
get(grains,'...')
```

Properties of grains

Geometric properties of grains

```
area(grains)
perimeter(grains)
diameter(grains)
centroid(grains)
shapefactor(grains)
aspectratio(grains)
equivalentradius(grains)
equivalentperimeter(grains)
principalcomponents(grains)
...
```

Other properties

```
grainSize(grains)
hasHole(grains)
isNotIndexed(grains)
```

Accessing grains

Accessing by phase

```
grains('mineral␣name')
grains({'fe','mg'})
```

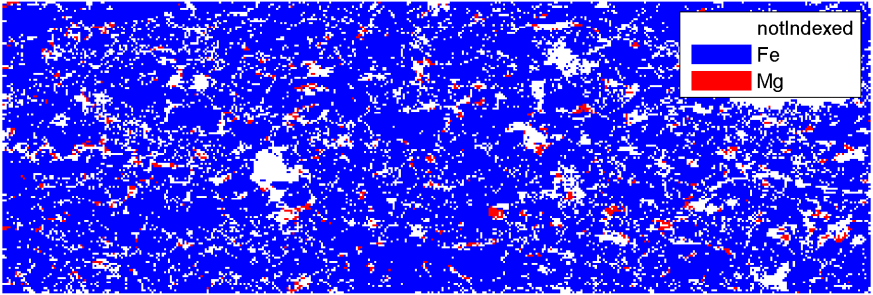
Accessing grains by indexing or logical expression

```
grains(1)
grains(1:10)
grains( area(grains) > 100 )
grains(diameter(grains)>10 | perimeter(grains)>10)
grains(diameter(grains)>10 & grains('fe'))
grains(grainSize(grains)>1 & ~grains('notindexed'))
```

Concatenation of grain

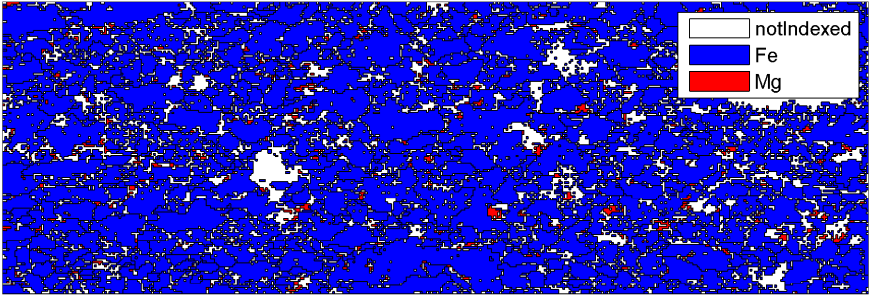
```
[grains('fe') grains('mg')]
```

Correcting EBSD and grains



1. Import EBSD.
2. Reconstruct grains.

Correcting EBSD and grains



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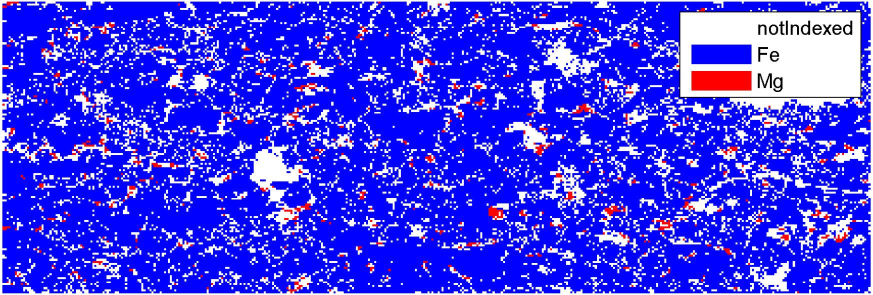
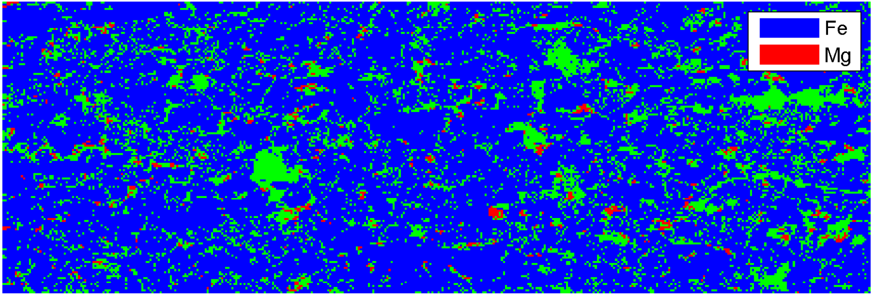
Correcting EBSD and grains



1. Import EBSD.
2. Remove badly indexed data and remove non-plausible grains, e.g. '1-pixel' grains.
3. Reconstruct grains.

Correcting EBSD and grains



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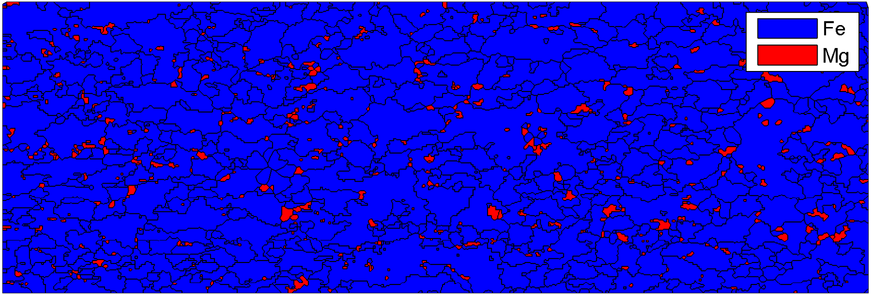
Correcting EBSD and grains



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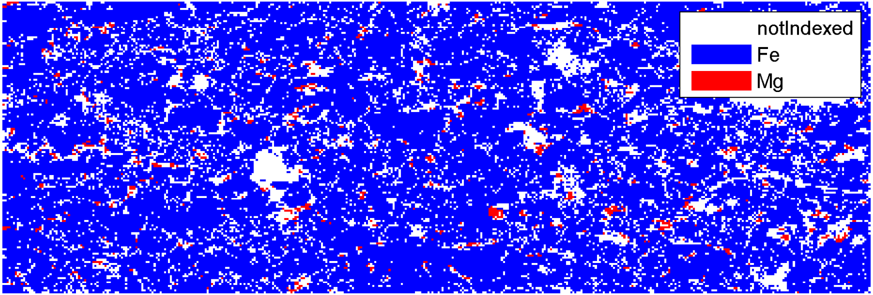
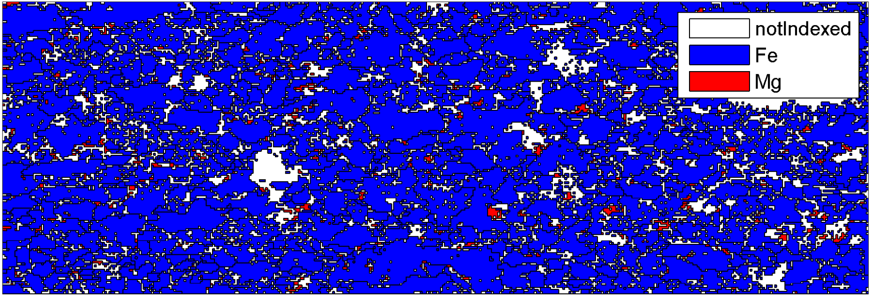
Correcting EBSD and grains



1. Import EBSD.
2. Reconstruct grains.
3. Remove non-plausible data but keep some dummy data.
4. Reconstruct grains again.

Correcting EBSD and grains



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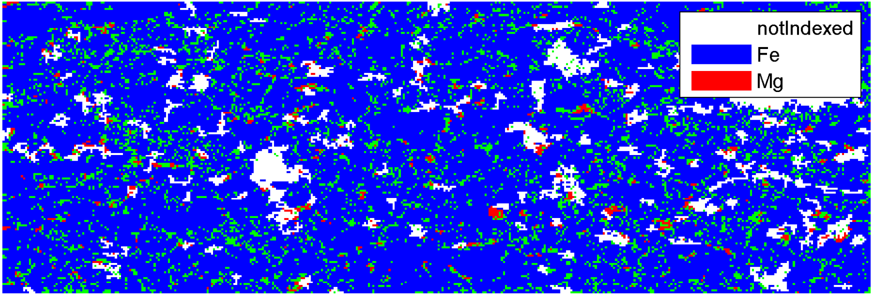
Correcting EBSD and grains



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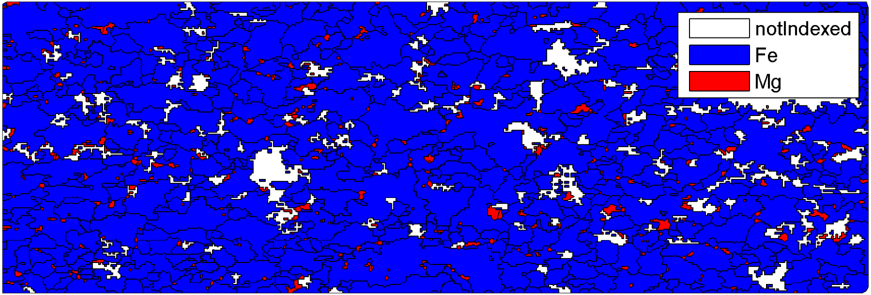
Correcting EBSD and grains

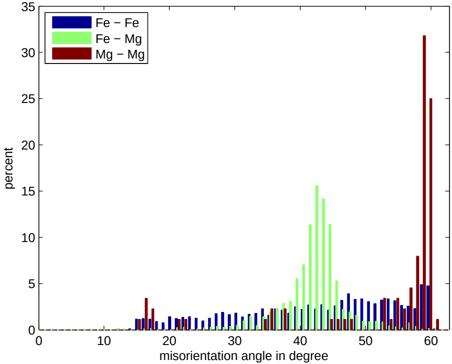


1. Import EBSD.
2. Reconstruct grains.
3. Remove non-plausible data but keep some dummy data.
4. Reconstruct grains again.

Grain boundaries and misorienation

via boundary misorientation angular distribution

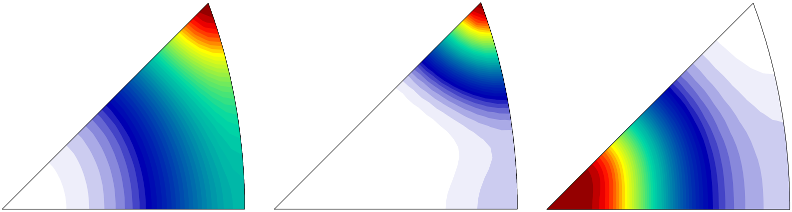
```
plotAngleDistribution(grains)
plotAngleDistribution(grains('fe'),63)
plotAngleDistribution(grains('fe'),grains('mg'),63)
```



Grain boundaries and misorienation

via boundary misorientation axis distribution

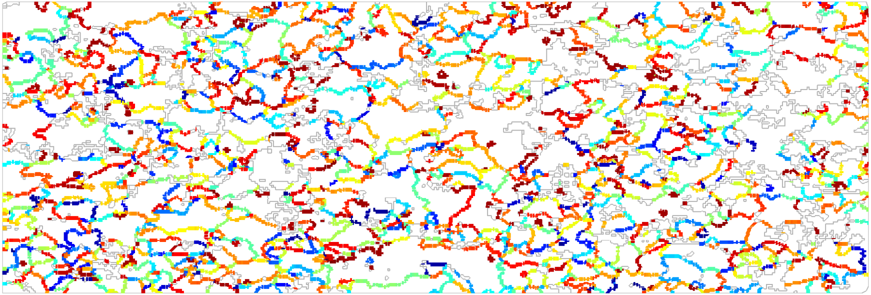
```
plotAxisDistribution(grains('fe'))
plotAxisDistribution(grains('mg'),...
                          'smooth','antipodal')
plotAxisDistribution(grains('mg'),grains('fe'))
```



Grain boundaries and misorienation

via spatial plots

```
plotBoundary(grains,'property','angle')
plotBoundary(grains,'property','misorientation')
plotBoundary(grains,'property',...
   orientation(...),'delta',2*degree)
plotBoundary(grains,'property',[2 10]*degree)
```



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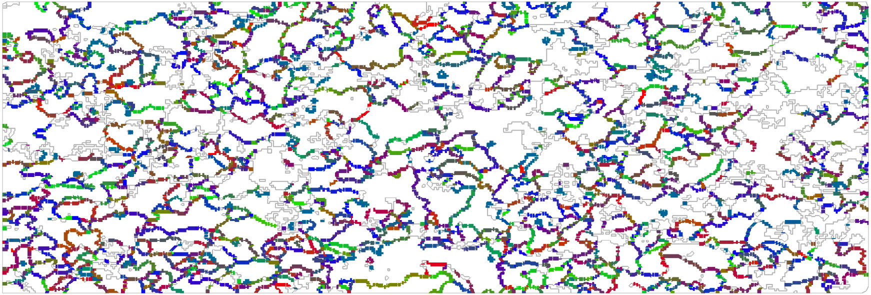

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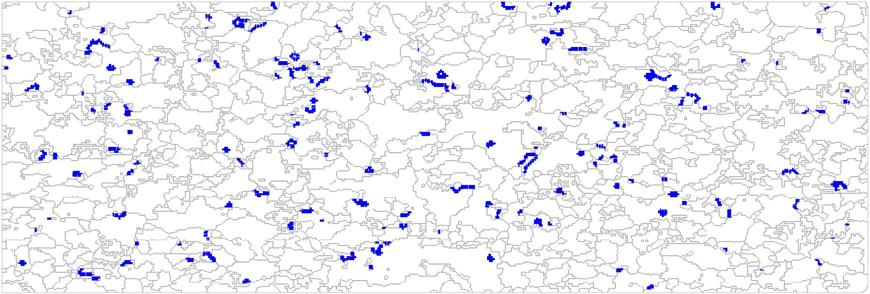

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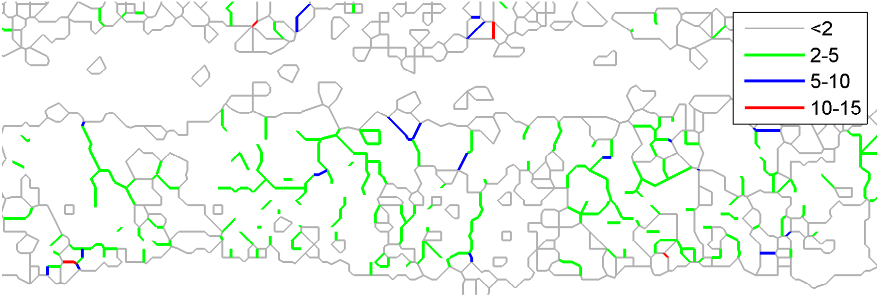
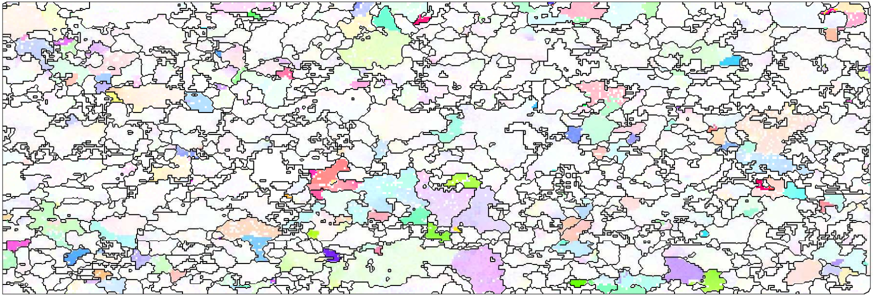


Grains and internal misorienation

Observe misorientation within a grain

```
plot(grains,'property','mis2mean')
plot(grains,'property','mis2mean',...
                    'colorcoding','angle')
```



Grains and internal misorienation

Observe misorientation within a grain

```
plot(grains,'property','mis2mean')
plot(grains,'property','mis2mean',...
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```
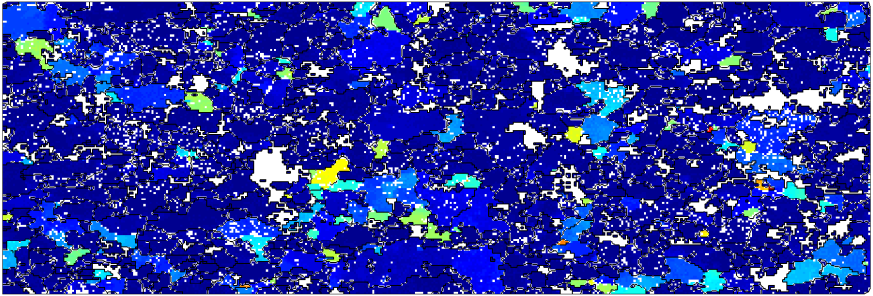
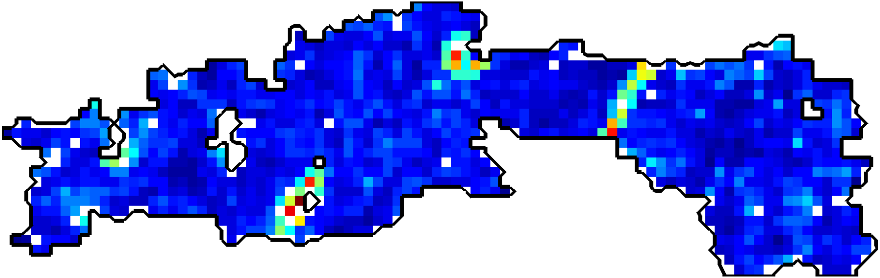



Grains and internal misorienation

Observe misorientation of grains individually

```
singlegrain = findByLocation(grains,[x y])
plotKAM(singlegrain)
spatialProfile(singlegrain,[x1 y1; x2 y2])
```



Grains and internal misorienation

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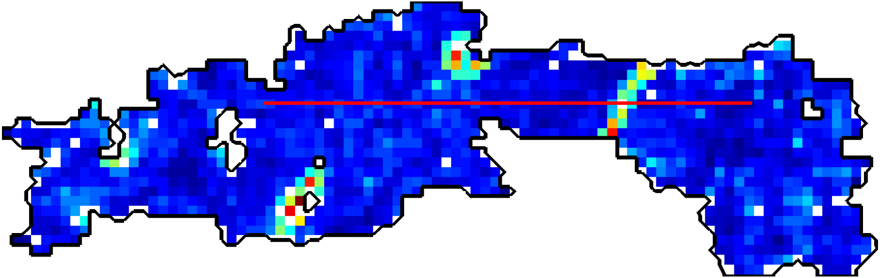

Grains and internal misorienation

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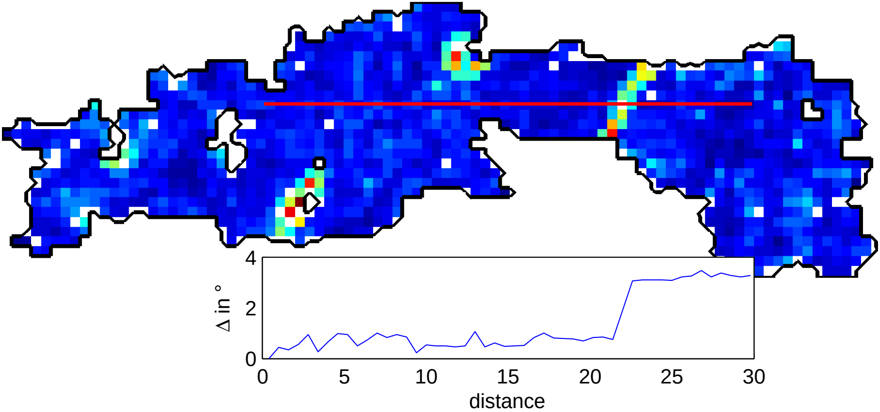

Grains and misorienation

via boundary misorientation angular distribution

```
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plotAngleDistribution(grains('fe'),63)
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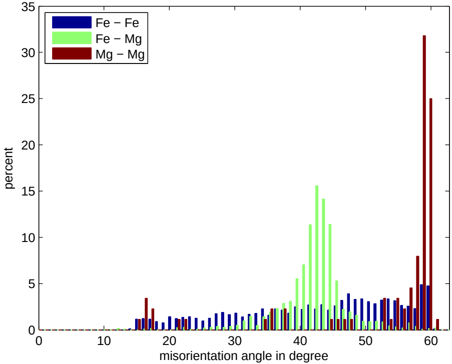


Organizing grains hierarchically

merging grains with certain misorientation angle

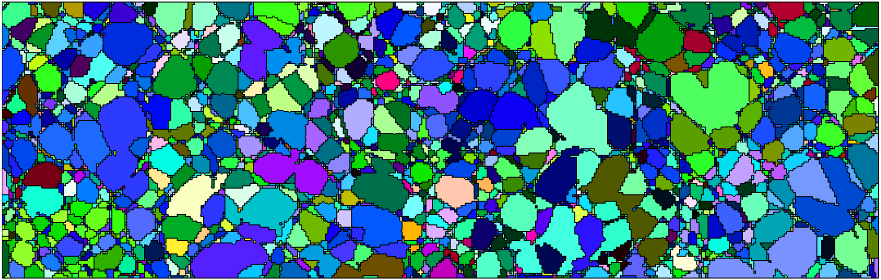
```
[grains5  I_5]  = merge(grains,5*degree);
[grains10 I_10] = merge(grains5,10*degree);

sum(I_5,2); sum(I_10,2);
sum(I_10*I_5,2);
```

Organizing grains hierarchically

merging grains with special boundary

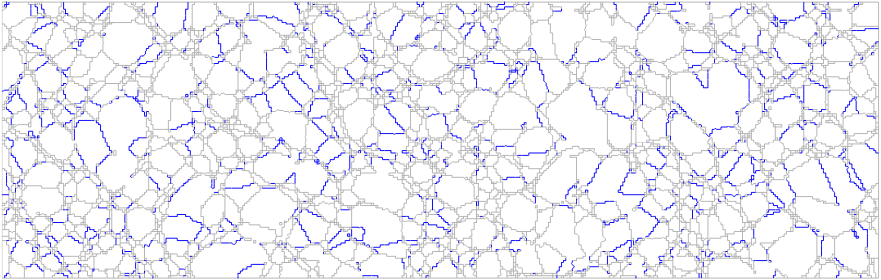
```
[grains_csl  I_csl] = merge(grains,CSL(3));
[grains_o    I_o  ] = merge(grains,...
                 orientation(...),'delta',2*degree);
```



Organizing grains hierarchically

merging grains with special boundary

```
[grains_csl I_csl] = merge(grains,CSL(3));
[grains_o   I_o  ] = merge(grains,...
                      orientation(...),'delta',2*degree);
```



Organizing grains hierarchically

merging grains with special boundary

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```

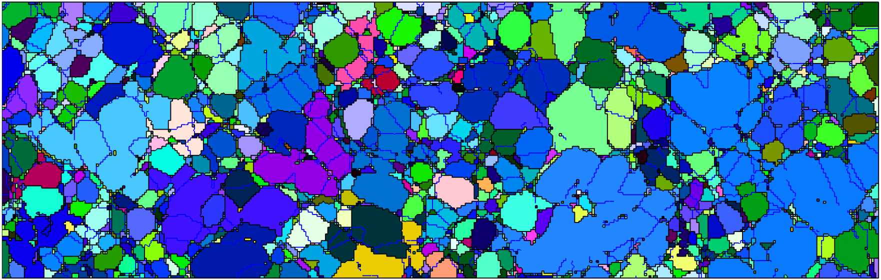

Organizing grains hierarchically

merging grains with special boundary

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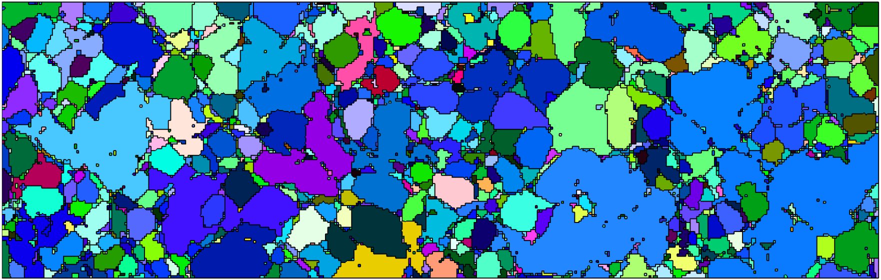

Exercises

Examine the EBSD data `mtexdata aachen`:

- Correct the EBSD data / grains.
- How does the correction influence the data analysis?

Examine the EBSD data `mtexdata mylonite`:

- Characterize special grain boundaries for all phases.
- Visualize your results.

Examine the EBSD data `ebsd_mergeCSL3.txt`:

- Which texture is present?
- Characterize special grain boundaries.
- Merge grains and investigate merged regions.
- What is wrong with the data?