Combining a front-tracking model (elle) with the finite element code OOF2

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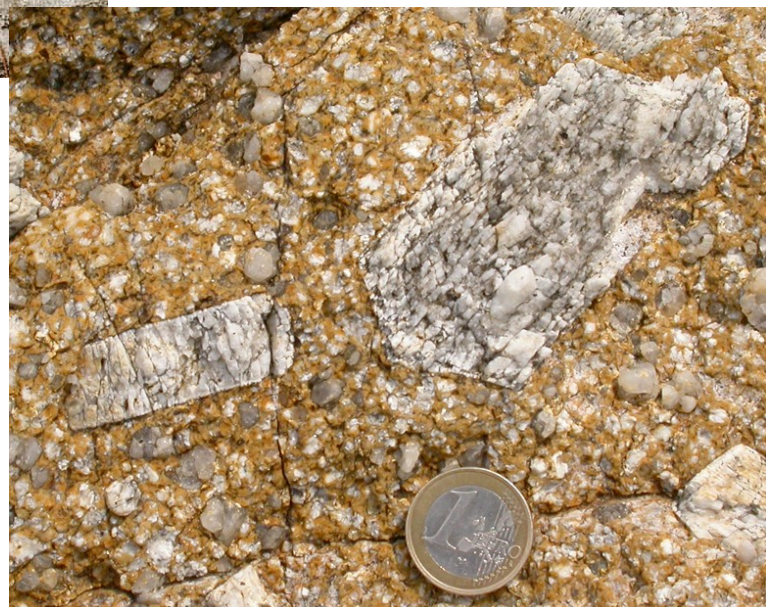
A geological multiphase material: rocks

The nice thing about rocks is that they come in absolutely every color, shape, setting, mixture etc. you can think of.

The bad thing about rocks is that they come in absolutely every color, shape, setting, mixture etc. you can think of.



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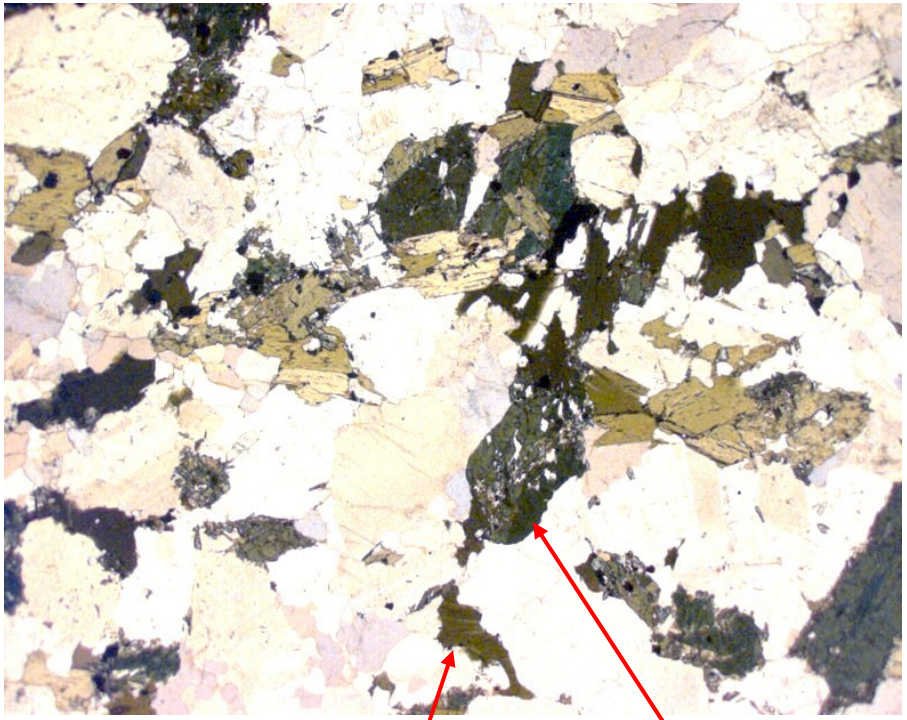
Thin sections of rocks

Tonalite (Kimberley, Australia)

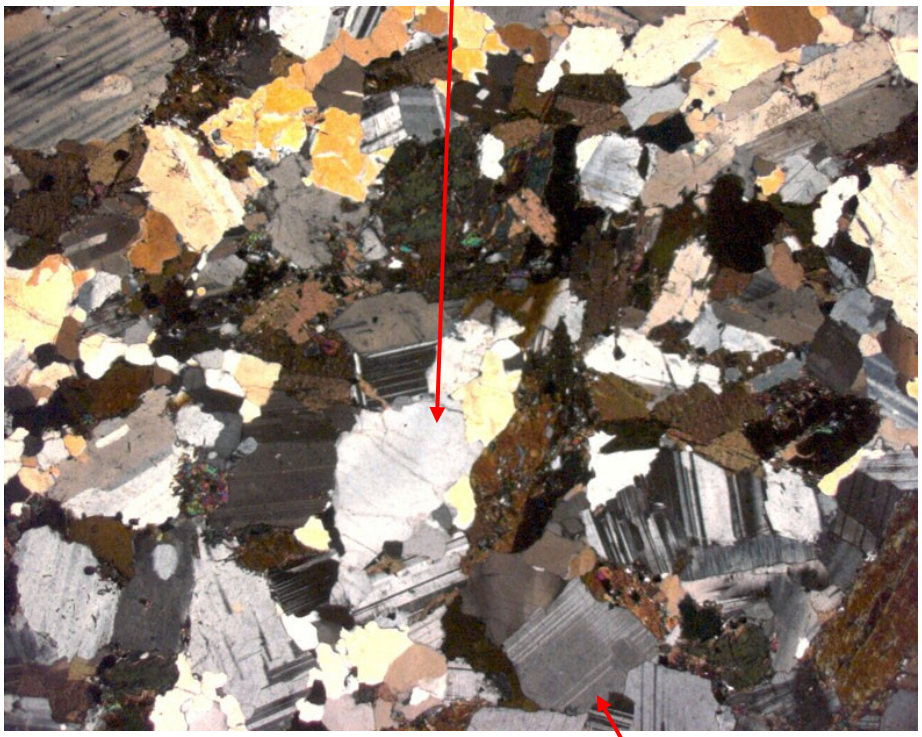
1 mm



biotite

hornblende

quartz



plagioclase

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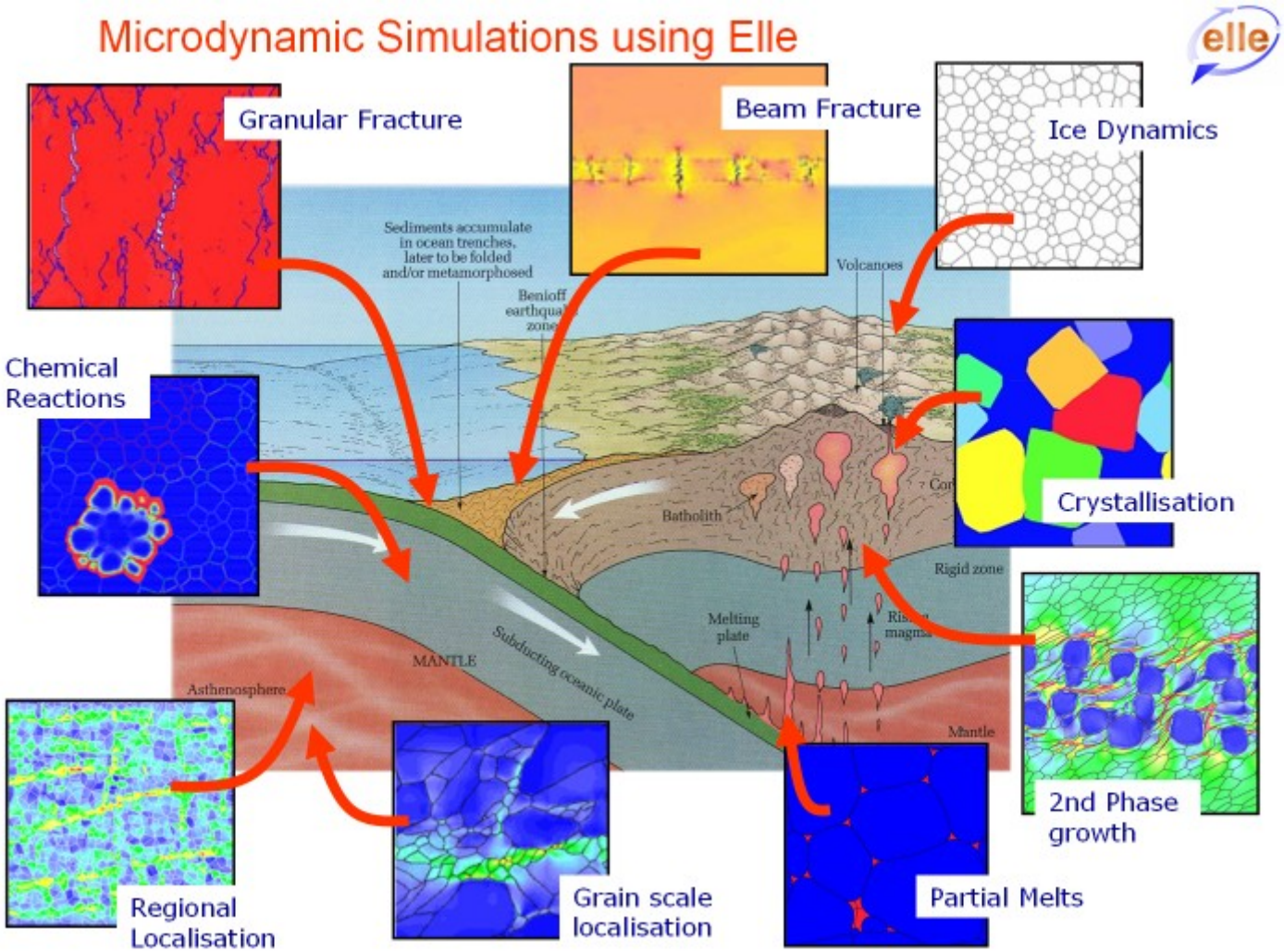
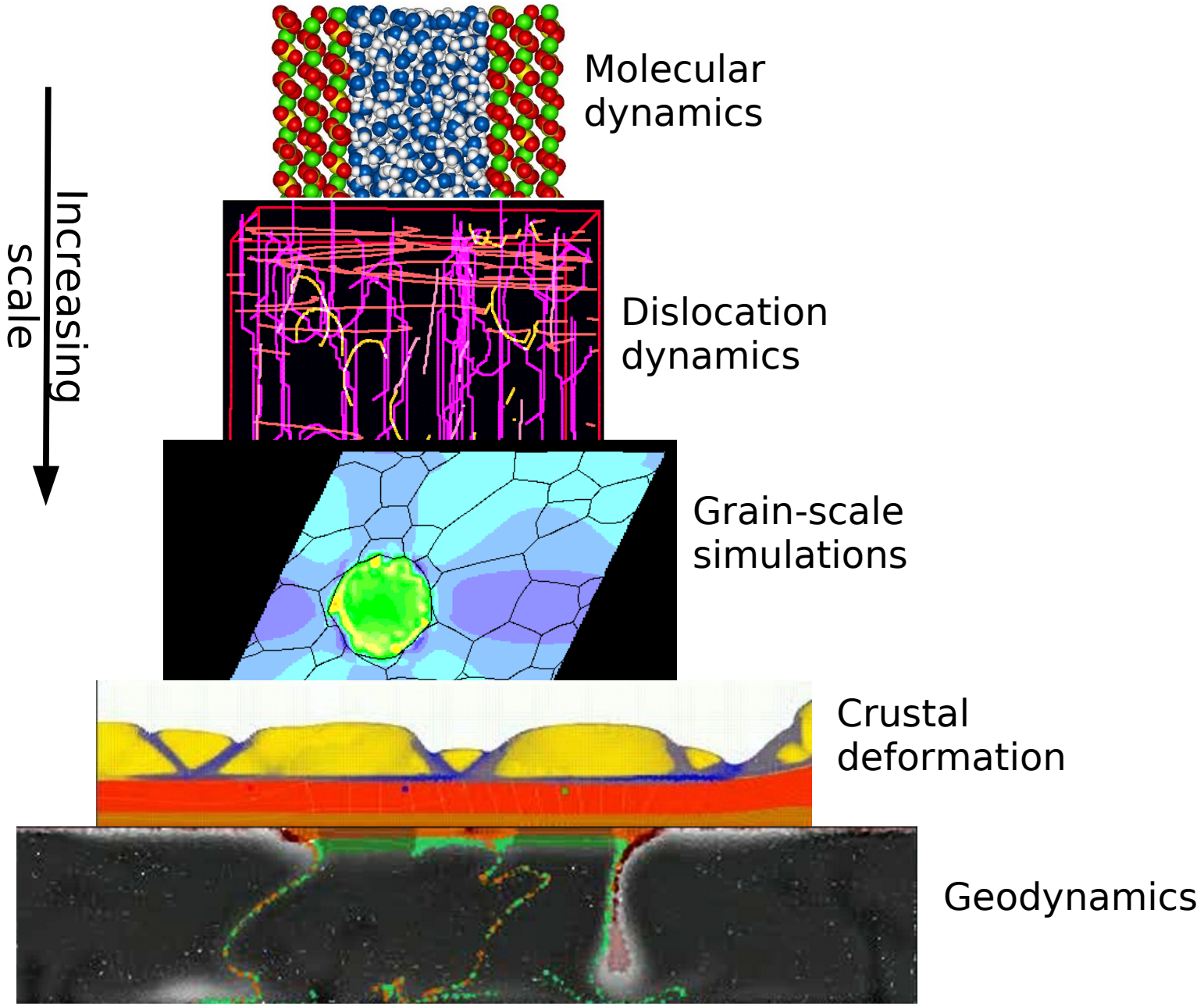
Different environments means different rocks

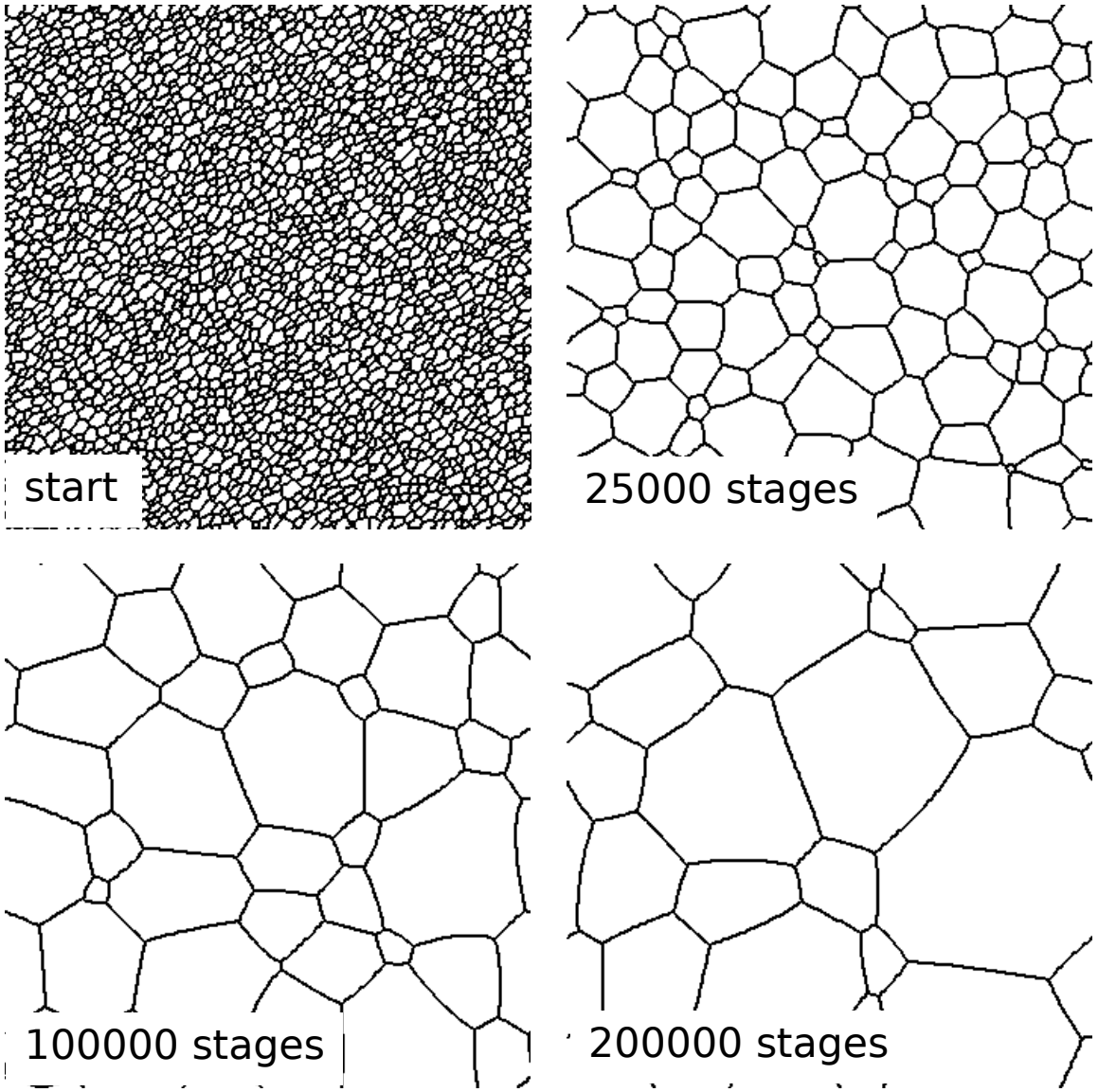


Elle is a versatile software-package that can be used to simulate different processes sequentially.

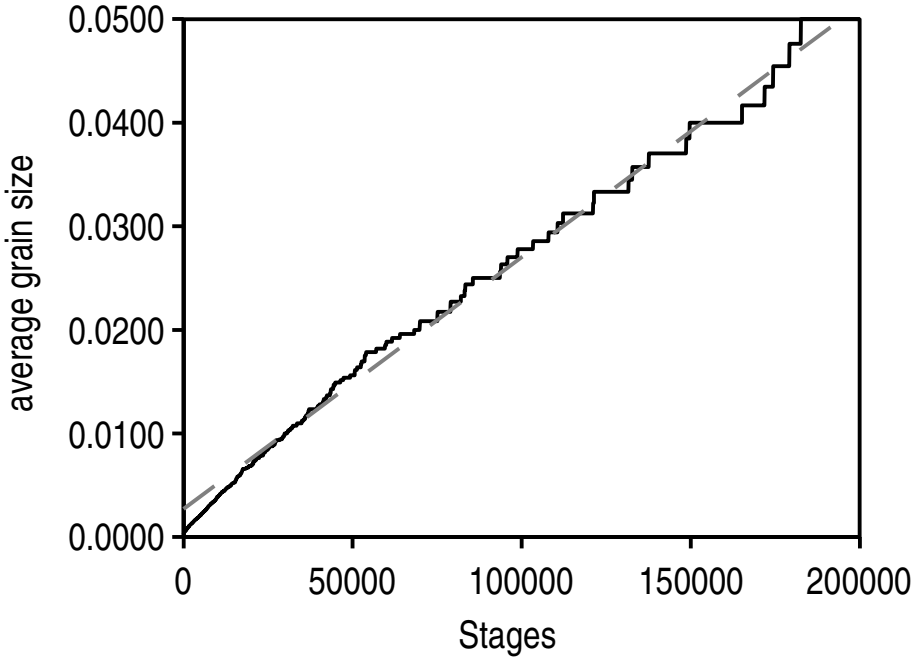
Elle is dimensionless



Examples of single processes: grain growth (1)



Example of simple grain growth



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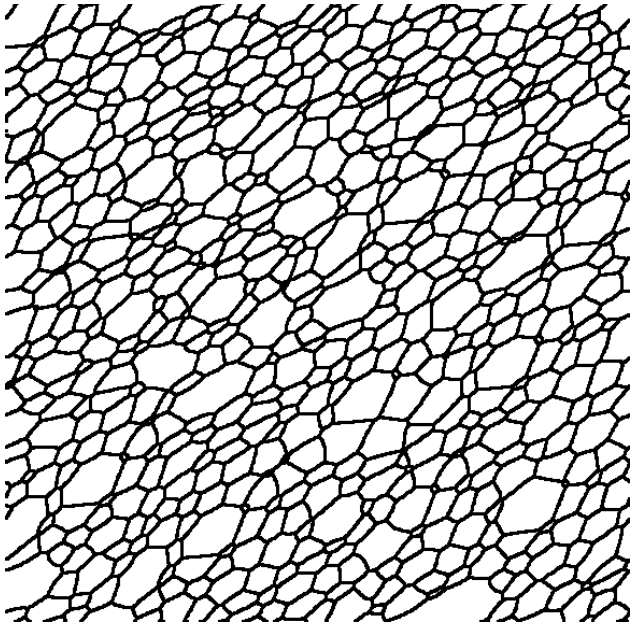
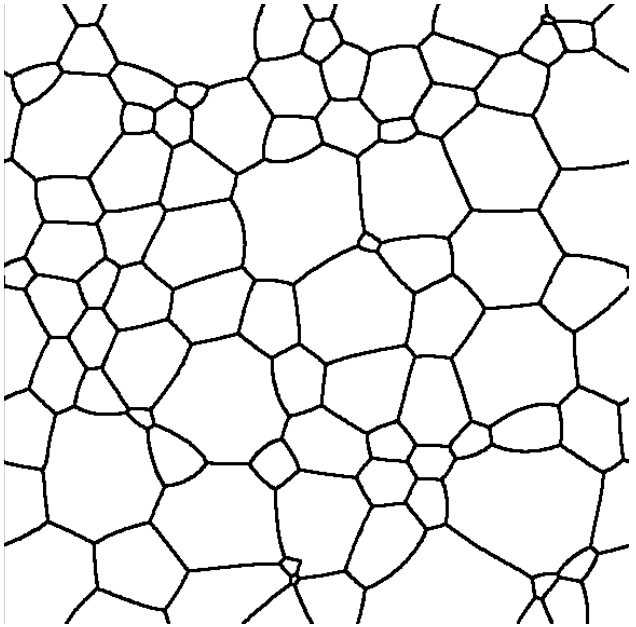
Examples of single processes: grain growth (2)



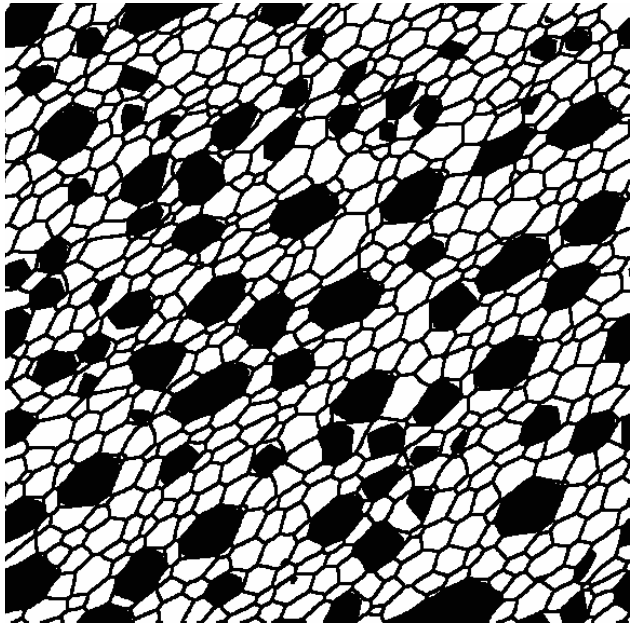
Grain boundary network

t=0



Grain boundary network

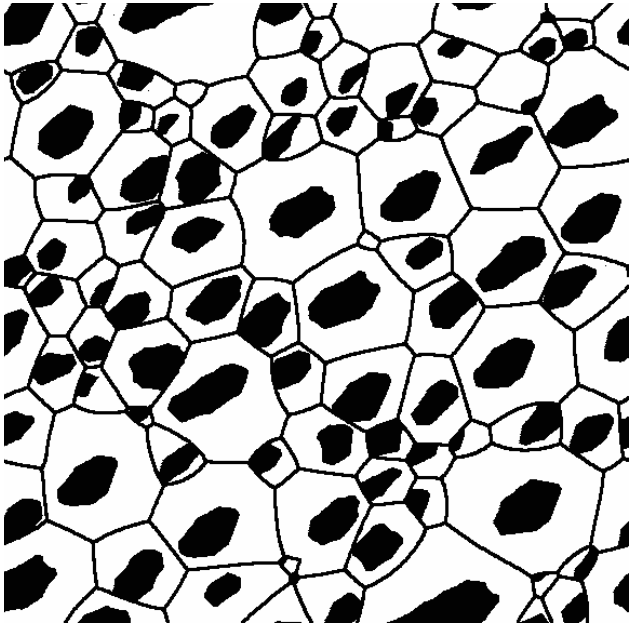
t=800



t=0

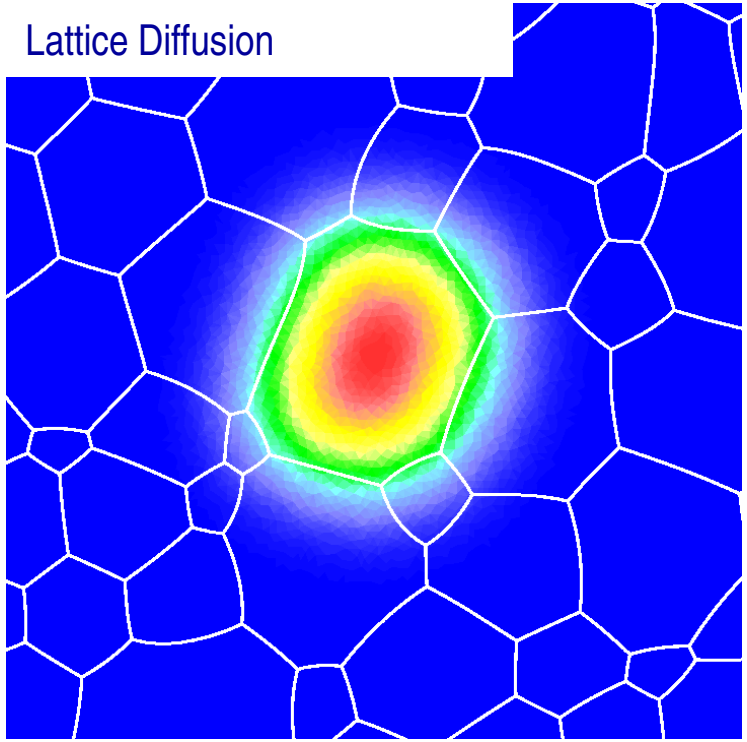
Unswept cores

Swept zones

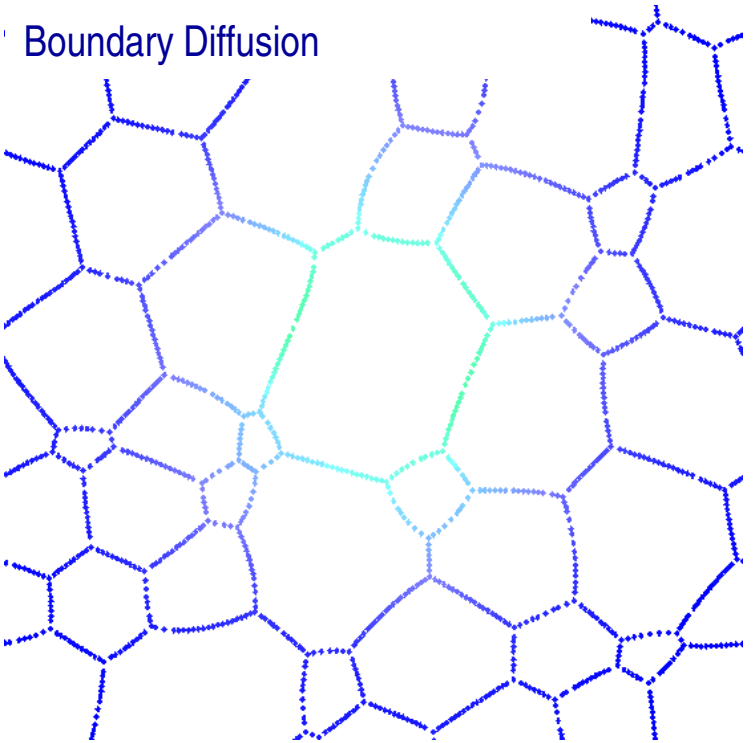


t=800

Examples of single processes: diffusion

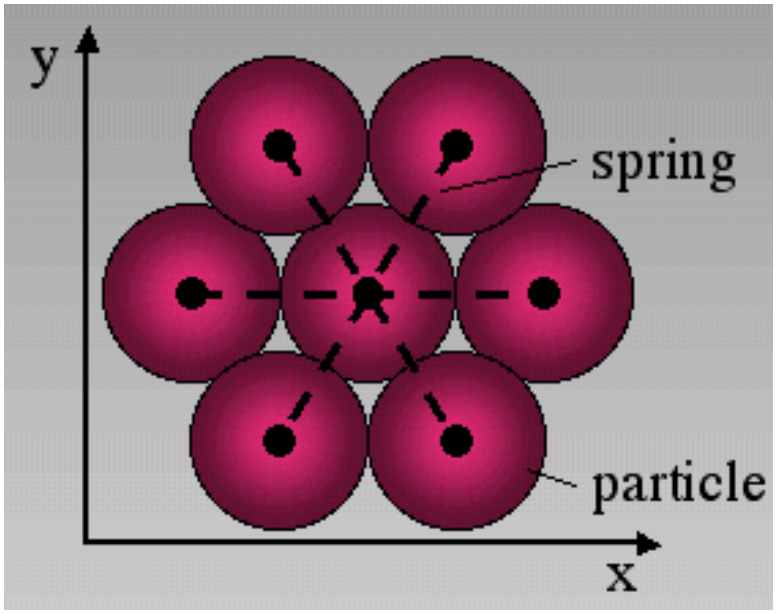


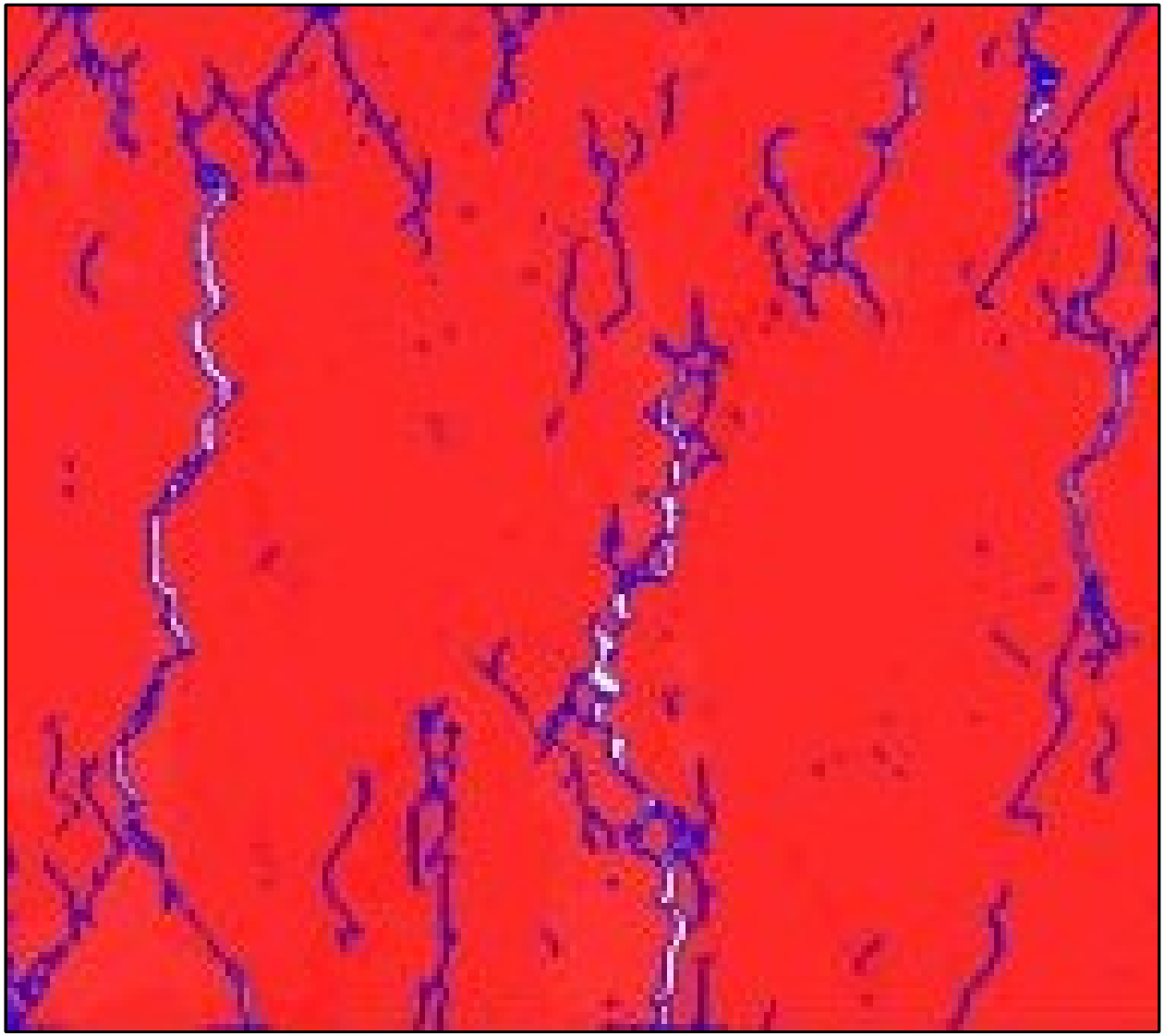
elle_diff



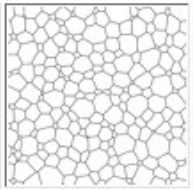
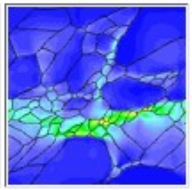
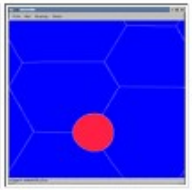
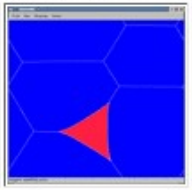
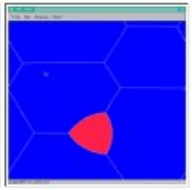
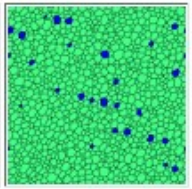
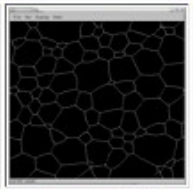
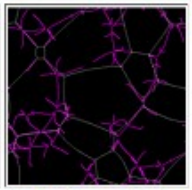
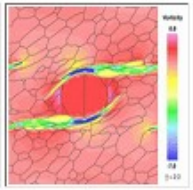
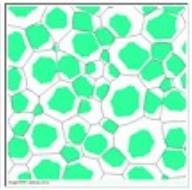
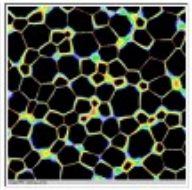
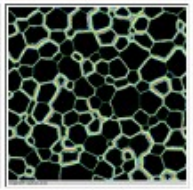
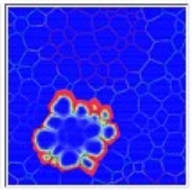
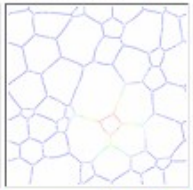
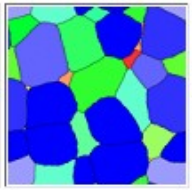
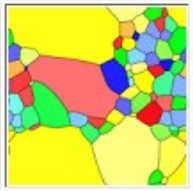
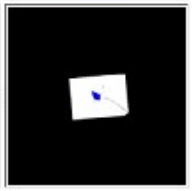
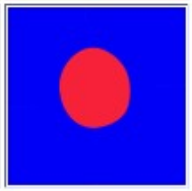
elle_gbdiff

Fracturing (using Latte)





Growing number of processes available

1		Layered ice grain growth	2		Localisation of deformation	3		Melt Pocket Angle=180
4		Melt Pocket Angle=0	5		Melt Pocket Angle=120	6		Ostwald Ripening
7		Grain boundary migration microstructures	8		Crystallisation from a melt	9		Triple junction trails
10		Porhyroblast Rotation?	11		Grain boundary sweeping	12		Cyclic grain growth bands
13		Defect energy driven gbm growth bands	14		Exchange Reaction	15		Sug-grain growth
16		Grain boundary diffusion	17		Dislocation density driven grain boundary migration	18		Grain Growth
19		Exaggerated Grain Growth	20		Crystallisation from a melt	21		Surface Energy Reduction of a Snowflake

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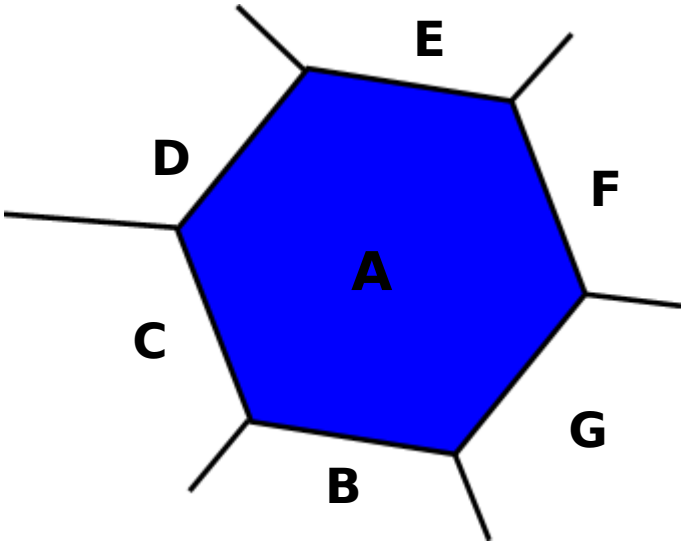
How does Elle work?

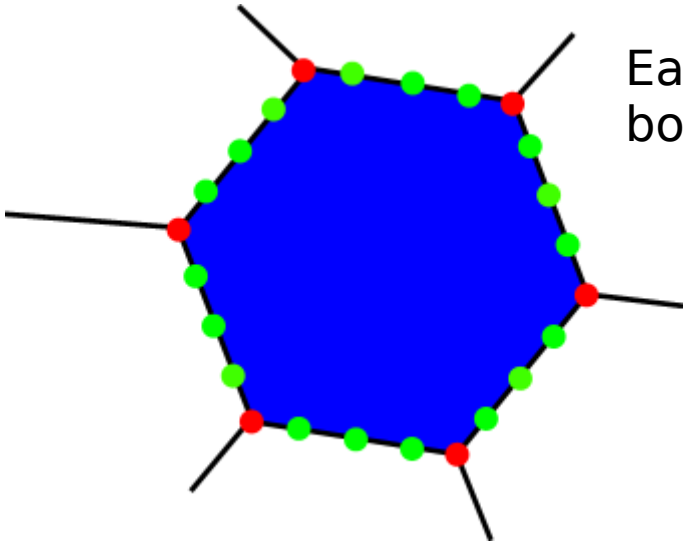
Elle uses a front-tracking approach. Very simply put this means it “just” calculates the changes of properties at the boundaries of polygons.



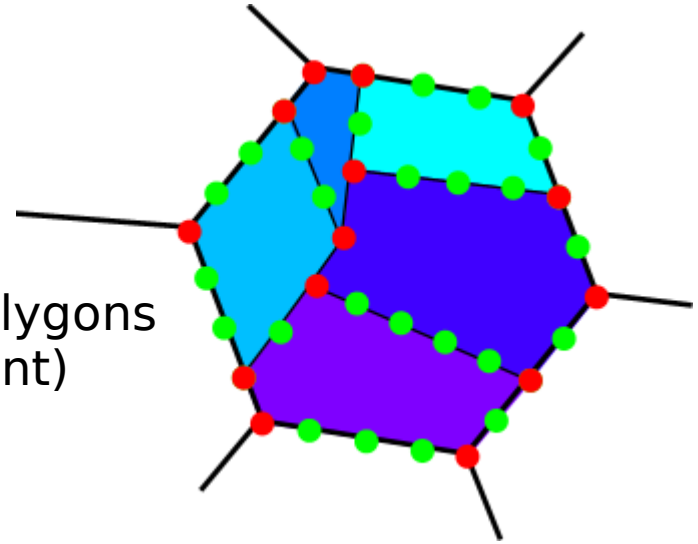
If A, B,C etc. is a material property that changes between the different polygons (can be a linear or non-linear change) then the difference between the two properties can be used as a driving force of some kind. This is obvious for surface energies of facet but maybe less obvious in case of e.g. chemical concentrations etc..

The trick is the way information about polygons is stored and cross-linked.

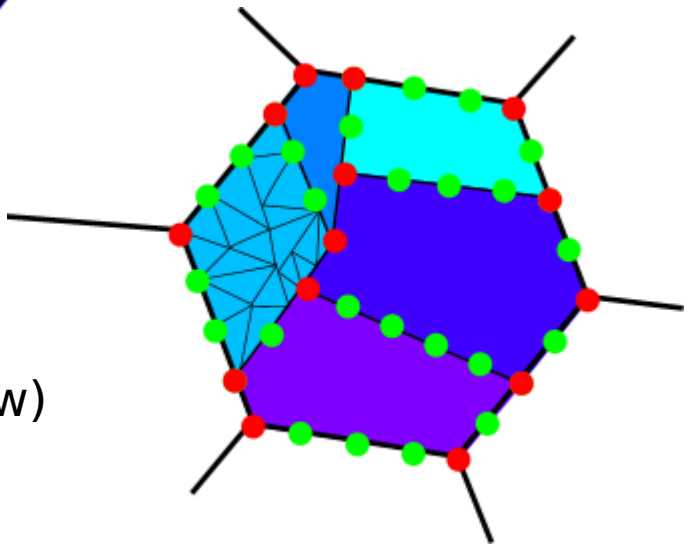
Hierarchical ordering of elements in Elle



Each polygon has a defined number of
boundary nodes (so called double and triple nodes)



We can have a set of sub-polygons
(children) in a polygon (parent)



We can triangulate parts or all of a polygon
(and now also calculate Voronoi-subsets now)

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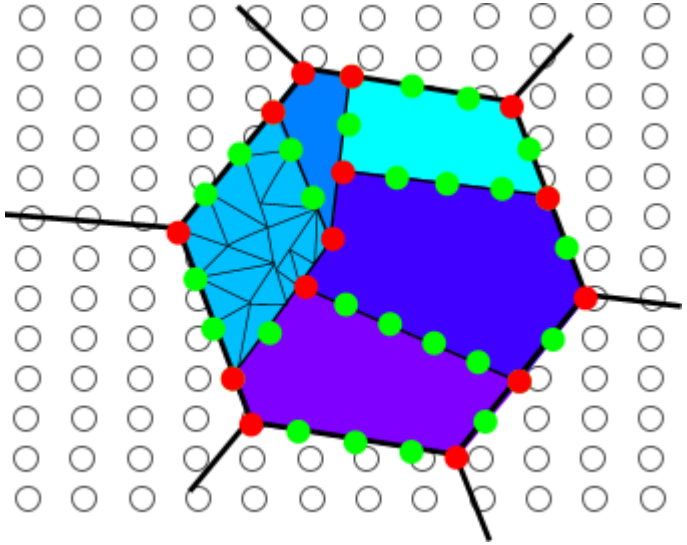
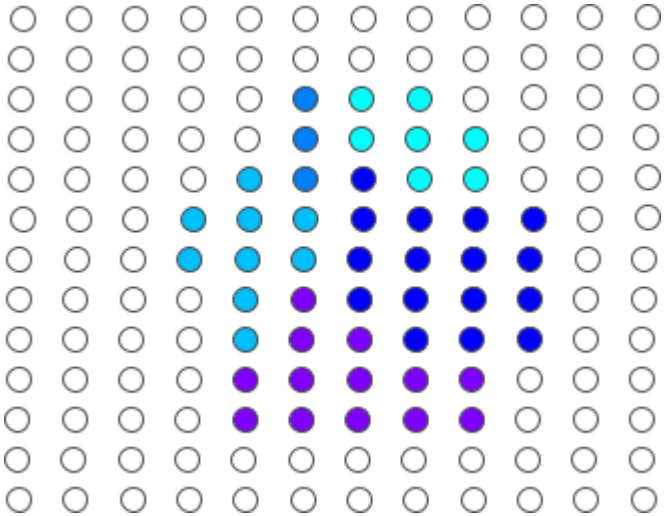
Underlying set of points: unconnected nodes



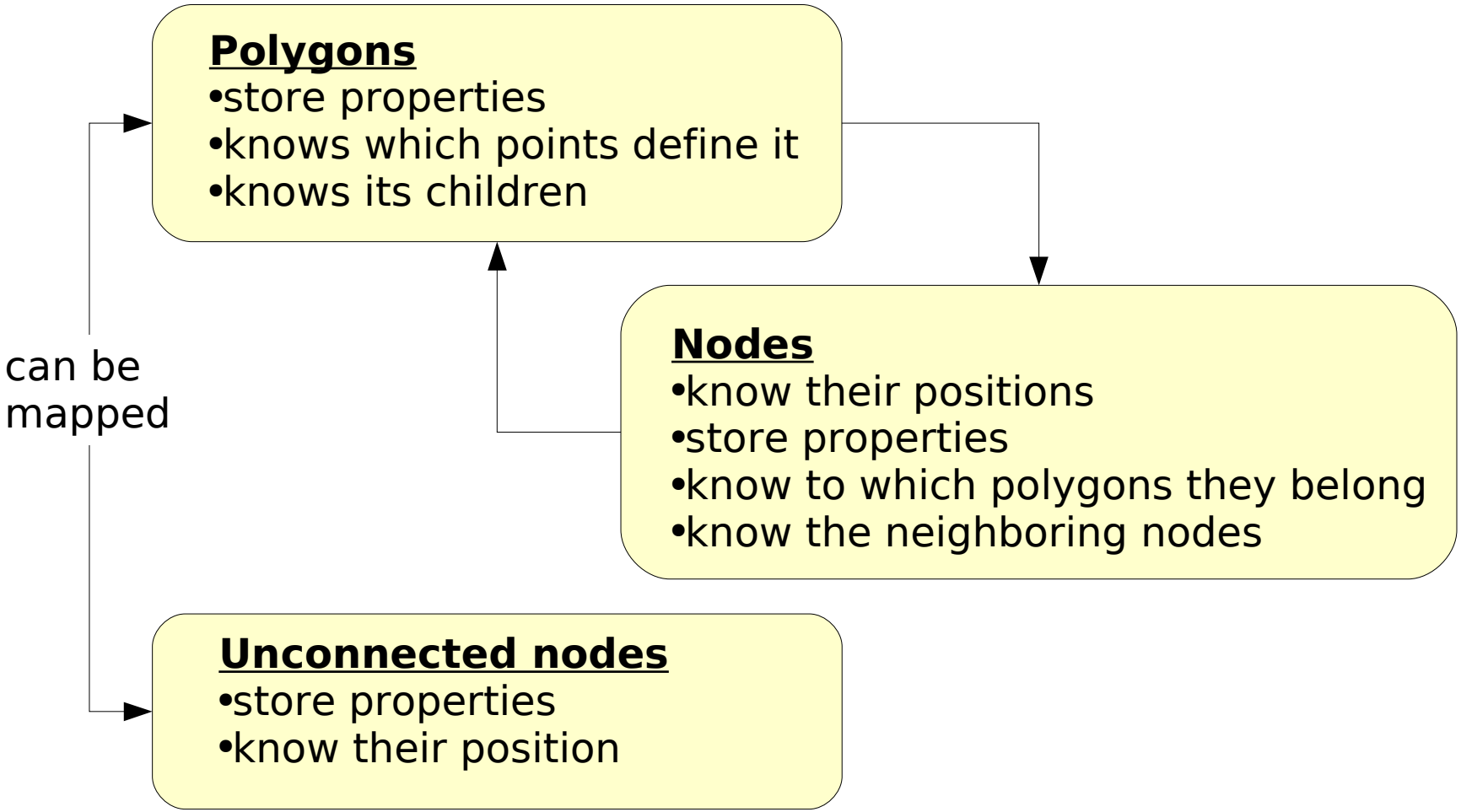
The unodes are not (unless you want to) related to the polygonal structure



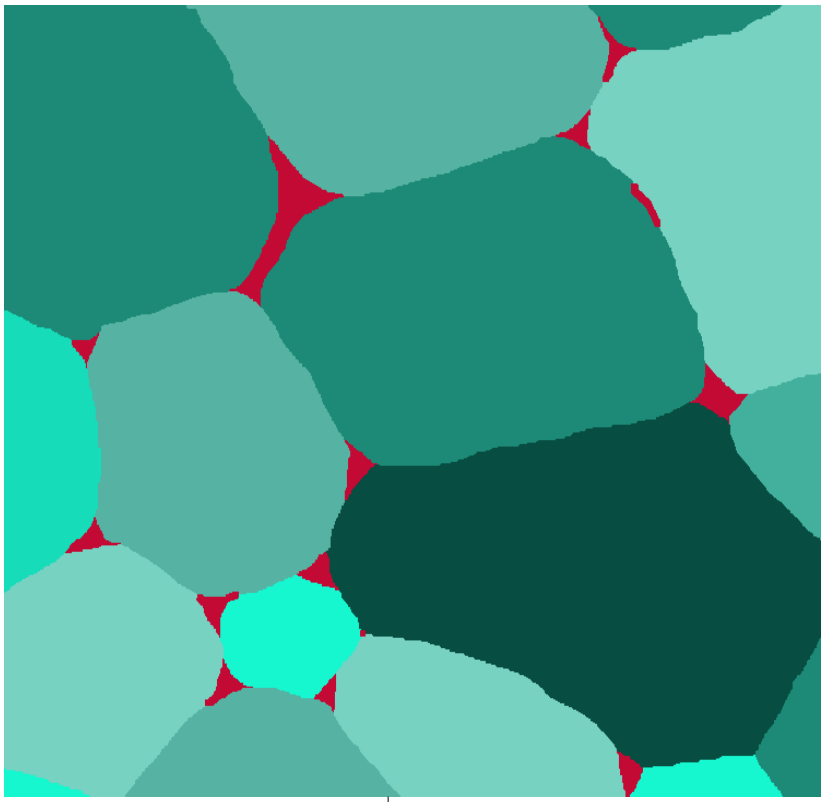
Polygon properties can be mapped to the unodes if necessary (therewith creating a regular or irregular spaced grid)

How to store properties

Each polygon, boundary node and unode can store material properties (such as chemical concentrations, stress/strain, mineral type etc.)



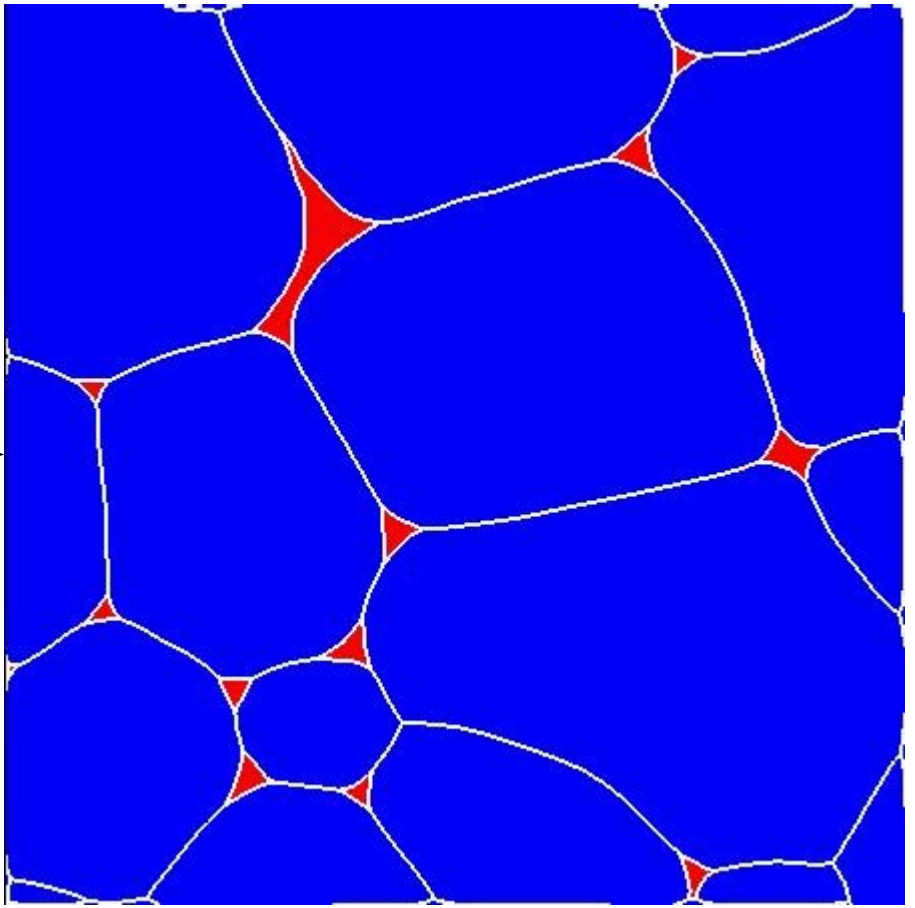
How to make an input file



Simple drawing from any program,
has to be in ppm-format.

ppm2elle

Elle-file

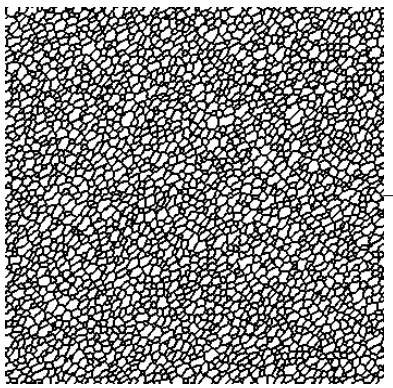


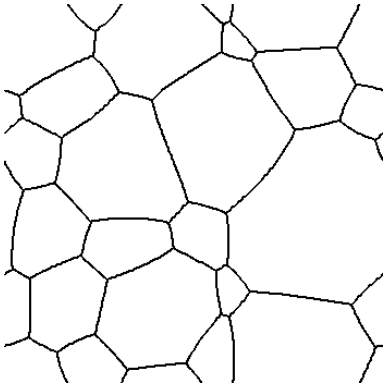
The input file

```
# Created by elle_melt: elle version 2.3.9  Thu Feb 27 10:40:46 2003

OPTIONS
SwitchDistance 5.00000000e-03
MaxNodeSeparation 1.10000000e-02
MinNodeSeparation 5.00000000e-03
[...]
FLYNNS
0 10 1687 1846 1847 1843 46 668 249 248 247 2938
2 187 3166 1300 344 343 342 341 340 339 337 335 334 332 331 330 329 327 325 324 323
[...]
37 28 2749 216 219 602 3282 220 221 222 223 224 226 229 231 232 234 236 237 667 2918 244
437 2798 592 2780 435 2758 434 2735
MINERAL
Default QUARTZ
7 MINERAL_A
[...]
32 MINERAL_A
35 MINERAL_A
F_ATTRIB_A
Default 0.00000000e+00
7 1.00000000e+00
8 1.00000000e+00
9 1.00000000e+00
[...]32 1.00000000e+00
35 1.00000000e+00
LOCATION
0 0.9981955322 0.9915783320
1 0.9989879113 0.9851930942
[...]
3283 0.9972380907 0.9970020920
```

Sequential application of different processes





10000 stages

grain growth

100 stages

output file

output file

2 stages

deformation

diffusion

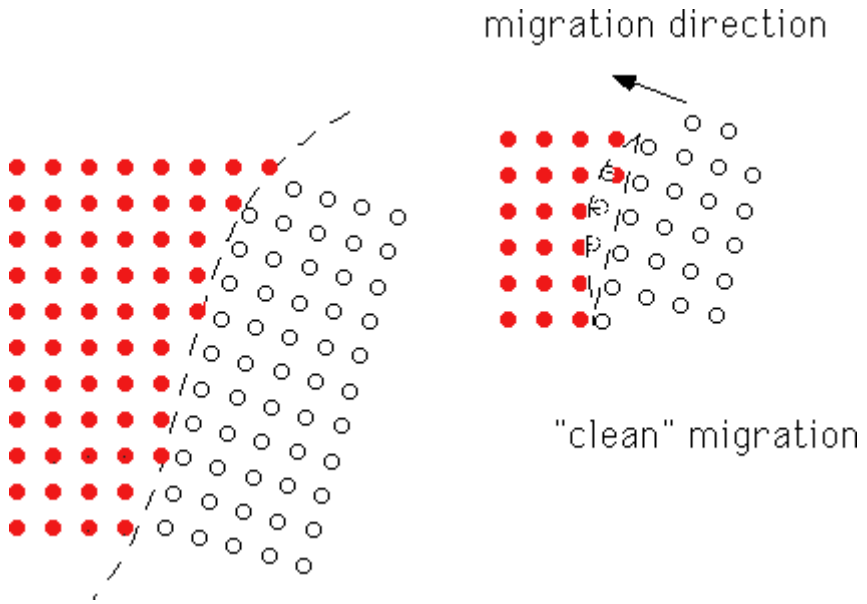
300 stages

output file

A simple example:
Grain Boundary Migration

Grain boundary migration can have several causes:

- diffusion of single atoms
- rotating and shuffling atoms from one lattice to the other
- possibly by the movement of whole clusters of atoms

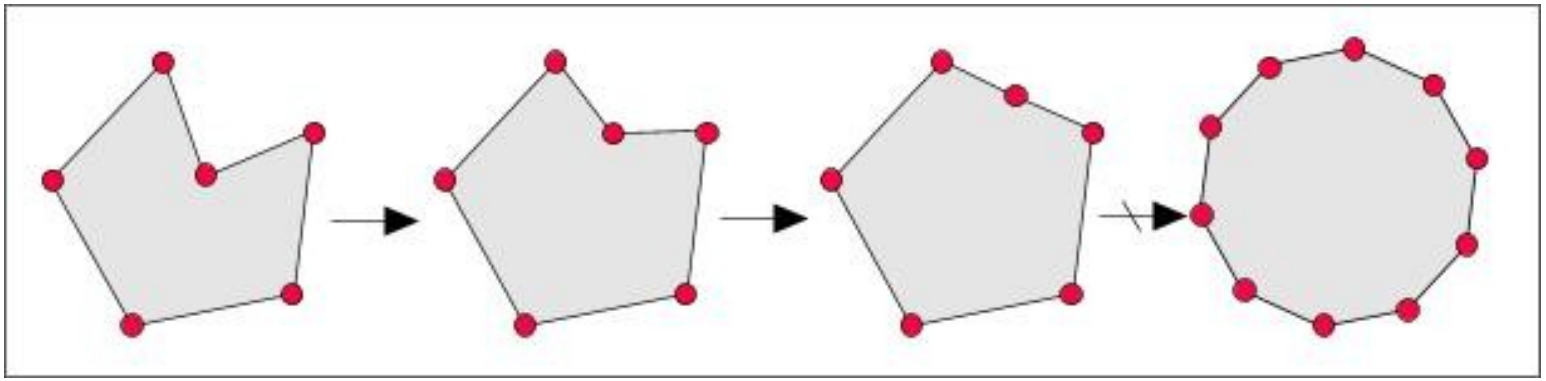


For the geologist, these processes are indistinguishable. We have to deal with the outcome and more general energies.

Driving forces for grain boundary migration

Elle uses only one driving force for grain boundary migration: surface energies. The total surface energy of a boundary is related to the boundary length. Therefore, the surface energy tries to minimize the circumference of a grain.

This may be modified by an energy-lookup-table.



What really happens

Basic equation:

- Work done = force x distance
- $W = \Delta E = \underline{F} \cdot \Delta \underline{p}$
- $\underline{F} = \Delta E / \Delta \underline{p}$, or better: $F = dE/d\underline{p}$

We can calculate the velocity of a node from:

- the mobilities of the segments
- the orientations and lengths of the segments
- the driving force F

The driving force F can be calculated for any kind of process where we can calculate the energy state as a function of position of a node

- chemical/metamorphic reactions
- GBM driven by dislocation density differences
- GBM driven by surface energy

Energy calculations

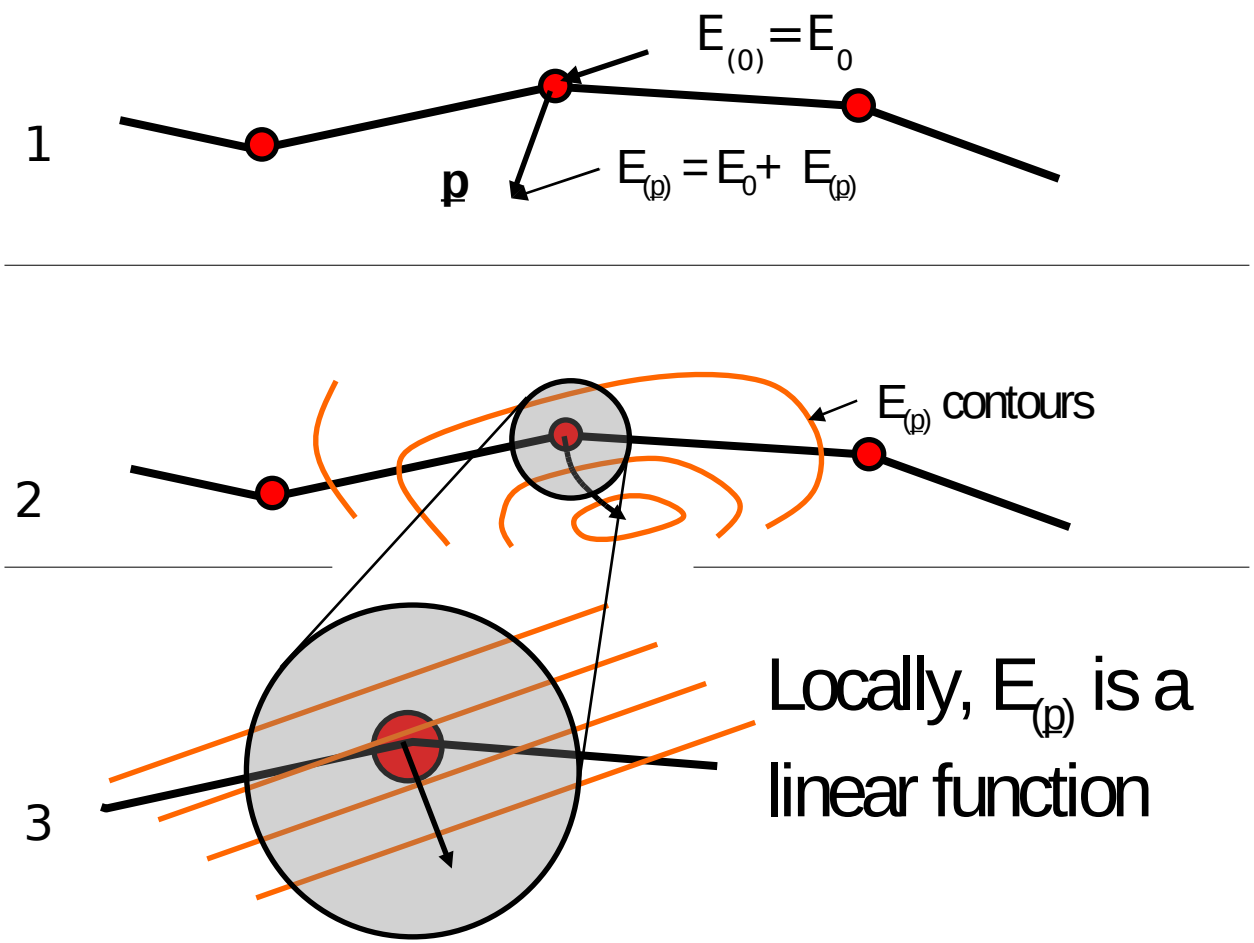


Fig. 1: A – A node should always move towards a point where the energy $E_{(p)}$ is lower than $E_{(0)}$. This can be achieved by calculating the local energy field (B). On a large scale, this field and its respective isolines can have any shape, however, locally, the isolines can be treated as linear (C). Therefore, the local energy function is a linear function. From 4 trial positions (D), the local energy function can be calculated according to the general equation shown in C and the node is moved along the gradient resembling the lowest energy (D).

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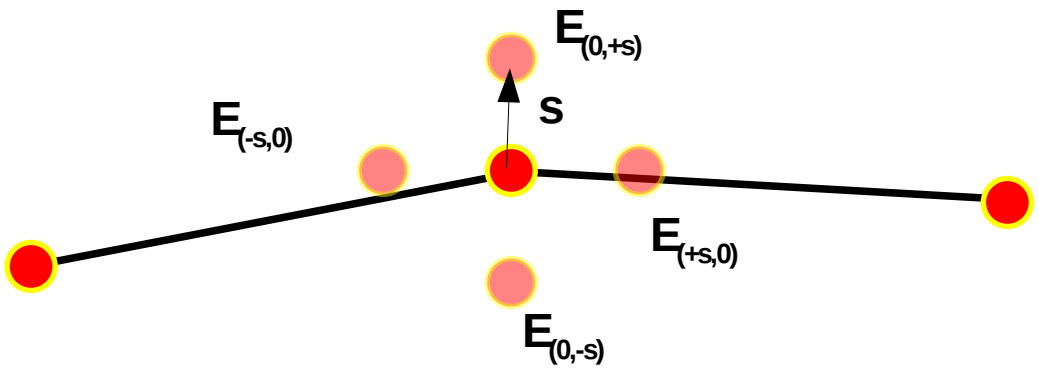
Energy calculations

We can calculate the energy of a node at different positions. We can do that with different equations. As long as their units are the same, we can just add them up and therewith combine different driving forces.



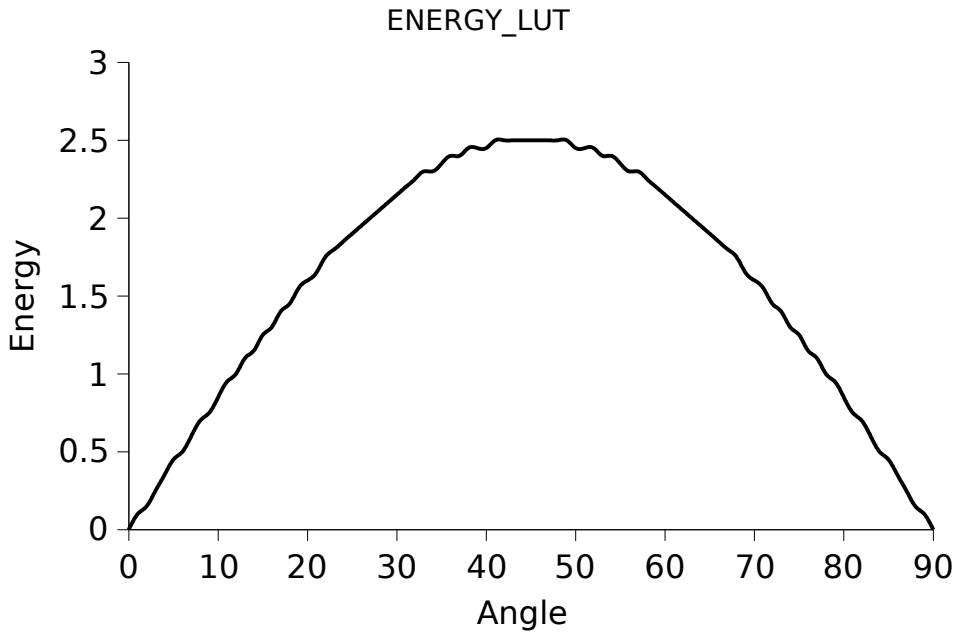
$$E_{(x/y)} = E_{gg} + E_{ss}$$

Boundaries also have a mobility. This is a material property that usually is poorly known. Once we have the direction of the movement, we need to know how far the node is going to move.

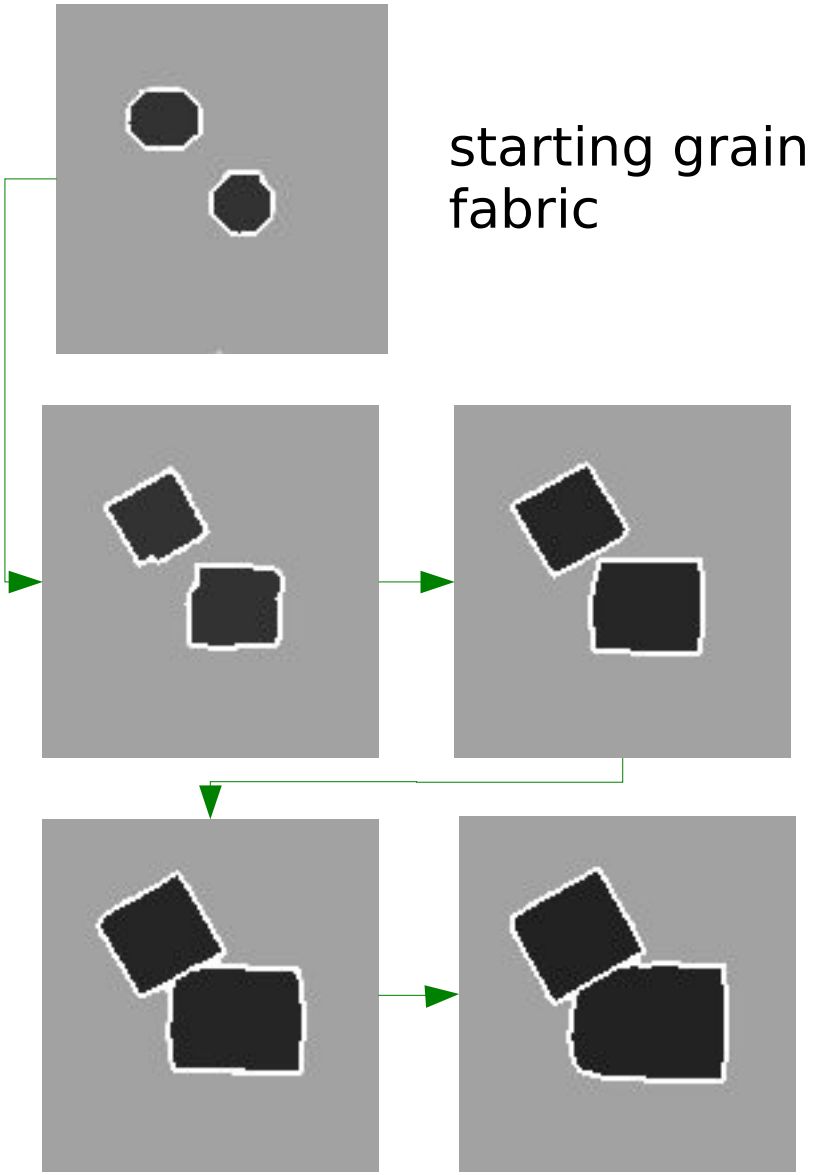
Anisotropy in elle

Anisotropic grain growth from a melt

Grains with anisotropic surface energies are not circular. Their shape depends on the surface energies.



Evolution of the grain fabric



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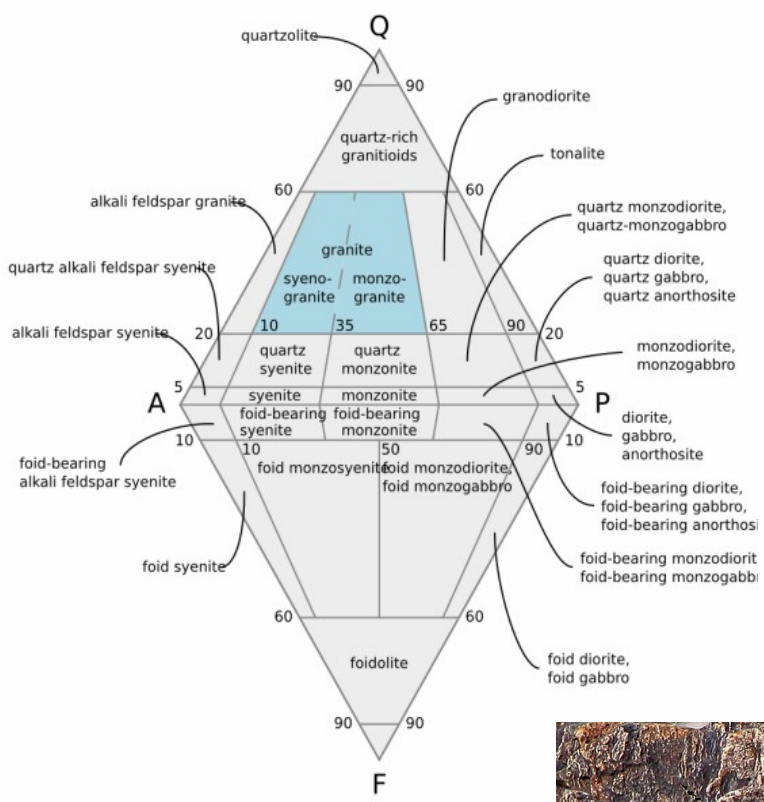
And now for something completely different:

What I am doing and why I want to use OOF2

What is a granite



There are lots of different types of granites. In the end, they are all characterized by only 4 different minerals:
Q – Quartz
A – Alkali-Feldspar
P – Plagioclase (another feldspar)
F – Foids (very rare)

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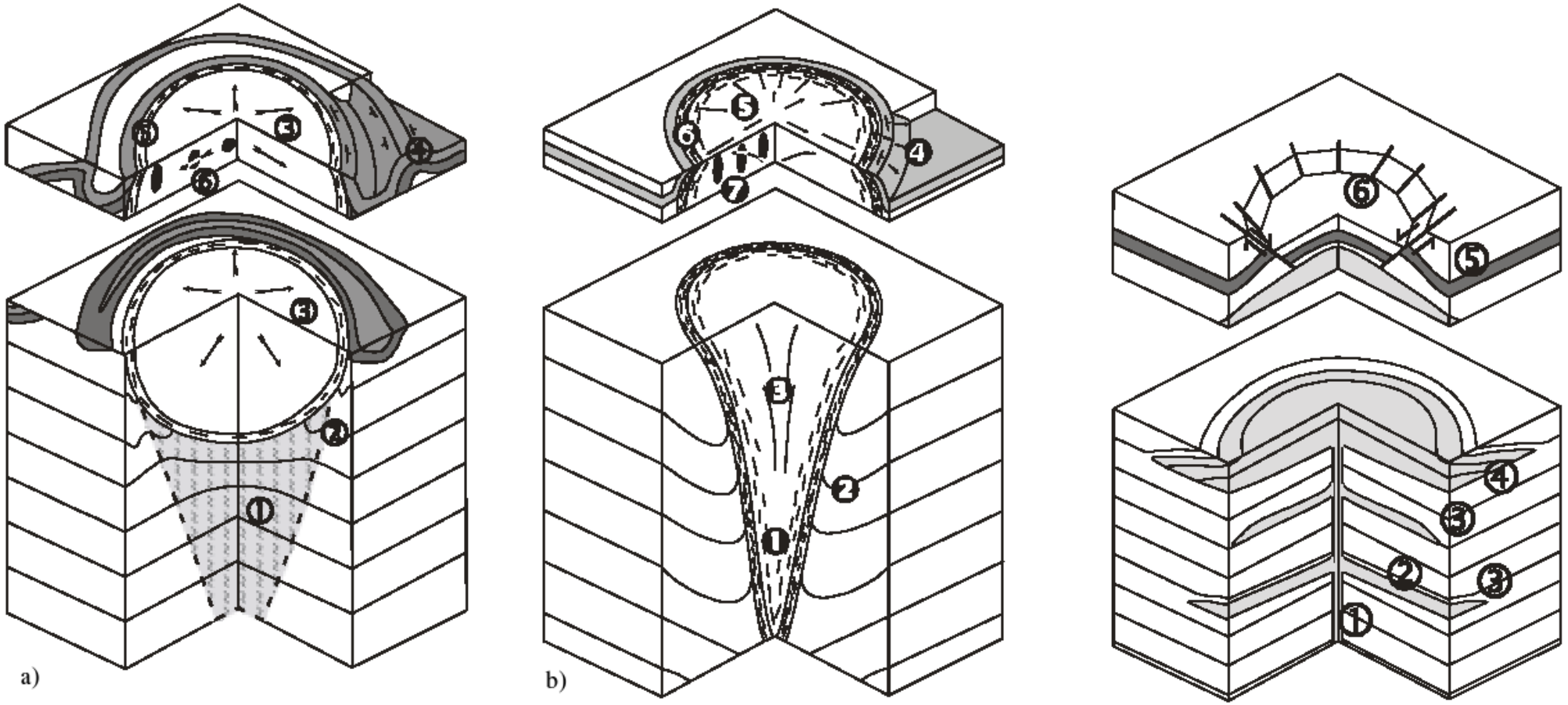
Emplacement of granitic bodies

From Wikipedia:

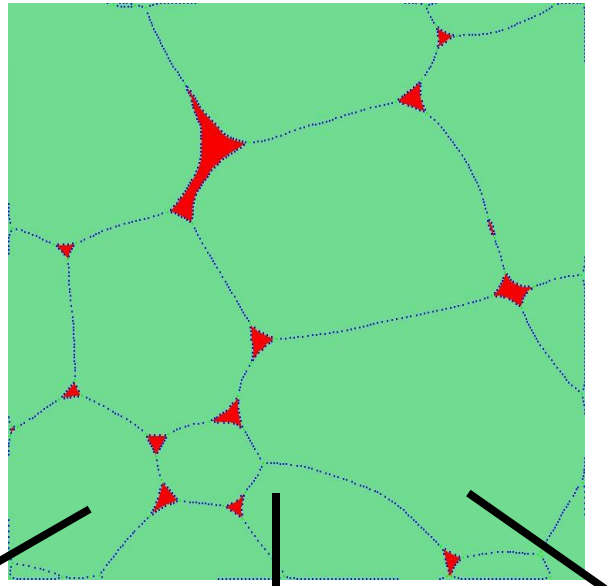
The problem of emplacing large volumes of molten rock within the solid Earth has faced geologists for over a century, and is not entirely resolved. Granite magma must make room for itself or be intruded into other rocks in order to form an intrusion, and several mechanisms have been proposed to explain how large batholiths have been emplaced.

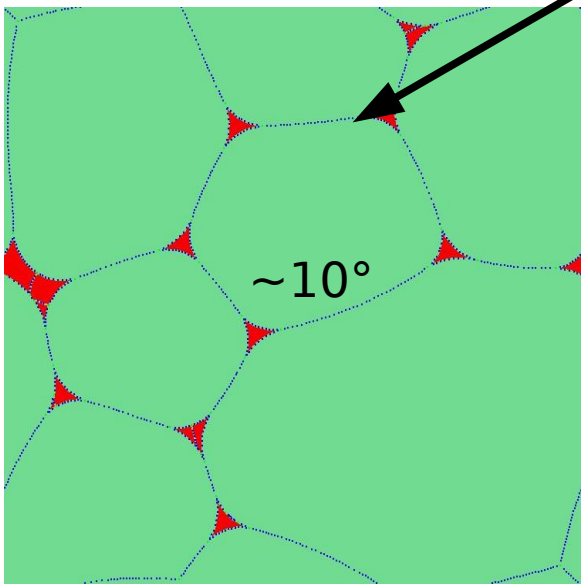


Behavior of melt (or more general a liquid)

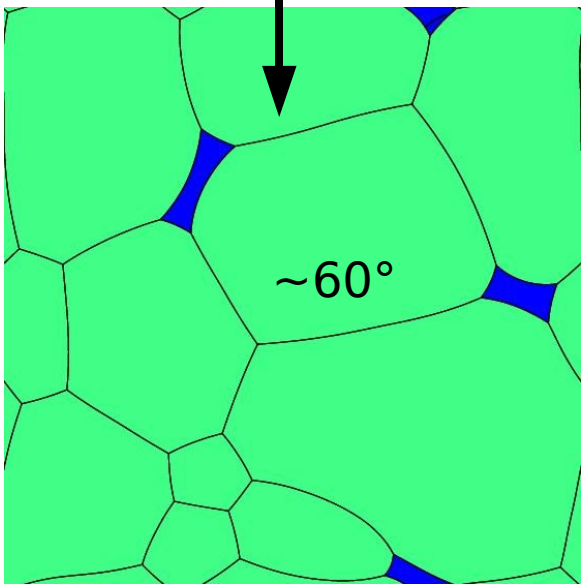
Using the same starting grain fabric with different wetting angles

Please see attached movies

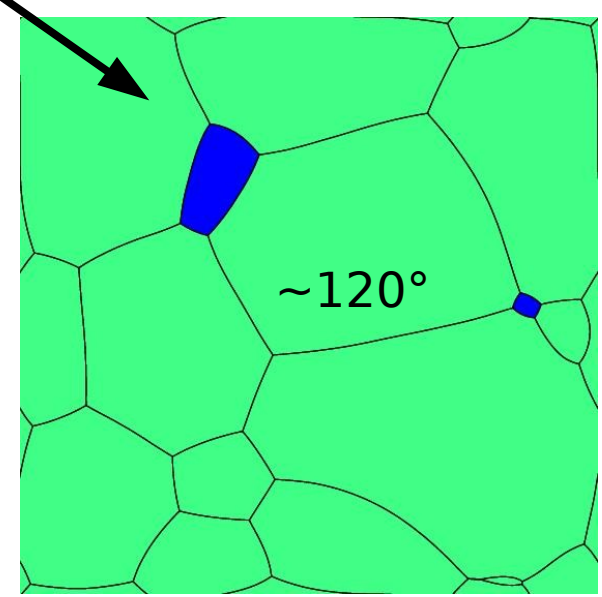




sim10a.mov



sim60.mov



sim120.mov

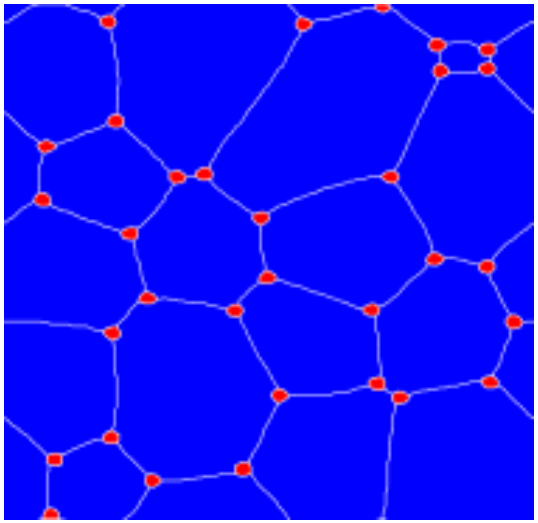
How to verify the results: Analog modeling

Since we cannot compare our results to real nature, we have to find other means of verifying our results. That is usually analoge modeling. The example movie shows an analoge experiment using norcamphor and ethanol (analog experiments were done by N. Walte). At room temperature norcamphor has the same material properties as quartz has at higher temperatures.

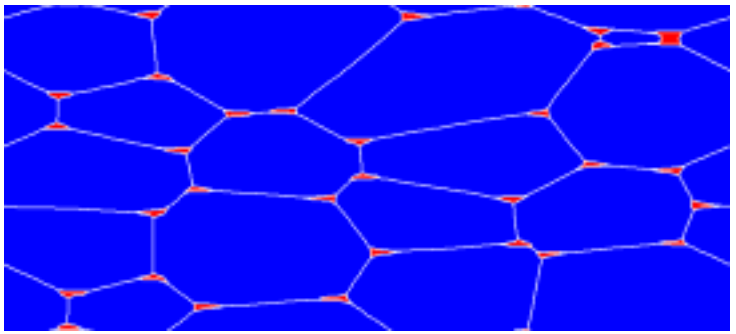
Please see attached movie: sim-ana.mov

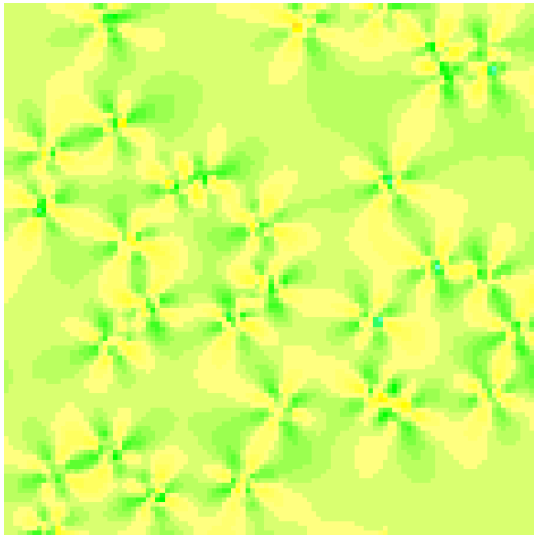
Deforming a partially molten rock in pure shear

At the depth these processes take place, rocks are very hot and under constant (hydrostatic) pressure.

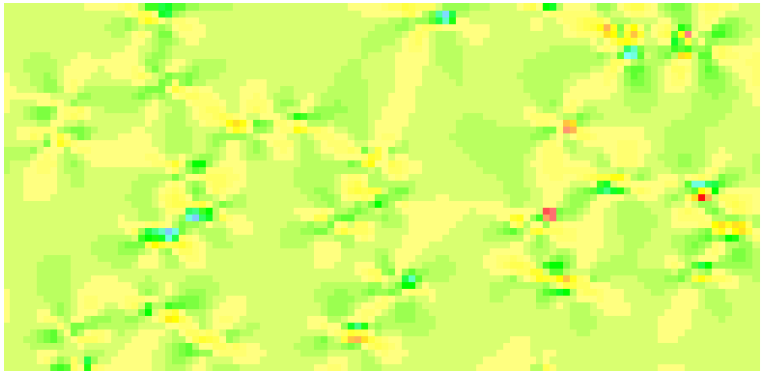


Topology





Strain (xy)



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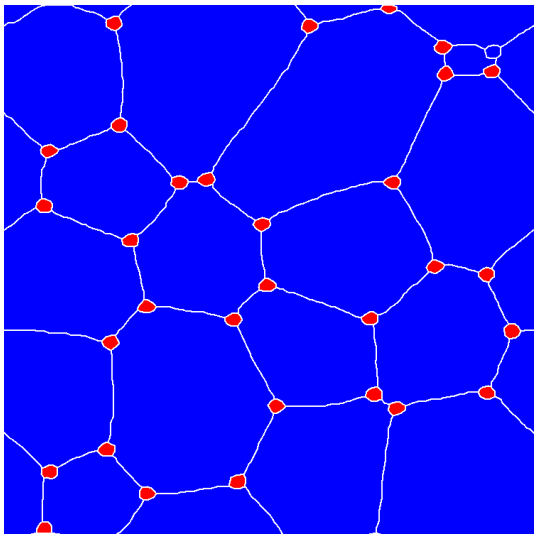
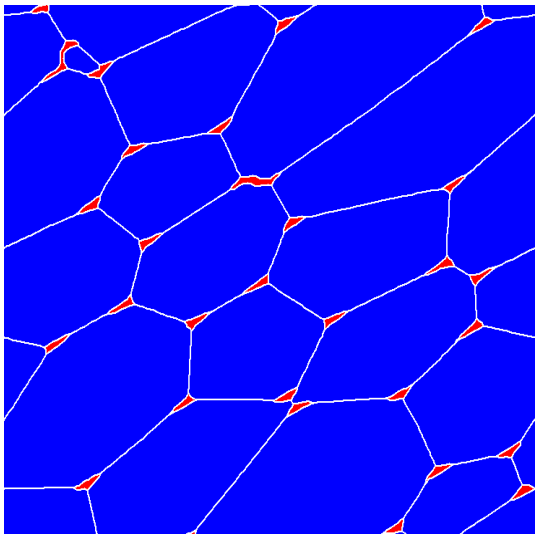
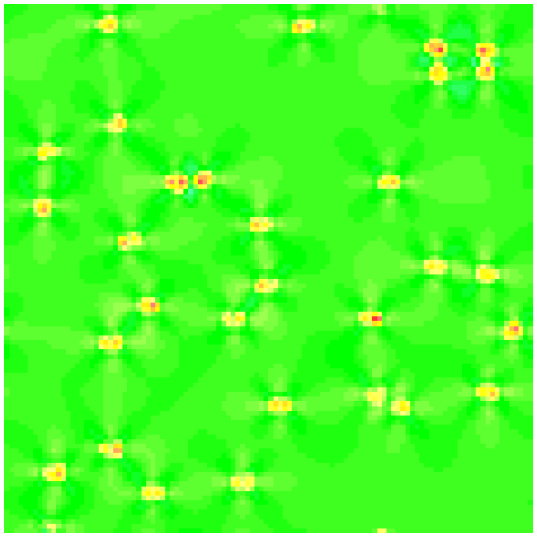
Using simple shear to deform a partially molten rock

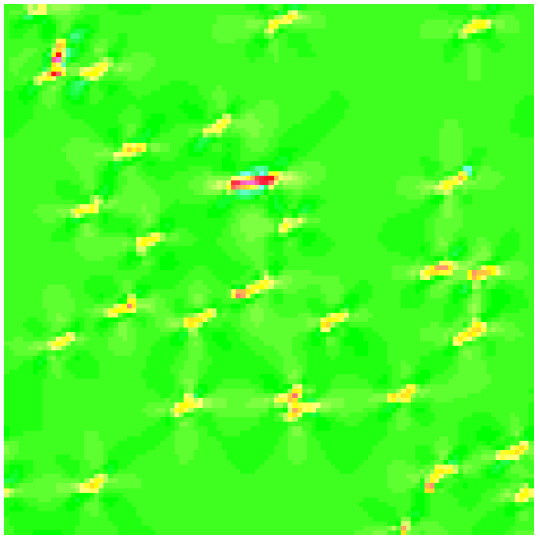


Topology





Strain
(xy)



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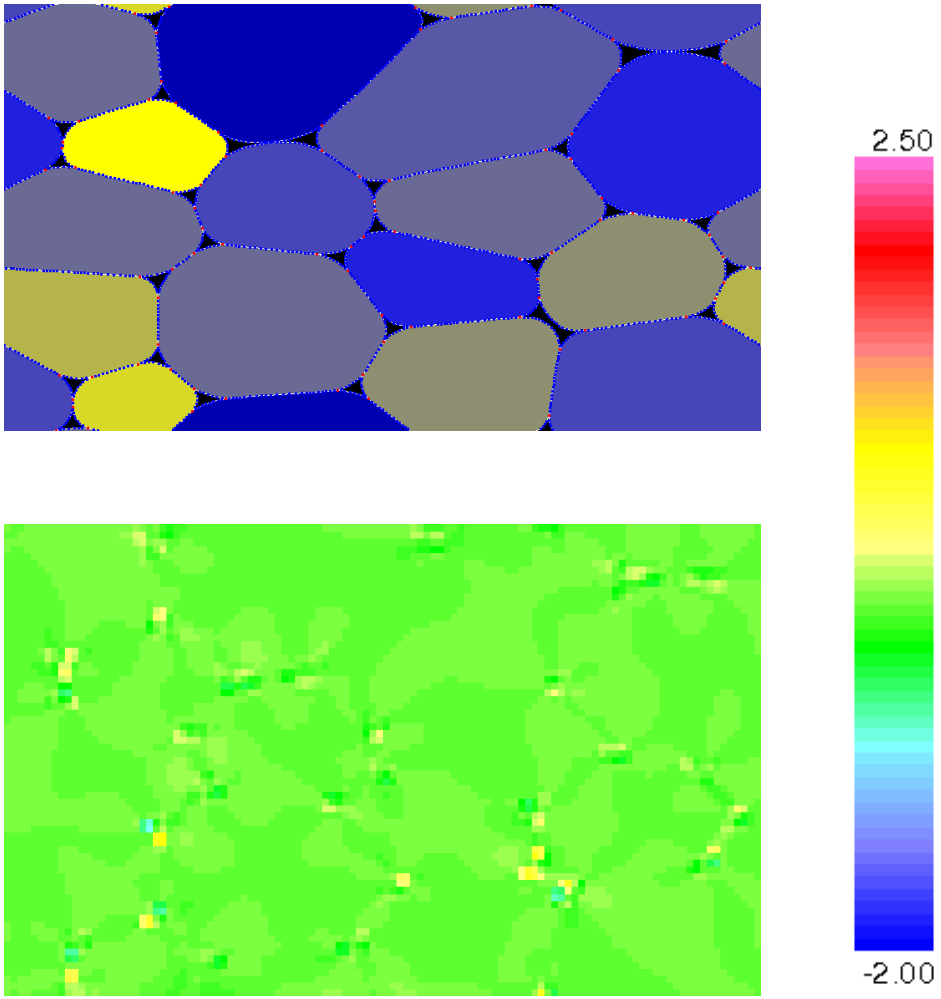
Variations of the above

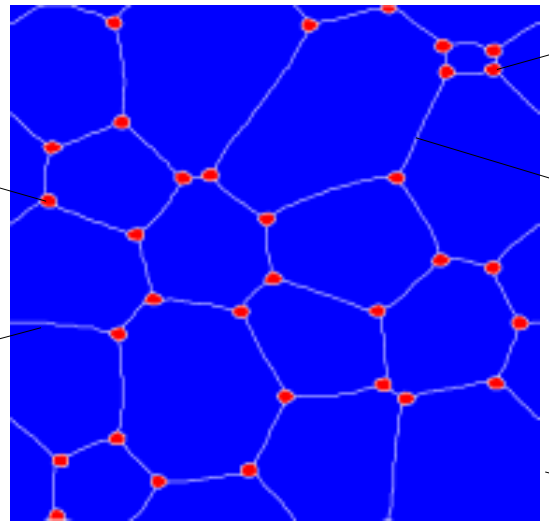
Different viscosities



How to combine elle with oof2

I will have to use the output files of elle and stick them into OOF2 then let OOF2 do its magic and save out that magic and one that sticks that magic back into Elle (we did all that for OOF).

if that works I will have to put visco-plastic (linear and or non-linear) deformation into OOF2.



Melt pocket evolution (Elle)

Grain boundary migration (Elle)

Assign internal boundary conditions to melt pockets (OOF2)

Assign internal boundary conditions to grain boundaries (OOF2)

Deform the microstructure (OOF2)