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

Dr. J.K. Becker
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.
Thin sections of rocks

Tonalite (Kimberley, Australia)

1 mm

biotite
hornblende
plagioclase
quartz
Different environments means different rocks

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

- Molecular dynamics
- Dislocation dynamics
- Grain-scale simulations
- Crustal deformation
- Geodynamics
Examples of single processes:

- **Grain growth (1)***

<table>
<thead>
<tr>
<th>Stages</th>
<th>Average Grain Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.0000</td>
</tr>
<tr>
<td>50000</td>
<td>0.0100</td>
</tr>
<tr>
<td>100000</td>
<td>0.0200</td>
</tr>
<tr>
<td>150000</td>
<td>0.0300</td>
</tr>
<tr>
<td>200000</td>
<td>0.0400</td>
</tr>
</tbody>
</table>

Example of simple grain growth
Examples of single processes: grain growth (2)

Grain boundary network

t=0

Grain boundary network

t=800

Unswept cores

Swept zones

t=0

t=800
Examples of single processes: diffusion

Lattice Diffusion

Boundary Diffusion

elle_diff

elle_gbdiff
Fracturing (using Latte)
<table>
<thead>
<tr>
<th></th>
<th>Description</th>
<th></th>
<th>Description</th>
<th></th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Layered ice grain growth</td>
<td>2</td>
<td>Localisation of deformation</td>
<td>3</td>
<td>Melt Pocket Angle=180</td>
</tr>
<tr>
<td>4</td>
<td>Melt Pocket Angle=0</td>
<td>5</td>
<td>Melt Pocket Angle=120</td>
<td>6</td>
<td>Ostwald Ripening</td>
</tr>
<tr>
<td>7</td>
<td>Grain boundary migration microstructures</td>
<td>8</td>
<td>Crystallisation from a melt</td>
<td>9</td>
<td>Triple junction trails</td>
</tr>
<tr>
<td>10</td>
<td>Porphyroblast Rotation?</td>
<td>11</td>
<td>Grain boundary sweeping</td>
<td>12</td>
<td>Cyclic grain growth bands</td>
</tr>
<tr>
<td>13</td>
<td>Defect energy driven grain growth bands</td>
<td>14</td>
<td>Exchange Reaction</td>
<td>15</td>
<td>Sug-grain growth</td>
</tr>
<tr>
<td>16</td>
<td>Grain boundary diffusion</td>
<td>17</td>
<td>Dislocation density driven grain boundary migration</td>
<td>18</td>
<td>Grain Growth</td>
</tr>
<tr>
<td>19</td>
<td>Exaggerated Grain Growth</td>
<td>20</td>
<td>Crystallisation from a melt</td>
<td>21</td>
<td>Surface Energy Reduction of a Snowflake</td>
</tr>
</tbody>
</table>
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).
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.)

**Polygons**
- store properties
- knows which points define it
- knows its children

**Nodes**
- know their positions
- store properties
- know to which polygons they belong
- know the neighboring nodes

**Unconnected nodes**
- store properties
- know their position

can be mapped
How to make an input file

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

ppm2elle

Elle-file
The input file

```plaintext
# 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 344 343 342 341 339 337 335 334 332 331 330 329 327 325 324 323

MINERAL
Default QUARTZ
7 MINERAL_A

F_ATTRIB_A
Default 0.00000000e+00
7 1.00000000e+00
8 1.00000000e+00
9 1.00000000e+00

LOCATION
0 0.9981955322 0.9915783320
1 0.9989879113 0.9851930942

3283 0.9972380907 0.9970020920
```
Sequential application of different processes

- Grain growth
- Diffusion
- Deformation

- 10000 stages
- 300 stages
- 2 stages
- 100 stages
- 300 stages
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
- $W = \Delta E = F \cdot \Delta \varphi$
- $F = \Delta E/\Delta \varphi$, or better: $F = dE/d\varphi$

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).
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.
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)
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

$\sim 10^\circ$

$\sim 60^\circ$

$\sim 120^\circ$

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)
Using simple shear to deform a partially molten rock

Topology

Strain (xy)
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)