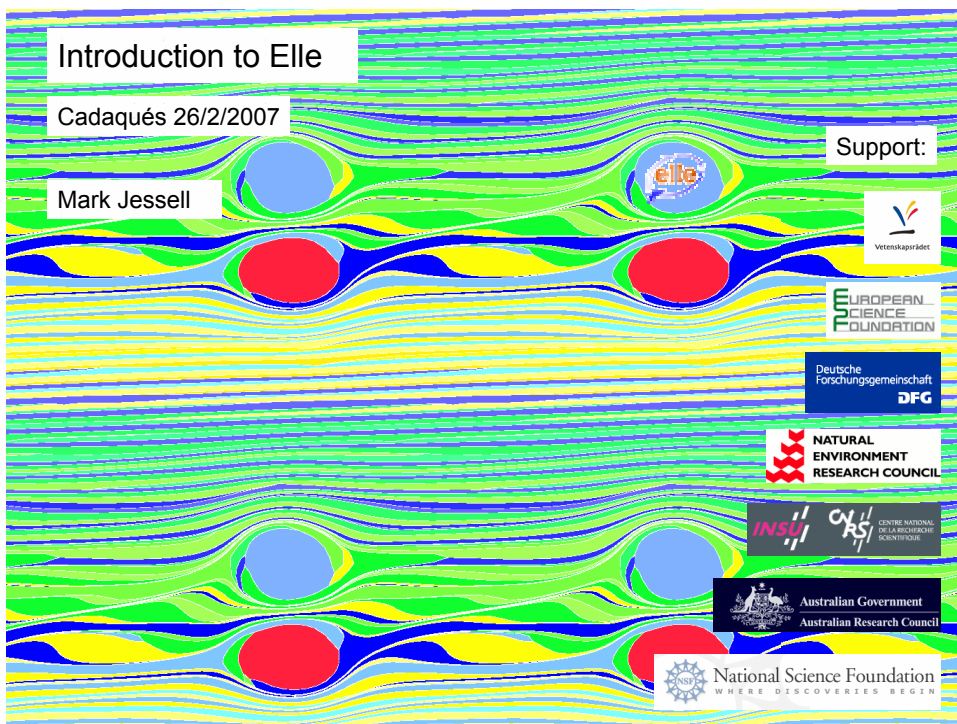


Introduction to Elle

Cadaqués 26/2/2007

Mark Jessell

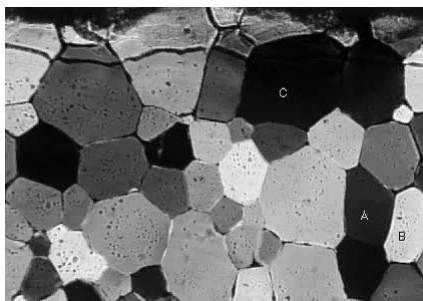
Support:



Support logos include: Vetenskapsrådet, EUROPEAN SCIENCE FOUNDATION, Deutsche Forschungsgemeinschaft DFG, NATURAL ENVIRONMENT RESEARCH COUNCIL, INSU / CNRS / CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE, Australian Government Australian Research Council, and National Science Foundation WHERE DISCOVERIES BEGIN.

### Background to Project

*In Situ* Observation of Process Coupling (Park et al 2000)



Crystalline Organic Chemical ( $C_3Cl_8$ ) deformed between thin sheets under an optical microscope (Park, Ree & Means 2000)

## Background to Project

### Developers Workshops:

Graz 1999

DRT 2001

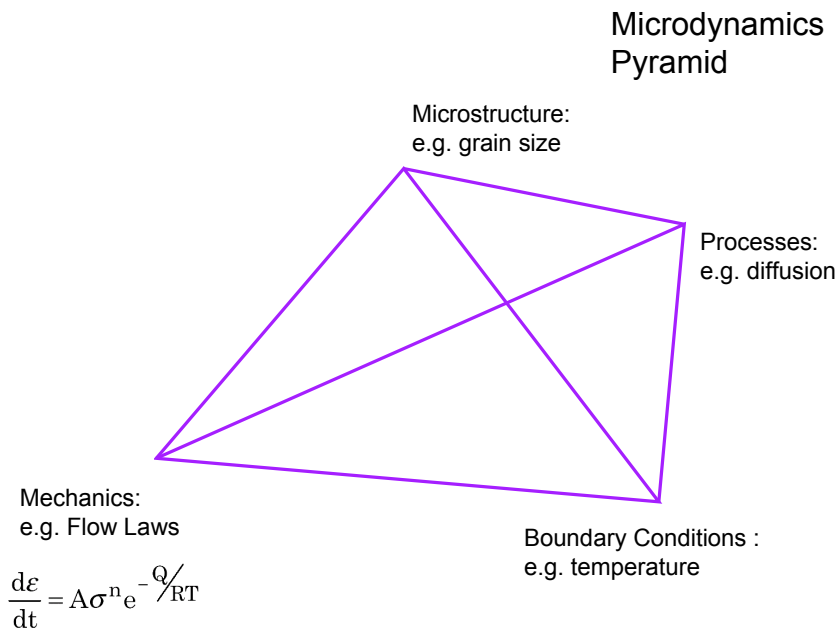
Estonia 2002

Estremoz 2004

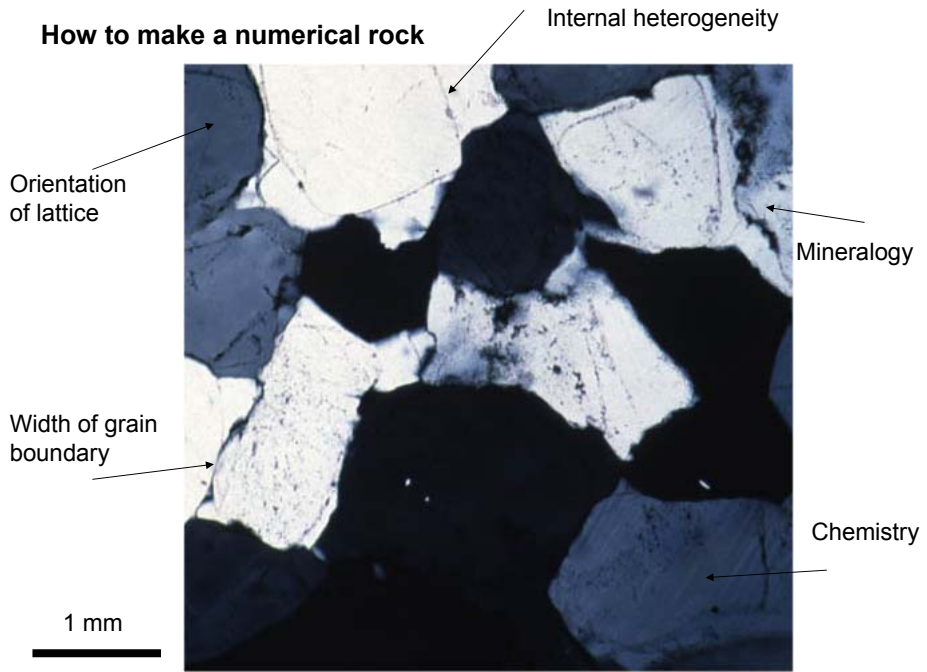
Toulouse 2005

### Short Courses:

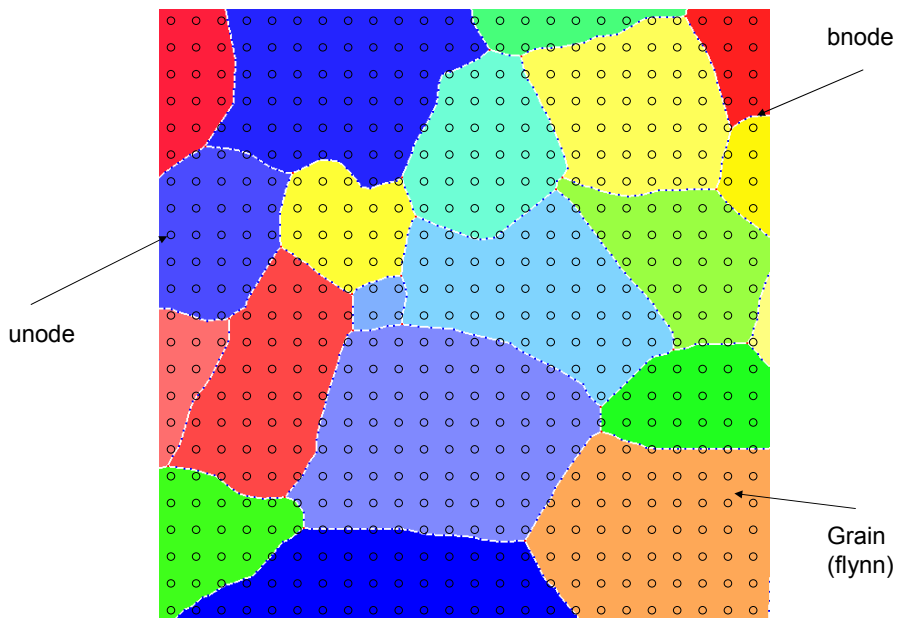
Tubingen, Melbourne, Mainz, Aachen, Leeds, Italy,  
Maine, Cadaqués, Minnesota



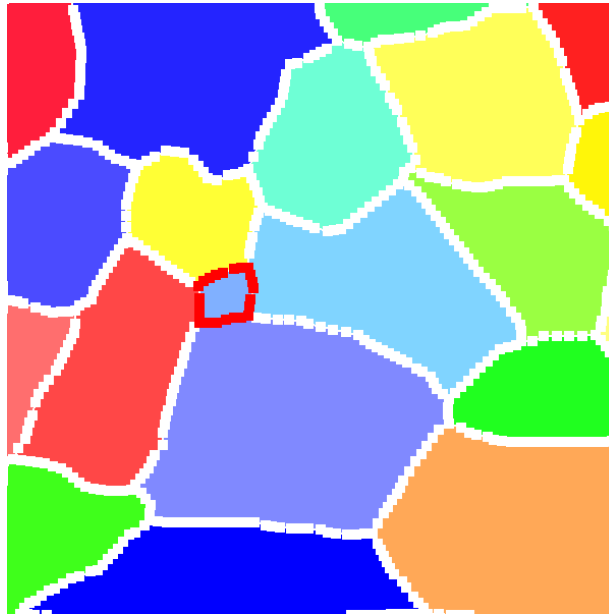
### How to make a numerical rock



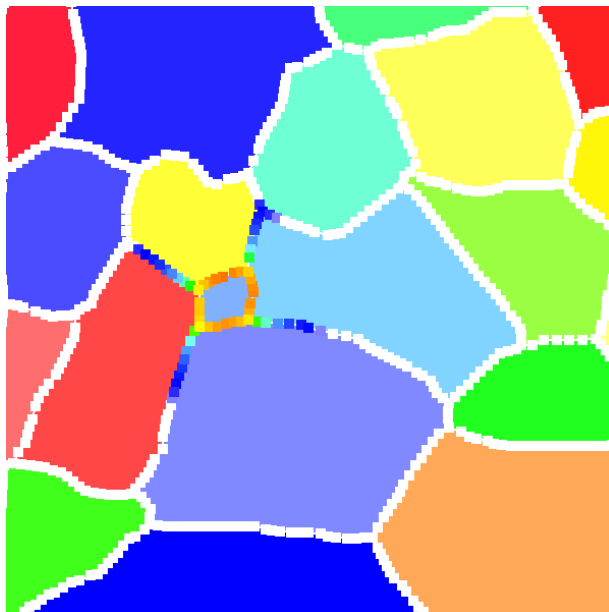
### How to make a numerical rock



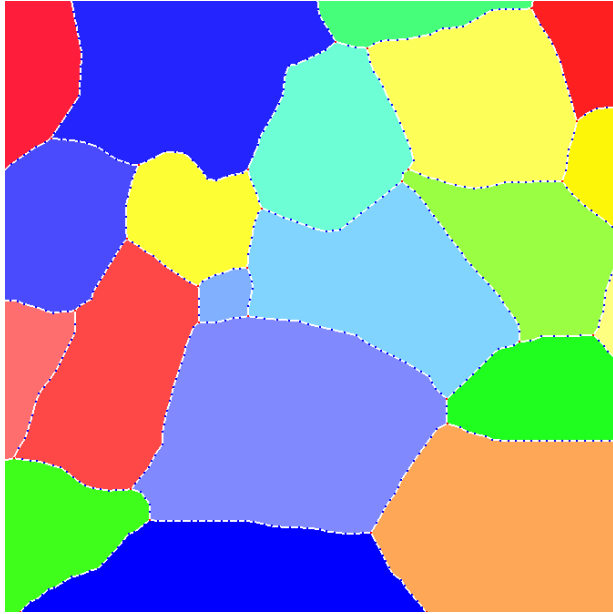
How to make a numerical rock diffuse



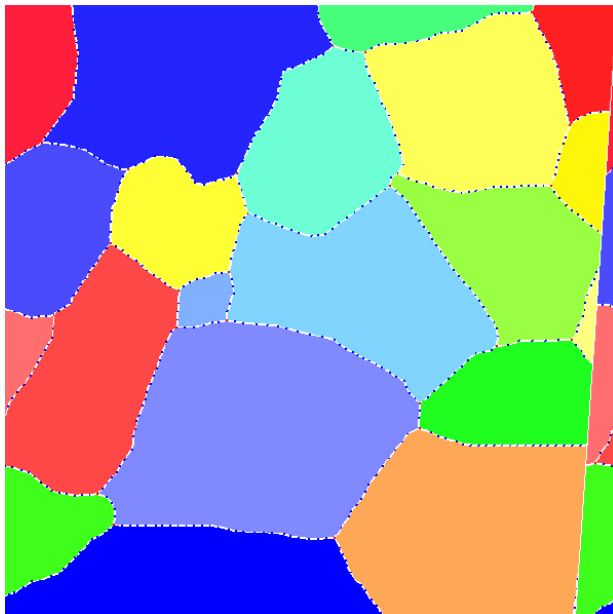
How to make a numerical rock diffuse



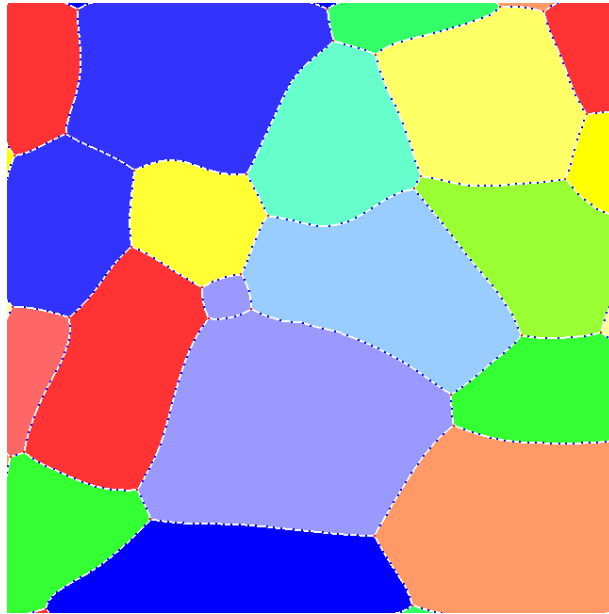
**How to make a numerical rock deform**



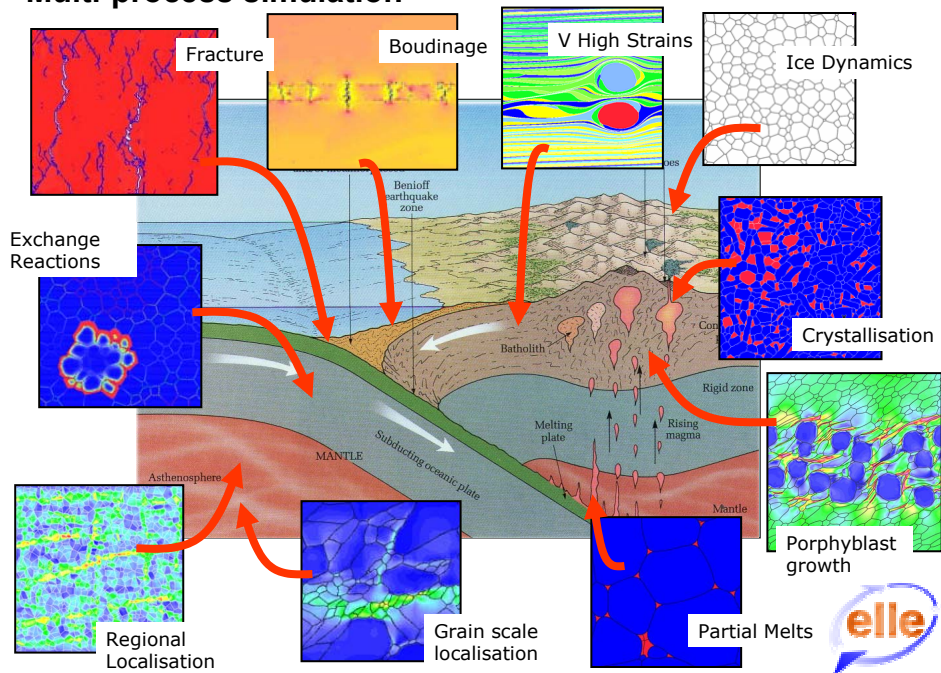
**How to make a numerical rock deform**



## How to make a numerical rock recrystallise

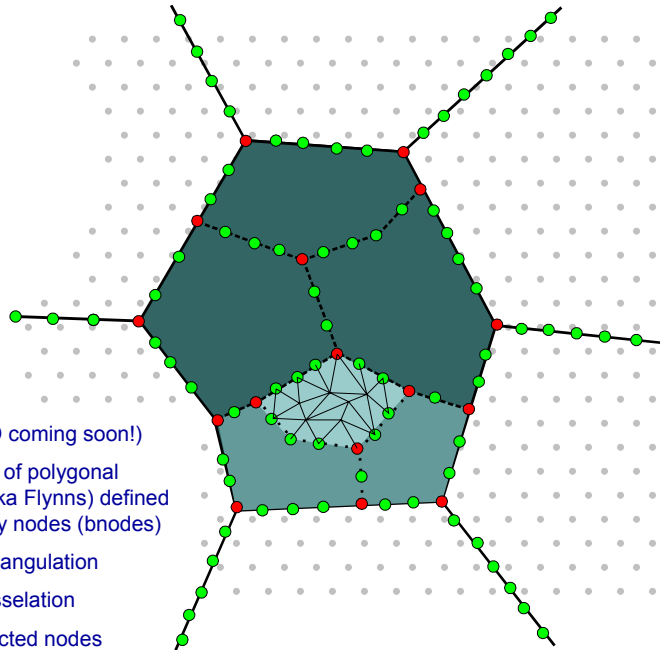


## Multi-process simulation



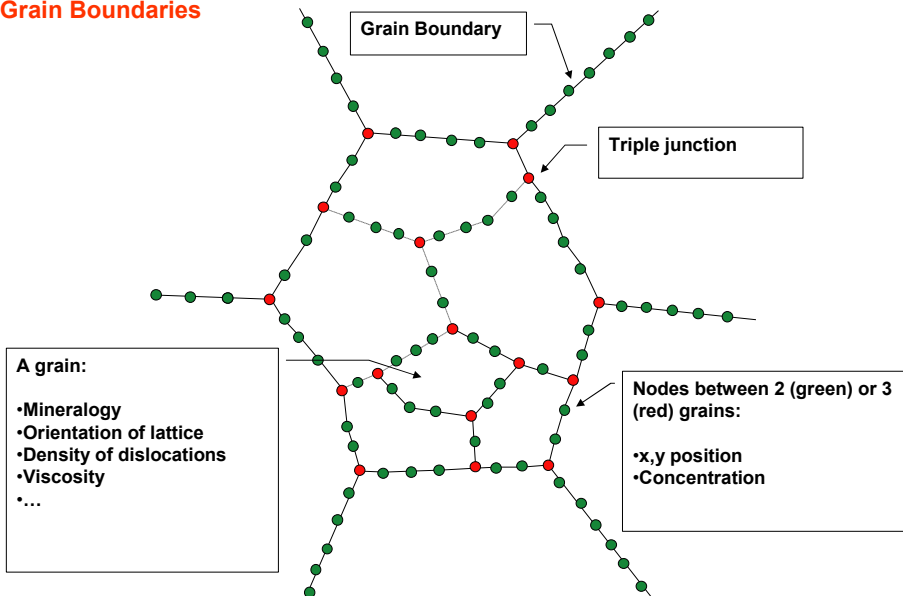
## Data Model

- Two-dimensional (3D coming soon!)
- Hierarchical ordering of polygonal domains (aka Flynns) defined by boundary nodes (bnodes)
- Optional Delaunay triangulation
- Optional Voronoi Tessellation
- Underlay of unconnected nodes (unodes)

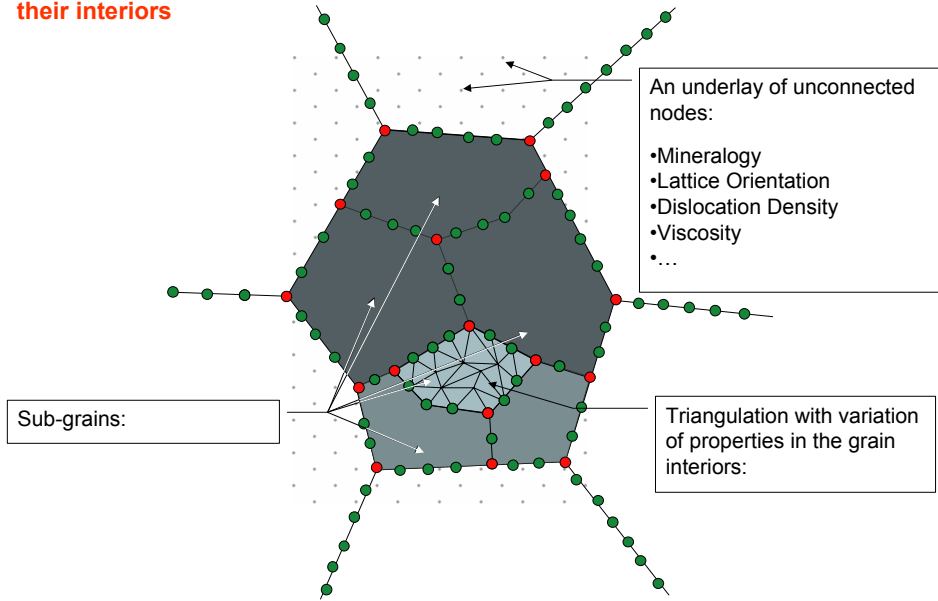


Jessell et al 2001

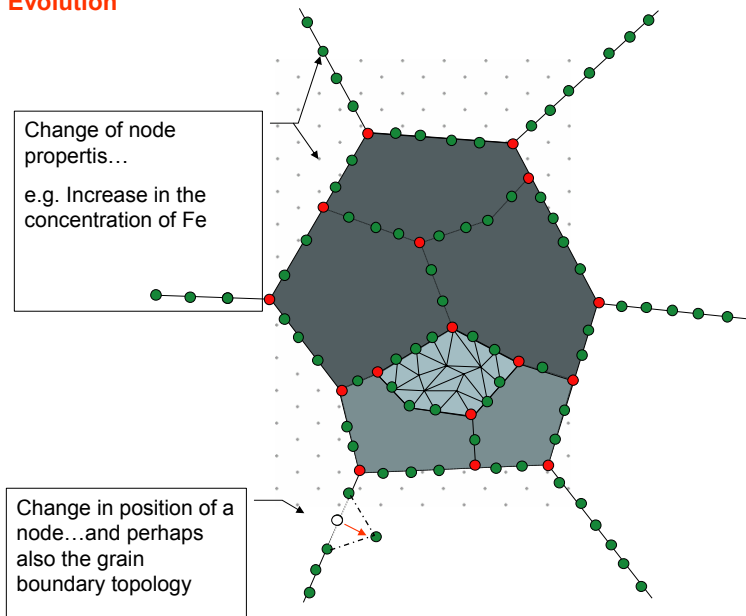
## Data Model- Nodes and Grain Boundaries



## Data Model- Sub-grains and their interiors



## Data Model- Microstructure Evolution

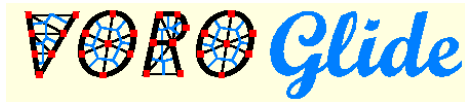


# Delaunay/Voronoi Networks

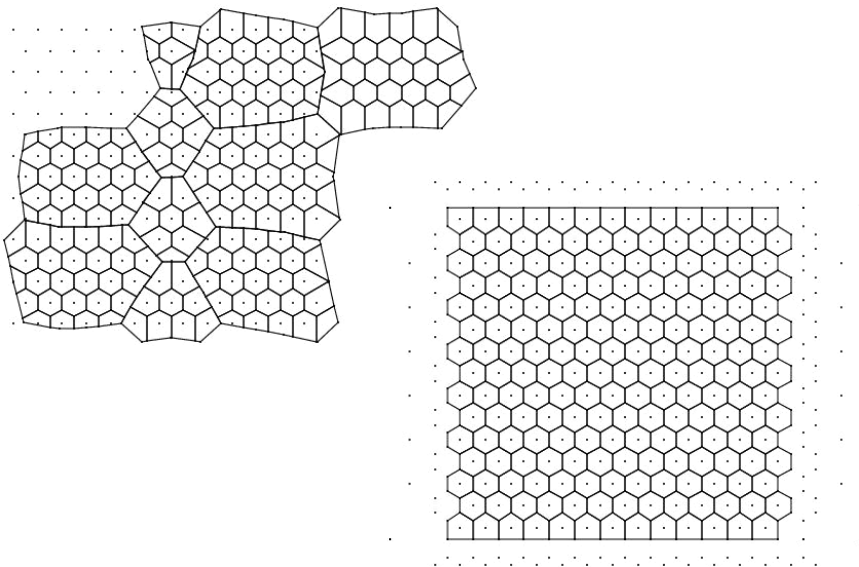
Delaunay triangles of whole grains or

Delaunay triangles and Voronoi cells based on unode positions

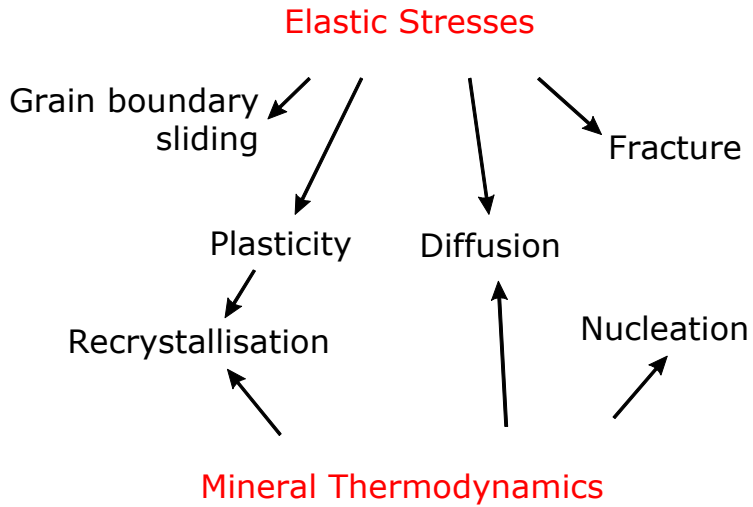
Voronoi cells clipped by grain boundaries (or not)



## Voronoi Cells



**Data Model- The forces:**



**Running Single Processes**

- Can be followed in real time
- Can save out files every  $n$  timesteps
- Can save out images as postscript
- Can be run in the background

## Command line primer

To run an individual process, one command line call is needed with options specifying information such as the number of steps to be simulated, the input and output file and the simulation mode.

Synopsis: process\_name [-cefhinsuv]

Options:

**c** the colourmap to use for the X window. Use the argument "greyscale" for a greyscale diagram which will give a better result on black-&-white printers.

**e** the next argument will be the filename of an extra data file (see tbh example)

**f** the next argument will set the frequency for saving the Elle data during a run i.e. 10 will mean that the data is saved after every 10th stage

**h** help, list the valid options

**i** the next argument will be the filename of an Elle data file

**n** no display (run without the graphical display)

**s** the number of stages to run (default 20)

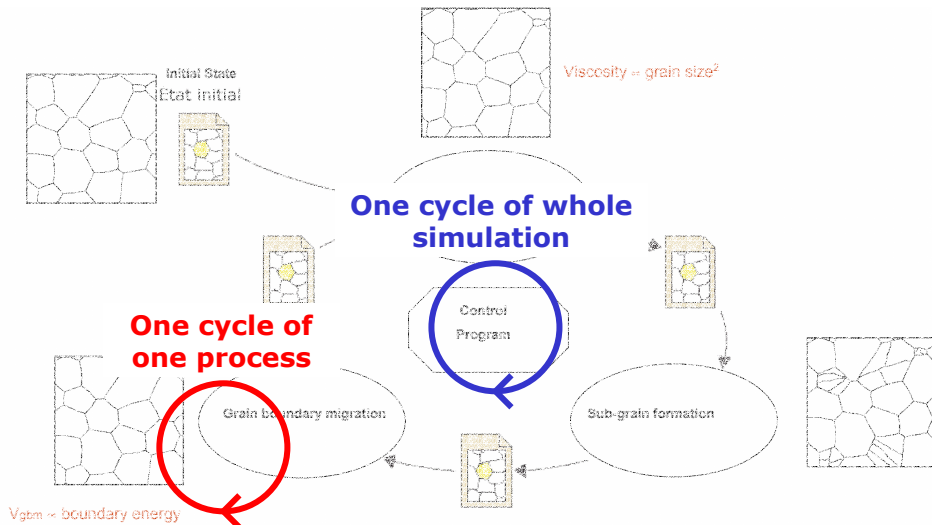
**u** may be followed by up to 5 numbers which allow the user to vary parameters defined for a particular process e.g. elle\_gbdiff interprets the first value as the diffusion rate.

**v** the boundary velocity (only used by elle\_manuel)

These are the only options which can currently be changed at runtime when executing in batch mode. An example of calling an *Elle* process:

```
elle_pblast -i start.elle -s 25 -f 25 -n
```

## Process Coupling: Time Scales

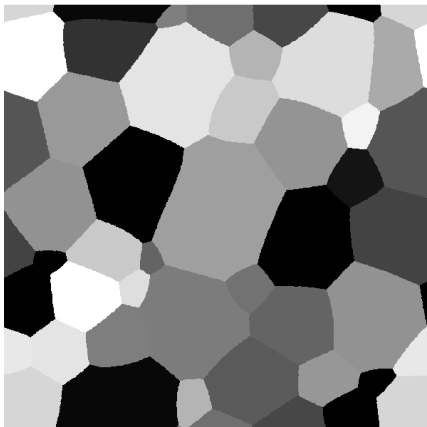


## shelle script

```
#!/bin/sh
#shell script generated by shelle v1.22
DEBUG= #for running
#DEBUG=echo #for debugging
LOCAL=/usr/local
BIN=$LOCAL/elle/bin #location of the Elle applications
STARTFILE=gsv.elle
TIME=0
LASTTIME=5
TIMESTEP=1
GGSTAGES=001
GSTAGES=000
PBSTAGES=000
.
.
.
.
SAVEALL=16
BASINFILE=intilt
ROOTNAME=gsv_loc
GV_SAVE=1
PLOTAX=0
LIST="1 2 3 13 98 16"
.
.
.
```

## Length Scales

- One side of the box is typically set to 1cm, but this is arbitrary
- Node spacing greatly affects accuracy but also speed of calculation



## Programming

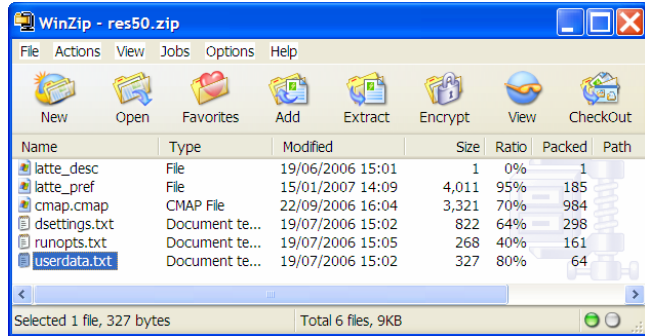
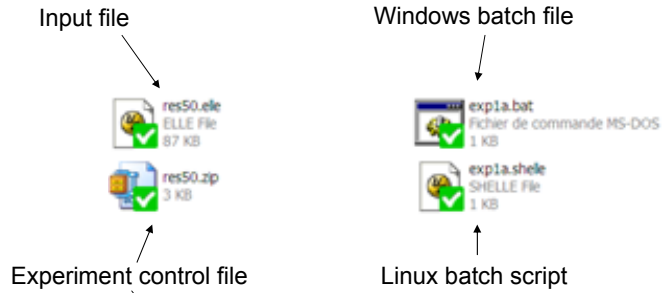
- Open Source code: <https://sourceforge.net/projects/elle/>
- Mostly C/C++
  - Base Libraries: move a node...
  - Process Code: Grain Boundary Migration...
  - Display Codes: Plot concentrations...
  - Analysis Codes: Statistics...
- Control Program & Control Program Generator (shelle script)
- External Codes: oof, BASIL, N-site FFT...

### Elle File Format

```
# Created by test_unodes: elle version 2.3.2 Fri Jun 8 13:38:25 2001
# LINES THAT START WITH A # ARE COMMENTS
# The OPTIONS BLOCK DEFINES GLOBAL PARAMETERS
OPTIONS
SwitchDistance 2.50000000e-02
MaxNodeSeparation 5.50000000e-02
MinNodeSeparation 2.50000000e-02
SpeedUp 1.0
CellBoundingBox 0.00000000e+00 0.00000000e+00
    1.00000000e+00 0.00000000e+00
    1.00000000e+00 1.00000000e+00
    0.00000000e+00 1.00000000e+00
SimpleShearOffset 0.00000000e+00
CumulativeSimpleShear 0.00000000e+00
Timestep 3.15000000e+07
UnitLength 1.00000000e-02
Temperature 2.50000000e+01
Pressure 1.00000000e+00
MassIncrement 0.00000000e+00
#THE NEXT BLOCK DEFINES THE POLYGONAL STRUCTURES: THE
FIRST NUMBER IS THE ID <E.G. 3>, THE SECOND THE NUMBER OF
NODES THAT DEFINE THE POLYGON <E.G. 23>, ANS FOLLOWED BY
AN ANTICLOCKWISE LIST OF NODE IDS E.G. <133 272 140 ETC.>
FLYNNS
3 23 133 272 140 146 112 174 87 15 147 150 211 129 17 39 62 94 119 20
13 8 72 135 7
7 36 21 76 31 29 73 107 279 302 166 280 167 30 224 156 209 27 131 25
16 77 132 2 0 141 4 121 1 10 86 122 155 227 22 3 37 105
11 24 20 119 94 62 39 17 33 165 34 48 49 162 51 50 88 36 38 56 78 29 31
76 21 142
17 25 50 123 110 204 164 158 64 53 67 115 128 85 68 24 91 180 40 23
185 182 284 96 38 36 88
#ETC.
#ETC.
#ETC.
#THE NEXT BLOCKS DEFINE FLYNN PAAMETERS SO TAHT FOR
EXAMPLE, AN EXPAND PARAMETER IS DEFINED FOR THESE
FLYNNS, THE DEFAULT VALUE IS 1 AND THE FLYNN WITH ID 17 IS
SET TO 1
EXPAND
Default 1
17 0
DISLOCDEN
Default 0.00000000e+00
```

```
MINERAL
Default QUARTZ
EULER_3
Default 0.00000000e+00 0.00000000e+00 0.00000000e+00
#THE LOCATION BLOCK DEFINES THE LOCATION OF BOUNDARY NODES. THE
FIRST NUMBER IT THE BNODE ID, THE SECOND IS X, THE THIRD IS Y
LOCATION
0 0.7157127300 0.0004124800
1 0.5647232500 0.9642747600
2 0.7517333600 0.9709875600
3 0.4205657800 0.7458517000
4 0.6626872400 0.9829956900
5 0.0854129600 0.0134190800
255 0.1195778800 0.1301631600
272 0.1584355500 0.756001600
279 0.5814173200 0.6308649800
280 0.6592591400 0.6547707300
284 0.5687853700 0.4511538400
289 0.1280806400 0.3809446100
293 0.2484257500 0.1165237400
302 0.6079290500 0.6402233800
#ETC.
#ETC.
#ETC.
#NEXT COMES BNODE PROPERTIES
CONC_A
Default 0.00000000e+00
29 4.0
#THE NEXT BLOCK DEFINES THE POSITION OF UNCONNECTED NODES. THE
FIRST NUMBER IT THE UNODE ID, THE SECOND IS X, THE THIRD IS Y
UNODES
0 0.000000 0.008660
1 0.020000 0.008660
2 0.040000 0.008660
3 0.060000 0.008660
4 0.080000 0.008660
5 0.100000 0.008660
6 0.120000 0.008660
7 0.140000 0.008660
#ETC.
#ETC.
#ETC.
#NEXT COMES UNODE PROPERTIES
U_CONC_A
Default 1
0 1.2
```

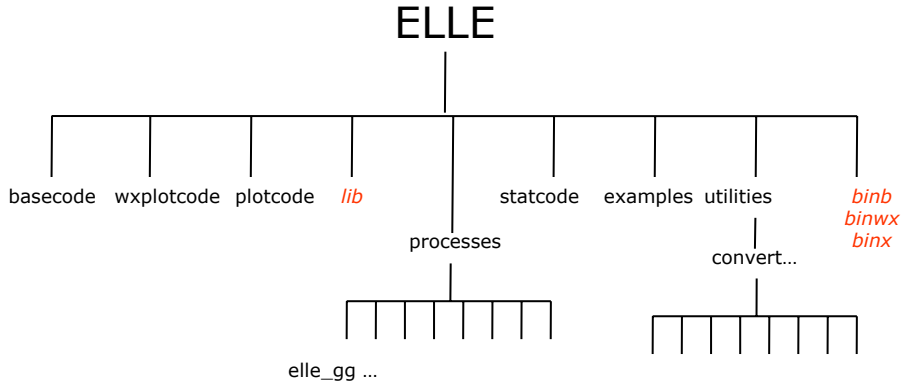
# Elle Experiments



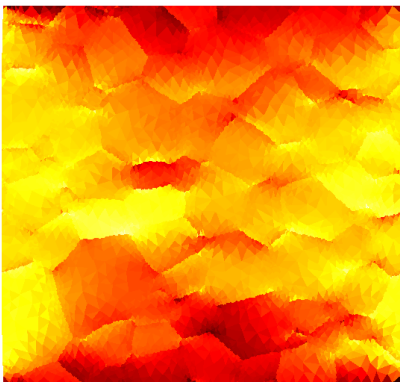
## Programming- Directory Structure

```
drwx-----+ 3 mark Aucun    0 Sep 28 15:11 basecode
drwx-----+ 2 mark Aucun    0 Sep 28 15:04 bin
drwx-----+ 2 mark Aucun    0 Jan 30 16:08 binwx
drwx-----+ 13 mark Aucun    0 Sep 25 13:16 examples
-rwx-----+ 1 mark Aucun   3640 Nov 30 2005 install.sh
-rwx-----+ 1 mark Aucun   3159 Jul  6 2006 install.win
drwx-----+ 2 mark Aucun    0 Sep 28 15:05 lib
drwx-----+ 3 mark Aucun    0 Sep 28 15:11 plotcode
drwx-----+ 27 mark Aucun    0 Sep 25 13:21 processes
drwx-----+ 3 mark Aucun    0 Sep 25 13:21 statscode
drwx-----+ 19 mark Aucun    0 Sep 25 13:22 utilities
drwx-----+ 4 mark Aucun    0 Sep 28 15:11 wxplotcode
```

## Programming- Directory Structure



## Anisotropic Elasticity (OOF & OOF2)



Elastic stress state in MgO in synthetic uniaxial compression experiment (OOF1)

OOF2 can potentially handle any problem of the form:

$$\text{Flux} = \text{Modulus times gradient of Field}$$

and

$$\text{divergence of Flux} = \text{Applied Force}$$

- Currently OOF2 actually only solves elasticity (Field=displacement, Gradient=strain, Modulus=Cijkl, Flux=stress) and thermal diffusion (Field=temperature, Modulus=thermal conductivity, flux=heat current), but can easily be extended to include electrical polarization, piezoelectricity, chemical diffusion, etc.

- New Fields, Fluxes and material properties can be added with only a few lines of Python code.

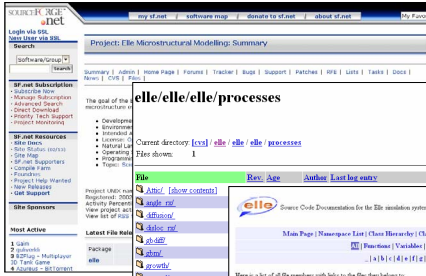
- Materials are built from a collection of Properties. Any logical combination of Properties is allowed.

- OOF2 contains a more powerful set of finite elements than does OOF1. OOF2 has 3 noded triangles, 4 node quadrilaterals, 6 noded sub- and superparametric triangles, and 8 noded sub- and superparametric quadrilaterals.

- OOF2 incorporates nonlinear solvers. (But not many non-linear material properties are yet present.)

<http://www.ctcms.nist.gov/oof/oof2/>

# Help



sourceforge

CVS

documentation

Main site

www.microstructure.info/elle



# Commercial Break

- Book
- Summer Schools

**Book** SPRINGER BOOK series "Lecture Notes in Earth Science".

**Microdynamic simulation – From microprocess to patterns in rocks**

**Editors: Bons, Koehn, Jessell**

**Preface (5 pages)**

**by Bons, Koehn & Jessell**

**1 Introduction (15 pages) by Bons & Jessell**

**2 Analysis and verification (10 pages) by Wilson & Piazzo**

**3 Numerical Methods (60 pages) by Bons, Jessell, Koehn, Stüwe**

**4 Processes (60 pages) Edited by Koehn** Edited chapter, with authored sub-chapters, going through those processes that are modelled with ELLE.

**5 Case studies (30 pages) edited by Jessell** Edited chapter with examples of the application of microdynamic simulation, involving coupling of two or more processes.

**6 Conclusions (5 pages) by Bons, Koehn, Jessell**

Little blurb, wrapping everything up. Expected future developments.

**References**

**Index (& glossary)**

**Appendix 1** How to use Elle: reproducing some of the section 3 & 4 results (Authors of chapters 4 & 5)

**Appendix 2** Data structures of Elle (Evans, Becker)

**Appendix 3** Elle & figures/movies CD, and weblink to current version (Evans, Becker, Bons)

**Total:** ca 185 pages + references, index & appendices



**Marie Curie Summer Schools**

*Interdisciplinary Materials Science*

The syllabus will use an integrated approach to materials, using the idea of a Materials Knowledge Lattice, where the three axes of Scale, Approach and Material encourage a cross-linked foundation for future research.

Aimed primarily at PhDs and early Postdocs from natural and manufactured materials sciences

The four summer schools will be organized by :

- 2005** Aachen (Günter Gottstein)
- 2006** Stockholm (Sandra Piazzo)
- 2007** Estremoz (Mark Jessell)
- 2008** Strasbourg (Karel Schulmann)

