Integrating N-site FFT and ELLE

M. Jessell[1], L. Evans[2], R. Lebensohn[3], A. Griera[1]

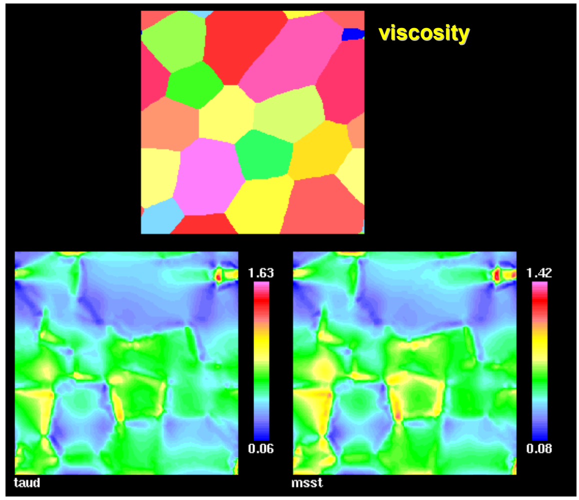
[1] LMTG (Toulouse), [2] University of Melbourne, [3] LANL (Los Alamos)

Outline

1) Why do we need upgrade the stress/strain process?
2) From single to a polycrystalline medium. What's the best choice to model it?
3) Coupling N-Site FFT and Elle
4) An example of possible process: recrystallisation driven by stored energy at dislocation (*at initial stage*)

Why do we need to upgrade the stress/strain process?

• Basil: 2D FEM non linear viscous but assume isotropic behaviour…



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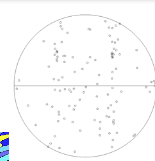
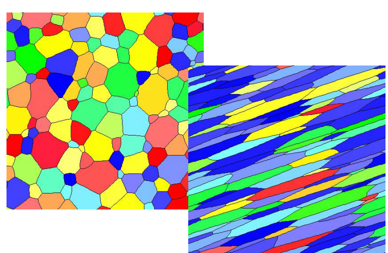
Upgrade the stress/strain process, Why?

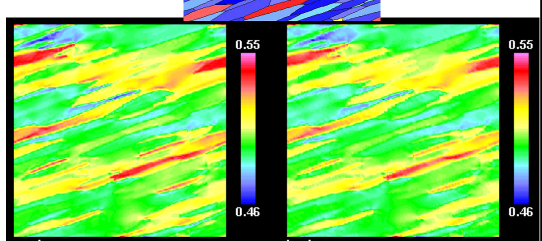
Why do we need to upgrade the stress/strain process?



• Basil: 2D FEM non linear viscous but assume isotropic behaviour…

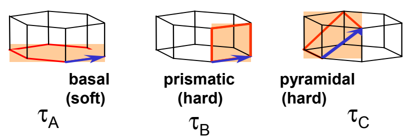


• Possible to define a "pseudo" anisotropy modifying effective viscosity as function of slip systems (e.g. TBH process)… but limited to a monomineralogical polycrystalline medium.



During plastic deformation, geologic materials show strong anisotropy and local high heterogeneous stress/strain fields at subgrain scale (in grain)…

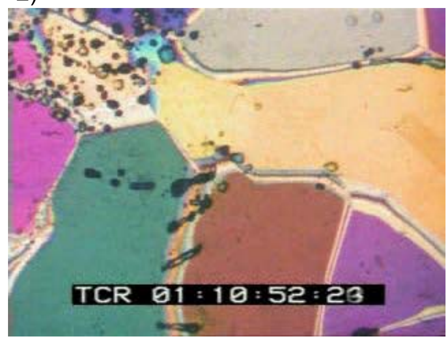
1) e.g. ICE
slip modes in ice crystals:
3 gliding systems, τ_i critical shear stress



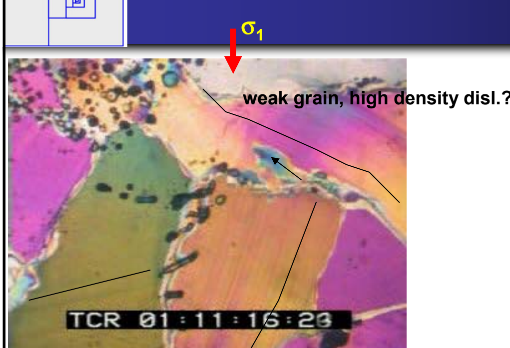
$$\tau_B = \tau_C = 70\tau_A$$

Castelnau et al., 1996

2)



Pure shear deformation of Ice -1ºC (Wilson 1999, www.earthsci.unimeb.edu.au/wilson/ice1)



-Bending of basal plane
-Recrystallisation, GBM, heterogeneous distribution in grain

In ice, "dislocation density is proportional to curvature of basal plane" but at rocks more complex…

- What does we need?

A numerical modelling that simulate an anisotropic polycrystalline medium.

- Polycrystal plasticity models are comprised of two parts:

1) A set of single crystal equations describing properties and orientations (similar for all modelling approaches).

2) A set of equations that link individual crystals together into a polycrystal (different modelling approaches).

Basic single crystal equations

1) Deformation rate is equal to a linear combination of the slip on α slip systems

$$D_{ij} = \sum_{\alpha} \dot{\gamma}_{\alpha}(\mathbf{b}_{\alpha} \otimes \mathbf{n}_{\alpha})$$

where γ is rate of shearing, **b** the slip direction and **n** the slip plane normal vector

A minimum of five independent slip systems are necessary for arbitrary homogeneous plastic deformation. (D_{ij} 6 components but 5 if we assume non volume change; von Mises criterion)

Basic single crystal equations

2) The constitutive relations at slip systems assume a rate-dependent behaviour. The relation between the resolved shear stress (τ_α) on a given α system slip is and the rate of shearing (γ_α),

$$\tau_\alpha = \tau_{cr} \frac{\dot{\gamma}_\alpha}{\dot{\gamma}_0} \left| \frac{\dot{\gamma}_\alpha}{\dot{\gamma}_0} \right|^{m-1}$$

where τ_{cr} is the critical shear stress, γ_0 is the reference rate of shearing and *m* represents the material strain rate sensitivity.

The use of a rate-dependent allows all slip system to be potentially active, although shear rates on some of them may be negligible.

Polycrystal interaction equations

• The difficult task:
How to partition the macroscopic strain into the crystal aggregate.

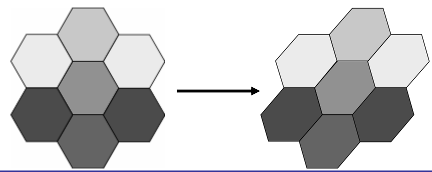
• Numerous models have been proposed (*fast review*):

1) **Classical FC Taylor** (non-dimensional)

"the microscopic strain rate is equal to the macroscopic strain rate, uniform lattice orientation"

$$\mathbf{l} = \mathbf{L}$$

$$P^* = \sum_{\alpha} \tau |\dot{\gamma}| = \min$$



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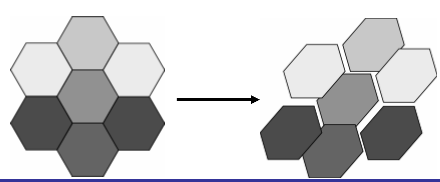
Crystal viscoplasticity: polycrystals

1) **Classical FC Taylor** (non-dimensional)
2) **Relaxed Constraints Models** (non-dimensional)

"all grains share some strain components, but GB mismatches in other orientations"

$$\mathbf{l} \neq \mathbf{L}, \ \mathbf{s} \neq \mathbf{S}$$

$$\mathbf{l} = \mathbf{L} - \sum_{1}^{R} K\dot{\gamma}$$

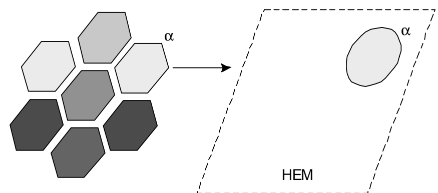


1) **Classical FC Taylor** (non-dimensional)
2) **Relaxed Constraints Models** (non-dimensional)
3) **Self-consistent models** (non-dimensional)

"Grains deform freely within an homogeneous effective medium (HEV) reflecting the ensemble of the system. Deviation of stress/strain rate in the crystal from interaction equation "

$$\bar{\mathbf{s}} = \frac{1}{N}\sum_{\alpha=1}^{N}\mathbf{s}_\alpha, \bar{\mathbf{d}} = \frac{1}{N}\sum_{\alpha=1}^{N}\mathbf{d}_\alpha$$

$$\mathbf{d}_\alpha - \bar{\mathbf{d}} = -\tilde{\mathbf{M}} : (\mathbf{s}_\alpha - \bar{\mathbf{s}})$$



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Crystal viscoplasticity: polycrystals

1) **Classical FC Taylor** (non-dimensional)
2) **Relaxed Constraints Models** (non-dimensional)
3) **Self-consistent models** (non-dimensional)

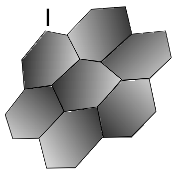
All are non-dimensional models, not possible to use to model 2D/3D microstructure evolution.

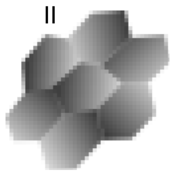
Solve the mechanical response by means of numerical methods: two mean options to solve the problem..

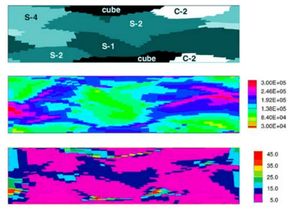
FEM,FDM or FFT ?

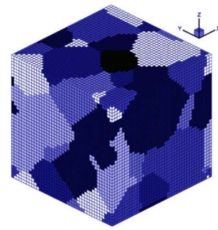
Crystal viscoplasticity: polycrystals

FEM, FDM examples

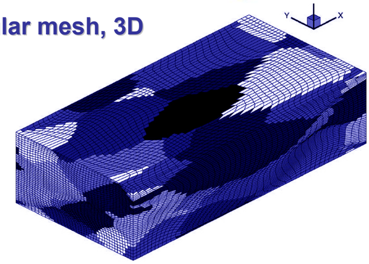




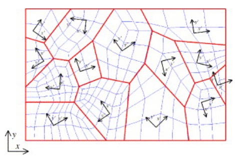


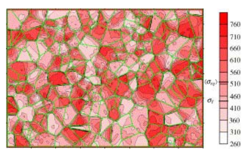


- Regular mesh, 3D



- **Grain adapted mesh,** complex topology at 3D

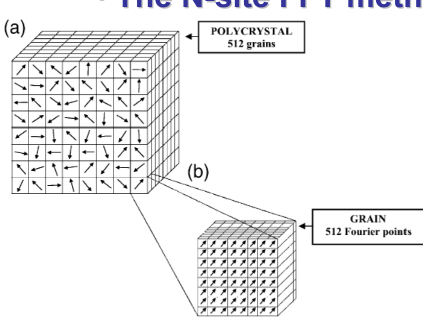




After Sarma and Radhakrishnan

Crystal viscoplasticity: FFT model

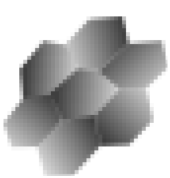
- **The N-site FFT method….. but what does it mean?**



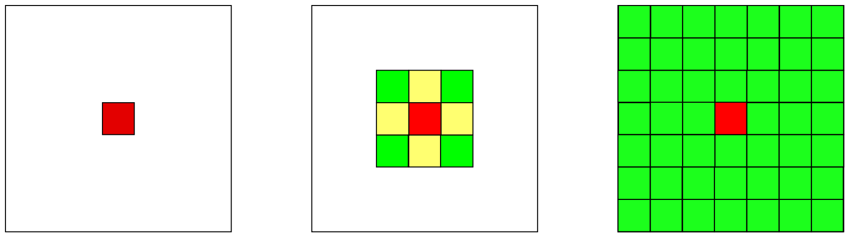
Developed by Lebensohn (2001)

Main characteristics:

1) 3D anisotropic polycrystal medium. Defined by discrete prismatic grains arranged in a regular fashion.
2) Periodic boundary conditions: Representative Volume Element (RVE).
3) Box size: N x M x L but 2^n



1) What's mean a N-site kind ? The neighbors problem



- **1-site : grain considered to deform embedded in a homogeneous medium with average properties.**
- **The first neighbours grains (Von Neumann, Moore)**
- **n-site kind: with no cutoff distance of interaction, all grains are considered.**

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Crystal viscoplasticity: FFT model

2) FFT: Fast Fourier Transform Method

Considering incompressibility, the system of differential equations to be solved In viscoplasticity becomes (motion equation),

$$L_{ijkl} v_{k,lj}(\mathbf{x}) + \tau_{ij,j} = 0$$

$$v_{k,k}(\mathbf{x}) = 0$$

The system is solved by,

1) The Green function associated to velocity field (G (x-x'))
2) Local fluctuation of velocity and stress fields respect to a reference medium.
3) Use of the Fourier transform.

Then,

$$L_{ijkl}G_{km,lj}(\mathbf{x}-\mathbf{x}')+\delta_{im}\delta(\mathbf{x}-\mathbf{x}')=0$$

$$G_{km,k}(\mathbf{x}-\mathbf{x}')=0$$

$$\tilde{v}_{i,j}=\int_{R^3}G_{ik,jl}(\mathbf{x}-\mathbf{x}')\tau_{kl}(\mathbf{x}')d\mathbf{x}'=G_{ijkl}*\tau_{kl}$$

"Real" Space

$$L_{ijkl}v_{k,lj}(\mathbf{x})+\tau_{ij,j}=0$$

$$v_{k,k}(\mathbf{x})=0$$

$$\longleftrightarrow$$

Fourier Space

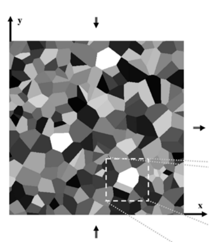
$$\xi_1\xi_j L_{ijkl}\hat{G}_{km}-i\xi_i\hat{H}_m=\delta_{im}$$

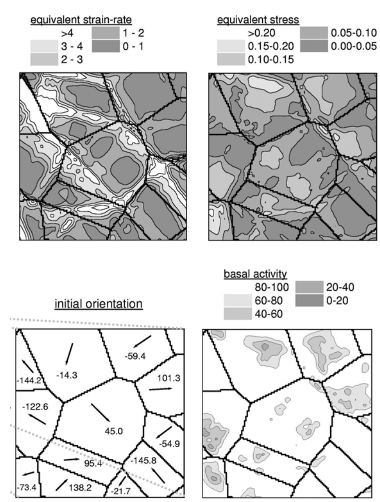
$$\xi_k\hat{G}_{km}=0$$

Iterative solved, convergence test

Lebensohn et al., submitted to Acta Mater.

FFT examples: ice deformation



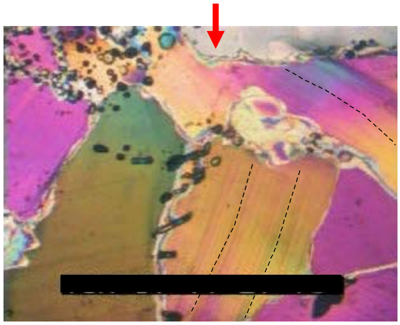


1) It gives the local stress and strain rate fields-It is well suited for strongly anisotropic materials

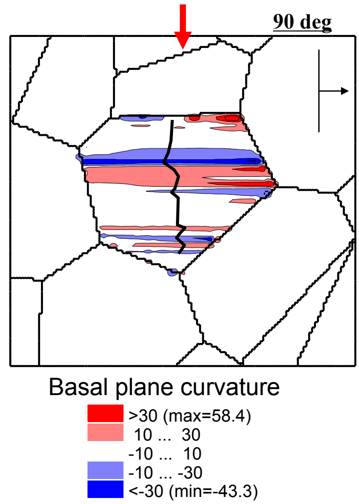
2) Local stress and strain rate fluctuations are related to the grain orientation and the neighbourhood.

Crystal viscoplasticity: FFT model

•The FFT model can reproduces the mechanical behaviour of ice.



From Wilson, 1999
(www.earthsci.unimeb.edu.au/wilson/ice1)



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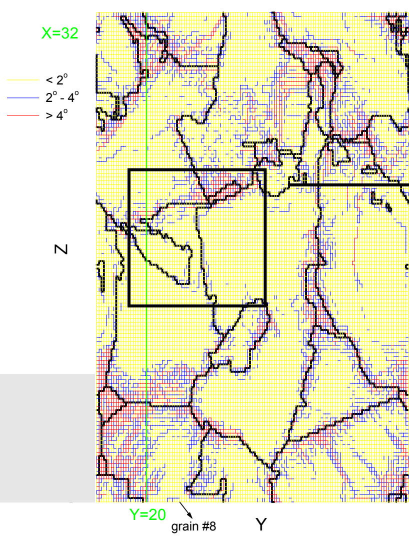
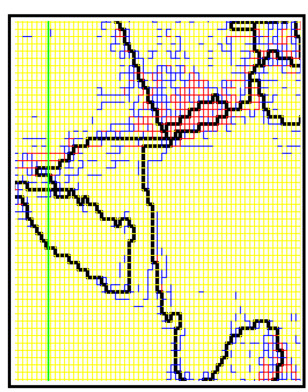
Crystal viscoplasticity: FFT model



It's possible to misorientation maps of lattice, texture predictions, control of type and activity of slip systems, etc… but grain boundaries are implicit and rectangular.



Lebensohn et al.,

Advantages of FFT

- Results are coherent with experiments, and well suited for strongly anisotropic materials.
- 3D easier, non topological limitations on mesh (avoid the problem of retetrahedralisation).
- Periodic boundary conditions similar than in Elle.
- Faster numerical performance than FEM, but 1 FFT step needs 1-2 minutes (?)… but is parallelisable (uff!)
- CPFEM based on commercial codes. Access to FFT, and mutual interest for coupled both codes…

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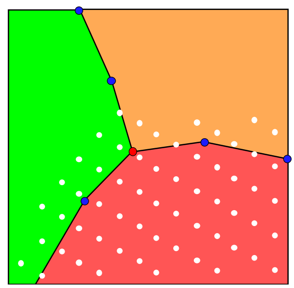
FFT vs. CPFEM models

Drawbacks of FFT

-Regular mesh of Fourier space, we need an interpolation between N-site FFT and Elle data.
- Large amount of unodes, and decrease of velocity of numerical performance.

1) Design a microstructure in Elle: periodic but irregular polygonal network



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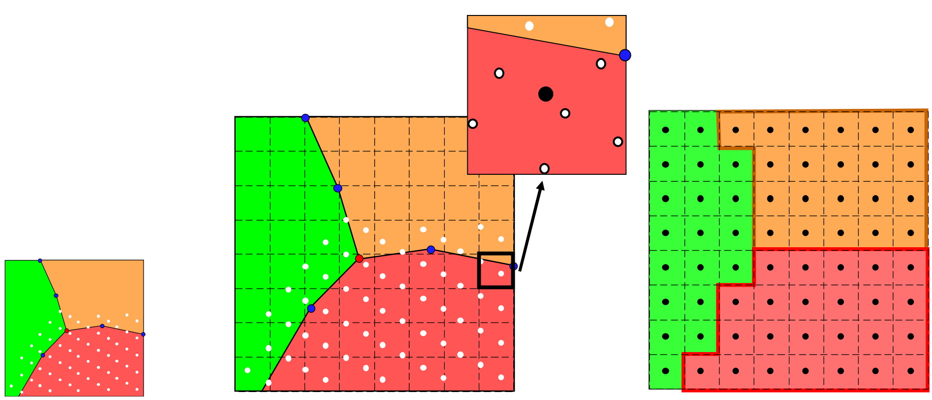
A cycle of couple FFT and Elle
Basic idea at 26/02, tomorrow?

1) Design a microstructure in Elle: periodic but irregular polygonal network.
2) Map network onto a regular grid and transfer properties information (regular unodes xyz, ownership unodes, variables, etc.)



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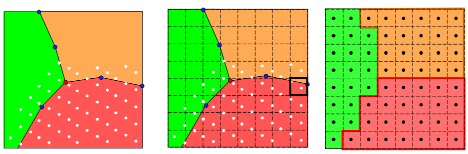
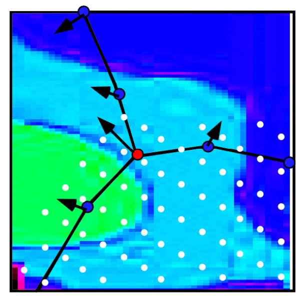
A cycle of couple FFT and Elle

Basic idea at 26/02, tomorrow?

1) Design a microstructure in Elle: periodic but irregular polygonal network.
2) Map network onto a regular grid and transfer properties information.
3) Run the FFT crystal viscoplastic calculation for a small strain increment.
4) Use the deformation fields to map the new positions of polygon network and unodes layer (regular unodes xyz, properties unodes, variables as work,etc)





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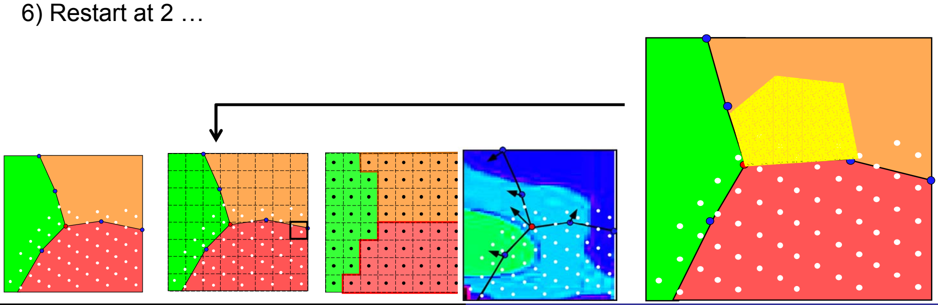
A cycle of couple FFT and Elle

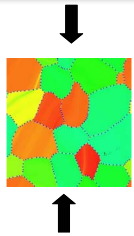
Basic idea at 26/02, tomorrow?

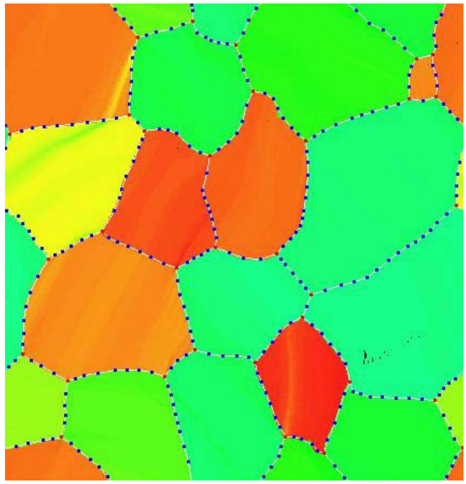
1) Design a microstructure in Elle: periodic but irregular polygonal network.
2) Map network onto a regular grid and transfer properties information.
3) Run the FFT crystal viscoplastic calculation for a small strain increment.
4) Use the deformation fields to map the new positions of polygon network and unodes layer.
5) Run whatever of the Elle process (grain boundary migration, lattice diffusion, recovery, etc).
6) Restart at 2 …



A cycle of couple FFT and Elle

First exercise: 1 cycle of fft2elle / elle2fft





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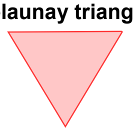
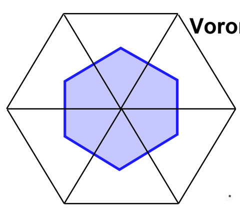
A cycle of couple FFT and Elle

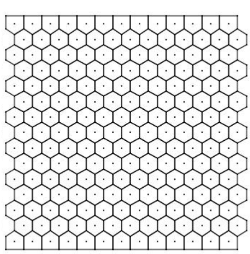
Parallel tools…

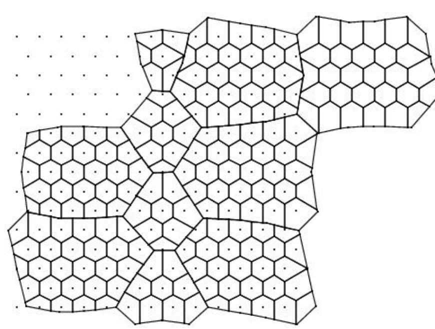
Delaunay triangles



Voronoi cells



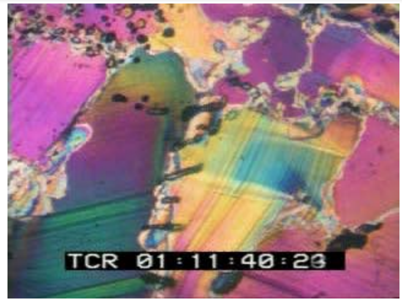




- Voronoi cells clipped along grain boundaries

GBM driving by differences of stored energy in dislocation (density dislocations, scalar)….

- Nodes network and unodes layer



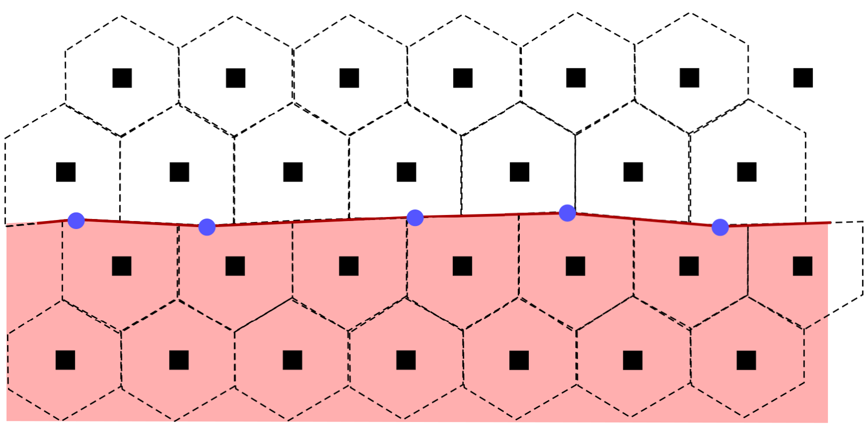
$$v_i \propto M p_i$$

$$p_i = \sum p_i = \vec{p}_{surface\ energy} + \vec{p}_{stored\ energy} + \vec{p}_{metamorphic} + \ldots$$

$$\vec{p}_{stored\ energy} = \frac{1}{2} \rho \mu b^2$$

M values, scale the models,..?

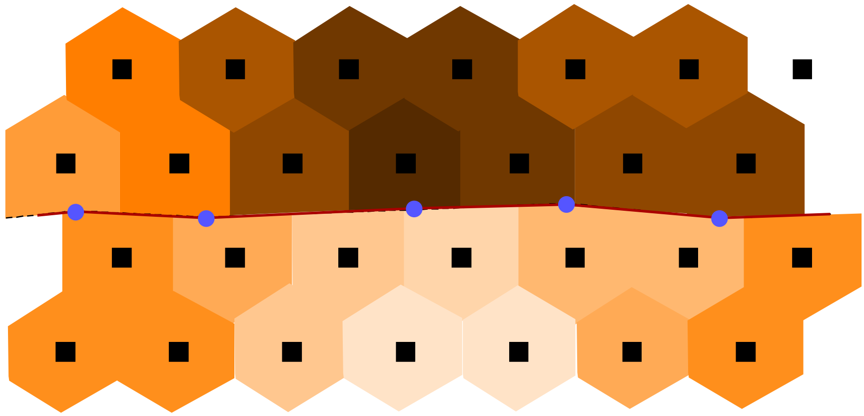
Preliminary fantasy…



A hypothetical grain boundary between two grains …

Preliminary fantasy…

low density → high density

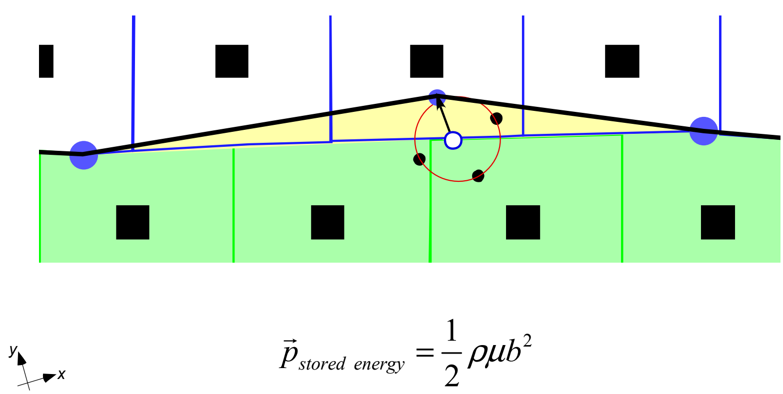


A hypothetical grain boundary between two grains with different dislocation density…

Preliminary fantasy…

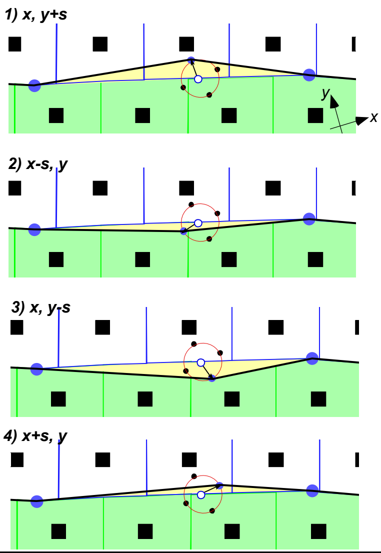
STEP 1, random pick of unodes, virtual step *s*, calculate the gradient,…

$$v_i \propto M p_i$$



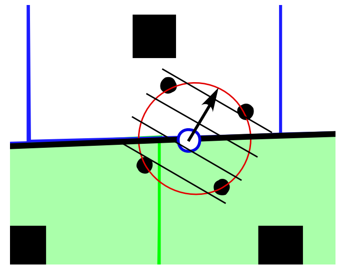
$$\vec{p}_{stored\ \ energy} = \frac{1}{2}\rho\mu b^2$$

Preliminary fantasy…



Calculate direction of maximum decrease of stored energy

$$E_{swept} \square \sum \rho_i A_i E_n$$



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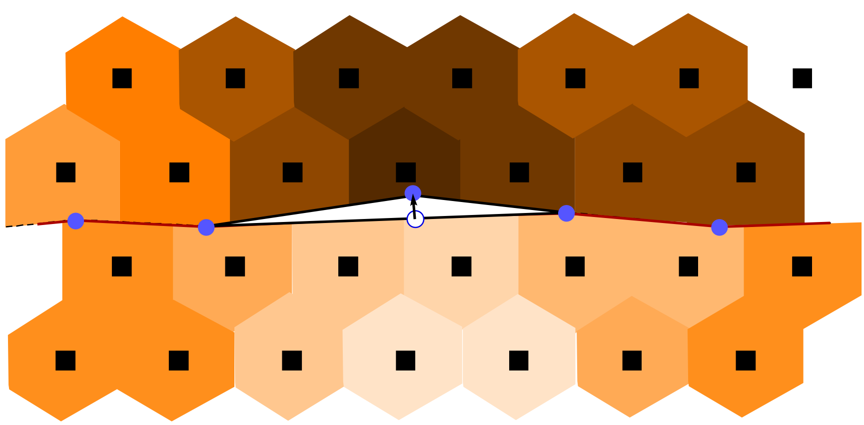
Preliminary fantasy…



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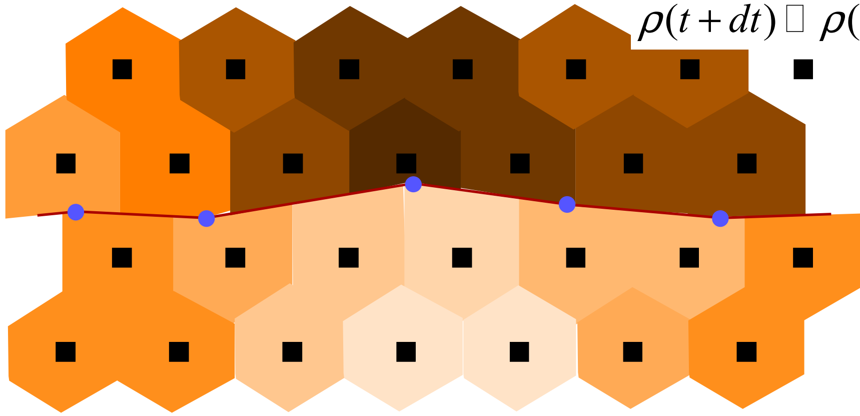
Preliminary fantasy…

Update dislocation density, local voronoi cells,…

$$\rho(t+dt) \approx \rho(t)$$



Local update voronoi cells, …

$$\rho(t+dt) = \rho(t)\frac{A(t)}{A(t+dt)} + \rho_{swept}\frac{A_{swept}}{A(t+dt)} \approx \rho(t)\frac{A(t)}{A(t+dt)}$$

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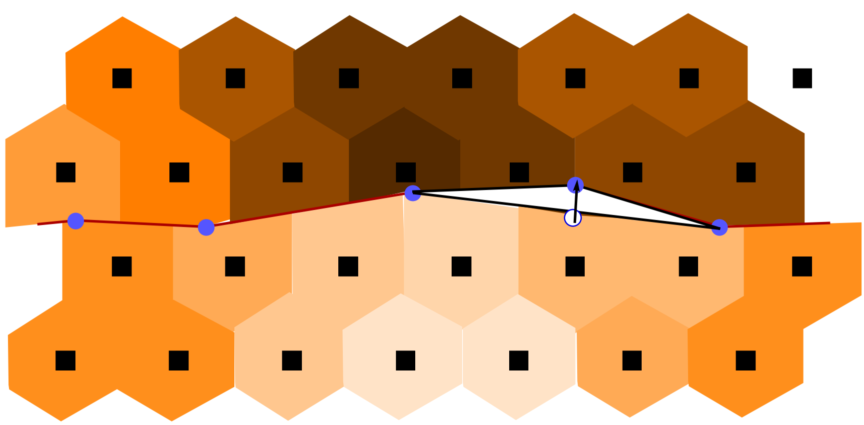
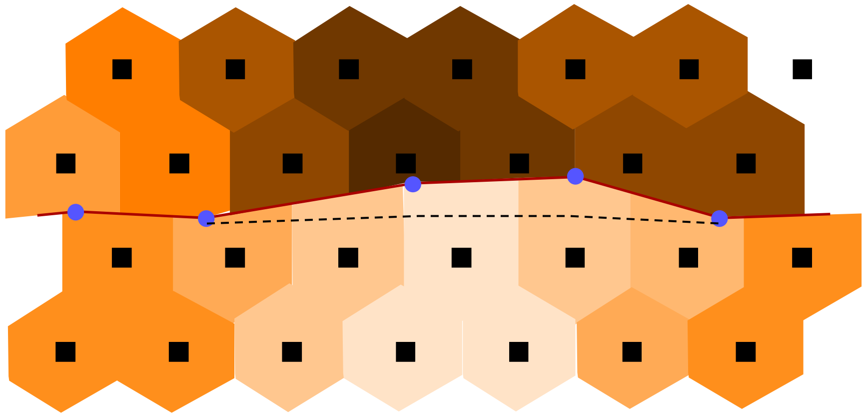
+ fantasy…



+ fantasy...



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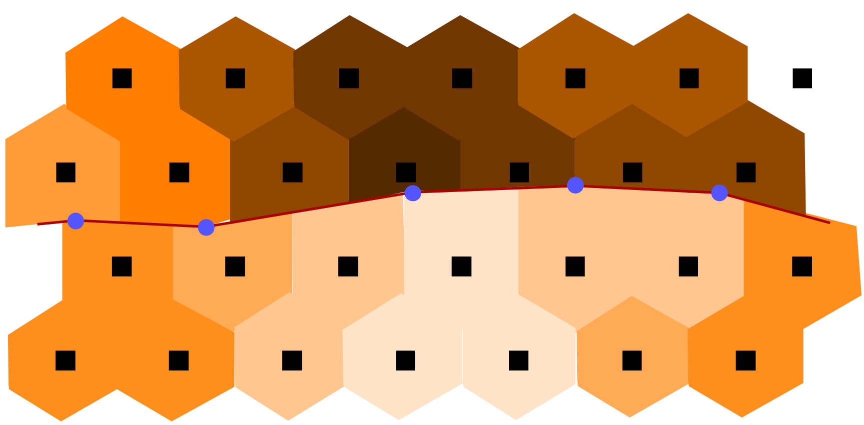
+ fantasy...



SubStructure Dynamics

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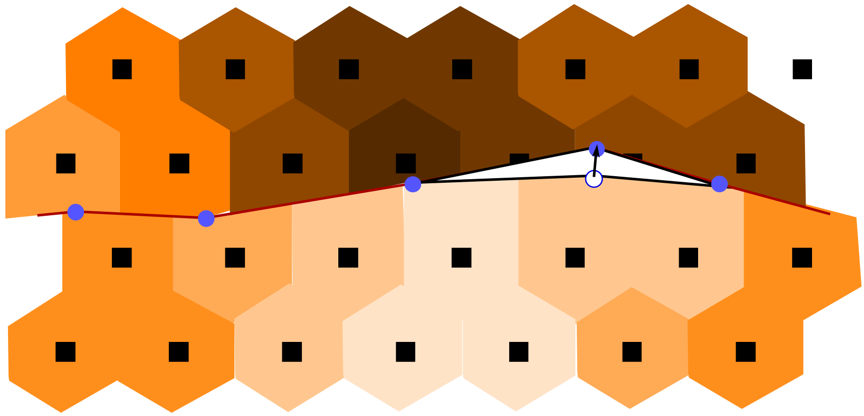
++ fantasy...

when GBM jumps an unode...



SubStructure Dynamics

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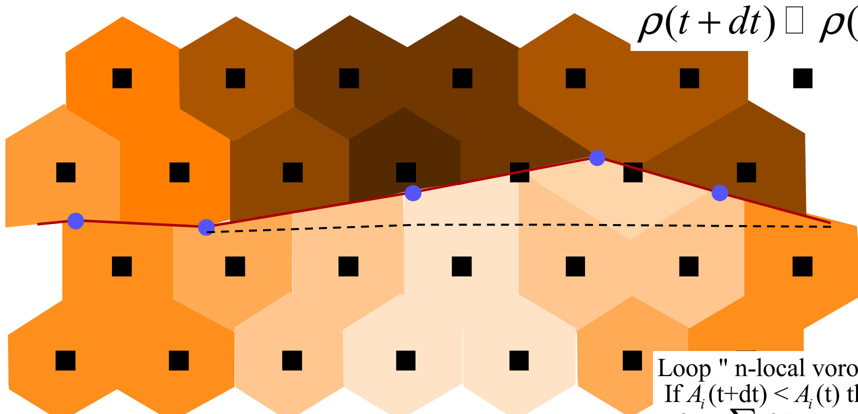
++ fantasy...

$$\rho(t+dt) \square \rho(t)$$



Loop " n-local voronoi "
If A_i(t+dt) < A_i(t) then

$$d\rho = \sum_n dA_i \rho_i$$

$$\rho(t+dt) \square \frac{d\rho}{A(t+dt)}$$

end_if
end_loop

SubStructure Dynamics

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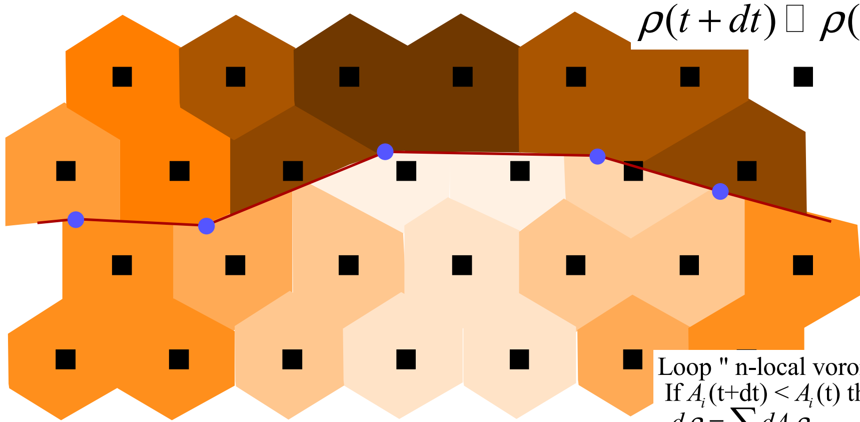
++ fantasy...

when GBM jumps *n* unodes...

$\rho(t+dt)$ □ $\rho(t)$



Loop " n-local voronoi "

If A_i(t+dt) < A_i(t) then

$d\rho = \sum_{n} dA_i \rho_i$

$\rho(t+dt)$ □ $\dfrac{d\rho}{A(t+dt)}$

end_if

end_loop

SubStructure Dynamics

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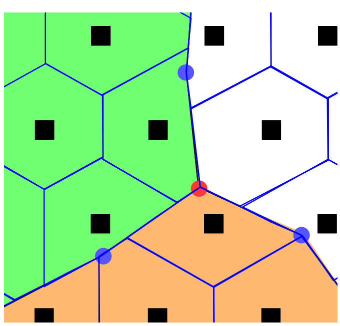
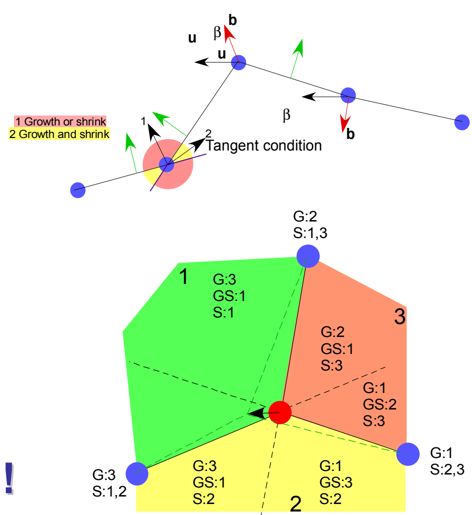
t-nodes, special topological events, etc..



...but another day!!



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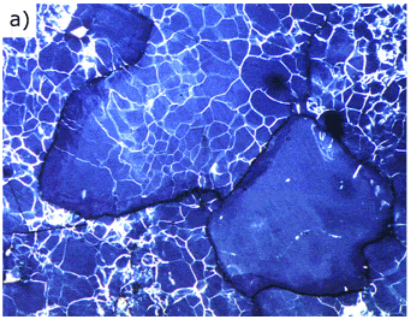
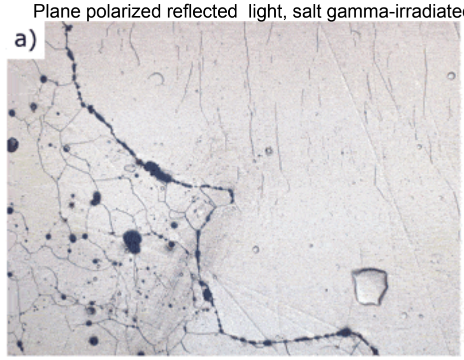
non fantasy… real rocks micro.



Plane polarized transmitted light, salt gamma-irradiated

But for models we will need M **values, scale the models,..?**

Plane polarized reflected light, salt gamma-irradiated



from Schléder and Urai ()

SubStructure Dynamics

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++ fantasy…