ON 2-D MESOSCOPIC MODELING OF A POLY-CRYSTAL

Fabrizio Cleri[1,2] and Gregorio D'Agostino[1]

1) ENEA, Divisione Materiali Avanzati
Centro Ricerche Casaccia, C.P. 2400, 00100 Roma, and
2) INFM, Unità di Ricerca Roma I

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Summary

- *Simulation of Microstructure evolution:*
  Meso-scale approach from nucleation to poly-crystal plasticity.

- *Stochastic Network versus Lattice Markov chain:*
  Free Henthalpy . Friction terms. Transition probability.

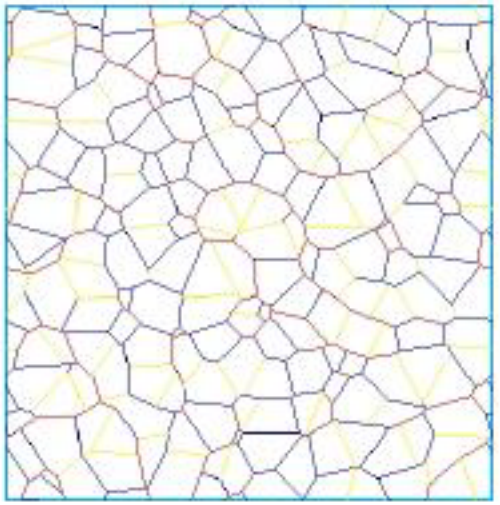
- *Vertex mode for Secondary Growth.*
  Interacting triple junctions. Scaling laws.

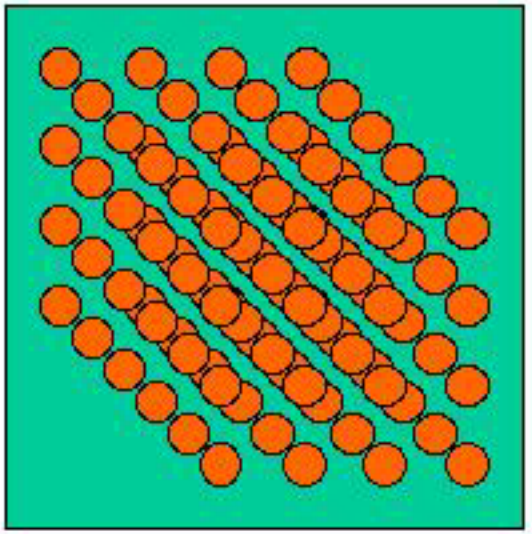
- *Nucleation and Primary Growth*
  Transition FreeHentalpy, Mobility and Nucleation Rate.

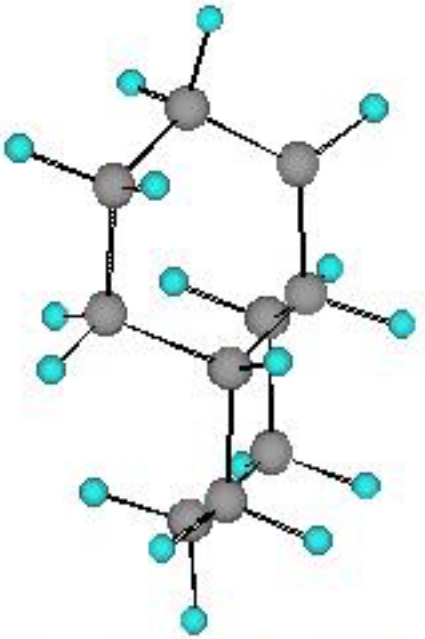
- *Anisotropy effects.*
  Grain Boundary versus mobility Anisotropy.

- *Elasticity and Dislocation plasticity.*
  Constitution equations. Local stresses.

Meso-scale







MesoscopicSimulations

Driving Functional Π

$$W(a \rightarrow b) = 1/\tau \, e^{-(\Delta \Pi_k \Delta t / k_B T)}$$

Atomistic Simulations

Classical Potential

$$m \cdot \ddot{x} = -\vec{\nabla} V$$

Quantum Simulations

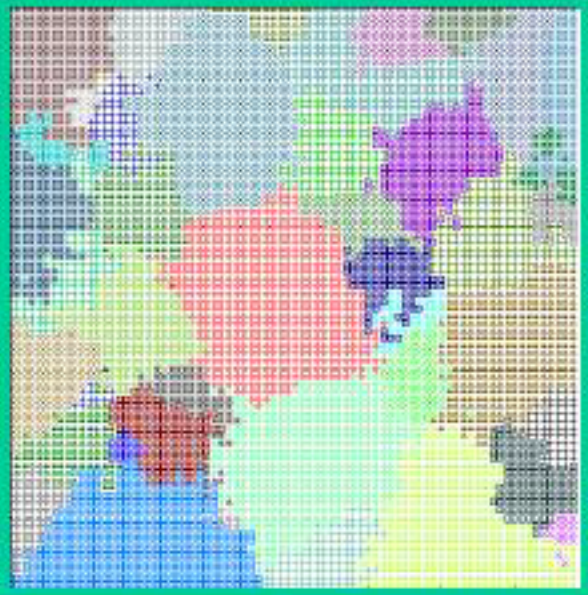
HeisembergEquation

$$i \frac{\partial}{\partial t} \Psi = H \Psi$$

Twofold Approach

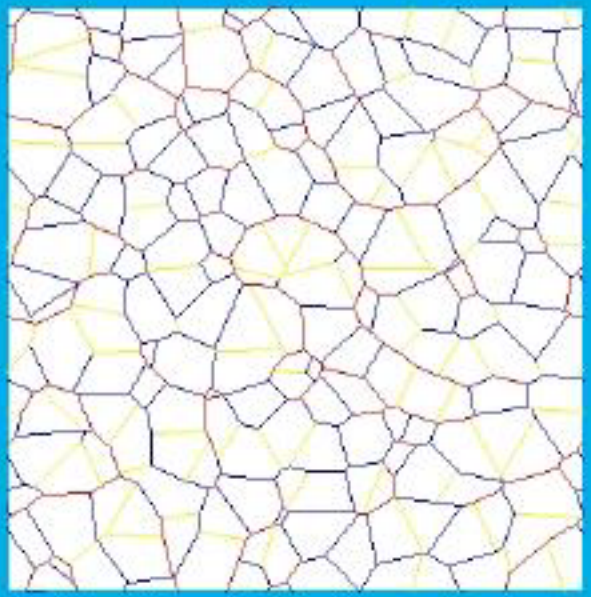
L.S.C
Lattice Stochastic Chain

Stochastic Lattice

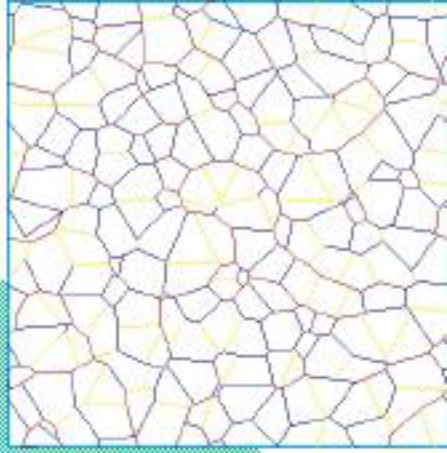


S.N.
Stochastic Network

Stochastic network



Stochastic Network



Modeling is based on a *"Network evolution"*

- Physical system is partitioned in cells of suitable size and shape. Discrete Time-step evolution is assumed. Cells are separated by interfaces.
- Each cell represents a homogeneous portion of matter.
- Each cell is assigned an order parameter (Index) representing the state of the system. Several other degrees of freedom are definite: average temperature, stress tensor, strain tensor etc.
- A 2-D crystal lattice orientation angle is assigned to "solid" celles.
- A driving Functional is indroduced that provides physical evolution via an Extremality Variational Principle.

Toward Equilibrium

Thermodynamics equilibrium is achieved a Free enthalpy minimum.

The way the system approaches equilibrium is a general problem that is solved by means of an ansatz.

Basic idea is to introduce a suited Functional depending on a small number of average physical quantities and a Variational Principle to achieve network motion.

The Functional consists of two terms: the Driving Force represented by the gradient of Free Enthalpy and a Friction Term that provides Inertia to the system:

$$\Pi = \frac{dG}{dt} + \Pi_{in}$$

Network evolution is described by Variational Equations:

$$\delta\Pi = 0$$

The Needleman-Rice Variational Functional

Solid state poly-crystalline Grain growth

A. Needleman and J.R. Rice, *Acta Met.* 28, 1315 (1980)
A.C.F. Cocks and S.P. Gill, *Acta Mater.* 44, 4765 (1996)

Free Enthalpy depends on Grain Boundaries (G.B.) degrees of freedom only i.e. surface energy (free enthalpy) γ and lenght L:

$$G = \sum_{N_{grb}} \int_{L_i} \gamma_i ds$$

Therefore **variational functional** Π depends only on the G.B. velocity field $v(s)$ as independent degrees of freedom defined on the collection of grain-boundaries:

$$\Pi[v] = \sum_{N_{grb}} \left(\int_{L_i} \gamma_i \kappa_i v_n(s) ds + \int_{L_i} \gamma_i \frac{\partial v_s(s)}{\partial s} ds + \int_{L_i} \frac{v_n^2(s)}{2\mu_i} ds \right)$$

The three terms describe **curvature-driven** boundary migration, **line tension imbalance** at triple junctions and **viscous resistance** to boundary motion. Parameter μ will be referred to as GB **mobility**

Additional terms to describe GB rotation, sliding, diffusion are already available....
(see: Pan-Cocks-Kucherenko, *Proc. R. Soc. London* A 453, 2161 (1997))

Velocity MonteCarlo Scheme

(F. Cleri, *Physica* A 282, 339 (2000))

Adopting a straight boundaries constraint, dynamics will depend on **Triple Junctions** ("*vertex-model*") only.

Extremality of (free enthalpy) energy dissipation rate is achieved by means of a MonteCarlo scheme. As a consequence, the ***probability*** per unit time of occurrence of a given configuration is written in terms of a ***transitionrate*** betweentwo microscopic configurations a and b, $W(a \rightarrow b)$, as a function of the energy dissipation rate:

$$W(a \rightarrow b) = 1/\tau \, e^{-(\Delta\Pi_k \Delta t / k_B T)} \qquad \text{if } \Delta\Pi_k > 0 \quad \text{for a variation of } \mathbf{v}_k \rightarrow \mathbf{v}_k'$$

$$W(a \rightarrow b) = 1/\tau \qquad \text{if } \Delta\Pi_k \leq 0$$

the Needleman-Rice functional reducing to a function of the discrete set $\{\mathbf{v}\}_k$, e.g. :

$$\Pi(\mathbf{v}_k) = \Sigma_{i=1,3} \{ \gamma_i (v_{s,i} - v_{s,k}) + (L_i/6\mu_i) [(v_{n,i})^2 + (v_{n,k})^2 + v_{n,i} v_{n,k}] \}$$

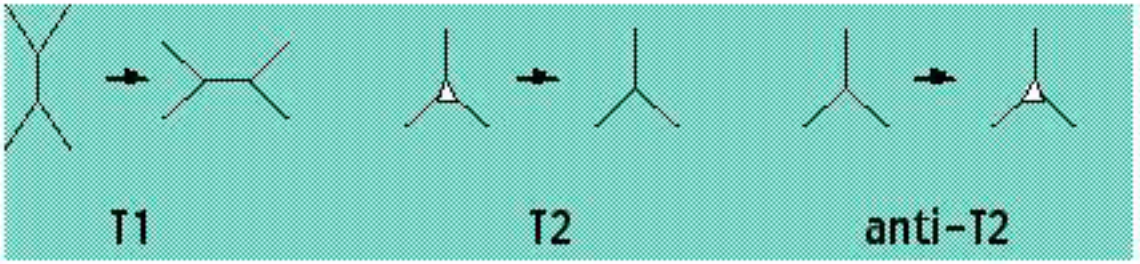
This is a "velocity" MC method!

For a random variation of $\mathbf{v}_k \rightarrow \mathbf{v}_k'$

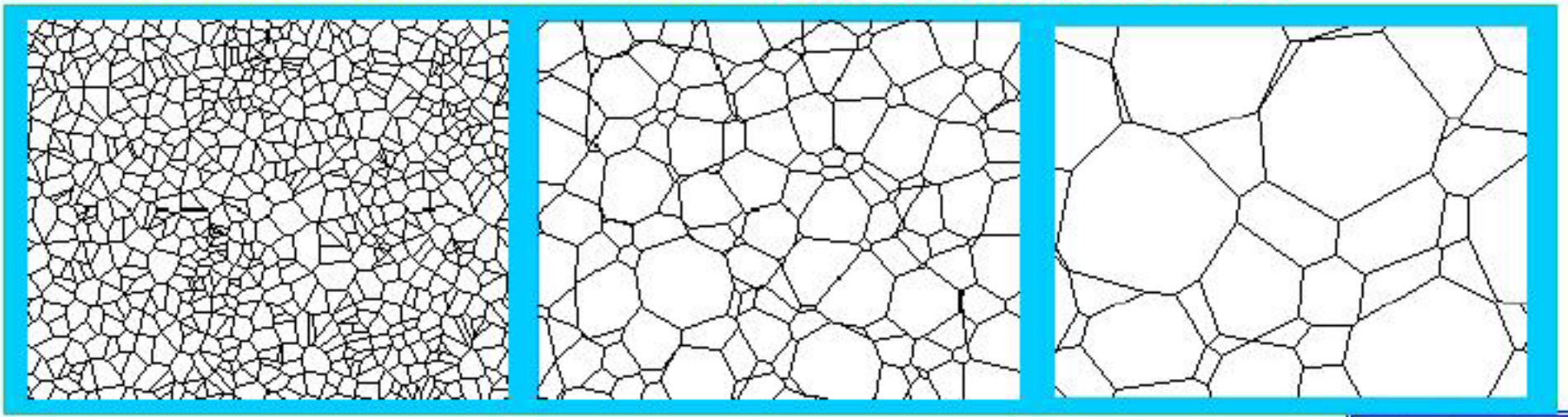
$$\Delta\Pi_k = \Pi(\mathbf{v}_k') - \Pi(\mathbf{v}_k)$$

Grain Growth

In order to account for grain and boundary annihilation or creation, three additional topological moves (or "rules") were also introduced:

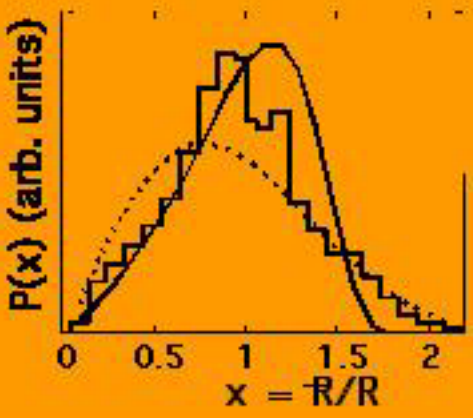


Typical example of **2D modeling of "normal" grain coarsening**

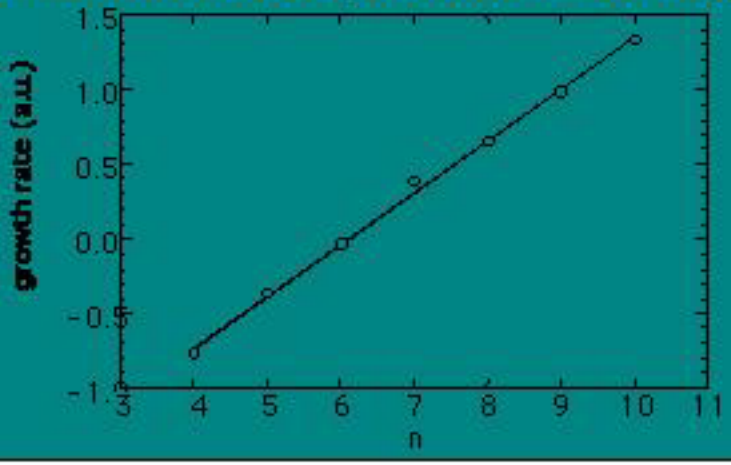


Scaling laws

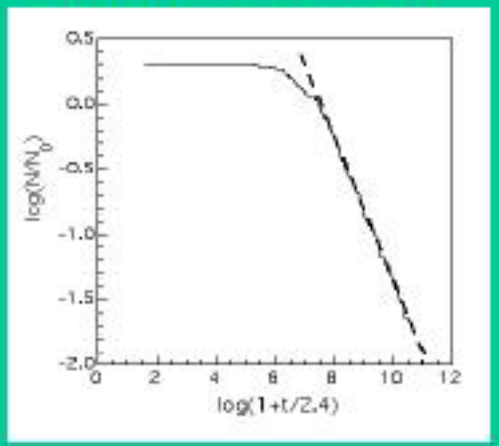
Grain size distribution



Growth velocityvs number of edges



Grain-size scaling



$$\frac{dA_n}{dt} \approx n - 6$$

Von Neuman law is respected:

$$< d > \approx t^{2.4}$$

Number of grains decrease as a power

Size distribution follows Reileight distribution initially and Hillert distribution at large diameters

Mobility and GB Energy anisotropy

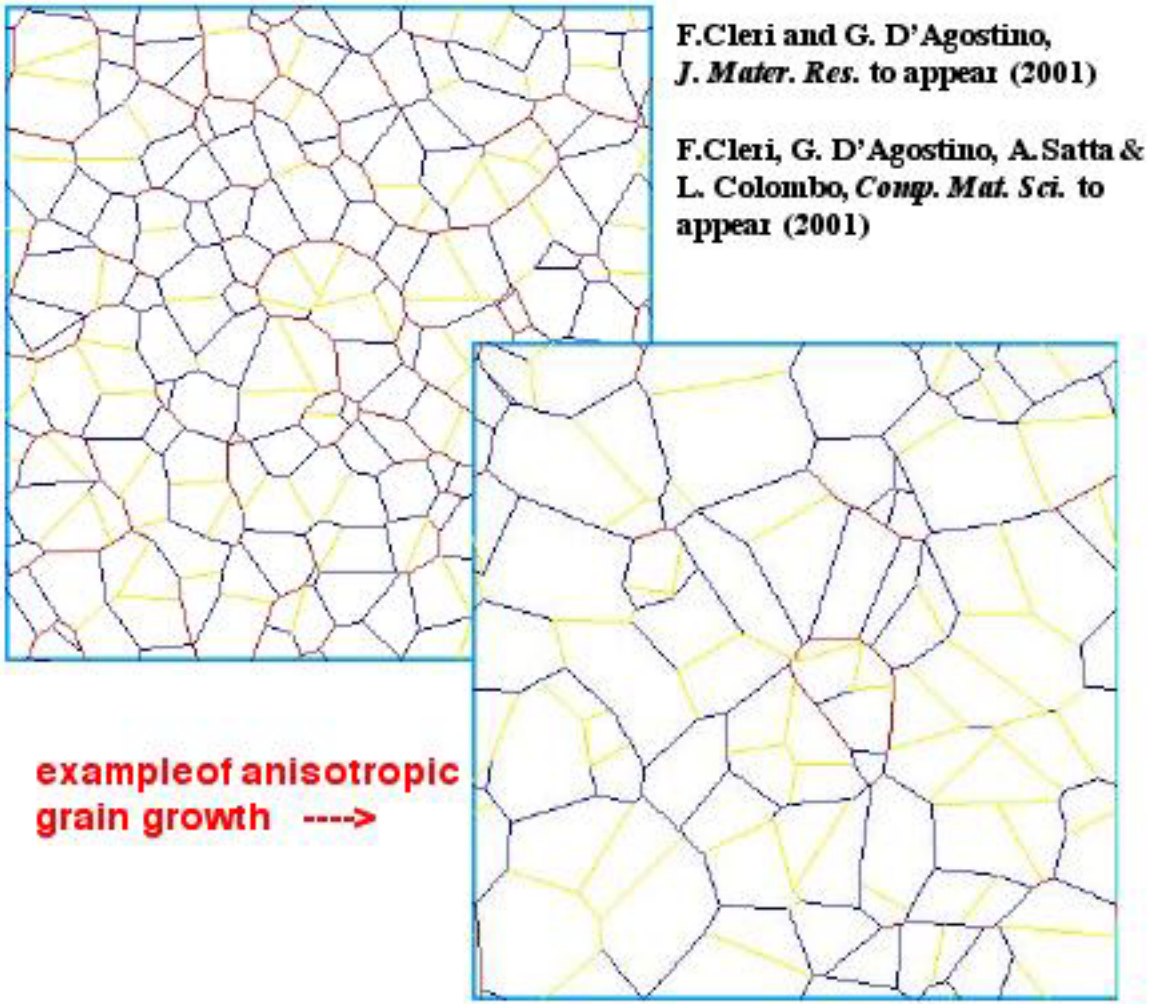
γ and μ depend on Misorientation

Both GB energy and mobility are assumed to be functions of the **relative misorientation** of grains. Each grain is assigned an absolute value of rotation θ_k with respect to the common polar axis.
The GB energy is given by the **Read-Shockley** formula as a function of $\Delta\theta=\theta_k-\theta_n$:

$$\gamma(\Delta\theta) = \gamma_0\,\Delta\theta\left[A - \log(\Delta\theta)\right]$$

For the GB mobility an expression already adopted also by other authors is:

$$\mu(\Delta\theta) = \mu_0\,\Delta\theta^{0.2}$$



F.Cleri and G. D'Agostino, *J. Mater. Res.* to appear (2001)

F.Cleri, G. D'Agostino, A.Satta & L. Colombo, *Comp. Mat. Sci.* to appear (2001)

example of anisotropic grain growth ---->

Mobility anisotropy only induces a different behavior

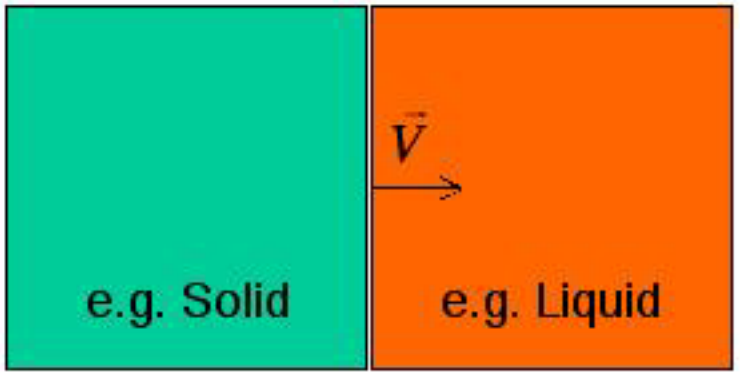
Multi-Phase Systems

So far single phase domainhave been involved. Whenthe system isphase in-homogeneous the total Free Enthalpy acquires a phase dependent "volume term" (actually, a surface term in D=2):

$$G = \sum_{i \in N_\phi} \int_i G_V(\phi_i)\, dV$$

As a consequence, the driving functional becomes:

$$\Pi_{P.T.}[v] = \Pi_{N.R.}[v] + \sum_{i \in N_{pl}} \int_{L_i} \Delta G_{L_i} v_n ds$$



Solving the equation for a planar interface:

$$\frac{v}{\mu} = \Delta G$$

Primary Growth

Single nucleus results

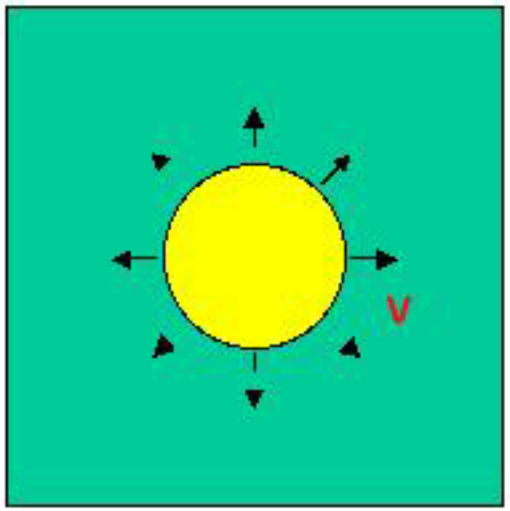
Applying the previous formalismto a spherical embryo creation one obtains the following functional:

$$\Pi_{P.T.}[v] = 2\pi \cdot R \cdot \frac{v^2}{2\mu} + 2\pi \cdot R \cdot v \cdot \Delta G_v - 2\pi \cdot v \cdot \gamma$$

Variationalprinciple provides nucleus evolution equations:

$$2\frac{1}{\mu}\frac{dR}{dt} = -\Delta G_v + \cdot\frac{\gamma}{R}$$

This behavior was firstpostulated by Hillert M. 1965 *Acta Metall* **13**,227



Primary growth law

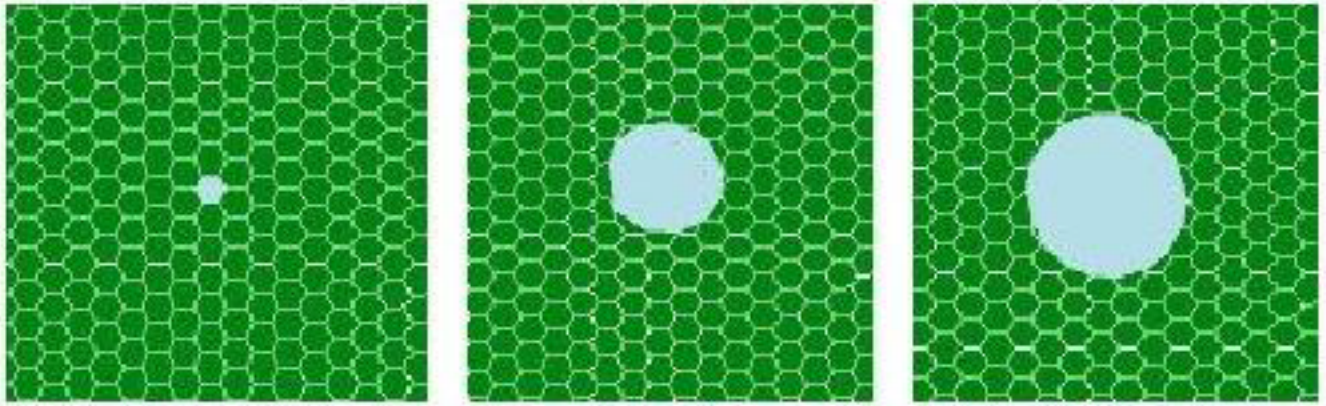
$$\frac{dr}{ds} = \pm\left(1 + \frac{1}{r}\right)$$

$$t = r - r_0 + \log\left(\frac{r-1}{r-r_0}\right) + t_0$$

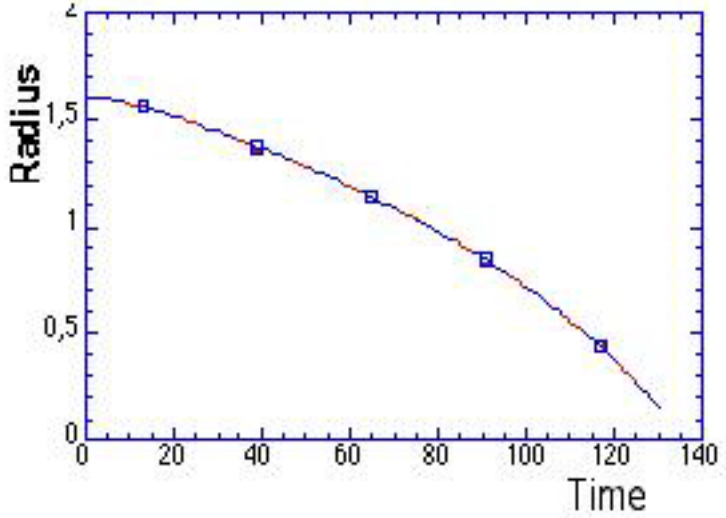
Scaled variables:
Critical radius: $R_c=\gamma/\Delta G$
Scaled time $s=\mu\ \Delta G/2R_c$
Reduced radius $r=R/R_c$

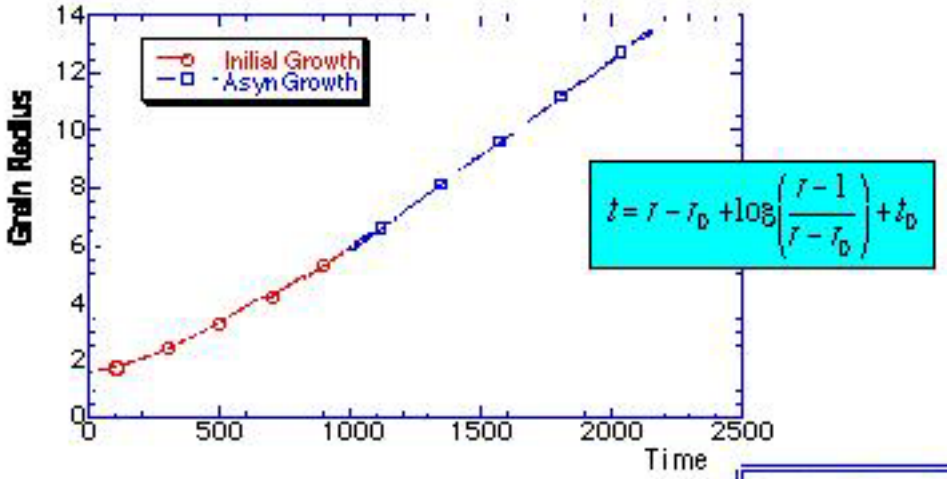
Embryo Evolution

Green cells cover aunique meta-stablephase domain (e.g. a overcooled liquid domain). Light blue cell represents amore stablenucleating phase.

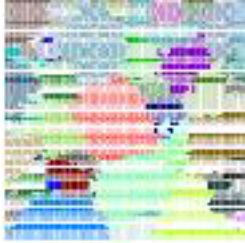


Edges separating greencells represent a computational artifact and do not contribute to physical quantities or network dynamics





Lattice Stochastic Chain



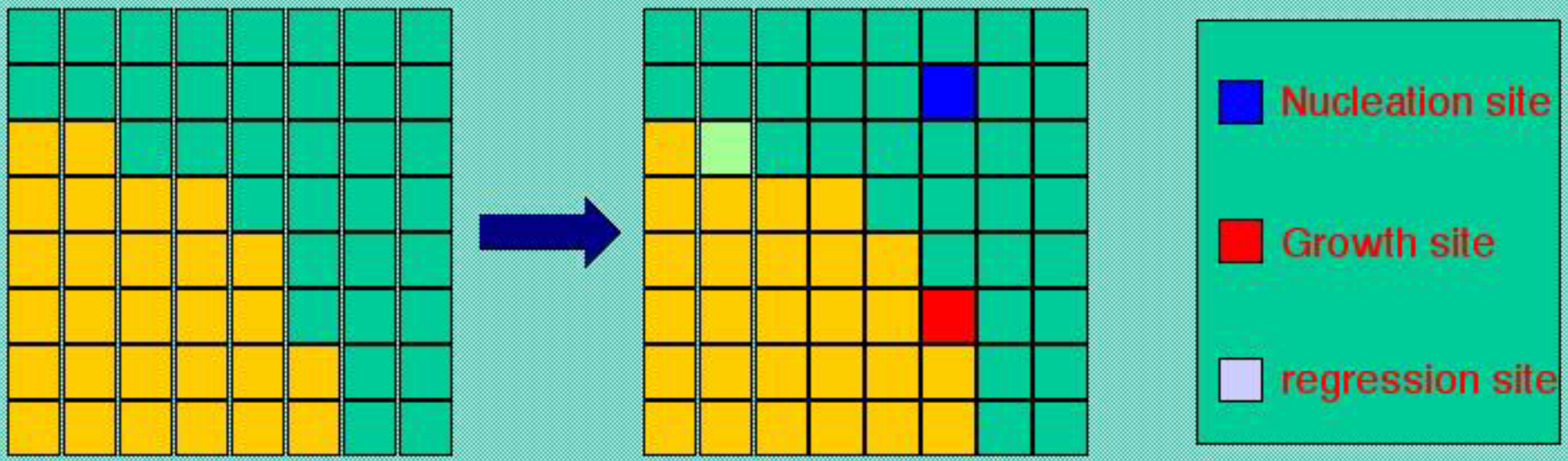
The model represents a *"discrete Markov chain"*

- Physical systems are partitioned by an assigned (squared) lattice. Discrete Time-step evolution is assumed.
- Each site represents a homogeneous portion of matter.
- Each site is assigned an order parameter (Index) representing the state of the system. Several other degrees of freedom are definite: average temperature, stress tensor, strain tensor etc.
- A 2-D crystal lattice orientation angle is assigned to "solid" sites.
- A stochastic transition matrix is defined accounting for nucleation and growth events.

Phase Transition Events

At any time step two possible processes have been accounted:

- Nucleation. Spontaneous phase transition.
- Phase growth Aggregation to an existing contiguous phase.

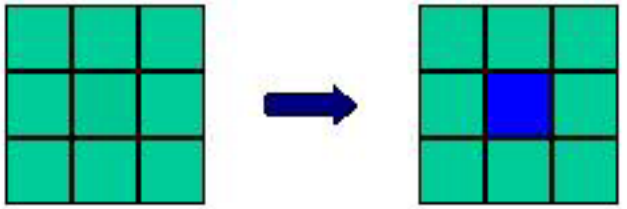


Transition Matrix

Lattice evolution is determined by the **transition probability matrix**

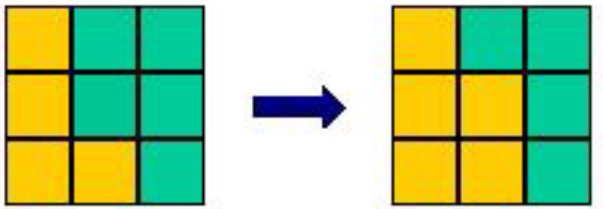
Assigned a **nucleation rate**: Γ, the critical nucleus formation probability per time step Δt is:

$$P_{nucl} = 1 - e^{-\Gamma \cdot \Delta t} \cong \Gamma \cdot \Delta t$$



Assigned a **growth probability** per unit length unit time: p the probability of including a site in a formed phase is:

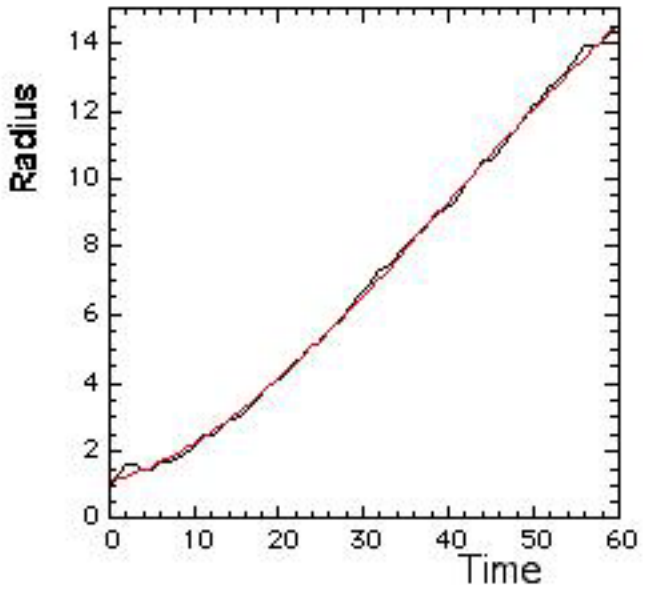
$$P_{incl} = 1 - \left[1 - \left(1 - e^{-p \cdot \Delta t}\right)\right]^N \cong N \cdot p \cdot \Delta t$$



N is number or neighboring sites of the growing phase.

Primary Growth

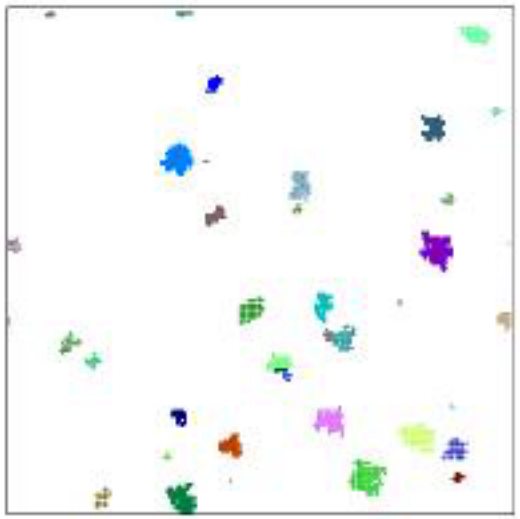
Single grain Growth



Quite surprising a single seed grows following the same universal law found for the Stochastic Network approach.

$$t = r - r_0 + \log\left(\frac{r-1}{r-r_0}\right) + t_0$$

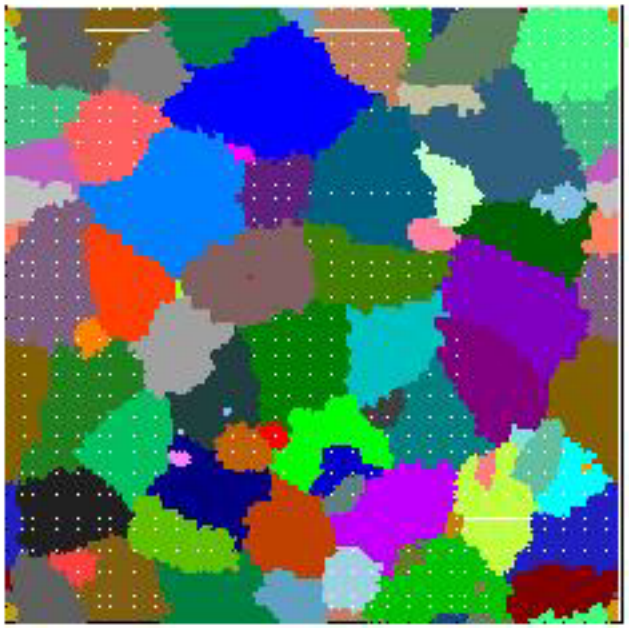
Typical Primary Growth

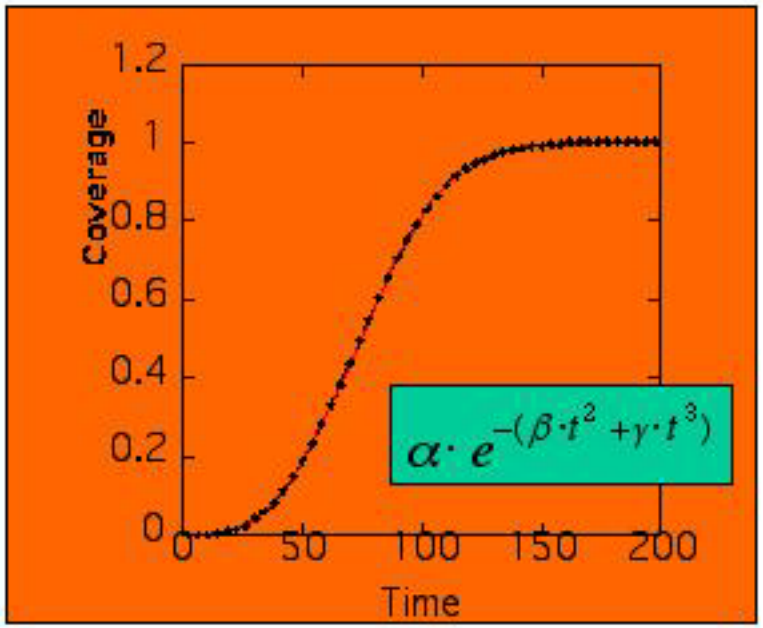


Space exhaustion

Primary growth stops when grains come in contact. By this way the space is totally filled.

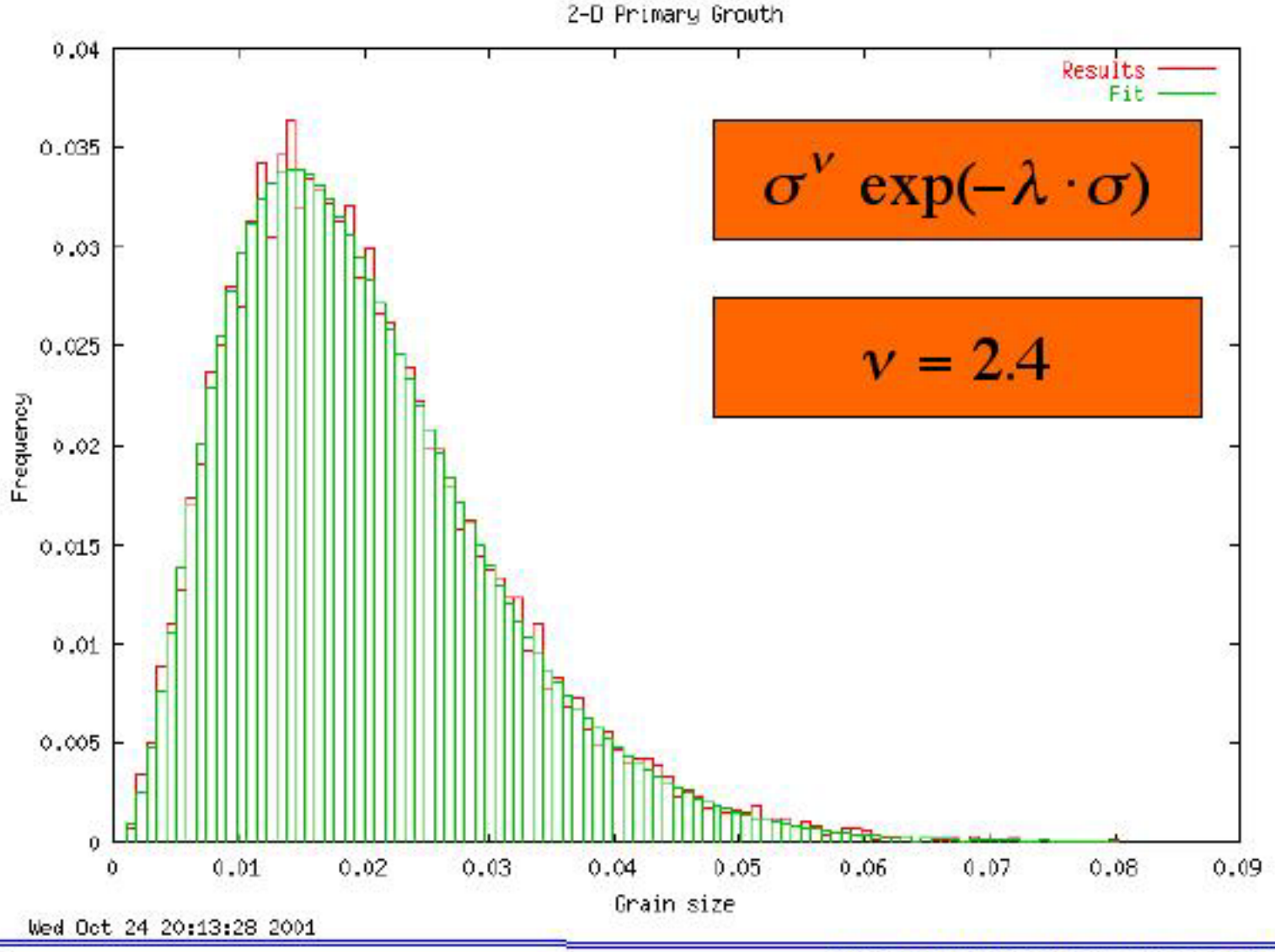
Space filling follows a (suitable variation of) Johnson, Mehl, Avrami, Kolmogorov Theory





Grain Size Distribution

Impurity dominated nucleation



Heat flow

Heat flow is accounted at any time step by solving deterministic

Fourier Equation: $\frac{\partial u}{c\partial t} = -\Delta u + W$

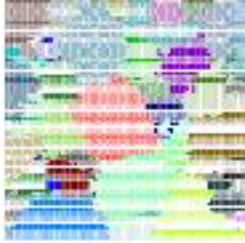
The variable *U* represents local internal energy (related to temperature) and

The constant C represents the product of specific heat times conductivity.
It contains all physical information as system local isotropy is assumed
W represents the resulting power:

$$W = W_{Ext} + W_{P.T.} + W_I$$

W_{ext} represents an external source term (e.g. laser supply)
$W_{P.T.}$ represents latent heat of possible (first order) Phase Transition
and
W_I represents heat released at interfaces and triple Junctions due to curvature or surface (i.e. length in D=2) reduction.

Temperature Evolution



Heat flow is accounted at any time step by an approximate solution of Fourier Equation:

$$u(t+\Delta t) - u(t) = \alpha[u_L(t) + u_R(t) + u_F(t) + u_B(t) - 4u(t)] + Q$$

B,F,L,R label neighbors, α is a suited function and Q represents power released during integration time (times c).

$$\alpha = \frac{1}{g}\left(1 - e^{-g\frac{c\Delta t}{\Delta x^2}}\right) \cong \frac{c\Delta t}{\Delta x^2}$$

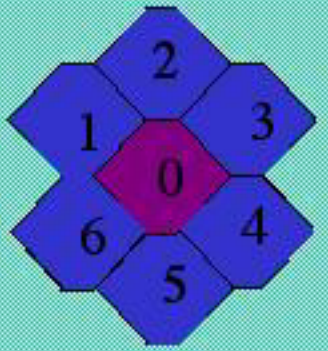
$$\alpha_\infty = \frac{1}{g}$$

g=5 (i.e. number of neighbors plus one) represents the correct asymptotic value for an isolate cluster as time interval goes to infinity. It allows energy conservation
g=4 represents the correct asymptotic value when an infinite system sustains neighbors temperature.

Deterministic Temperature Evolution S.N.

Iterative temperature evolution for a stochastic net

$$u(t+\Delta t) - u(t) = \alpha \cdot \left[\sum_{i=1}^{N} L_i \cdot u_i - L \cdot u(t) \right] + Q$$



Index i *spans on all neighboring cells*
α *is a time interval dependent function*

$$\alpha = \frac{1}{g}\left(1 - e^{-g\frac{c\Delta t}{\Delta x^2}}\right) \qquad g \approx L + L_0$$

$$i = 1, \cdots, Neighbors$$

$$L = \sum_{i=1}^{N} L_i$$

L_i can be length or surface of neighboring cells

Present ansatz represents a rough approximation for large cell sizes.

To improve temperature control ghost cells are introduced

Including Dislocations

A continuum distribution of dislocations in each grain

Application of an external load results into **additional energy-dissipation terms** in the functional $\Pi[v]$:

$$\Pi_D[v] = \Pi[v] + \sum_{N_g} \{ \int_S \Omega_{elastic}(\varepsilon_{kl}, \dot{\varepsilon}_{kl}) dS + \int_S \Omega_D(\dot{\varepsilon}_{kl}) dS \} - \int_{L_{ext}} (T \cdot v) ds$$

elastic deformation energy — **plastic deformation energy** — **external loading**

The **elastic energy dissipation** is trivially obtained by calculating the effective strain in each grain:

$$W_{elastic} = \frac{1}{2} C_{\alpha\beta\gamma\delta} \varepsilon^{(k)}_{\gamma\delta} \varepsilon^{(k)}_{\alpha\beta} \quad \Rightarrow \quad \Omega_{elastic} = \frac{\partial W}{\partial t} = C_{\alpha\beta\gamma\delta} \varepsilon^{(k)}_{\gamma\delta} \dot{\varepsilon}^{(k)}_{\alpha\beta}$$

The **plastic energy dissipation** is obtained from a non-linear-viscous stress strain relation as:

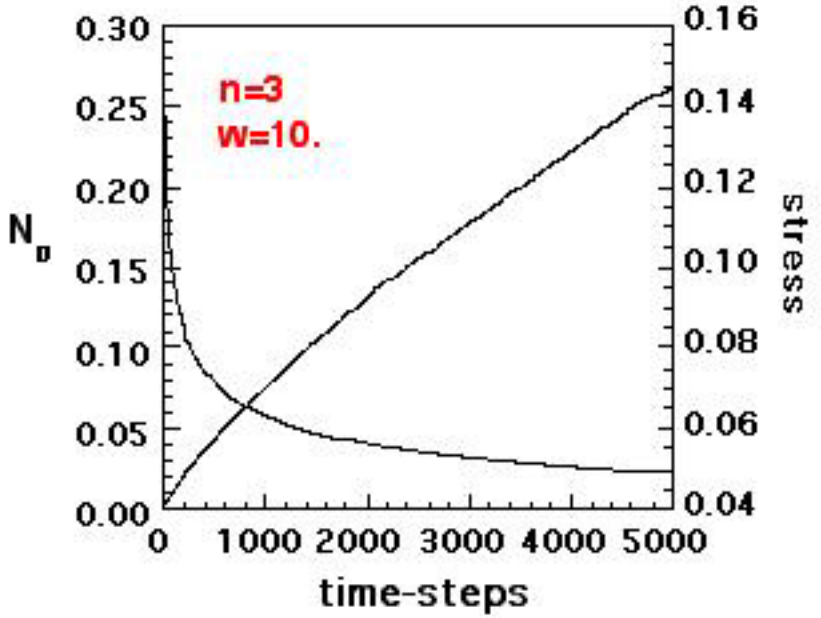
$$\int_0^{\dot{\varepsilon}_{kl}} \sigma_{ij} \, d\dot{\varepsilon}_{ij} = \Omega_D(\dot{\varepsilon}_{kl}) = \frac{n}{1+n} B(N_D) \dot{\varepsilon}^{(1+n)/n}$$

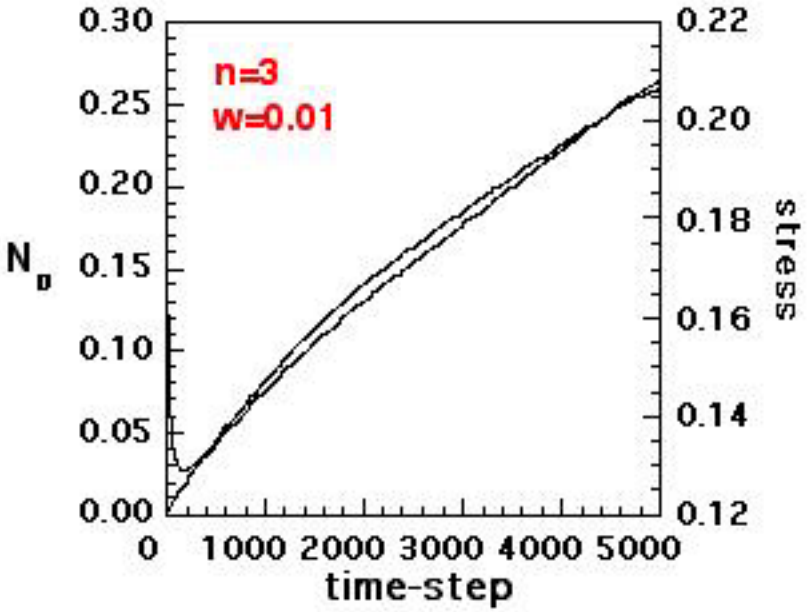
for a continuously-evolving **dislocation density** in each grain:

$$\frac{dN_D}{dt} = kN_D(\tau - AN_D^{1/2})^{m+1} \exp(-U/kT)$$

Preliminary results

The model is still in its infancy. We are still checking that under simple conditions (e.g. a few steps of straining at constant rate) the average quantities evolve as expected:





Evolution of the grain-averaged dislocation density and internal plastic stress for two different sets of model parameters.

Conclusions

- We have assessed a versatile bi-dimensional tool that allows (qualitative) reproduction of different phenomena such as: Phase Nucleation, Primary Growth, Grain Coarsening, Elastic and Plastic Deformation of poly-crystalline systems. Heath flow control is also accounted.

- Consistent Results from both Stochastic Network and Lattice Markov Chain were presented concerning 2-D primary growth.

- Future theoretical work on the subject will possibly focus on:
  - -Dendridic primary growth simulation.
  - -A deeper understanding of dislocation dynamics.
  - -Improving temperature control
  - -Extension to 3D System (ongoing for Lattice Markov Chain)