

METRO

MEtallurgical TRaining On-line



# Numerical modelling of micro-scale phenomena and micro-structure

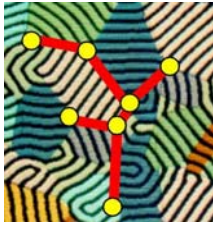
Interface tracking and interface non-tracking techniques

Olga Wodo

CzUT



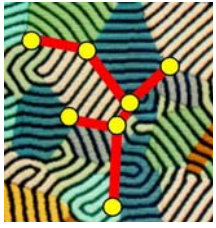
Education and Culture



# Outline



- Introduction
- Cellular automata technique
- Phase Field Method
- Summary
- Keypoints and sources

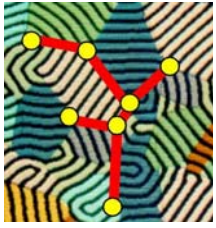


# Motivation



- grain structure influence the mechanical properties (Hall-Petch relation)
- micro-structure modelling gives the possibilities to simulate evolution of the grain morphology
- understanding and quantitatively description of mechanism controlling development of the structure are essential in designing the welding and casting technologies

$$\sigma_y = \sigma_0 + k_y \cdot d^{-1/2}$$

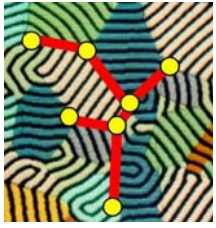


# Introduction



## Different - scale structure:

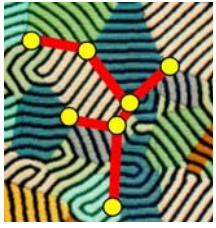
- micro-scale - micro-structure
- nano-scale - nano-phenomena  
like: growth atom attachment to the interface
- meso-scale - grain



# Physical introduction



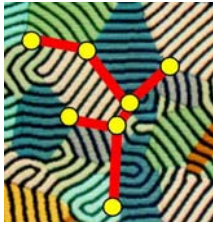
- nucleation and growth processes + grain orientation should be considered in the model
- coupling between macro and micro- scale
- micro-structure is defined by many parameters, like: the phases, grains, defects, volume fractions, the morphologies, etc.
- micro-structure depends on many factors, like: properties of the phases, and on local solidification processing condition.



# Micro-structure modelling methods



- **Deterministic**
- **Stochastic**



# Micro-structure modelling methods

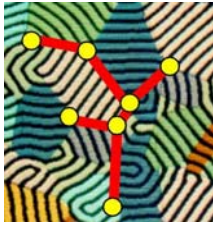


- interface tracking methods  
(e.g. Cellular Automaton - CA)
- interface non-tracking techniques  
(e.g. Phase Field method - PF)



# Cellular Automata Method





# Cellular Automata

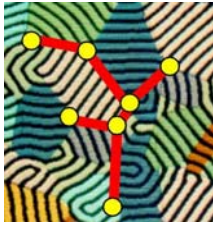


## CA (M,S,T)

**M** – mesh of cells (neighbourhood defined)

**S** – states (solid, liquid, interface ect.)

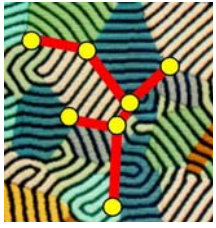
**T** – transition rules from one state to another  
(deterministic, probabilistic)



# Cellular Automata



- CA as a technique originally proposed in the **1940s** by Ulam and von Neumann
- Utilized for microstructure modelling in the **1990s** by Rappaz, Gandin and Sasikumar, Sreenivasan

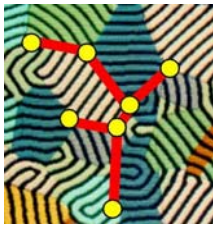


# Cellular Automata

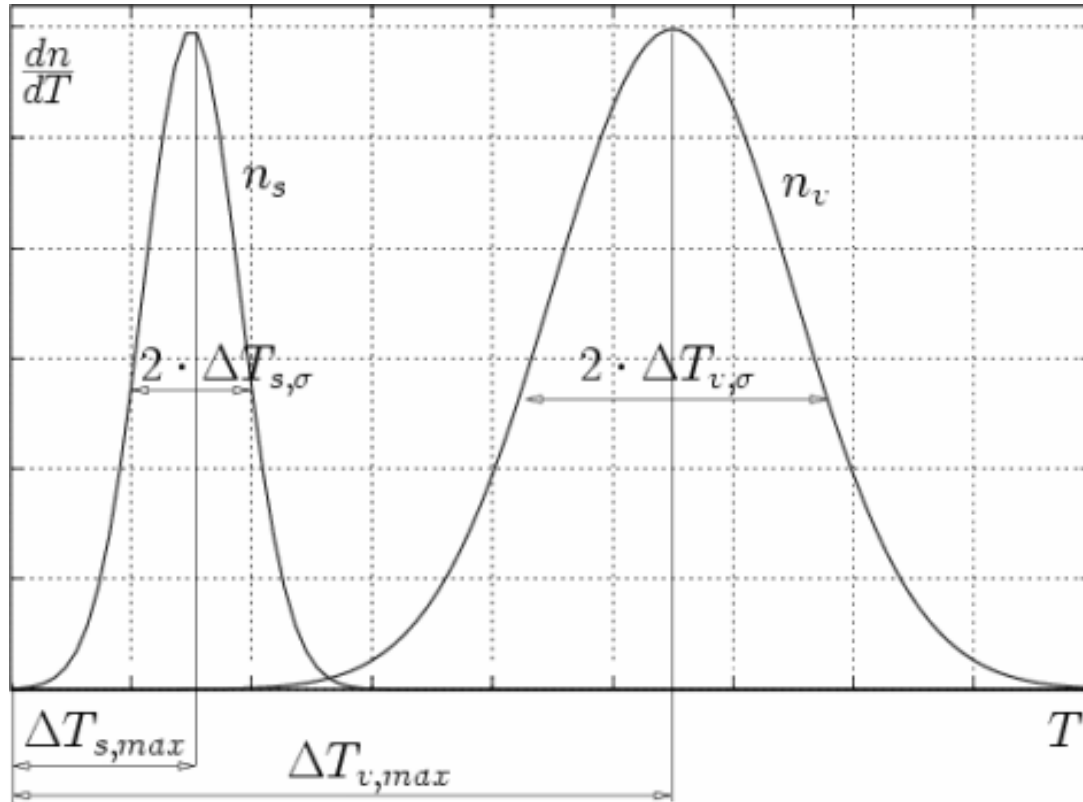


## Micro-structure modelling:

- “classical” CA model - CA
- “modified” CA model - MCA



# Classical CA model

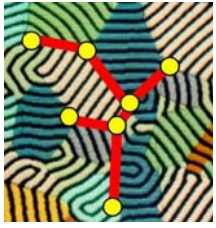


Nucleation process:  
Gaussian distribution

$$n_s = \frac{\pi}{4} [n_s^*]^2$$

$$n_v = \sqrt{\frac{\pi}{6}} [n_v^*]^{3/2}$$

$$n(\Delta T) = S \int_0^{\Delta T} \left[ \frac{n}{\Delta T_{\sigma} \sqrt{2\pi}} \exp\left(-\left(\frac{\Delta T' - \Delta T_{max}}{\sqrt{2}\Delta T_{max}}\right)^2\right) \right] d(\Delta T')$$

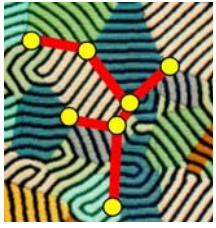


# Classical CA model



## Preferential crystallographic orientation:

- grains are growing along the random orientation
- type of metal determines the crystallographic directions
- 48 classes of orientation between  $-45^\circ \div 45^\circ$



# Classical CA model

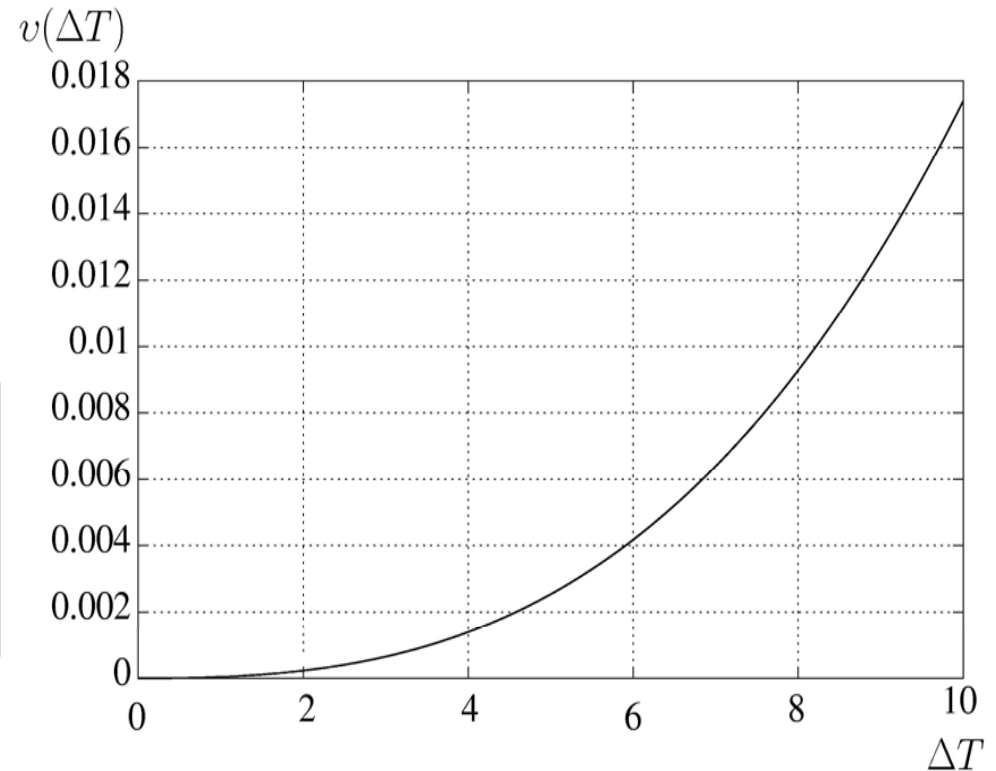


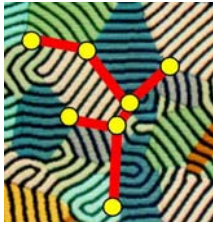
## Growth algorithm

- utilizes the KGT model

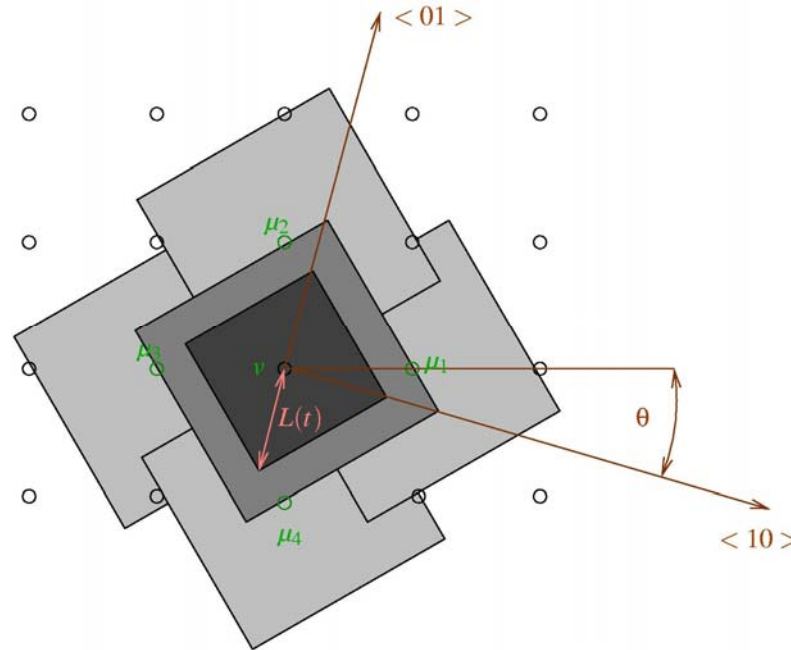
$$\Delta T = \Delta T_c + \Delta T_t + \Delta T_k + \Delta T_r$$

$$v = a_2 \Delta T^2 + a_3 \Delta T^3$$





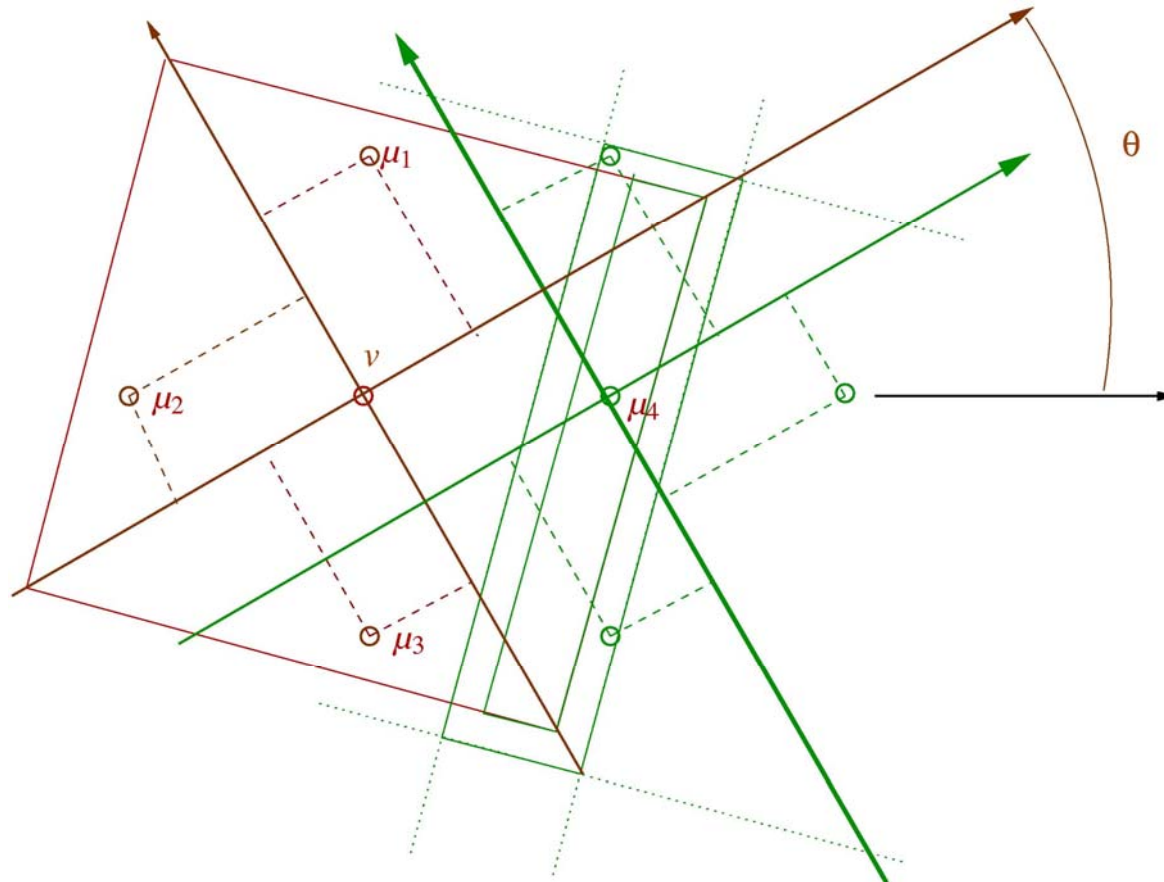
# Classical CA model



$$L(t) = \int_{t_N}^t v[\Delta T(t')] dt'$$

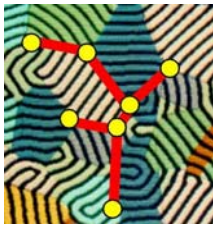


# Classical CA model

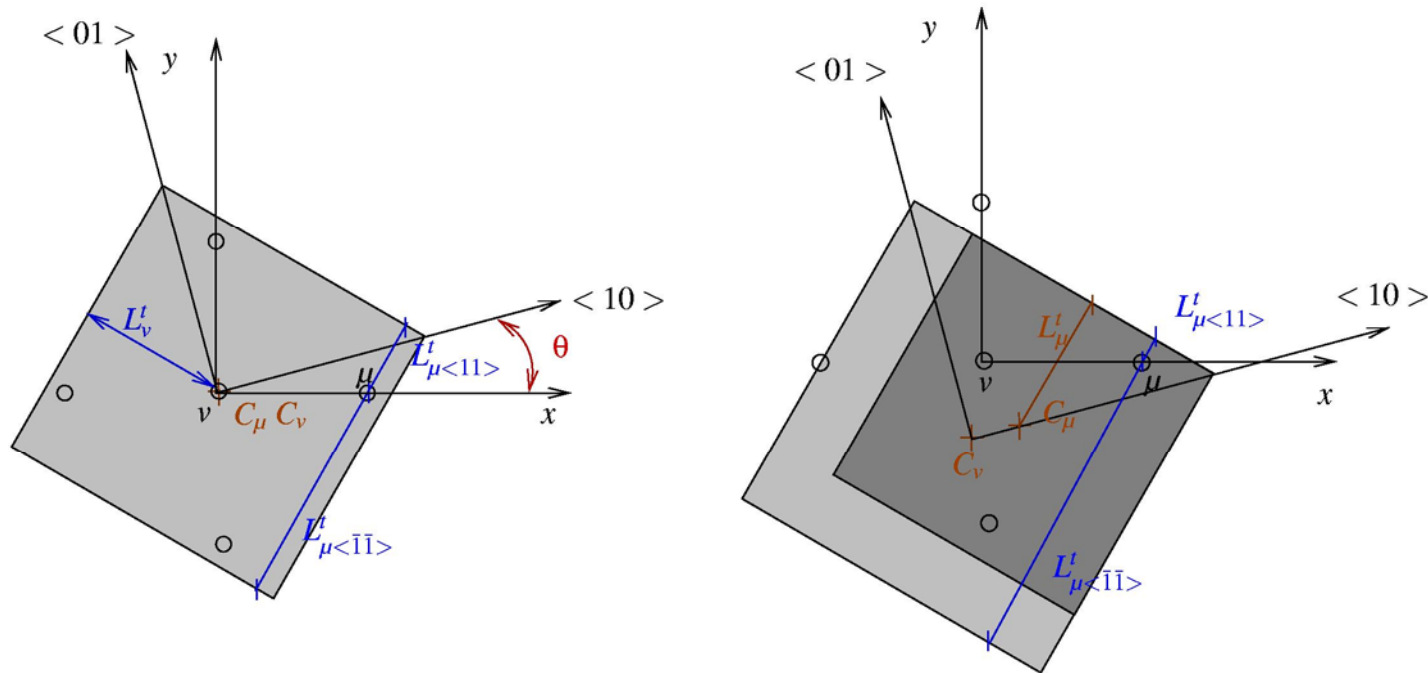


[2] Gandin, Ch.-A. and Rappaz, M. Acta metall. mater., Vol.42, No.7, pp.2233-2246, 1994



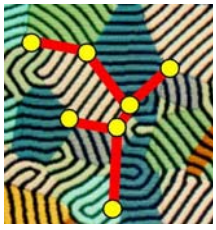


# Classical CA model

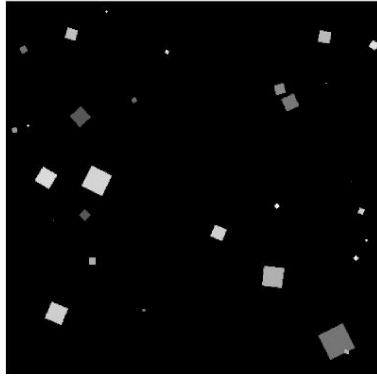


$$L_{\mu}^t = \frac{1}{2} [\text{Min}(L_{\mu\langle 11 \rangle}^t, \sqrt{2} \cdot dl) + \text{Min}(L_{\mu\langle \bar{1}\bar{1} \rangle}^t, \sqrt{2} \cdot dl)]$$

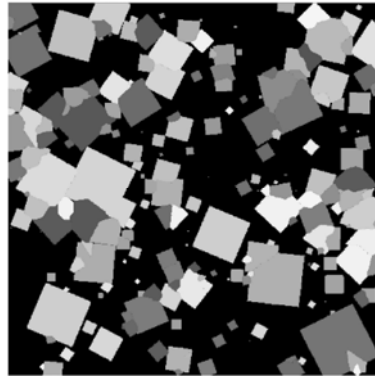
[3] Gandin, Ch.-A., Rappaz, M. Acta mater., Vol.45, No.5, pp.2187-2195, 1997



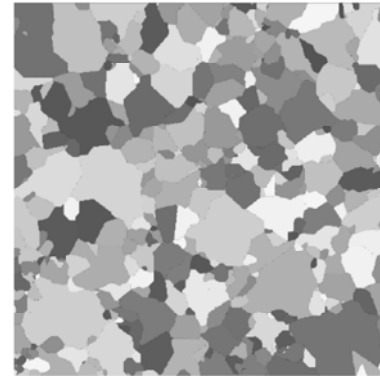
# Classical CA model



(a)



(b)



(c)

$n$	$5.5 \cdot 10^{10}$	$[m^{-3}]$
$\Delta T_{\sigma}$	0.1	$[K]$
$\Delta T_{\max}$	10.5	$[K]$
$a_2$	$2.9 \cdot 10^{-6}$	$[\frac{m}{sK^2}]$
$a_3$	$1.49 \cdot 10^{-6}$	$[\frac{m}{sK^3}]$



# Classical CA model



(a)

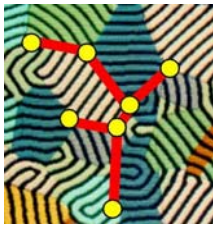


(b)



(c)

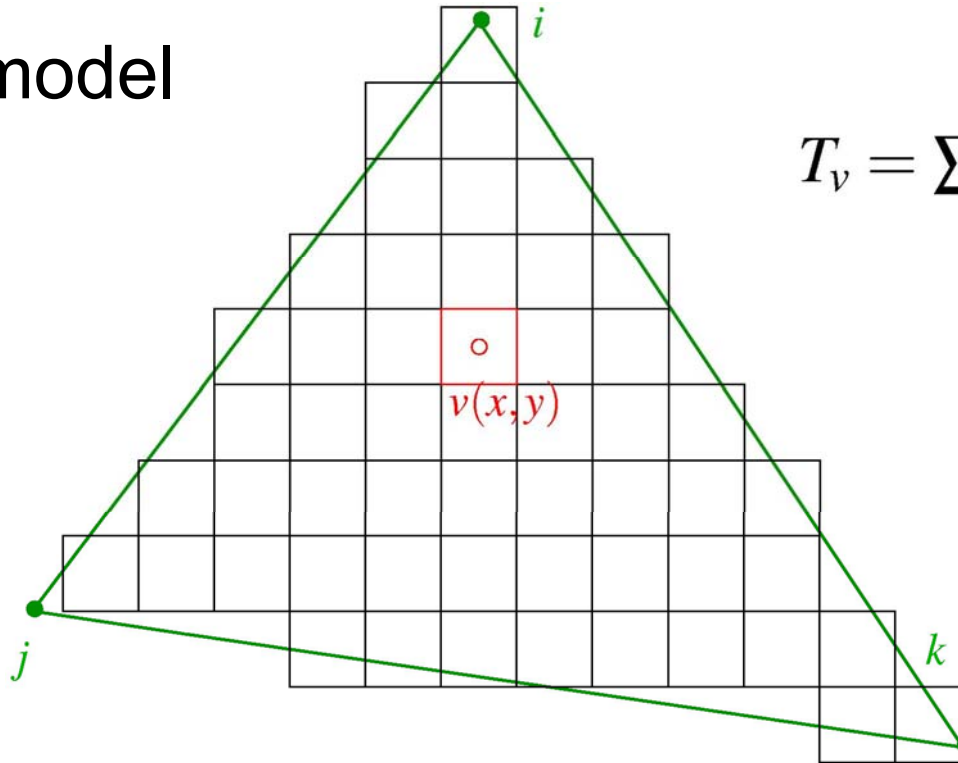
	$\Delta T_{s,max} [K]$	$\Delta T_{v,max} [K]$
(a)	0.5	6.0
(b)	0.5	8.0
(c)	0.5	10.5



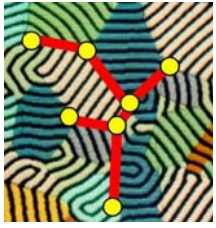
# Classical CA model



## CAFE model



$$T_v = \sum_n \phi_{vn} T_n^t$$



# Classical CA model

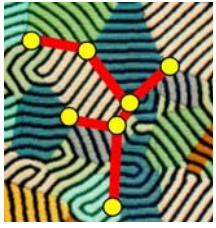


- 1) no variation of the volume fraction
- 2) increase of solid fraction of the already mushy zone

$$\delta f_{s,v} = \frac{-\delta H_v}{\rho c_p (T_L - T_m) (k-1) [1 - f_{s,v}^t]^{k-2} + \Delta H_f}$$

- 3) increase of solid fraction of cell which was liquid

$$\delta f_{s,v} = 1 - \left[ \frac{T_v^t - T_m}{T_L - T_m} \right]^{1/(k-1)}$$



# Classical CA model



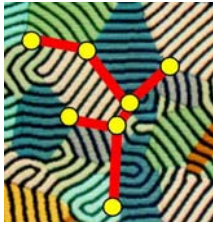
Solid fraction update in nodes:

$$\delta f_{s,n} = \frac{\sum_v \phi_{vn} \cdot \delta f_{s,n}}{\sum_v \phi_{v,n}}$$

Temperature update in nodes:

$$\delta H_n = \rho c_p [T_n^{t+\delta t} - T_n^t] - \Delta H_f [f_{s,n}^{t+\delta t} - f_{s,n}^t]$$

[2] Gandin, Ch.-A. and Rappaz, M. Acta metall. mater., Vol.42, No.7, pp.2233-2246, 1994



# Classical CA model



## CAFE model advantages:

- ability to predict grain structure using local rules – CA
- physical mechanisms involved in the dendritic growth
- coupled with the macro-scale temperature calculation
- predicts satisfactory the grain structure in various solidification processes
- ability to predict CET
- predict as-cast structure thanks to the 3D model
- it is utilized in commercial software – CalcoSoft



# Classical CA model



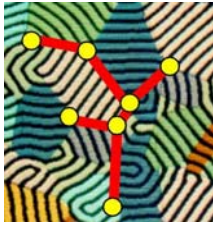
## CAFE model drawbacks:

- ability to predict only grain structure,
- some assumption:  
nucleation radius of grain is neglected, KGT model.

## Numerical problems:

- two time steps,
- memory requirement - the dynamic allocation of cells.





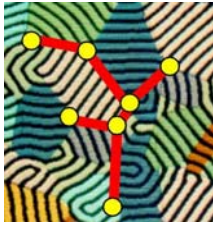
# Modified Cellular Automata



## Modified Cellular Automata

(include also solute distribution):

- first type (based on the numerical solutions of the transport equations including boundary condition on the interface)
- second type (based on the analytic solutions of dendritic growth)



# Modified Cellular Automata

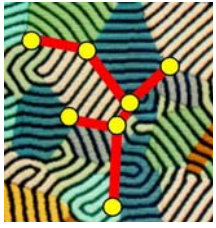


Transport processes:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( K \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( K \frac{\partial T}{\partial y} \right) - \rho L \frac{\partial f_l}{\partial t}$$

$$\frac{\partial C_l}{\partial t} = \frac{\partial}{\partial x} \left( D_l \frac{\partial C_l}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_l \frac{\partial C_l}{\partial y} \right)$$

$$\frac{\partial C_s}{\partial t} = \frac{\partial}{\partial x} \left( D_s \frac{\partial C_s}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_s \frac{\partial C_s}{\partial y} \right)$$



# Modified Cellular Automata

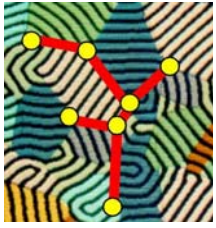


Solid-liquid interface:

$$C_s^* = kC_l^*$$

$$V_n^* C_l (k - 1) = [-D_l (\frac{\partial C_l}{\partial x} + \frac{\partial C_l}{\partial y}) + D_s (\frac{\partial C_s}{\partial x} + \frac{\partial C_s}{\partial y})] n$$

$$T^* = T_l^{eq} + (C_l^* - C_0) m_l - \Gamma \bar{\kappa} f(\gamma, \theta)$$



# Modified Cellular Automata



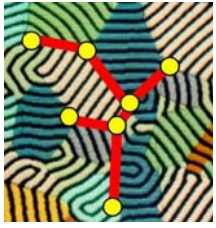
## Stochastic element:

- nucleation (e.g. Gaussian distribution)
- growth

all cells in the neighbourhood are change into interface  
probability determines if it is change into interface state

$$p_c = \frac{1}{\sqrt{\tan^2\theta + 1}}$$

- artificial anisotropy

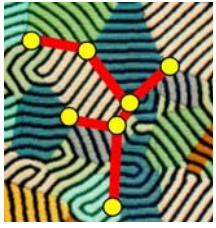


# Modified Cellular Automata



$$V_x(i, j) = \frac{D_l}{dl(1-k)} \left[ \left( 1 - \frac{C_l(i-1, j)}{C_l^*(i, j)} \right) f_l(i-1, j) + \left( 1 - \frac{C_l(i+1, j)}{C_l^*(i, j)} \right) f_l(i+1, j) \right] \\ + \frac{kD_s}{dl(1-k)} \left[ \left( 1 - \frac{C_s(i-1, j)}{kC_l^*(i, j)} \right) f_s(i-1, j) + \left( 1 - \frac{C_s(i+1, j)}{kC_l^*(i, j)} \right) f_s(i+1, j) \right]$$

$$\delta f_s = \frac{\delta t}{dl} (V_x + V_y - V_x V_y \frac{\delta t}{dl}) \\ f_s^n = f_s^o + \delta f_s \\ V_n^* = \delta f_s \frac{dl}{\delta t}$$



# Modified Cellular Automata

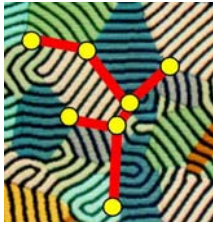


$$C_l^* = C_0 + \frac{T^* - T_l^{eq} + \Gamma \bar{\kappa} f(\gamma, \theta)}{m_l}$$

$$\bar{\kappa} = \frac{1}{dl} \left( 1 - 2 \frac{f_s + \sum_{k=1}^N f_s(k)}{N + 1} \right)$$

$$f(\gamma, \theta) = 1 + \delta(4(\gamma - \theta))$$

$$\cos \gamma = \frac{V_x}{\sqrt{V_x^2 + V_y^2}}$$



# Modified Cellular Automata

Read Database, Generate Mesh;

**repeat**

Assign State to Cells;

Compute *time step*;

Compute temperature distribution;

**if**  $T < T_l$  **then**

Nucleation and Growth considered;

Compute  $V_x, V_y$ ;

Compute  $\delta f_s, f_s$ ;

Compute  $\bar{\kappa}, f(\gamma, \theta)$ ;

Compute  $C_l^*$  ;

Compute solute distribution ;

**until** *All cells in solid phase ;*

[6] Nastac. L. Acta mater., Vol. 47, No. 17, pp. 4253-4262, 1999



# Modified Cellular Automata



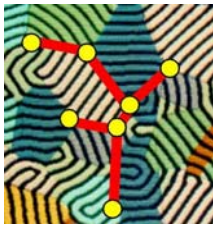
## Second type of MCA:

- nucleation - Gaussian distribution
- 48 classes of crystallographic orientation
- growth kinetics – KGT model
- undercooling

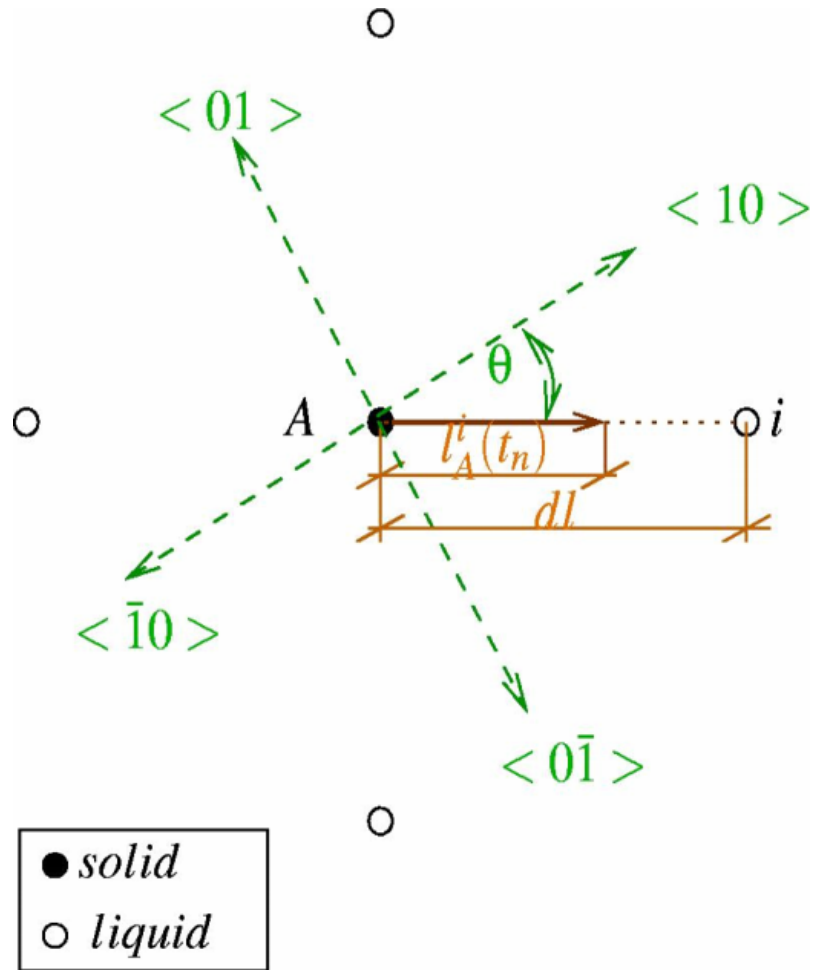
$$\Delta T_i(t_n) = T_l - T_i(t_n) + (C_i(t_n) - C_0)m - \Gamma \bar{\kappa}_i(t_n)$$

$$\bar{\kappa}_i = \frac{1}{dl} \left[ 1 - 2 \frac{f_s(i) + \sum_{j=1}^n f_s(j)}{n+1} \right]$$





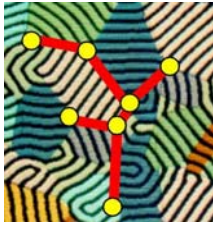
# Modified Cellular Automata



$$l_A^i(t_n) = \frac{\sum_{n=1}^N v_n(\Delta T(t_n))\Delta t_n}{\cos\theta + |\sin\theta|}$$

$$f_s^i(t_n) = \frac{l_A^i(t_n)}{dl}$$

$$\delta T_L = \frac{\delta H_v dl^2}{\rho c_p d X_{cv}^2}$$



# Modified Cellular Automata



Generate Mesh;

Compute *CV time step*;

**repeat**

    Compute temperature distribution;

    Compute *CA time step*;

**if** *cell state changed from liquid to solid* **then**

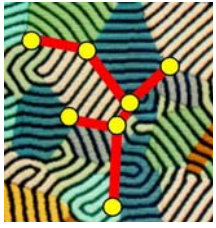
        Partition solute and liberate latent heat;

        Update the temperature within the CV;

    Compute solute diffusion;

**until** *All cells in solid phase* ;

[8] Zhu, M.F. and Hong C.P. ISIJ International, Vol.41, No.5, pp.436-445, 2001

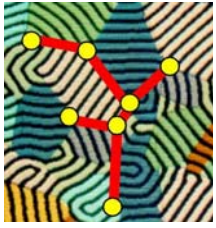


# Modified Cellular Automata



## Prons:

- the growth of the morphology inside the grains can be observed (the curvature and the anisotropy of the interface are taken into account)
- dependence of solid fraction from temperature and solute concentration is easy to derived from the simulations.
- these techniques can be considered as a bridge between the microscopic and mesoscopic simulations.
- no assumptions about the final shape of the interface are made. The shape is determined as a result of computations.
- it helps us to visualise the development of the structure (great educational value)

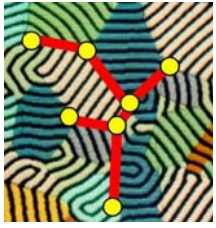


# Modified Cellular Automata



## Cons:

- the anisotropy introduced by the square shape of cell
- application of empirical oriented procedures for calculating the anisotropy and the curvature
- necessity to track the interface



# Modified Cellular Automata

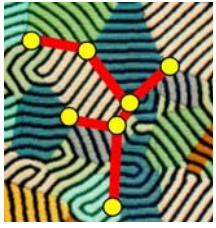


## Eutectic morphology

(two phases, diffusion of both solute and surface energy, competitive growth and the cooperative growth should be embedded):

Zhu and Hong extended model:

$$\Delta T(t_n) = T_E - T_i(t_n) + (C_i(t_n) - C_0)m - \Gamma \bar{\kappa}(t_n)$$



# Modified Cellular Automata

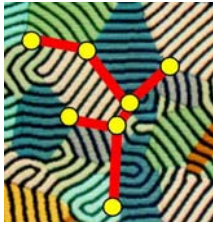


Solute distribution:

$$\frac{\partial C}{\partial t} = D\nabla^2 C + C(1 - k_\alpha) \frac{\partial f_{s,\alpha}}{\partial t} + (C - C_{\beta 0}) \frac{\partial f_{s,\beta}}{\partial t}$$

The branching, competitive and cooperative growth were embedded.

Model which couples dendritic growth with interdendritic eutectics was also proposed.



# Phase Field Method



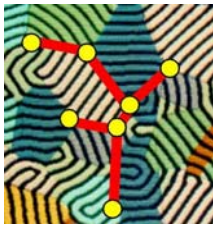
# Phase Field



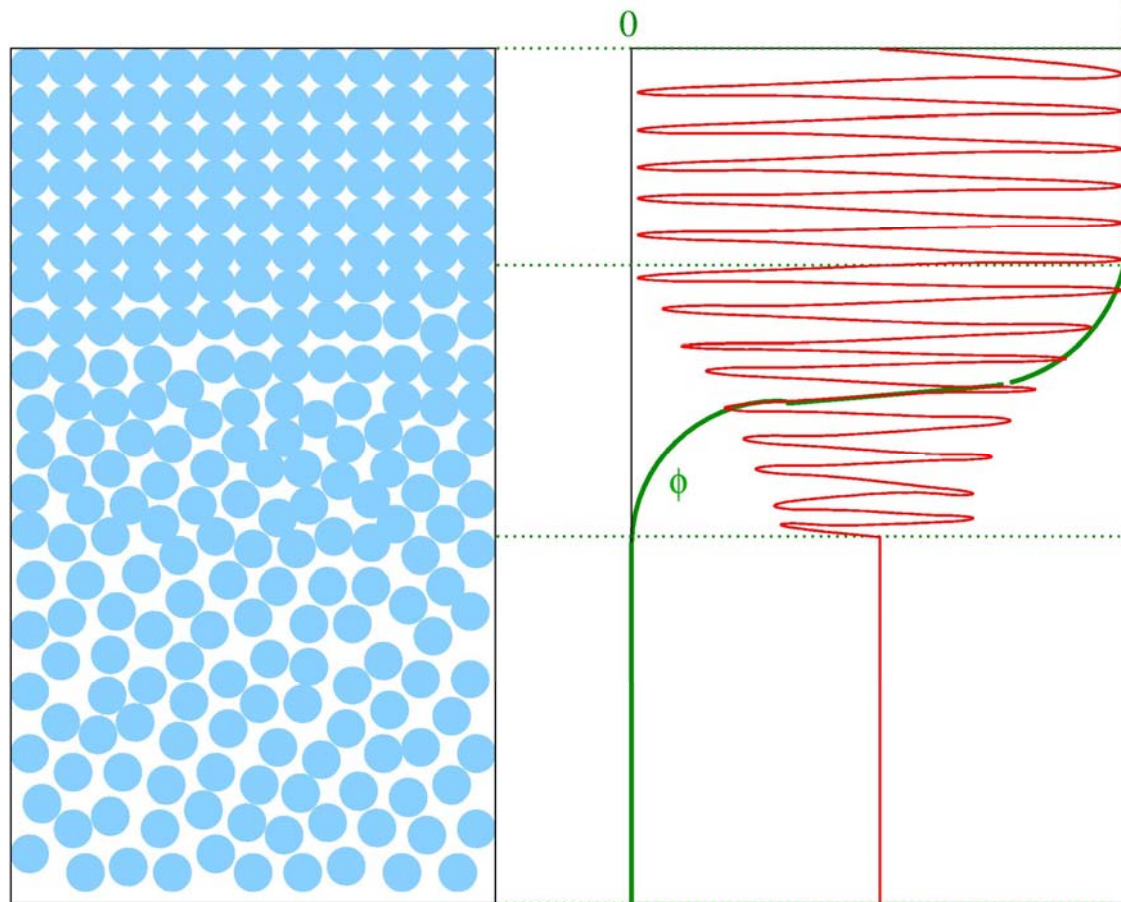
- PF introduced by the Collins, Levine and Caginalp and Fife in 80s.
- the basis proposed earlier by Landau and Chalatkow in 50s

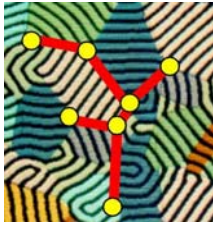
The theory of Landau states that free energy of Gibbs is continuous function of pressure, temperature and so called “order parameter”





# Phase Field





# Phase Field

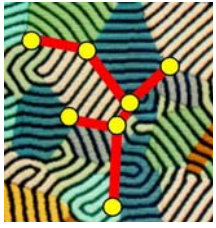


- equation of motion for the phase field parameter

$$\tau \frac{\partial \phi}{\partial t} = - \frac{\delta F}{\delta \phi}$$

- free energy functional

$$F = \int \left( \frac{W^2}{2} |\nabla \phi|^2 + f(\phi, T) \right) dV$$



# Phase Field

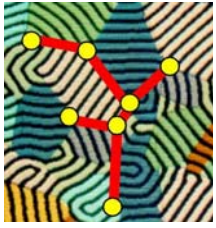


- equation of motion for the phase field parameter

$$\tau \frac{\partial \phi}{\partial t} = W^2 \nabla^2 \phi + f_\phi(\phi, T)$$

- heat transfer equation

$$\lambda \nabla^2 T = c_p \frac{\partial T}{\partial t} + \frac{L}{2} \frac{\partial \phi}{\partial t}$$



# Phase Field



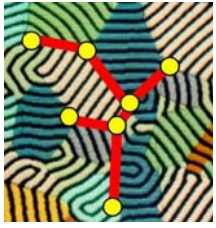
## Free energy density - double-well potential

- Langer and Caginalp [13] (minima at -1, 1)

$$f(\phi, T) = \frac{(\phi^2 - 1)^2}{16a} + \alpha(T - T_M)\phi$$

- Kobayashi [13] (minima at 0 and -1)

$$f(\phi, T) = W \int_0^\phi p(p-1)[p - \frac{1}{2} - \beta(T)]dp$$



# Phase Field

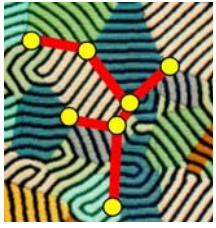


- Wang et al. [17](minima at 0 and 1)

$$f(\phi, T) = f(\theta) + \lambda T g(\phi)$$

- Entropy formulation [13]

$$S = \int \left[ -\frac{W^2}{2} |\nabla \phi|^2 + s(\phi, e) \right] dV$$



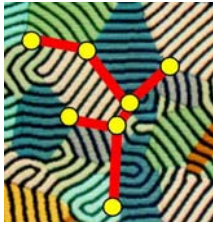
# Phase Field



**Anisotropy** introduce by:

- modification of the square gradient term in the free energy functional
- inclusion of the nearest-neighbour-interactions
- width of the interface depend on the angle of the normal vector of phase field gradient to a fixed direction

$$W(\theta) = \xi\eta(\theta)$$



# Phase Field



Example introduction of the anisotropy:

$$W = \bar{W}\eta = \bar{W}(1 + \gamma_w \cos(k_w \theta))$$

$$\tan \theta = \frac{\phi_y}{\phi_x}$$

Motion equation for phase field with anisotropy effect:

$$-\tau \frac{\partial \phi}{\partial t} = \frac{\partial f}{\partial \phi} + \bar{W}^2 \nabla \cdot (\eta^2 \nabla \phi) - \bar{W}^2 \frac{\partial}{\partial x} (\eta \eta' \frac{\partial \phi}{\partial y}) + \bar{W}^2 \frac{\partial}{\partial y} (\eta \eta' \frac{\partial \phi}{\partial x})$$

$$\eta' = \frac{\partial \eta}{\partial \phi}, \quad \theta_x = \frac{\phi_x \phi_{xy} - \phi_y \phi_{xx}}{|\nabla \phi|^2}, \quad \theta_y = \frac{\phi_x \phi_{yy} - \phi_y \phi_{yx}}{|\nabla \phi|^2}$$



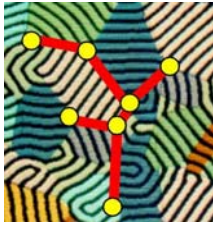
# Phase Field



Sharp-interface model  
is limiting case of the phase-field model

- asymptotic analysis
- thickness of the interface
- the grid spacing



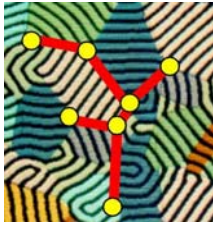


# Phase Field



## Other models:

- models for binary alloys
- isothermal growth and non-isothermal growth of dendrites
- peritectic and eutectic growth
- polycrystalline material
  - free energy density has  $N$  minima
  - introduce  $N$  order parameter
  - introducing new terms into free energy functional



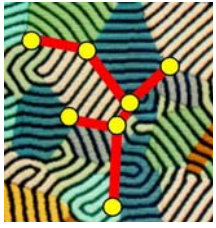
# Phase Field



No unique phase field model - family of phase field models

## Advantages:

- may allow to simulate the plane, cellular and dendritic interface growth
- models include such processes like: diffusion of heat and solute, the coarsening of the dendritic structure
- omits necessity to track the location of interface
- gives opportunity for better understanding the dynamics of the process
- allows to model growth of pure metals, binary alloys, eutectic solidification, peritectic solidification.

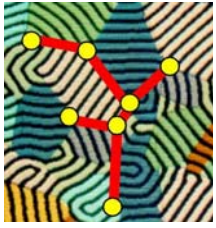


# Phase Field



## Drawbacks:

- asymptotic analysis must be done
- large computational requirement for the width of the interface several grid points should be spread over thickness region
- system of equations is strong non-linear

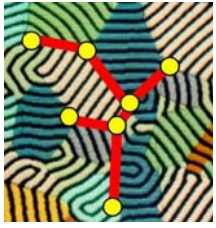


## PF+CA model



Modified cellular automata model with the diffuse interface:

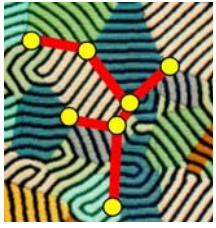
- the solid fraction is first evaluated by the classical sharp interface
- then is diffuse in the cells around the solid/liquid interface.
- the continuum model for species and momentum transfer solved
- convection can be examine.



# Keypoints



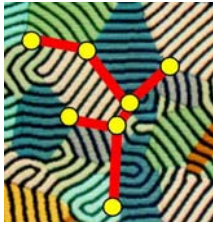
- to understand the micro-structure formation we can use the experimental techniques, analytical and numerical methods
- two types of the techniques have been presented: cellular automata and phase field method.
- they begin to be developed in the same period of time.
- PF the phase field method does not require the interface tracking.
- the cellular automata method the tip of the dendritic arm or the interface is tracking



# Keypoints - CA



- CA is a triple of: mesh, states, and transition rules
- three states are usually defines: S, L, I
- nucleation and growth processes considered
- preferential orientation take into account
- temperature solute fields are determined
- MCA takes into account also curvature and anisotropy
- CAFE model is utilized in real-life applications
- CA is reasonable less consuming comparing to PF
- two time stops may be utilized.



## Keypoints - PF



- there is no unique phase field method, but rather a family of the models,
- introduces the order parameter called phase field, which is changed smoothly from one value into another,
- the equation of motion is utilized for this parameter,
- the functional of free energy or the entropy must be formulated,
- the anisotropy may be introduced in several different ways,
- the sharp interface model is limiting case of the phase field method,
- several models for polycrystalline micro-structure were also proposed.

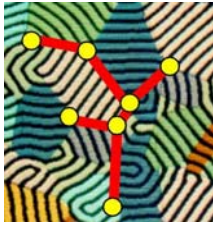


# Summary



- **PF** and **CA** can give the same qualitative results
- Suffers from:
  - **CA** – anisotropy introduced by cell mesh
  - **PF** – interface width, several grid points within the interface region.

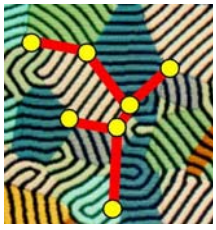




# Summary



Due to the continuous development in the computer science and numerical methods, more and more models are proposed and many limitations are being eliminated. More factors are included in the models, however, we are still far from the complex multi-scale analysis.

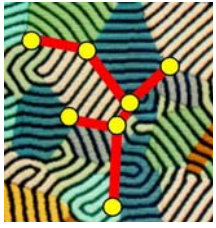


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## Phase Field

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## CA+PF

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