Modeling of dendritic growth –

are there alternatives to the phase field method?

Markus Rettenmayr, Klemens Reuther
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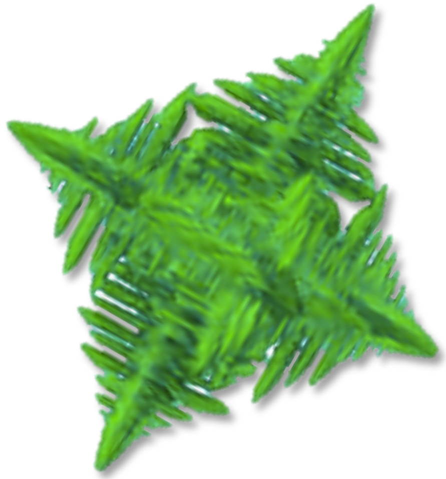
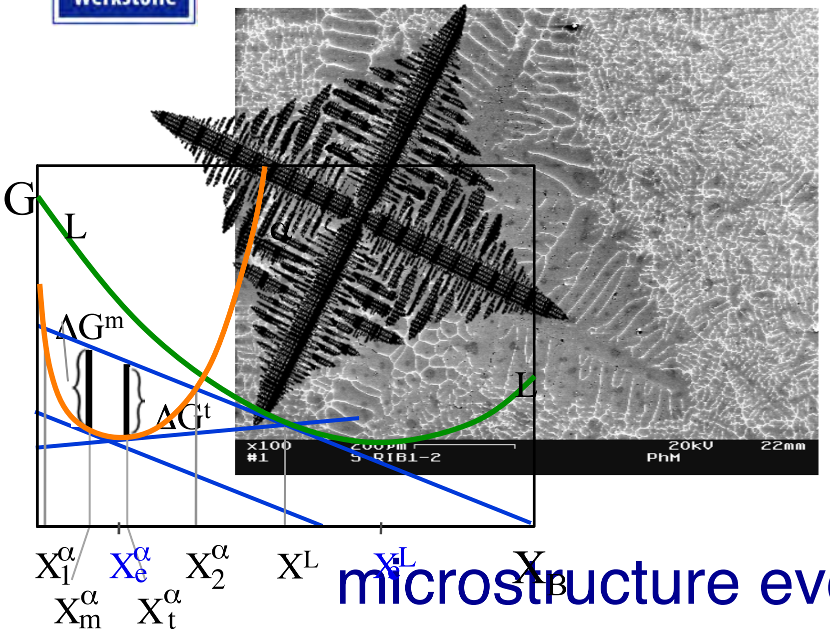
Chair of Metallic Materials



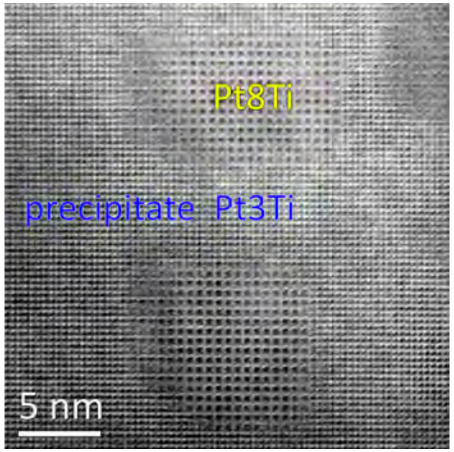
Nova Gorica, 27.3.2014

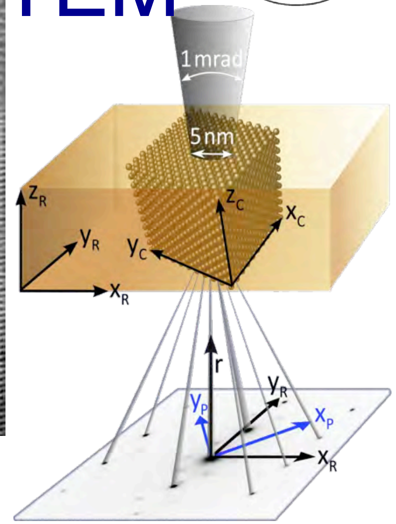
Metallic Materials – research fields

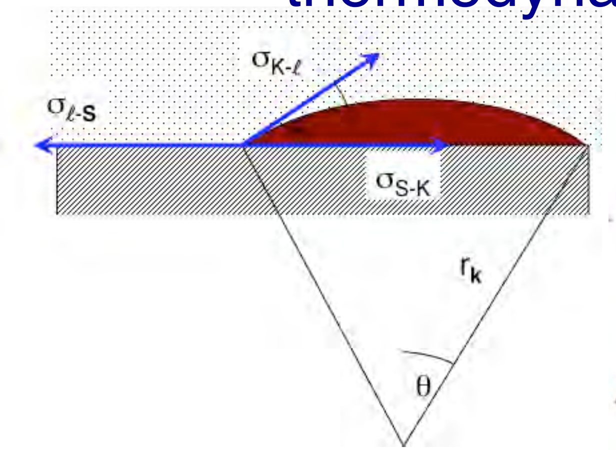


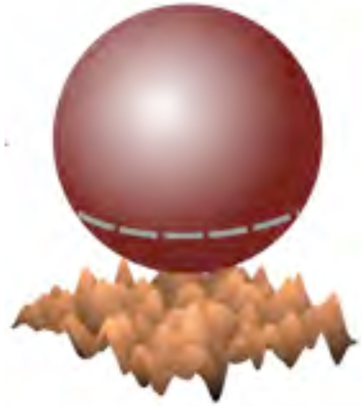
microstructure evolution
thermodynamics/kinetics

TEM









interfaces

alloy development

acknowledgements

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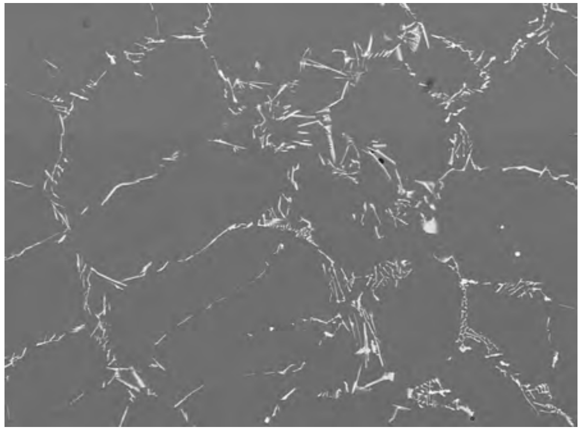
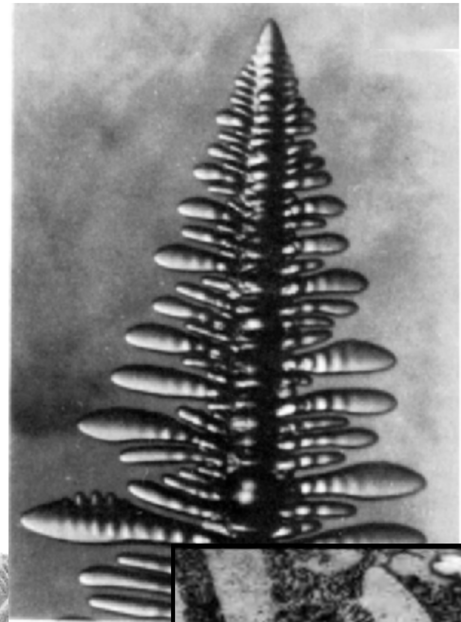
Prof. Michel Rappaz
Prof. Hans Eckart Exner †
Prof. Martin Glicksman

solidification microstructures

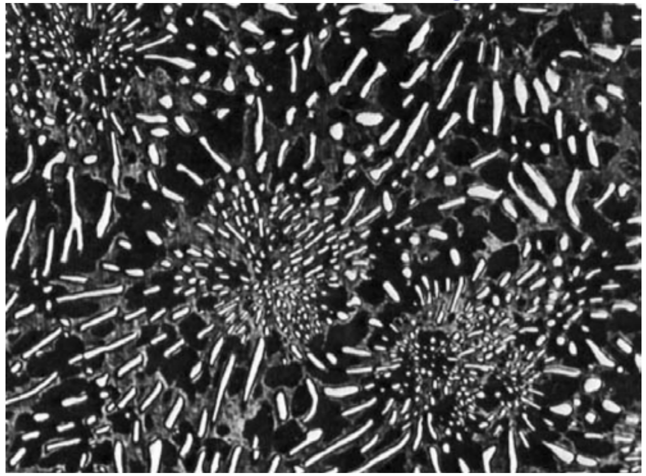


Al-Fe-Si

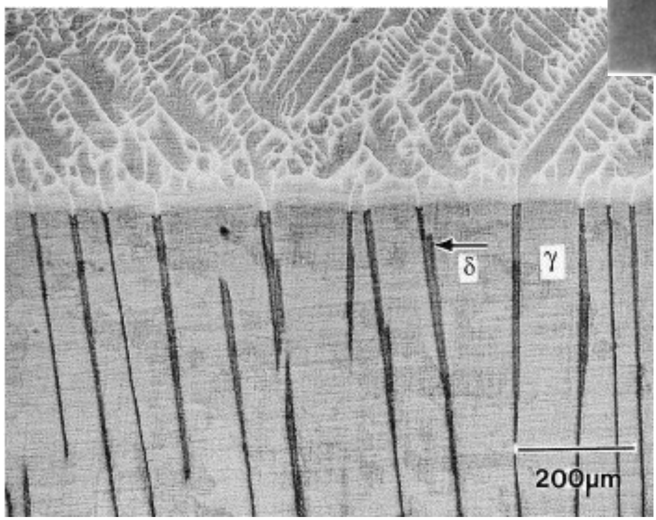
SCN

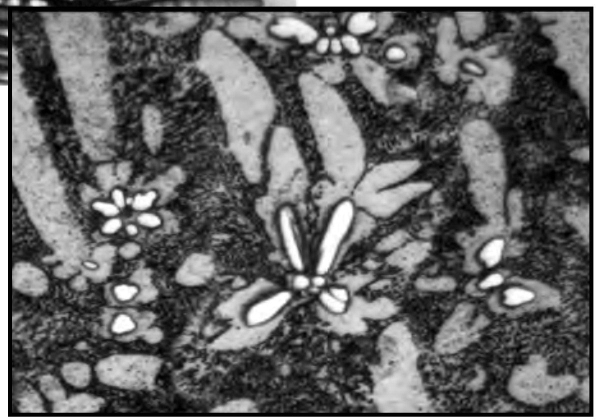


Cd-Cu-Ag

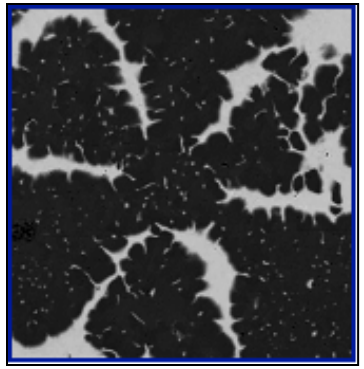


Fe-Ni





Pb-Sn-Ag-Cu



Ag-Bi

10^{14} dendrites in castings solidify worldwide per second

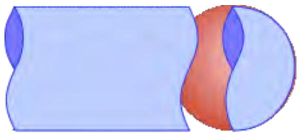
size: micrometers to meters

growth in crystallographic direction

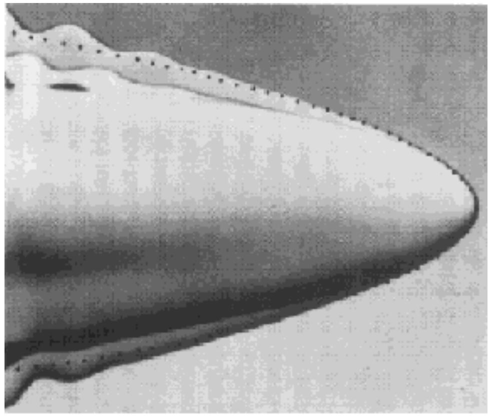
→ cubic lattice: 4-fold symmetry

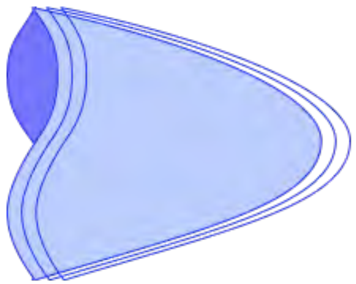
experimental observation: dendrite tip = paraboloid of revolution

first analytical model

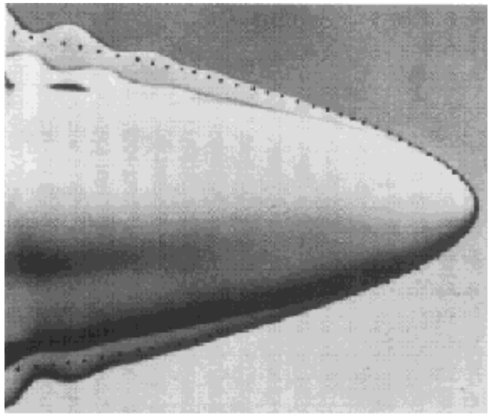


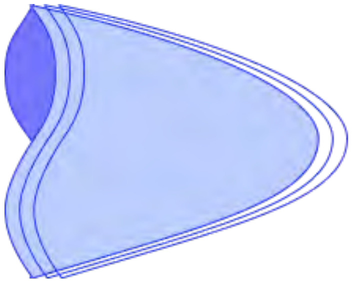
‘hemispherical needle ‘

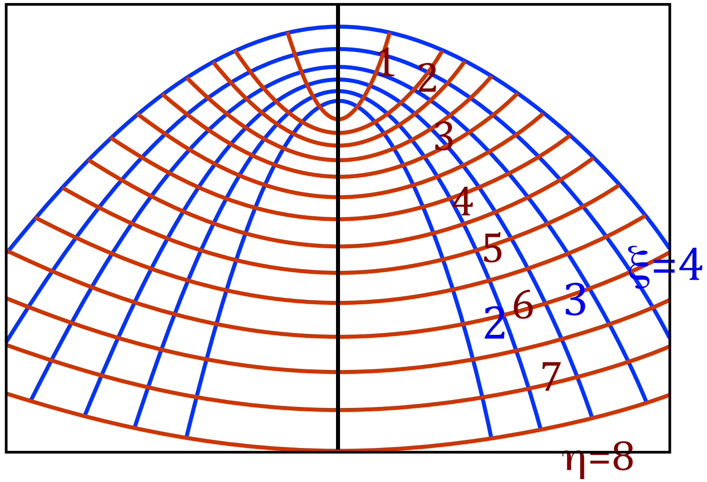




diffusion at a dendrite tip



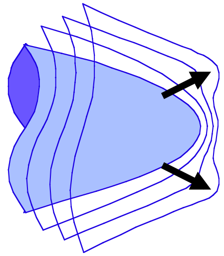




analytical solution 1940ies:

”Ivantsov transport solution“

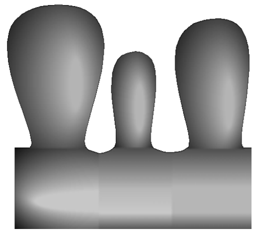
(parabolic coordinate system)



influence of interfacial energy not included

→ tip shape not realistic

→ secondary arms not at all included

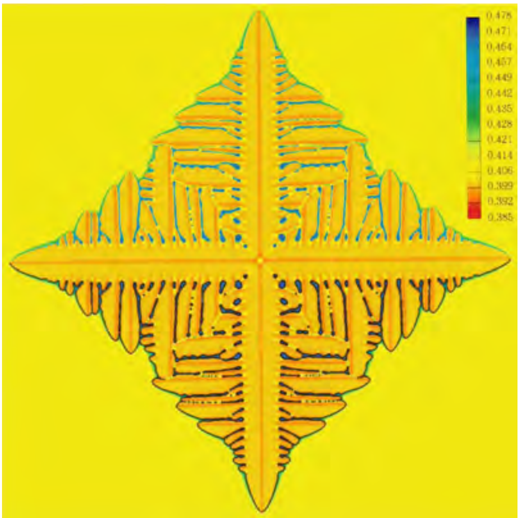


State of the art: phase field models

solves diffusion equation in the vicinity of a moving boundary

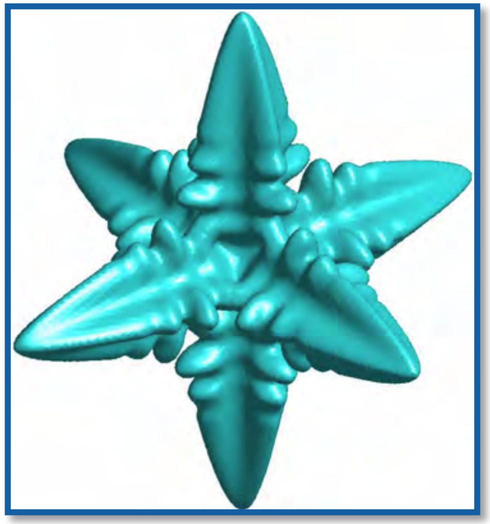
describes complex morphologies

includes interface energy and its anisotropy



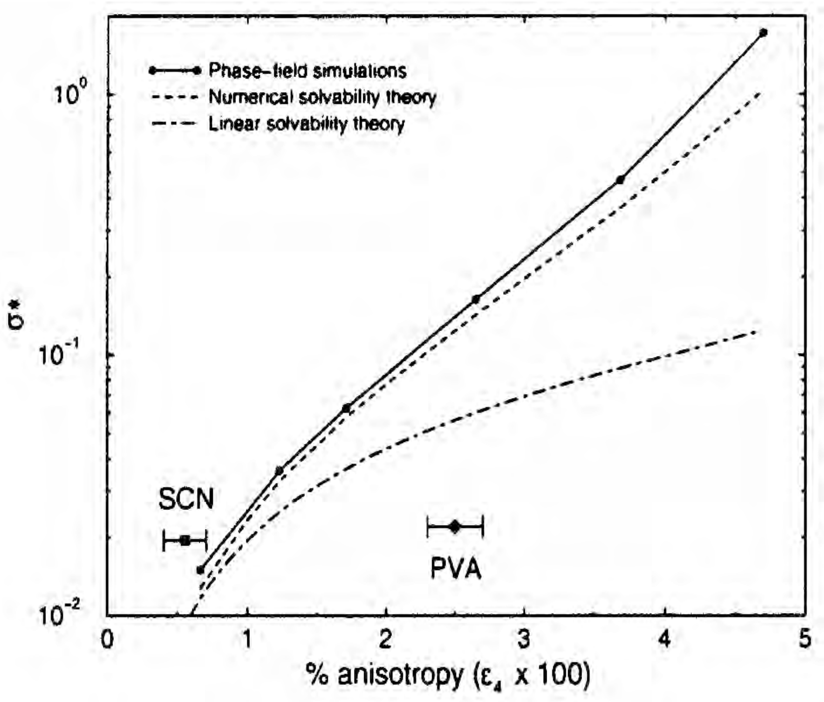
J. Warren, W.Boettinger

René Magritte



A. Karma, M. Rappaz

phase field dendrites, solved problems



physical interface thickness only in 1D (otherwise simulation too slow)

→ thicker interface, "anti-trapping current"

weak grid anisotropy remains

→ empirical corrections, choice of grid

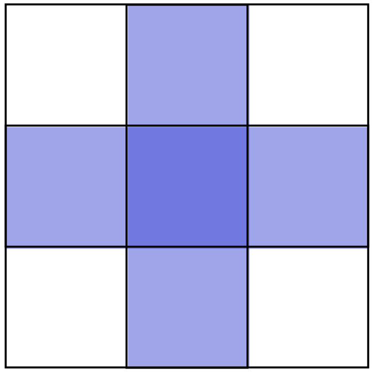
high computational cost

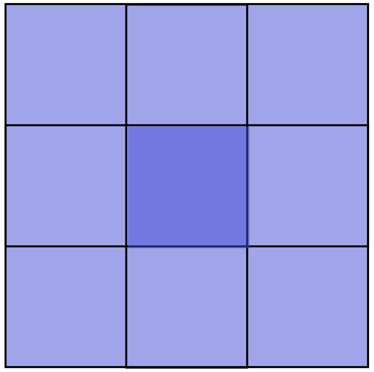
→ avoid slow (technical) processes

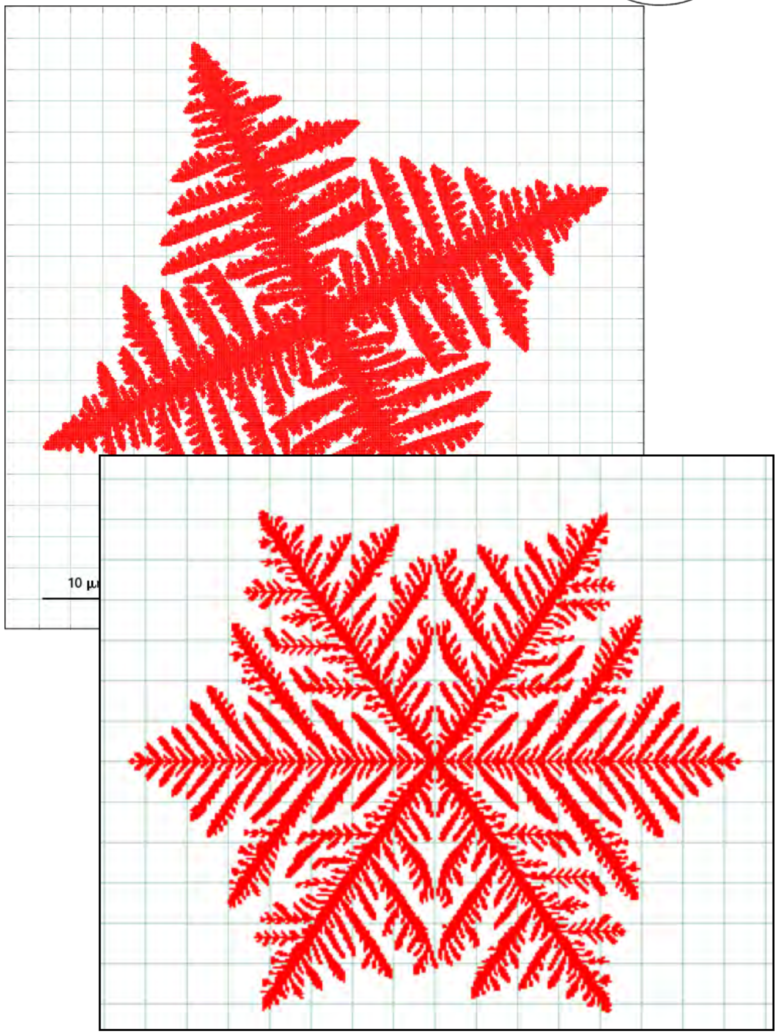
interface energy anisotropy considered, but not in agreement with experiments

→ attack experimentalists

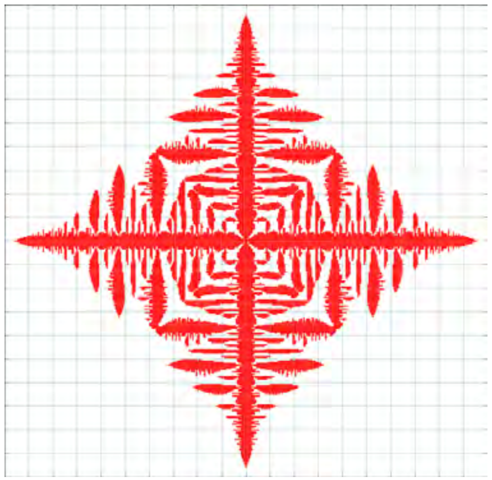
alternate method: Cellular Automata





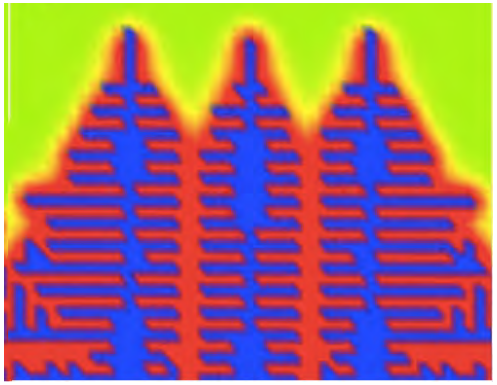


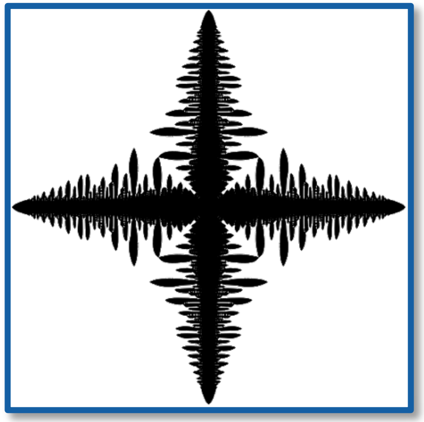
von Neumann or *Moore* neighborhoods
very very strong grid anisotropy

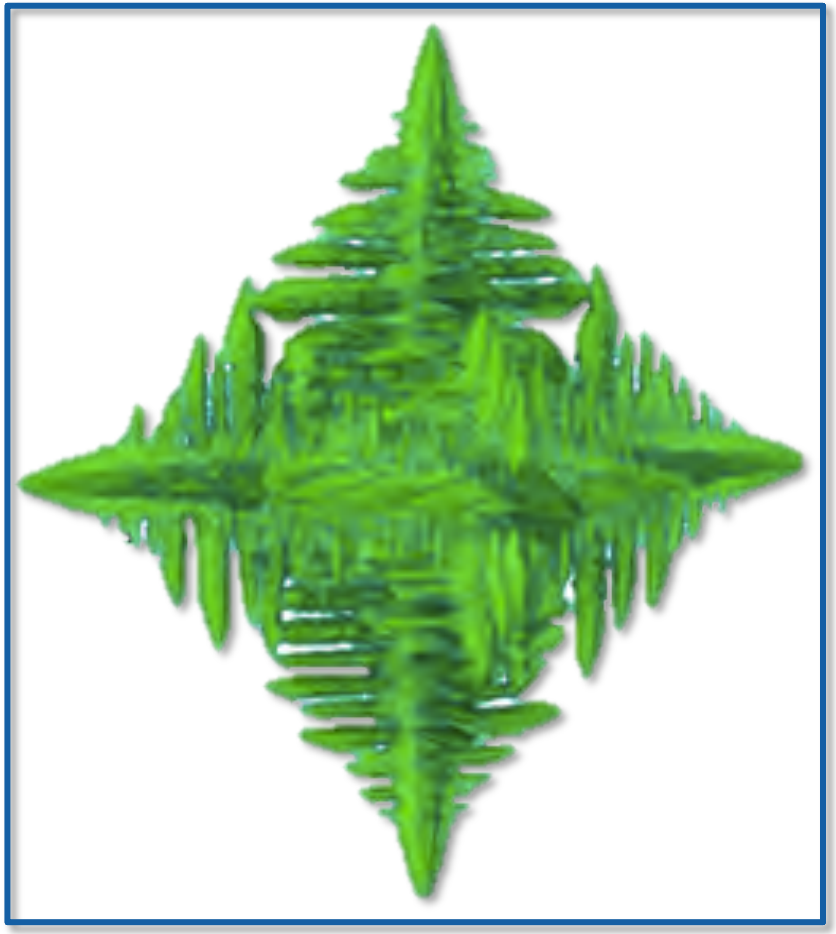


hybrid neighborhoods ? → work of A. Lorbiecka, B. Sarler

Cellular Automata – state of the art



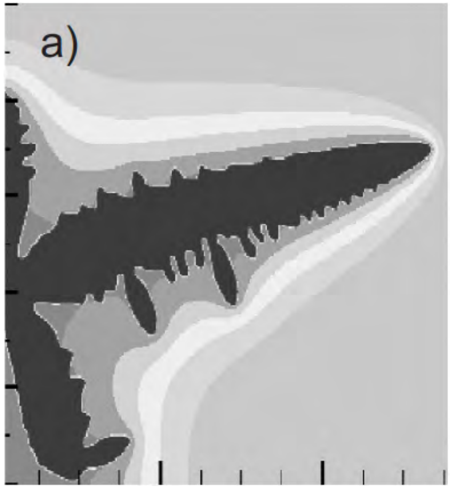


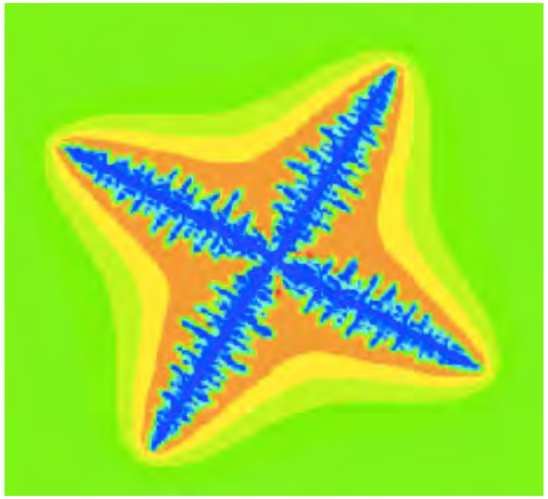


- level set method for interface position
- sophisticated curvature treatment

CA dendrite, K. Reuther, M. Rettenmayr, Comp. Mater. Sci. 2012

growth in off-grid direction





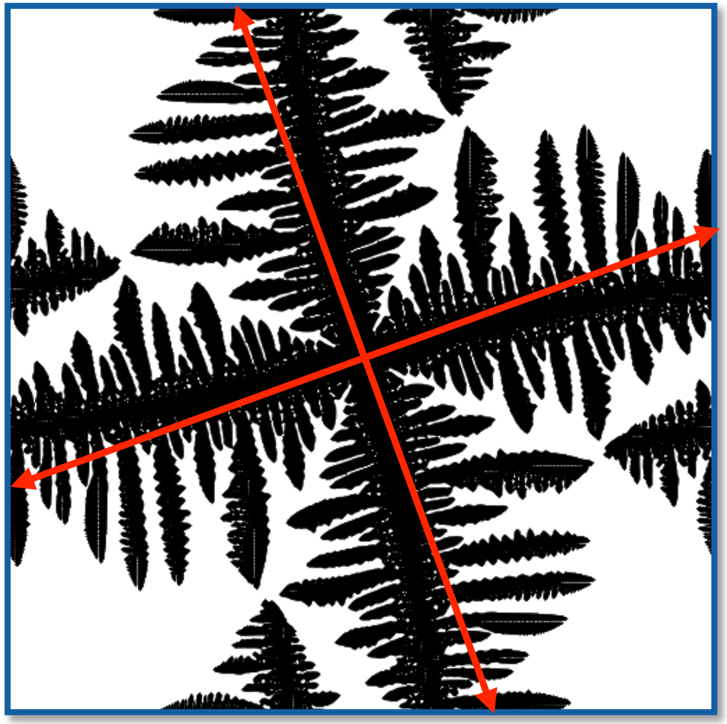
grid with mesh size of ≈1μm

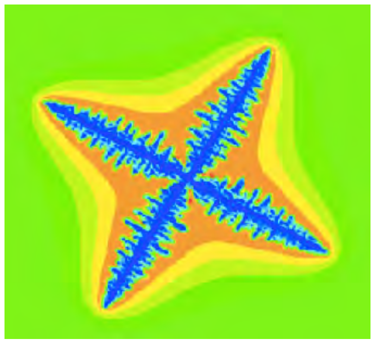
growth in **any** direction with respect to the grid*

arm surfaces along different grid directions
→ direction dependent branching behavior

*... to be honest →

growth in off-grid direction





growth in **any** off-grid direction
only for short distances
(but better in 3D)

→ **conclusion on CA:**

- fast (1% of CPU of Phase Field)
- grid anisotropy reduced,
  but essentially unavoidable
- secondary arms mostly unrealistic

conclusion on phase field:

- large community
- far developed
- precise
- slow
- low (but non-zero) grid anisotropy

→ new attempt: meshless method

"a computer algorithm is most benign on regular or almost regular grids"

(experienced modeller)

commonly used method:

start with regular grid

displace each node by small amount

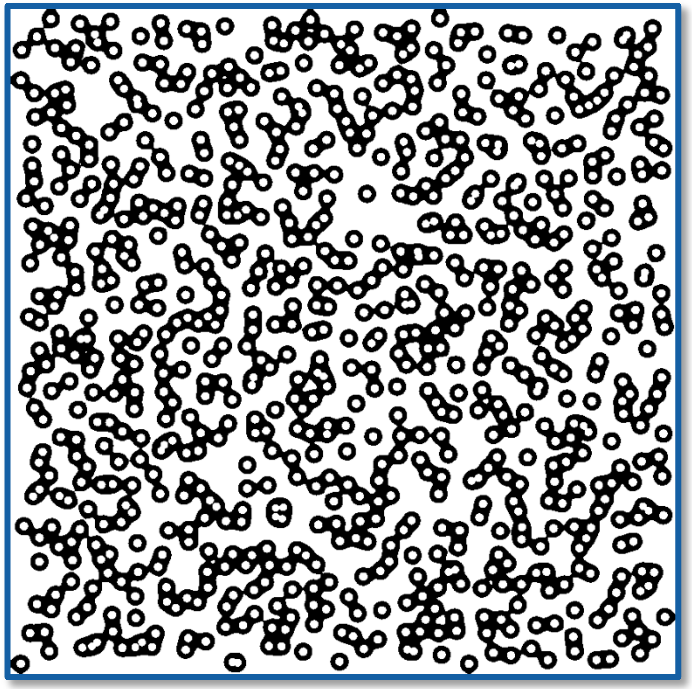
→ retains neighborhoods from cartesian grid

→ retains bookkeeping

known problems:

numerical instabilities

local divergence

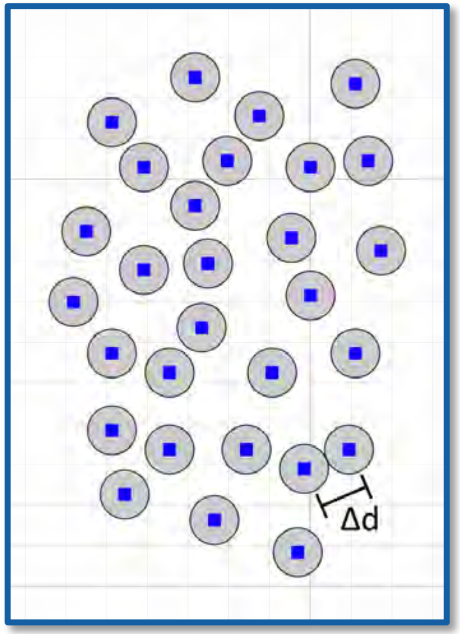


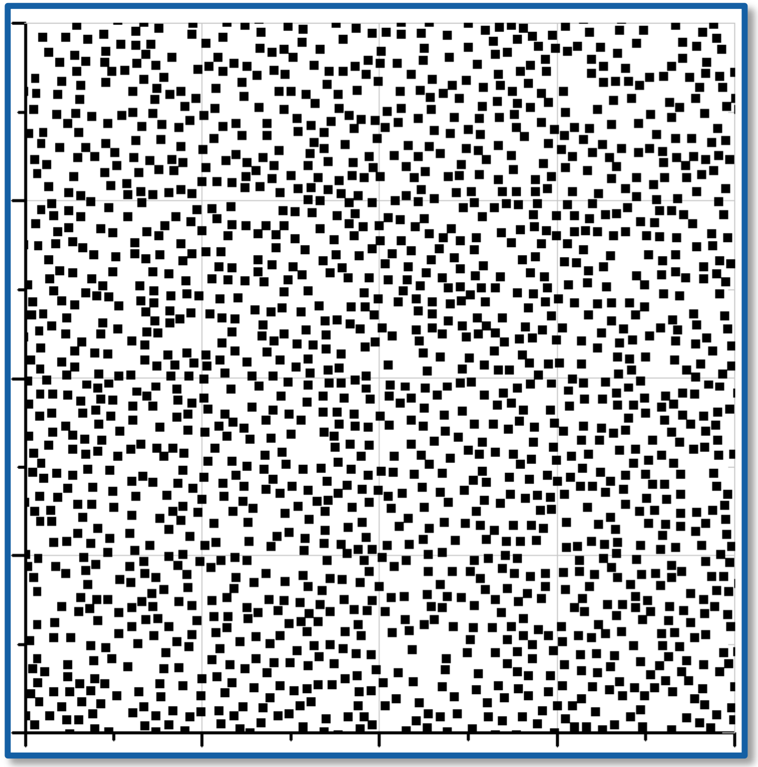
(Perko, CMES 2007)

random positioning of nodes

minimum distance *Δd* between every node for improved homogeneity

➔ no preferred direction, isotropic at length scales >*Δd*





(Reuther, Sarler, Rettenmayr 2012, IJTS) point based solver of partial differential equations

”Point Automata“

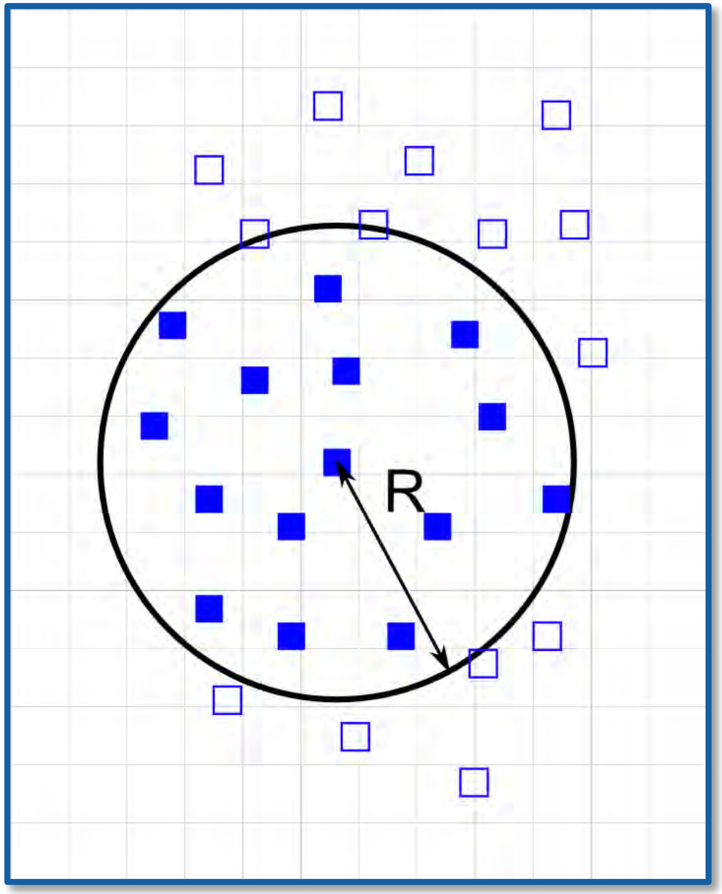
example: diffusion equation

interpolation of the concentration field by a **distance weighted least squares fit** within radius *R*

Taylor series of 2nd degree:

$$c(x,y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 y^2 + a_5 xy$$

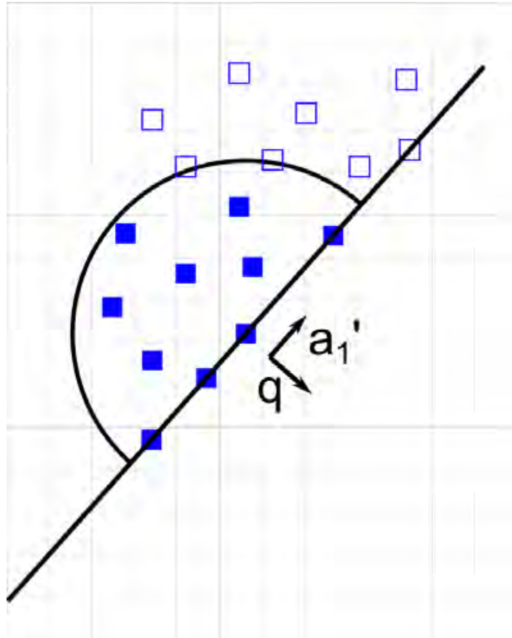
$$\nabla^2 c = 2(a_3 + a_4)$$



e.g. Neumann boundary conditions

$$c(x,y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 y^2 + a_5 xy$$

$$\frac{\partial c}{\partial n} = n_x(a_1 + y a_5) + n_y(a_2 + x a_5) \equiv q$$



find *c* such that the coefficients from the least squares fit satisfy the boundary condition

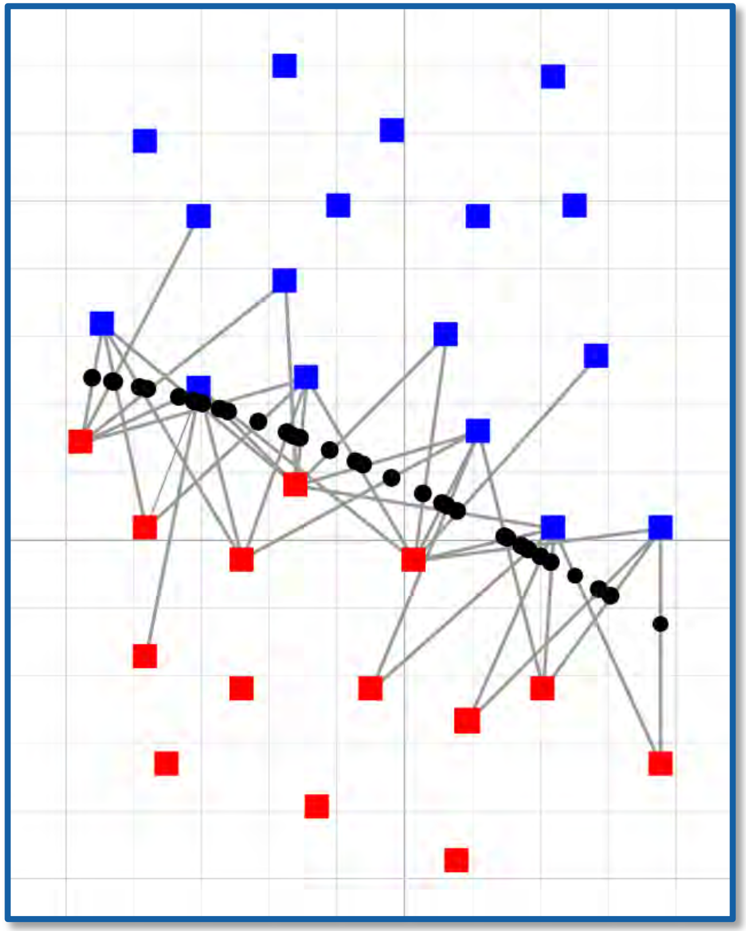
tangential flow not treated explicitely at boundary

$$c(x,y) = a_0 + a_1'(n_y x - n_x y) + q(n_x x + n_y y) + a_3 x^2 + a_4 y^2 + a_5 xy$$

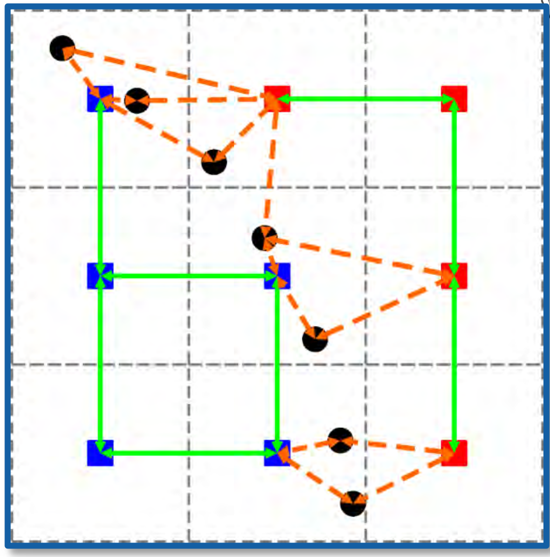
normal term: given from boundary condition
tangential term: included in the fit

major problem: position of interface

- grid node ■:
  solid or liquid
- interface ● :
  ”particles” between nodes
  with different state

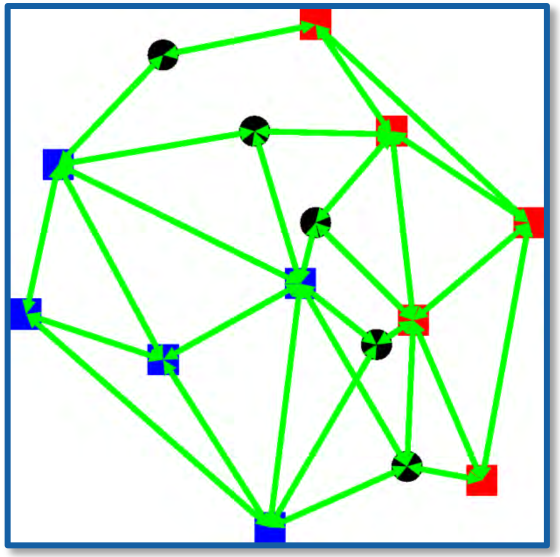


Reuther, Rettenmayr, Acta Mater 2013



”particles“ on a fixed, regular grid:

→ interpolation/extrapolation scheme outside finite difference method

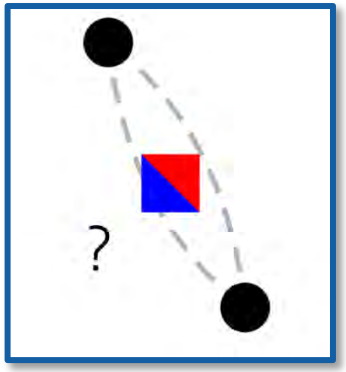


particles on an irregular grid

→ interpolation scheme is inherent to point based meshless method

front tracking with particles

particle movement in point automata:



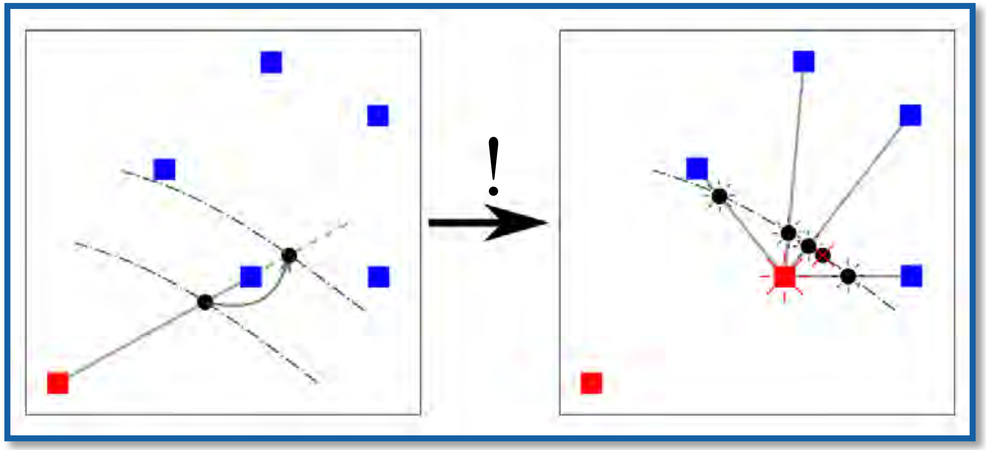
introduction of ”free“ particles requires special attention for the node bookkeeping

→ particle-node coupling

trapping:

new particles introduced

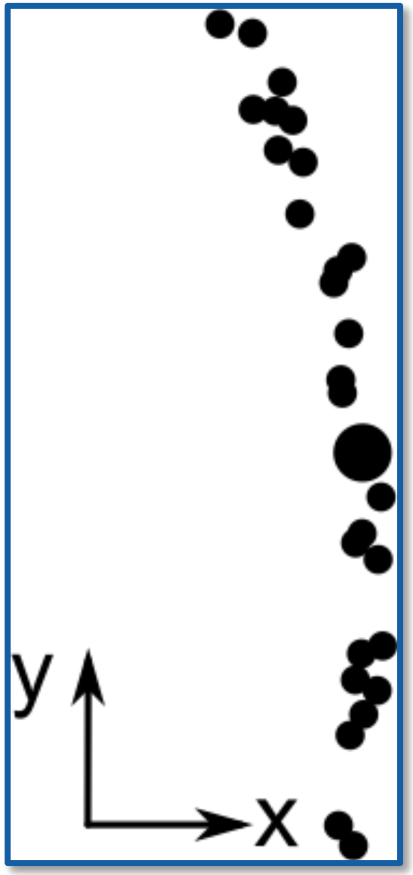
old particle deleted



interface **normal**

total least square fit

$$n = \begin{pmatrix} 1 \\ a \end{pmatrix}$$



$$a = \frac{1}{2}\Sigma_{yy} - \Sigma_{xx} \pm \sqrt{\left(\Sigma_{yy} - \Sigma_{xx}\right)^2 + 4\Sigma_{xy}^2} \,/\, \Sigma_{xy}$$

with

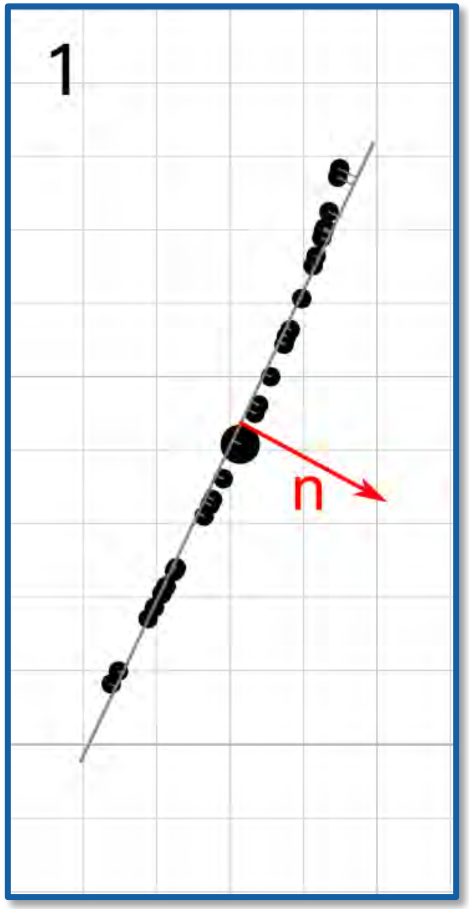
$$\Sigma_{xy} = \sum_i w_i x_i y_i$$

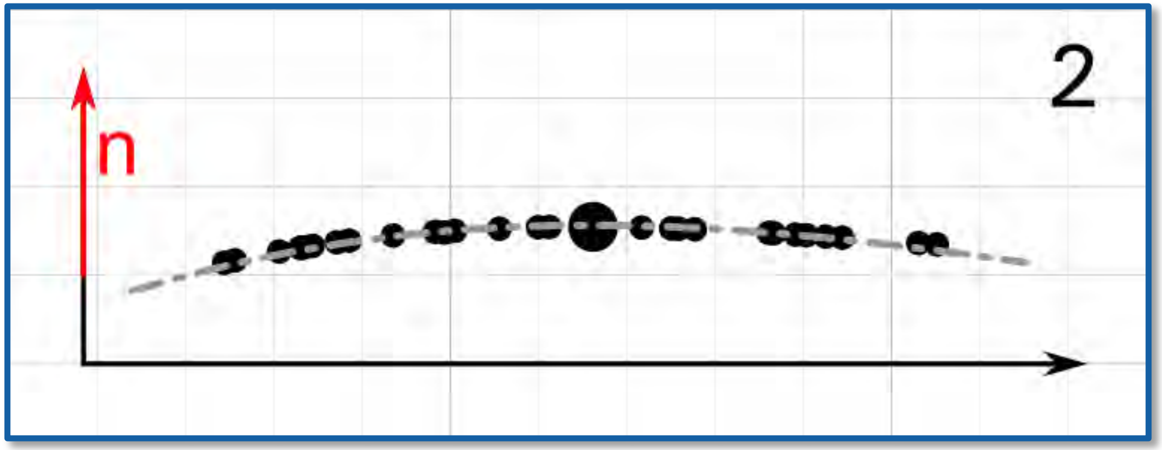
etc.

interface **shape** and **curvature**

least square fit

in the cartesian coordinate system



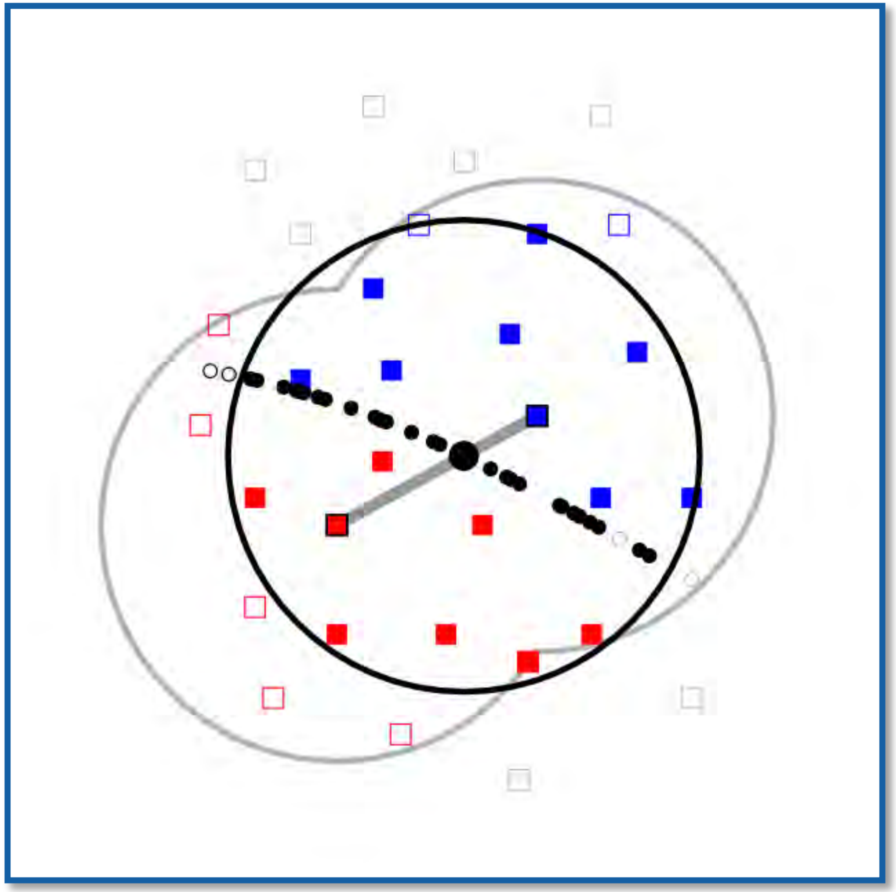


$$\Delta T = \Gamma(\theta) \cdot K$$

local undercooling dependent on
interface geometry:
curvature (K)
angle (θ) to normal direction

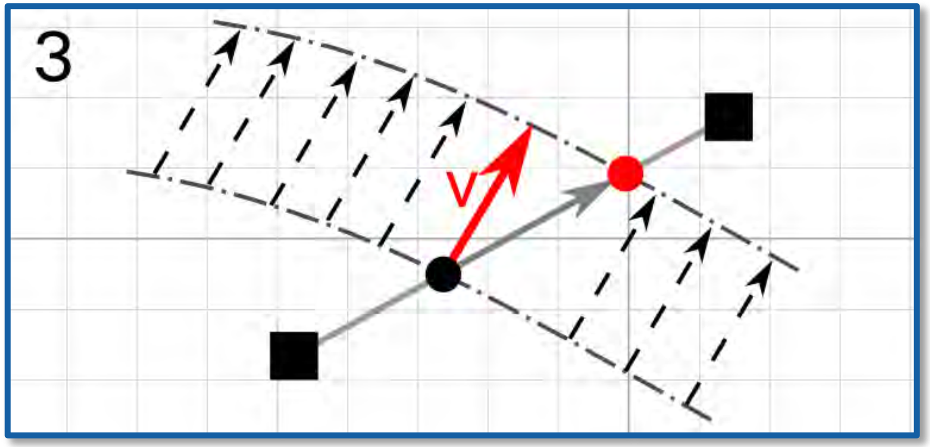
interface **velocity**
defined by mass balance

$$\vec{v}\cdot\left(c_l^* - c_s^*\right) = D_l \frac{\partial c_l}{\partial \vec{n}_{l\to s}} + D_s \frac{\partial c_s}{\partial \vec{n}_{l\to s}}$$



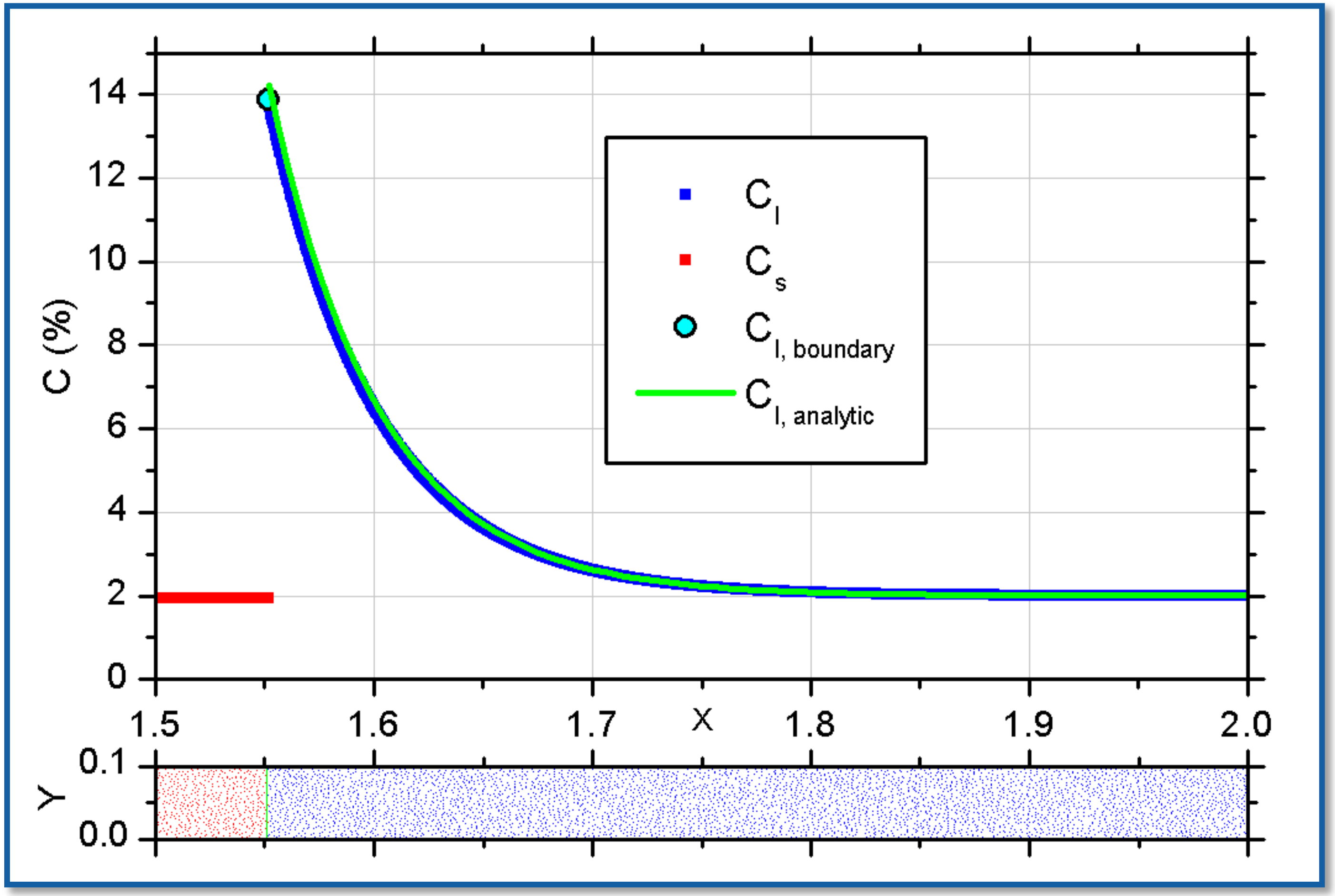
Reuther and Rettenmayr, Acta Mater. 2013 interface migration **direction**

defined by translation of the fit



Reuther and Rettenmayr, Acta Mater. 2013 steady state solidification, concentration profile in the liquid

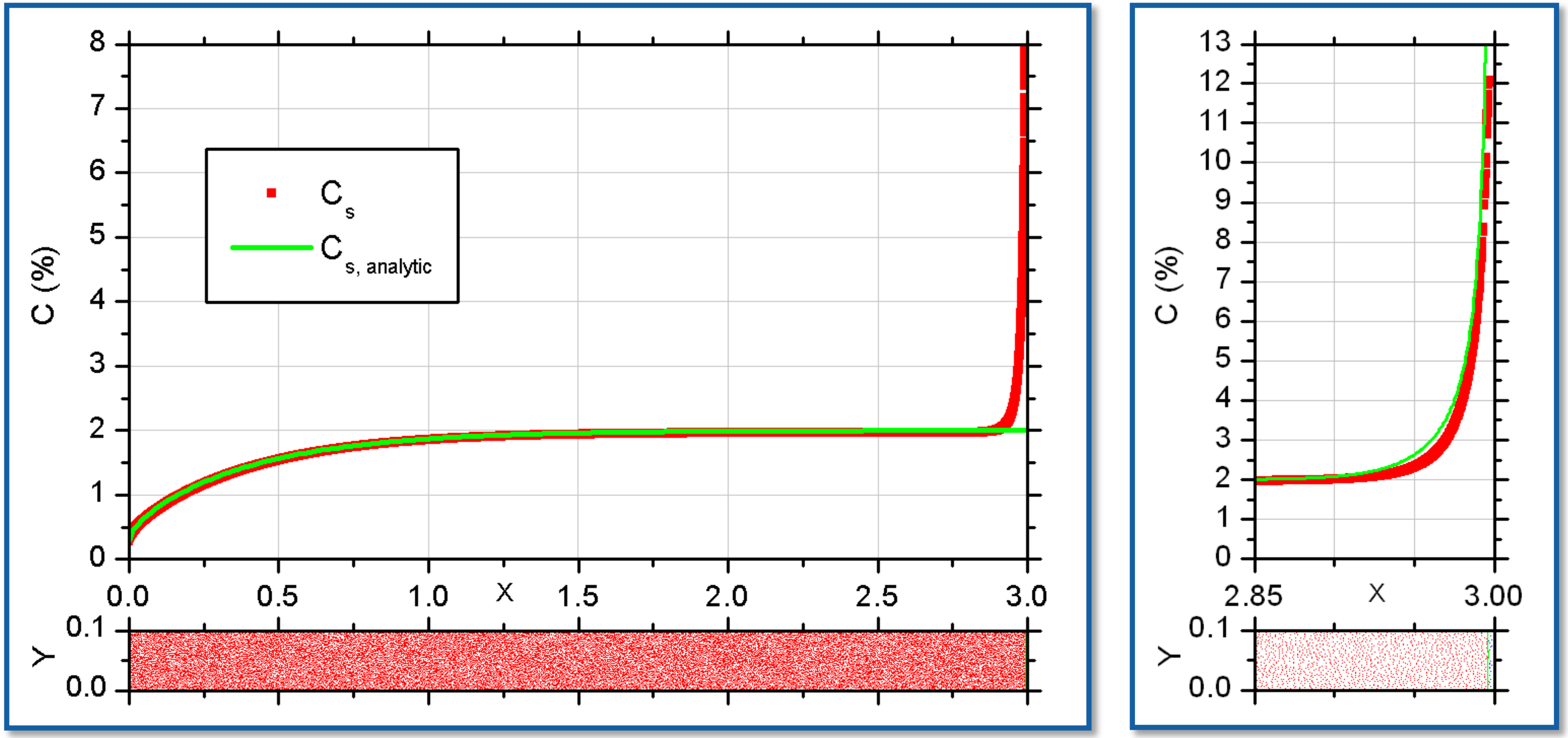
$C_0 = 2\%$
$k = 0,14$



Acta Mater. 2013

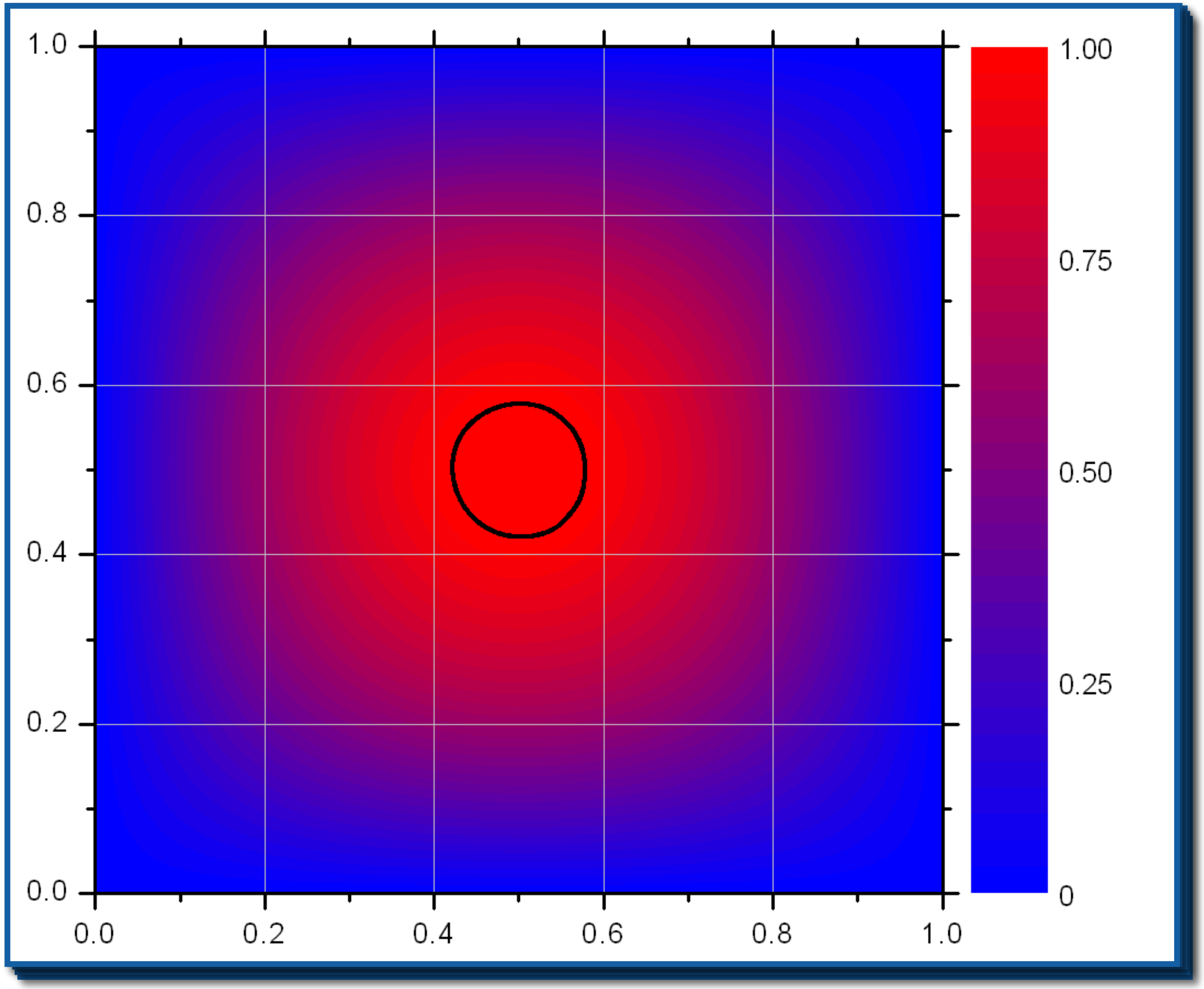
first results – comparison with analytical model

steady state solidification, initial and final transients

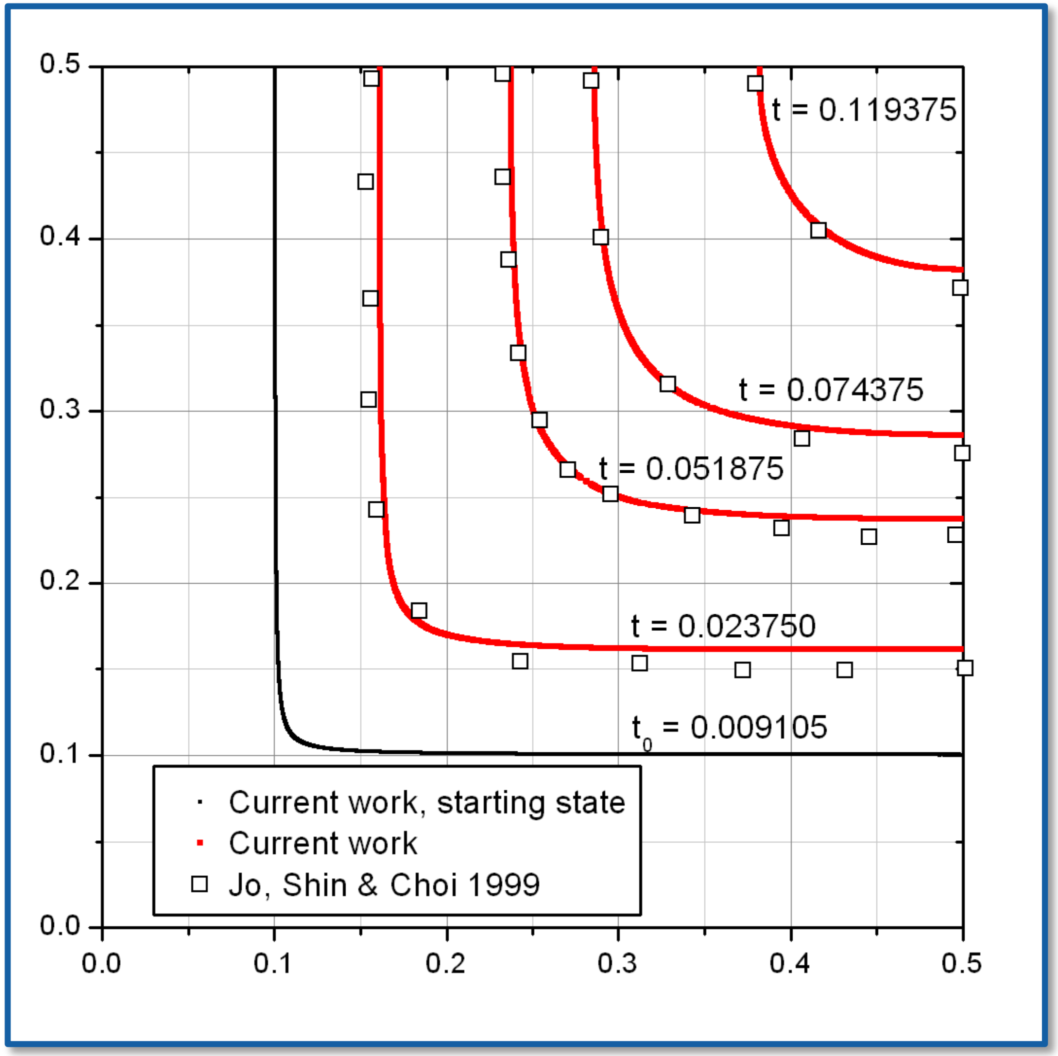


Acta Mater. 2013

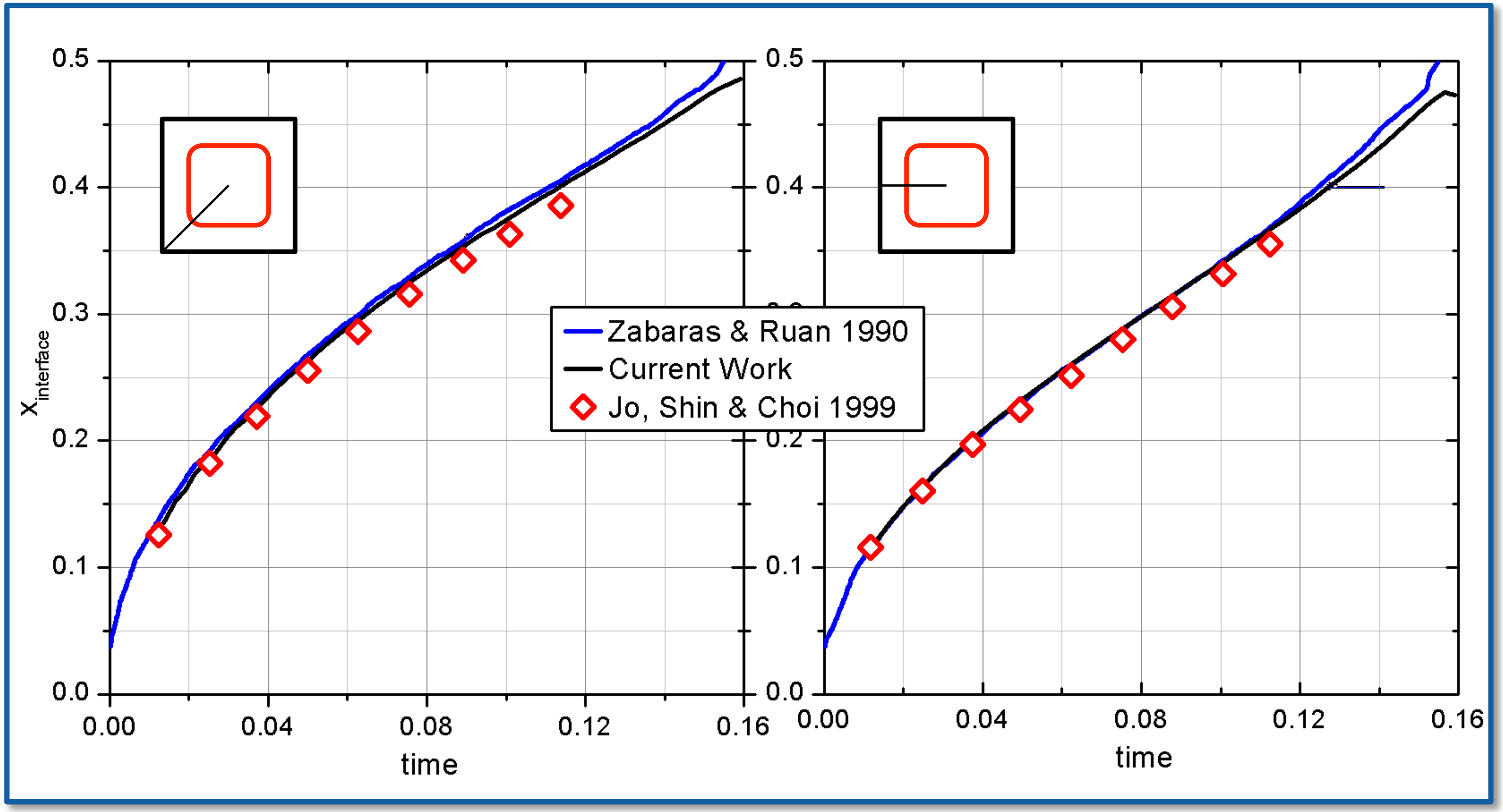
inward solidification in a square mold

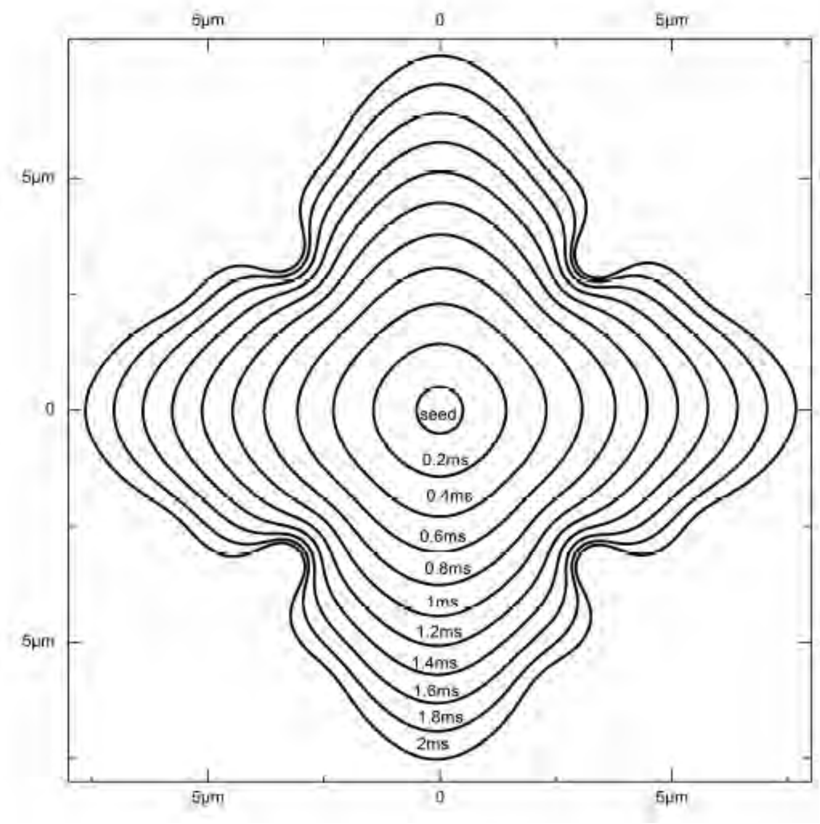


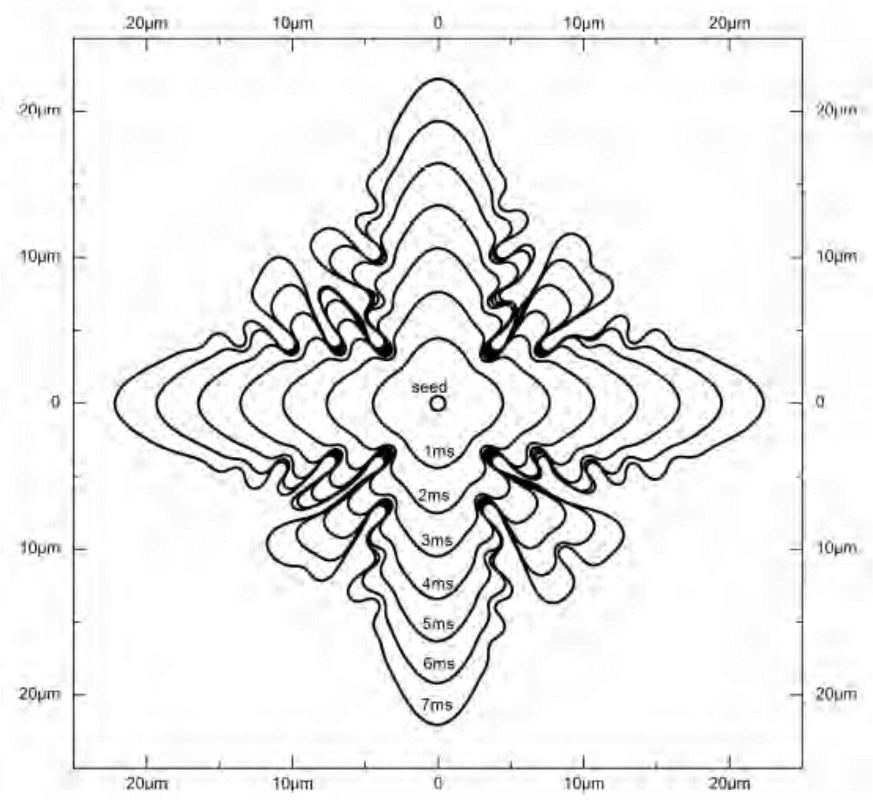
comparison with literature data



comparison with literature data




5µm
0
5µm
seed
0.2ms
0.4ms
0.6ms
0.8ms
1ms
1.2ms
1.4ms
1.6ms
1.8ms
2ms


20µm
10µm
0
seed
1ms
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conclusion

simulation of complex morphologies with Cellular Automata

- fast (→ 100times faster than Phase Field)
- similarities with real growth morphologogies undeniable

simulation of complex morphologies with Point Automata

- not very slow (→ 10 times faster than Phase Field)
- excellent reproduction of growth morphologogies

simulation of complex morphologies with Phase Field

- far developed
- slow (→ not faster than Phase Field)
- very good reproduction of growth morphologogies