PHASE-FIELD MODELING OF CELLULAR AND DENDRITIC SOLIDIFICATION MICROSTRUCTURES

DAMIEN TOURRET*, YOUNGGIL SONG, ALAIN KARMA

dtourret@lanl.gov you.song@neu.edu a.karma@neu.edu

Department of Physics, Northeastern University, Boston, MA

* Currently at: Los Alamos National Laboratory, MST-6: Metallurgy, Los Alamos, NM

Northeastern University

INTRODUCTION, CONTEXT, OBJECTIVE

- ✓ Solidification microstructures crucial to metallurgical R&D
- ✓ Existing quantitative crystal growth phase-field (PF) model [1]
- ✓ Emerging highly-parallel calculation architectures (GPUs)
- ⇒ *Objective: Implement a computationally efficient PF code of crystal growth capable of quantitative prediction, and use it extensively to study complex solidification scenarios*
- *Approach: Systematic quantitative comparisons with state-of-the-art well-controlled experiments and literature*

PHASE-FIELD MODEL [1]

- Quantitative model for dilute binary alloy directional solidification [1]
- Graphic Processing Units (GPU) massively parallel implementation

Model equations

Preconditioned phase-field ψ

$$\left[1-(1-k)\frac{x-\tilde V_p t}{\tilde l_T}\right] a_s(\theta)^2 \frac{\partial\psi}{\partial t} = \vec\nabla\cdot\left[a_s(\theta)^2\vec\nabla\psi\right] + \sum_{m=x,y}\left[\partial_m\left(|\vec\nabla\psi|^2 a_s(\theta)\frac{\partial a_s(\theta)}{\partial(\partial_m\psi)}\right)\right] + \varphi\sqrt2\left(1-a_s(\theta)^2|\vec\nabla\psi|^2\right) - \lambda(1-\varphi^2)\sqrt2\left[U+\frac{x-\tilde V_p t}{\tilde l_T}\right]$$

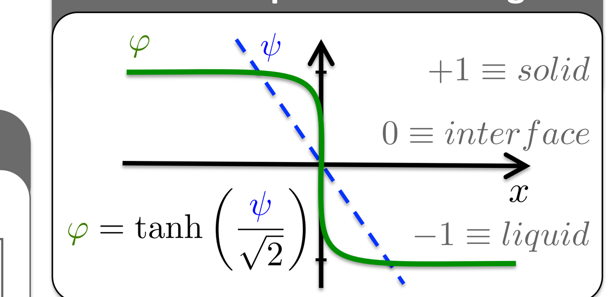
Solute supersaturation, U

$$\left(1+k-(1-k)\varphi\right)\frac{\partial U}{\partial t} = \tilde D\,\vec\nabla\cdot\left[(1-\varphi)\vec\nabla U\right] + \vec\nabla\cdot\left[\left(1+(1-k)U\right)\frac{(1-\varphi^2)}{2}\frac{\partial\psi}{\partial t}\frac{\vec\nabla\psi}{|\vec\nabla\psi|}\right] + \left[1+(1-k)U\right]\frac{(1-\varphi^2)}{\sqrt2}\frac{\partial\psi}{\partial t}$$

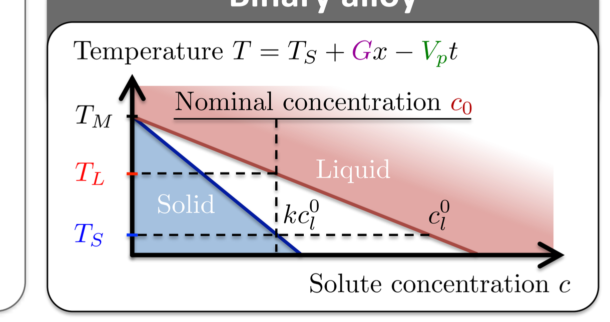
where the supersaturation derives from the solute concentration, c, as $U=\frac{1}{1-k}\left[\frac{c/c_l^0}{(1-\varphi)/2+k(1+\varphi)/2}-1\right]$

and c_l^0, k, $\tilde D$, $\tilde\lambda$, $\tilde V_p$ and $\tilde l_T$ are alloy/process/computational parameters.

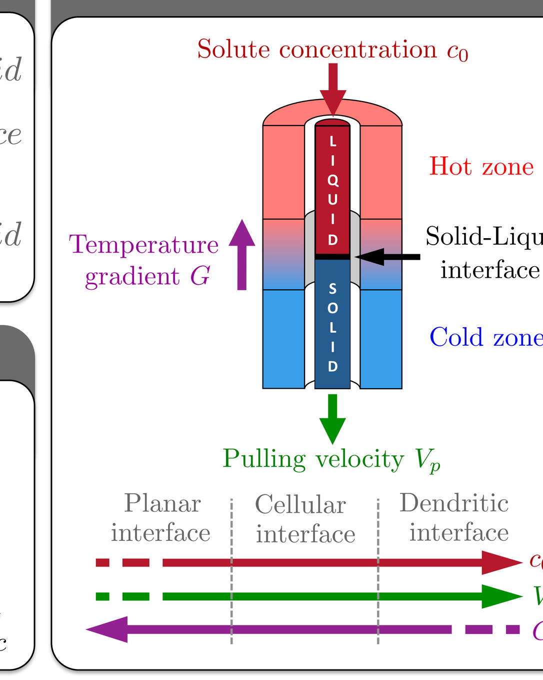
Phase-field preconditioning [2]



Binary alloy

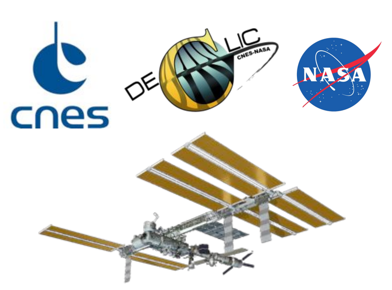


Directional solidification



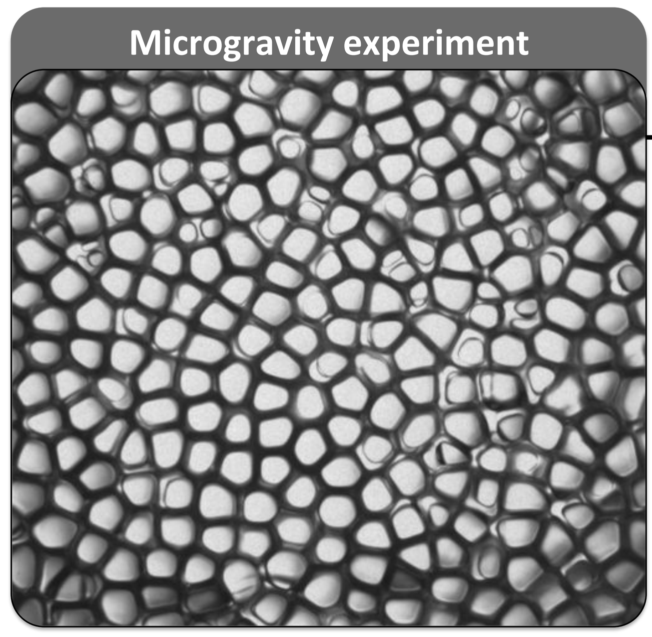
CELLULAR OSCILLATORY GROWTH DYNAMICS [3]

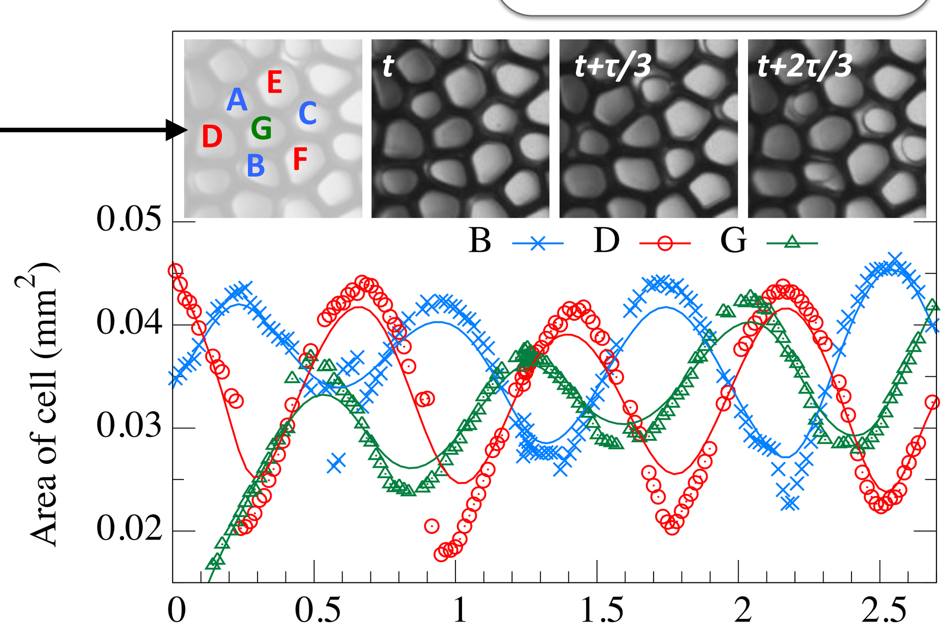
- DEvice for the study of Critical LIquids and Crystallization (*DECLIC*)
  - Microgravity onboard the International Space Station
  - Directional Solidification Insert
- *In situ* observation of SCN-Camphor alloy
  - Oscillatory behavior of entire cellular arrays
  - Phase coherence only in ordered regions
    - ⇒ Localized breathing mode oscillations
  - Tip splitting instabilities prevent global order



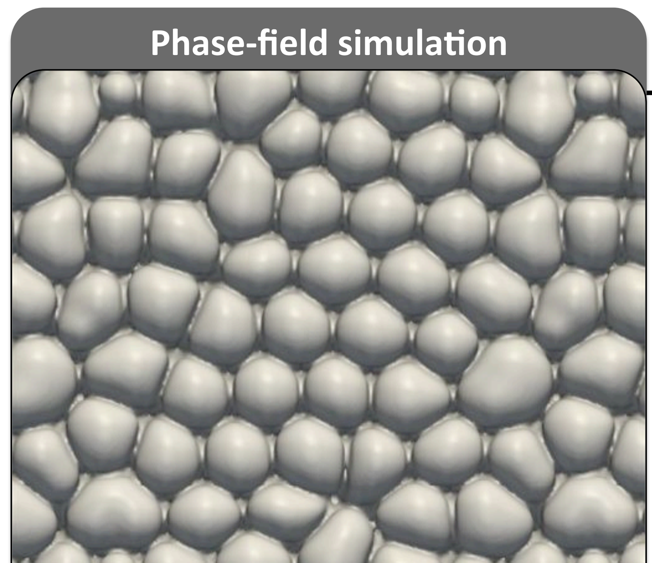
Oscillation period
Experiment: τ ≈ 46 min
Simulation: τ ≈ 48 min

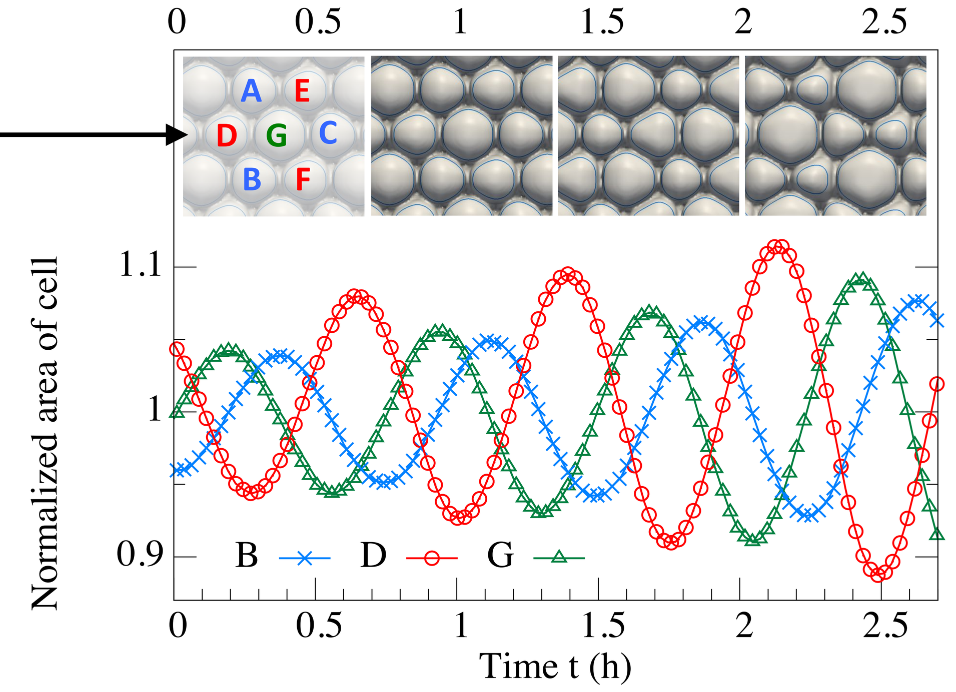
Microgravity experiment





Phase-field simulation





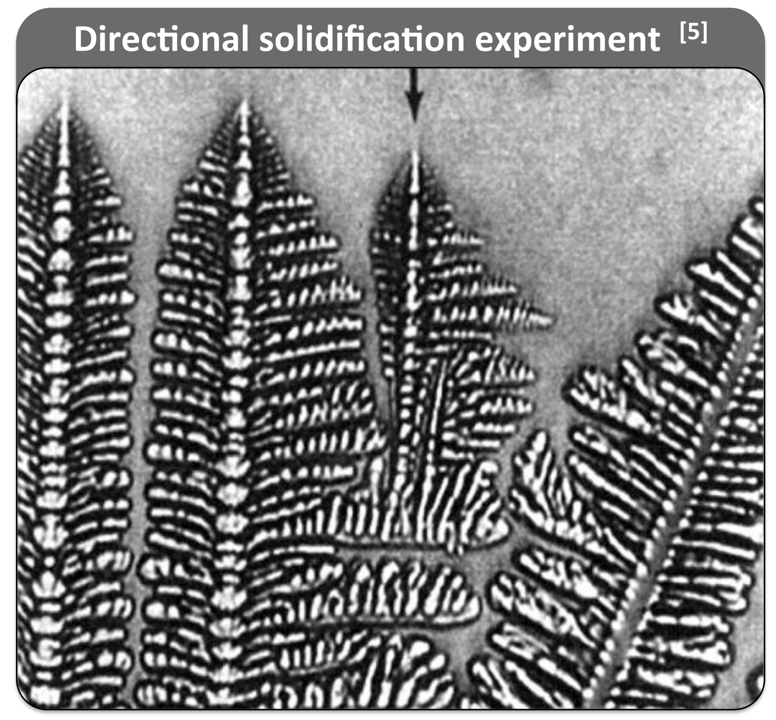
SCN-0.24wt%Camphor, G=28K/cm, V=1μm/s

Collaborators:
R. Trivedi — Iowa State University
N. Bergeon, B. Billia, L. Chen, A. Ramirez, J.-M. Debierre, R. Guérin — Aix*Marseille Université, CNRS

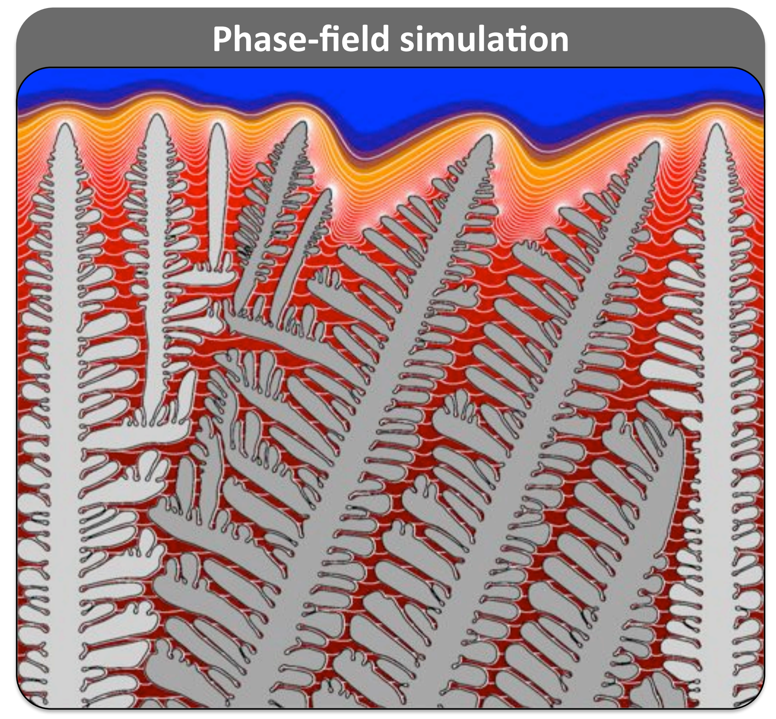
DENDRITIC GRAIN GROWTH COMPETITION [4]

- Computationally intensive study of a bi-crystal SCN-acetone alloy
  - *Influence of the temperature gradient and crystal orientation*
- Quantitative comparison to experimental values and scaling laws
  - *Selection of primary spacing and dendrite growth direction*
- Microscopic thermal fluctuations at the origin of sidebranching critically influences the macroscopic grain boundary orientations
- Grain elimination rate is not monotonic with crystal misorientation
- Spacing selected by branching > spacing after planar destabilization

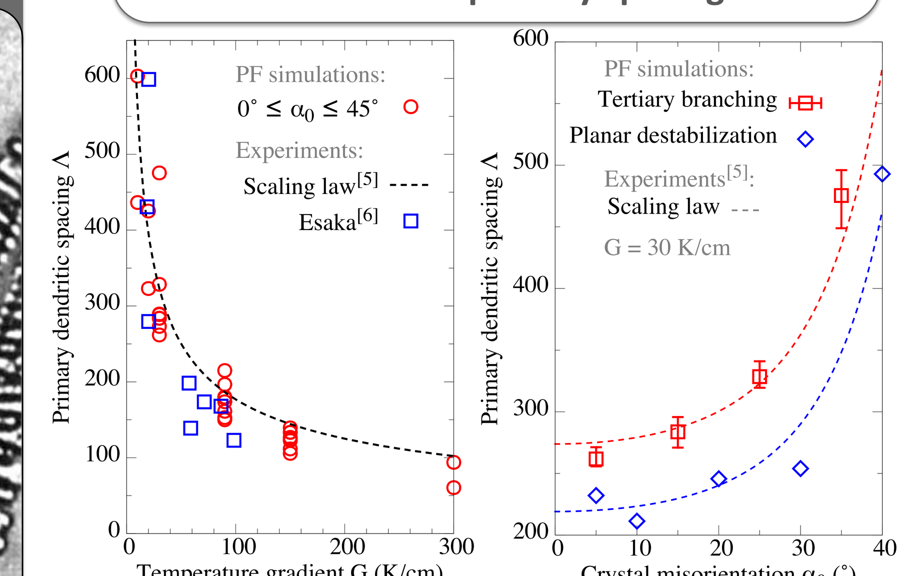
Directional solidification experiment [5]



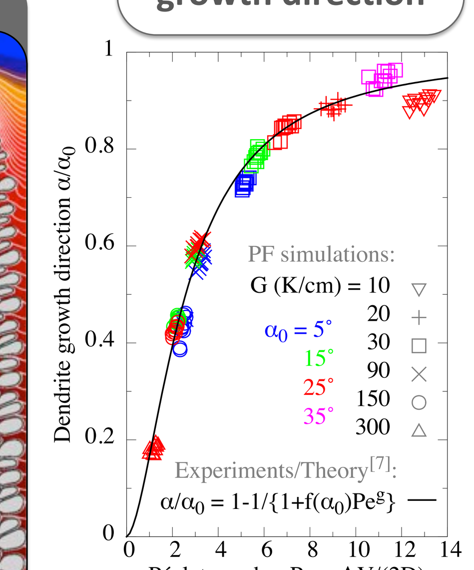
Phase-field simulation



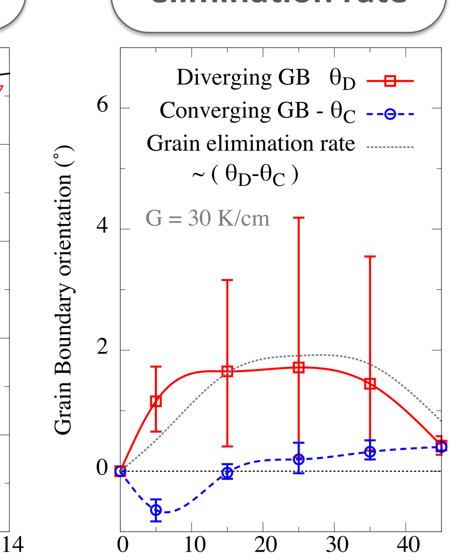
Selection of primary spacing



Selection of growth direction



Misoriented grain elimination rate

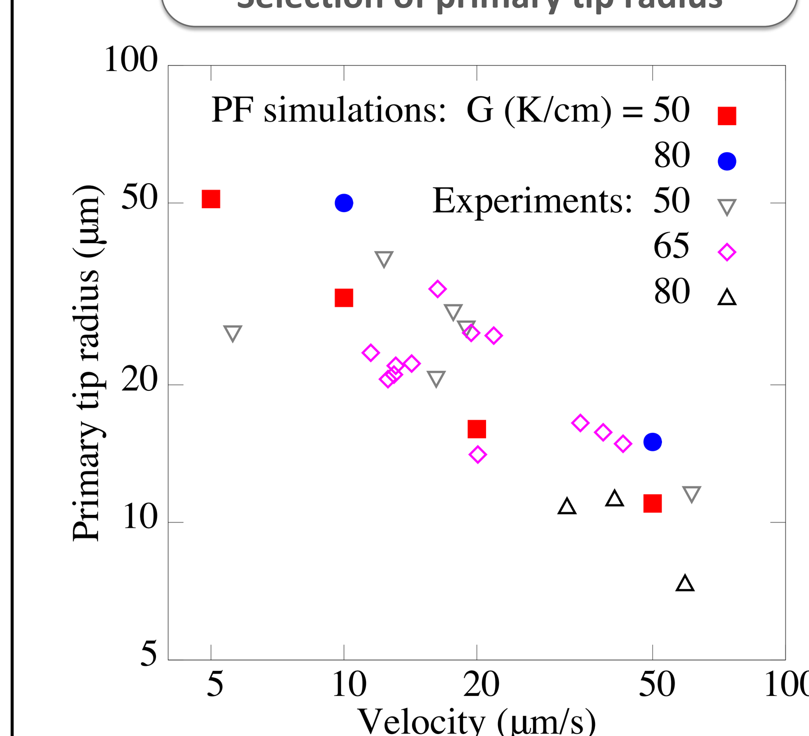


SCN-0.4wt%Acetone, G = 10-300 K/cm, V = 25 μm/s

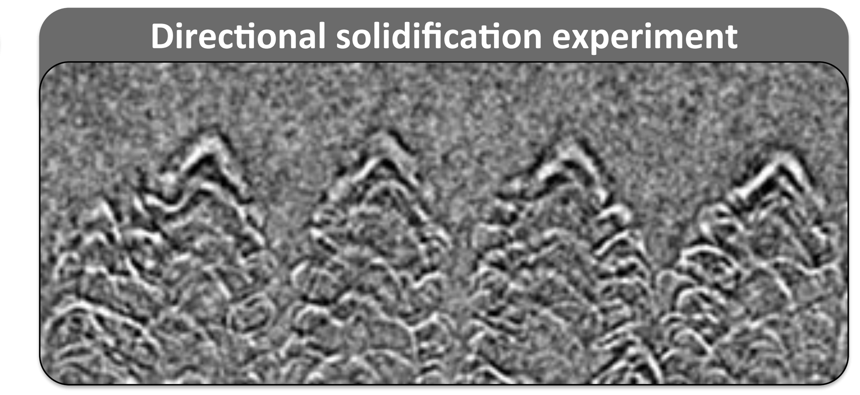
DENDRITE TIP SELECTION IN METALLIC ALLOYS

- X-ray imaging of thin sample Al-Cu directional solidification
  - Measure of dendritic tip radius at different growth velocities

Selection of primary tip radius



Directional solidification experiment



Phase-field simulation

Al-1.4wt%Cu, G = 80 K/cm, V ≈ 40-50 μm/s

Collaborators:
A. Clarke, P. Gibbs, S. Imhoff
Los Alamos National Laboratory — U.S. Department of Energy, Office of Science — Argonne National Laboratory

SUMMARY, CONCLUSIONS, OUTLOOK

- ✓ Phase-Field model parallel implementation on GPUs
  ⇒ Quantitative predictions at the scale of experiments
- Cellular oscillations in 3D more complex than quasi-2D experiments: Long range coherence linked to spatial order
- Stochastic selection of dendritic GB orientation in polycrystals
- *Outlook:*
  - *Dendritic regime in microgravity experiments*
  - *Dendritic growth competition in 3D*
  - *Effect of convection on microstructure selection*

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[1] Echebarria, Folch, Karma, Plapp; Phys Rev E 70, 061604 (2004) [2] Glasner; J Comput Phys 174, 695 (2001) [3] Bergeon, Tourret, Chen, Debierre, Guérin, Ramirez, Billia, Karma, Trivedi; Phys Rev Lett 110, 226102 (2013)
[4] Tourret, Karma; Acta Mat, *in press* (2014) [5] Gandin, Eshelman, Trivedi; Metall & Mat Trans A 27, 2727 (1996) [6] Esaka; PhD thesis, EPFL, Lausanne, Switzerland (1986) [7] Deschamps, Georgelin, Pocheau; Phys Rev E 78, 011605 (2008)