Directional Solidification Model for Additive Manufacturing Testbed Problem

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1 Microscopic model

We consider the Echebarria model [?, ?, ?, ?] with frozen temperature approximation, i.e., fixed G, R,

$$T(z,t) = T_0 + G(z - Rt), \tag{1}$$

where $T_0 = T_m - |m|c_l^0$ and $c_l^0 = c_\infty/k$.

The compute set of phase-field equations are

$$\tau_\phi(\hat{n}, z)\frac{\partial \phi}{\partial t} = W_0^2 \left\{ \nabla \cdot [a_s(\hat{n})^2 \nabla \phi] + \partial_x \left(|\nabla \phi|^2 a_s(\hat{n}) \frac{\partial a_s(\hat{n})}{\partial(\partial_x \phi)} \right) + \partial_z \left(|\nabla \phi|^2 a_s(\hat{n}) \frac{\partial a_s(\hat{n})}{\partial(\partial_z \phi)} \right) \right\}$$
$$+ \phi - \phi^3 - \lambda(1-\phi^2)^2 \left(U + \frac{z - Rt}{l_T} \right), \tag{2}$$

$$\tau_U \frac{\partial U}{\partial t} = \nabla \cdot [D_l d(\phi) \nabla U + \vec{j}_{at}] + [1 + (1-k)U] \frac{1}{2} \frac{\partial \phi}{\partial t}, \tag{3}$$

where

$$U = \frac{1}{1-k} \left(\frac{c/c_l^0}{(1-\phi)/2 + k(1+\phi)/2} - 1 \right), \quad d(\phi) = (1-\phi)/2. \tag{4}$$

Other parameters and terms are defined as

$$\tau_\phi(\hat{n}, z) = \tau_0(a_s(\hat{n}))^2\left[1-(1-k)\frac{(z-Rt)}{l_T}\right] \tag{5}$$

$$\tau_U = \frac{1+k}{2} - \frac{1-k}{2}\phi \tag{6}$$

$$\vec{j}_{at} = \frac{1}{2\sqrt{2}}W_0[1+(1-k)U]\frac{\nabla\phi}{|\nabla\phi|}\frac{\partial\phi}{\partial t} \tag{7}$$

$$a_s(\hat{n}) = (1-3\delta)\left\{1+\frac{4\delta}{1-3\delta}(\hat{n}_x^4+\hat{n}_z^4)\right\} \tag{8}$$

$$\hat{n} = \frac{\nabla\phi}{|\nabla\phi|} \tag{9}$$

$$l_T = \frac{|m|c_\infty(1/k-1)}{G} \tag{10}$$

$$\lambda = \frac{5\sqrt{2}}{8}\frac{W_0}{d_0} \tag{11}$$

$$d_0 = \frac{\Gamma}{|m|c_\infty(1/k-1)} = \frac{\gamma T_m/L}{|m|c_\infty(1/k-1)} \tag{12}$$

$$\tau_0 = \frac{0.6267\lambda W_0^2}{D_l} \tag{13}$$

The boundary conditions are periodic in the x-direction and no-flux in the z-direction.

1.1 Non-dimensionalized equations

We use the interfacial width W_0 as the length scale and τ_0 as the time scale to non-dimensionalize the equations:

$$\begin{aligned}\left[1-(1-k)\frac{(z-\tilde{R}t)}{\tilde{l}_T}\right]a_s(\hat{n}^2)\frac{\partial\phi}{\partial t} &= \nabla\cdot[a_s(\hat{n})^2\nabla\phi]+ \\ &\partial_x\left(|\nabla\phi|^2 a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_x\phi)}\right)+\partial_z\left(|\nabla\phi|^2 a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_z\phi)}\right) \\ &+\phi-\phi^3-\lambda(1-\phi^2)^2\left(U+\frac{z-\tilde{R}t}{\tilde{l}_T}\right)\end{aligned} \tag{14}$$

$$\left(\frac{1+k}{2}-\frac{1-k}{2}\phi\right)\frac{\partial U}{\partial t} = \nabla\cdot[\tilde{D}_l d(\phi)\nabla U+\vec{j}_{at}]+[1+(1-k)U]\frac{1}{2}\frac{\partial\phi}{\partial t}, \tag{15}$$

where the non-dimensional parameters are $\tilde{R} = R\tau_0/W_0$, $\tilde{D}_l = D_l\tau_0/W_0^2$ and $\tilde{l}_T = l_T/W_0$.

1.2 Noise

2 Micro model discretization

2.1 ϕ-equation

We first discretize the ϕ-equation in **??**. The challenge is to discretize the anisotropic surface tension term. We will make a few simplications. First, note the anisotropic surface tension can be parametrized by $\theta \equiv \arctan(\phi_y/\phi_x)$, i.e.,

$$a_s(\theta) = 1 + \delta\cos(4\theta) \tag{16}$$
$$a_s'(\theta) = -4\delta\sin(4\theta) \tag{17}$$

By using some trigonometric identities (check), and $\cos(\theta) = \phi_x/|\nabla\phi|$ and $\sin(\theta) = \phi_y/|\nabla\phi|$, we have

$$\cos(4\theta) = 1 - 8\cos^2(\theta)\sin^2(\theta) = 1 - 8\frac{\phi_x^2\phi_z^2}{|\nabla\phi|^4} \tag{18}$$
$$\sin(4\theta) = 4\sin(\theta)\cos(\theta)(\cos^2(\theta) - \sin^2(\theta)) = 4\frac{(\phi_x^3\phi_z - \phi_x\phi_z^3)}{|\nabla\phi|^4}. \tag{19}$$

We can also write (see Appendix B of [?])

$$\partial_x\left(|\nabla\phi|^2 a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_x\phi)}\right) = \partial_x(-a_s'(\theta)a_s(\theta)\partial_z\phi) \tag{20}$$
$$\partial_z\left(|\nabla\phi|^2 a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_z\phi)}\right) = \partial_z(a_s'(\theta)a_s(\theta)\partial_x\phi). \tag{21}$$

Therefore,

$$\begin{aligned}&\nabla\cdot[a_s(\hat{n})^2\nabla\phi] + \partial_x\left(|\nabla\phi|^2 a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_x\phi)}\right) + \partial_z\left(|\nabla\phi|^2 a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_z\phi)}\right)\\ &= \partial_x\underbrace{\left[a_s^2(\theta)\partial_x\phi - a_s'(\theta)a_s(\theta)\partial_z\phi\right]}_{=:F} + \partial_z\underbrace{\left[a_s^2(\theta)\partial_z\phi + a_s'(\theta)a_s(\theta)\partial_x\phi\right]}_{=:J}\end{aligned} \tag{22}$$

We define $\phi(i,j)$ on the cell nodes. Therefore, **??** is discretized as

$$\frac{F(i+1/2,j) - F(i-1/2,j)}{\Delta x} + \frac{J(i,j+1/2) - J(i,j-1/2)}{\Delta z} \tag{23}$$

Note F, J are defined on cell edges. For example, to evaluate $F(i+\frac{1}{2},j)$, we need to evaluate

$$a_s(\theta)\Big|_{i+1/2,j} = \left(1 - 3\delta + 4\delta\frac{\phi_x^4 + \phi_z^4}{|\nabla\phi|^4}\right)\Big|_{i+1/2,j} \tag{24}$$
$$a_s'(\theta)\Big|_{i+1/2,j} = -16\delta\frac{(\phi_x^3\phi_z - \phi_x\phi_z^3)}{|\nabla\phi|^4}\Big|_{i+1/2,j} \tag{25}$$
$$\partial_x\phi\Big|_{i+1/2,j} = \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x} \tag{26}$$
$$\partial_z\phi\Big|_{i+1/2,j} = \frac{\phi_{i,j+1} + \phi_{i+1,j+1} - \phi_{i,j-1} - \phi_{i+1,j-1}}{4\Delta z} \tag{27}$$

Note evaluating $\partial_z\phi|_{i+1/2,j}$ requires averaging nearby cells. Please work out the details for $F(i-1/2,j)$, $J(i,j+1/2)$ and $J(i,j-1/2)$. Many of them are redundant. I think you only need $\partial_x\phi|_{i,j+1/2}$ and $\partial_z\phi|_{i,j+1/2}$.

2.2 Divide-by-zero in anisotropy

On page 66 of [?], whenever $|\nabla\phi(i,j)|^2 \leq \epsilon$, say $\epsilon = 10^{-8}$, we just set

$$\begin{aligned} a_s(\hat{n}) &= 1 - 3\delta, \\ a_s'(\hat{n}) &= 0. \end{aligned}$$

In [?], Karma explained the need for $a_s(\hat{n})$ in the definition τ_ϕ on the LHS of **??** because it is related to the correct kinetics in the Stefan problem. Fortunately this term is never zero so it is safe to divide.

2.3 Misorientation

We denote α_0 the misorientation angle, and introduce a rotated coordinate $(\tilde{x}, \tilde{z})$,

$$\begin{pmatrix} \phi_{\tilde{x}} \\ \phi_{\tilde{z}} \end{pmatrix} = \begin{bmatrix} \cos\alpha_0 & -\sin\alpha_0 \\ \sin\alpha_0 & \cos\alpha_0 \end{bmatrix} \begin{pmatrix} \phi_x \\ \phi_z \end{pmatrix} \tag{28}$$

$$\cos(4\tilde{\theta}) = \cos(4(\theta - \alpha_0)) = 1 - 8\frac{\phi_{\tilde{x}}^2\phi_{\tilde{z}}^2}{|\widetilde{\nabla}\phi|^4} \tag{29}$$

$$\sin(4\tilde{\theta}) = \sin(4(\theta - \alpha_0)) = 4\frac{(\phi_{\tilde{x}}^3\phi_{\tilde{z}} - \phi_{\tilde{x}}\phi_{\tilde{z}}^3)}{|\widetilde{\nabla}\phi|^4} \tag{30}$$

$$a_s(\widetilde{\nabla}\phi) = a_s(\tilde{\theta}) = 1 + \delta\cos(4(\theta - \alpha_0)) \tag{31}$$

$$\tag{32}$$

We replace $a_s(\nabla\phi)$ in **??** by $a_s(\widetilde{\nabla}\phi)$

$$\begin{aligned} \left[1 - (1-k)\frac{(z - \tilde{R}t)}{\tilde{l}_T}\right] a_s(\widetilde{\nabla}\phi)^2\frac{\partial\phi}{\partial t} &= \nabla\cdot[\tilde{a}_s(\widetilde{\nabla}\phi)^2\nabla\phi] + \phi - \phi^3 - \lambda(1-\phi^2)^2\left(U + \frac{z - \tilde{R}t}{\tilde{l}_T}\right) \\ &\partial_x\left(|\nabla\phi|^2 a_s(\widetilde{\nabla}\phi)\frac{\partial a_s(\widetilde{\nabla}\phi)}{\partial(\partial_x\phi)}\right) + \partial_z\left(|\nabla\phi|^2 a_s(\widetilde{\nabla}\phi)\frac{\partial a_s(\widetilde{\nabla}\phi)}{\partial(\partial_z\phi)}\right) \end{aligned} \tag{33}$$

2.4 U-equation

- A routine that takes in edge-centered vector data and outputs the divergence at cell nodes, i.e.,

$$\nabla\cdot\mathbf{u} = \frac{u_{i+1/2,j} - u_{i-1/2,j}}{\Delta x} + \frac{v_{i,j+1/2} - v_{i,j-1/2}}{\Delta z} \tag{34}$$

- we need the following terms at $(i+1/2, j)$ and $(i, j+1/2)$

$$[(1-\phi)U_x]_{i+1/2,j} = \left(1 - \frac{\phi_{i+1,j} + \phi_{i,j}}{2}\right)\frac{U_{i+1,j} - U_{i,j}}{\Delta x} \tag{35}$$

$$[(1-\phi)U_z]_{i,j+1/2} = \left(1 - \frac{\phi_{i,j+1} + \phi_{i,j}}{2}\right)\frac{U_{i,j+1} - U_{i,j}}{\Delta z} \tag{36}$$

$$\tag{37}$$

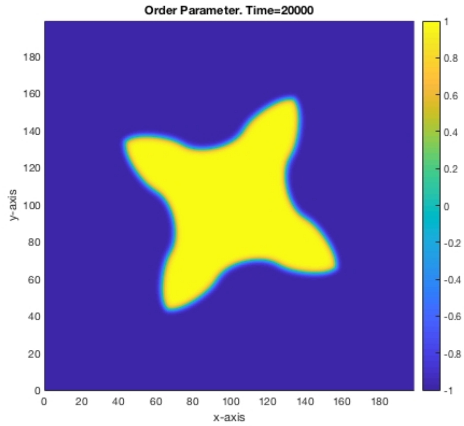


Fig. 1: Misorientation angle $\alpha_0 = \pi/3$

- Similarly, for the anti-trapping flux $\vec{j}_{at}$, we need

$$\left[[1+(1-k)U]\frac{\phi_x}{|\nabla\phi|}\frac{\partial\phi}{\partial t}\right]_{i+1/2,j} = \frac{1}{2}\left[[1+(1-k)U_{i+1,j}]\partial_t\phi_{i+1,j} + [1+(1-k)U_{i,j}]\partial_t\phi_{i,j}\right]\frac{\phi_x}{|\nabla\phi|}\bigg|_{i+1/2,j} \tag{38}$$

$$\left[[1+(1-k)U]\frac{\phi_y}{|\nabla\phi|}\frac{\partial\phi}{\partial t}\right]_{i,j+1/2} = \frac{1}{2}\left[[1+(1-k)U_{i,j+1}]\partial_t\phi_{i,j+1} + [1+(1-k)U_{i,j}]\partial_t\phi_{i,j}\right]\frac{\phi_x}{|\nabla\phi|}\bigg|_{i,+1/2j} \tag{39}$$

2.5 Initial condition

The initial condition is a planar interface perturbed with sinusoidal bumps:

$$\phi(x,z,t=0) = -\tanh\left(\frac{z-z_0-A_0\sin(2n\pi x/L_x)}{W_0}\right), \tag{40}$$

where z_0 is the initial height, A_0 is the amplitude to initial perturbation, and n is the number of sinusoidal bumps.

For the initial condition of U, we set $c_l = c_\infty, c_s = kc_l$ [?], which with the definition of $c_l^0 = c_\infty/k$, corresponds to $U \equiv -1$ in the whole system!

3 Simulation results

3.1 α_0=0, no noise

Use parameters in [?], ie. table **??**

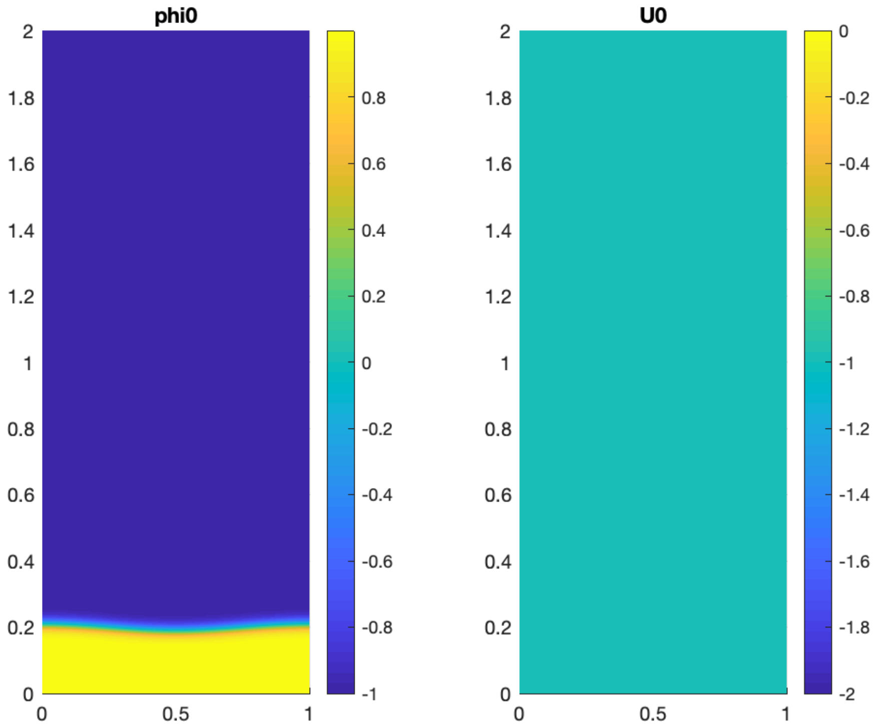


Fig. 2: sample initial condition for ϕ and U

Table 1: Parameters for SCN.

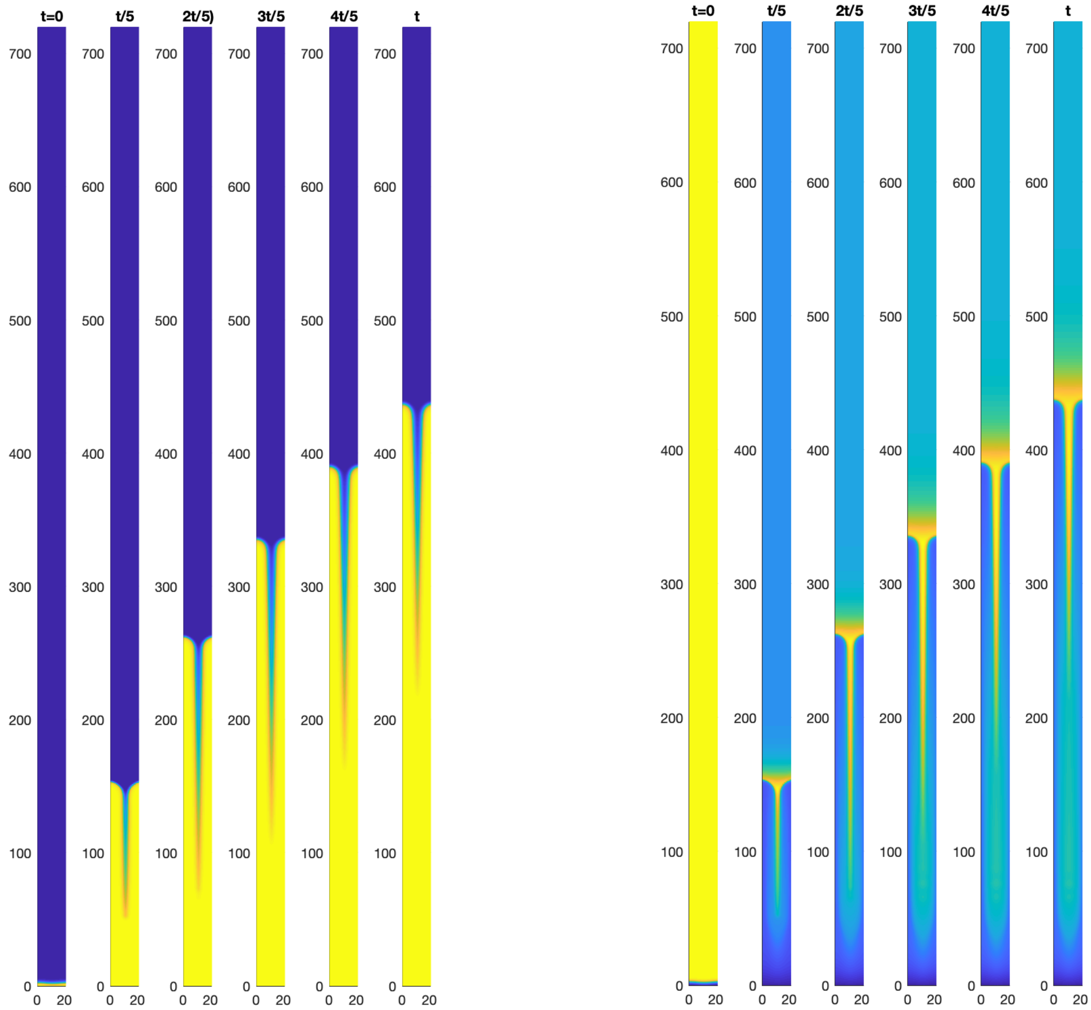
symbol	meaning	values	units
$c_\infty m$	nominal solute concentration	2	K
k	interface solute partition coefficient	0.3	
δ	strength of the surface tension anisotropy	0.007	
Γ	Gibbs-Thompson coefficient	6.48×10^{-8}	Km
d_0	capillary length	1.3×10^{-2}	μm
G	thermal gradient	140	K/cm
R	pulling speed	32	μm/s
D_l	solute diffusion coefficient	10^3	$\mu\text{m}^2/\text{s}$
W_0	interface thickness	40-90	d_0
Δx	mesh size	0.4-0.8	W_0

Table 2: Parameters forAl-Cu.

symbol	meaning	values	units
$c_\infty m$	nominal solute concentration	7.8	K
k	interface solute partition coefficient	0.14	
δ	strength of the surface tension anisotropy	0.01	
Γ	Gibbs-Thompson coefficient	2.4×10^{-7}	Km
d_0	capillary length	5×10^{-3}	μm
G	thermal gradient	700	K/cm
R	pulling speed	1000	μm/s
D_l	solute diffusion coefficient	3000	μm^2/s
W_0	interface thickness	22.6	d_0
Δx	mesh size	0.5	W_0

Table 3: Simulation parameters

symbol	meaning	values	units
ϵ	divide-by-zero	1e-4	
Δx	mesh size	0.8	W_0
Δt	time step size	0.0005	τ_0
Λ	primary spacing	22.5	μm
A_p	amplitude of initial perturbation	0.2	W_0
L_x	length of computation domain	1	Λ
M_t	time steps	120000	



(a) ϕ (b) c/c_∞

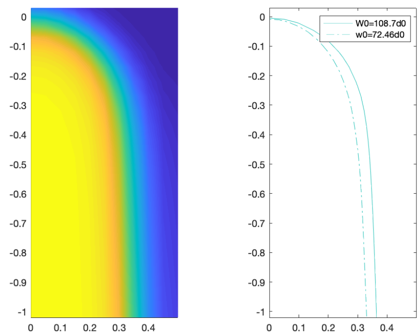
Fig. 3: phase field and concentration for SCN. $W_0 = 108.7d_0$

3.2 Convergence study on Δ x and Δ t

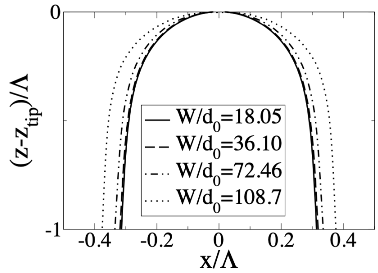
3.3 α_0=30, no noise

3.4 α_0=30, increase primary spacing

3.5 Increase number of initial pertubations

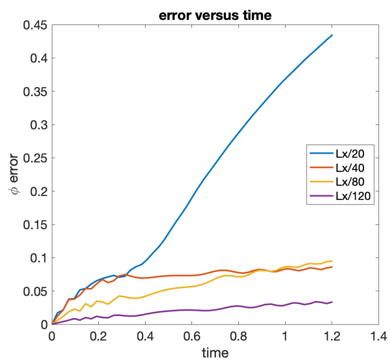


(a) results

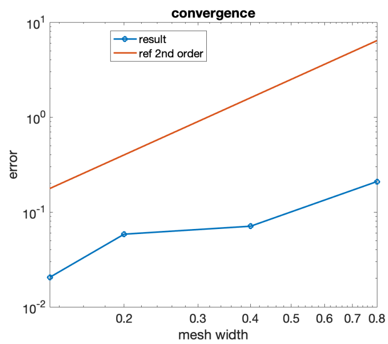


(b) reference

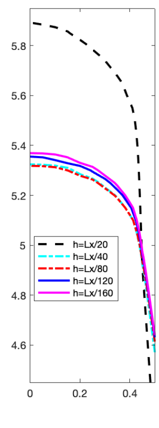
Fig. 4: phase field shape convergence for different W0



(a) error

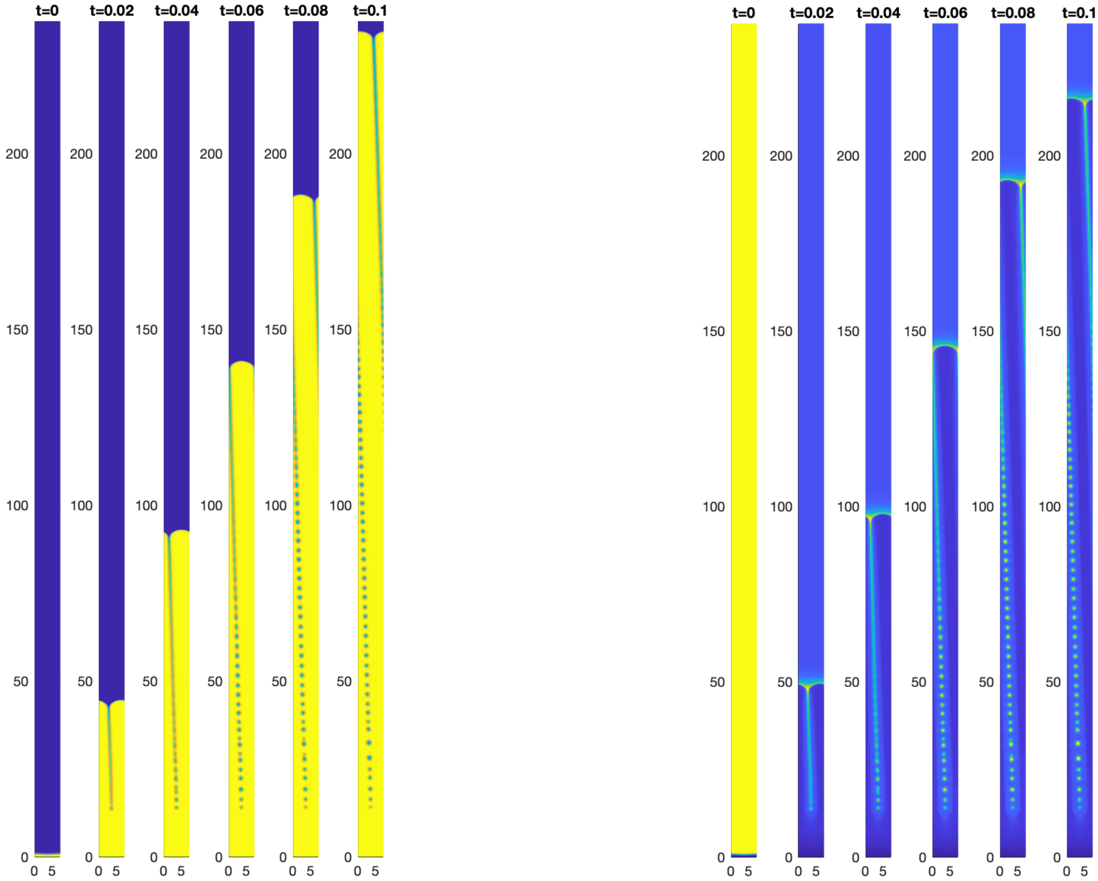


(b) convergence



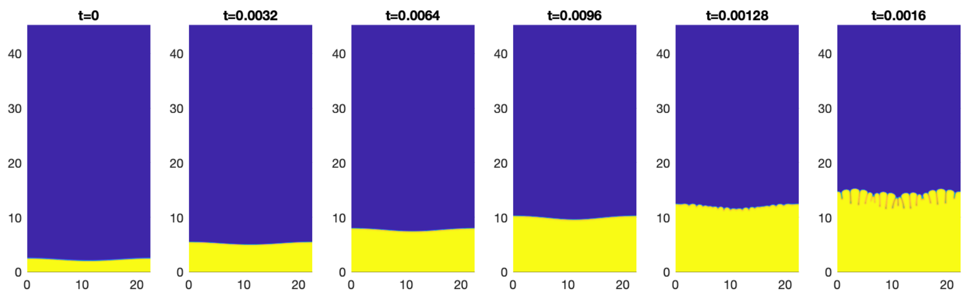
(c) shape

Fig. 5: convergence



(a) ϕ (b) c/c_∞

Fig. 6: tilted growth of Al-Cu alloy at α_0=30°



(a) ϕ

Fig. 7: tilted growth of Al-Cu alloy at α_0=30°,larger spacing

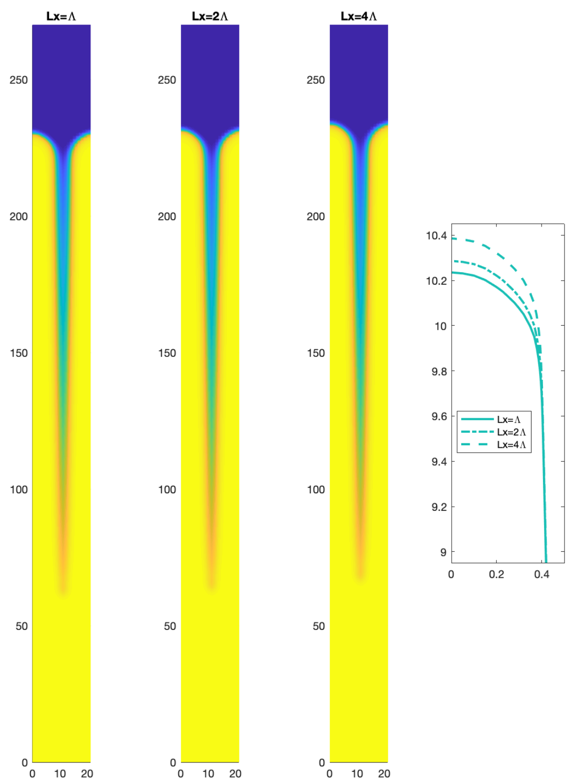


Fig. 8: phase field for different Lx with same Λ