Macroscopic Heat Transfer Model for Additive Manufacturing Testbed Problem

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1 Macroscopic model

We model the macroscopic heat transfer in the rectangular domain Ω

$$\frac{\partial \rho c_p T}{\partial t} = \nabla \cdot (K \nabla T) - \frac{\partial \rho L f_l(T)}{\partial t} \quad \text{in } \Omega \tag{1}$$

$$\frac{\partial T}{\partial t} = \alpha \Delta T - \frac{L}{c_p} \frac{\partial f_l(T)}{\partial t} \quad \text{in } \Omega \tag{2}$$

with boundary conditions

$$(-K\nabla T) \cdot \hat{n} = -q_s + h(T - T_e) + \epsilon\sigma(T^4 - T_e^4) \quad \text{on } \Gamma_{top} \tag{3}$$

$$(-K\nabla T) \cdot \hat{n} = 0 \quad \text{on } \Gamma \backslash \Gamma_{top} \tag{4}$$

where K is the heat conductivity, α is thermal diffusivity, h is the convective heat transfer coefficient, ϵ is the thermal radiation coefficient, σ is the Stefan-Boltzmann constant, and L is the latent heat. The fluid mass fraction f_l is modeled as

$$f_l(T) = \begin{cases} 1 & T > T_l \\ \frac{T - T_s}{T_l - T_s} & T_s \leq T \leq T_l \\ 0 & T < T_s \end{cases} \tag{5}$$

where T_l and T_s are the liquidus and solidus temperature, respectively. The heat source q_S is modeled as a moving Gaussian

$$q_s(x,t) = \frac{2Q\eta}{\pi r_b^2} \exp\left(-\frac{2(x - V_s t)^2}{r_b^2} \right), \tag{6}$$

where Q is the source of heat power, η is the absorption coefficient, r_b is the radius of heat source and V_s is the scanning speed.

2 Macroscopic model 2

We consider the following macroscopic heat transfer model

$$\rho C_p(T)\frac{\partial T}{\partial t} = K\nabla^2 T, \tag{7}$$

where $C_p(T)$ is the heat capacity which can be modeled as

$$C_p(T) = C_{p,solid}(1-\alpha(T)) + C_{p,liquid}\alpha(T) + L_{s\to l}\frac{d\alpha}{dT}, \tag{8}$$

where $\alpha(T)$ is the phase transition function

$$\alpha(T) = \begin{cases} 0 & T < T_s, \\ \frac{1}{2}(1-\cos(\pi(T-T_s)/(T_l-T_s))) & T_s \leq T \leq T_l, \\ 1 & T > T_l. \end{cases} \tag{9}$$

with boundary conditions

$$(-K\nabla T)\cdot\hat{n} = -q_s + h(T-T_e) + \epsilon\sigma(T^4 - T_e^4) \quad \text{on } \Gamma_{top} \tag{10}$$

$$(-K\nabla T)\cdot\hat{n} = 0 \quad \text{on } \Gamma\backslash\Gamma_{top} \tag{11}$$

where K is the heat conductivity, α is thermal diffusivity, h is the convective heat transfer coefficient, ϵ is the thermal radiation coefficient, σ is the Stefan-Boltzmann constant, and $L_{s\to l}$ is the latent heat.

The heat source q_S is modeled as a moving Gaussian

$$q_s(x,t) = \frac{2Q\eta}{\pi r_b^2}\exp\left(-\frac{2(x-V_s t)^2}{r_b^2}\right), \tag{12}$$

where Q is the source of heat power, η is the absorption coefficient, r_b is the radius of heat source and V_s is the scanning speed.

The microscopic model is coupled to the macroscopic model through the temperature field, where:

$$G = ||\nabla T||_2 \tag{13}$$

$$R = \frac{1}{G}\frac{\partial T}{\partial t} \tag{14}$$

3 Macro model discretization

3.1 Forward Euler scheme

We discretize the domain Ω using $(N+1)\times(M+1)$ grid with meshwidth h. Lx = Nh, x = ih. Let $T_{ij}^n = T(ih, jh, t_n)$ for $i = 0,\ldots,N$ and $j = 0,\ldots,M$.

$$\frac{T_{i,j}^n - T_{i,j}^{n-1}}{\Delta t} = \alpha\frac{T_{i,j+1}^n + T_{i,j-1}^n + T_{i-1,j}^n + T_{i+1,j}^n - 4T_{i,j}^n}{h^2} - L_m\frac{\partial f_l(T)}{\partial t}\bigg|_{t=t_n} \tag{15}$$

At the top boundary ($j=0$), we treat the convection and radiation term explicitly,

$$-K\frac{T^n_{i,-1}-T^n_{i,1}}{2h} = -q_s(ih,t_{n-1}) + h(T^{n-1}_{i,0}-T_e) + \epsilon\sigma((T^{n-1}_{i,0})^4 - T_e^4),\ i=0,\dots,N \tag{16}$$

$$T^n_{i,-1} = T^n_{i,1} - \frac{2h}{K}\left(-q_s(ih,t_{n-1}) + h(T^{n-1}_{i,0}-T_e) + \epsilon\sigma((T^{n-1}_{i,0})^4 - T_e^4)\right) = T^n_{i,1} + U^{n-1}_i,\ i=0,\dots,N \tag{17}$$

Other boundaries:

$$T^n_{i,M+1} = T^n_{i,M-1},\ i=0,\dots,N \tag{18}$$
$$T^n_{-1,j} = T^n_{1,j},\ j=0,\dots,M \tag{19}$$
$$T^n_{N-1,j} = T^n_{N+1,j},\ j=0,\dots,M \tag{20}$$

Eventually, the linear system of equation should look like

$$(\mathbf{I}-C\mathbf{L})\mathbf{T}^n + \mathbf{N}(\mathbf{T}^n) = \mathbf{T}^{n-1} + \mathbf{N}(\mathbf{T}^{n-1}) + \text{BC terms} \tag{21}$$

where C is CFL number, $\mathbf{L}$ is the discrete 2D laplacian with Neumann BCs and $\mathbf{N}$ is a nonlinear function due the implicit treatment of latent heat term. If we treat the latent heat term explicitly, we need two starting values initially.

3.2 Crank-Nicolson

First, we absorb the latent heat to the left hand side, rewrite the equation in Crank-Nicolson scheme:

$$\mathbf{La}(T^{n-1}_{i,j})\left(T^n_{i,j}-T^{n-1}_{i,j}\right) = \frac{C}{2}\left(T^n_{i,j+1}+T^n_{i,j-1}+T^n_{i-1,j}+T^n_{i+1,j}-4T^n_{i,j}\right) + \frac{C}{2}\left(T^{n-1}_{i,j+1}+T^{n-1}_{i,j-1}+T^{n-1}_{i-1,j}+T^{n-1}_{i+1,\ldots}\right. \tag{22}$$

$$\mathbf{La}(\mathbf{T}^{n-1})\left(\mathbf{T}^n-\mathbf{T}^{n-1}\right) = \frac{C}{2}\mathbf{L}(\mathbf{T}^n) + \frac{C}{2}\mathbf{L}(\mathbf{T}^{n-1}) \tag{23}$$

Add boundary condition (check if the convergence is right)

$$(\mathbf{La}(\mathbf{T}^{n-1}) - \frac{C}{2}\mathbf{L})\mathbf{T}^n = (\mathbf{La}(\mathbf{T}^{n-1}) + \frac{C}{2}\mathbf{L})\mathbf{T}^{n-1} + \text{BC terms} \tag{24}$$

If there is no latent heat, $\mathbf{La}=\mathbf{I}$

3.3 Symmetrization

$\mathbf{La}(\mathbf{T}^{n-1})$is diagonal, in order to make the system symmetric, pre-multiply a matrix Q.

$$Q\left((\mathbf{La}(\mathbf{T}^{n-1}) - \frac{C}{2}\mathbf{L})\mathbf{T}^n\right) = Q\left((\mathbf{La}(\mathbf{T}^{n-1}) + \frac{C}{2}\mathbf{L})\mathbf{T}^{n-1} + \text{BC terms}\right) \tag{25}$$

4 Macro model numerical tests

4.1 No latent heat term

$$\frac{T^n_{i,j} - T^{n-1}_{i,j}}{\Delta t} = \alpha \frac{T^n_{i,j+1} + T^n_{i,j-1} + T^n_{i-1,j} + T^n_{i+1,j} - 4T^n_{i,j}}{h^2} \tag{26}$$

for top boundary (j=0)

$$\frac{T^n_{i,0} - T^{n-1}_{i,0}}{\Delta t} = \alpha \frac{T^n_{i,1} + T^n_{i,-1} + T^n_{i-1,0} + T^n_{i+1,0} - 4T^n_{i,0}}{h^2} = \alpha \frac{2T^n_{i,1} + U^{n-1}_i + T^n_{i-1,0} + T^n_{i+1,0} - 4T^n_{i,0}}{h^2} \tag{27}$$

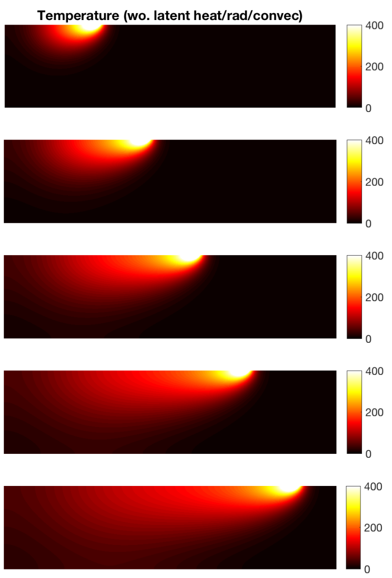
$$\text{BC terms} = CU^{n-1}_i, \quad j = 0, \; i = 0, \dots, N \tag{28}$$

$$U^{n-1}_i = -\frac{2h}{K}\left(-q_s(ih, t_{n-1}) + h_c(T^{n-1}_{i,0} - T_e) + \epsilon\sigma((T^{n-1}_{i,0})^4 - T^4_e)\right), \; i = 0, \dots, N \tag{29}$$

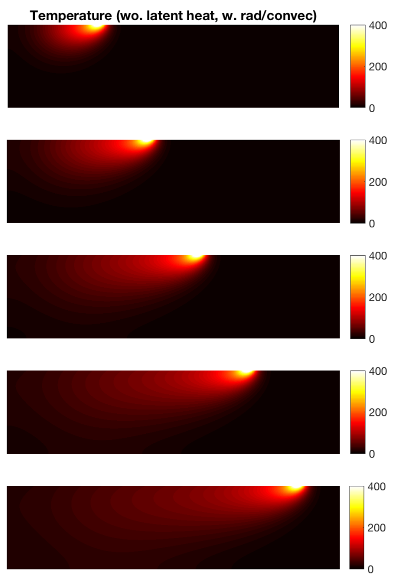
$$q_s(ih, t_n) = q_0 \exp\left(-\frac{2(ih - V_s t_n)^2}{r^2_b}\right) = q_0 \exp\left(-\frac{2(i - {V_s}' t_n)^2}{{r_b}'^2}\right), \; i = 0, \dots, N \tag{30}$$

4.1.1 Test 1

Parameters: K = 0.01, $\rho = 1.0$, $C_p = 1.0$, Q = 3, $\eta = 1$, $r_b = 0.2$, $V_s = 0.075$.
Up boundary cooling parameters: h_c= 0.005, $\epsilon = 0.005$, σ = 5.67E-8, $T_e = 0$.
Computation domain: $L_x = 8$, $L_y = 2$.



(a) no surface cooling h_c= 0, $\epsilon = 0$

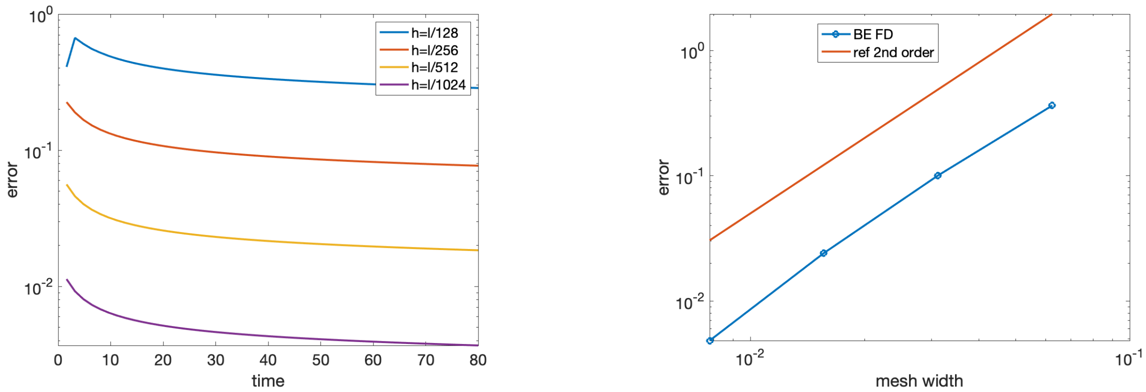


(b) h_c= 0.005, $\epsilon = 0.005$

Fig. 1: Temperature distribution without latent heat.

4.1.2 Self Convergence Study (with convection and radiation)

Ground truth: dt = 0.00625, h = $L_x/2048$
Trial: dt = 0.025, 0.1, 0.4, 1.6; h = $L_x/1024, L_x/512, L_x/256, L_x/128$



(a) L^2 error (b) convergence order 2.076

Fig. 2: Self convergence.

4.2 Latent heat term implicit-explicit

Implicit:

$$\frac{\partial f_l(T)}{\partial t} = \frac{f_l^n(T) - f_l^{n-1}(T)}{\Delta t} \tag{31}$$

Explicit:

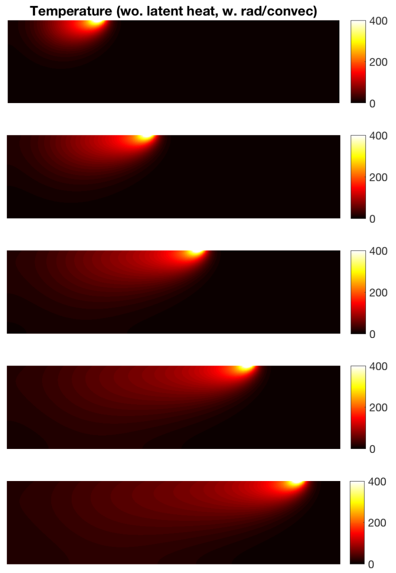
$$f_l^n(T) = \begin{cases} 1 & T^{n-1} > T_l \\ \frac{T^n - T_s}{T_l - T_s} & T_s \leq T^{n-1} \leq T_l \\ 0 & T^{n-1} < T_s \end{cases} \tag{32}$$

$$f_l^{n-1}(T) = \begin{cases} 1 & T^{n-1} > T_l \\ \frac{T^{n-1} - T_s}{T_l - T_s} & T_s \leq T^{n-1} \leq T_l \\ 0 & T^{n-1} < T_s \end{cases} \tag{33}$$

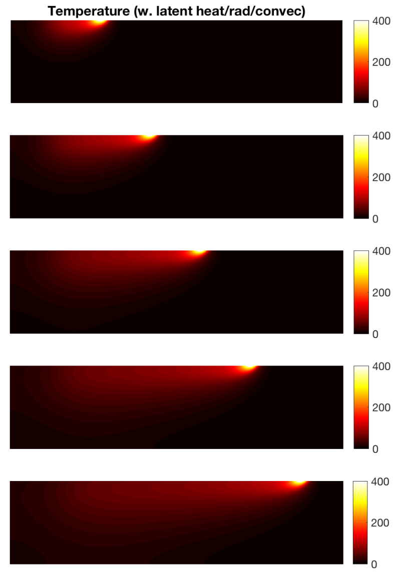
$$\text{Latent heat term} = \begin{cases} 0 & T^{n-1} > T_l \\ -\frac{L_m}{\Delta t}\frac{T^n - T^{n-1}}{T_l - T_s} & T_s \leq T^{n-1} \leq T_l \\ 0 & T^{n-1} < T_s \end{cases} \tag{34}$$

4.2.1 Test2

Parameters: L=200, T_s=40, T_l=110

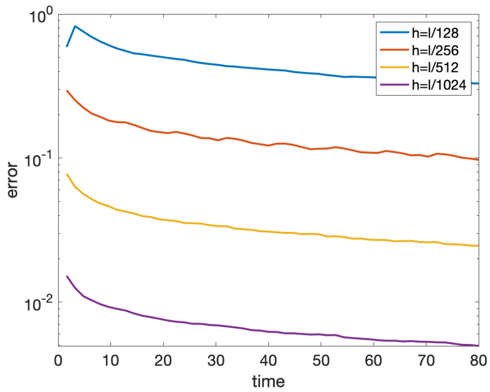


(a) Without latent heat

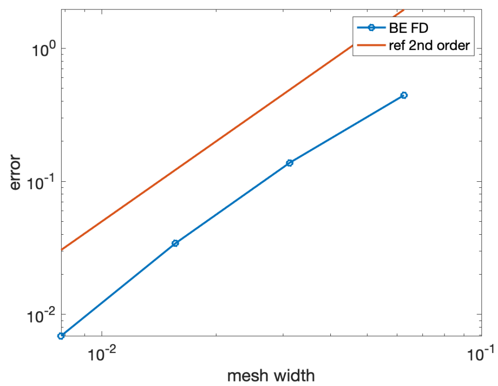


(b) With latent heat

Fig. 3: Temperature distribution with and without latent heat. Surface cooling is included.



(a) L^2 error



(b) convergence order

Fig. 4: Self convergence.

GMRES solver (Tol = 1e-9):
For mesh width h = $L_x/1024, L_x/512, L_x/256, L_x/128$
Iterations per time step without precondtioner: 58, 54, 48, 49, 50
Iterations per time step with precondtioner: 20, 17, 16,... but took longer time to run

5 Microscopic model

This model also makes the frozen temperature approximation [?, ?, ?, ?]:

$$T(z,t) = T_0 + G(z - Rt), \tag{35}$$

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

The compute set of phase-field equations are

$$\begin{aligned}\tau_\phi(\hat{n},z)\frac{\partial\phi}{\partial t} &= W_0^2\left\{\nabla\cdot[a_s(\hat{n})^2\nabla\phi] + \partial_x\left(|\nabla\phi|^2 a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_x\phi)}\right) + \partial_z\left(|\nabla\phi|^2 a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_z\phi)}\right)\right\}\\ &\quad + \phi - \phi^3 - \lambda(1-\phi^2)^2\left(U + \frac{z-Rt}{l_T}\right), \qquad (36)\\ \tau_U\frac{\partial U}{\partial t} &= \nabla\cdot[D_l d(\phi)\nabla U + \vec{j}_{at}] + [1+(1-k)U]\frac{1}{2}\frac{\partial\phi}{\partial t}, \qquad (37)\end{aligned}$$

where

$$U = \frac{1}{1-k}\left(\frac{c/c_l^0}{(1-\phi)/2 + k(1+\phi)/2} - 1\right), \quad d(\phi) = (1-\phi)/2. \tag{38}$$

Other parameters and terms are defined as

$$\tau_\phi(\hat{n},z) = \tau_0(a_s(\hat{n}))^2\left[1 - (1-k)\frac{(z-Rt)}{l_T}\right] \tag{39}$$

$$\tau_U = \frac{1+k}{2} - \frac{1-k}{2}\phi \tag{40}$$

$$\vec{j}_{at} = \frac{1}{2\sqrt{2}}W_0[1+(1-k)U]\frac{\nabla\phi}{|\nabla\phi|}\frac{\partial\phi}{\partial t} \tag{41}$$

$$a_s(\hat{n}) = (1-3\delta)\left\{1 + \frac{4\delta}{1-3\delta}(\hat{n}_x^4 + \hat{n}_z^4)\right\} \tag{42}$$

$$\hat{n} = \frac{\nabla\phi}{|\nabla\phi|} \tag{43}$$

$$l_T = \frac{|m|c_\infty(1/k-1)}{G} \tag{44}$$

$$\lambda = \frac{5\sqrt{2}}{8}\frac{W_0}{d_0} \tag{45}$$

$$d_0 = \frac{\Gamma}{|m|c_\infty(1/k-1)} = \frac{\gamma T_m/L}{|m|c_\infty(1/k-1)} \tag{46}$$

$$\tau_0 = \frac{0.6267\lambda W_0^2}{D_l} \tag{47}$$

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

symbol	meaning	values	units
c_∞	nominal solute concentration	0.4	wt.%
c_l^0	equilibrium concentration	c_∞/k	wt.%
m	liquidus slope	-3.02	K wt./%
k	interface solute partition coefficient	0.1-0.3	
T_0	reference solidus temperature		
T_m	melting temperature of pure material A		
l_T	thermal length		mm
γ	average surface tension		
δ	strength of the surface tension anisotropy	0.007 or 0.011	
Γ	Gibbs-Thompson coefficient	6.4×10^{-8}	Km
d_0	capillary length	$\approx 10^{-3}$	μm
G	thermal gradient	10-300	K/cm
R	pulling speed	8-32	μm/s
D_l	solute diffusion coefficient	10^{-9}	m^2/s
L	latent heat		
W_0	interface thickness	40-90	d_0
Δx	mesh size	0.4-0.8	W_0

5.1 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:

$$\left[1-(1-k)\frac{(z-\tilde{R}t)}{\tilde{l}_T}\right]a_s(\hat{n}^2)\frac{\partial\phi}{\partial t}=\nabla\cdot[a_s(\hat{n})^2\nabla\phi]+$$
$$\partial_x\left(|\nabla\phi|^2a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_x\phi)}\right)+\partial_z\left(|\nabla\phi|^2a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_z\phi)}\right)$$
$$+\phi-\phi^3-\lambda(1-\phi^2)^2\left(U+\frac{z-\tilde{R}t}{\tilde{l}_T}\right) \tag{48}$$

$$\left(\frac{1+k}{2}-\frac{1-k}{2}\phi\right)\frac{\partial U}{\partial t}=\nabla\cdot[\tilde{D}_l d(\phi)\nabla U+\vec{j}_{at}]+[1+(1-k)U]\frac{1}{2}\frac{\partial\phi}{\partial t}, \tag{49}$$

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

5.2 Micro model discretization

5.2.1 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.,

$$a_s(\theta)=1+\delta\cos(4\theta) \tag{50}$$
$$a_s'(\theta)=-4\delta\sin(4\theta) \tag{51}$$

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

$$\cos(4\theta)=1-8\cos^2(\theta)\sin^2(\theta)=1-8\frac{\phi_x^2\phi_z^2}{|\nabla\phi|^4} \tag{52}$$
$$\sin(4\theta)=4\sin(\theta)\cos(\theta)(\cos^2(\theta)-\sin^2(\theta))=4\frac{(\phi_x^3\phi_z-\phi_x\phi_z^3)}{|\nabla\phi|^4}. \tag{53}$$

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

$$\partial_x\left(|\nabla\phi|^2a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_x\phi)}\right)=\partial_x(-a_s'(\theta)a_s(\theta)\partial_z\phi) \tag{54}$$
$$\partial_z\left(|\nabla\phi|^2a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_z\phi)}\right)=\partial_z(a_s'(\theta)a_s(\theta)\partial_x\phi). \tag{55}$$

Therefore,

$$\nabla\cdot[a_s(\hat{n})^2\nabla\phi]+\partial_x\left(|\nabla\phi|^2a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_x\phi)}\right)+\partial_z\left(|\nabla\phi|^2a_s(\hat{n})\frac{\partial a_s(\hat{n})}{\partial(\partial_z\phi)}\right)$$
$$=\partial_x\underbrace{\left[a_s^2(\theta)\partial_x\phi-a_s'(\theta)a_s(\theta)\partial_z\phi\right]}_{=:F}+\partial_z\underbrace{\left[a_s^2(\theta)\partial_z\phi+a_s'(\theta)a_s(\theta)\partial_x\phi\right]}_{=:J} \tag{56}$$

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

$$\frac{F(i+1/2,j)-F(i-1/2,j)}{\Delta x}+\frac{J(i,j+1/2)-J(i,j-1/2)}{\Delta z} \tag{57}$$

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

$$a_s(\theta)\Big|_{i+1/2,j} = \left(1-3\delta+4\delta\frac{\phi_x^4+\phi_z^4}{|\nabla\phi|^4}\right)\Big|_{i+1/2,j} \tag{58}$$

$$a_s'(\theta)\Big|_{i+1/2,j} = -16\delta\frac{(\phi_x^3\phi_z-\phi_x\phi_z^3)}{|\nabla\phi|^4}\Big|_{i+1/2,j} \tag{59}$$

$$\partial_x\phi\Big|_{i+1/2,j} = \frac{\phi_{i+1,j}-\phi_{i,j}}{\Delta x} \tag{60}$$

$$\partial_z\phi\Big|_{i+1/2,j} = \frac{\phi_{i,j+1}+\phi_{i+1,j+1}-\phi_{i,j-1}-\phi_{i+1,j-1}}{4\Delta z} \tag{61}$$

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 $\partial_z\phi|_{i,j+1/2}$.

Bao: Note that you need both $a_s(\nabla\phi_{i\pm1/2,j\pm1/2})$ for $a_s(\hat{n})$ on the right-hand-side and $a_s(\nabla\phi_{i,j})$ for $\tau_\phi(\hat{n},z)$ on the left-hand-side.

Once we discretize **??**, the rest is straightforward. Please fill in the details.

5.2.2 Misorientation

$$\partial_{x'}\phi = \cos\alpha_0\partial_x\phi+\sin\alpha_0\partial_y\phi \tag{62}$$

$$\partial_{z'}\phi = -\sin\alpha_0\partial_x\phi+\cos\alpha_0\partial_z\phi \tag{63}$$

$$\cos(4(\theta-\alpha_0)) = 1-8\frac{\phi_{x'}^2\phi_{z'}^2}{|\nabla\phi|^4} \tag{64}$$

$$\sin(4(\theta-\alpha_0)) = 4\frac{(\phi_{x'}^3\phi_{z'}-\phi_{x'}\phi_{z'}^3)}{|\nabla\phi|^4}. \tag{65}$$

5.2.3 Divide-by-zero in anisotropy

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

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

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.

5.2.4 U-equation

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

$$\nabla \cdot \mathbf{u} = \frac{u_{i+1/2,j} - u_{i-1/2,j}}{\Delta x} + \frac{v_{i,j+1/2} - v_{i,j-1/2}}{\Delta z} \tag{66}$$

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

$$[(1-\phi)U_x]_{i+1/2,j} = \left(1 - \frac{\phi_{i+1,j} + \phi_{i,j}}{2}\right) \frac{U_{i+1,j} - U_{i,j}}{\Delta x} \tag{67}$$

$$[(1-\phi)U_z]_{i,j+1/2} = \left(1 - \frac{\phi_{i,j+1} + \phi_{i,j}}{2}\right) \frac{U_{i,j+1} - U_{i,j}}{\Delta z} \tag{68}$$

$$\tag{69}$$

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

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

$$\frac{1}{2} \left[[1 + (1-k)U_{i+1,j}]\partial_t \phi_{i+1,j} + [1 + (1-k)U_{i,j}]\partial_t \phi_{i,j}\right] \frac{\phi_x}{|\nabla \phi|}\bigg|_{i+1/2,j} \tag{70}$$

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

$$\frac{1}{2} \left[[1 + (1-k)U_{i,j+1}]\partial_t \phi_{i,j+1} + [1 + (1-k)U_{i,j}]\partial_t \phi_{i,j}\right] \frac{\phi_x}{|\nabla \phi|}\bigg|_{i,+1/2j} \tag{71}$$

Bao: The bottom line with finite difference is that: whenever the quantity is not defined on the target grid points, you just average nearby cell data.

Bao: I strongly recommend you read the appendices of [?], and page 65, page 101-102 of [?].

5.2.5 Initial condition

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

$$\phi(x, z, t = 0) = 1 - \tanh\left(\frac{z - z_0 - A_0 \sin(2n\pi x/L_x)}{W_0}\right), \tag{72}$$

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!

5.2.6 Noise

5.3 Simulation results

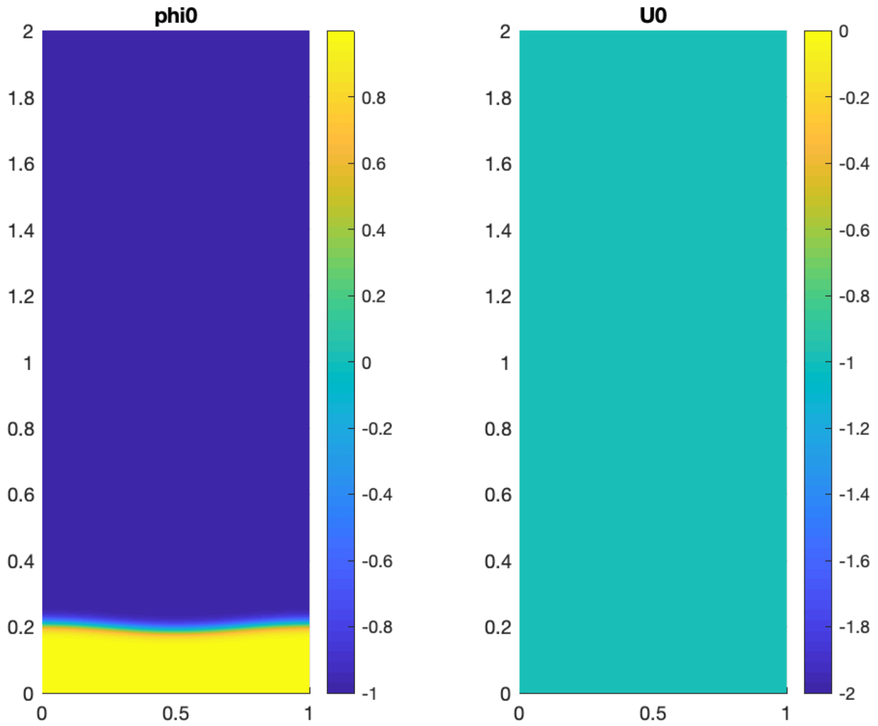


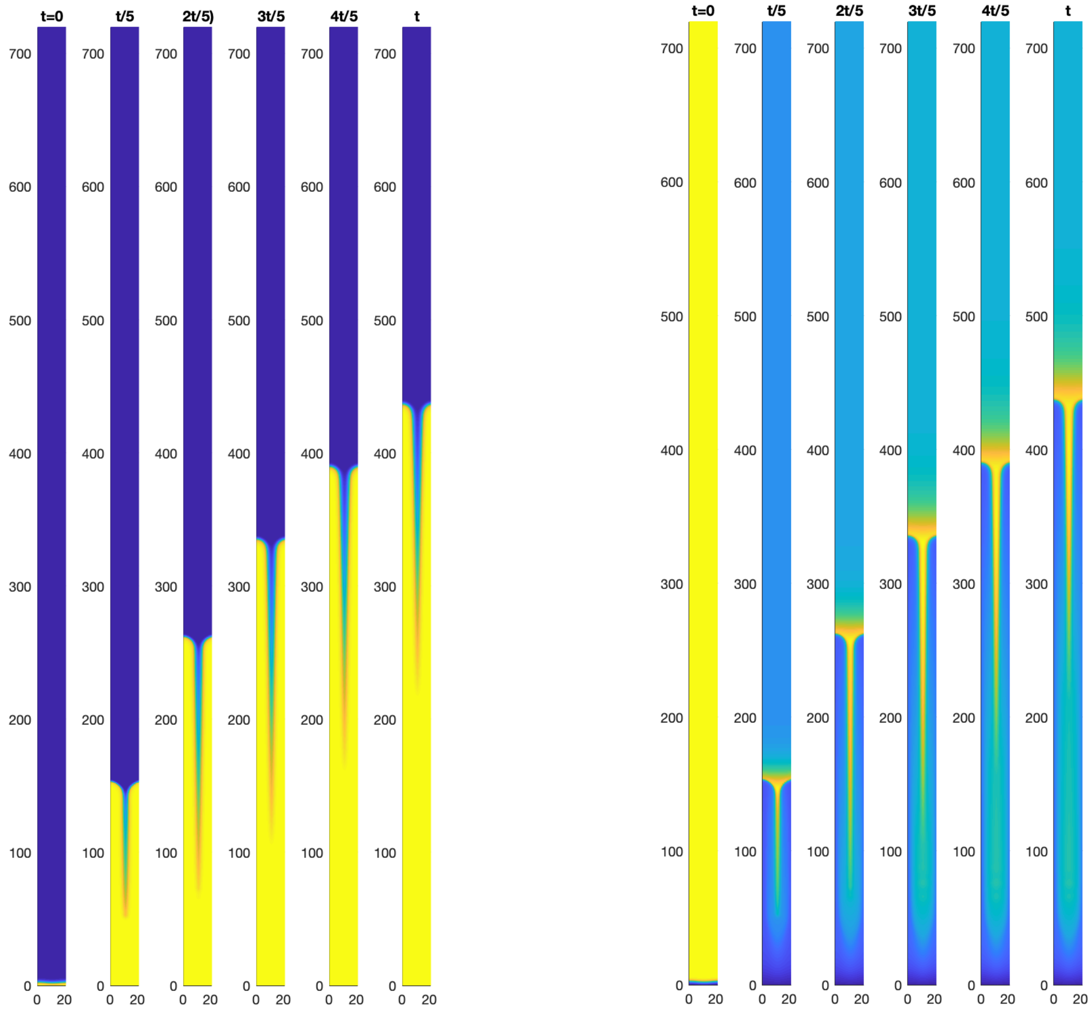
Fig. 5: sample initial condition for ϕ and U

Table 1: Parameters for SCN.

symbol	meaning	values	units
$c_\infty m$	nominal solute concentration	2	K
c_l^0	equilibrium concentration	c_∞/k	wt.%
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	μm^2/s
W_0	interface thickness	40-90	d_0
Δx	mesh size	0.4-0.8	W_0

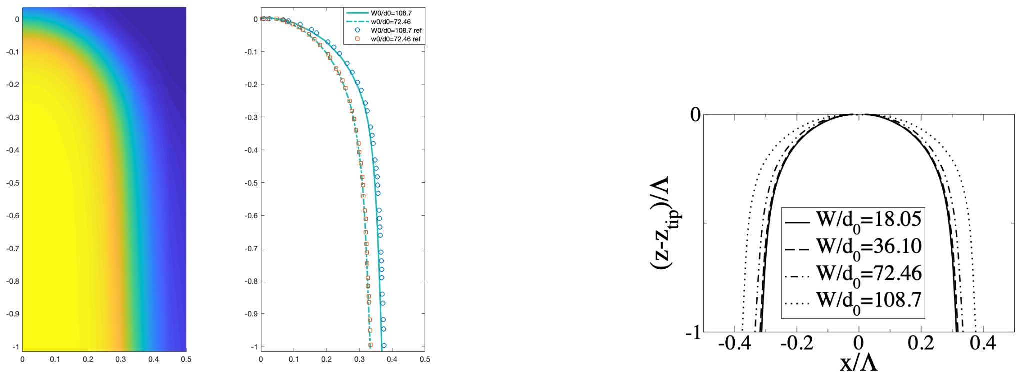
Table 2: Simulation parameters

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. 6: phase field and concentration for SCN.



(a) results

(b) reference

Fig. 7: phase field shape