Mesoscale Multi-Physics Simulation of Solidification in Selective Laser Melting Process Using A Phase Field and Thermal Lattice Boltzmann Model

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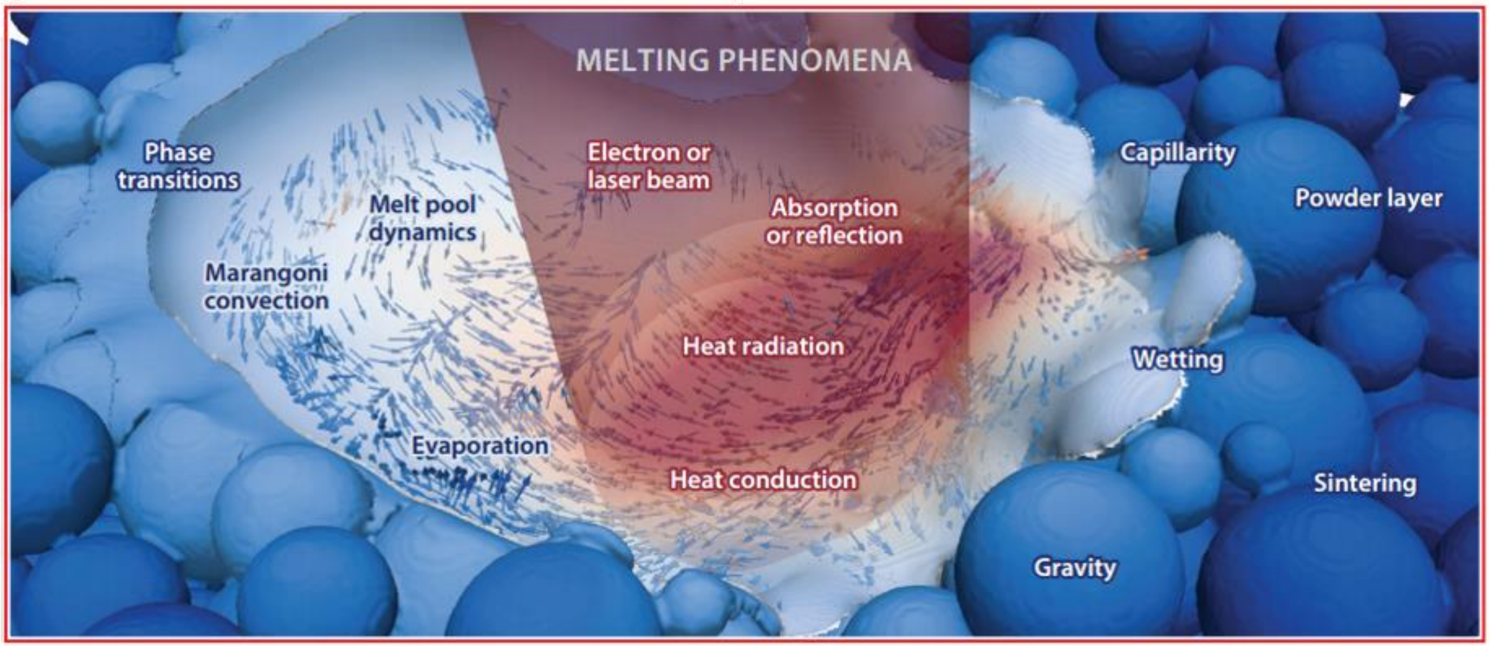
Outline

- **Background**
- **Methodology**
  - Phase Field Method
  - Thermal Lattice Boltzmann
  - Motion of Grain
  - Simulation Algorithm
- **Simulation Results**
  - Effect of Flow
  - Effect of Cooling Rate
- **Summary**

Background

- Solidification of melt in SLM process is very complicated, which involves multiple physical phenomena
- Challenge: Create a multi-physics based model to investigate the Process-Structure relationship



Markl, M., & Körner, C. (2016)

Single-Physics Simulation – Phase Field Method

- Phase field method has been used to simulate the microstructure evolution and solute concentration of Ti-6Al-4V alloy during solidification in powder-bed electron beam AM process (Gong & Chou 2015; Sahoo & Chou 2016)

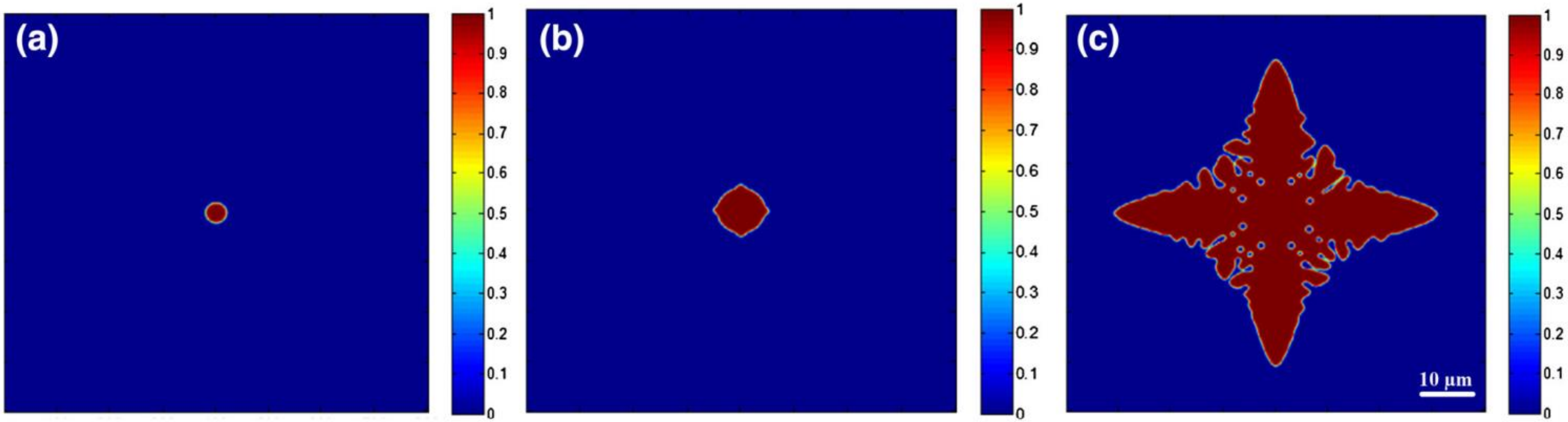
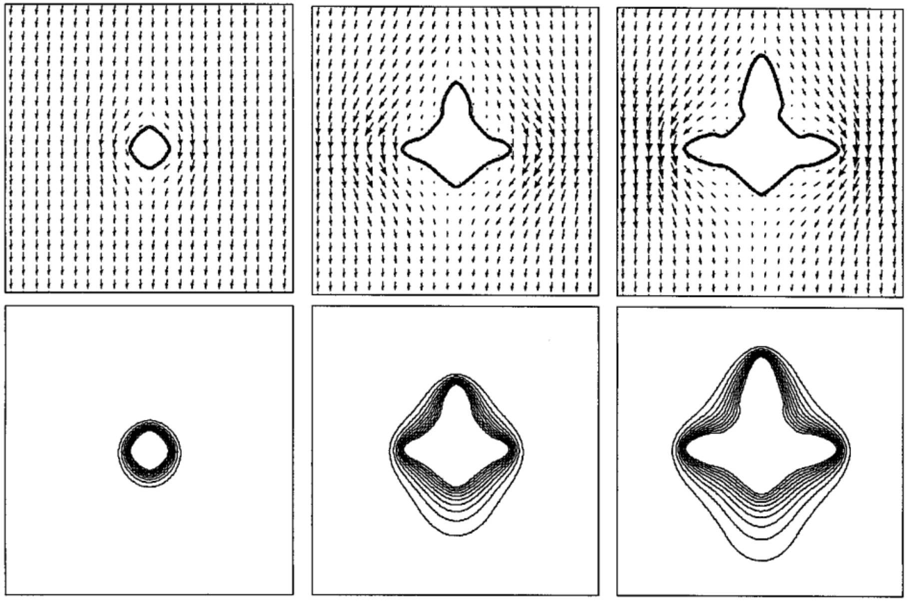


Fig. 1. Simulated dendrite structure growth at different times: (a) 0.01 ms, (b) 0.2 ms, and (c) 1.6 ms.

  - Isothermal assumption without considering the effect of the latent heat
  - No effect of melt flow

Multi-Physics Simulation
– Phase Field + Convection

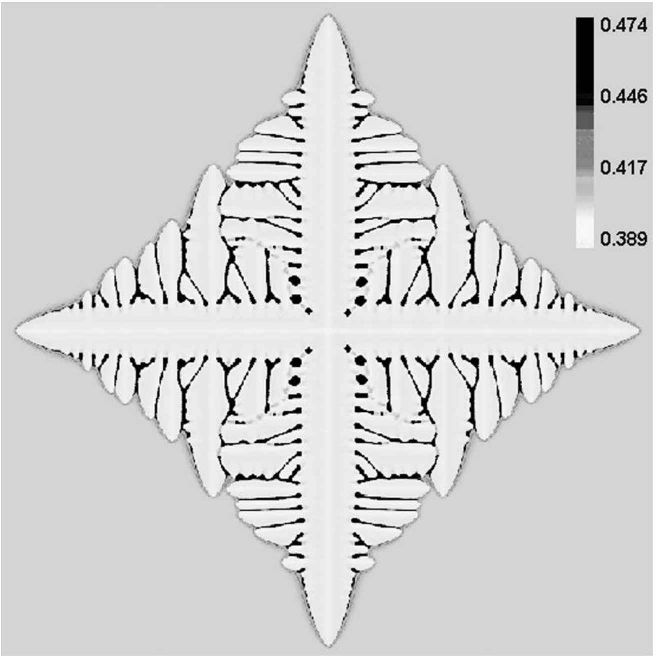
- Navier-Stokes equation to predict fluid flow velocity (Beckermann et al. 1999)
- Advection-Diffusion



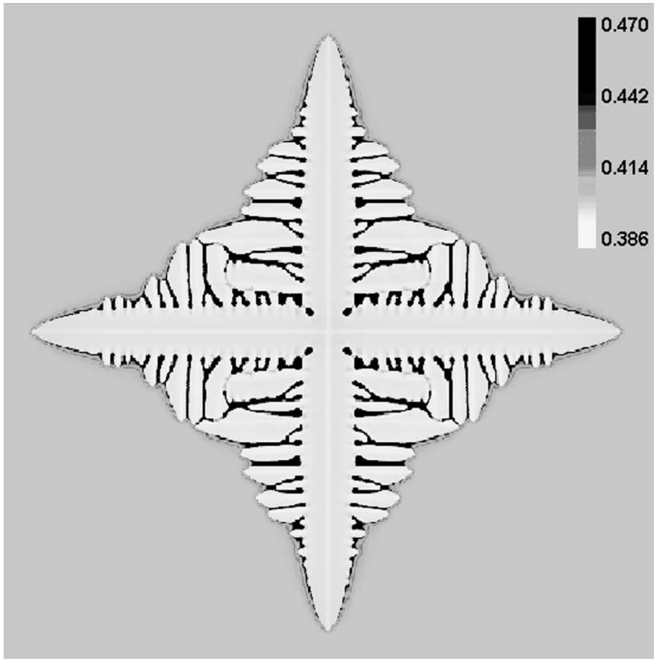
(Beckermann et al. 1999)

Multi-Physics Simulation
– Phase Field + Non-isothermal

- Heat transfer with high cooling rates (Loginova et al. 2001; Grujicic et al. 2002; Echebarria et al. 2004)



Isothermal

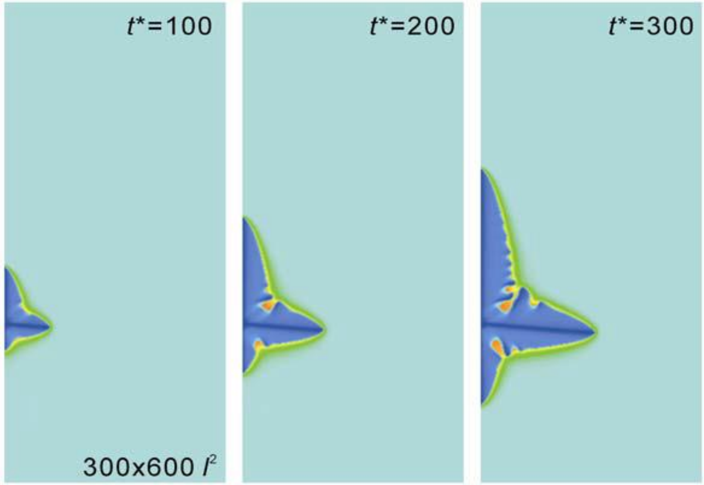


Non-isothermal

(Loginova et al., 2001)

Multi-Physics Simulation
– Phase Field + Convection + Non-isothermal

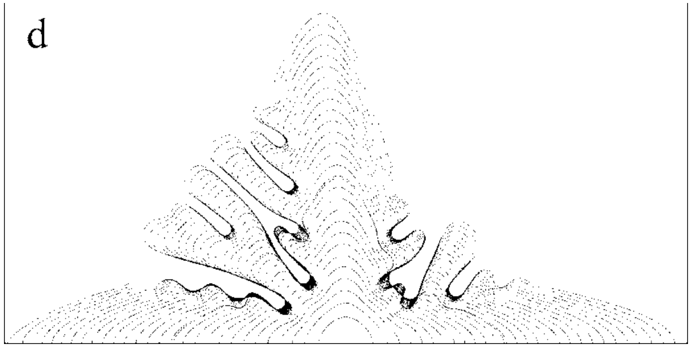
- Navier-Stokes equation is applied to predict fluid flow velocity, thermal conduction (Lan & Shih, 2004; Du & Zhang, 2014; Holfelder et al. 2016)
- Advection-diffusion



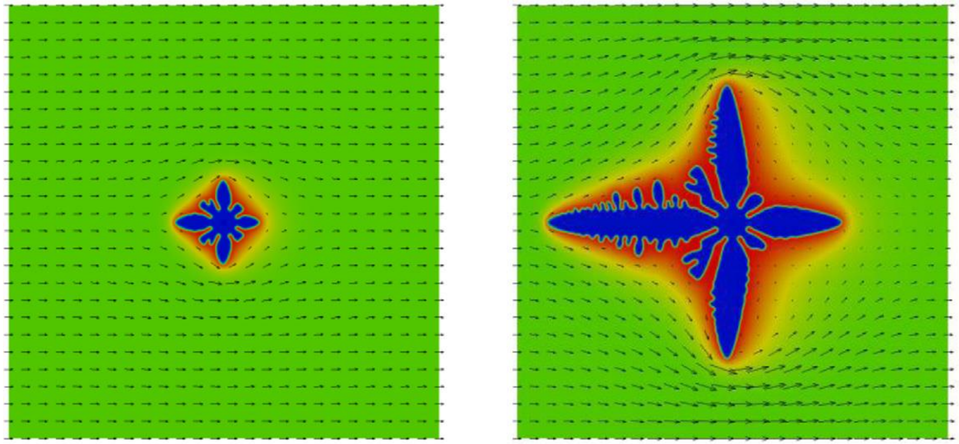
(Lan & Shih, 2004)

Multi-Physics Simulation
– Phase field + lattice Boltzmann method

- Lattice Boltzmann method simulates fluid flow (Medvedev & Kassner 2005; Miller et al. 2006; ; Rojas et al. 2015; Böttger et al. 2016; Cartalade et al. 2016)



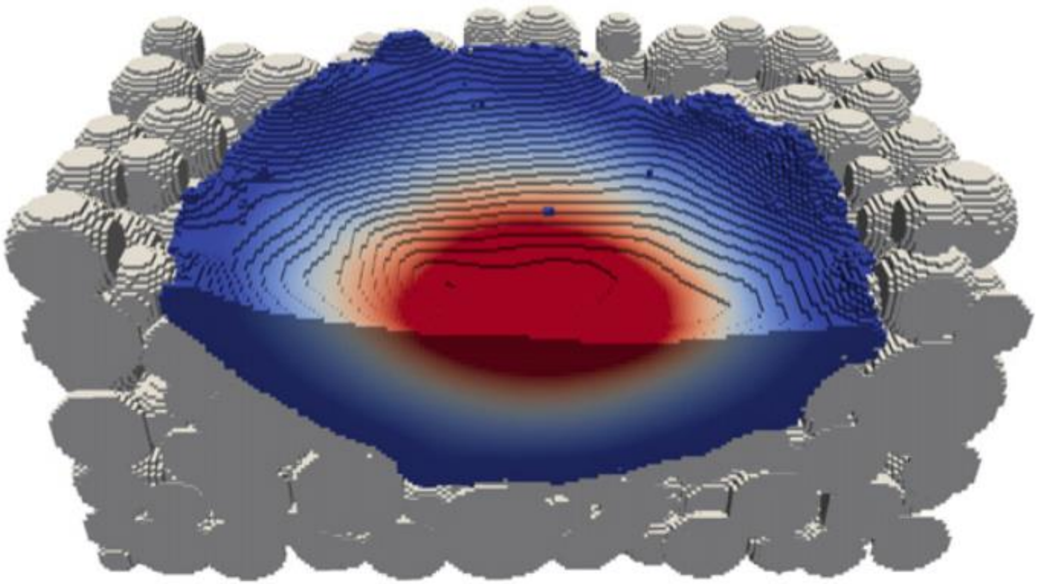
(Medvedev & Kassner 2005)



(Rojas et al. 2015)

Multi-Physics Simulation
– thermal lattice Boltzmann method

- 3D thermal lattice Boltzmann method to simulate the evolution of temperature and velocity field in electron beam melting processes (Ammer et al., 2014)



(Ammer et al., 2014)

  – The evolution of dendrite structure is not simulated

- **Methodology**
  - Phase Field Method
  - Thermal Lattice Boltzmann
  - Motion of Grain
  - Simulation Algorithm

Proposed Multi-Physics Model

- Phase Field + Thermal Lattice Boltzmann Method (**PF-TLBM**) integrates:
  - solute transport,
  - heat transfer,
  - phase transition,
  - fluid dynamics,
  - motion of the solid phase

Phase Field

- Solute transport
- Phase transition

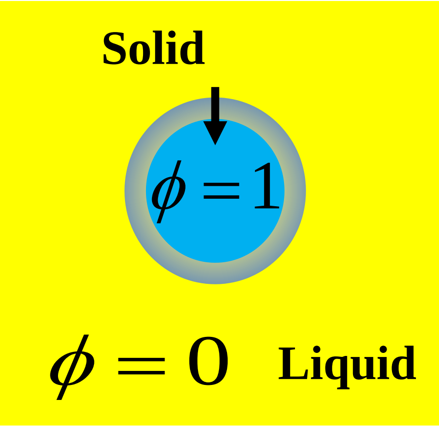
↔

Thermal Lattice Boltzmann

- Fluid dynamics
- Heat transfer
- Motion of grain

Phase Field Method

- Phase Field Method (PFM) is a versatile and accurate numerical tool to simulate solidification (Boettinger et al., 2002; Chen, 2002; Singer-Loginova and Singer, 2008; Moelans et al., 2008; Steinbach, 2009)
- *Phase field* or *order parameter* ϕ describes the distribution of phase
- Free energy functional drives the evolution of microstructure



$$F = \int_{\Omega} (f^{GB} + f^{CH}) dV$$

$$f^{GB} = \frac{4\sigma(\mathbf{n})}{\eta} \left\{ |\nabla \phi|^2 + \frac{\pi^2}{\eta^2} \phi(1-\phi) \right\}$$

$$f^{CH} = h(\phi) f_s(C_s) + h(1-\phi) f_l(C_l) + \mu\left(C - (\phi_s C_s + \phi_l C_l)\right)$$

Our Implemented PFM

- Kinetic equation for the phase field

$$\dot{\phi}+\boxed{\mathbf{u}_s\cdot\nabla\phi}=M_\phi\left\{\sigma(\mathbf{n})\left[\nabla^2\phi+\frac{\pi^2}{\eta^2}\left(\phi-\frac{1}{2}\right)\right]+\frac{\pi}{\eta}\sqrt{\phi(1-\phi)}\Delta G\right\}$$

- Kinetic equation for the composition field

$$\dot{C}+\boxed{\mathbf{u}_l\cdot\nabla\left(\left(1-\phi\right)C_l\right)+\mathbf{u}_s\cdot\nabla\left(\phi C_s\right)}=\nabla\cdot\left(D_l\left(1-\phi\right)\nabla C_l\right)+\boxed{\nabla\cdot\mathbf{j}_{at}}$$

  - Advection effect is considered in solute transport and phase transition
  - Anti-trapping current

$$\mathbf{j}_{at}=\frac{\eta}{\pi}\sqrt{\phi(1-\phi)}\left(C_l-C_s\right)\dot{\phi}\frac{\nabla\phi}{\left|\nabla\phi\right|}$$

Thermal Lattice Boltzmann Method

- Coupling of melt flow with heat transfer

$$\nabla \cdot (\phi_l \mathbf{u}_l) = 0$$

$$\frac{\partial}{\partial t}(\phi_l \mathbf{u}_l) + \nabla \cdot (\phi_l \mathbf{u}_l \mathbf{u}_l) = -\frac{\phi_l}{\rho} \nabla P + \nabla \cdot [\nu \nabla (\phi_l \mathbf{u}_l)] + \mathbf{F}$$

$$\frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{u}_l T) = \nabla \cdot (\alpha \nabla T) + q$$

- Kinetic equations for *density* and *temperature* particle distributions

Density: $$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = \frac{1}{\tau_f}\left(f_i^{eq}(\mathbf{x}, t) - f_i(\mathbf{x}, t)\right) + F_i(\mathbf{x}, t)$$

Temperature: $$g_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) - g_i(\mathbf{x}, t) = \frac{1}{\tau_g}\left(g_i^{eq}(\mathbf{x}, t) - g_i(\mathbf{x}, t)\right) + Q_i(\mathbf{x}, t)$$

  – Macroscopic quantities of density, velocity, and temperature are calculated from f_i's and g_i's.

Thermal Lattice Boltzmann Method

- Latent heat

$$q = \frac{L_H}{c_p}\frac{\partial \phi}{\partial t}$$

- Force source

$$F_i = \left(1 - \frac{1}{2\tau_f}\right)\omega_i\left(\frac{\mathbf{e}_i - \mathbf{u}_l}{c_s^2} + \frac{\mathbf{e}_i \cdot \mathbf{u}_l}{c_s^4}\mathbf{e}_i\right)\cdot \mathbf{F}$$

- Heat source

$$Q_i = \left(1 - \frac{1}{2\tau_g}\right)\omega_i q$$

  - weights (for D2Q9)

$$\omega_i = \begin{cases} 4/9, & i = 0 \\ 1/9, & i = 1,\ldots,4 \\ 1/36, & i = 5,\ldots,8 \end{cases}$$

Motion of Grain

- Motion of grain includes rigid translation and rotation of the grains.
  - Total force and torque acting on a grain

$$\mathbf{F} = -\sum \mathbf{F}_d, \ \mathbf{M} = -\sum \left(\mathbf{r} - \mathbf{R}_{cm}\right) \times \mathbf{F}_d$$

  - Translation of the grain (center of mass)

$$\dot{\mathbf{R}}_{cm} = \mathbf{U}_{cm}, \ \dot{\mathbf{U}}_{cm} = \mathbf{F} / \mathrm{m}$$

  - Rotation of the grain

$$\theta = \omega, \ \dot{\omega} = \mathbf{M} / \mathbf{I}$$

  - Local velocity of the grain

$$\mathbf{u}_s = \mathbf{U}_{cm} + \omega \times \left(\mathbf{r} - \mathbf{R}_{cm}\right)$$

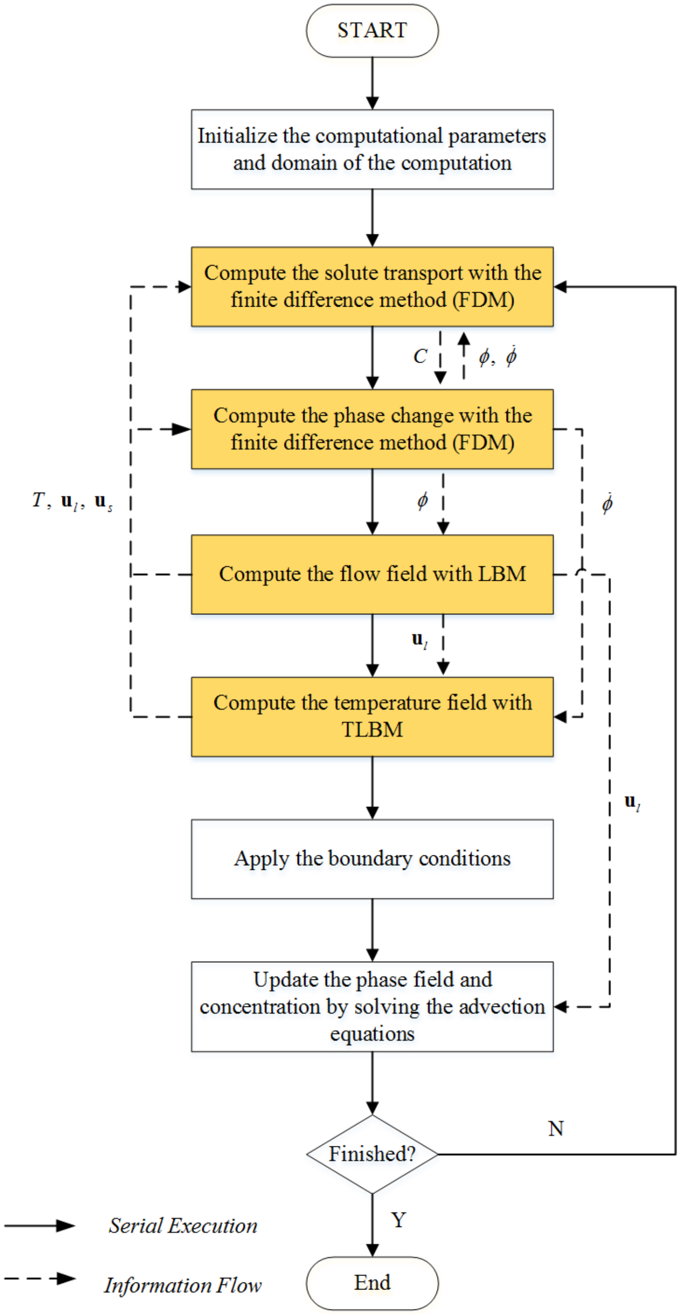
PF-TLBM Algorithm

- Different variables are coupled

$$\phi \quad \dot{\phi} \quad C \quad T \quad \mathbf{u}_l \quad \mathbf{u}_s$$

- The algorithm is implemented in C++ programming language and integrated with OpenPhase

- The OpenMP shared-memory parallel programming framework is used to accelerate the computation

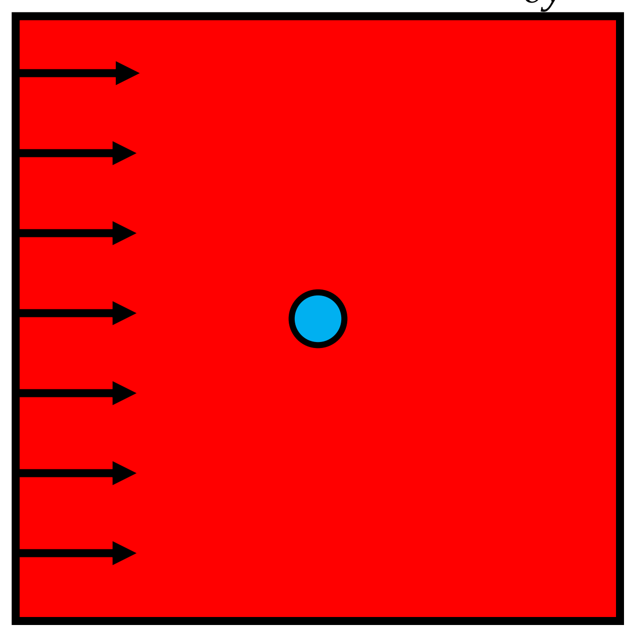


Simulation Results: Al-Cu

- A single nucleus is put at the center of Al-4wt%Cu alloy melt flow
- Zero Neumann conditions are applied at all boundaries for phase field ϕ and composition C.
- For melt flow, periodic boundary conditions are applied at the left and right boundary
- Given a constant cooling rate $\dot{T} = 2\times10^4$ K/s , a fixed heat flux $q_H = \rho c_p \dot{T} L_y / 2$ is set at the upper and lower boundaries

$$u_x = 5\times10^{-4} \text{ m/s},\ q_H = -k\frac{\partial T}{\partial y}$$

$$\frac{\partial T}{\partial x} = 0$$



$$\frac{\partial T}{\partial x} = 0$$

$$u_x = 5\times10^{-4} \text{ m/s},\ q_H = -k\frac{\partial T}{\partial y}$$

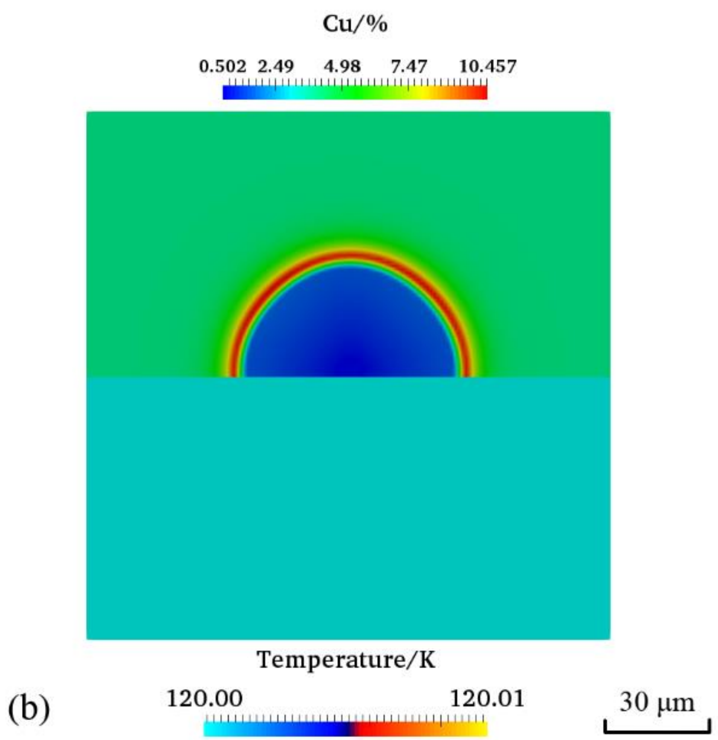
Physical properties

TABLE 1: Physical properties of Al-4wt%Cu alloy

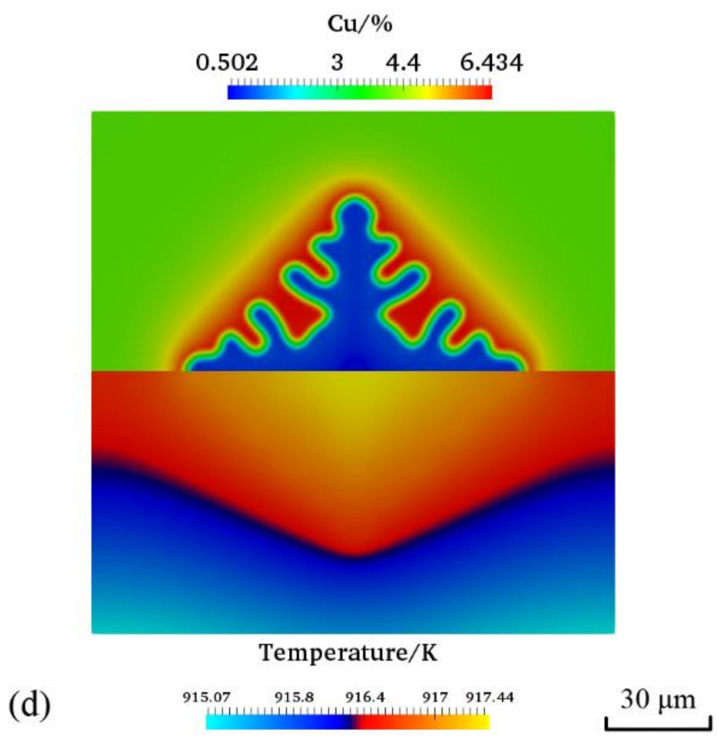
Melting point Al	T_m [K]	933.6
Liquidus slope	m_l [K/%]	-2.6
Partition coefficient	k	0.14
Liquid diffusivity	D_l [m²/s]	3.0×10^{-9}
Interface energy	σ_0 [J/ m²]	0.24
Interface energy anisotropy	ε	0.35
Kinematic viscosity	ν [m²/s]	5.7×10^{-7}
Thermal diffusivity	α [m²/s]	4.9×10^{-5}
Latent heat of fusion	L_H [J/kg]	3.98×10^{5}
Specific heat capacity	c_p [J/(kg•K)]	1450

Simulation Results: Al-Cu

- isothermal

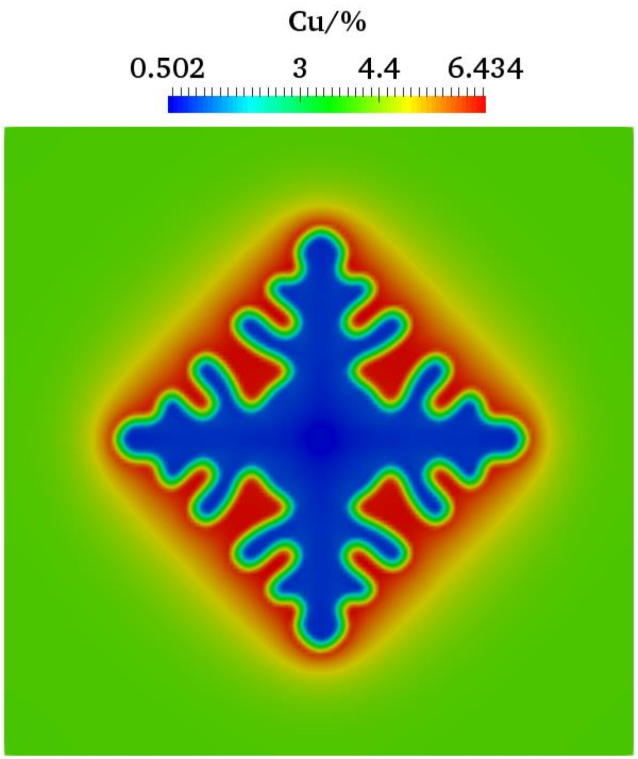


- Non-isothermal

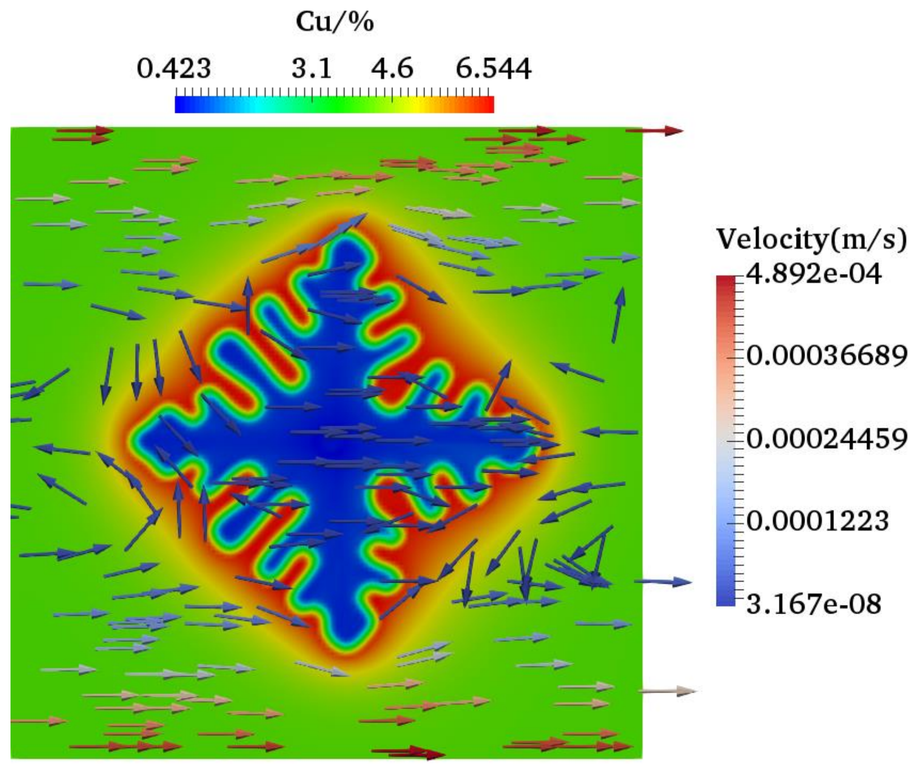


Effect of Flow

- With flow, the upstream portion of dendrite grows faster than the downstream portion, and the primary arm against the flow is deflected



100ms

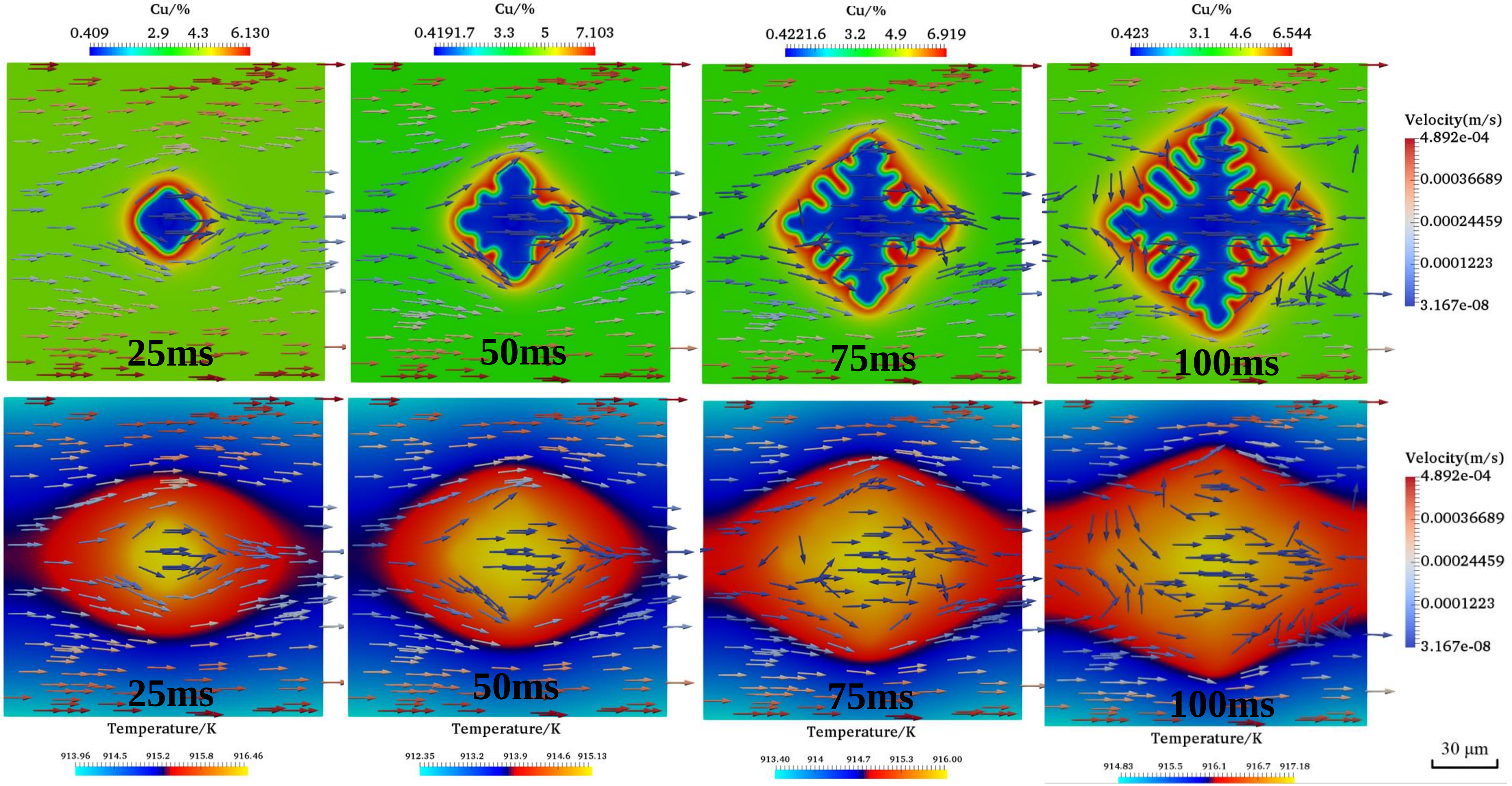


100ms

30 μm

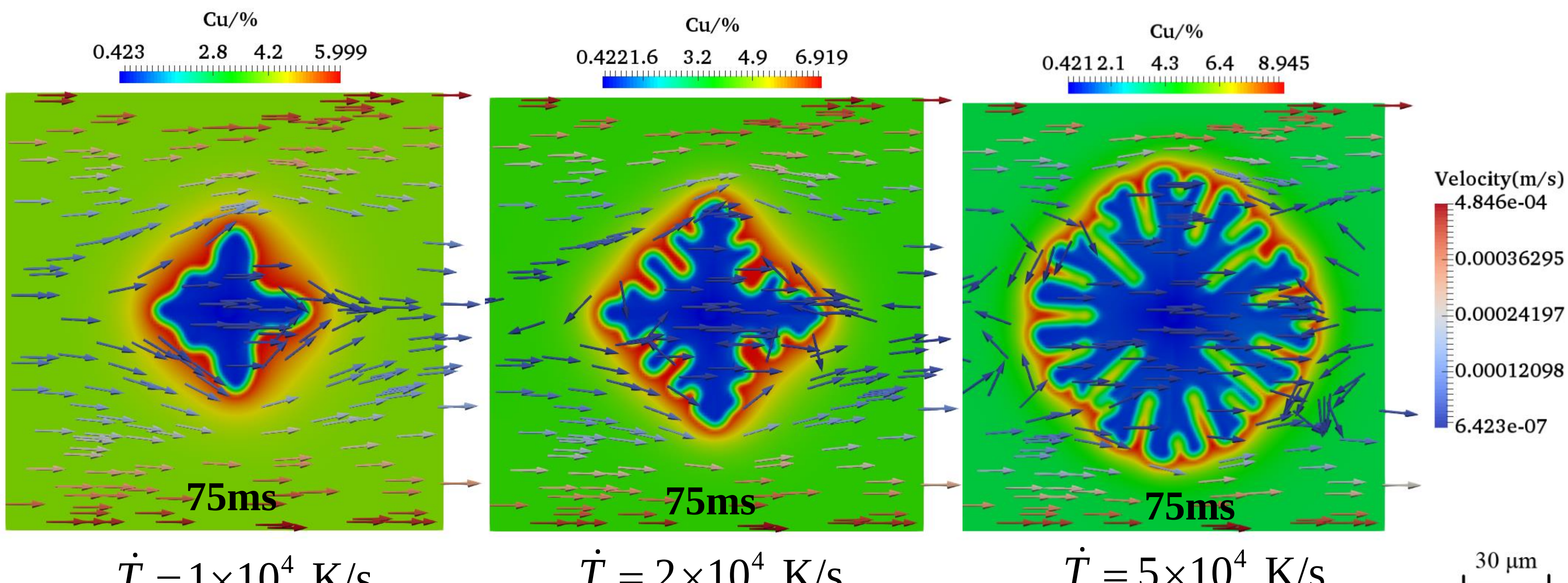
Effect of Flow

- The flow brings fresh material to its vicinity, which also increases the undercooling



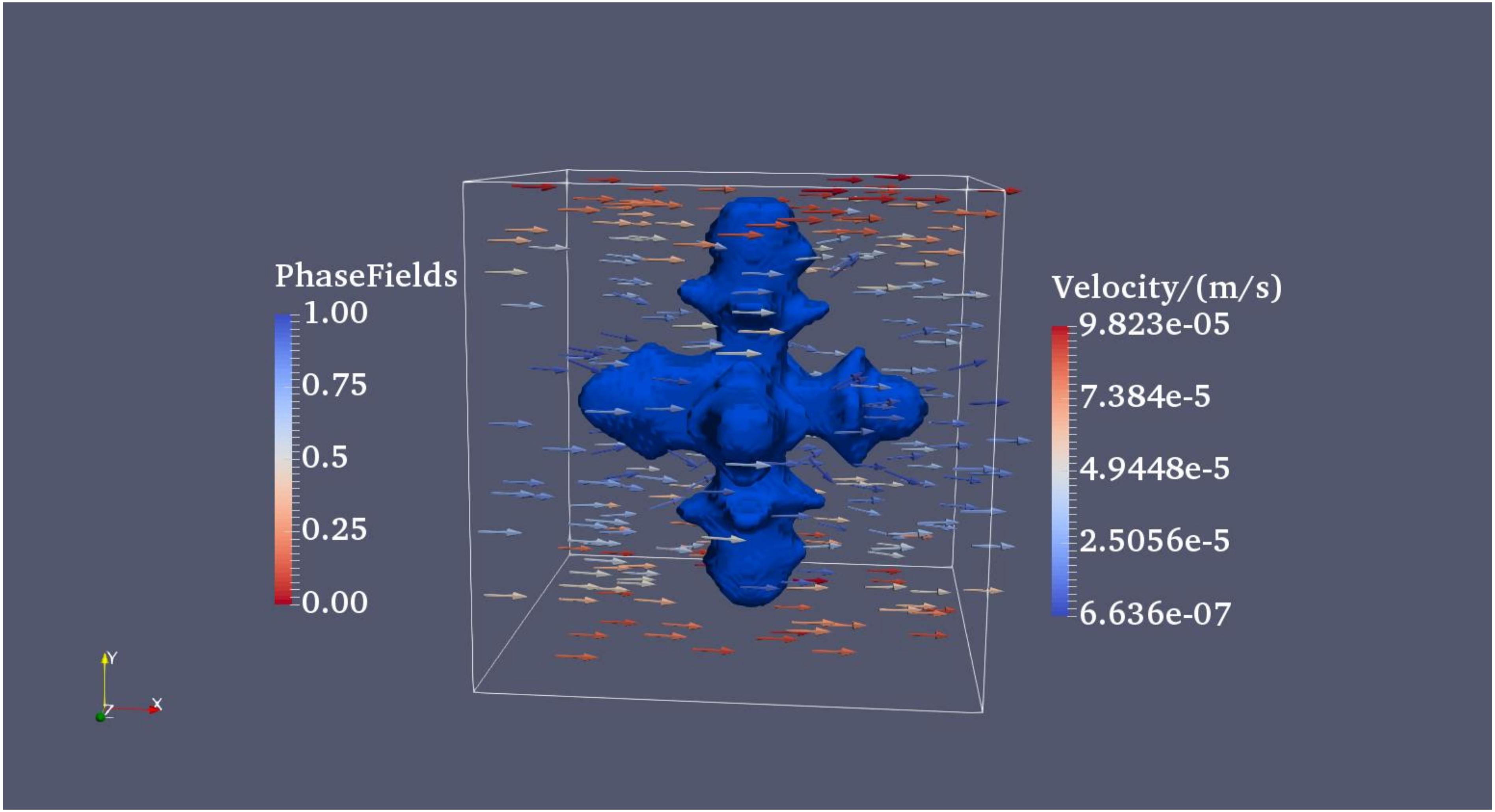
Effect of Cooling Rate

- Higher cooling rate increases the growth rate of secondary arms of dendrite
- A higher cooling rate also results in higher segregation of Cu at the solid-liquid interface



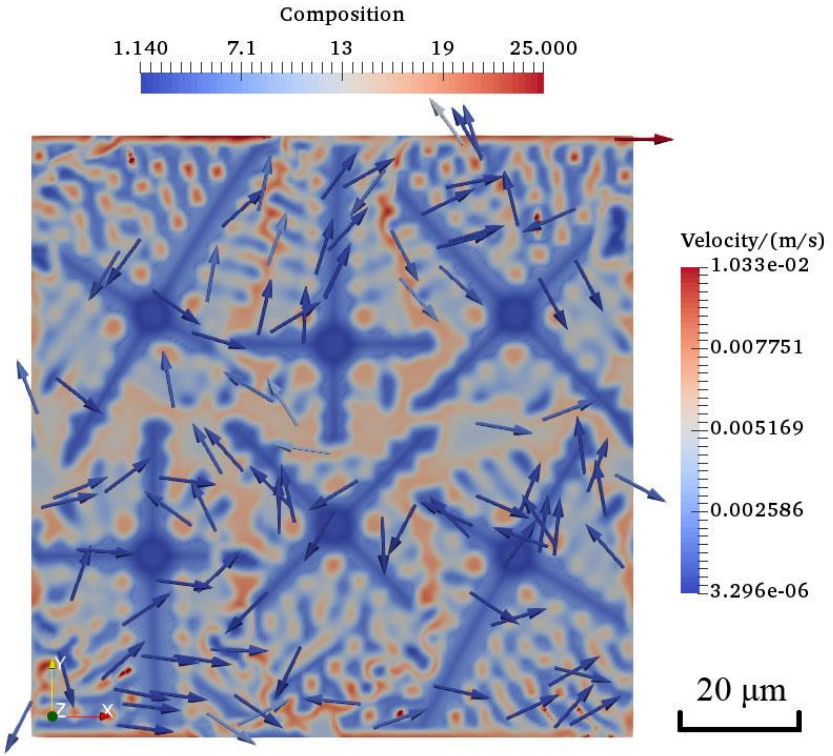
$\dot{T} = 1\times10^4$ K/s $\quad$ $\dot{T} = 2\times10^4$ K/s $\quad$ $\dot{T} = 5\times10^4$ K/s

3D Dendrite Growth

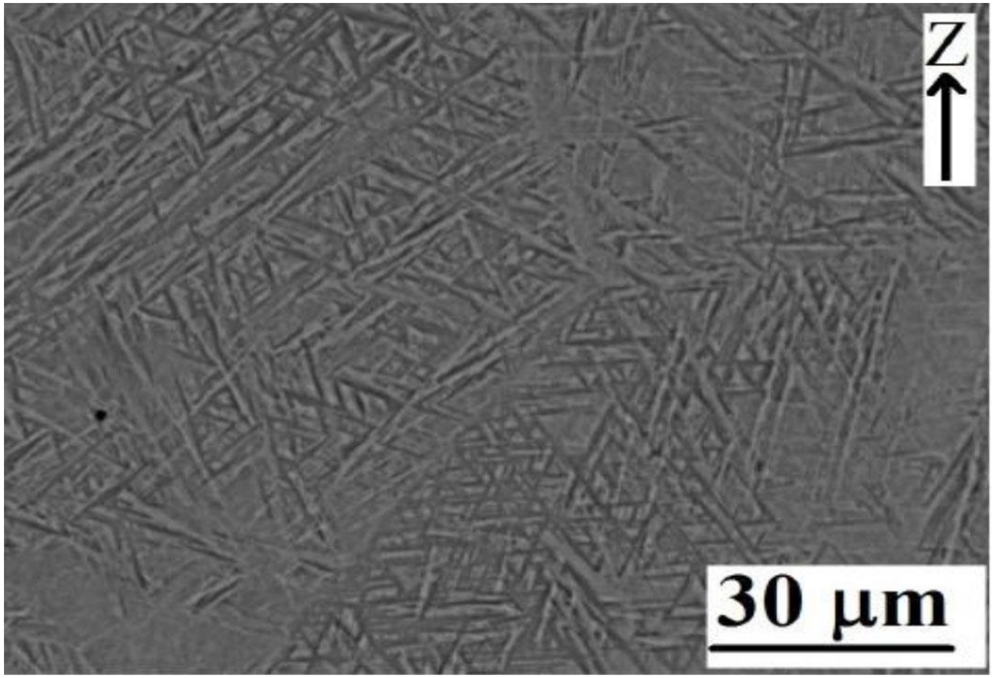


Simulation Results: Ti-6Al-4V

- Multigrain growth
- Cooling rate: $\dot{T} = 2 \times 10^5$ K/s
- Flow speed: 50 mm/s



Simulated microstructure



SEM image of Ti64 microstructure produced by SLM

Research Issues

- How to improve computational efficiency
  - parallelization
- How to improve accuracy
  - Uncertainty quantification
    - Parameter uncertainty
    - Model form uncertainty
- How to use simulation in process planning and optimization
  - Establishing Process-Structure-Property (P-S-P) relationship

Summary

- A mesoscale multi-physics model is developed to simulate the solidification process in SLM based on Phase Field and Thermal Lattice Boltzmann Methods

- The PF-TLBM model incorporates solute transport, heat transfer, fluid dynamics, kinetics of phase transformation, and grain growth.

- It simulates systems at a reasonable time scale for manufacturing processes while providing fine-grained material phase and composition information.

köszönöm
!תודה
děkuji
mahalo
고맙습니다
thank you
merci
谢谢
danke
Ευχαριστώ
شكرا
どうもありがとう
gracias

Thanks!