中国科学技术大学
University of Science and Technology of China

Basilisk (Gerris) Users' Meeting 2025

Simulation of melting/icing problems with the phase-field method

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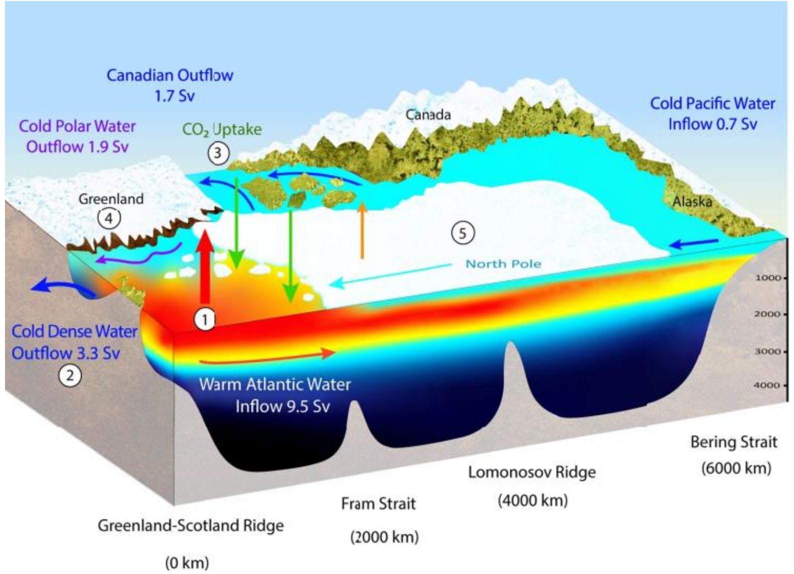
Content Outline

- **Research Background and Present Scenario**
- **Limitations of Phase Field Models and Improvements**
- **Verification Cases**
  - Stefan Problem
  - Rayleigh-Bénard Convection
  - Ice Growth on Cylinder in Flow
  - Vertical Convection
- **Conclusion & Outlook**

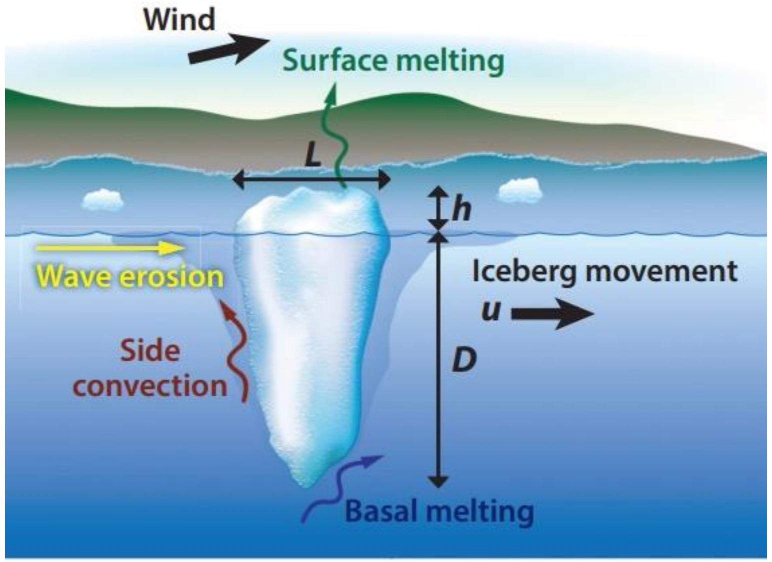
Research Background

Melting and icing phenomena are common in nature and human life.



Smedsrud, L. H. *et al.* (2022)
Rev. Geophys.

➢ Atlantic inflow cooling and sea ice variation



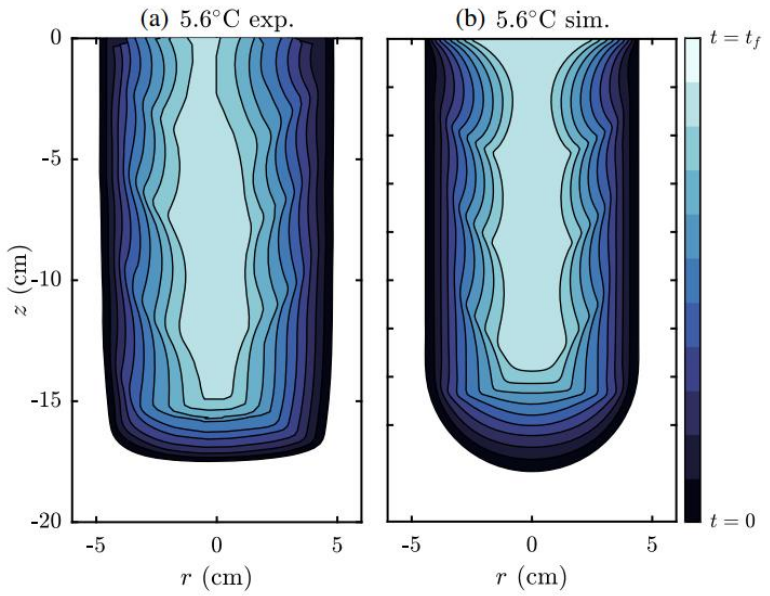
Cenedese, C. *et al.* (2023)
Annu. Rev. Fluid Mech.

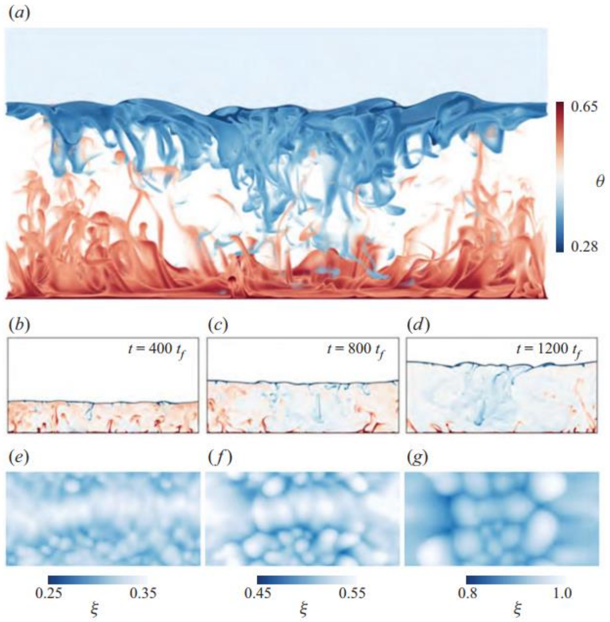
➢ Iceberg Melting

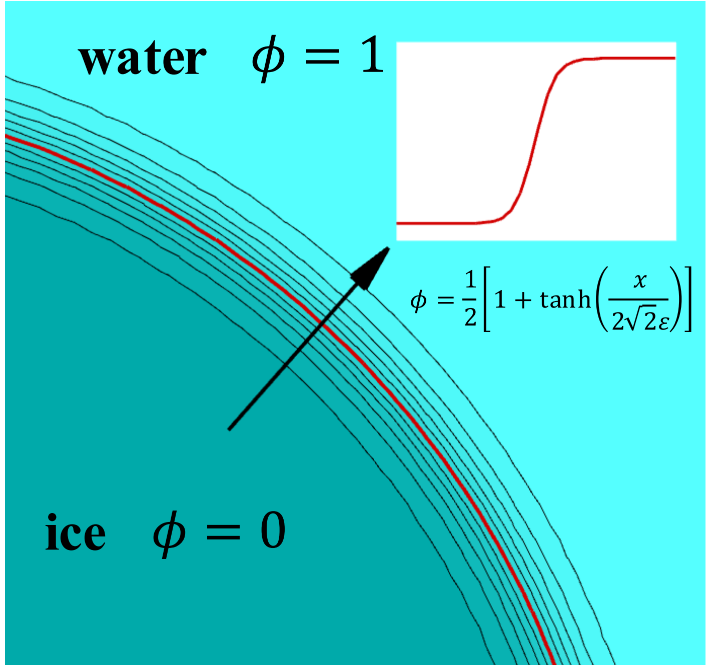
➢ Icing on aircraft wings

Current State of Research

Phase-field methods have been widely adopted for studying melting and icing problems.







Weady, S. *et al.* (2022)
Phys. Rev. Lett.

Yang, R. *et al.* (2023)
J. Fluid Mech.

ice front
$\phi = 0.5$

Current State of Research

Phase-field methods can yield non-physical results.

Advantages:

- Easy topological change handling
- Exact energy conservation
- Easy multiphase extension

Disadvantages:

Non-physical motion of the ice front

- High local curvature
- Low Stefan number

Phase-Field Method for Ice–Water Change

Traditional phase-field methods have difficulty with
accurate temperature boundary conditions at the ice front.

Navier-Stokes Equations

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)=-\nabla \mathrm{P}+\frac{1}{Re}\nabla^2\boldsymbol{u}-\frac{\rho}{Fr}\boldsymbol{e_g}+\boldsymbol{f_p} \qquad \nabla\cdot\boldsymbol{u}=0$$

Energy Equation

$$\frac{\partial\theta}{\partial t}+\boldsymbol{\nabla}\cdot(\boldsymbol{u}\theta)=\frac{1}{\rho C_p}\nabla[k_{\mathrm{T}}\nabla\theta]-St\frac{\lambda_\rho}{\rho C_p}\frac{\partial\phi}{\partial t}$$

Phase-Field Model
（Allen-Cahn Equation）

$$\boxed{\frac{\partial\phi}{\partial t}=M\left[\nabla^2\phi-\frac{1}{4\varepsilon^2}\frac{dg}{d\phi}\right]+\frac{M}{\varepsilon^2}\frac{df}{d\phi}(\theta-\theta_m)}$$

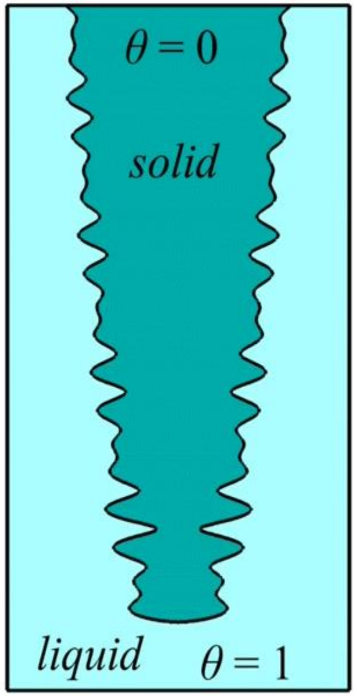
$$\Downarrow$$

at the ice front: $\theta_\Gamma \neq \theta_m$

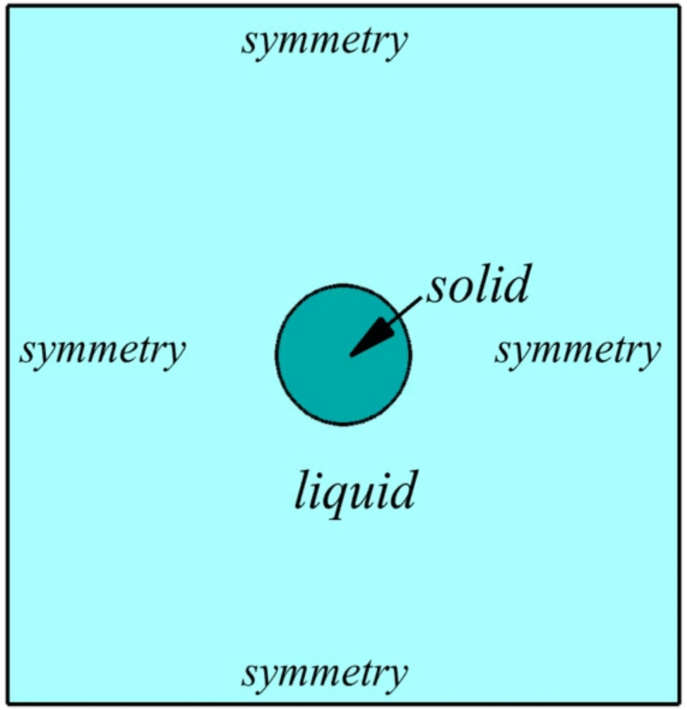
Temperature Boundary Effects on Ice Front

Challenges faced by traditional phase field methods

Melting of an icicle



Ice–Water Coexistence Validation



- **Small-scale structures are smoothed**
- **Ice and water cannot coexist at melting point**

Temperature boundary conditions at the ice front:

$$\theta_\Gamma \neq \theta_m$$

Significant non-physical motion of the interface occurs in regions with high local curvature

Improved Phase-Field Model

- **Original Phase-Field Model:**

$$\frac{\partial\phi}{\partial t} = M\left[\nabla^2\phi - \frac{1}{4\varepsilon^2}\frac{dg}{d\phi}\right] + \frac{M}{\varepsilon^2}\frac{df}{d\phi}(\theta - \theta_m)$$

- **Improved Phase-Field Model:**

$$\frac{\partial\phi}{\partial t} = M\nabla^2\phi - M\nabla\cdot\left[\frac{\phi(1-\phi)}{\sqrt{2}\varepsilon}\boldsymbol{n}\right] + \frac{M}{\varepsilon^2}\phi(1-\phi)\left(\theta - \theta_m^{eff}\right)$$

Remove curvature effect

Introduce effective melting point θ_m^{eff}

- **At the ice front:**

$$\theta_\Gamma - \theta_m = 0$$

- **Maintain the original equilibrium form and stability:**

$$\phi = \frac{1}{2}\left[1 + \tanh\left(\frac{x}{2\sqrt{2}\varepsilon}\right)\right]$$

- **Energy conservation.**

Improved Phase-Field Method Steps

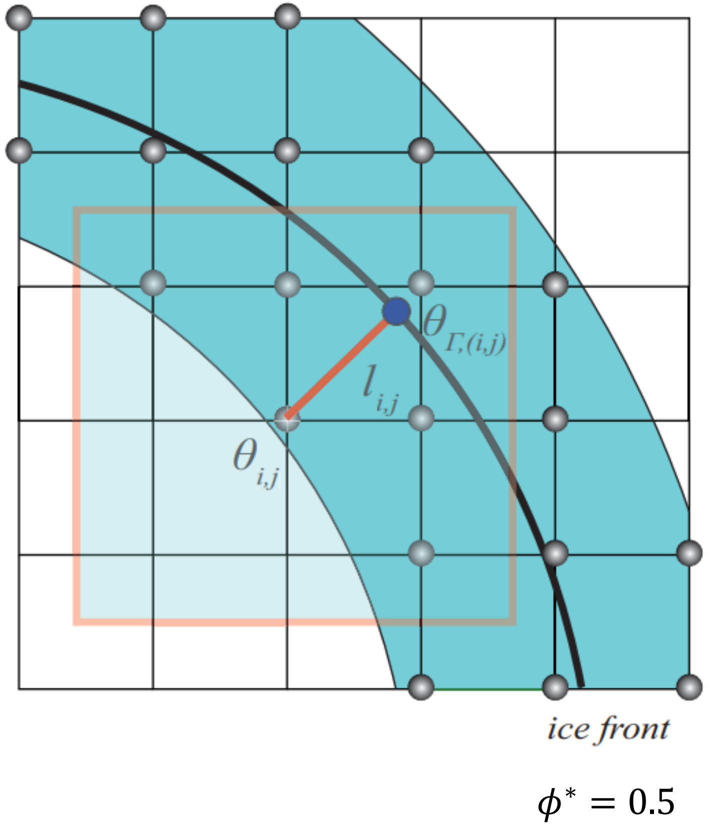
- **Initialization:** Set $\theta_m^{eff,0} = \theta_m$
- **Prediction step :**

• Advance ϕ^n using $\theta_m^{eff,n}$ to obtain ϕ^*;

• Compute the temperature at the ice front and use its deviation from the melting point to update the effective melting point.

$$\theta_\Gamma = \theta_{i,j} + l\nabla\theta_{i,j} \cdot \boldsymbol{n_{i,j}}$$

$$\theta_m^{eff,n+1} = \theta_m^{eff,n} - (\theta_\Gamma - \theta_m)$$

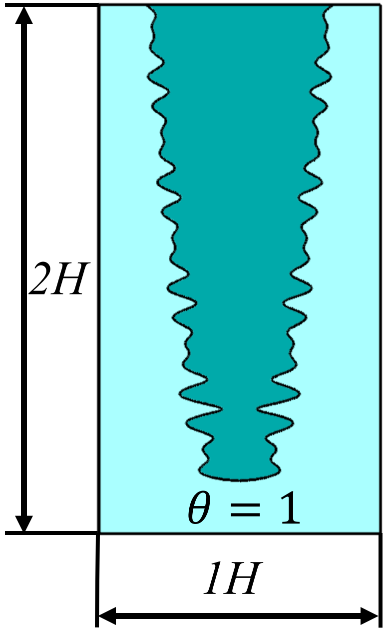


- **Correction step:**

• Advance ϕ^{n+1} using the updated effective melting point $\theta_m^{eff,n+1}$.

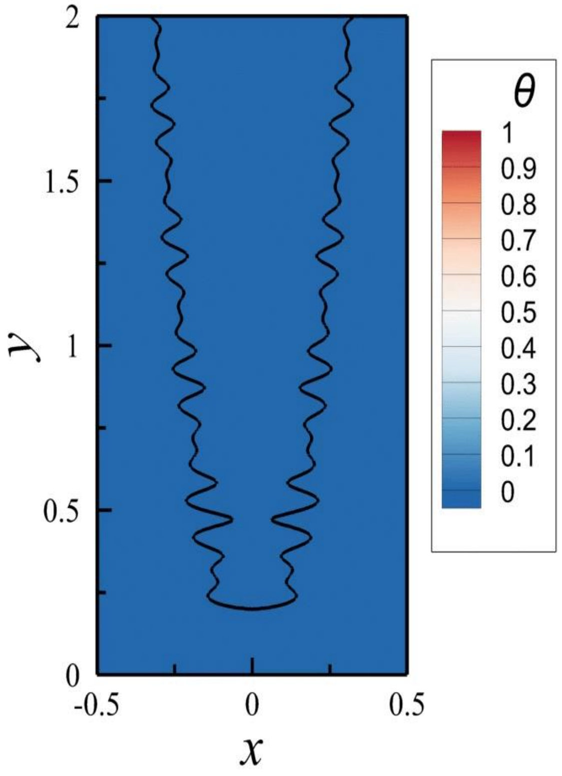
The improved phase-field model accurately captures small-scale structures.

- **Melting of an icicle**

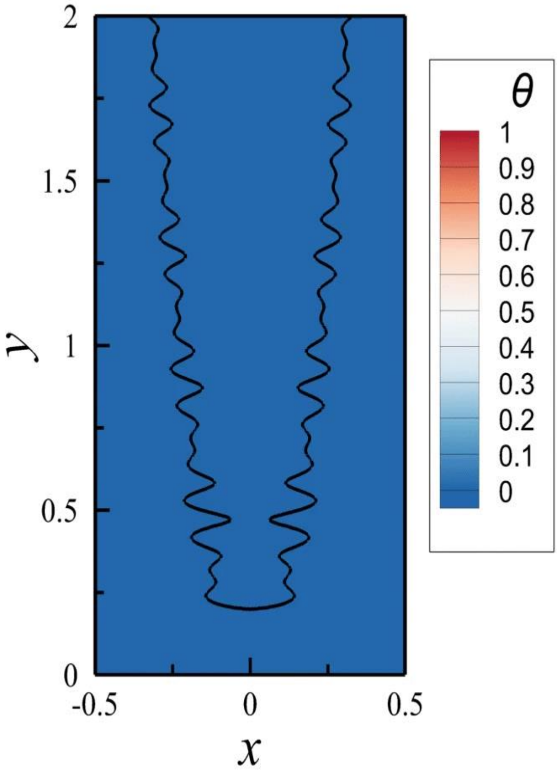


$$y+\frac{1}{\gamma}\cos(3\gamma\pi y)+\frac{1}{\gamma}\sin(4\gamma\pi y)=4\gamma x^2$$

Uniform initial temperature: $\theta=\theta_m$



- **Improved Phase-Field Model**



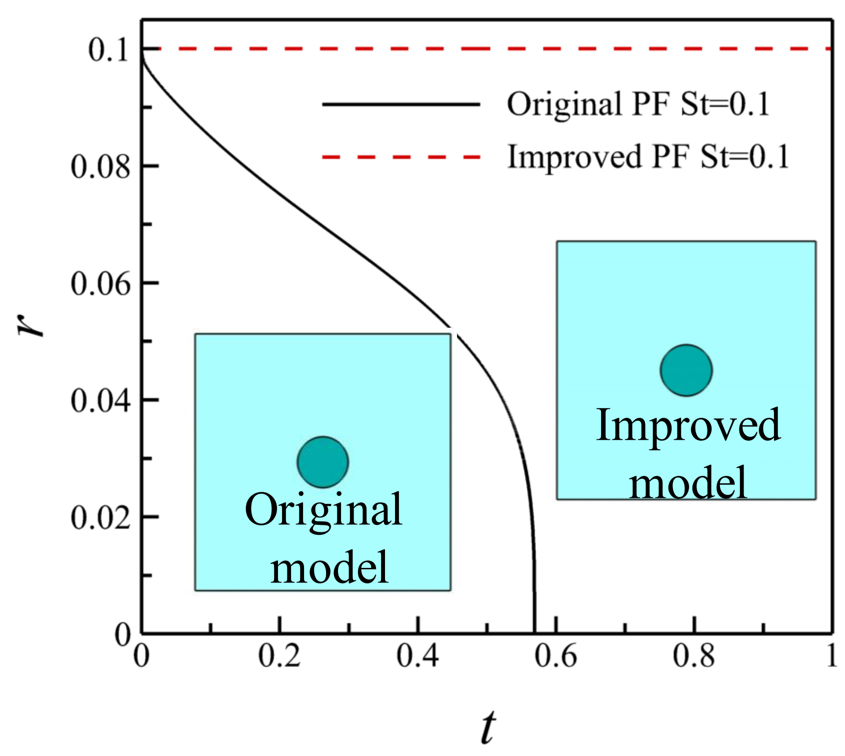
- **Original Phase-Field Model**

Case: 2D Stefan Problem

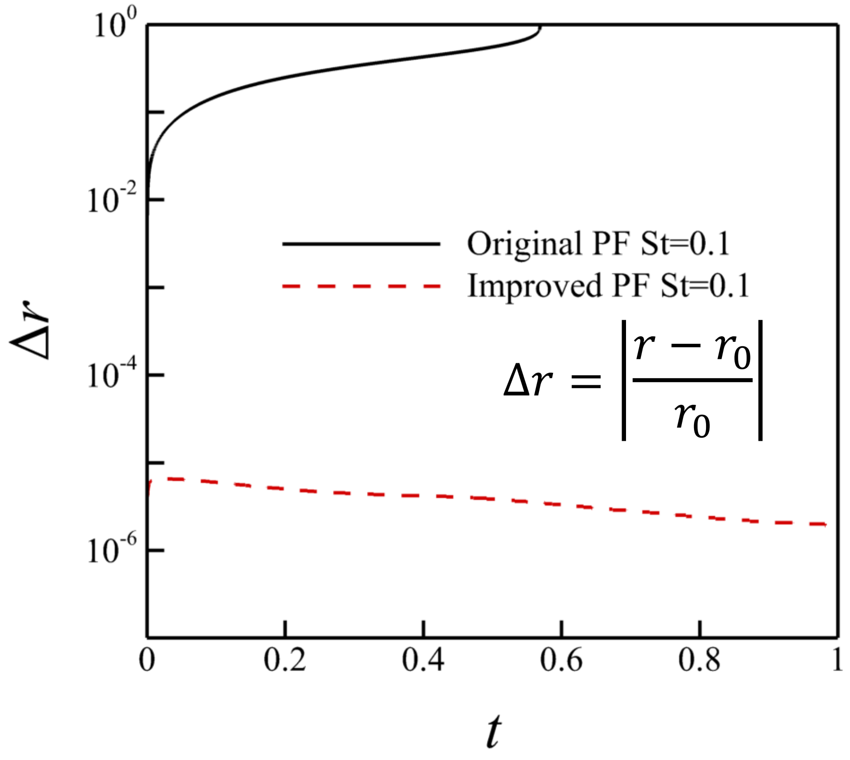
Improved phase-field model removes curvature effects and ensures ice–water coexistence.

➢ Ice–Water Coexistence Validation

Uniform initial temperature: $\theta = \theta_m$



- **Ice circle radius evolution**

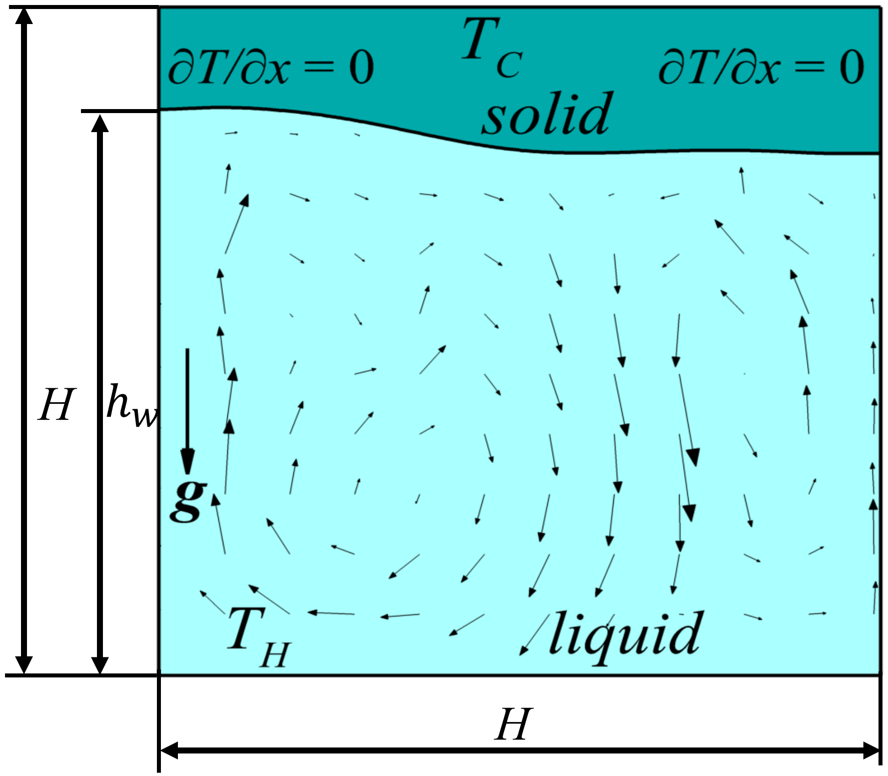


- **Ice circle radius change ratio**

Case: Rayleigh-Bénard Convection

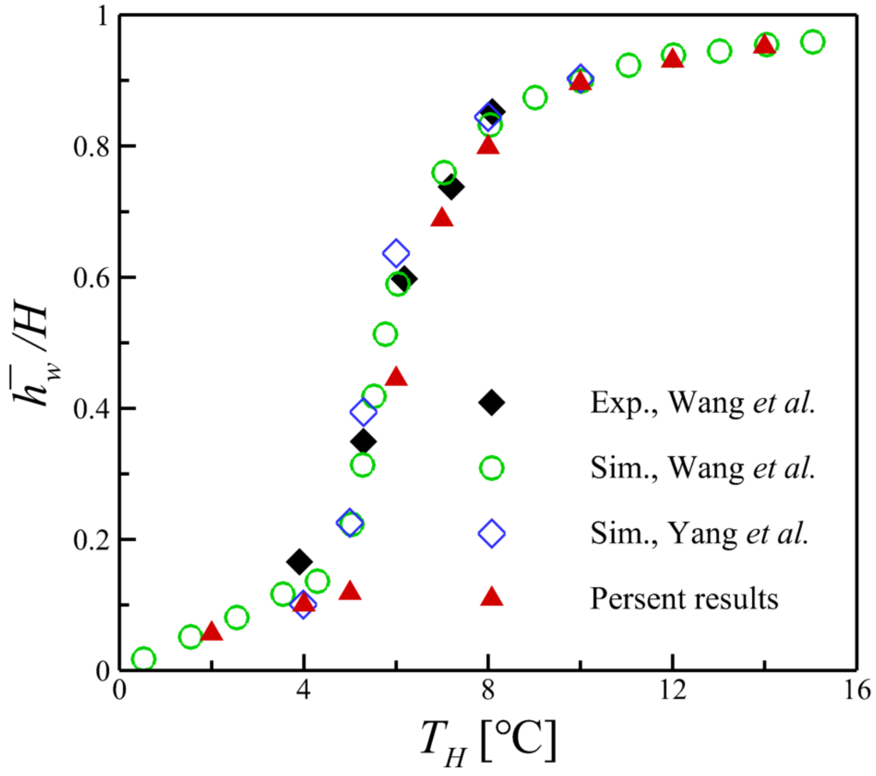
Good agreement with previous results

$T_c = -10$℃



$T_H = 2\sim14$℃

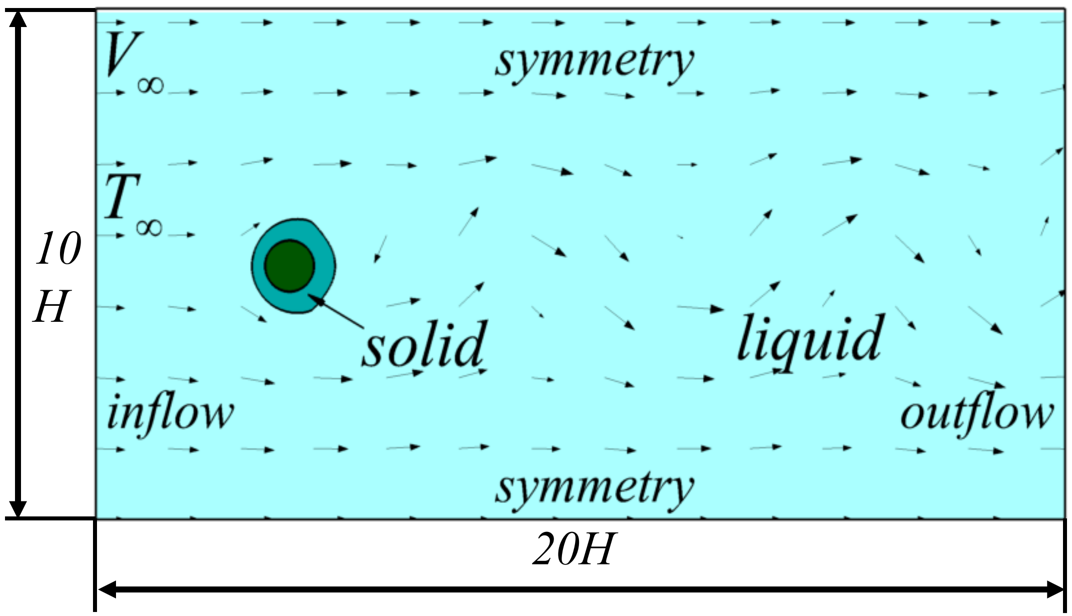
Rayleigh number $\frac{\beta g H^3 (T_H - T_C)^q}{\nu k} \sim 10^9$



- **Average water height at steady state**

Case: Ice Growth on Cylinder in Flow

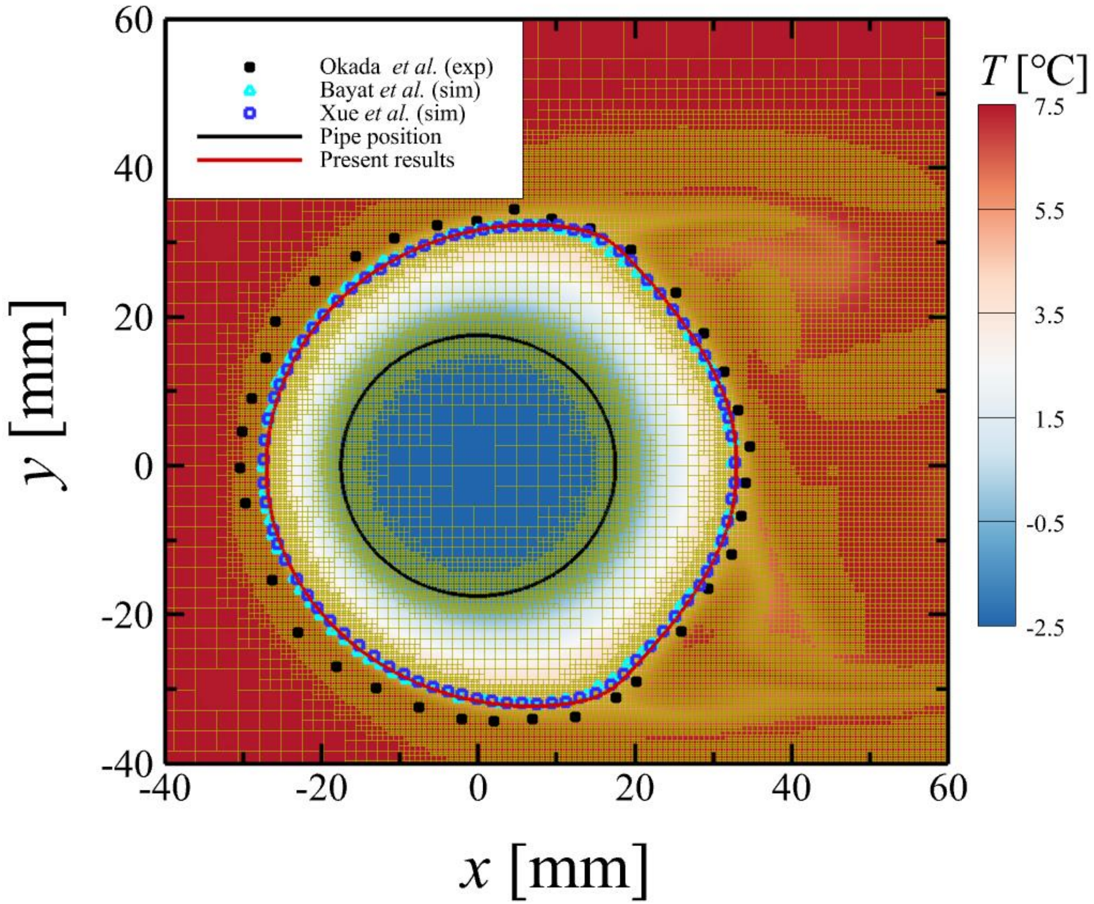
Adaptive mesh refinement near the ice front



Inflow temperature $T_\infty = 2.5°C$

Cooled pipe temperature $-7.5°C$

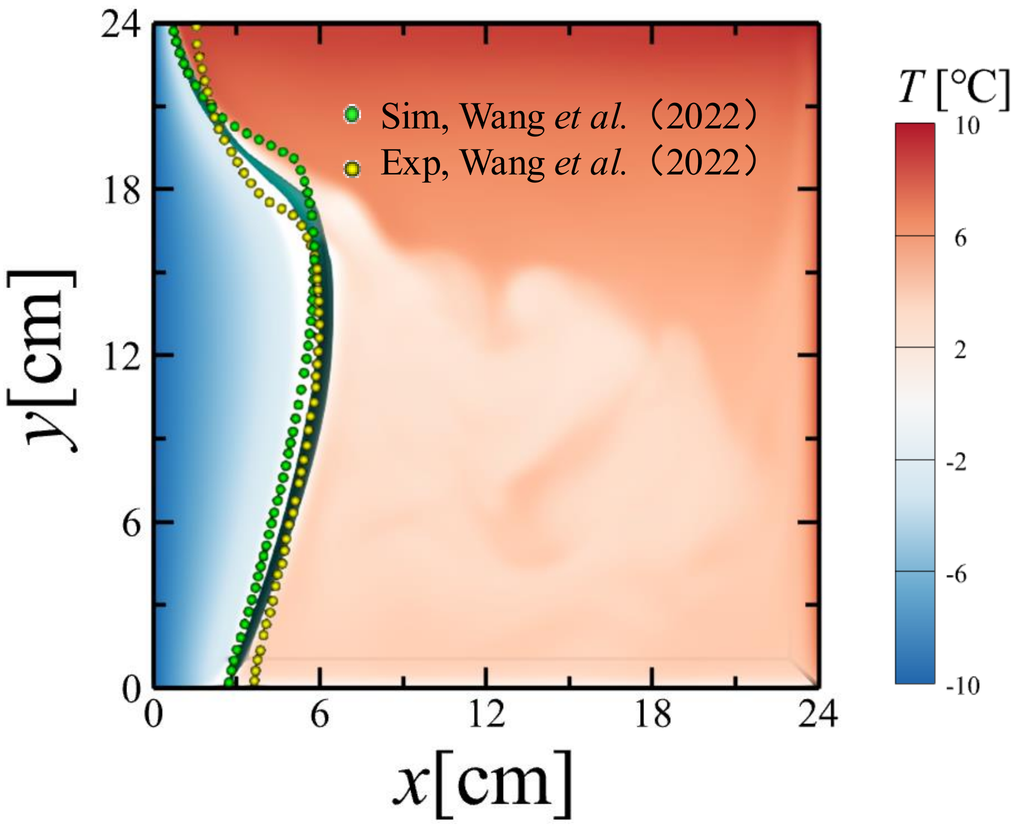
Inflow velocity $V_\infty = 0.01 m/s$



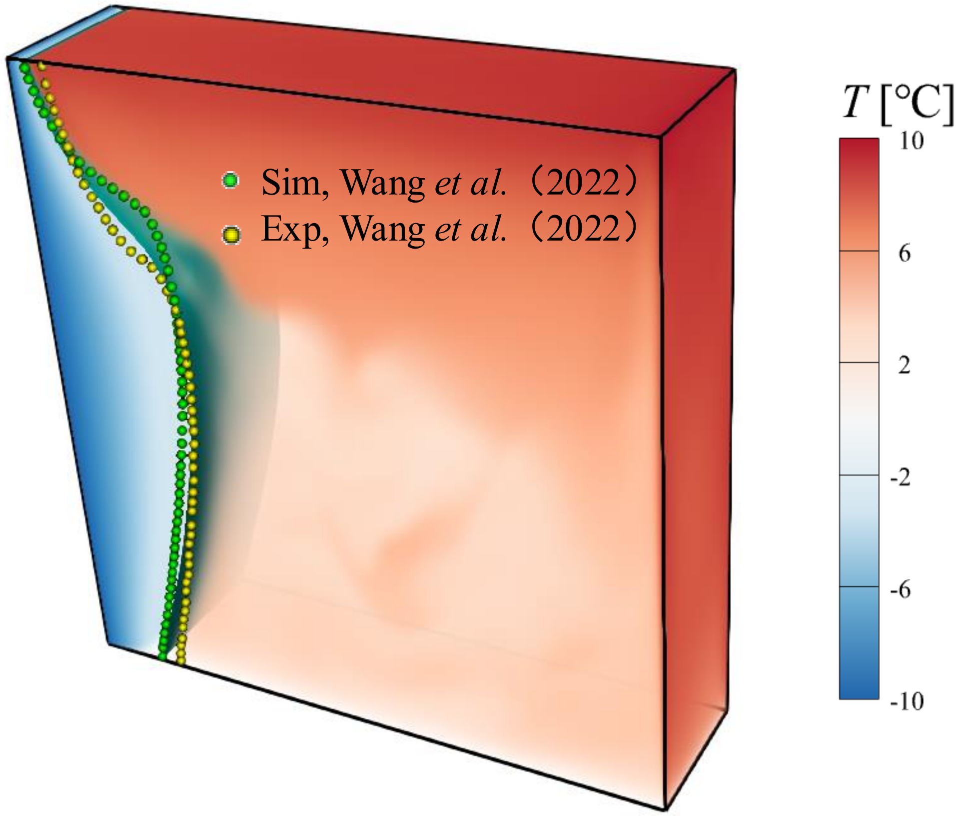
- **Ice front profile comparison**

Case: Vertical Convection

Suitable for 3D simulations



- **Front View**



- **Side View**

Conclusion

- An improved phase-field model is proposed to eliminate curvature-induced artifacts and introduce an effective melting point, ensuring that the temperature at the ice front equals the melting point.

- The improved model demonstrates superior performance in both classical Stefan problems and complex flow simulations.

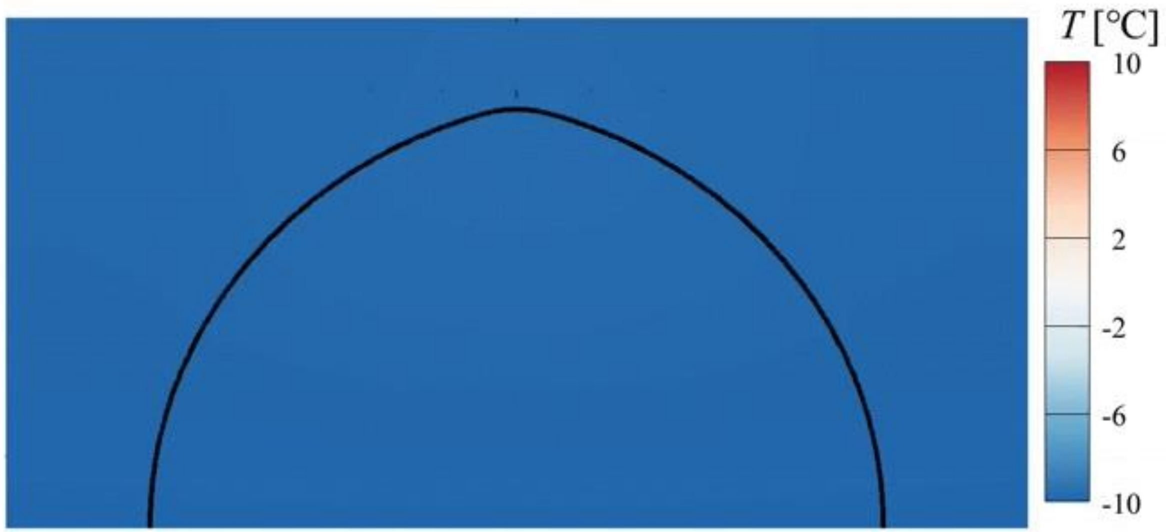
- The code will be released soon on Sandbox.

" The development of an improved phase-field method for simulating freezing/melting problems in turbulent environments" to be submitted to the *J. Comput. Phys.*

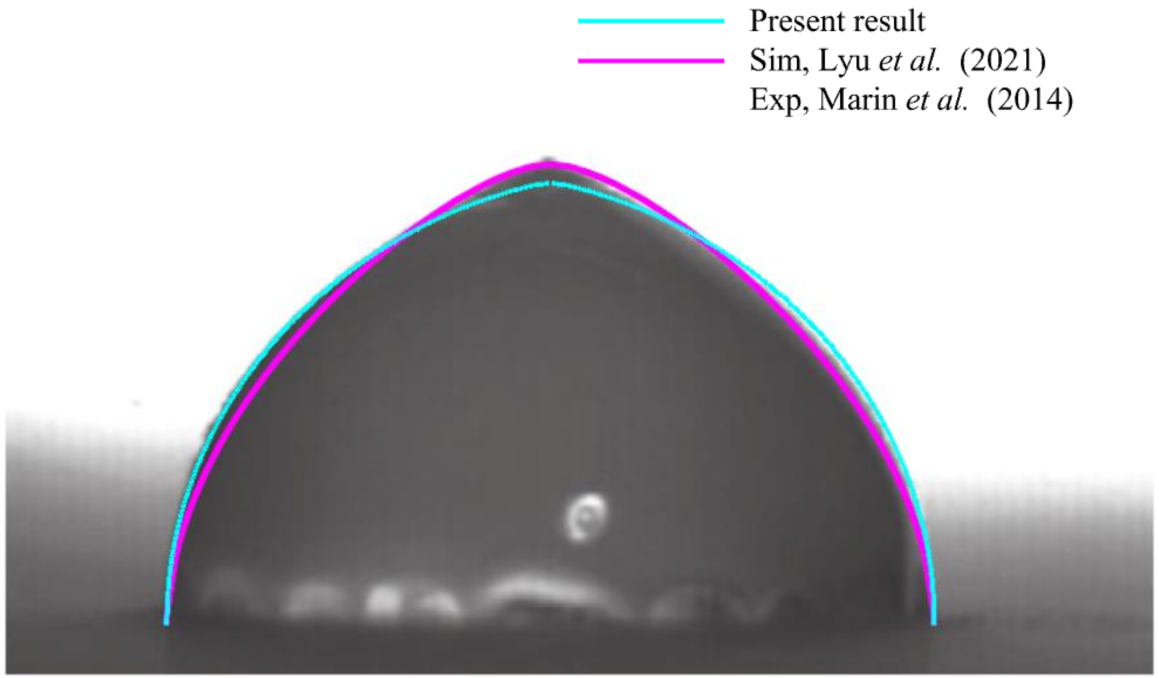
Outlook

Future Work: ice–water phase transition in the presence of air

- **Droplet freezing**



	ρ [kg/m^3]	μ [Pa·s]	α [m^2/s]	C_p [J/(kg°C)]
Air	1.29	1.70×10^{-5}	2.00×10^{-5}	1.00×10^{3}
Water	1.00×10^{3}	1.70×10^{-3}	1.32×10^{-7}	4.21×10^{3}
Ice	9.17×10^{2}	1.70×10^{-3}	1.18×10^{-6}	2.03×10^{3}



- **Ice front profile comparison**

Thank You for Your Attention

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