Numerical Simulation of Dendritic Solidification

Outline

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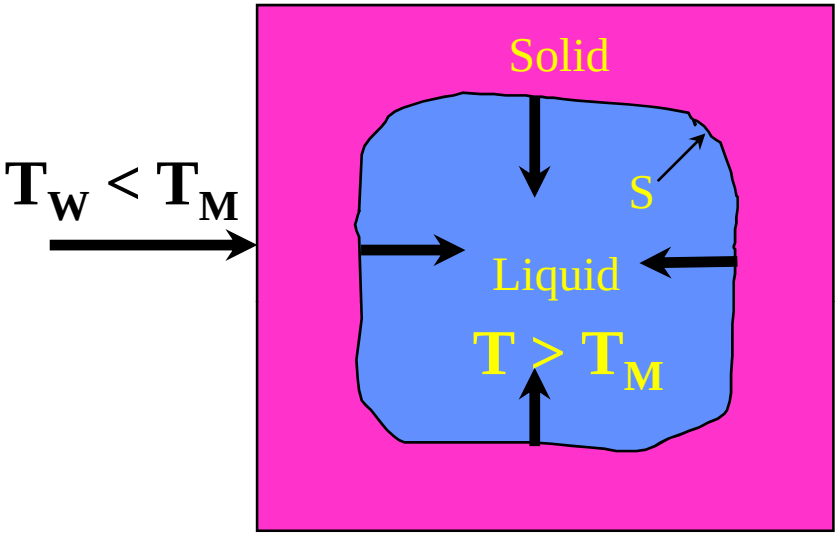
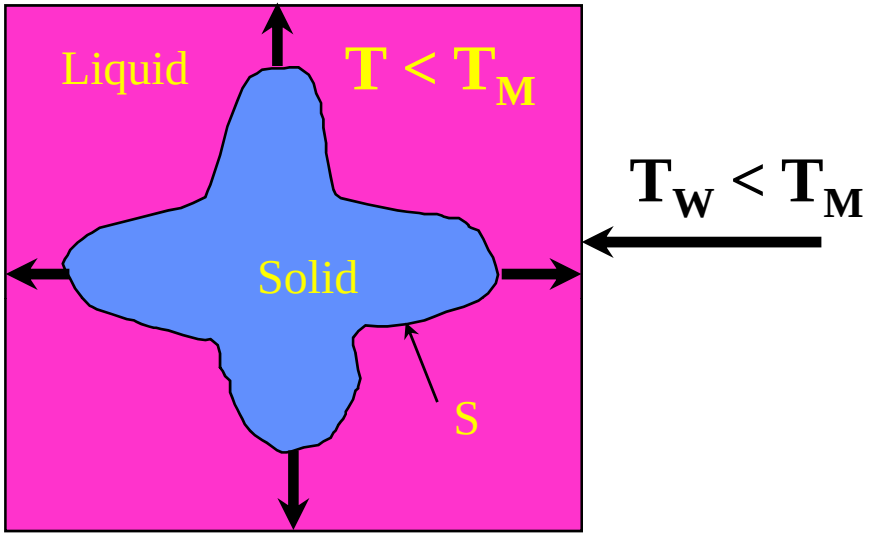
- Solution strategies
- Governing equations
- FEM formulation
- Numerical techniques
- Results
- Conclusion

Problem Statement



When the solidification front grows into a superheated liquid, the interface is stable, heat is conducted through the solid



When the solidification front grows into an undercooled melt, the interface is unstable, heat is conducted through the liquid

Solution Strategies

Most analytical solutions are limited to parabolic cylinder or a paraboloid of revolution

Experimental studies are usually limited to transparent materials with ideal thermal properties such as succinonitrile

Numerical solution can change the various material characteristics and modify the governing equations to gain more insight to the actual underlying physics

Governing Equations

Heat conduction is the dominant mode of thermal transport:

$$c \frac{\partial T}{\partial t} = \nabla \bullet k \nabla T$$

The interface temperature is modified by local capillary effects:

$$T(S(t)) = -\frac{\gamma T_m}{L} K$$

The second boundary conditions on the interface preserves the sensible heat transported away from the interface and the latent heat of fusion released at the interface:

$$L \vec{V} \bullet \vec{n} = [(k \nabla T)_s - (k \nabla T)_L] \bullet \vec{n}$$

Finite Element Formulation

For the energy equation in each domain,

$$c\frac{\partial T}{\partial t} = \nabla \bullet k\nabla T$$

the Galerkin Weighted Residual finite element method formulation can be expresses as:

$$\iint c\frac{\partial (T_j N_j)}{\partial t} W_i + \iint k\nabla W_i \nabla (T_j N_j) = \int k\nabla T \bullet \vec{n} W_i ds$$

Finite Element Formulation - Continued

Since a moving mesh is used to track the interface, the motion of the coordinate system must be incorporated:

$$\frac{\partial (T_j N_j)}{\partial t} = \frac{\partial T_j}{\partial t} N_j + T_j \frac{\partial N_j}{\partial t} \qquad \frac{DN_j}{Dt} = 0 = \frac{\partial N_j}{\partial t} + V \bullet \nabla N_j$$

$$\frac{\partial N_j}{\partial t} = -V \bullet \nabla N_j \qquad \frac{\partial (TN)_j}{\partial t} = -(\vec{V} \bullet \nabla N_j)\{T_j\} + N_j \frac{dT_j}{dt}$$

The FEM formulation of the heat equation can be rewritten as:

$$\iint c \frac{\partial T_j}{\partial t} N_j W_i - \iint c\vec{V} \nabla (N_j T_j) W_i + \iint k \nabla W_i \nabla (T_j N_j) = \int k \nabla T \bullet \vec{n} W_i ds$$

The time derivative is treated in standard finite difference form,

$$\frac{dT}{dt} = \frac{T^{k+1} - T^{k}}{t^{k+1} - t^{k}}$$

and the heat equation is evaluated at time:

$$t^{k+\theta} = \theta t^{k+1} + (1-\theta) t^{k}$$

with:

$$T^{k+\theta} = \theta T^{k+1} + (1-\theta) T^{k}$$

Finite Element Formulation - Continued

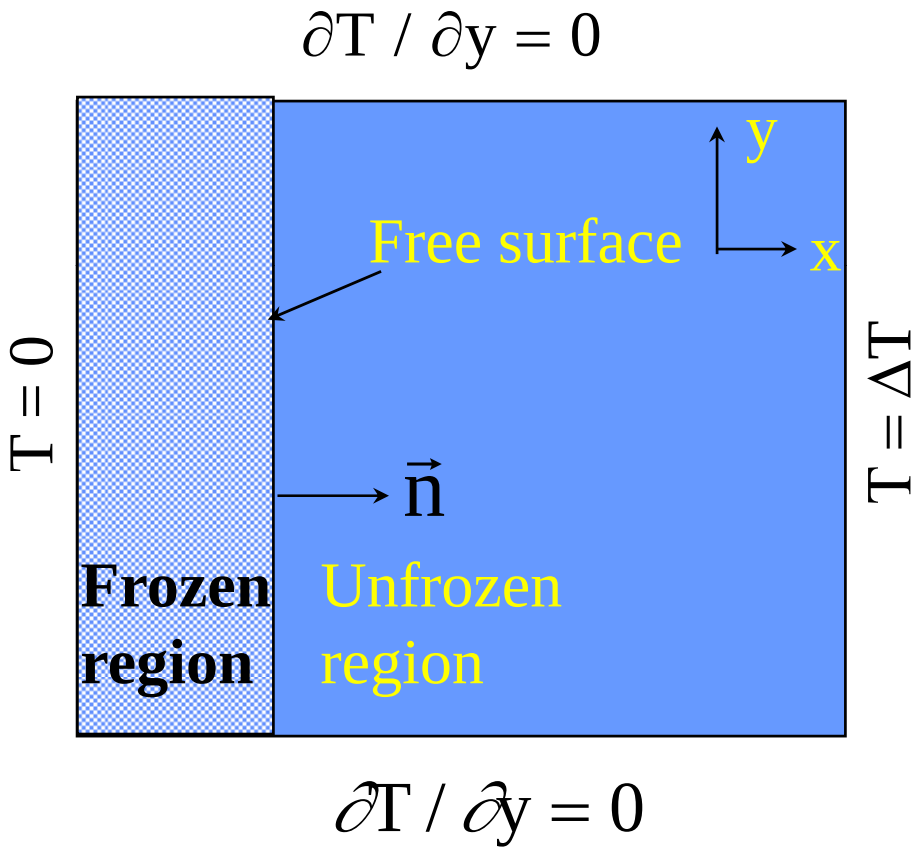
The interface motion balances the heat diffused from the front and the heat liberated at the front:

$$L\vec{V} \bullet \vec{n} = \left[(k\nabla T)_s - (k\nabla T)_L \right] \bullet \vec{n}$$

Numerically:

$$\int \{ L\vec{V} \bullet \vec{n} - \left[(k\nabla T)_s - (k\nabla T)_L \right] \bullet \vec{n} \} W_i ds = 0$$

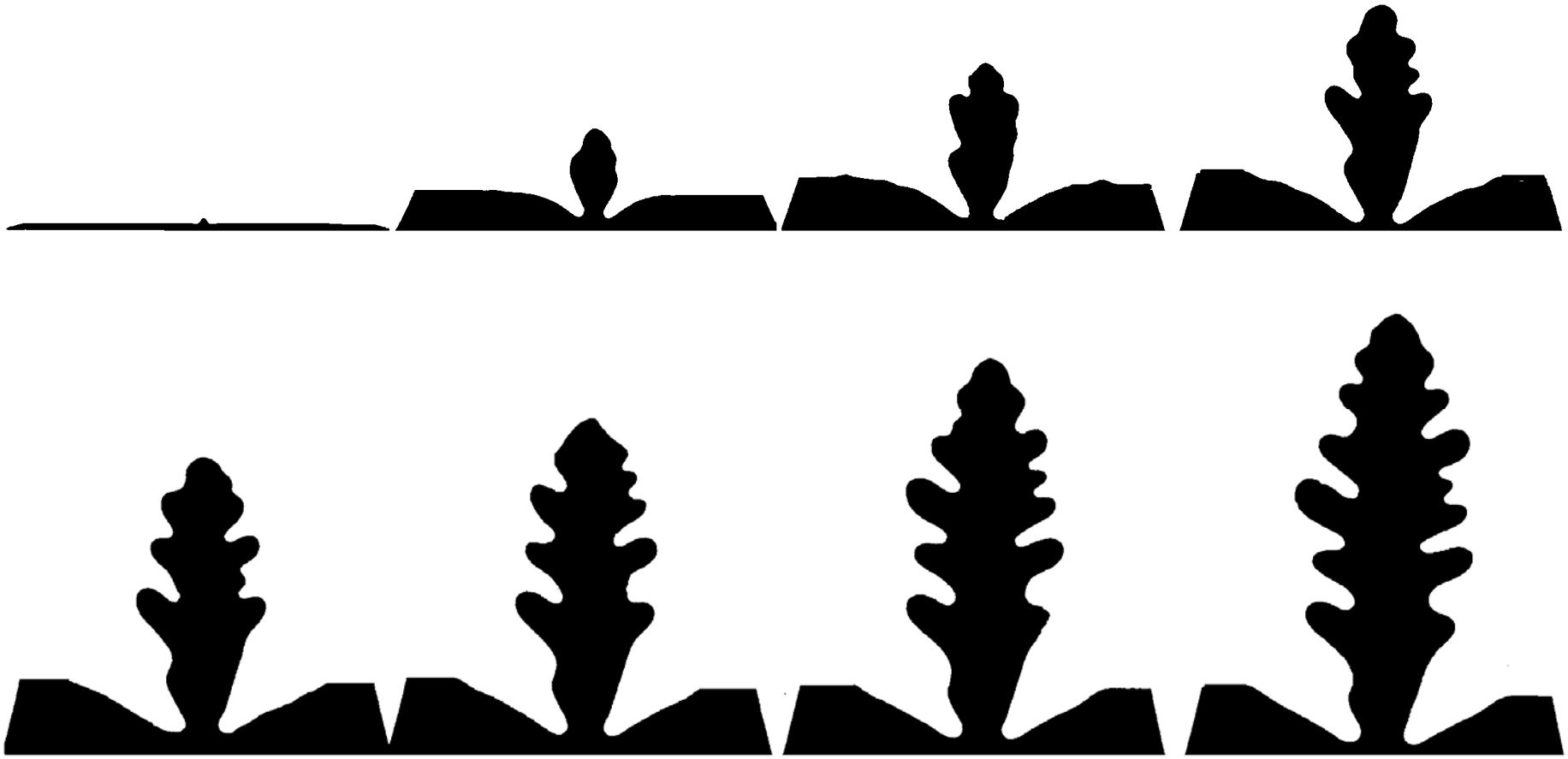
Numerical Simulation Domain



- As the solidification front advances into the undercooled melt, unstable perturbations emerge and develop into dendrite
- Infinitesimal perturbation is seeded in the middle of the interface
- Boundaries are extended far enough to simulate a relatively unconfined environment

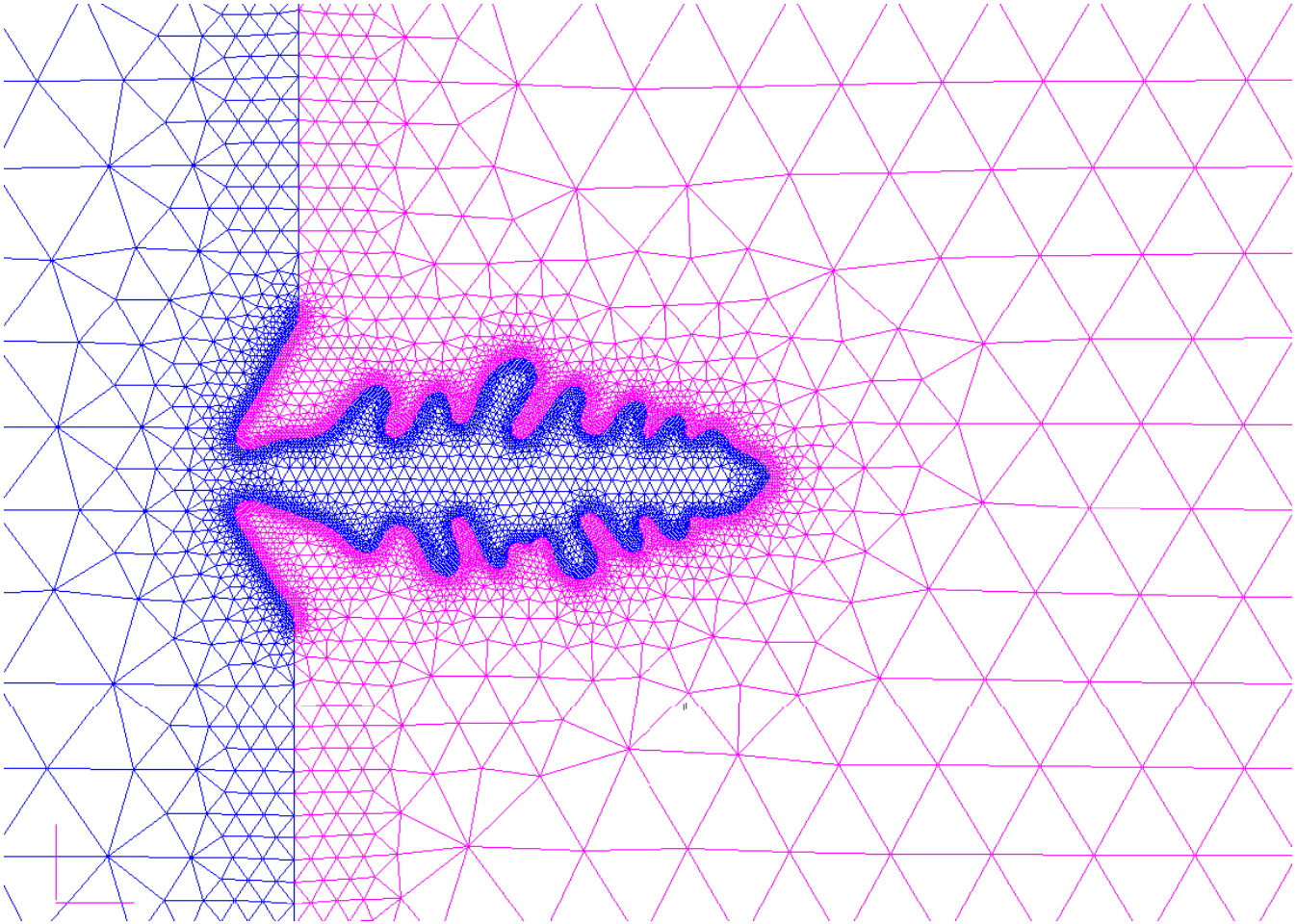
Simulation Results

Sequences of Dendrite Growth from a Crystallization Seed



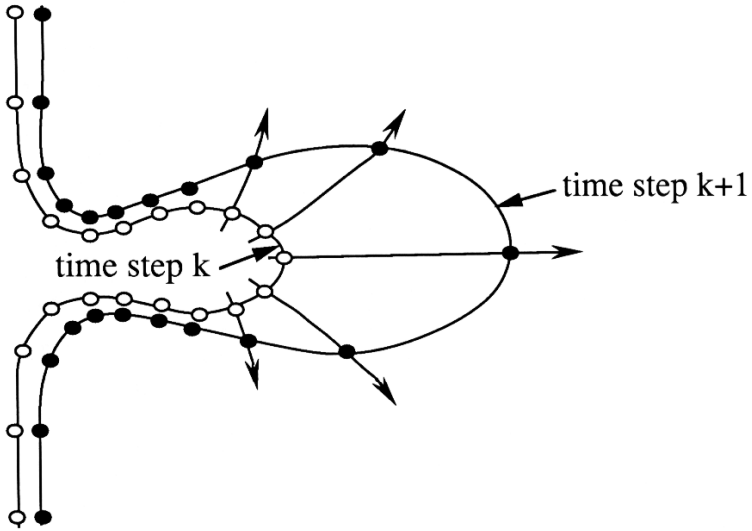
Finite Element Mesh

Solid

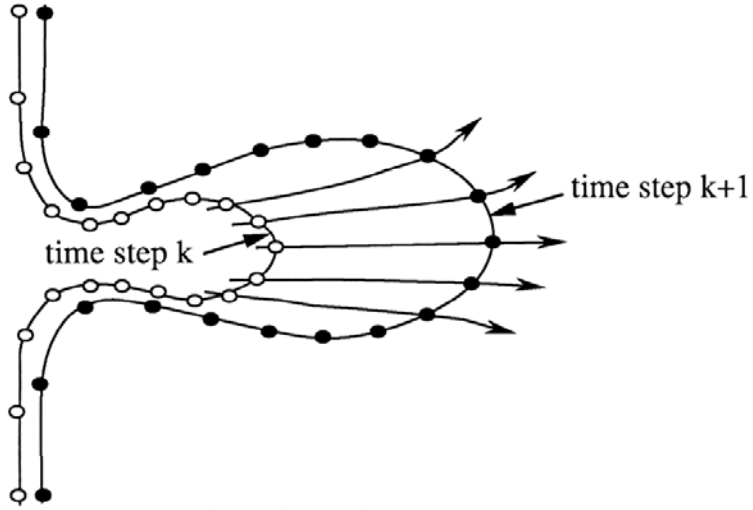


Liquid

Numerical Technique -- Interface node adjustment

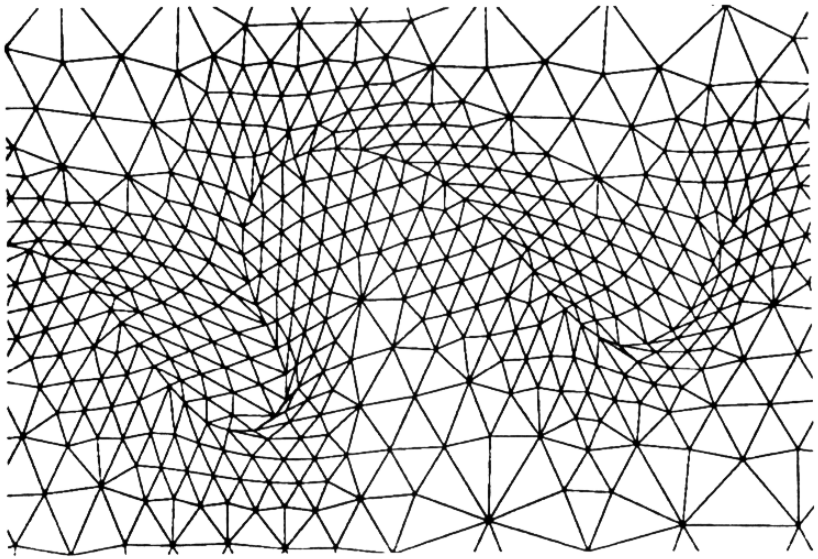


Coarse Interface Resolution

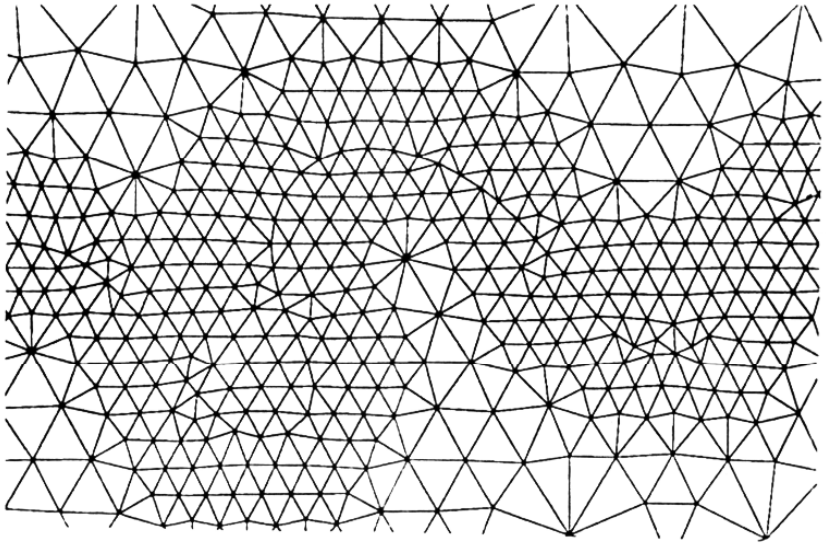


Refined Interface Resolution

Numerical Technique --Remeshing

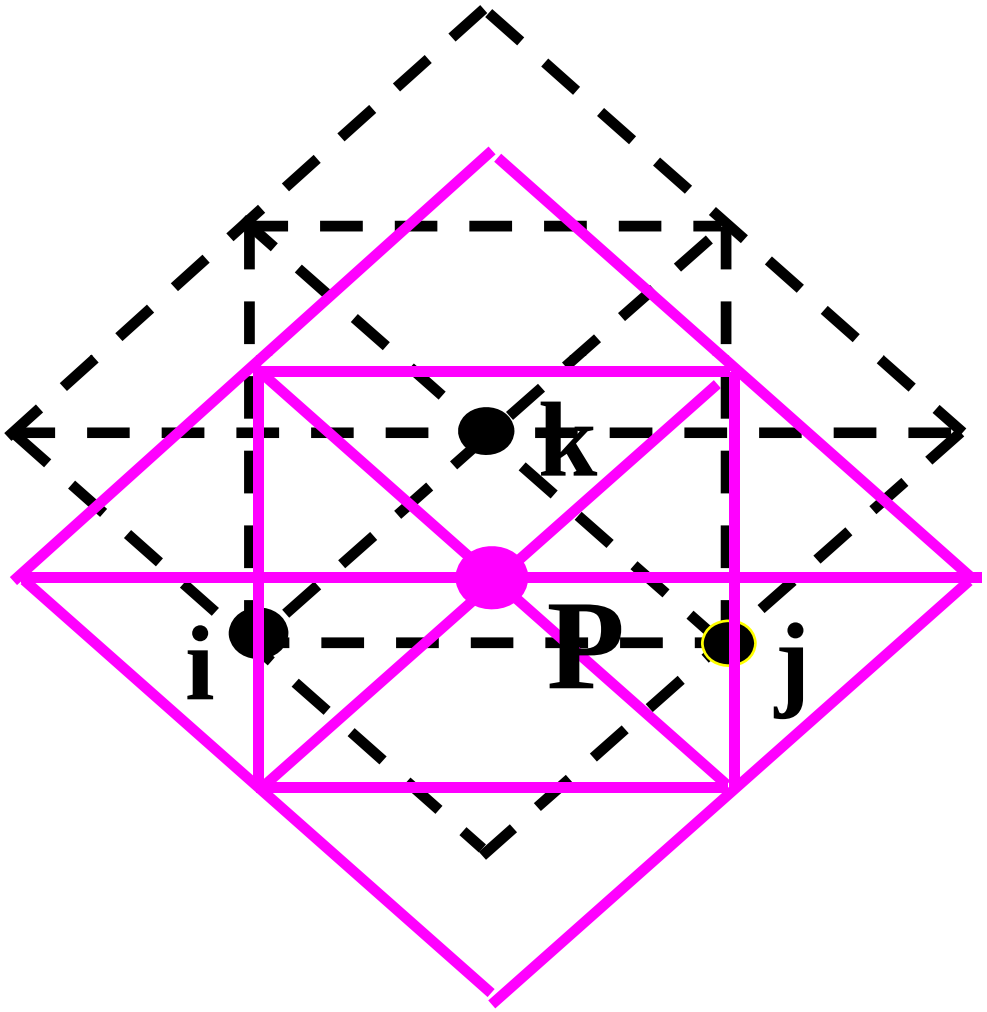


Distorted Mesh

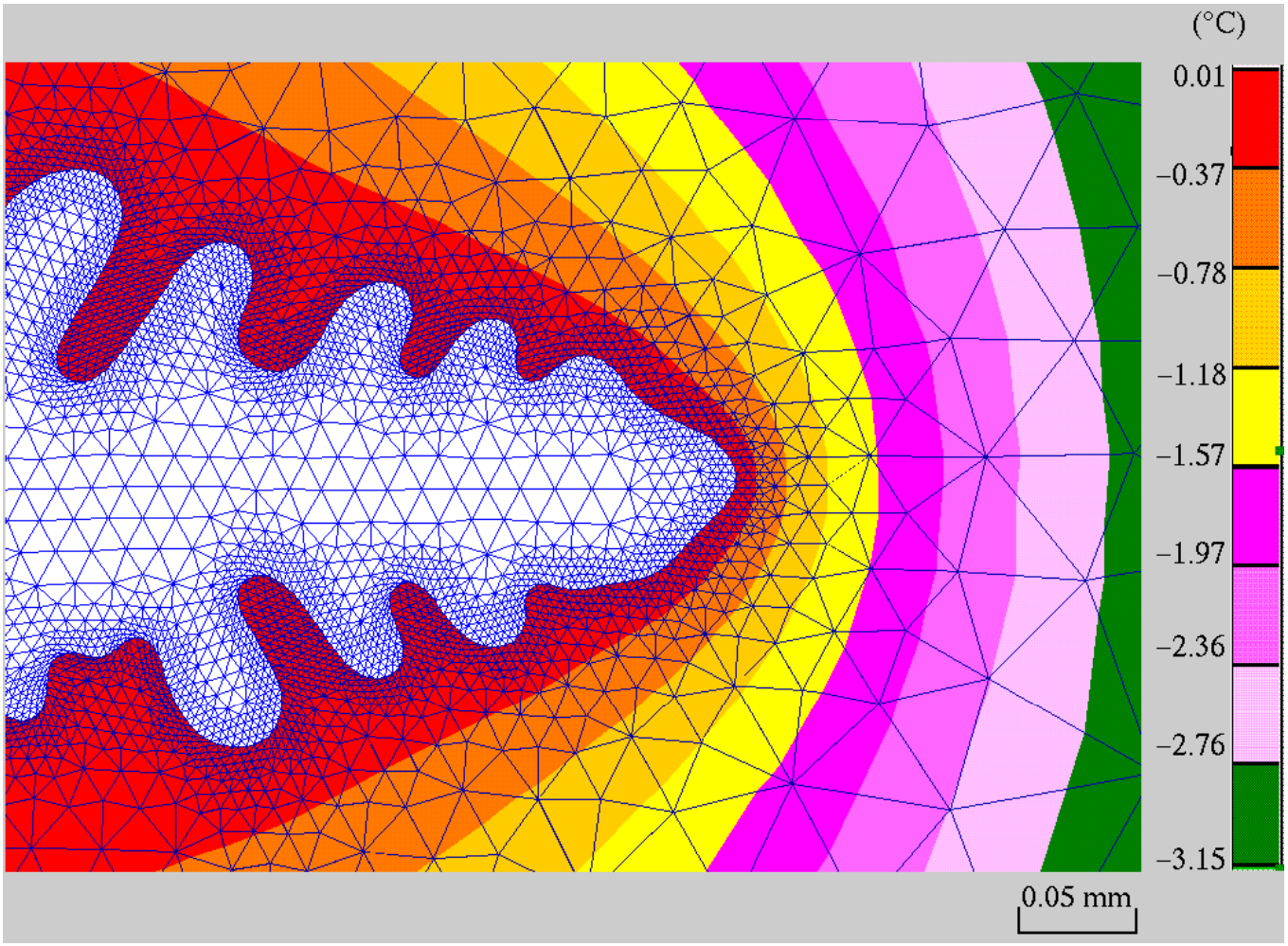


Remeshed Mesh

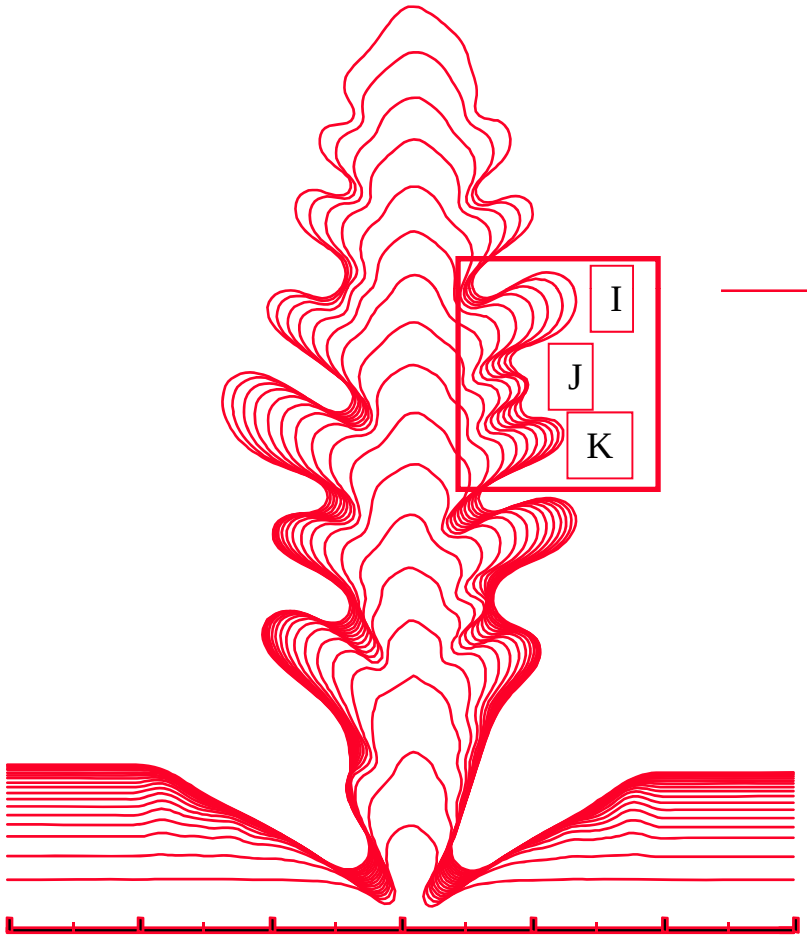
Numerical Technique -- Solution Mapping

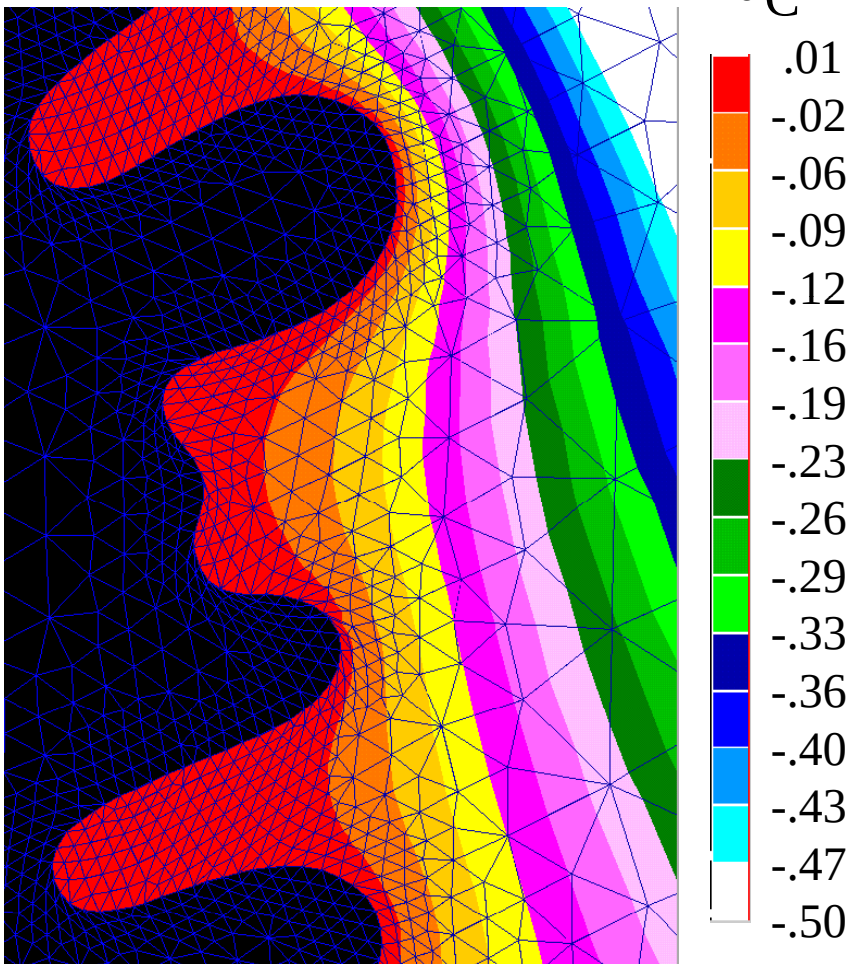


Simulation Results --Thermal Field in the Vicinity of the Dendrite Tip



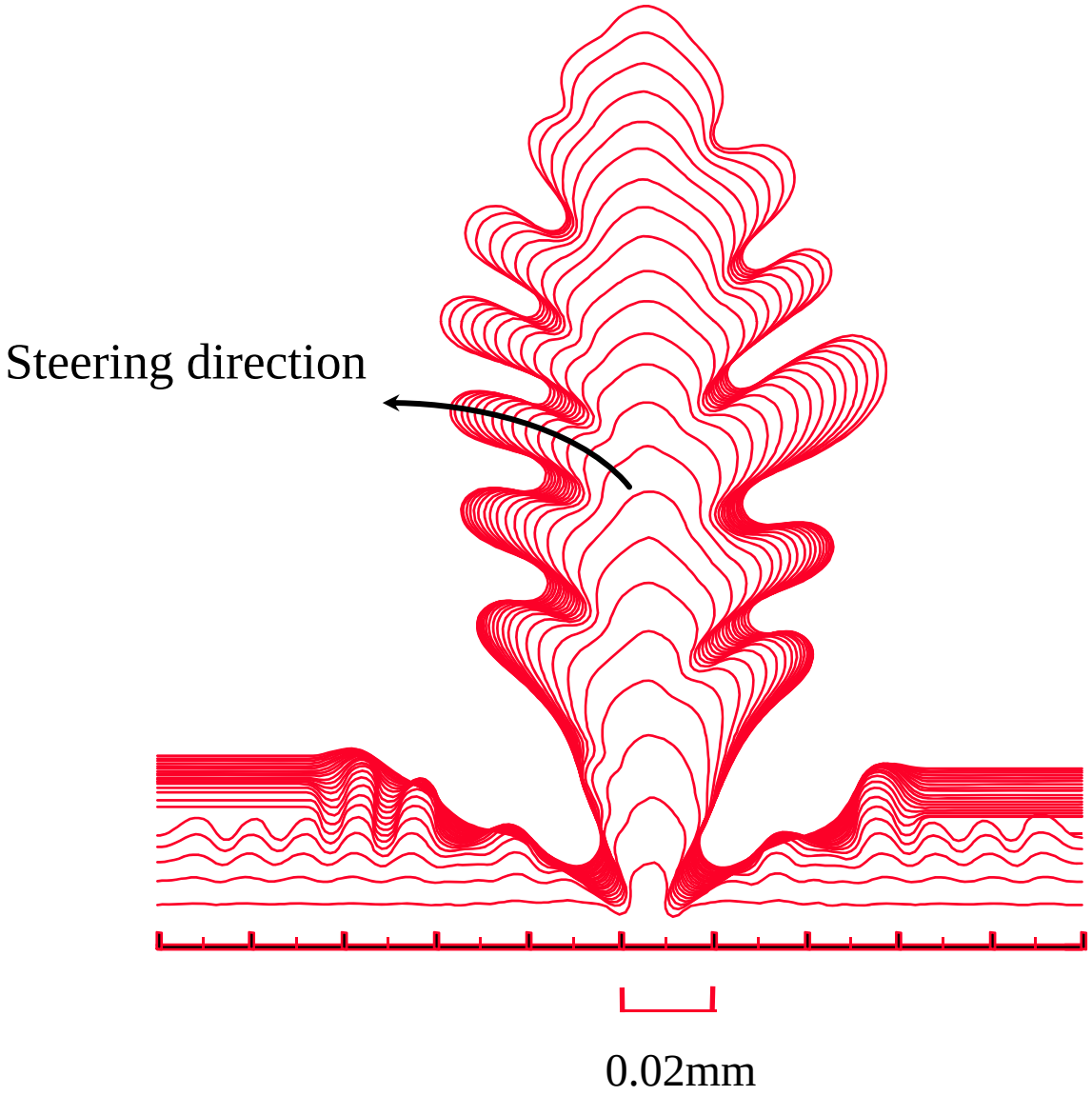
Simulation Results -- Isotherm Coarsening



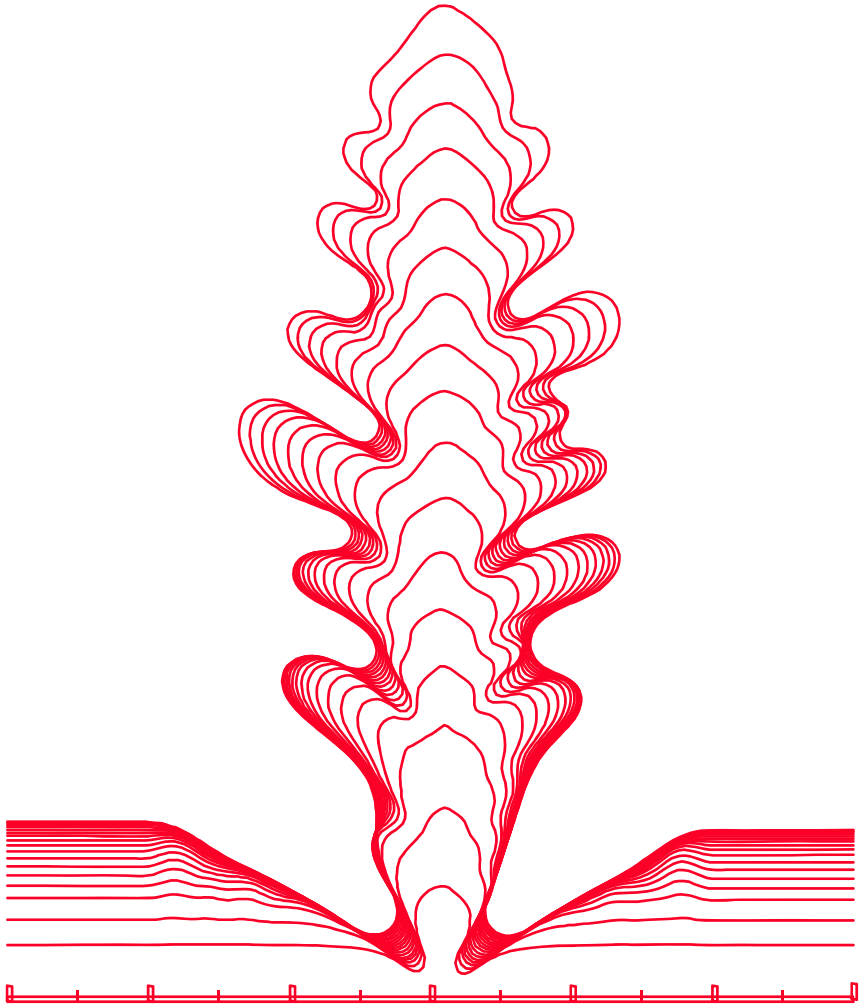


0.1 mm

Side Branch Steering



Simulation Results

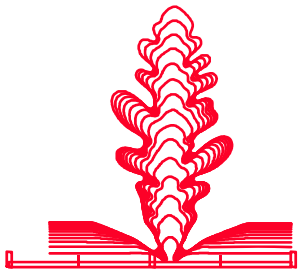


0.1 mm

ΔT: 5.92 °C

Scaling Relationship of Dendrite Size with the Critical Instability Wavelength

--- Dimensional

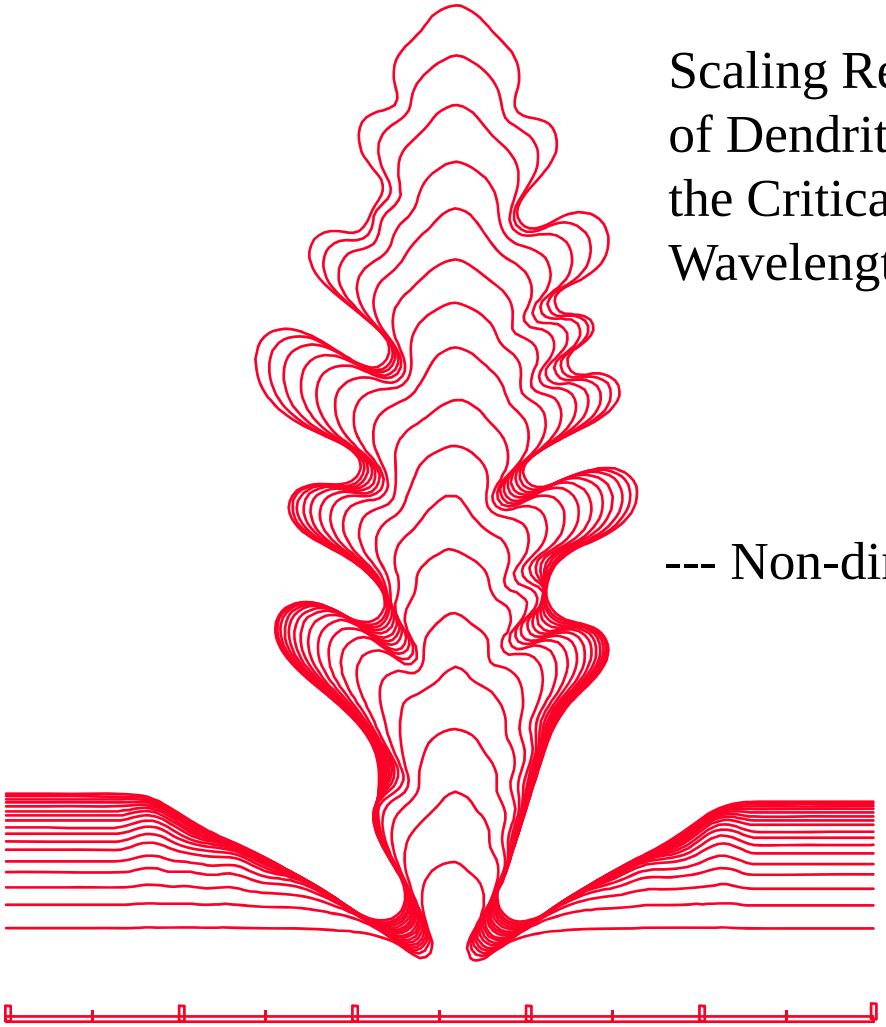


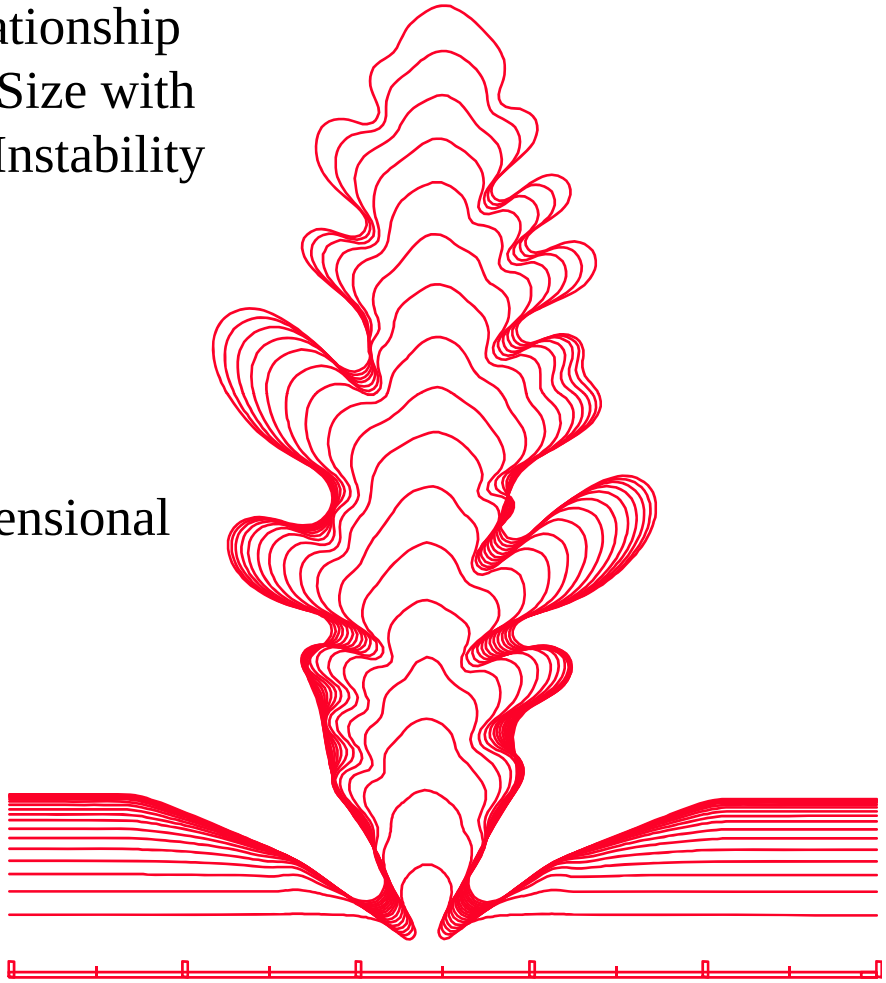
ΔT: 10 °C

Simulation Results

Scaling Relationship of Dendrite Size with the Critical Instability Wavelength

--- Non-dimensional





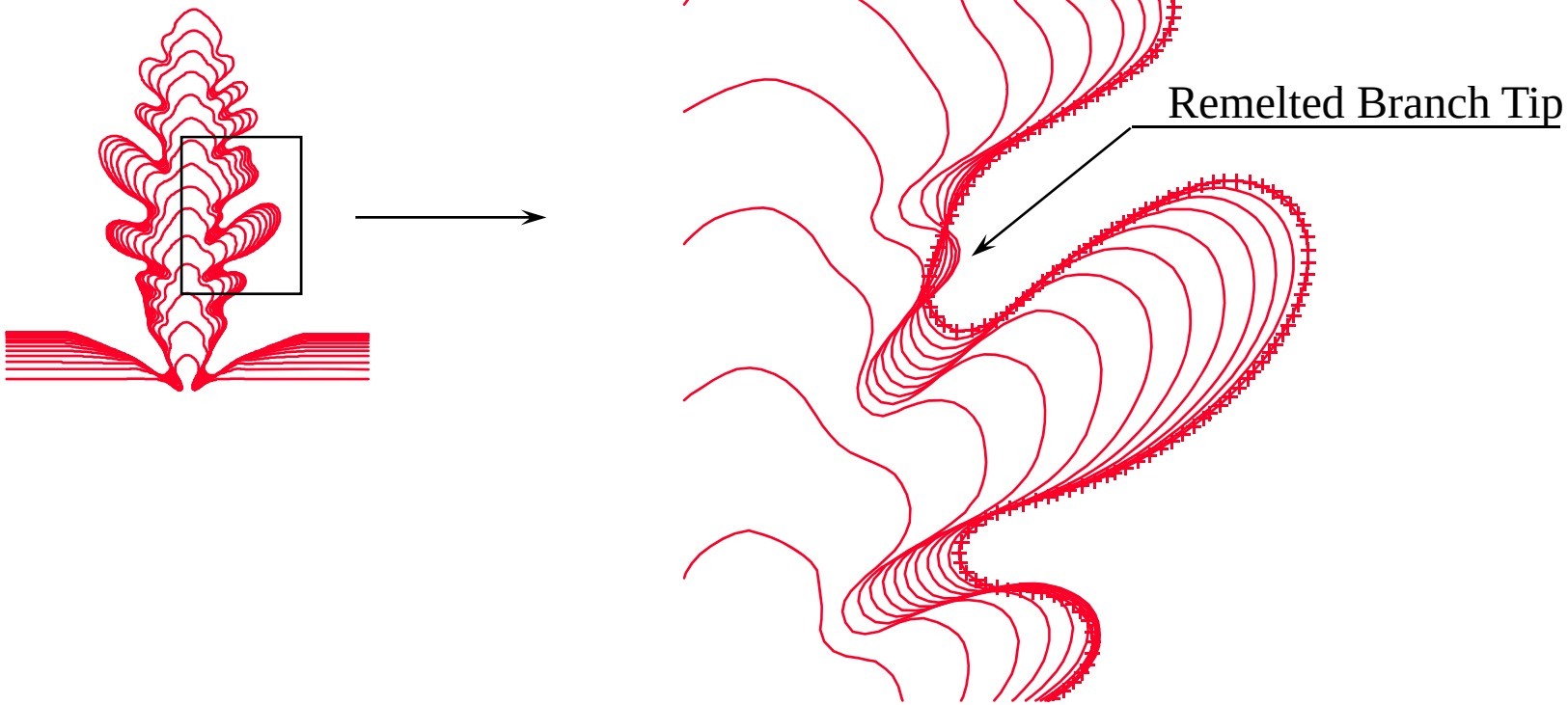
10

ΔT: 5.92 °C (ΔU: 0.25)

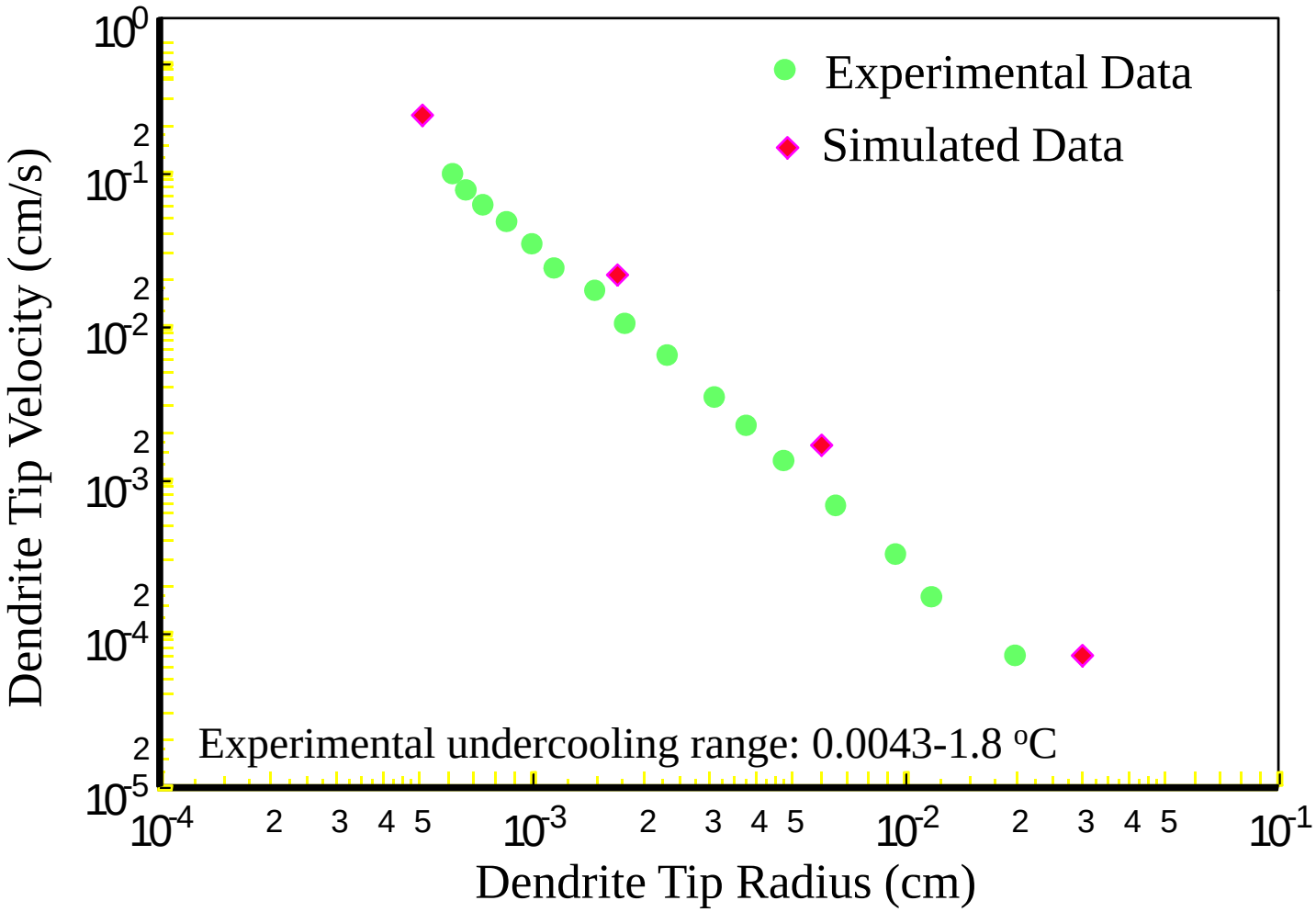
ΔT: 10 °C (ΔU: 0.42)

Simulation Results

Remelting



Simulation Results -- Dendrite Tip Velocity and Tip Radius Relationship



Conclusions

- A numerical model was developed for dendritic growth simulation during solidification based on the physics governing the conduction of heat.

- The model accounts for interfacial curvature, surface energy, and the latent heat of fusion released during solidification.

- The moving interface was tracked with moving mesh, automatic remeshing and refinement techniques.

- The simulated dendrite growth characteristics agree with experimental observation:
  - dendrite growth tip velocity and radius relationship
  - dendrite size scaling relationship
  - side branch competition and remelting, isothermal coarsening.