Phase field models with evaporation & condensation

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Today's talk:

Part 1)
Liquid- Gas :
Spreading & Evaporation

Part2)
Liquid-solid with inhomogeneous T

Latent heat is crucial in these examples

Phase changes in inhomogeneous T are still unsolved . Usual GL theory is inapplicable.

Part1: Gas-Liquid in one-component fluids:

n: number density, e: internal energy density

Entropy $\mathcal{S} = \int d\mathbf{r}[ns(n,e) - C|\nabla n|^2/2]$

regular (bulk) *gradient*

Internal energy $\mathcal{E} = \int d\mathbf{r}\hat{e}$

internal energy density $\hat{e} = e + K|\nabla n|^2/2$

regular (bulk) *gradient*

Definition of T: at fixed n $1/T = \delta\mathcal{S}/\delta e$

valid for inhomogeneous T

van der Waals $(v_0, \epsilon = \text{const})$

$$s = k_B \ln[(e/n + \epsilon v_0 n)^{d/2}(1/v_0 n - 1)] + \textbf{const.}$$

$$e = dnk_B T/2 - \epsilon v_0 n^2$$

$$p = nk_B T/(1 - v_0 n) - \epsilon v_0 n^2$$

Stress tensor for K=0

$$\Pi_{ij} = p\delta_{ij} - CT[n\nabla^2 n + (\nabla n)^2/2]\delta_{ij}$$
$$+ CT\nabla_i n \nabla_j n - \sigma_{ij}$$

reversible stress + viscous stress (η,ζ)

Korteweg stress (1901)

$$\frac{\partial}{\partial t}\rho = -\nabla(\rho\mathbf{v}), \;\; (\rho = mn)$$

$$\rho(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla)\mathbf{v} = -\nabla\cdot\Pi - \rho g\mathbf{e}_z$$

$$\frac{\partial}{\partial t}e_T = -\nabla\cdot(e_T + \Pi\cdot)\mathbf{v}$$

$$+\nabla\lambda\nabla T - \rho g v_z, \;\; (e_T = \hat{e} + \rho v^2/2)$$

Stress* Π *contains gradient terms

Entropy production >0 if no heat from outside.

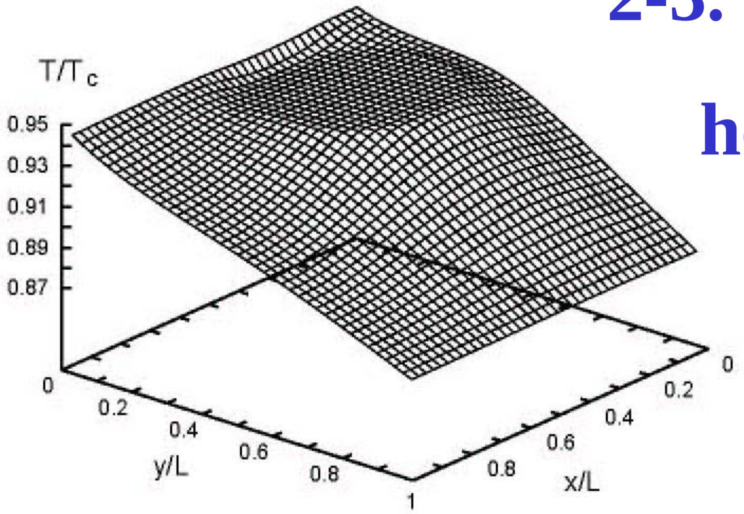
We require

$$\frac{\partial}{\partial t}\mathcal{S} = \int d\boldsymbol{r}\frac{1}{T}[\nabla\cdot\lambda\nabla T + \sum_{ij}\sigma_{ij}\nabla_i v_j]$$

Gradient terms are automatically determined

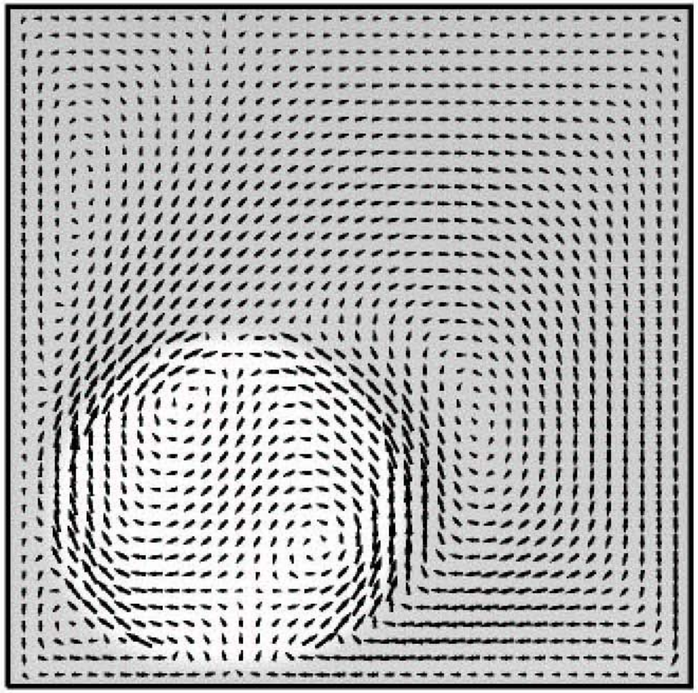
2D simulations (Onuki PRE 2004)

2-3. Bubble is attracted to heated wall. Apparent partial wetting



$T_{\rm bot}/T_c$ is changed from 0.875 to 0.945

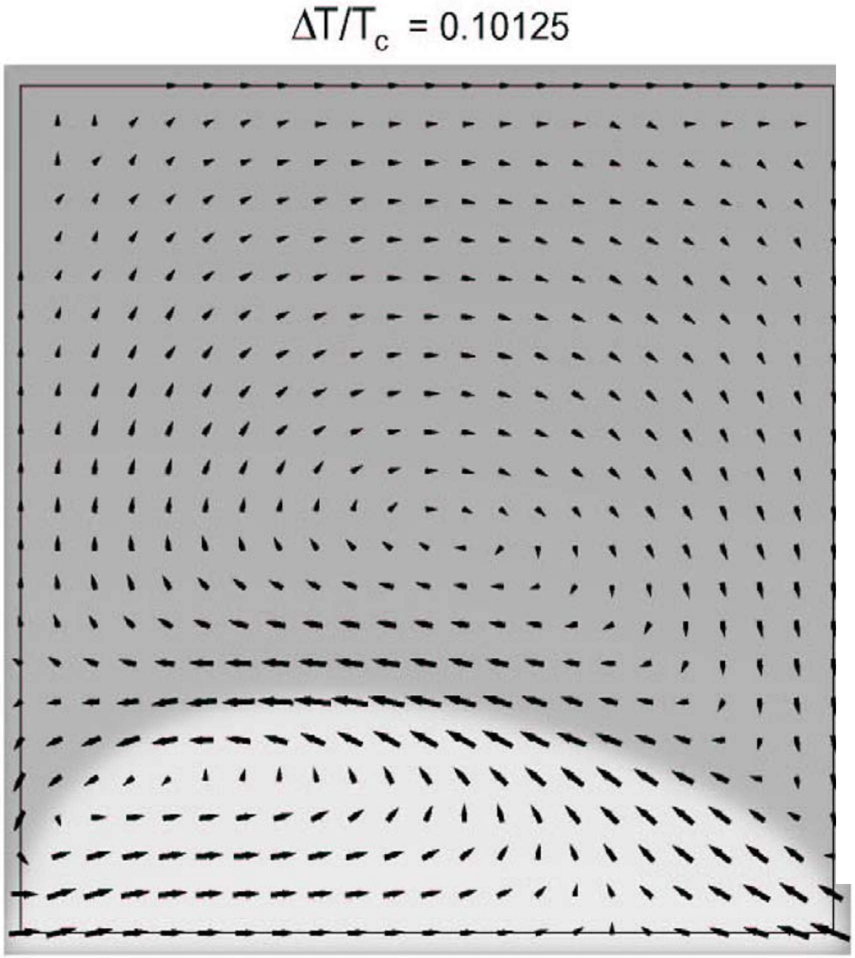
$T_{\rm top}/T_c = 0.875$

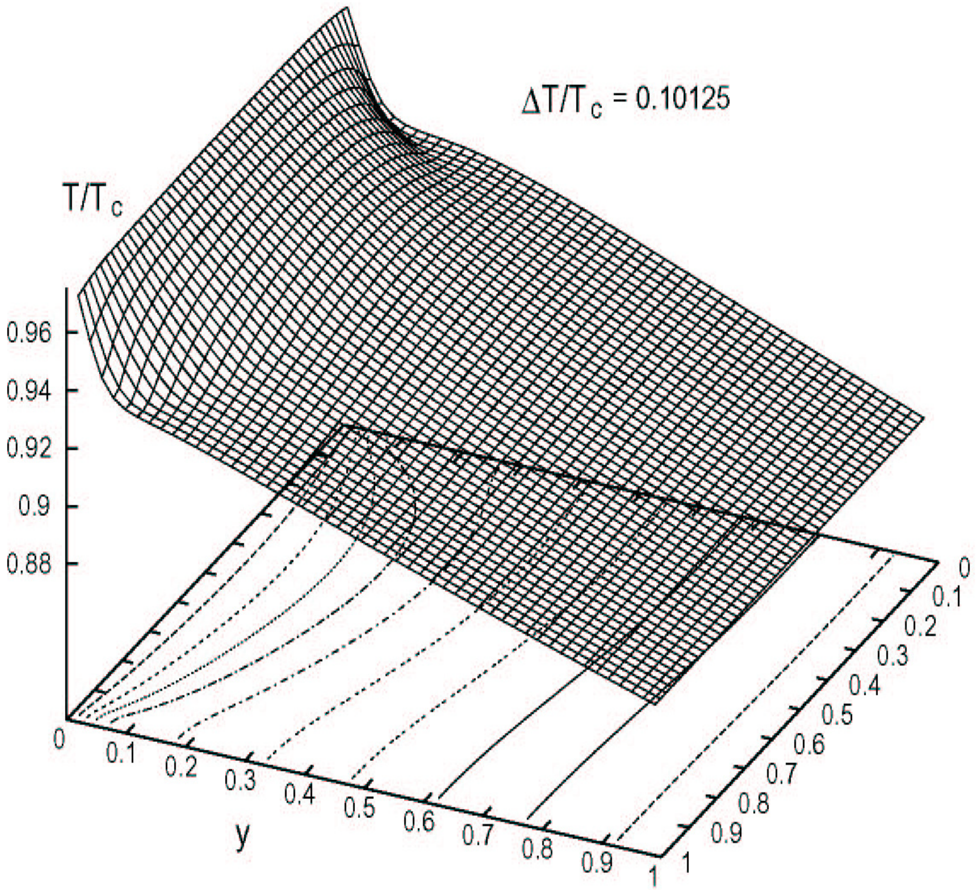


Pressure is nearly homogeneous. Interface is nearly on the coexistence curve.

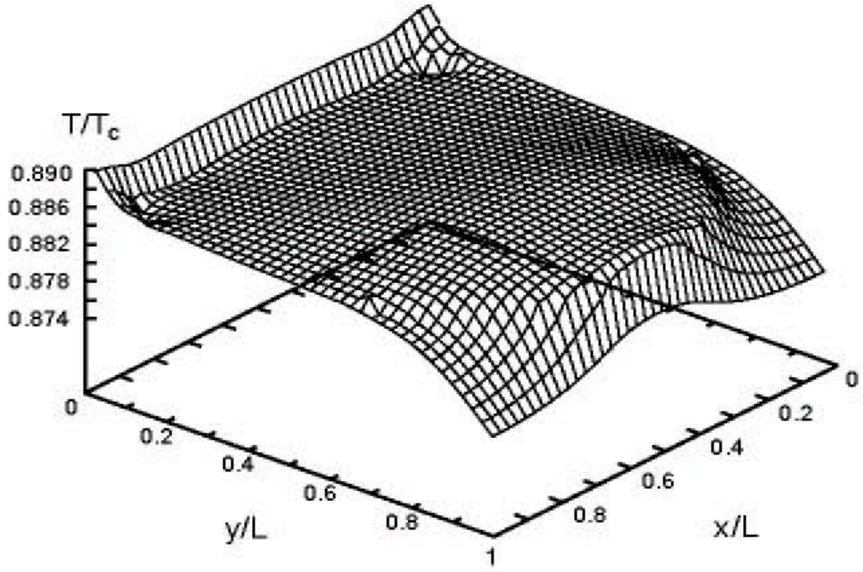
T is flat within bubble = Tcx(p) due to latent heat convection

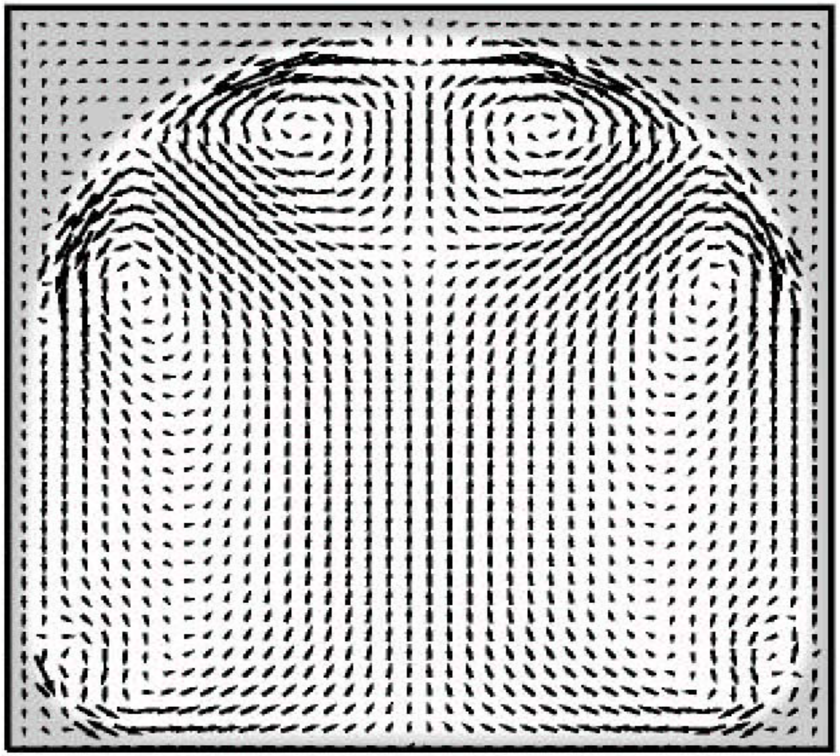
2-4. Wall is covered by gas. Latent heat transport is suppressed Large gradient in gas film





$\lambda = An \quad (\lambda_{liq}/\lambda_{gas} = 5)$





2.5 Efficient heat transport by flow along wetting layer, no gravity

$$\lambda_{\mathrm{liq}} = 5\lambda_{\mathrm{gas}}$$

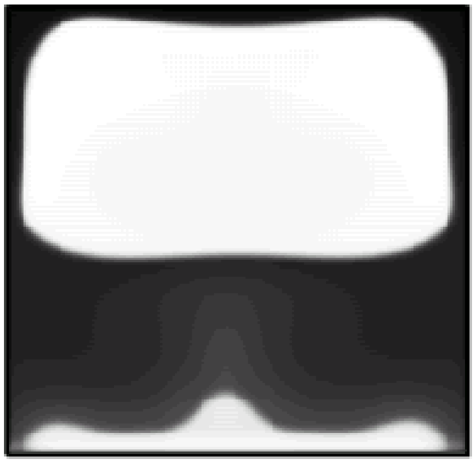
$$Nu = \frac{\lambda_{\mathrm{eff}}}{\lambda_{\mathrm{liq}}} = 5$$

$$T_{\mathrm{bot}}/T_c = 0.895$$

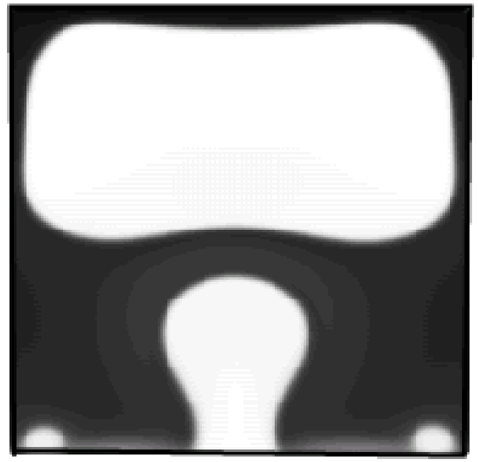
$$T_{\mathrm{top}}/T_c = 0.875$$

Steady flow, but drying for larger Tbot.
Heat pipe mechanism.

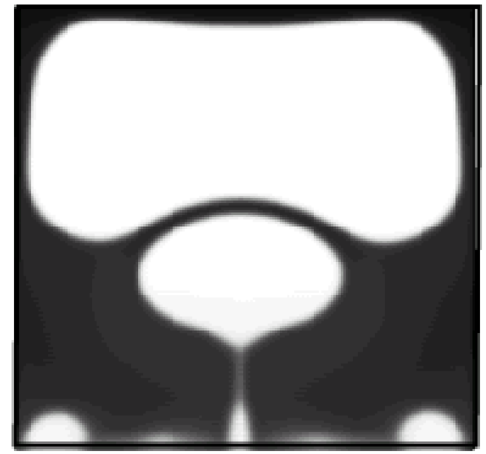
8-1. Boiling: gravity applied , Tt/Tc=0.77 , Tb/Tc is changed from 0.94 to 1 at t=34000



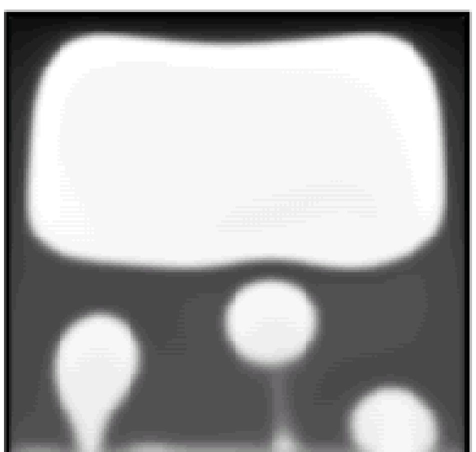
t=34600



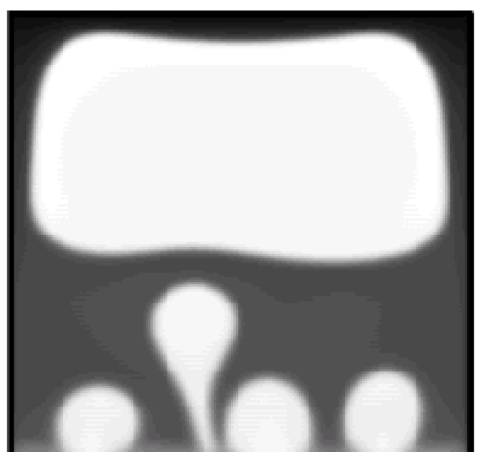
t=35100



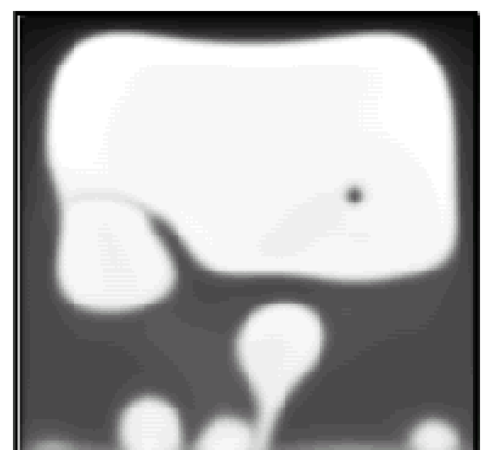
t=35230



t=66300

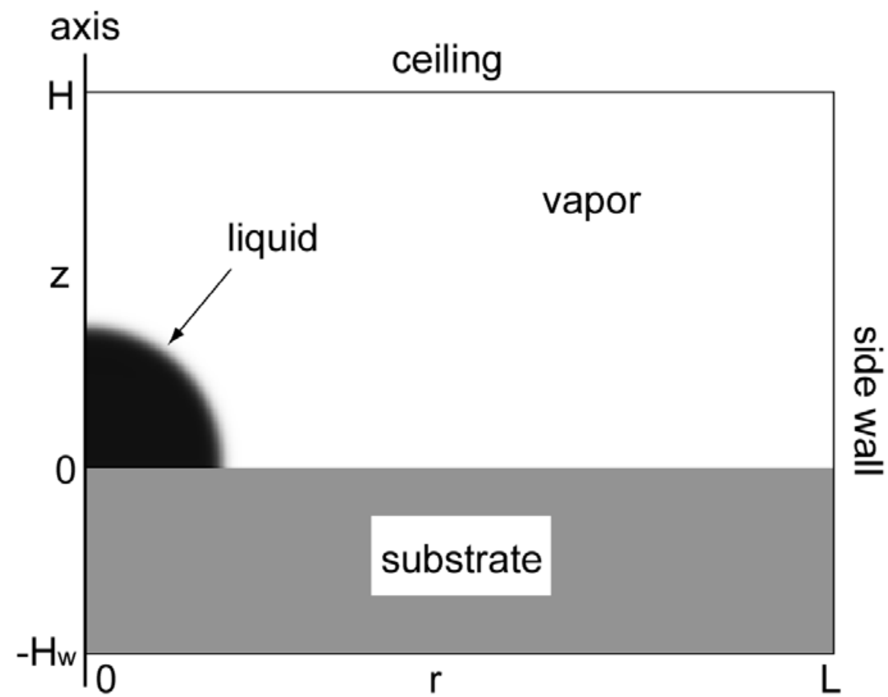


t=71000



t=74100

Simulation: axysymmetric (3D) 600 x 600
Teshigawara &Onuki PRE2011



- **temperature**

Bottom of the substrate : given constant

Ceiling : given constant

Side wall : insulating

- **density**

Boundary condition on number density

substrate

$$\frac{d}{dz}n(z,r)\bigg|_{z=0} = -\Phi_1/CT(0,r)$$

side wall $$\frac{dn}{dz}\bigg|_{z=H} = 0$$

ceiling $$\frac{dn}{dr}\bigg|_{r=L} = 0$$

T=Tw :wall bottom z= -Hw

Thermal diffusion equation in solid

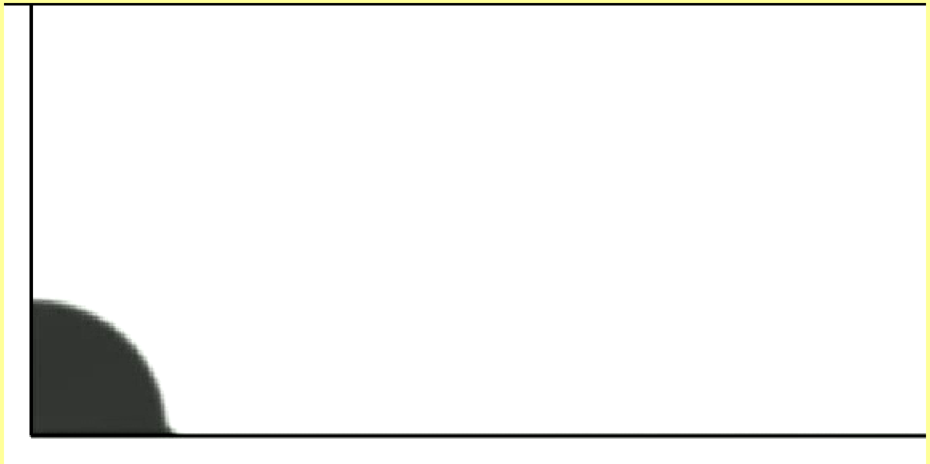
$$C_w\frac{\partial T}{\partial t} = \lambda_w \nabla^2 T,$$

thermal conductivity ratio : $\Lambda = \lambda/(nv_0\lambda_w)$

a) Precursor film formation in complete wetting

Plate temperature Tw was not higher than initial liquid temperature

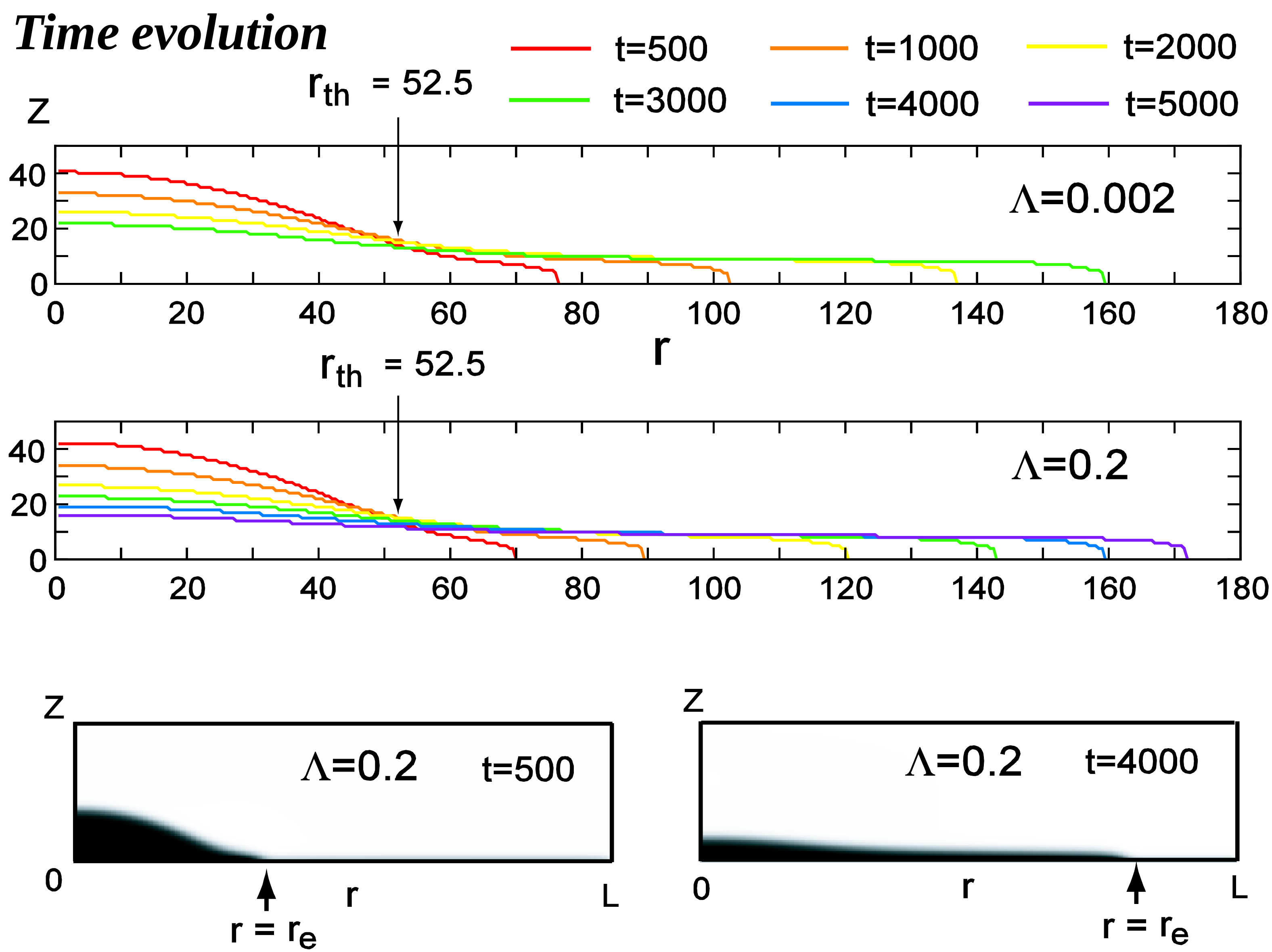
Complete wetting case



Precursor film

Fast growth of precurser film due to evaporation and condensation

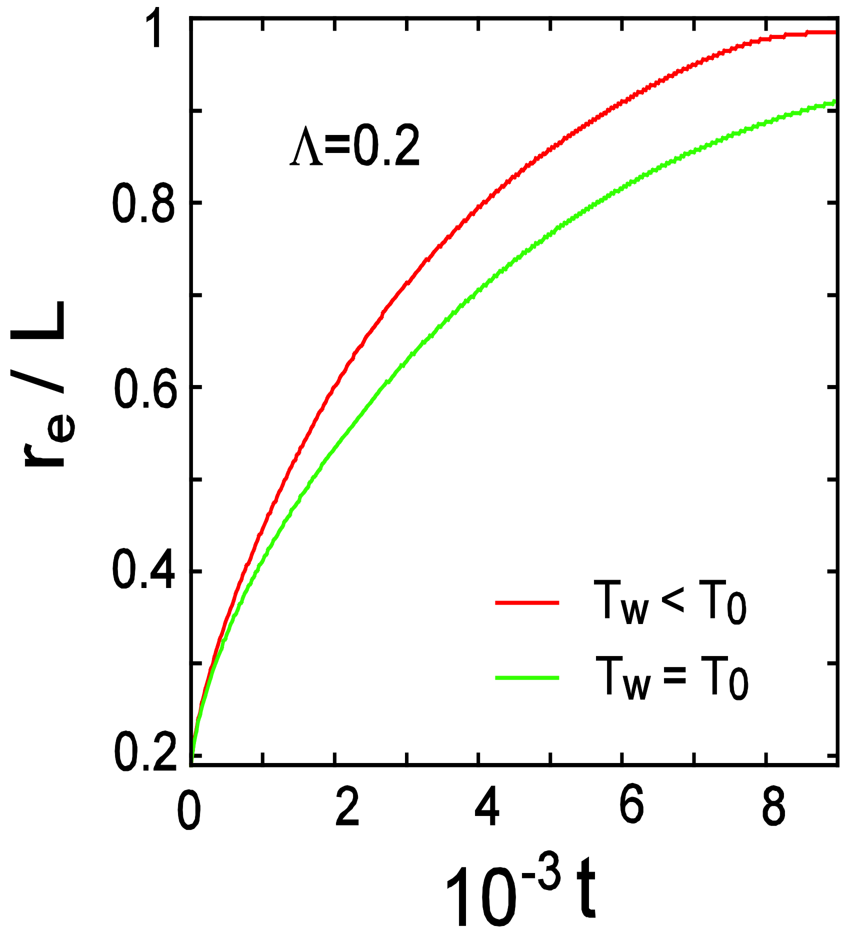
Large wetting parameter Φ_1 ⇒ Precursor film extension

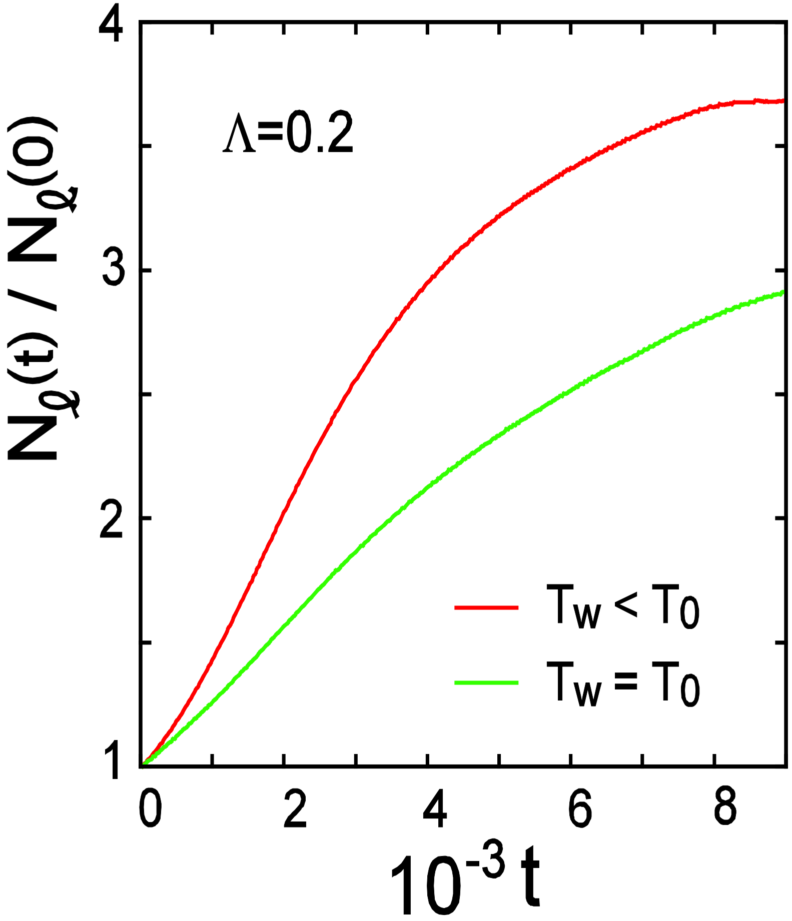


Film thickness = constant. Film expands mainly due to condensation (or flow from the droplet body is smaller).

Condensation occurs for cooled wall

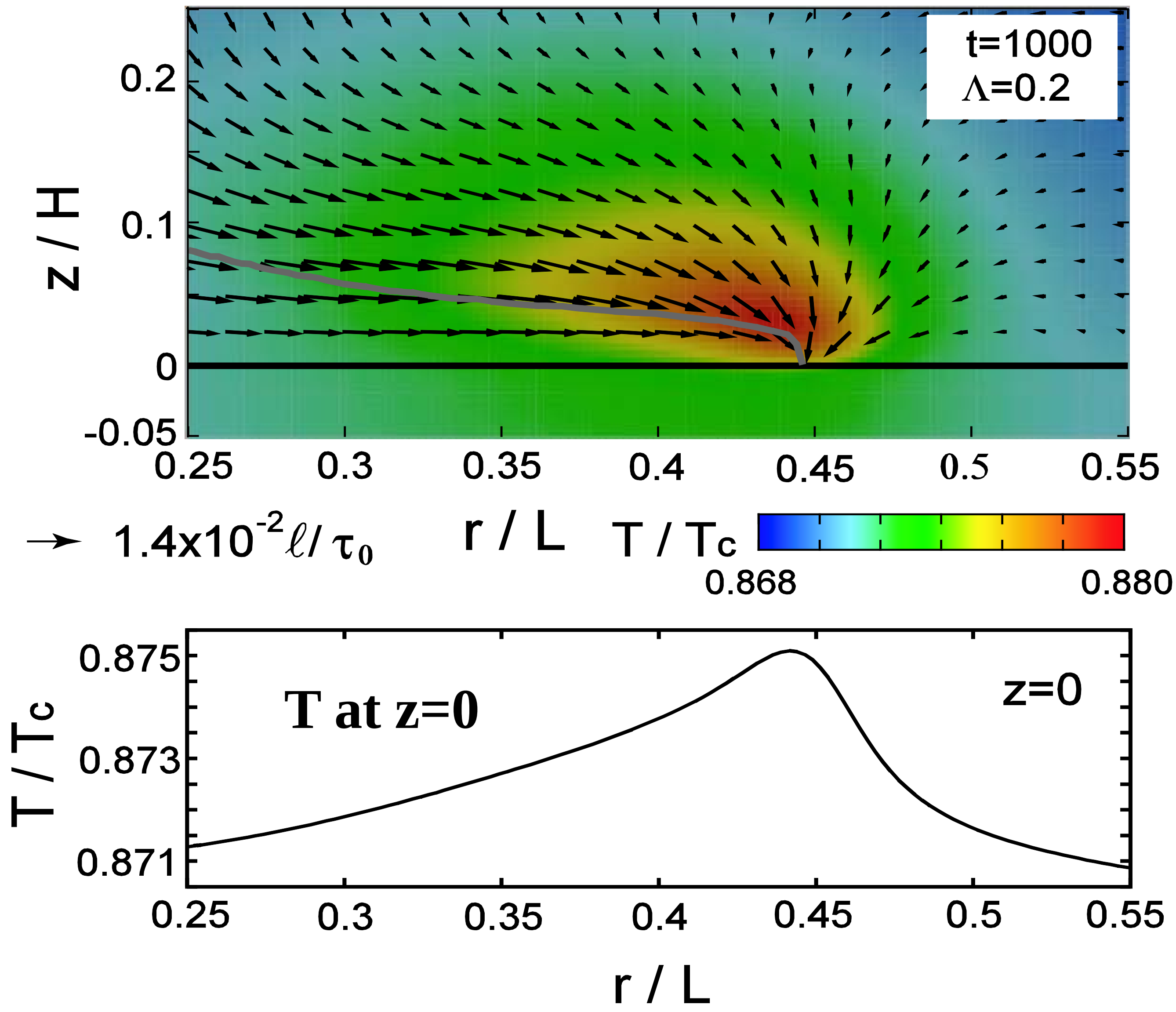
re (t) : edge radius **Nl (t) :particle number in liquid**





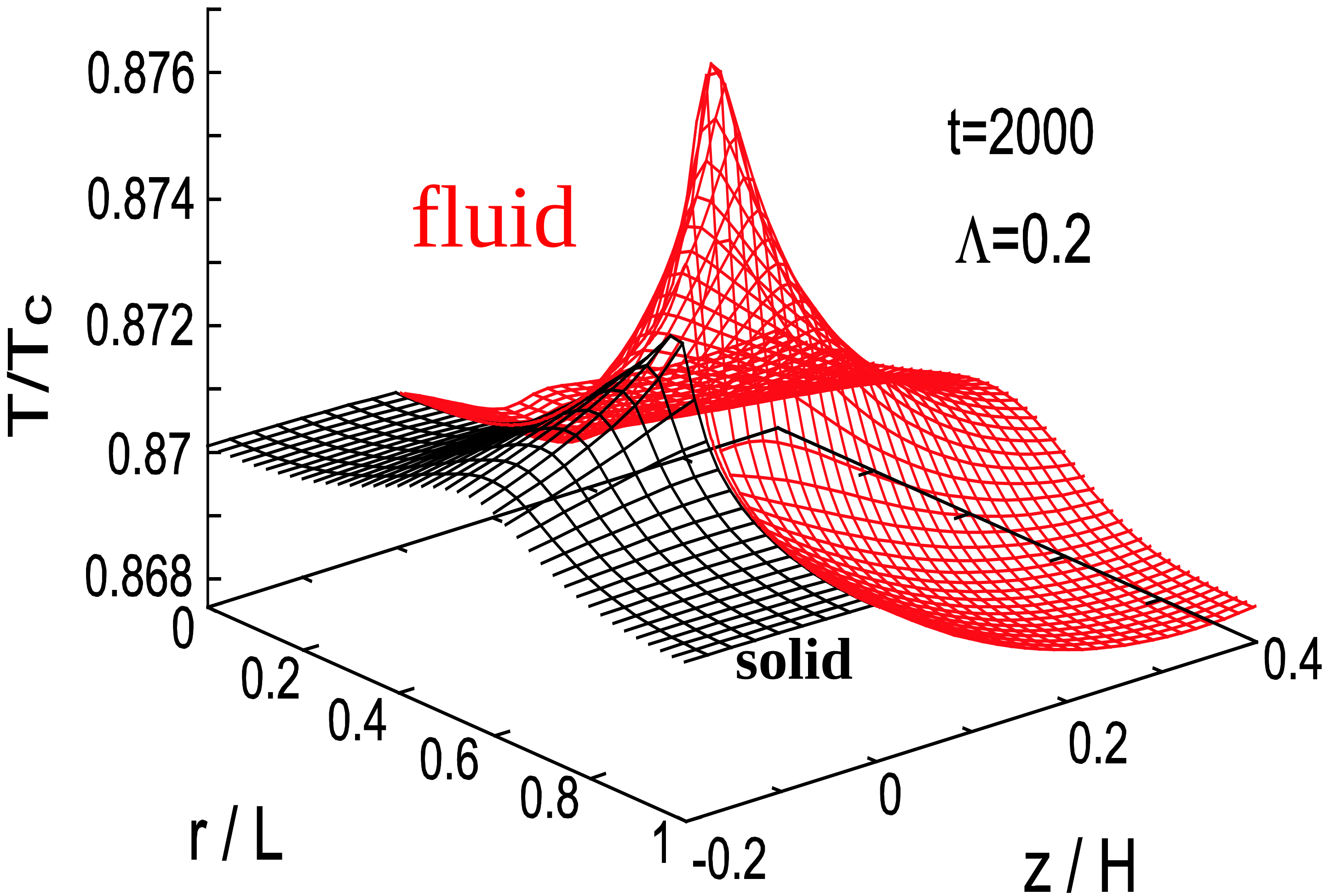
T0= 0.875 Tc , Tw = 0.870 Tc

A hot spot appears due to condensation at edge on a cooled wall

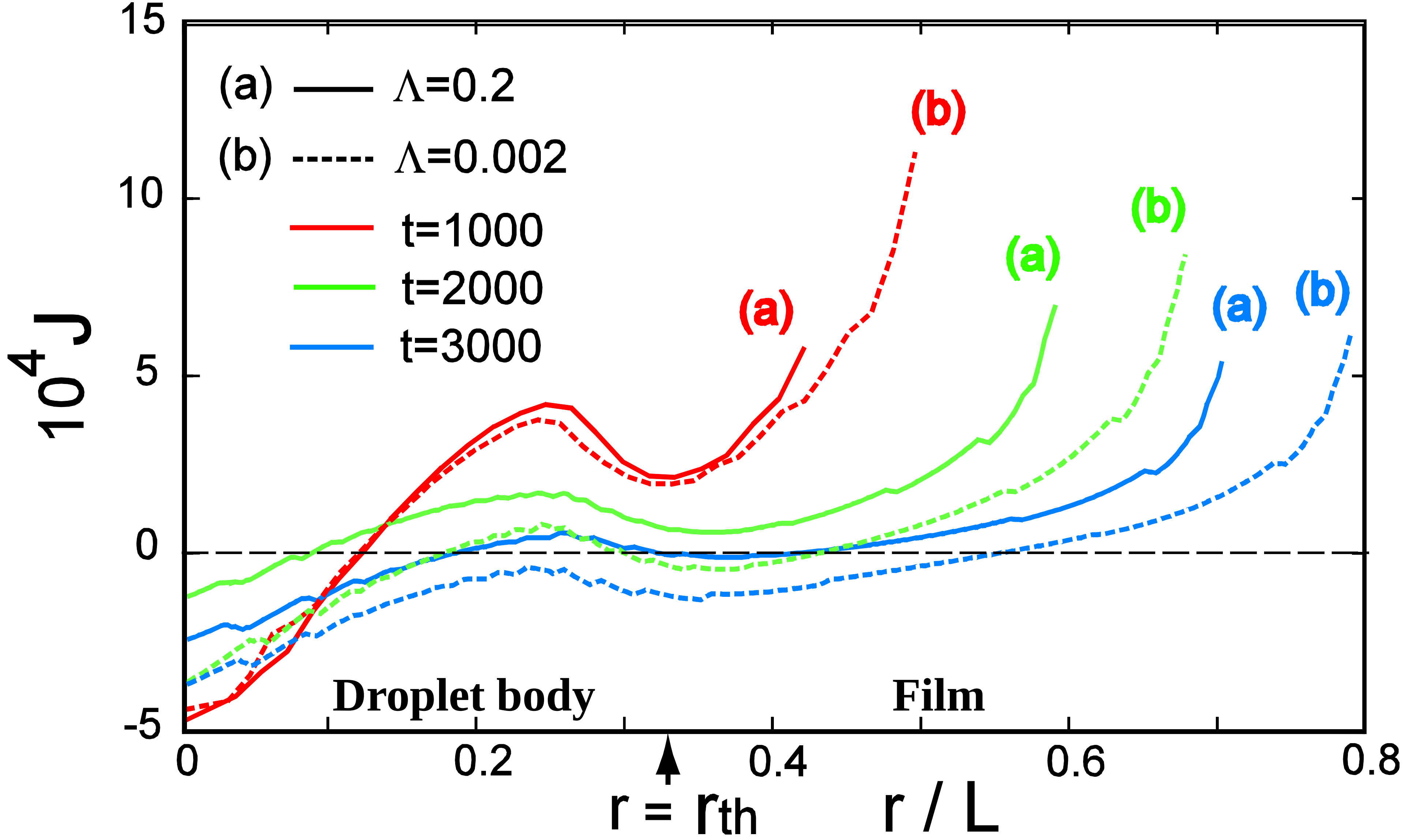


Substrate temperature is inhomogeneous

Bird view of temperature around hot spot

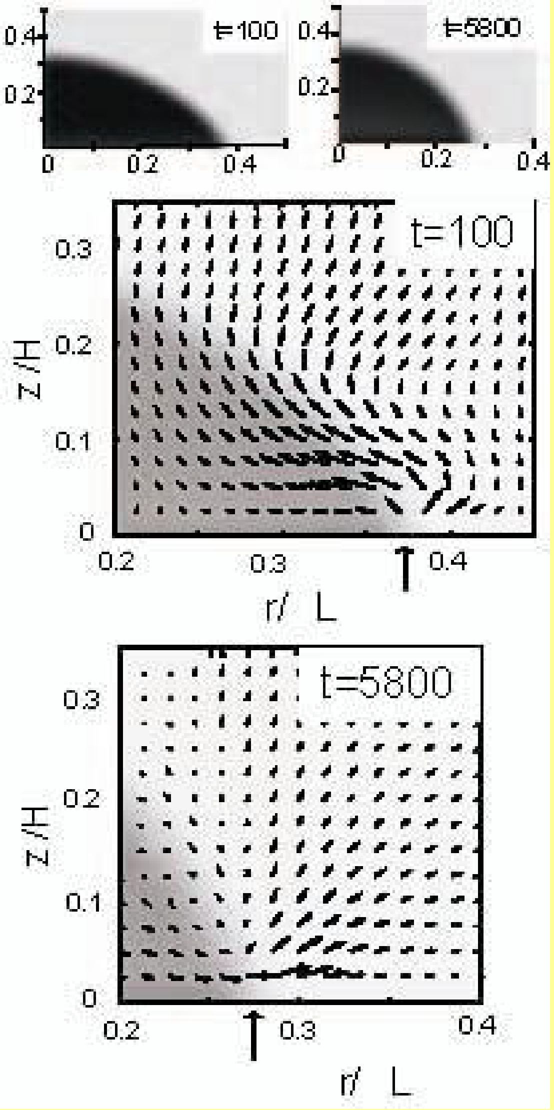


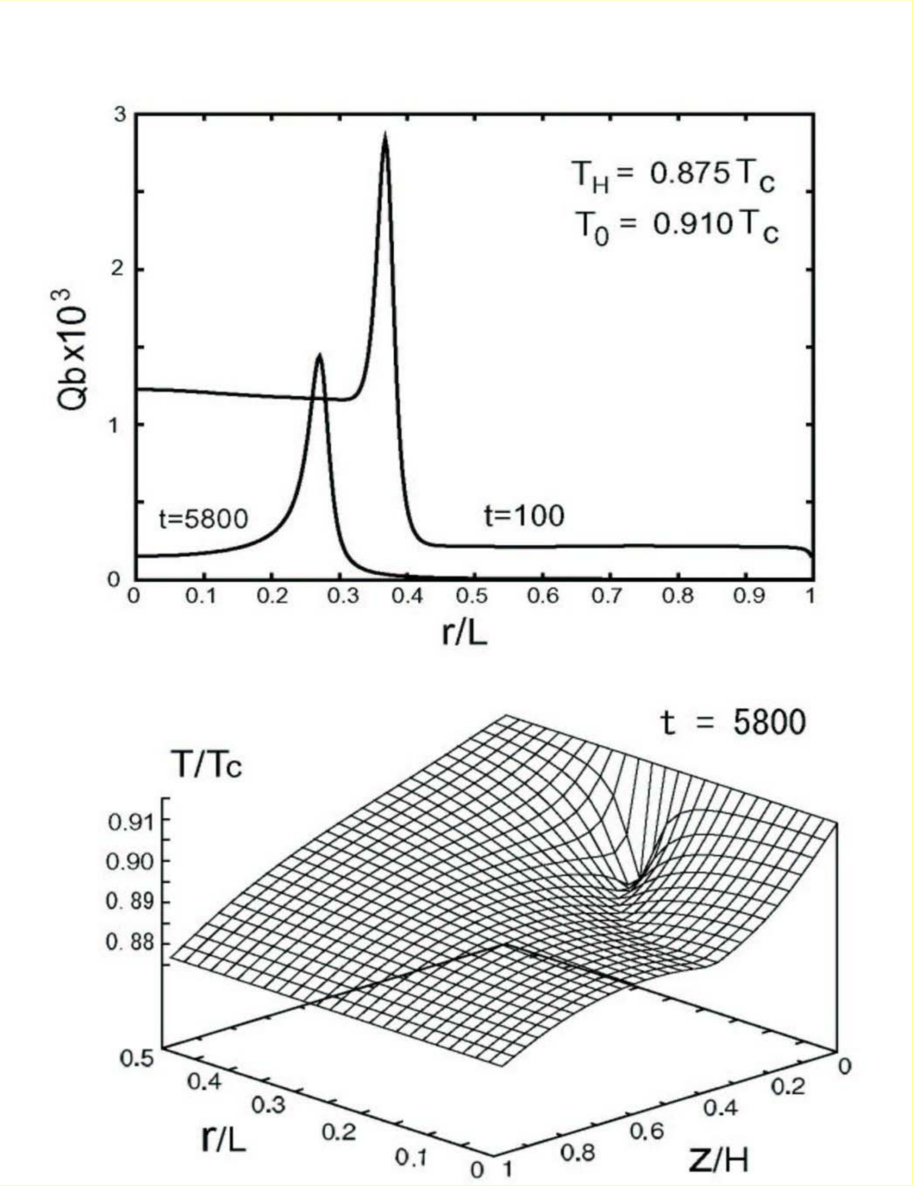
Local evaporation rate J= n (v int –v). normal vector



J>0: condensation, J <0: evaporation

b) Droplet evaporation in partial wetting



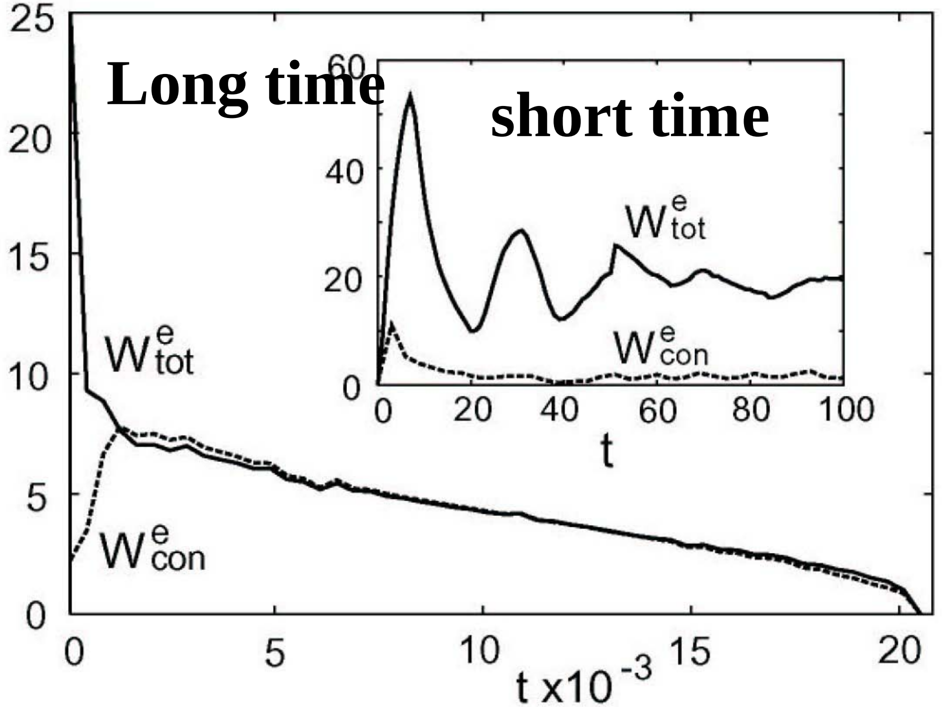


J: $T\Delta s J - \boldsymbol{\nu}\cdot[(\lambda\nabla T)_{\text{gas}} - (\lambda\nabla T)_{\text{liq}}] = 0,$

Evaporation rates

All surface $$W^e_{\text{tot}} = 2\pi\int_0^{r_\text{c}} dr\, r J/\sin\theta.$$

Near contact line $$W^e_{\text{con}} = 2\pi\int_{r_\text{c}-r_w}^{r_\text{c}} dr\, r J/\sin\theta.$$



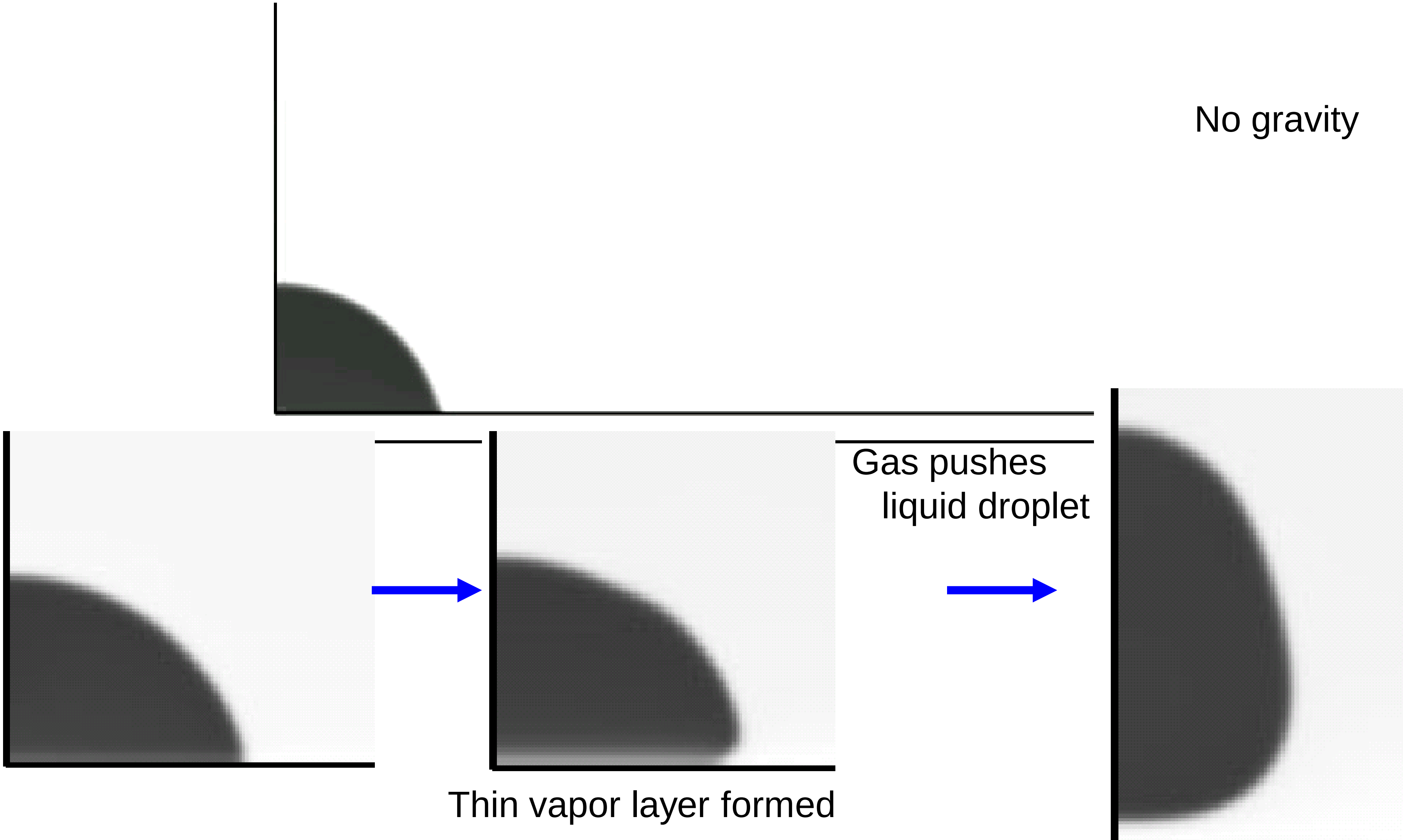
J:mass flux through interface

$r_w = 2\times$interface width

On long times evaporation occurs only at contact line

Leidenfrost effect: droplet detachment by strong heating

On wall T/T_c is changed from 0.875 to 0.975



Part 2) solid-liquid (one-component)

anisotropic strains e_2 & e_3

Takae & Onuki, Pre (2011)

ϕ: Phase field

emtropy density : $\hat{S} = S(\rho, e, \phi) - \frac{1}{2} C |\nabla \phi|^2$

energy density : $e_{\rm T} = e + \rho |\boldsymbol{v}|^2/2 + G(\phi)(e_2^2 + e_3^2)/2$

e_2:elongational strain, e_3:shear strain,

Here linear elasticity

$G = G_0 \phi^2$:shear modulus

Expand S up to second order at a reference state:

$$S = S_{0\ell} + \frac{\delta e - \mu_0 \delta \rho}{T_0} - C_V^0 \frac{\tau^2}{2} - \frac{\zeta^2}{2 T_0 K_T^0} - W(\phi)$$

We introduce two field variables

$$\tau = (\delta e - \beta_0 \delta \rho)/T_0 C_V^0 - a_1 \theta(\phi)$$

$$\zeta = \delta \rho / \rho_{0\ell} - a_2 \theta(\phi)$$

$$W(\phi) = \frac{1}{2} A \phi^2 (1-\phi)^2, \quad \theta(\phi) = \phi^2 (3 - 2\phi)$$

Hydrodynamics + elasticity+ phase transition 2D

Phase-field hydrodynamics for solid-liquid:

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}),$$

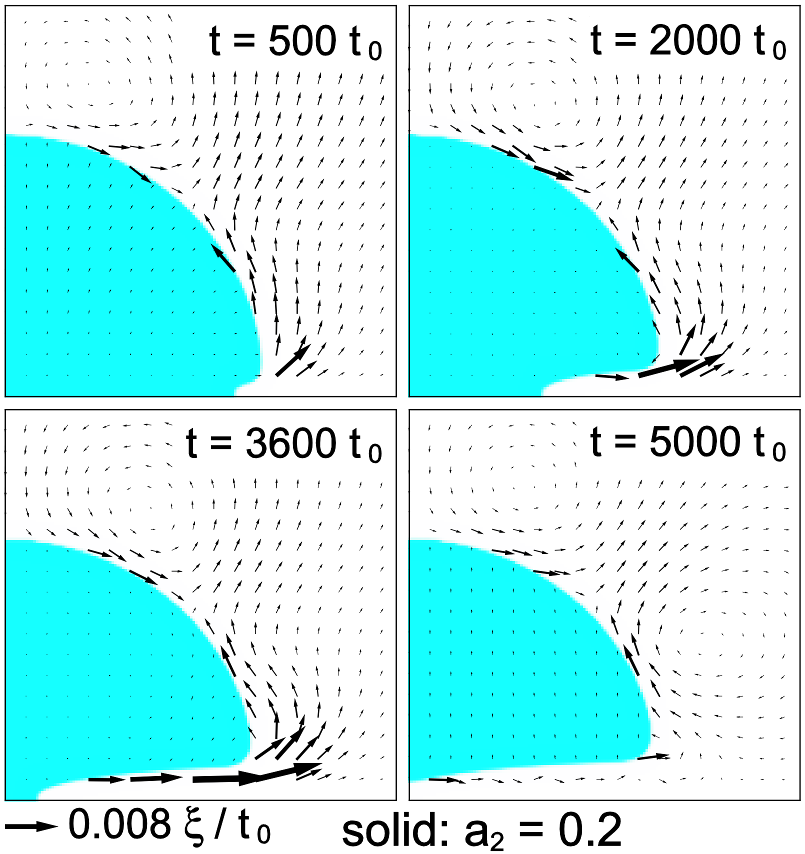
$$\frac{\partial \rho \boldsymbol{v}}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} + \overleftrightarrow{\boldsymbol{\Pi}} - \overleftrightarrow{\boldsymbol{\sigma}}),$$

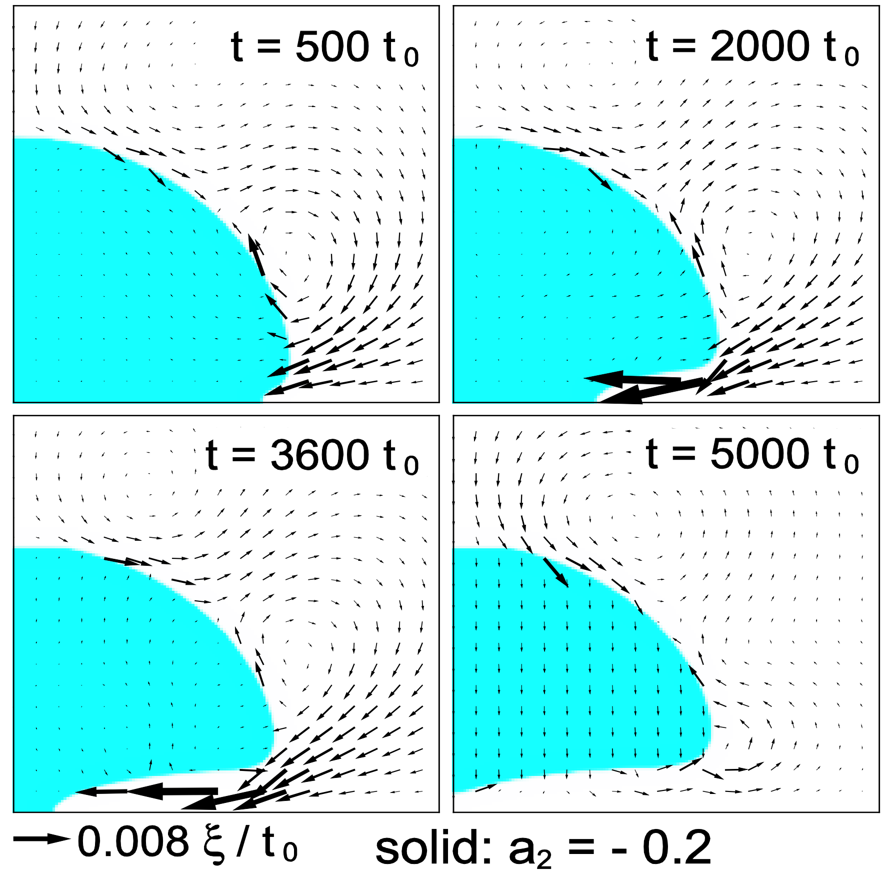
$$\frac{\partial e_T}{\partial t} = -\nabla \cdot [e_T \boldsymbol{v} + (\overleftrightarrow{\boldsymbol{\Pi}} - \overleftrightarrow{\boldsymbol{\sigma}}) \cdot \boldsymbol{v} - \lambda \nabla T]$$

$$\frac{\partial}{\partial t} e_2 = -\boldsymbol{v} \cdot \nabla e_2 + \nabla_x v_x - \nabla_y v_y$$

$$\frac{\partial}{\partial t} e_3 = -\boldsymbol{v} \cdot \nabla e_3 + \nabla_x v_y + \nabla_y v_x.$$

Example1) “Ice on a hot plate”





$\rho_{\mathrm{lsolid}} > \rho_{\mathrm{liq}}$

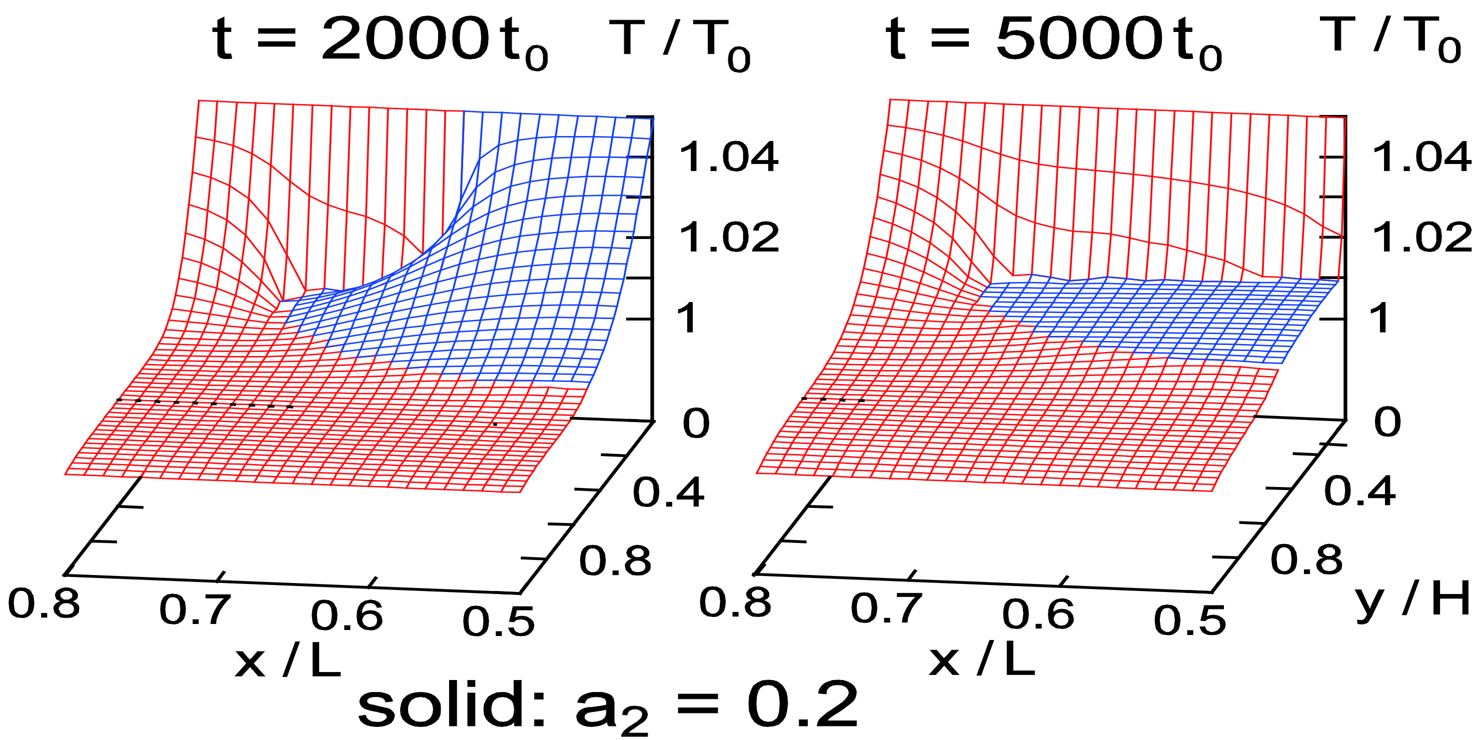
outgoing flow

$\rho_{\mathrm{liq}} < \rho_{\mathrm{solid}}$

incoming flow

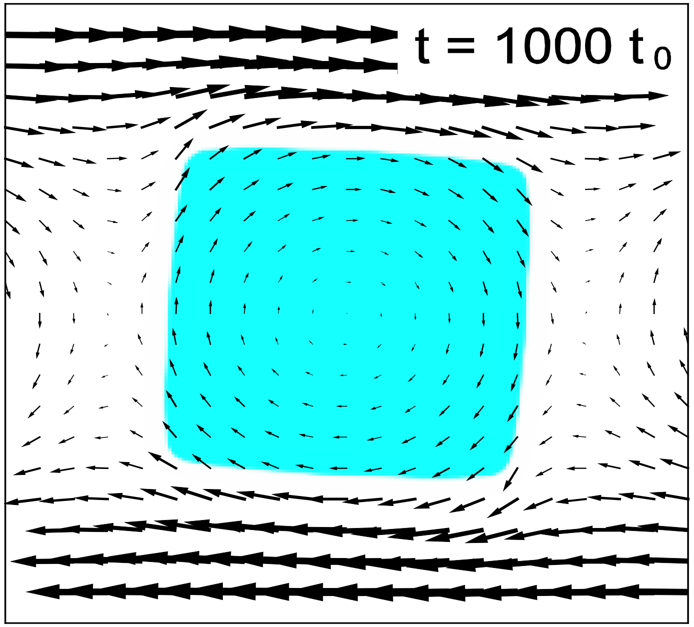
Temperature around heated ice

Blue: solid, red: liquid



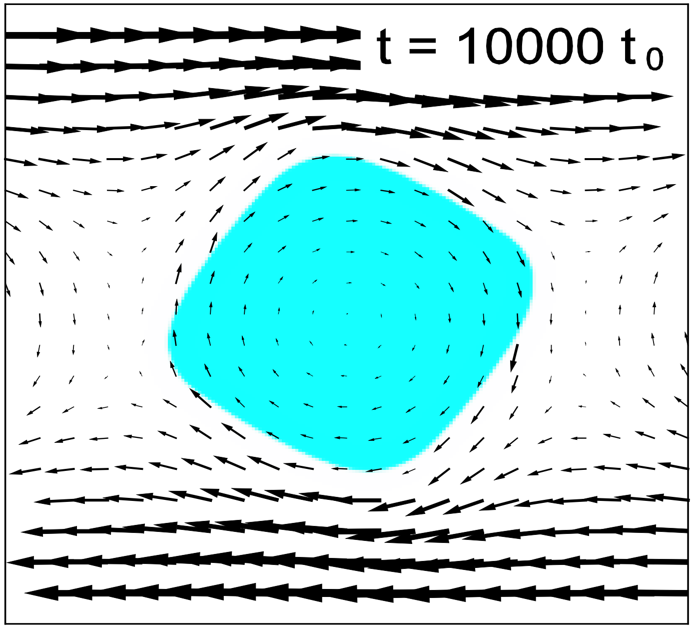
attached to wall **detached from wall**

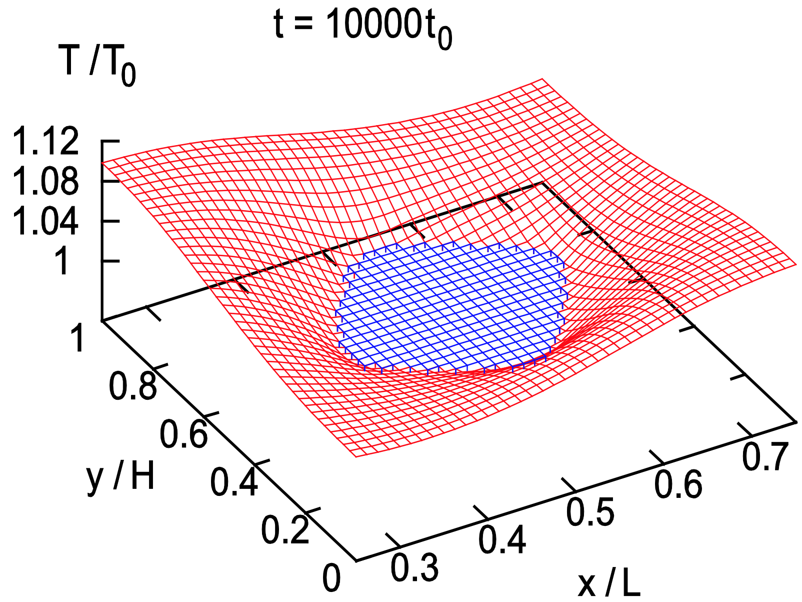
Latent heat cools the liquid region



Example2)Ice cube in warm liquid in shear flow

Latent heat due to melting cools liquid
Shear flow accelerates melting





Generalization to account for plasticity

Nonlinear elasticity (periodic in e_2 and e_3)

$$e_2 = \nabla_x u_x - \nabla_y u_y, \quad e_3 = \nabla_x u_y + \nabla_y u_x.$$

elastic energy $= K(\nabla \cdot \boldsymbol{u})^2/2 + G(\phi)\Phi(e_2, e_3)$

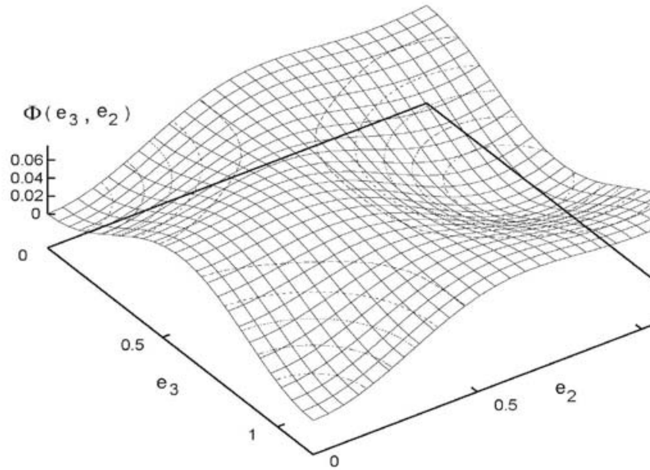
$$\Phi = \frac{1}{6\pi^2}\left[3 - \cos(2\pi e_2) - \cos(2\pi e_+) - \cos(2\pi e_-)\right]$$

$(e_\pm = (\sqrt{3}e_3 \pm e_2)/2)$

(invariant with respect to $\pm\pi/6$ rotations)

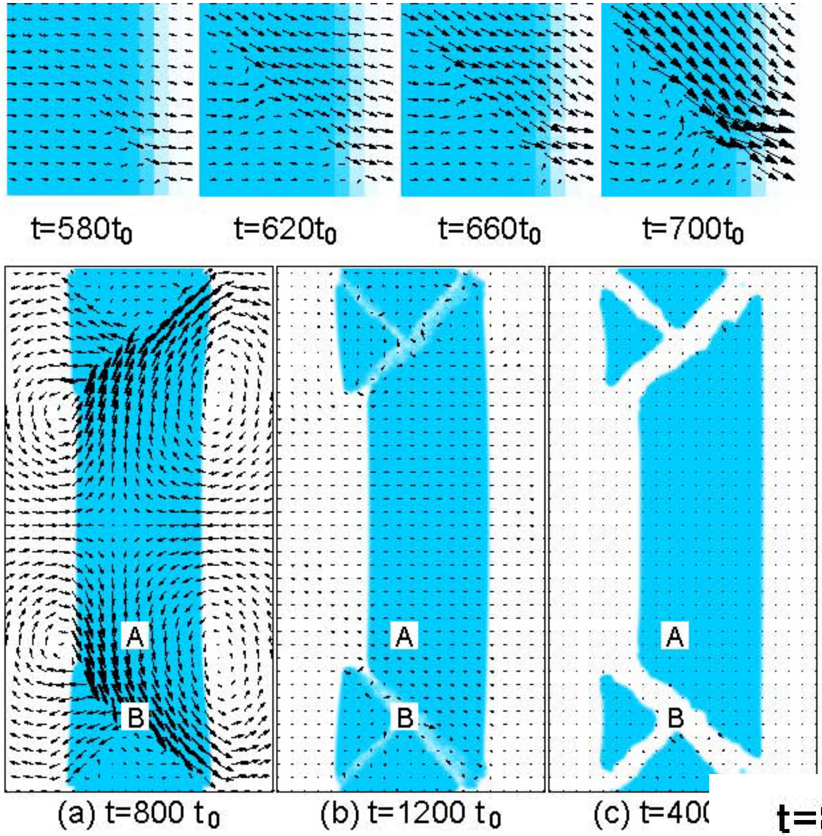
For small e_2 and e_3, linear elasticit

$$\Phi \cong (e_2^2 + e_3^2)/2$$

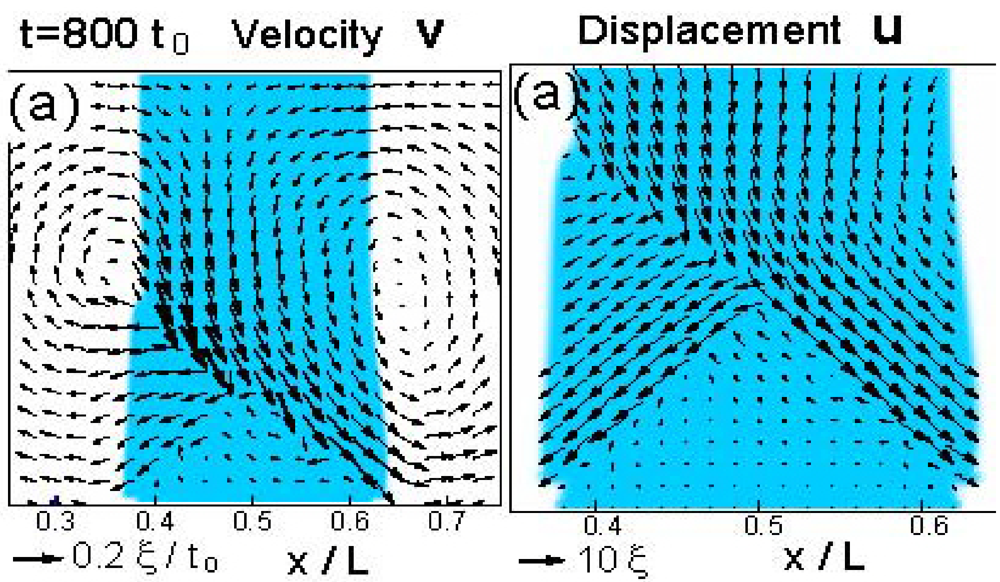


Jumps among multiple minima induce dislocations

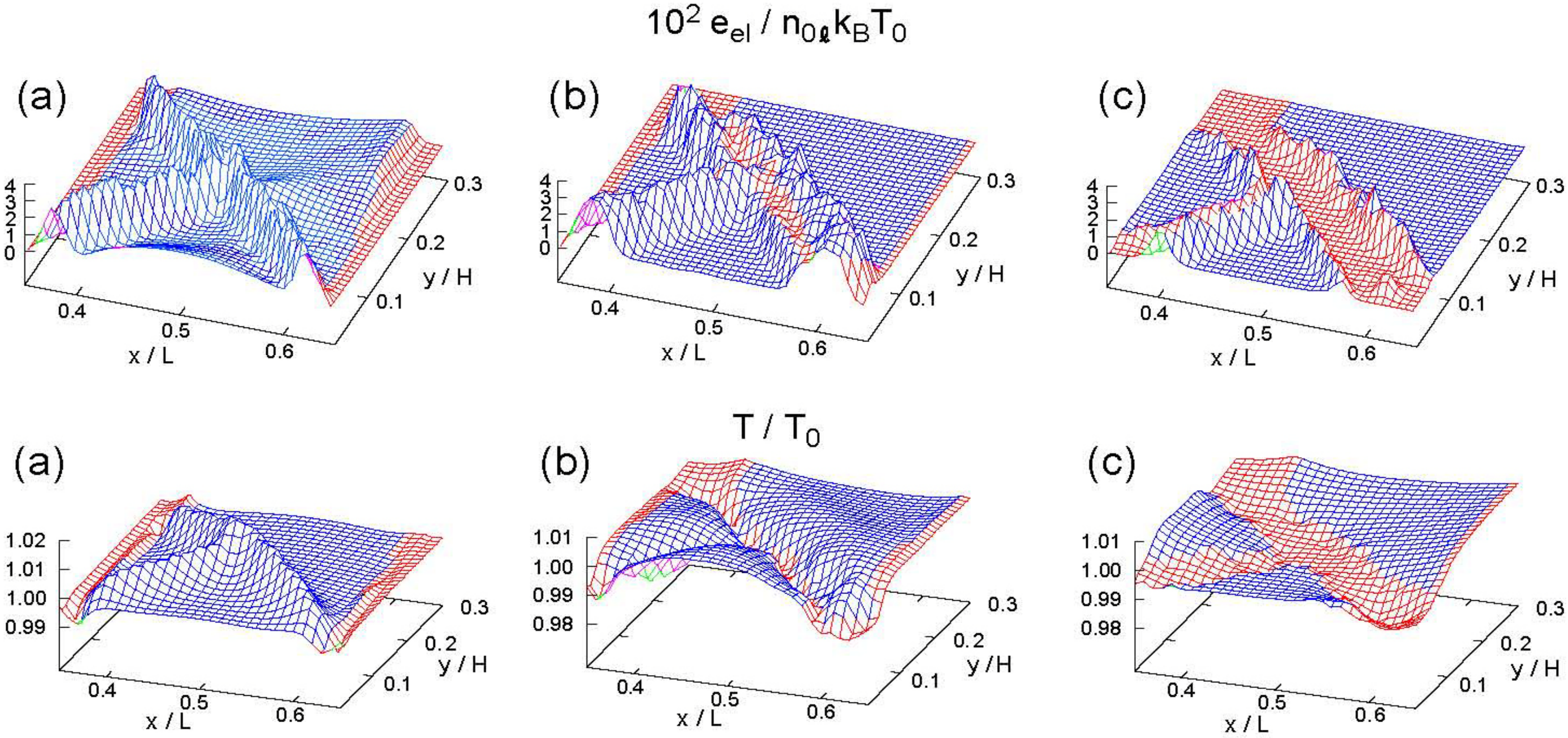
Compressed crystal rod undergoes plastic deformation and subsequent melting



Dislocations induce slip.



Elastic energy density and temperature around plastically deformed region (botom)



Viscous heating **Latent heat cooling upon melting**

Summary

1. Two-phase dynamics with evaporation and condensation

2. Wetting dynamics: evaporation, spreading,….

3 Solid-liquid with elasticity in flow

Many important problems in future:

In real systems: multi-component fluids !

Boiling (water+air), Marangoni convection