Advanced Inverse Techniques for the Design of Directional Solidification processes

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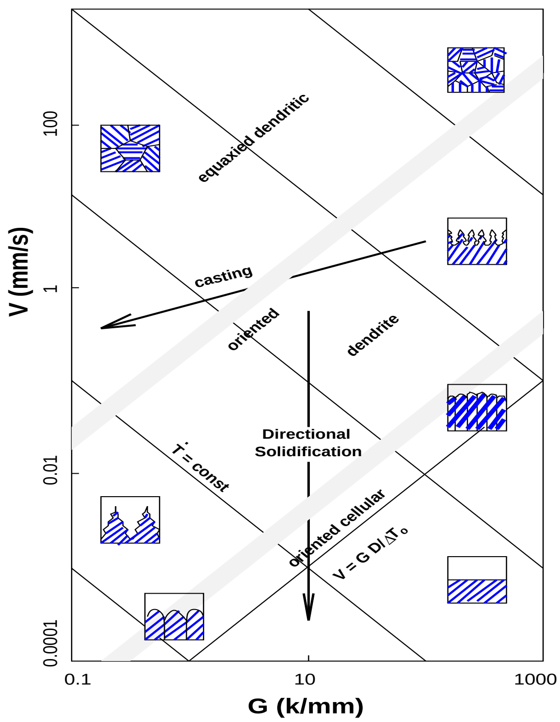
Modeling of Casting, Welding and
Advanced Solidification Processes
San Diego, California
June 7-12, 1998

Supported by NSF grants CTS-9115438
and DDII-9157189

Outline of the presentation

- Motivation and objectives
- Background and related work
- Inverse design techniques
- Solidification design for stable growth
- Numerical results
- Forthcoming developments

Inverse solidification design problems



Motivation:

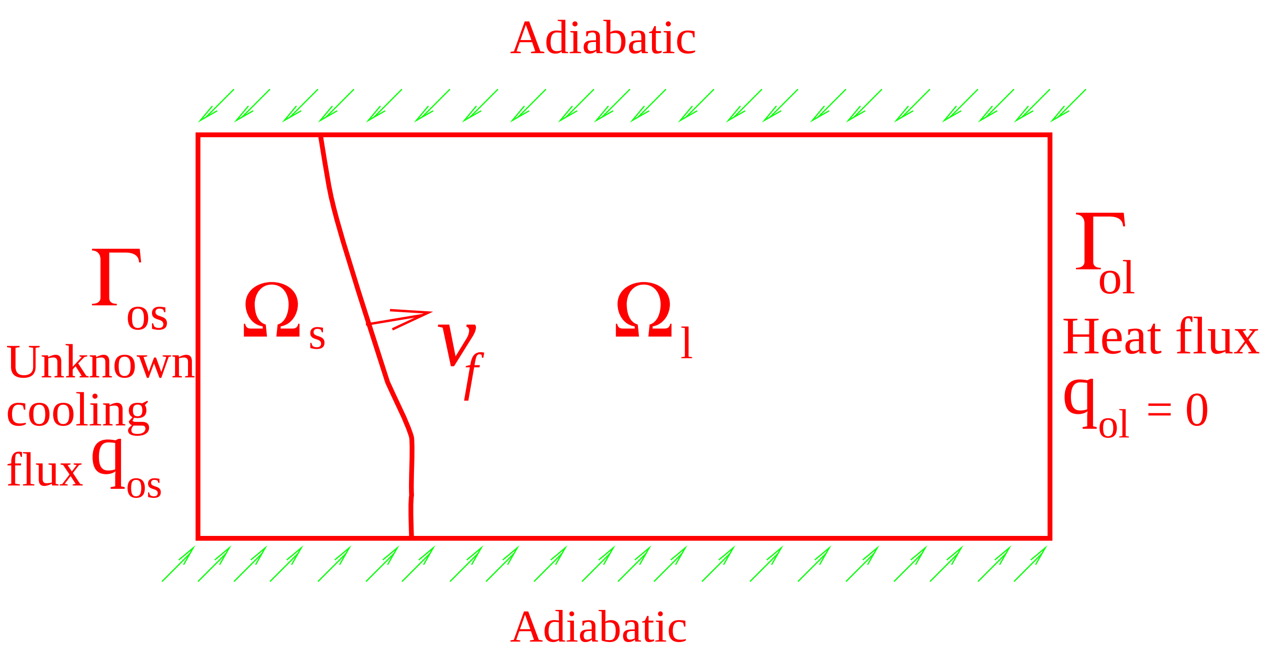
Solidification micro-
-structures depend on
the parameters G and V

- Kurz and Fisher (1984)

Progress :

- Inverse and design Stefan problems
  - Rubinski and Katz (1984)
  - Zabaras (1990)
  - Zabaras and Ruan (1992)
- Inverse conduction based solidification problem with data supplied from a direct melt convection problem
  - Zabaras and Nguyen (1995)
- Inverse convection based solidification design problems
  - Zabaras and Yang (1997, 1998)

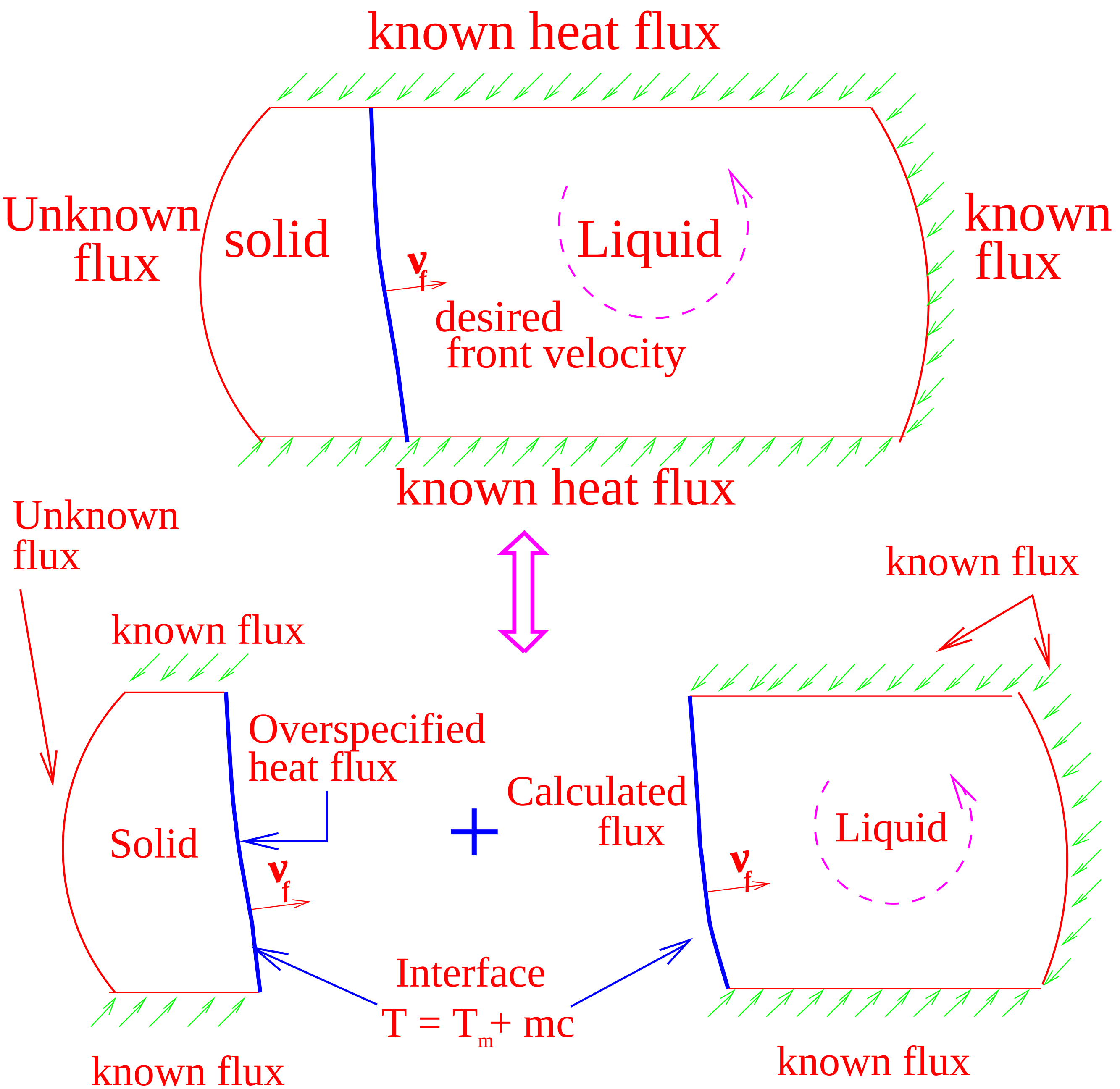
A reference design problem in the directional solidification of a dilute binary alloy



Define the following objective:

" Find appropriate cooling flux q_{os} at the solid mold wall such that the solid-liquid interface advances with a given spatially uniform velocity v_f (t) into the liquid "

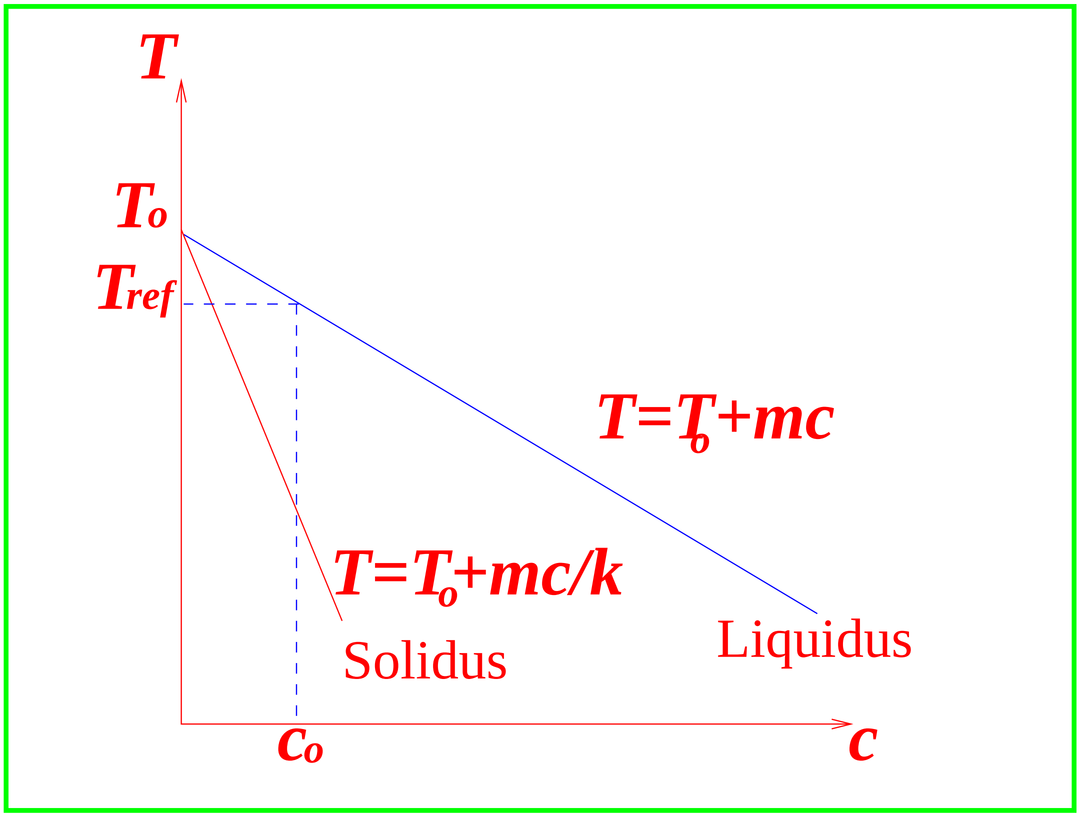
Solution technique for the inverse reference design problem

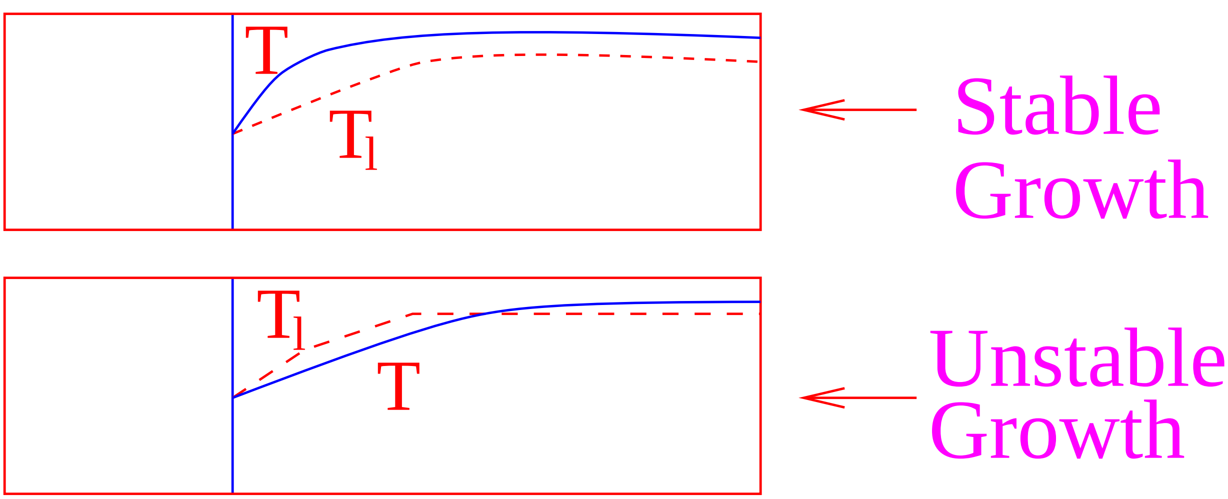


Inverse problem in solid

Quasi direct problem in liquid

Phase diagram and constitutional stability



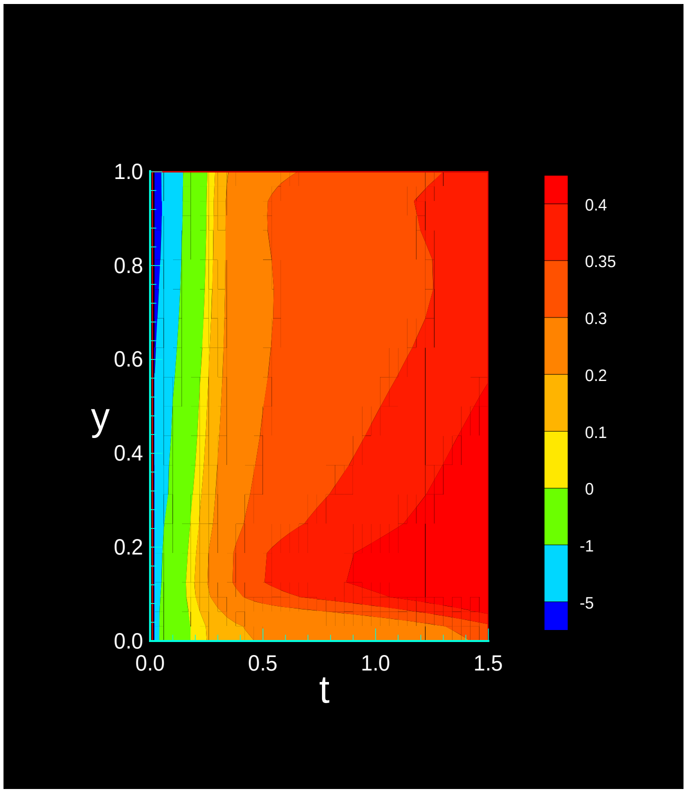


Kurz and Fisher (1984)

Violation of the a-priori assumption of stable growth!!

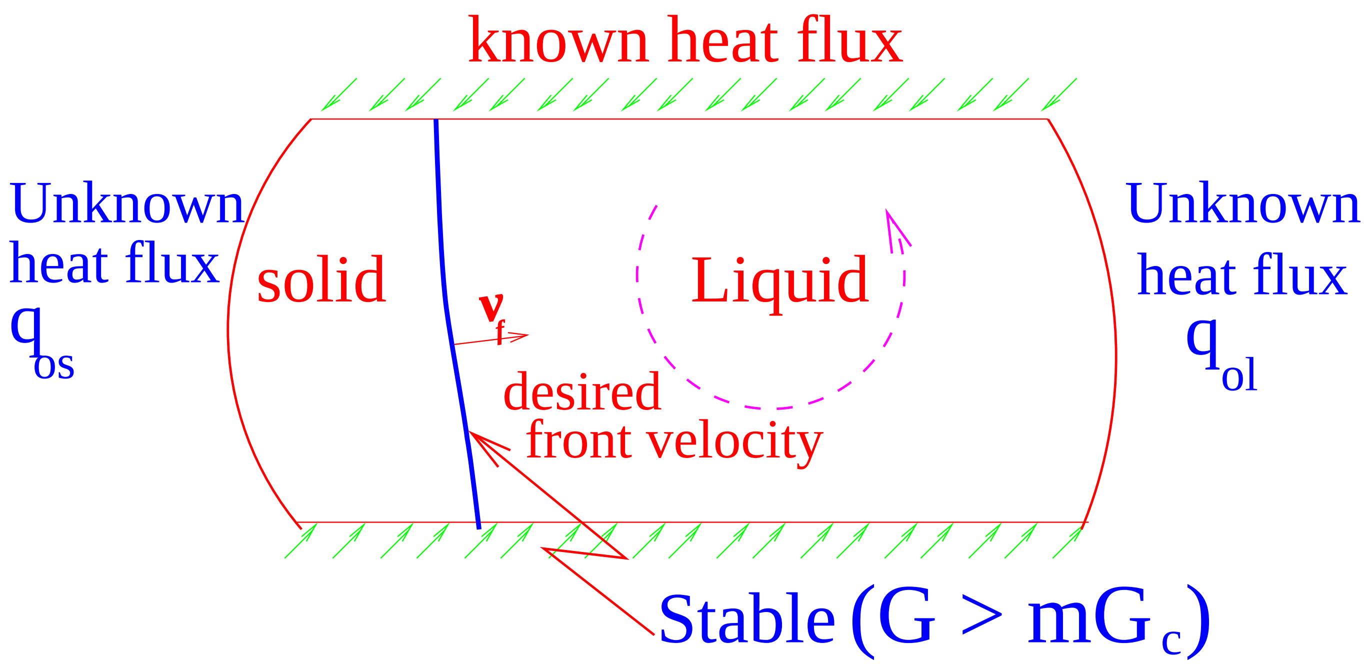
The solution of the reference design problem violates the constitutional stability criterion

$G > mG_c$ - Kurz and Fisher (1984)



Only a small region to the left is stable

Inverse binary alloy solidification under stable desired growth conditions



Recast the inverse design problem as:

"Find the 'cooling conditions' at Γ_{os} *as well as* the 'heating conditions' at Γ_{ol} such that a *desired growth* is achieved that is ensured to be *constitutionally stable*"

Enforcement of the stability constraint

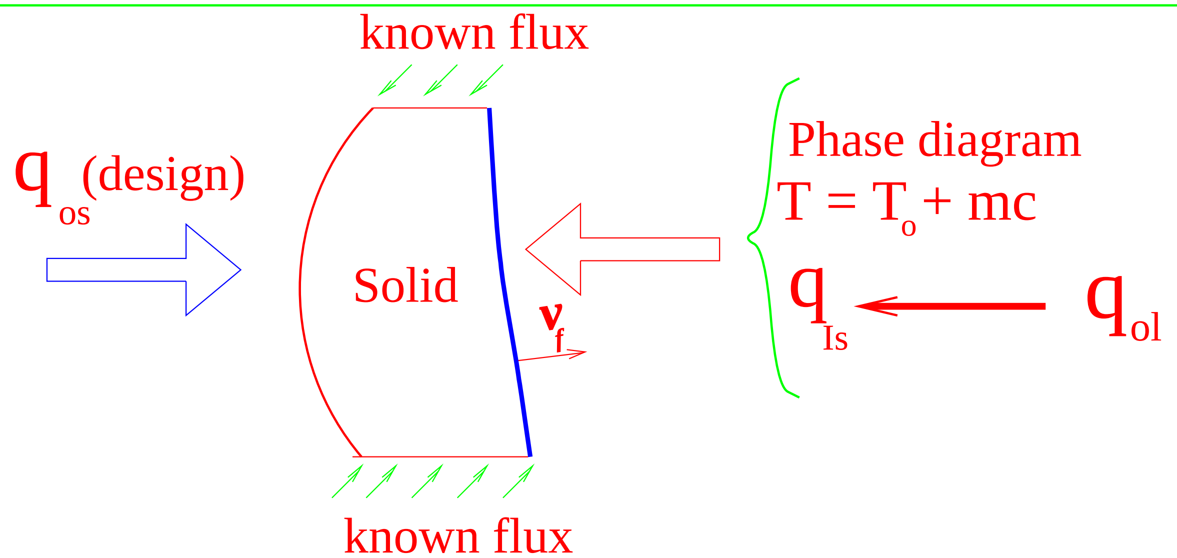
- Stability condition is enforced as follows:

$$G > mG_c \quad \longrightarrow \quad G = mG_c + \varepsilon(y,t)$$

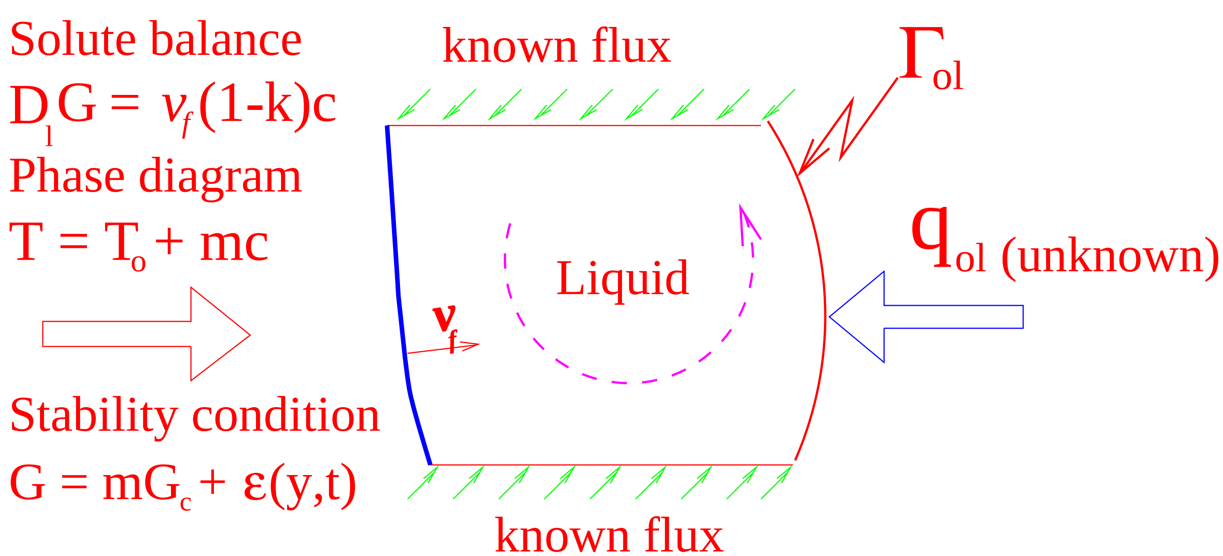
- The "over-stability" parameter $\varepsilon(y,t)$ is here chosen so as to ‘minimize’ the energy input to the system

$$\varepsilon(y,t) = -\, m\,\delta(1\text{-}k)\; v_f\, c_o/D_l,\;\; \delta \rightarrow 0$$

Decompose into two sub-inverse problems



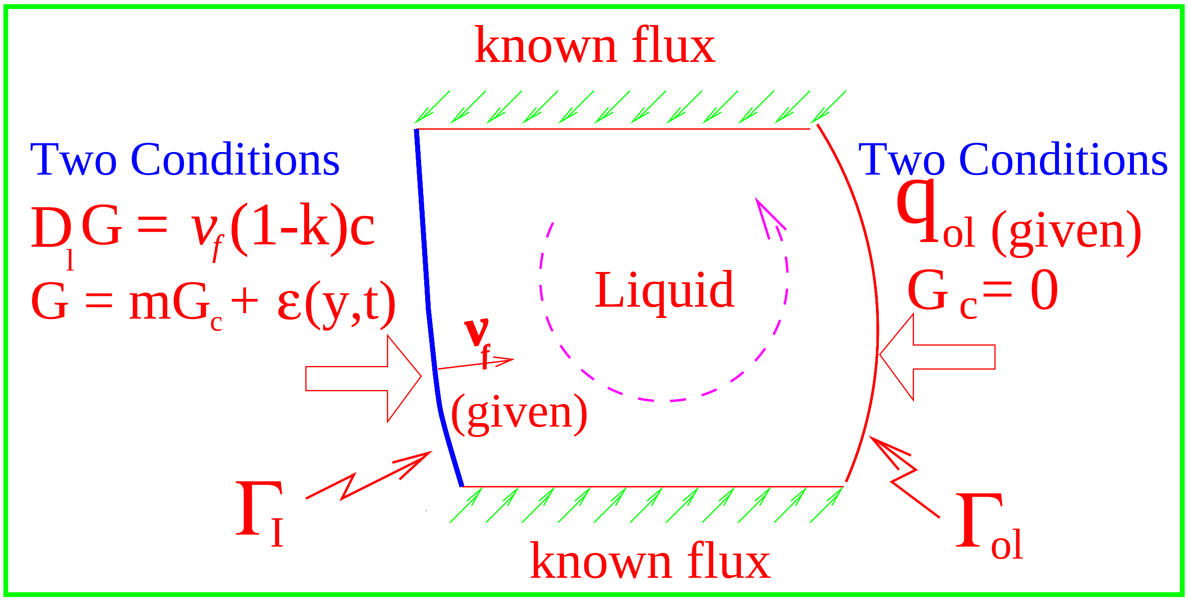
Solid: Inverse heat conduction problem



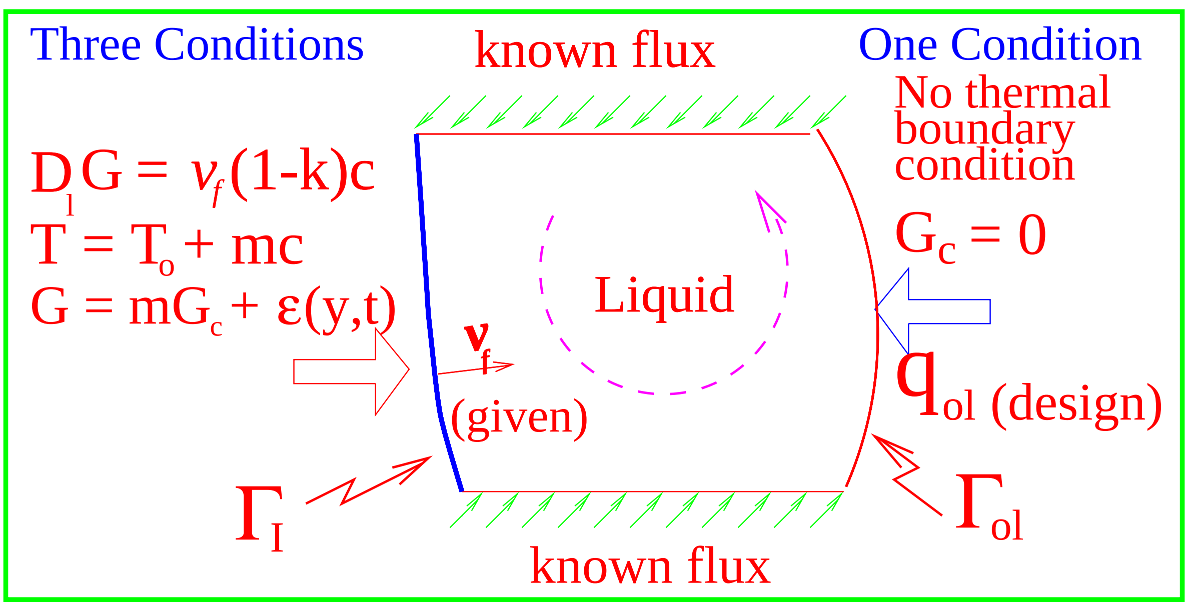
Liquid: Inverse design with coupled heat, flow and mass transport

Direct versus Inverse Thermo-solutal Convection problem

"Well -Posed Direct Problem"

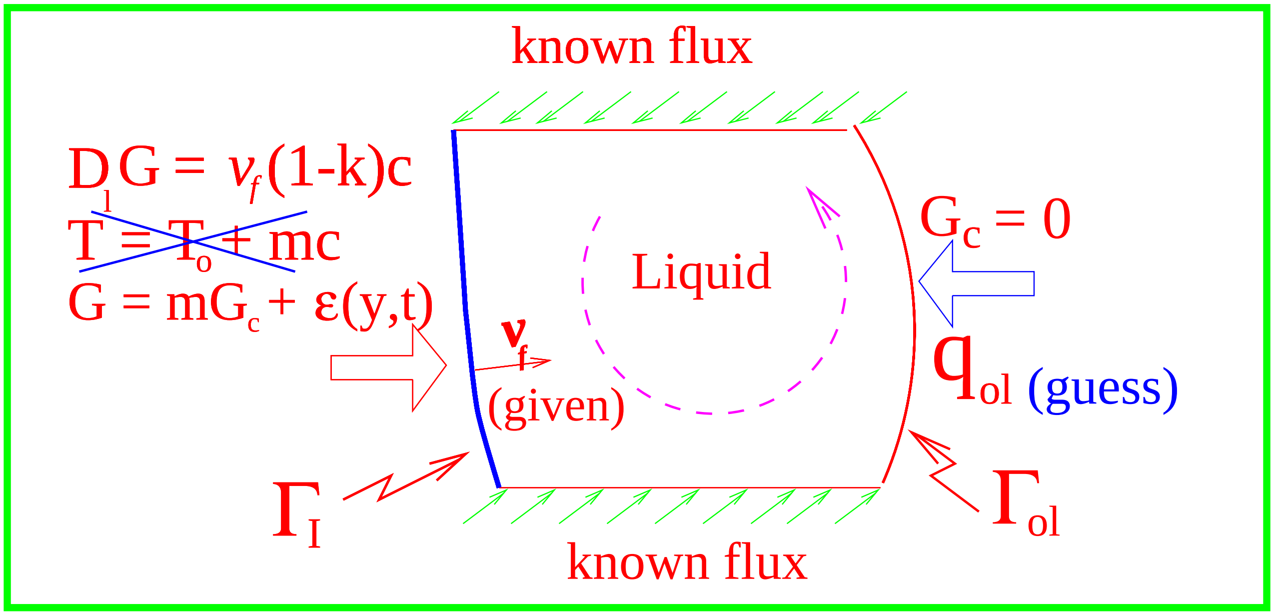


"Ill-Posed Inverse Problem"



Inverse design thermo-solutal convection problem

- With a *guessed heat flux* and without using the equilibrium condition solve the following direct problem



- Define the cost functional as a measure of deviation from thermodynamic equilibrium :

$$S(q_{ol}) = \frac{1}{2}\int_0^{t_{max}}\int_{\Gamma_I}\Big[T(\mathbf{x}, t; q_{ol}) - [T_m + mc(\mathbf{x}, t; q_{ol})]\Big]^2 d\Gamma\, dt$$

Inverse design thermo-solutal convection problem

- Define the inverse problem in the liquid domain in a minimization sense:

Find a *quasi solution* $\bar{q}_{ol} \in L_2(\Gamma_{ol} \times [0, t_{max}])$ such that :

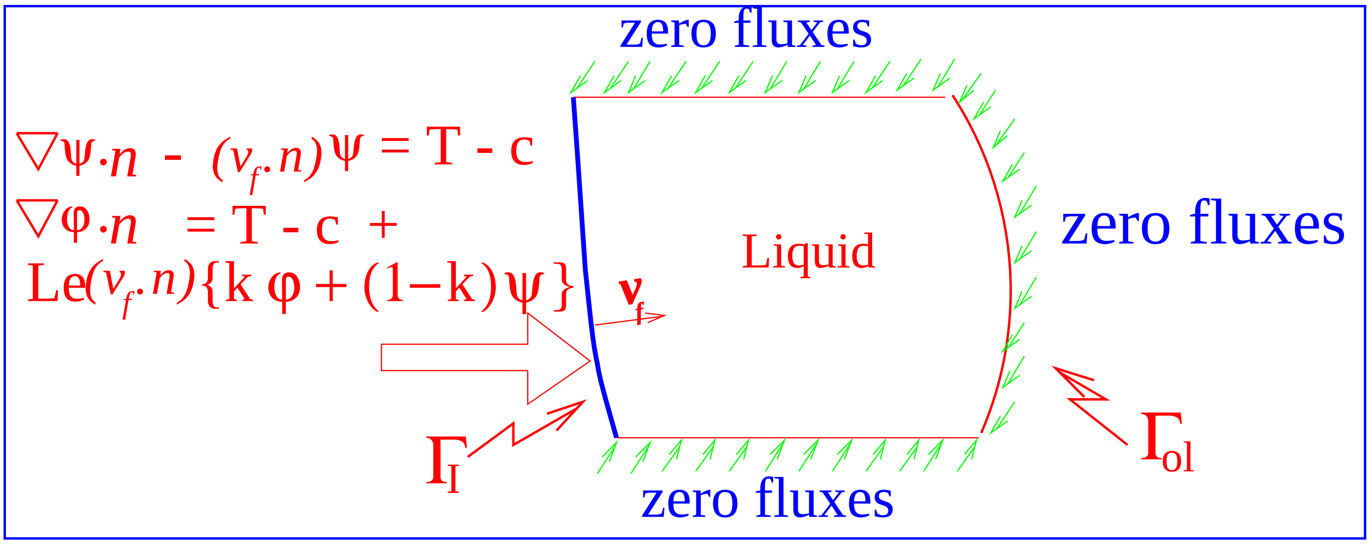
$$S(\bar{q}_{ol}) \leq S(q_{ol}) \quad \forall \quad q_{ol} \in L_2(\Gamma_{ol} \times [0, t_{max}])$$

- Solve the above minimization problem using the Conjugate Gradient method

Needs Gradient Information → Adjoint Problem

The adjoint problem

Gradient: $S'(q_{ol}) = \psi(\boldsymbol{x}, t; q_{ol})$ on Γ_{ol}



Definition of adjoint fields : $\phi(\boldsymbol{x}, t; q_{ol})$, $\psi(\boldsymbol{x}, t; q_{ol})$, $\varphi(\boldsymbol{x}, t; q_{ol})$

$$\frac{\partial \psi}{\partial t} + \boldsymbol{u} \cdot \nabla \psi = -\nabla^2 \psi + \boldsymbol{\phi} \cdot \boldsymbol{e_g}$$

$$\frac{\partial \varphi}{\partial t} + \boldsymbol{u} \cdot \nabla \varphi = -Le^{-1} \left[\nabla^2 \varphi + \frac{\gamma Ra_C}{Ra_T} \boldsymbol{\phi} \cdot \boldsymbol{e_g} \right]$$

$$\frac{\partial \boldsymbol{\phi}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{\phi} - [\nabla \boldsymbol{u}]^T \boldsymbol{\phi} = -Pr \nabla^2 \boldsymbol{\phi} - \nabla \pi + Pr\, Ra_T \left[\psi \nabla T - Le \varphi \nabla c \right]$$

$$\nabla \cdot \boldsymbol{\phi} = 0$$

$$\psi(\boldsymbol{x}, t_{max}; q_o) = \boldsymbol{\phi}(\boldsymbol{x}, t_{max}; q_o) = \varphi(\boldsymbol{x}, t_{max}; q_o) = 0$$

$$\frac{\partial \psi}{\partial n} - (\boldsymbol{v}_f \cdot \boldsymbol{n}) \psi = T - c, \quad (\boldsymbol{x}, t) \in \Gamma_I \times [0, t_{max}]$$

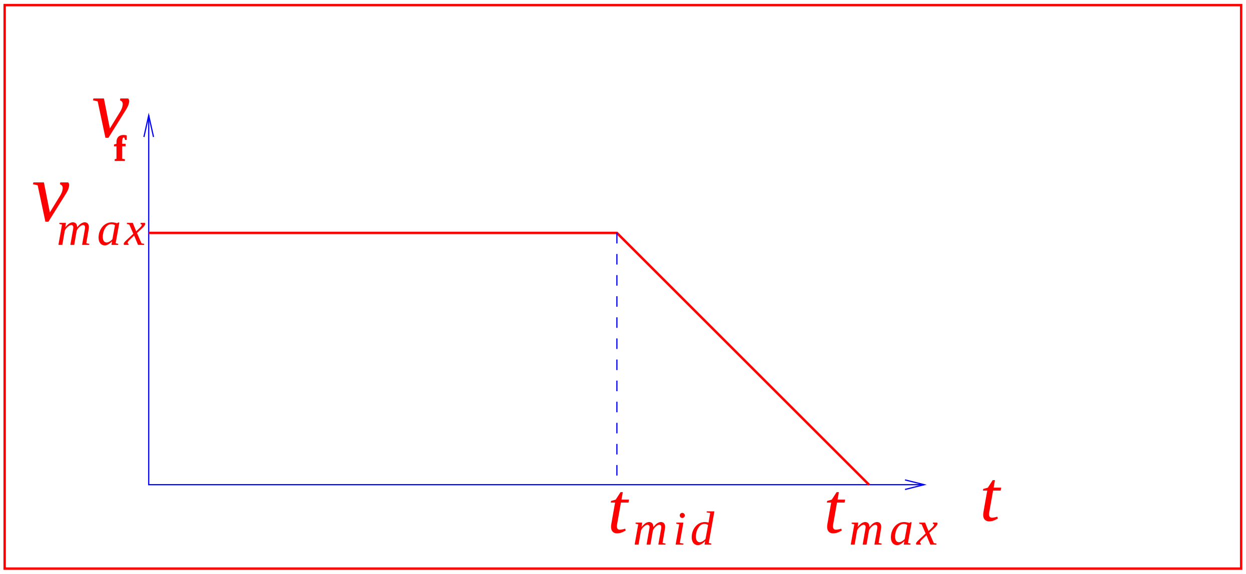
$$\frac{\partial \varphi}{\partial n} = Le(\boldsymbol{v}_f \cdot \boldsymbol{n}) [k \varphi + (1-k) \psi] + T - c, \quad (\boldsymbol{x}, t) \in \Gamma_I \times [0, t_{max}]$$

$$\frac{\partial \psi}{\partial n} = 0, \ \frac{\partial \varphi}{\partial n} = 0, \quad (\boldsymbol{x}, t) \in (\Gamma_{o\ell} \cup \Gamma_{h\ell}) \times [0, t_{max}]$$

$$\boldsymbol{\phi} = 0, \quad (\boldsymbol{x}, t) \in \Gamma_\ell \times [0, t_{max}]$$

Numerical Example

- Solidification of NH_4Cl - H_20 (1.5 wt% and overheat of 20^oC)
- Design to achieve "a flat desired interface growth"
- The prescribed front velocity is chosen as shown below:



Non-dimensionalization and parameters

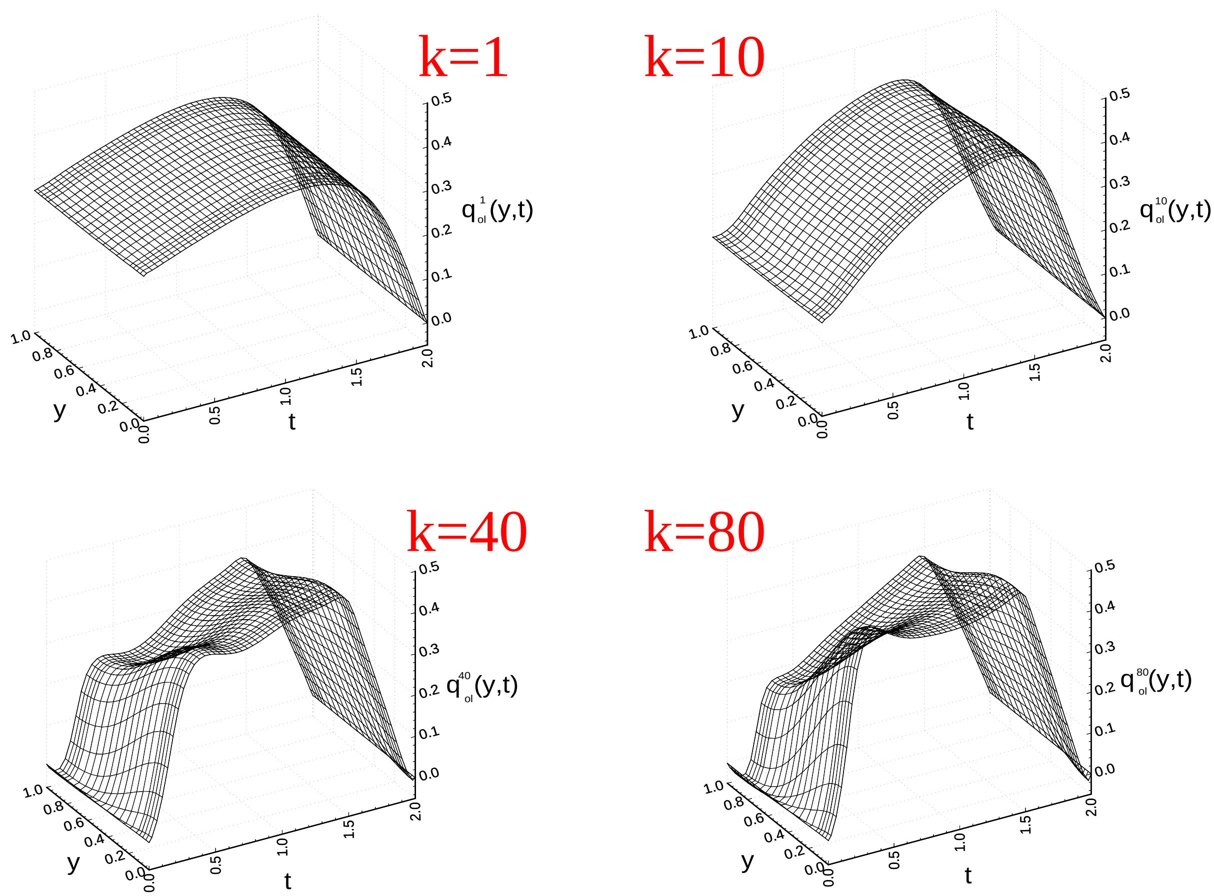
$$\bar{x} = x/L,\ \bar{t} = \alpha_l t/L^2,\ T_{ref} = T_o - mc_o$$

$$\bar{T} = \frac{T - T_{ref}}{T_i - T_{ref}},\ \bar{u} = \frac{uL}{\alpha_l},\ \bar{c} = \frac{c_o - c}{\gamma c_o}$$

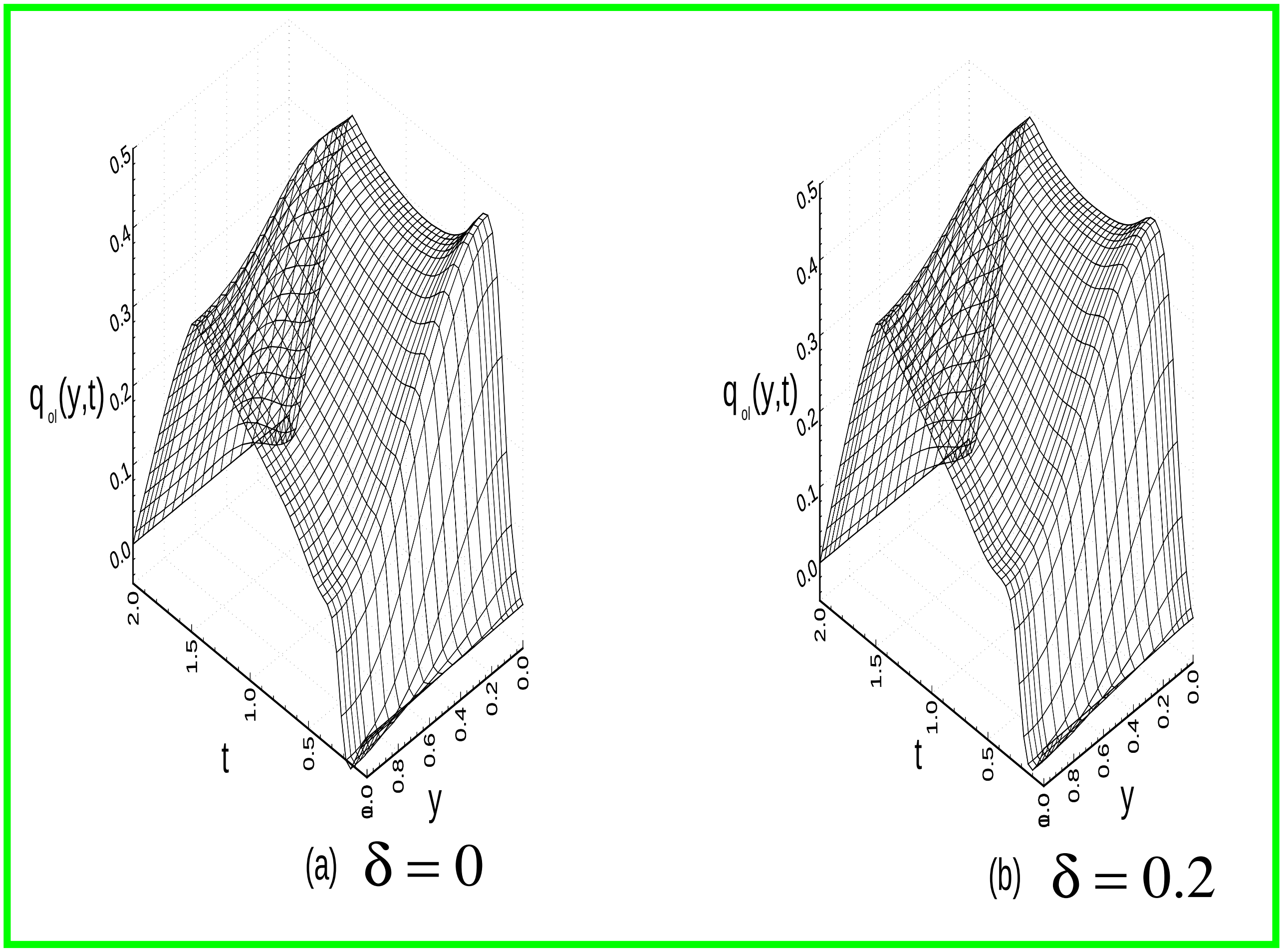
Parameter	Definition	Value
Prandtl number	ν/α_l	9.025
Lewis number	α_l/D_l	27.845
Partition ratio	c_s/c_l	0.3
Initial overheat	$(T_i - T_o)/mc_o + 1$	18.152
Thermal Rayleigh number	$g\beta_T \Delta T L^3/\nu\alpha_l$	2.0×10^4
Solutal Rayleigh number	$g\beta_c \Delta c L^3/\nu\alpha_l$	1.0×10^4

Heat flux solutions at intermediate iterations

* The temporal features are captured early whereas the spatial variation needs more iterations

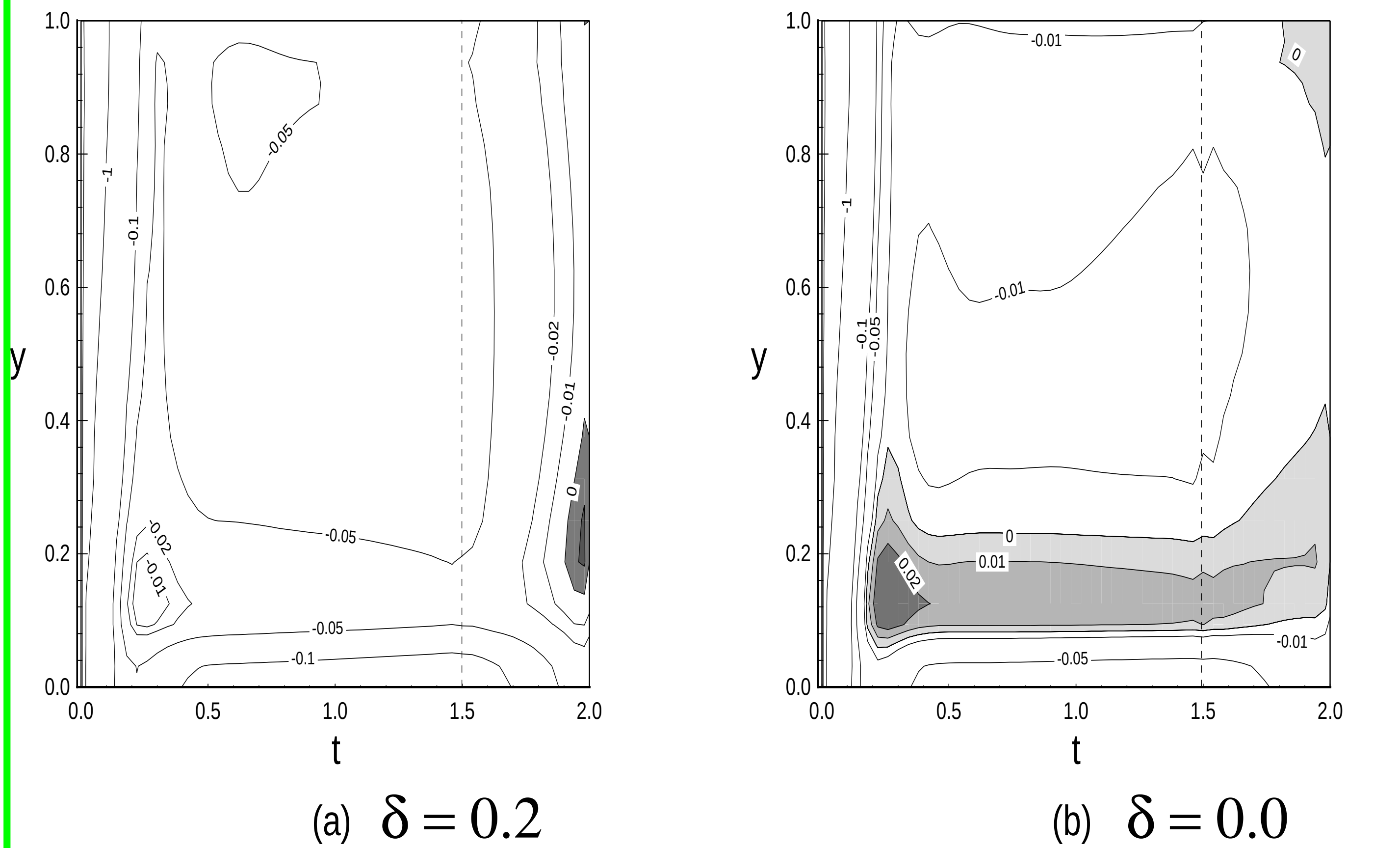


Inverse design optimal solution: $\bar{q}_{ol}$



- Requires heating flux at the liquid side with greater heating at the base than at the top
- More energy input is needed as "over-stable" parameter (δ) increases

Interface stability validation of the inverse solution

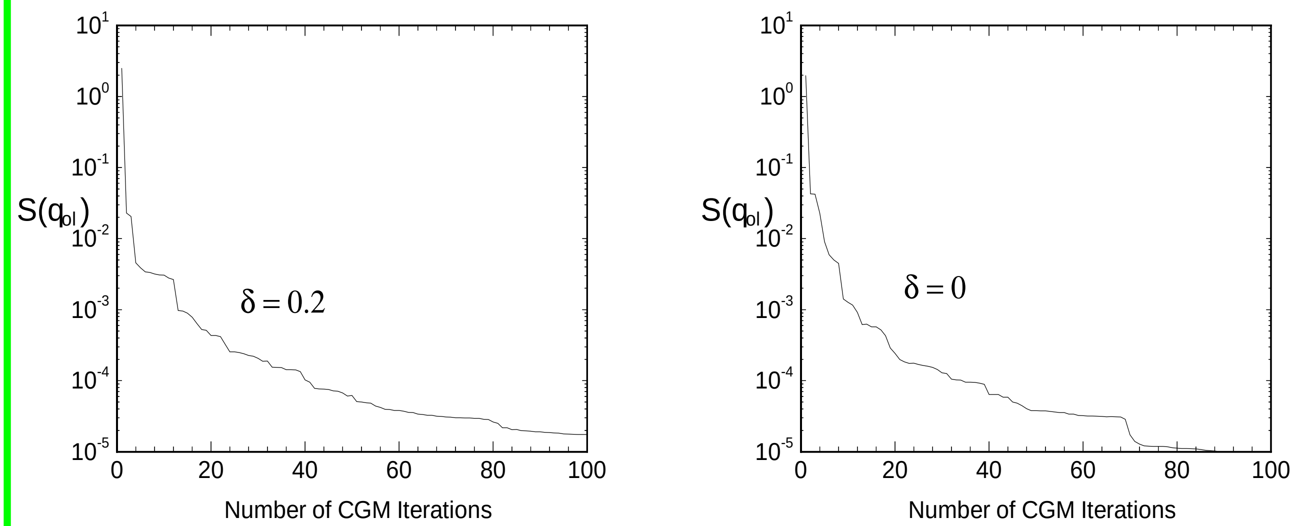


(a) $\delta = 0.2$ (b) $\delta = 0.0$

* The case $\delta = 0$ leads to an unstable process

* $\delta > 0$ is thus necessary to maintain stability during the "whole" process

Convergence of the inverse design algorithm



* Rapid drop in the cost functional initially but slower at later steps

* Convergence is better for lower values of δ

Determination of the solid side heat flux q_{os}

Additional Parameters

Inverse problem in the liquid

q_{ol}

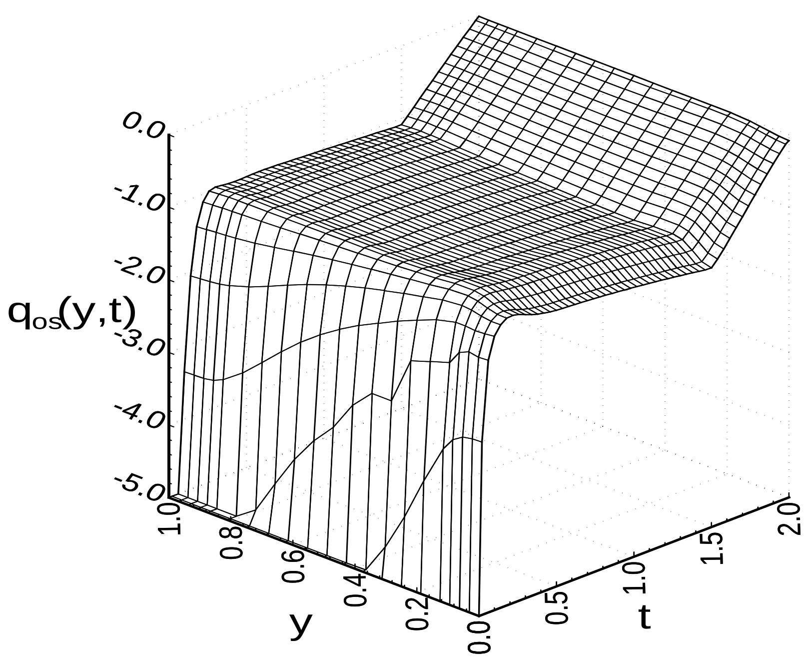
Inverse problem in the solid

$R_k = 1$

$R_\alpha = 1$

$Ste = 0.3$

q_{os}



Salient features and limitations

Salient features :

- ☆ New innovative adjoint technique to control binary alloy solidification systems
- ☆ Control parameters chosen based on factors governing the formation of microstructures
- ☆ Enforces stability to ensure physically valid results

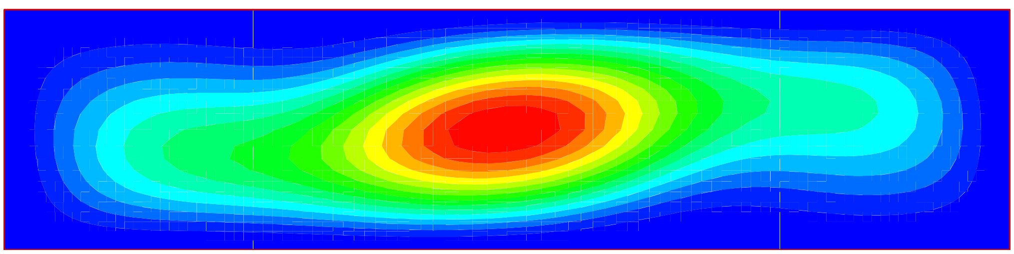
Limitations :

- ☆ Industrial implementation of optimal heat flux solution is quite challenging
- ☆ Only a "quasi solution" is guaranteed
- ☆ The "optimal solution" may lead to side effects that are undesirable

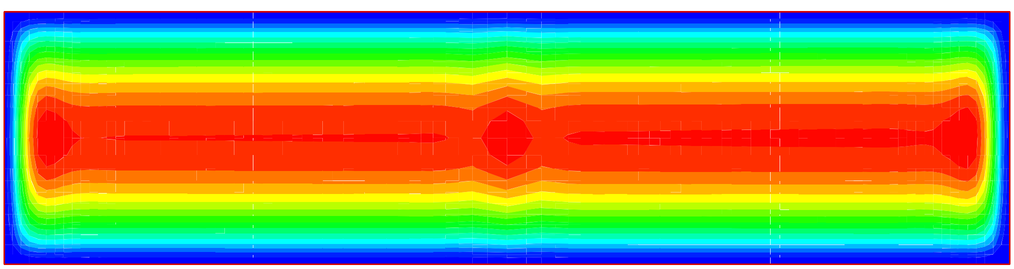
Forthcoming developments

Thermo-Electromagnetic control:

☆ The presence of a strong magnetic field effectively damps the melt flow



Ha = 0, Ψ_{max} = 0.55

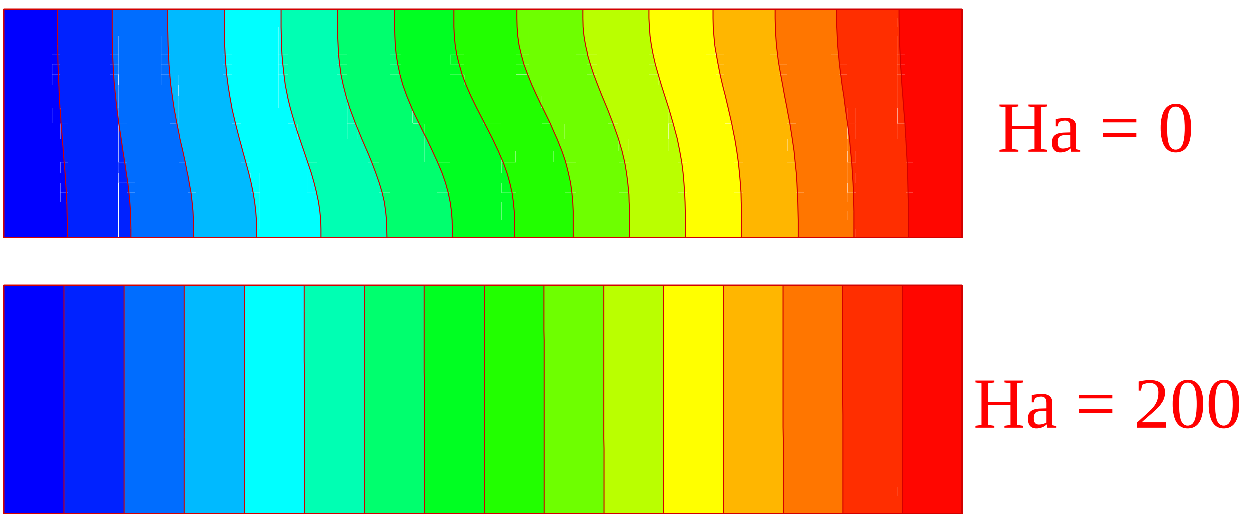


Ha = 200, Ψ_{max} = 0.00063

Stream function plot showing distinct drop in flow circulation

Forthcoming developments

☆ Magnetic control can make the optimal heat flux solutions smoother as the damping of the flow reduces the curving of the interface.



Curved isotherms get flatter with increasing Hartmann number

☆ Due to magnetic damping we can expect to have lesser solute variation in the crystal