COMPUTATIONAL TECHNIQUES FOR THE ANALYSIS AND DESIGN OF OPEN-BOAT DIRECTIONAL SOLIDIFICATION PROCESSES

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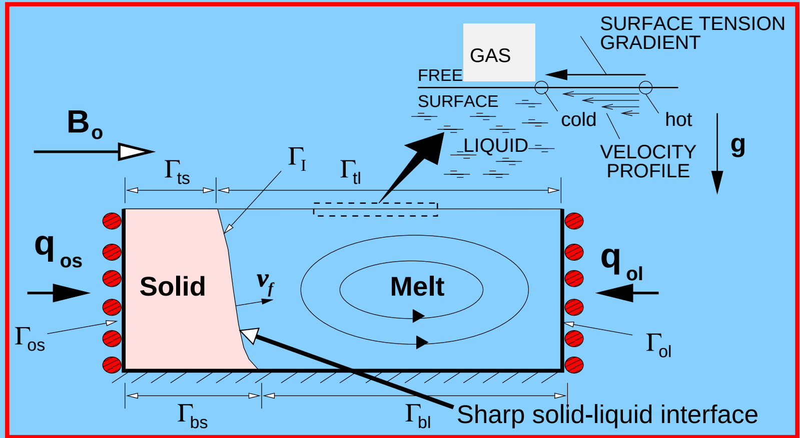
DIRECTIONAL SOLIDIFICATION OF A BINARY ALLOY DRIVEN BY BUOYANCY, SURFACE TENSION, AND ELECTROMAGNETIC FORCES



GOVERNING PHYSICS

SOLID

- Heat conduction

MELT

- Heat and solute transport
- Incompressibility
- Navier-Stokes equation with Lorentz and buoyancy body force terms
- Traction force on free surface due to surface tension variation

SOLID-LIQUID INTERFACE

- Interfacial heat and solute balance
- Local thermodynamic equilibrium conditions

FINITE ELEMENT SOLUTION METHODS

- SUPG/PSPG fluid flow formulation with additional terms from buoyancy, surface tension, and electromagnetic forces
- Consistent SUPG formulation for transport equations
- Moving/deforming FEM to explicitly track the advancing solid-liquid interface
- Predictor-corrector scheme for time integration of heat and solute transport equations
- T1 formulation for time integration of flow equations
- Mass lumping and LU-factorized preconditioner to improve the computational performance of various algorithms
- A preconditioned stabilized bi-conjugate gradients method (Bi-CGSTAB) for the solution of linear systems at each step
- Object-oriented programming (OOP) techniques for efficient implementation of various solution schemes

DETRIMENTAL ROLE OF CONVECTION AND PROPOSED MEANS FOR CONTROLLING ITS EFFECTS ON THE SOLIDIFIED CRYSTAL

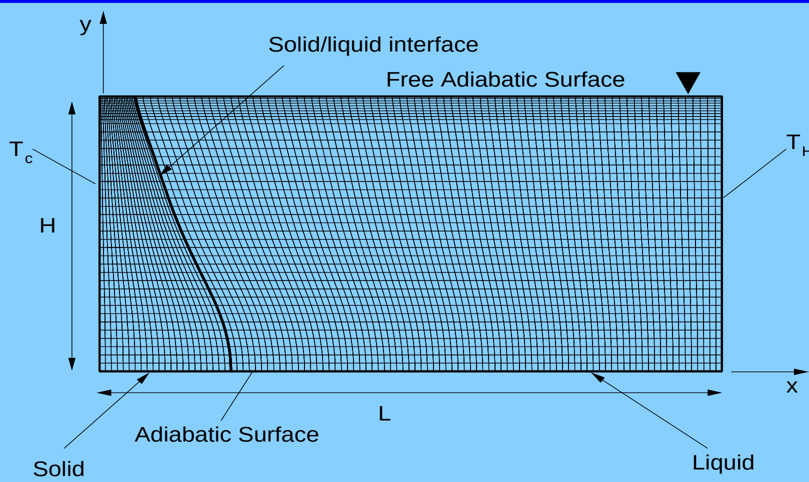
INFLUENCE OF COUPLED THERMOCAPILLARY AND BUOYANCY DRIVEN CONVECTION ON THE SOLIDIFICATION SYSTEM

- Coupled capillary and buoyancy forces increase the strength of melt convection leading to more distorted solid-liquid interface
- Transition to unsteady behaviour is hard to control due to the presence of capillary convection
- Buoyancy and thermocapillary forces can couple in a complicated manner leading to hydrodynamic instabilities
- Complex fluid flow pattern in the melt leads to solute variation on macro and micro scales resulting in poor crystal quality

SALIENT FEATURES OF THE CURRENT SOLIDIFICATION DESIGN STUDY

- Parametric preliminary design study to understand the effects of gravity and magnetic field on convection in the solidification system
- Formulation and implementation of a mathematically rigorous inverse design method for achieving "diffusion-based stable growth" in the presence of melt convection through application of optimal boundary thermal fluxes
- Simultaneous application of a strong magnetic field in order to suppress melt flow and thus help in achieving the design goals

DIRECT SOLIDIFICATION STUDY - REFERENCE PROBLEM



MATERIAL SYSTEM

Germanium melt with minute amounts of Antimony dopants

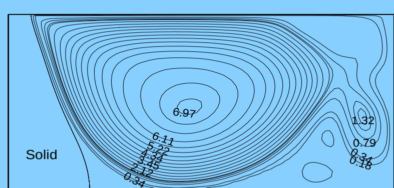
FINITE ELEMENT MESH

Solid: 880 bi-linear elements
943 nodes

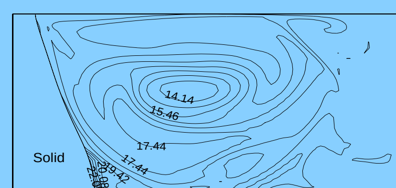
Melt: 3200 bi-linear elements
3321 nodes

GROWTH CONDITIONS

Normal gravity
No applied magnetic field

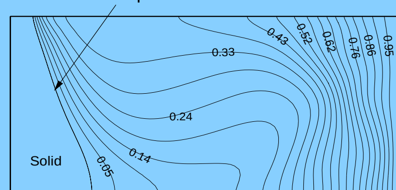


FLOW FIELD



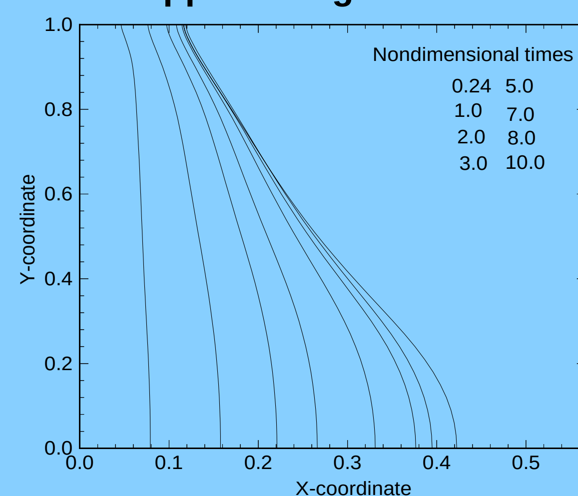
CONCENTRATION

solid/liquid interface



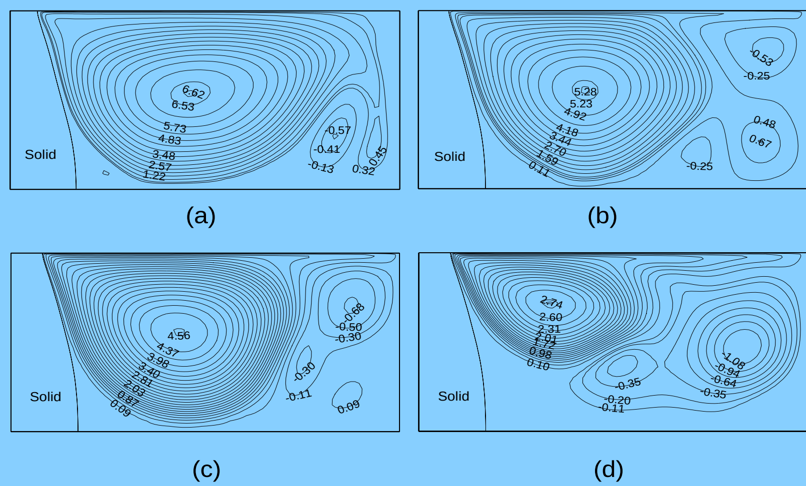
TEMPERATURE

Continuum fields at dimensionless time $\tau = 1$ (55.0 s)



Predicted solid-liquid interface locations at intermediate times

PARAMETRIC STUDY: EFFECTS OF VARYING GRAVITY AND MAGNETIC FIELD CONDITIONS ON THE REFERENCE SOLIDIFICATION PROBLEM



EFFECTS OF VARYING GRAVITY LEVELS

Streamlines at time t = 27.5 s for growth under varying gravity levels and zero magnetic field

(a) 0.5 g_{earth} (c) 0.01 g_{earth}

(b) 0.1 g_{earth} (d) 10^{-5} g_{earth}

EFFECTS OF VARYING MAGNETIC FIELD STRENGTH

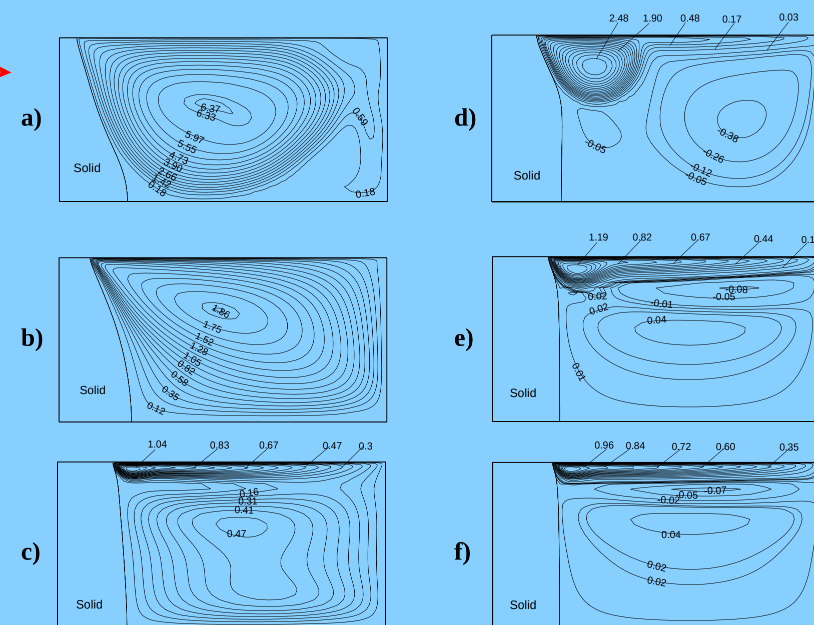
Streamlines at time t = 55 s for growth under the influence of an external magnetic field applied along the positive x-direction

Growth under normal gravity conditions

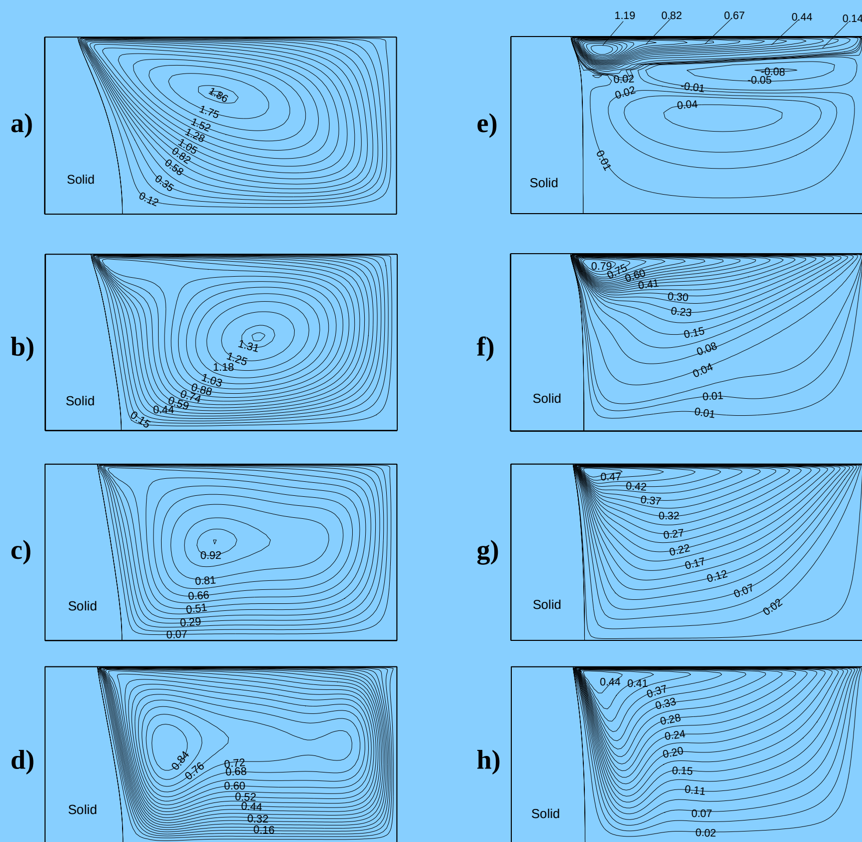
(a) B_o = 5 G (b) B_o = 50 G (c) B_o = 100 G

Growth under reduced gravity conditions (g = 10^{-5} g_{earth})

(d) B_o = 5 G (e) B_o = 50 G (f) B_o = 100 G



PARAMETRIC STUDY: EFFECTS OF VARYING GRAVITY AND MAGNETIC FIELD CONDITIONS ON THE REFERENCE SOLIDIFICATION PROBLEM



EFFECTS OF VARYING THE MAGNETIC FIELD ORIENTATION

Streamlines at time t = 55 s for solidification under the influence of an imposed horizontal magnetic field (B_o = 50 G) at various magnetic field inclinations

Growth under normal gravity conditions

(a) along the x-axis (b) 30^occw to x-axis
(c) 60^occw to x-axis (d) along the y-axis

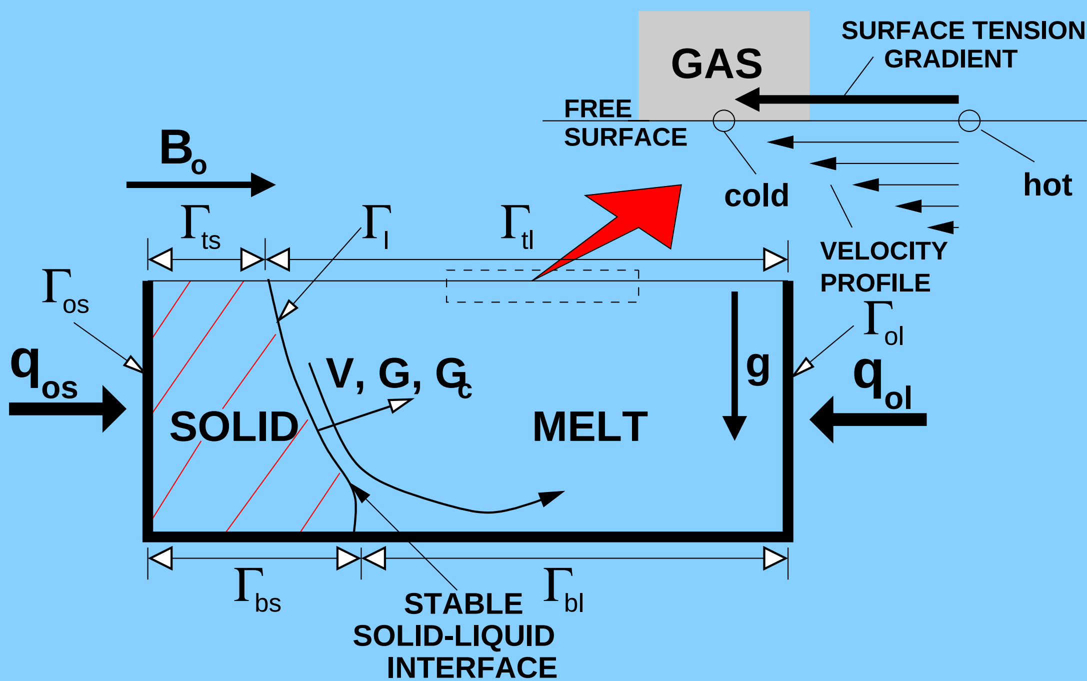
Growth under reduced gravity conditions ($g = 10^{-5} g_{earth}$)

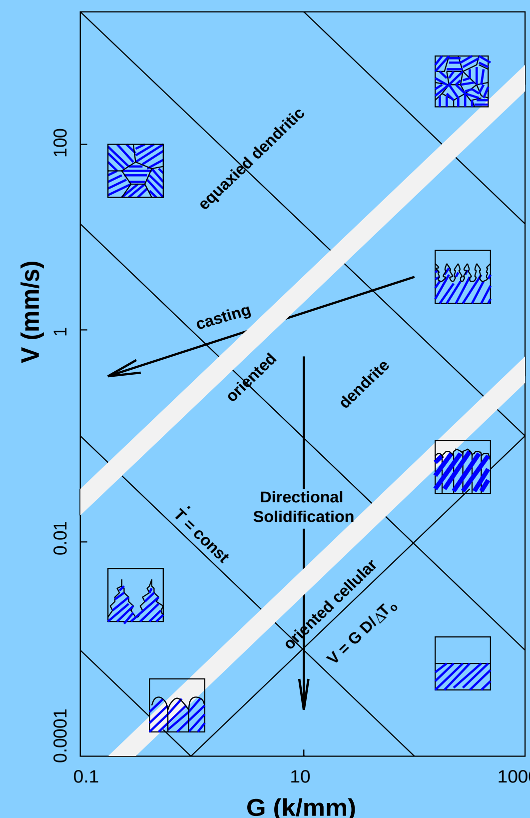
(e) along the x-axis (f) 30^occw to x-axis
(g) 60^occw to x-axis (h) along the y-axis

COUPLING THIS PARAMETRIC DESIGN WITH INVERSE THERMAL DESIGN

PARAMETRIC DESIGN APPROACH SUCH AS THE ONE ILLUSTRATED HERE CAN BE VERY EFFECTIVE AND COST-EFFICIENT IN CHOOSING APPROPRIATE MAGNETIC FIELD AND GRAVITY CONDITIONS, WHICH IN COMBINATION WITH OPTIMAL BOUNDARY HEAT FLUXES CAN LEAD TO DESIRED STABLE GROWTH CONDITIONS

THERMAL DESIGN OF STABLE BINARY EUTECTIC ALLOY SOLIDIFICATION PROCESSES WITH DESIRED G/V STATE

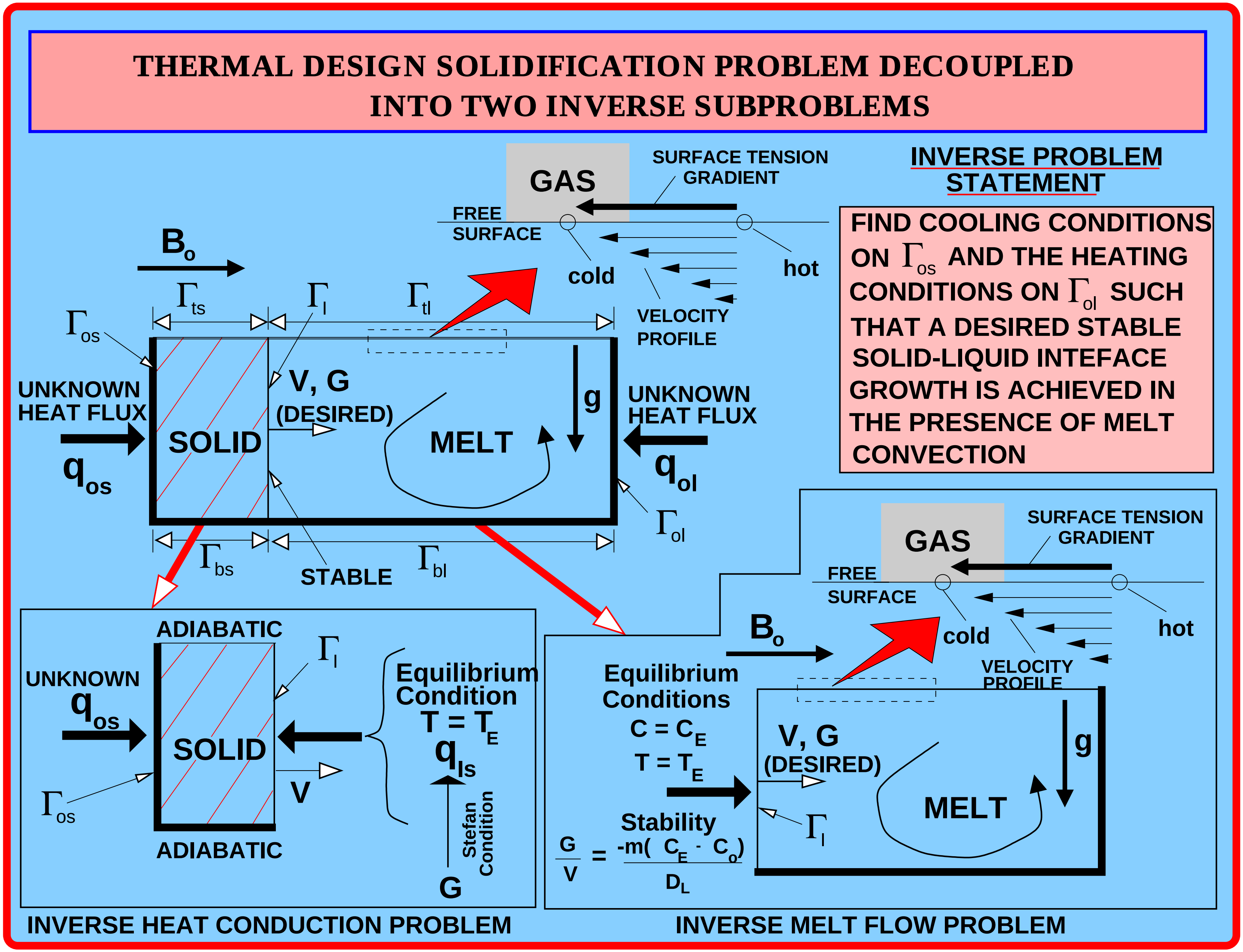




DESIGN OBJECTIVES

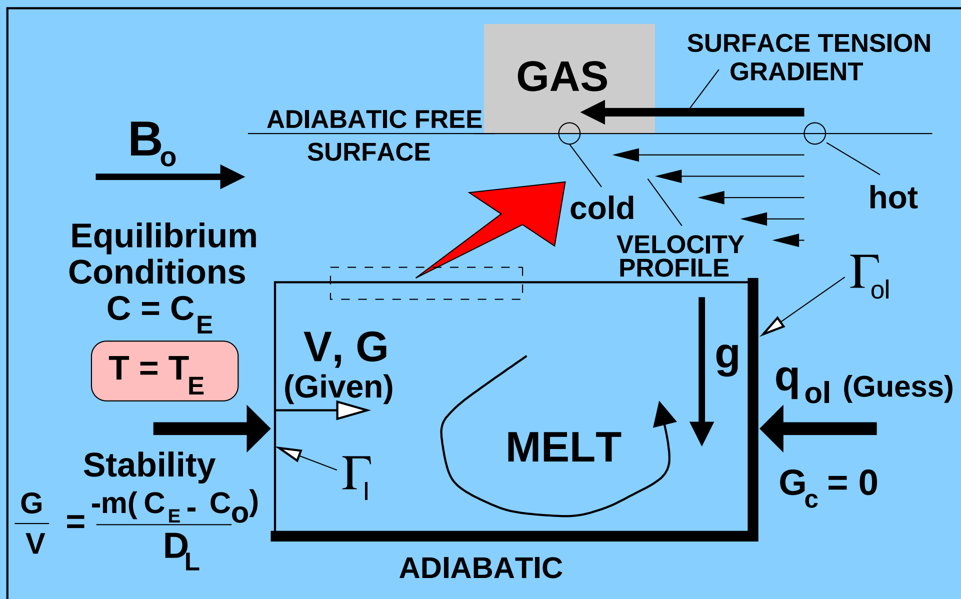
" Find the optimal solid side flux q_{os} *and the liquid side flux* q_{ol} *such that, in the presence of coupled thermocapillary, buoyancy, and electromagnetic convection in the melt, a flat solid-liquid interface with desired flux G and velocity V is achieved that is ensured to be morphologically stable"*

Thermal gradient (G) and growth velocity (V) are the main parameters that set the form and scale of cast microstructures



THERMAL DESIGN SOLIDIFICATION PROBLEM DECOUPLED INTO TWO INVERSE SUBPROBLEMS
INVERSE PROBLEM STATEMENT
FIND COOLING CONDITIONS ON Γos AND THE HEATING CONDITIONS ON Γol SUCH THAT A DESIRED STABLE SOLID-LIQUID INTEFACE GROWTH IS ACHIEVED IN THE PRESENCE OF MELT CONVECTION
GAS
SURFACE TENSION GRADIENT
FREE SURFACE
cold
hot
VELOCITY PROFILE
Bo
Γts
Γl
Γtl
Γos
UNKNOWN HEAT FLUX
qos
SOLID
V, G
(DESIRED)
MELT
g
UNKNOWN HEAT FLUX
qol
Γol
Γbs
STABLE
Γbl
ADIABATIC
UNKNOWN
qos
SOLID
Γl
V
Γos
ADIABATIC
Equilibrium Condition
T = TE
qls
Stefan Condition
G
INVERSE HEAT CONDUCTION PROBLEM
GAS
SURFACE TENSION GRADIENT
FREE SURFACE
cold
hot
VELOCITY PROFILE
Bo
Equilibrium Conditions
C = CE
T = TE
V, G
(DESIRED)
MELT
g
Γl
Stability
G/V = -m(CE - Co)/DL
INVERSE MELT FLOW PROBLEM

INVERSE PROBLEM IN THE MELT INCLUDING EFFECTS OF THERMOCAPILLARY, BUOYANCY, AND ELECTROMAGNETIC FORCES



With a guessed heat flux q_{ol} and without using the temperature boundary condition on Γ_I, solve the following direct problem for the temperature field $T(x, t; q_{ol})$, the concentration field $c(x, t; q_{ol})$, and the velocity field $v(x, t; q_{ol})$

Next, define the cost functional as follows:

$$J(q_{ol}) = \frac{1}{2}\left\| T(x, t, q_{ol}) - T_E \right\|^2_{L_2(\Gamma_I \times [0, t_{max}])} + \frac{\gamma}{2}\left\{ \left\| q_{ol} \right\|^2_{L_2(\Gamma_{ol} \times [0, t_{max}])} + \left\| \nabla q_{ol} \right\|^2_{L_2(\Gamma_{ol} \times [0, t_{max}])} \right\}$$

Measure of deviation from thermodynamic equilibrium

H^1 Regularization terms

NONLINEAR OPTIMIZATION APPROACH TO THE INVERSE MELT CONVECTION PROBLEM

- **Define the inverse convection problem in the melt as a unconstrained spatio-temporal optimization problem**

Find a quasi-solution $\bar{\mathbf{q}}_{ol} \in \mathbf{L}_2(\Gamma_{ol} \times [0, t_{max}])$ **such that**

$$\mathbf{J}(\bar{\mathbf{q}}_{ol}) \leq \mathbf{J}(\mathbf{q}_{ol}) \quad \forall \quad \mathbf{q}_{ol} \in \mathbf{L}_2(\Gamma_{ol} \times [0, t_{max}])$$

- **Solve the above unconstrained minimization problem using the nonlinear Conjugate Gradient Method (CGM)**

Needs design gradient information

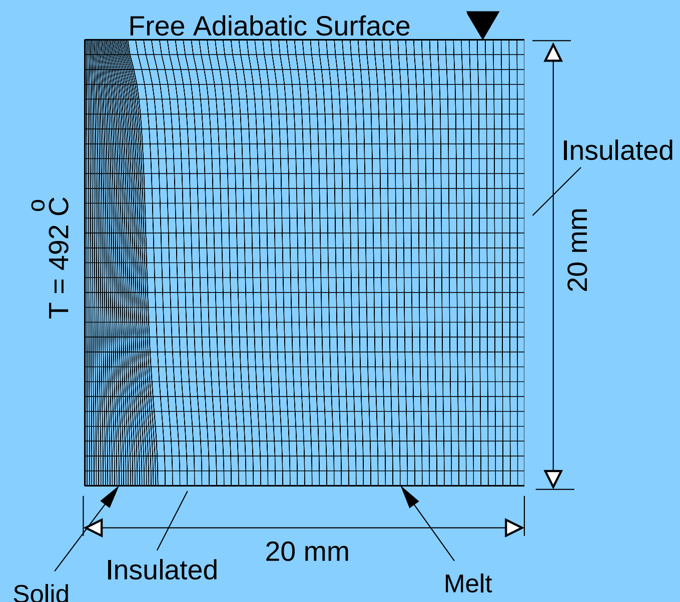
Needs descent step size

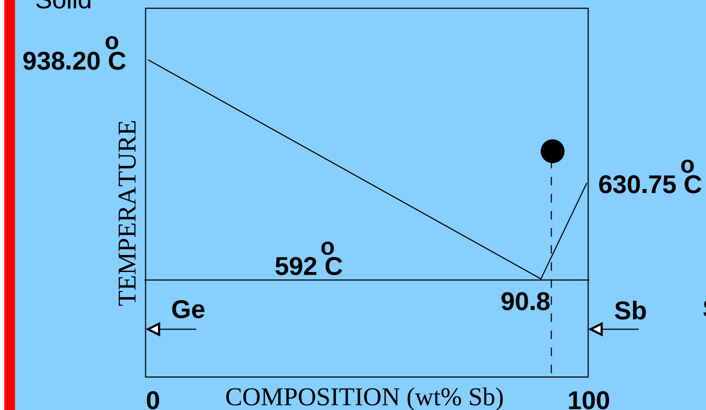
Continuum adjoint problem

Continuum sensitivity problem

NUMERICAL SOLIDIFICATION DESIGN EXAMPLE

REFERENCE BINARY ALLOY SOLIDIFICATION PROBLEM UNDER NORMAL GROWTH CONDITIONS (NORMAL GRAVITY, NO MAGNETIC FIELD)





FINITE ELEMENT MESH

Solid: 960 bi-linear elements
1023 nodes

Melt: 1500 bi-linear elements
1581 nodes

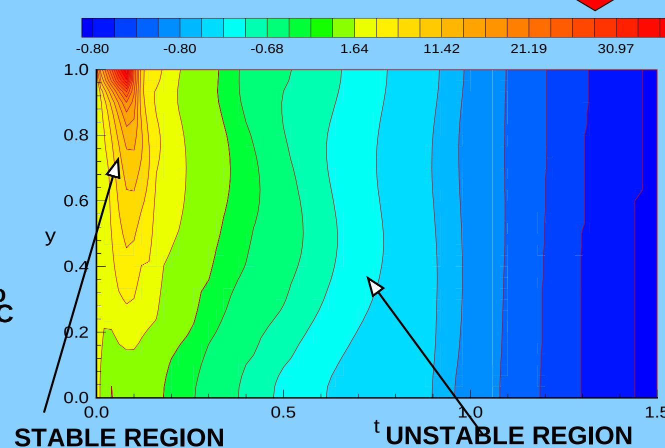
MATERIAL SYSTEM

Sb - 8.6% Ge (near-eutectic composition)

DIMENSIONLESS GROUPS

Prandtl number 0.017
Lewis number 319.0
Stefan number 0.1348
Solutal Rayleigh number 6.275e+04
Thermal Marangoni number -3982.02
Thermal Rayleigh number 1.644e+05

DIRECT FE SIMULATION → **POST PROCESS**



Examination of constitutional stability assumption on the solid-liquid interface

Dimensionless contours of

$$\boxed{\Delta = \frac{G}{V} + \frac{m}{D_L}(C_E - C_o)}$$

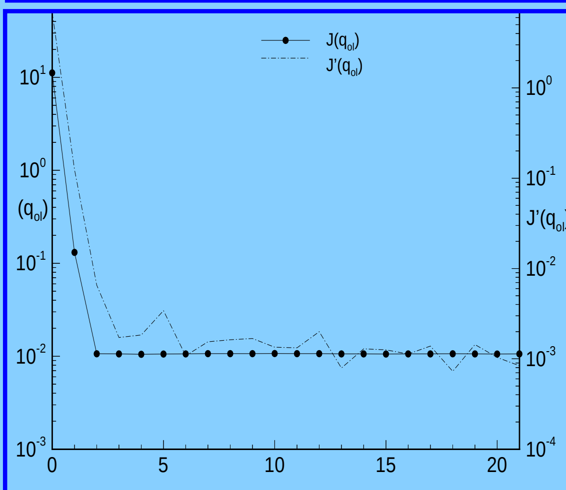
$\Delta < 0$ **corresponds to unstable growth**

THE WELL-POSED DIRECT SIMULATION RESULTS DO NOT SATISFY A-PRIORI ASSUMPTION OF STABILITY !

NUMERICAL SOLIDIFICATION DESIGN EXAMPLE

INVERSE SOLIDIFICATION PROBLEM TO ACHIEVE DIFFUSION-BASED STABLE GROWTH

Find the solid side optimal flux q_{os} as well as the liquid side optimal flux q_{ol} such that, in the presence of coupled thermocapillary, buoyancy, and electromagnetic convection in the melt, a stable interface growth with V corresponding to a diffusion-based problem and G/V corresponding to marginal stability is achieved

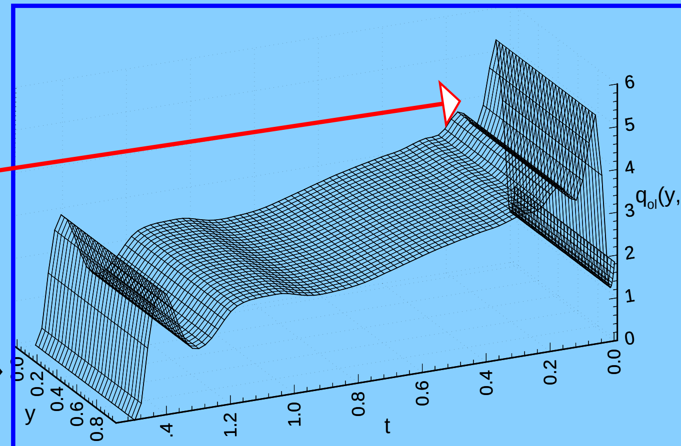


OBJECTIVE FUNCTION VARIATION FOR THE INVERSE PROBLEM IN MELT REGION

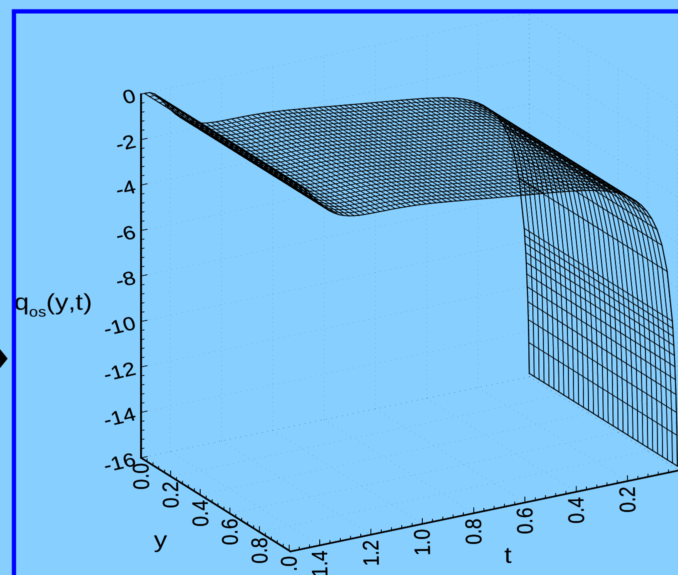
COUNTERACTS THE STRONG EFFECTS OF THERMOCAPILLARY FLOW AT EARLY TIMES

BASED ON THE RESULTS OF THE PARAMETRIC STUDIES REPORTED, A STRONG HORIZONTAL MAGNETIC FIELD WAS SELECTED IN ORDER TO FACILITATE THE THERMAL DESIGN PROCESS THROUGH DAMPING OF MELT FLOW

LIQUID SIDE OPTIMAL FLUX



SOLID SIDE OPTIMAL FLUX



FORTHCOMING RESEARCH EFFORTS

- Develop advanced numerical analysis tools to improve the performance of the computationally-taxing inverse problem solution in the melt region
- Improve the performance of the algorithms to address more complicated solidification systems with multiple length and time scales
- Develop inverse design methods to include the applied magnetic field (direction and magnitude) as an additional design variable
- Develop a computational framework for the design of solidification processes with continuum mushy zone solidification models

REFERENCES

- Yang, G. Z. and Zabaras, N. "The adjoint method for an inverse design problem in the directional solidification of a binary alloy", J. Comp. Phys., (1998) 432-452.
- Sampath, R. and Zabaras, N. "Inverse design of direction solidification processes in the presence of a strong magnetic field", Int. J. Numer. Methods Engr., (2000), in press
- Zabaras, N. "Adjoint methods for inverse free convection problems with applications to solidification processes", Computational Methods for Optimal Design and Control, (1998) 391-426.
- Yang, G. Z. and Zabaras, N. "An adjoint method for the inverse design of solidification processes with natural convection", Int. J. Numer. Methods Engr., (1998) 1121-1144.

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