THE ADJOINT METHOD FOR THE DESIGN OF DIRECTIONAL BINARY ALLOY SOLIDIFICATION PROCESSES IN THE PRESENCE OF A STRONG MAGNETIC FIELD

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OUTLINE OF THE PRESENTATION

- Ill-posed inverse thermal problems
- Directional solidification of a binary alloy
- Main objectives in solidification process control
- Various available means for control of casting microstructures
- Previous works on solidification process design

PRESENT STUDY

- Inverse magneto-convection problem
- Design of binary alloy solidification processes under the influence of external magnetic fields
- Design of two-dimensional binary eutectic solidification processes driven by buoyancy, surface-tension and electromagnetic forces

- Conclusions and suggestions
BACKGROUND: ILL-POSED INVERSE PROBLEMS

HISTORICAL PERSPECTIVE

- Hadamard (1902, 1923): Formal definition of well and ill-posed problem
  - Existence, Uniqueness and Stability
  Examples:
    (a) Backward heat conduction
    (b) Cauchy problem for Laplace equation

- Tikhonov (1950’s and 1960’s)
  Regularization using a-priori information

INVERSE HEAT CONDUCTION PROBLEMS

  - Sequential function specification method
  - Use of "future time information" for stabilization

- Alifanov et al (1980’s):
  - Finite dimensional optimization method
  - Whole time domain adjoint method
DIRECTIONAL SOLIDIFICATION OF A BINARY ALLOY

GOVERNING MATHEMATICAL PROBLEM

- Solid domain: Heat conduction
- Liquid domain: a) Heat conduction and convection  
  b) Solute diffusion and convection  
  c) Fluid flow
- Solid/liquid interface: Heat and solute balance

NOTE: The above well-posed problem may lead to unphysical results! Reason → Morphological instability
PHASE DIAGRAM AND CONSTITUTIONAL STABILITY

CONSTITUTIONAL STABILITY CRITERION FOR STABLE GROWTH

STABLE GROWTH

G > mG_c

SOLUTAL GRADIENT

THERMAL GRADIENT

G < mG_c

UNSTABLE GROWTH
MORPHOLOGICAL INSTABILITY AND FORMATION OF DENDRITIC MICROSTRUCTURE

- Violation of the constitutional stability criterion leads to an unstable solid-liquid interface
- Small perturbations to the solid-liquid interface are amplified leading to the formation of cells and dendrites

CELLS

COLUMNAR DENDRITES

EQUIAXED DENDRITES
The ratio $G/V$ controls the type of microstructures. The cooling rate $GV$ controls the scale of the microstructure. Thermal gradient ($G$) and growth velocity ($V$) determine the form and scale of microstructures. The cooling rate $GV$ controls the scale of the microstructure. The ratio $G/V$ controls the type of microstructures.
Control interface velocity $V$ and heat flux $G$ during the entire solidification process
   - important topic in furnaces for single-crystal growth and directional solidification
Find means of delaying or eliminating morphological instability
Eliminate or reduce the effects of convection on the solidification morphology
Improve macroscopic and microscopic homogeneity of the final crystal

MAIN OBJECTIVES IN CONTROL OF SOLIDIFICATION
STRATEGIES FOR INTELLIGENT CONTROL OF SOLIDIFICATION MICROSTRUCTURE

- Proper adjustment of cooling/heating furnace conditions
- Use of electromagnetic fields for conducting melts in order to suppress the melt flow
- Time-harmonic or moving magnetic fields to induce melt stirring
- Controlled rotation of the furnace/crucible to control melt flow and solute distribution (Hurle, 1993)
- Solidification in reduced or gravity free environment to reduce the effects of buoyancy driven melt flow - NASA experiments in space
- Vibration of the solidification system (Garimella et al., 1995)
PREVIOUS WORK ON INVERSE THERMAL DESIGN OF PURE SOLIDIFICATION PROCESSES

- Inverse and design Stefan problems
  - Zabaras (1990)
  - Zabaras and Ruan (1992)

- Inverse conduction based solidification problem with data supplied from a direct melt convection problem
  - Zabaras and Nguyen (1995)

Find the ‘cooling conditions’ on $\Gamma_{os}$ as well as the ‘heating conditions’ on $\Gamma_{ol}$ such that a desired growth is achieved that is ensured to be morphologically stable.
ENFORCEMENT OF THE CONSTITUTIONAL STABILITY CONDITION

The constitutional stability criterion is enforced as follows:

\[ G > m G_c \quad \Rightarrow \quad G = m G_c + \varepsilon(x,t) \]

The "over-stability function" \( \varepsilon(x,t) \) is a part of the inverse problem definition and can be chosen according to various problem specific design requirements.
DIVIDE INTO TWO SUB-INVERSE PROBLEMS

SOLID

\[ q_{os} \text{ (Unknown)} \]

\[
\begin{align*}
\Gamma_{os} & \quad \text{INSULATED} \\
\Gamma_{I} & \quad \text{SOLID}
\end{align*}
\]

PHASE DIAGRAM

\[ T = T_o + mc \]

\[ q_{Is} \leftarrow q_{ol} \]

LIQUID

\[ q_{ol} \text{ (Unknown)} \]

\[
\begin{align*}
\Gamma_{I} & \quad \text{INSULATED} \\
\Gamma_{ol} & \quad \text{LIQUID}
\end{align*}
\]

PHASE DIAGRAM

\[ T = T_o + mc \]

INVERSE DESIGN WITH COUPLED HEAT, MOMENTUM AND MASS TRANSPORT

STABILITY CONDITION

\[ G = mG_c + \varepsilon(y,t) \]

SOLUTE BALANCE

\[ D_v G_v = V(1-k)c \]

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DIRECT vs INVERSE THERMAL-SOLUTAL CONVECTION PROBLEM

TWO CONDITIONS

SOLUTE BALANCE
\( D_1 G_c = V(1-k)c \)

STABILITY CONDITION
\( G = mG_c + \varepsilon(y,t) \)

INSULATED

TWO CONDITIONS

\( G_c = 0 \)

\( q_{ol} \) (Known)

WELL-POSED DIRECT PROBLEM

THREE CONDITIONS

SOLUTE BALANCE
\( D_1 G_c = V(1-k)c \)

PHASE DIAGRAM
\( T = T_0 + mc \)

INSULATED

One CONDITION

No thermal boundary condition
\( G_c = 0 \)

\( q_{ol} \) (Unknown)

ILL-POSED INVERSE PROBLEM

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Define the cost functional as the measure of deviation from thermodynamic equilibrium

\[
J(q_{ol}) = \frac{1}{2} \left\| T(x,t;q_{ol}) - [T_m + mc(x,t;q_{ol})] \right\|^2_{L^2(0,t_{max})}
\]
INVERSE THERMAL-SOLUTAL CONVECTION PROBLEM

- Define the inverse problem in the liquid domain in an optimization sense

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

\[
J(\overline{q}_{\text{ol}}) \leq J(q_{\text{ol}}) \quad \forall \quad \overline{q}_{\text{ol}} \in L_2(\Gamma_{\text{ol}} \times [0, t_{\text{max}}])
\]

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

Needs gradient information

Needs descent step size

Continuum adjoint problem

Continuum sensitivity problem
INTERACTION OF AN APPLIED STRONG MAGNETIC FIELD WITH FLUID FLOW IN A BOUNDED DOMAIN

MODEL ASSUMPTIONS

- Walls of the cavity are electric insulators
- Magnetic Reynolds number is sufficiently small that the induced magnetic field is negligible in comparison to the imposed constant magnetic field $B_0$

ELECTROMAGNETIC RELATIONS GOVERNING THE MHD FLOW PROBLEM

- Lorentz body force term in the Navier-Stokes equations
  \[ \mathbf{F} = \mathbf{J} \times \mathbf{B} + \frac{\rho_e}{\sigma_e} \mathbf{E} \]
- Ohm’s law for moving medium
  \[ \mathbf{J} = \sigma_e \left( \nabla \phi + \mathbf{v} \times \mathbf{B} \right) + \frac{\rho_e}{\sigma_e} \mathbf{v} \]
- Conservation of electric current
  \[ \nabla \cdot \mathbf{J} = 0 \]

Neglected as $\rho_e$ is small in liquid metals
PREVIOUS WORK ON INVERSE FLUID FLOW PROBLEMS

- Moutsoglou (1989)
  - steady state inverse free convection problem

- Gunzburger and Lee (1994)
  - addressed control of temperature peaks along bounding surfaces of containers
  - flow field was decoupled from the heat transfer analysis

- Berggren, Glowinski and Lions (1996)
  - controllability issues of flow related models (e.g. viscous Burgers equation)

- Zabaras and Yang (1997)
  - inverse natural convection problems
  - applications to design of directional solidification processes

- Berggren (1998)
  - vorticity control problem
MATHEMATICAL DEFINITION OF THE INVERSE MAGNETO-CONVECTION PROBLEM

Pose the inverse problem as an unconstrained spatio-temporal optimization problem

Find a (quasi-) solution $\theta_{o} \in L_2(\Gamma_{ho} \times [0, t_{\text{max}}])$ such that:

$$J(\theta_{o}) \leq J(\tilde{q}), \quad \forall \tilde{q} \in L_2(\Gamma_{ho} \times [0, t_{\text{max}}]),$$

where

$$J(\tilde{q}) = \frac{1}{2} \left\| \theta(x,t;\tilde{q}) - \theta_m(x,t) \right\|_{L_2(\Gamma_i \times [0, t_{\text{max}}])}^2$$

$$= \frac{1}{2} \int_0^{t_{\text{max}}} \int_{\Gamma_i} [\theta(x,t;\tilde{q}) - \theta_m(x,t)]^2 d\Gamma dt$$

Solution of a direct magneto-convection problem for a given guessed heat flux $q_o$ on the boundary $\Gamma_{ho}$
WELL-POSED DIRECT MAGNETO-CONVECTION PROBLEM
FOR A GIVEN HEAT FLUX $q_0$ ON THE BOUNDARY $\Gamma_{ho}$

MATHEMATICAL PROBLEM
- Incompressibility condition
- Navier-Stokes equations with body force terms involving Lorentz force as well as buoyancy effects
- Thermal transport equation
- Electromagnetic potential equation
- No-slip condition on all boundaries
- Electrically insulating condition on all boundaries
- Problem specific temperature/flux thermal boundary condition
CALCULATION OF THE GRADIENT OF THE OBJECTIVE FUNCTION

From the definition: \( J(q_o) = \frac{1}{2} \left\| \theta(x,t;q_o) - \theta_m(x,t) \right\|^2_{L_2(I_0 x [0, t_{\text{max}}])} \)

\[
D_{\Delta q_o} J(q_o) \equiv \left( J'(q_o), \Delta q_o \right)_{L_2(I_0 x [0, t_{\text{max}}])}
\]

\[
= (\theta(x,t;q_o) - \theta_m(x,t), \Theta(x,t;q_o,\Delta q_o))_{L_2(I_0 x [0, t_{\text{max}}])}
\]

Sensitivity temperature field \( \Theta(x,t;q_o,\Delta q_o) \equiv D_{\Delta q_o} \theta(x,t;q_o) \)
Sensitivity velocity field \( \mathbf{V}(x,t;q_o,\Delta q_o) \equiv D_{\Delta q_o} \mathbf{v}(x,t;q_o) \)
Sensitivity potential field \( \Phi(x,t;q_o,\Delta q_o) \equiv D_{\Delta q_o} \phi(x,t;q_o) \)

Expression for the exact gradient is determined through the solution of an appropriate continuum adjoint problem and is given by

\[
J'(q_o) = \psi(x,t;q_o) \quad \text{for} \ (x,t) \in (I_0 x [0, t_{\text{max}}])
\]

Adjoint temperature field
SENSITIVITY MAGNETO-CONVECTION PROBLEM

Boundary $\Gamma_1 - \Gamma_t, \partial \Theta / \partial n = 0$

On all boundaries $V = 0, \partial \phi / \partial n = 0$

ADJOINT MAGNETO-CONVECTION PROBLEM

Boundary $\Gamma_1 - \Gamma_t, \partial \psi / \partial n = 0$

On all boundaries $\phi = 0, \partial \eta / \partial n = 0$
**HIGHLIGHTS OF THE FINITE ELEMENT METHOD**

- PSPG/SUPG stabilized fluid flow formulation with additional terms from buoyancy and Lorentz body force terms
- Consistent SUPG formulation for heat equation
- Decoupled solution methodology for the subproblems at a given time step
- One-step time integration (T1 formulation) for the fluid flow problem and Newmark scheme for the heat equation
- Symmetrized coefficient matrix for the pressure equation and use of lumped mass matrix
- Flow fields are obtained after 2 passes per time step
- LU-factorization of the stiffness matrix is performed only once for fixed domain problems
- For deforming domain problems (applications in solidification process design):
  - Preconditioned Bi-CGSTAB algorithm is employed
  - LU-factorization of the stiffness matrix is calculated at regular time intervals and is used as an effective preconditioner in Bi-CGSTAB algorithm
- Identical time integration and finite element solution procedures is used for direct, adjoint, and sensitivity problems
- "Backward in time" solution of the adjoint problem requires that the entire history of the direct problem solution be stored
**H¹ REGULARIZATION TO HANDLE RANDOM ERRORS IN INPUT TEMPERATURE DATA**

**MODIFIED COST FUNCTIONAL**

\[
J(q_o) = \frac{1}{2} \left\| \theta(x,t;q_o) - \theta_m(x,t) \right\|_{L^2(G \times [0, t_{max}] )}^2 + \frac{\gamma}{2} \left\| q_o \right\|_{L^2(G \times [0, t_{max}] )}^2 + \frac{\gamma}{2} \left\| \nabla q_o \right\|_{L^2(G \times [0, t_{max}] )}^2
\]

**DIRECTIONAL DERIVATIVE**

\[
D_{\Delta q_o} J(q_o) \equiv (\Psi(x,t;q_o), \Delta q_o)_{L^2(G_{\text{ho}} \times [0, t_{max}] )} + \gamma (q_o(x,t), \Delta q_o)_{L^2(G_{\text{ho}} \times [0, t_{max}] )} + \gamma (\nabla q_o(x,t), \nabla (\Delta q_o))_{L^2(G_{\text{ho}} \times [0, t_{max}] )}
\]

**EXPRESSION FOR MODIFIED GRADIENT**

\[
J'(q_o) = z + \gamma q_o
\]

Solution of the variational equation:

\[-\Delta z(x,t) + z(x,t) = \Psi(x,t;q_o)\]
NUMERICAL EXAMPLE

Two-dimensional unit square cavity

DIMENSIONLESS PARAMETERS

- Prandtl number (Pr) 0.01
- Rayleigh number (Ra) 2x10⁴
- Hartmann number (Ha) 75 (applied at 45° inclination to the x-axis)
- Initial temperature (θ₁) 1.0
- Measured temperature (θₘ) 0.0

Given heat flux history q_I applied on the left vertical wall of the cavity

Calculated from the solution of a direct magneto-convection problem with flux q_o(y,t) = 1 - t applied on the right wall and the left wall maintained at θₘ

OBJECTIVE OF THE INVERSE PROBLEM

Reconstruct the exact flux solution \( \overline{q}_o(y,t) = 1 - t \) using the overspecified conditions \( q_I(y,t) \) and \( \theta_m \), starting from any arbitrary initial guess heat flux
CONVERGENCE OF THE HEAT FLUX SOLUTION

INITIAL GUESS $q_0^0 = 0$ AND INTERMEDIATE FLUXES $q_0^k(y,t)$ AT ITERATIONS 1, 10, 20

(a) (b) (c) (d)
CONVERGENCE OF THE CONJUGATE GRADIENT METHOD

IMPORTANT TRENDS IN THE NUMERICAL SOLUTION

- Monotonic reduction of the cost functional
- Norm of the gradient decreases with CG iterations (but not monotonically)
- Maximum inaccuracy in the calculated solution is at $t = t_{\text{max}}$
EFFECTS OF THE INITIAL GUESS HEAT FLUX

INITIAL GUESS $q^0 = 1 - t^4$ AND INTERMEDIATE FLUXES $q^k(y,t)$ AT ITERATIONS 1, 5, 20
CONVERGENCE OF THE CG METHOD FOR INITIAL GUESS

\[ q_0^*(y,t) = 1 - t^4 \]

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EFFECTS OF LARGE MEASUREMENT ERRORS

Reconstruct a close approximation of the optimal solution \( \hat{q}_o = 1 - t \) using the inexact temperature measurements and the given flux \( q_I(y,t) \), starting from any arbitrary initial guess heat flux.

\[
\theta_m(y,t) = \theta_m(y,t) + \varepsilon \omega_h
\]

Uniformly distributed random numbers in the interval \([-1, 1]\).

OBJECTIVE OF THE INVERSE PROBLEM

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INVERSE DESIGN OF ALLOY SOLIDIFICATION UNDER THE INFLUENCE OF AN EXTERNAL MAGNETIC FIELD

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INVERSE PROBLEM STATEMENT

Find the ‘cooling conditions’ on \( \Gamma_{os} \) as well as the ‘heating conditions’ on \( \Gamma_{ol} \) so that in the presence of an externally applied magnetic field, a desired growth is achieved that is ensured to be constitutionally stable.
HIGHLIGHTS OF THE SOLIDIFICATION DESIGN PROBLEM INCLUDING EFFECTS OF A MAGNETIC FIELD

- The new **inverse magneto-alloy solidification** problem is decoupled into two sub-inverse problems.

- The inverse problem in the solid domain is a inverse heat conduction problem, as in the previous works.

- The inverse problem in the liquid domain is a new **inverse magneto-thermo-solutal convection** problem.

New adjoint formulation involving coupled effects of buoyancy and electro-magnetic convection.
FINITE ELEMENT SIMULATION OF THE DIRECT ALLOY SOLIDIFICATION PROBLEM

- Moving/deforming finite element method to explicitly track the advancing solid-liquid interface
- Energy preserving formulation for calculating the front velocities
- Decoupled solution methodology for the sub-problems at a given time step
- Stabilized Petrov-Galerkin formulation for the fluid flow sub-problem
- Upwind FE formulation for the thermal and solute transport equations
- Diffpack C++ library of finite element classes provided the basic FEM and Linear algebra environment
The adjoint and sensitivity problems are similar in form to the direct problem except for boundary terms.

Form of the adjoint problem necessitates a *backward in time* solution approach.

The entire history of the direct problem is stored as the solution, and the sensitivity and adjoint problems need the direct solution for their formulation.

Due to highly nonlinear and coupled nature of the solidification problem, a ‘differentiate-then-discretize’ approach is employed.

Convergence of the CG method is affected due to memory-intensive computations.
OBJECT ORIENTED FRAMEWORK FOR THE FINITE ELEMENT SIMULATION OF THE DIRECT PROBLEM

MagAlloySolidification

- Potential
- MagnetoFlow
- NonlinearHeatAlloy (Melt)
- NonlinearHeatAlloy (Solid)
- ConvectionDiffusion
- SoluteConcentration
- Stefan

LinearSolver
MenuUDC
Store4Plotting

FEM
MenuUDC
Store4Plotting
OBJECT-ORIENTED FRAMEWORK FOR THE FEM IMPLEMENTATION OF THE OPTIMIZATION PROBLEM
FINITE ELEMENT CODE VALIDATION

- 2D/3D Lid-driven cavity problem at $Re = 400$ (Tezduyar et al., 1992)
- Unsteady flow past a circular cylinder at $Re = 100$ (Tezduyar, 1992)
- Viscous flow around a tube bundle at $Re = 100$ (Zienkiewicz & Taylor, 1991)
- Rayleigh Benard problem (Argyris et al., 1992)
- Natural convection in a rectangular cavity $Ra = 10^4 - 10^6$ (Marshall et al., 1978)
- Natural convection in horizontal circular cylinder (Heinrich & Yu, 1988)
- Double-diffusive convection in a vertical/inclined slot (Heinrich, 1984)
- Magneto-convection in a cavity at various strength/orientation (Ben Hadid et al., 1997)
- Surface tension and buoyancy driven flow in a cavity (Shyy et al., 1994)
- Surface tension, buoyancy and magnetically driven flow in a cavity (Ben Hadid et al., 1997, Kuhlmann, 1999)
- Solidification of aluminum in a square region (McDaniel & Zabaras, 1994)
- Melting of gallium (Gau and Viskanta, 1986)
- Solidification of aqueous solution (Thompson & Szekely, 1987)
- Solidification of pure metal with liquid phase buoyancy and surface tension forces (Bergman et al., 1992)
SOLIDIFICATION DESIGN EXAMPLE

REFERENCE DIRECT ALLOY SOLIDIFICATION PROBLEM
UNDER THE INFLUENCE OF EXTERNAL MAGNETIC FIELD

\[ \theta = -0.5 \]

\[ B_0 \]

MATERIAL
Germanium + dopants
- Properties from Brown et al., 1988

FE MESH
800 bi-linear quadrilateral elements in the solid and liquid domains

MORPHOLOGICAL INSTABILITY
THE WELL POSED MATHEMATICAL PROBLEM VIOLATES THE A-PRIORI ASSUMPTION OF STABILITY!
OBJECTIVE OF THE INVERSE SOLIDIFICATION DESIGN PROBLEM

- Achieve a desired flat interface growth
- Ensure that the solid-liquid interface is constitutionally stable

STATEMENT OF THE INVERSE PROBLEM

Find the thermal conditions on the solid wall as well as liquid wall such that with convection in the melt, a flat interface stable growth is achieved that corresponds to a conduction driven solidification problem.

Ensures that effects of convection are removed.
SOLIDIFICATION DESIGN EXAMPLE

OBJECTIVE FUNCTION vs CGM ITERATIONS

TRENDS IN THE NUMERICAL SOLUTION

- Optimal flux distributions clearly show that much of the corrective action takes place at early times.
- Slower convergence compared to inverse magneto-convection problems addressed earlier.

LIQUID SIDE
OPTIMAL HEAT FLUX

SOLID SIDE
OPTIMAL HEAT FLUX

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SOLIDIFICATION DESIGN EXAMPLE

STABILITY VALIDATION OF THE INVERSE DESIGN SOLUTION

Solid side optimal heat flux $q_{os}$

Liquid side optimal heat flux $q_{ol}$

Direct alloy solidification solver including the effects of an external magnetic field

POST PROCESS

STABLE GROWTH FOR THE ENTIRE DURATION OF THE SOLIDIFICATION PROCESS
COMPUTATIONAL ISSUES

- Solution of the inverse magneto-thermal-solutal fluid flow problem was the computationally intensive part of the whole solution process.
- Optimal heat flux was obtained after 40 CG iterations when the norm of the gradient was below 1e-4.
- Each conjugate gradient iteration took about 3.5 hours of CPU time which includes "file operations".
- IBM RS-6000 machines provided by the Cornell Theory Center was used for all computations.
In addition to buoyancy and magnetic forces, convection is induced due to surface tension gradients on the free surface (Marangoni convection).

Action of Marangoni convection is undesirable as the transition to unsteady behavior is hard to control.
DECOUPLED INVERSE SOLIDIFICATION PROBLEM

FIND COOLING CONDITIONS ON $\Gamma_{os}$ AND THE HEATING CONDITIONS ON $\Gamma_{ol}$ SUCH THAT A DESIRED STABLE SOLID-LIQUID INTERFACE GROWTH IS ACHIEVED IN THE PRESENCE OF MELT CONVECTION.
With a guessed heat flux $q_{ol}$ and without using the temperature boundary condition on $\Gamma_{l}$, 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:

$$J(q_{ol}) = \frac{1}{2} \left\| T(x, t; q_{ol}) - T_{E} \right\|_{L_{2} (\Gamma_{l} \times [0, t_{\text{max}}])}^{2} + \frac{\gamma}{2} \left\{ \left\| q_{ol} \right\|_{L_{2} (\Gamma_{l} \times [0, t_{\text{max}}])}^{2} + \left\| \nabla q_{ol} \right\|_{L_{2} (\Gamma_{ol} \times [0, t_{\text{max}}])}^{2} \right\}$$

Measure of deviation from thermodynamic equilibrium

$H^{1}$ Regularization terms
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
Solutal Rayleigh number 6.275e+04
Lewis number 319.0
Thermal Marangoni number -3982.02
Stefan number 0.1348
Thermal Rayleigh number 1.644e+05

DIRECT FE SIMULATION

POST PROCESS
Examination of constitutional stability assumption on the solid-liquid interface
Dimensionless contours of
\[
\Delta = \frac{G}{v} + \frac{m}{D_L} (c_E - c_o)
\]
\[\Delta < 0\] 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 thermodiffusion, 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

STRONG HEATING AT EARLY TIMES TO OVERCOME THE UNDERCOOLING EFFECTS

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

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SOLIDIFICATION DESIGN EXAMPLE

NUMERICAL VALIDATION OF THE INVERSE DESIGN SOLUTION

Dimensionless contours of

\[ \Delta = \frac{G}{\nu} + \frac{m}{D_L} (C_E - C_o) \]

\( \Delta < 0 \) corresponds to unstable growth

STABLE GROWTH IS ACHIEVED FOR THE ENTIRE DURATION OF SOLIDIFICATION

Standard deviation representing the deviation of the calculated interface velocity from the desired growth conditions

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SUGGESTIONS FOR FUTURE STUDIES

- Develop advanced numerical analysis tools to improve the performance of the computationally-taxing inverse problem solution in the melt domain.
- Improve the performance of the algorithms to address more complicated solidification systems with multiple length and time scales.
- Develop inverse methods to include other means of control as additional design variables (e.g. strength and orientation of the applied magnetic field).
- Develop a computational framework for the design of solidification processes with continuum mushy zone solidification models.
- Extend and improve the present design techniques to address final state thermal design problems (e.g. reduction/optimization of residual stresses).