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**INVERSE THERMAL DESIGN OF THERMO-MAGNETICALLY  
DRIVEN BOUSSINESQ FLOWS**

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## OUTLINE OF THE PRESENTATION

- Review of previous work on inverse fluid flow problems
- Interaction of an externally applied magnetic field with fluid flow
- Mathematical definition of the inverse magneto-convection problem
- Adjoint method formulation for the solution of the inverse problem posed as a functional optimization problem
- Highlights of the FEM techniques used for the solution of the direct, adjoint and sensitivity problems
- $H^1$  regularization to handle large errors in input data
- Numerical results
- Extension of the developed method to address the design of directional solidification processes
- Summary

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## **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)

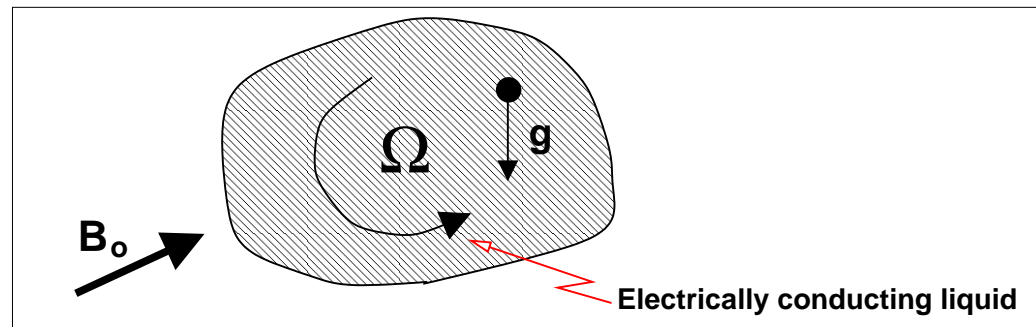
### **■ Zabaras and Yang (1997)**

- inverse natural convection problems
- applications to design of directional solidification processes

### **■ Berggren (1998)**

- vorticity control problem

# 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

$$\mathbf{F} = \mathbf{J} \times \mathbf{B} + \underbrace{\rho_e \mathbf{E}}_{\uparrow}$$

← Neglected as  $\rho_e$  is small in liquid metals

- Ohm's law for moving medium

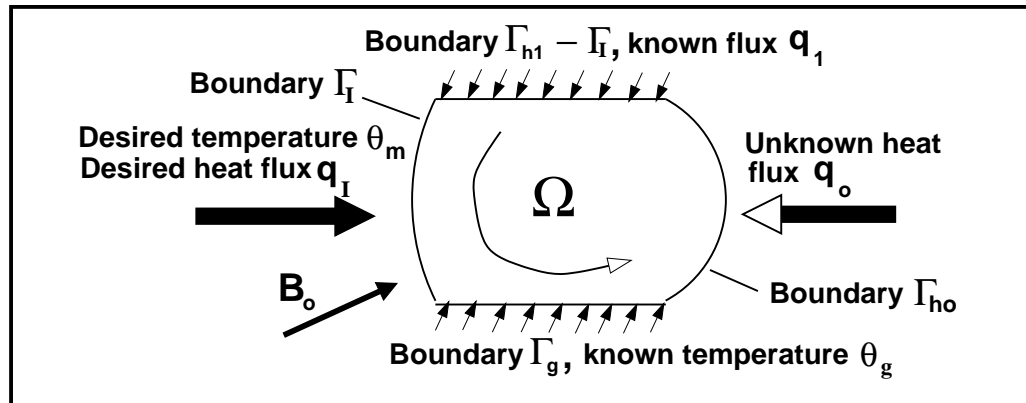
$$\mathbf{J} = \sigma_e (-\nabla\phi + \mathbf{v} \times \mathbf{B}) + \underbrace{\rho_e \mathbf{v}}_{\uparrow}$$

← Neglected as  $\rho_e$  is small in liquid metals

- Conservation of electric current

$$\nabla \cdot \mathbf{J} = 0$$

## MATHEMATICAL DEFINITION OF THE INVERSE MAGNETO-CONVECTION PROBLEM



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

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

$$J(\bar{q}_o) \leq J(q_o), \quad \forall \bar{q}_o \in L_2(\Gamma_{ho} \times [0, t_{max}]),$$

where

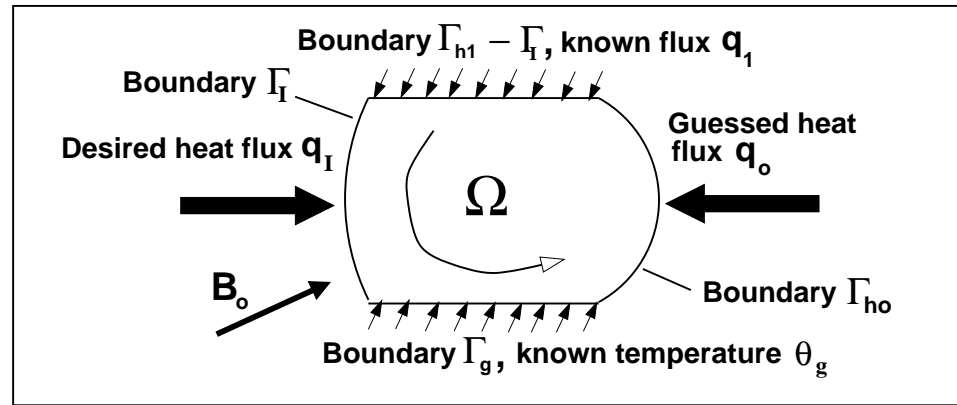
$$J(q_o) = \frac{1}{2} \left\| \theta(x,t;q_o) - \theta_m(x,t) \right\|_{L_2(\Gamma_I \times [0, t_{max}])}^2$$

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

Measured/desired temperature

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:  $J(q_o) = \frac{1}{2} \|\theta(x,t;q_o) - \theta_m(x,t)\|_{L_2(\Gamma_I \times [0, t_{max}])}^2$

$$\begin{aligned} D_{\Delta q_o} J(q_o) &\equiv (J'(q_o), \Delta q_o)_{L_2(\Gamma_{h0} \times [0, t_{max}])} \\ &= (\theta(x,t;q_o) - \theta_m(x,t), \Theta(x,t;q_o, \Delta q_o))_{L_2(\Gamma_I \times [0, t_{max}])} \end{aligned}$$

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

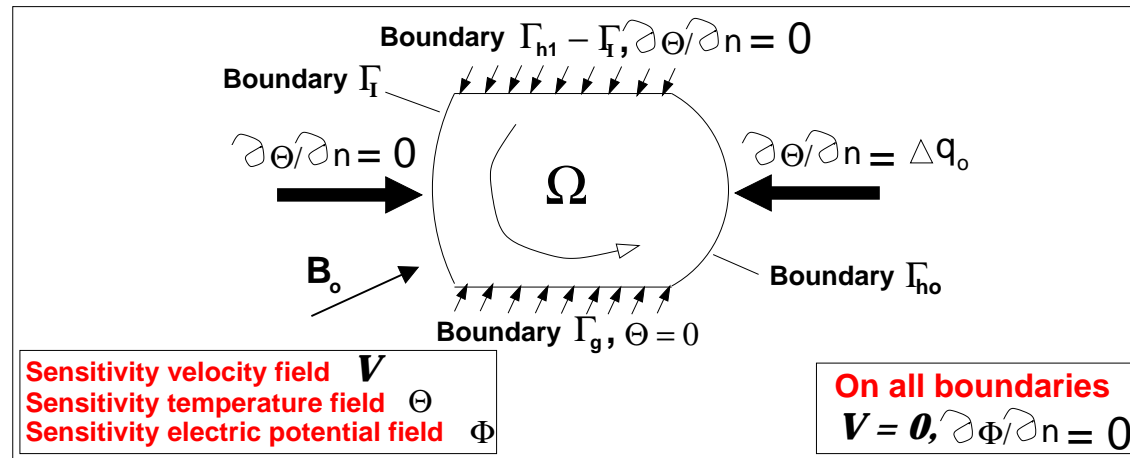
Determined through the solution of an appropriate linear **continuum sensitivity problem**

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

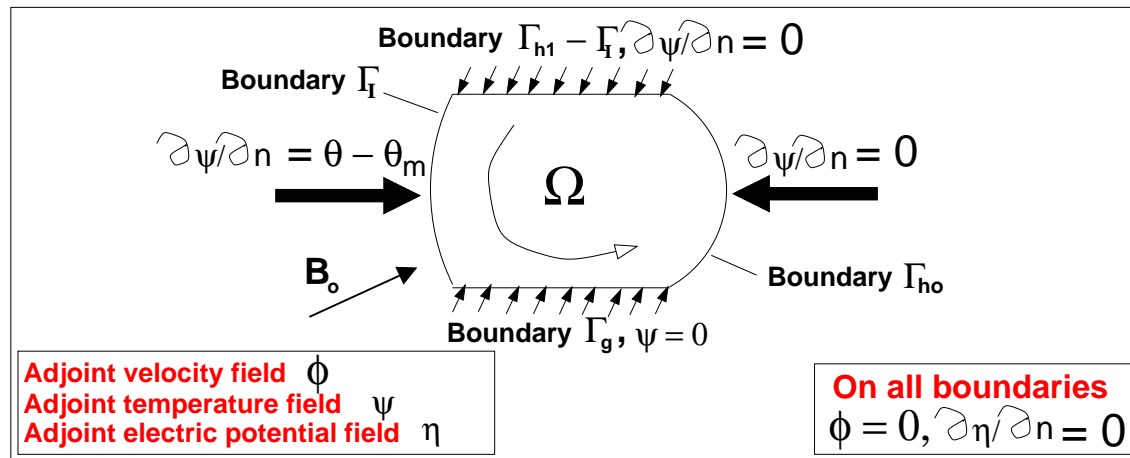
$$J'(q) = \psi(x,t;q_o) \text{ for } (x,t) \in (\Gamma_{h0} \times [0, t_{max}])$$

↑  
Adjoint temperature field

## SENSITIVITY MAGNETO-CONVECTION PROBLEM



## ADJOINT MAGNETO-CONVECTION PROBLEM



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## **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**

# H<sup>1</sup> REGULARIZATION TO HANDLE RANDOM ERRORS IN INPUT TEMPERATURE DATA

## MODIFIED COST FUNCTIONAL

$$J(q_o) = \frac{1}{2} \|\theta(x,t;q_o) - \theta_m(x,t)\|_{L_2(\Gamma \times [0, t_{\max}])}^2 + \frac{\gamma}{2} \|q_o\|_{L_2(\Gamma_{ho} \times [0, t_{\max}])}^2 + \frac{\gamma}{2} \|\nabla q_o\|_{L_2(\Gamma_{ho} \times [0, t_{\max}])}^2$$

## DIRECTIONAL DERIVATIVE

Regularization parameter

$$D_{\Delta q_o} J(q_o) \equiv (\Psi(x,t;q_o), \Delta q_o)_{L_2(\Gamma_{ho} \times [0, t_{\max}])} + \gamma (q_o(x,t), \Delta q_o)_{L_2(\Gamma_{ho} \times [0, t_{\max}])} + \gamma (\nabla q_o(x,t), \nabla (\Delta q_o))_{L_2(\Gamma_{ho} \times [0, t_{\max}])}$$

## EXPRESSION FOR MODIFIED GRADIENT

$$J'(q_o) = z + \gamma q_o$$

↑ Solution of the variational equation ←

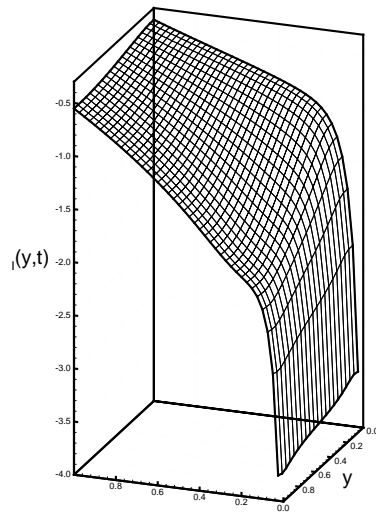
$$-\Delta z(x,t) + z(x,t) = \Psi(x,t;q_o)$$

## NUMERICAL EXAMPLE

### ■ Two-dimensional unit square cavity

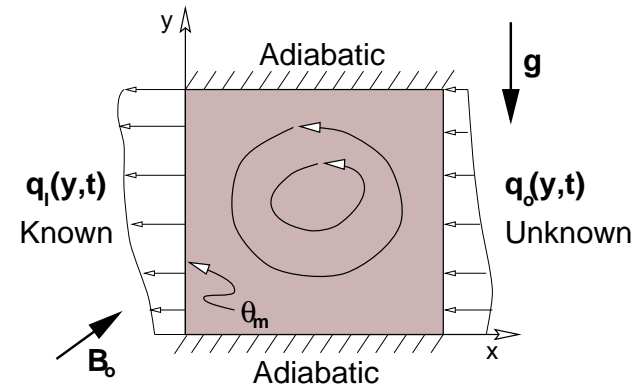
#### DIMENSIONLESS PARAMETERS

- Prandtl number (Pr) 0.01
- Rayleigh number (Ra)  $2 \times 10^4$
- Hartmann number (Ha) 75 (applied at  $45^\circ$  inclination to the x-axis)
- Initial temperature ( $\theta_i$ ) 1.0
- Measured temperature ( $\theta_m$ ) 1.0



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  $\theta_m$

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

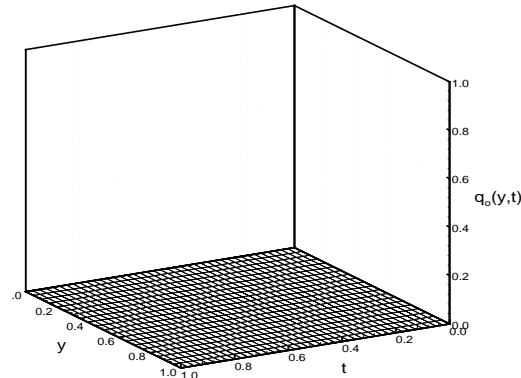


#### OBJECTIVE OF THE INVERSE PROBLEM

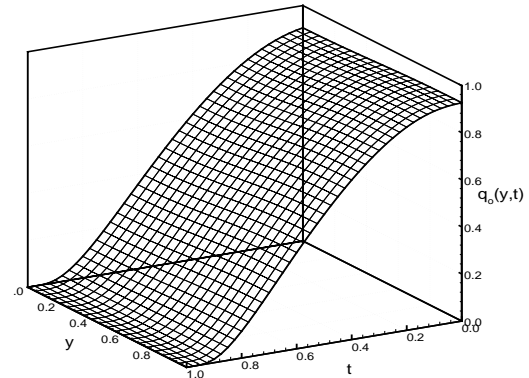
RECONSTRUCT THE EXACT FLUX SOLUTION  $\bar{q}_o(y,t) = 1 - t$  USING THE OVERSPECIFIED CONDITIONS  $q_I(y,t) = 1 - t$  AND  $\theta_m$ , STARTING FROM ANY ARBITRARY INITIAL GUESS HEAT FLUX

## CONVERGENCE OF THE HEAT FLUX SOLUTION

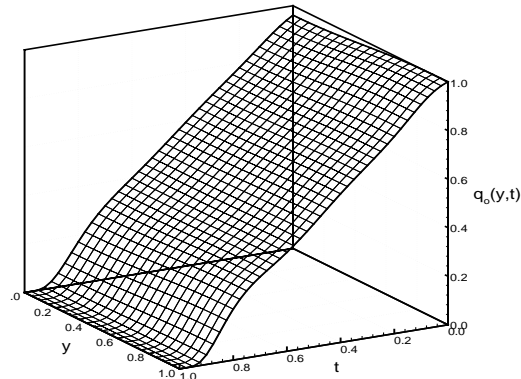
INITIAL GUESS  $q_0^0 = 0$  AND INTERMEDIATE FLUXES  $q_0^k(y,t)$  AT ITERATIONS 1, 10, 20



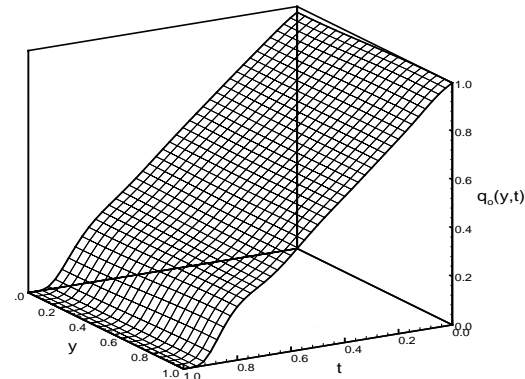
(a)



(b)

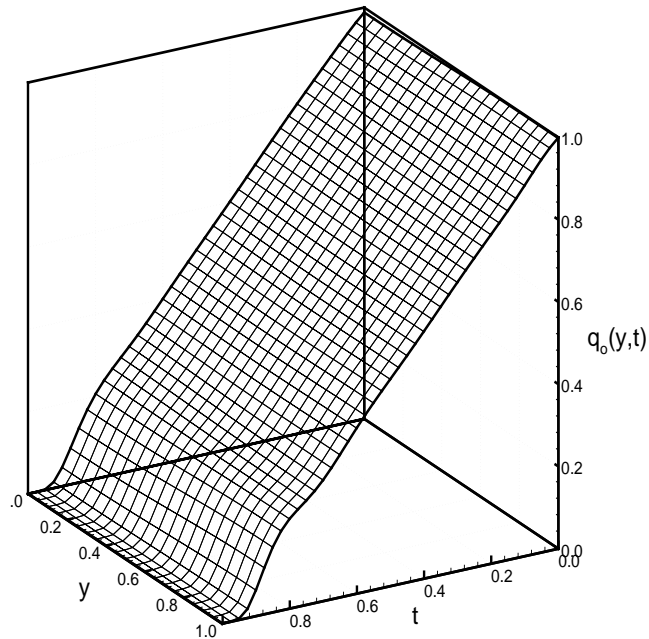


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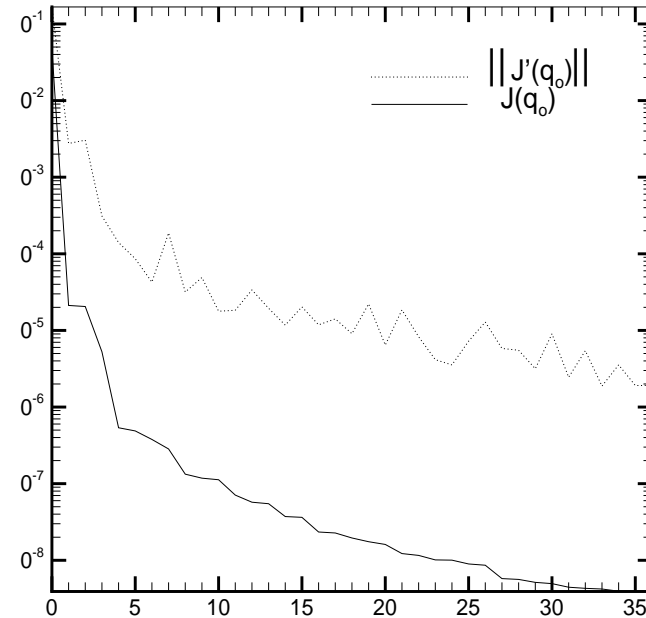


(d)

# CONVERGENCE OF THE CONJUGATE GRADIENT METHOD



OPTIMAL HEAT FLUX DISTRIBUTION CALCULATED AT THE 35th CONJUGATE-GRADIENT ITERATION



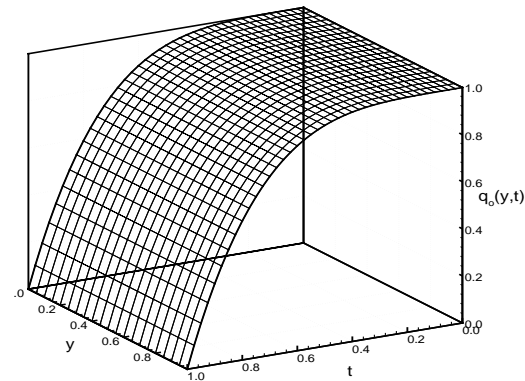
VARIATION OF THE COST FUNCTIONAL AND THE NORM OF THE GRADIENT WITH CG ITERATIONS

## IMPORTANT TRENDS IN THE NUMERICAL SOLUTION

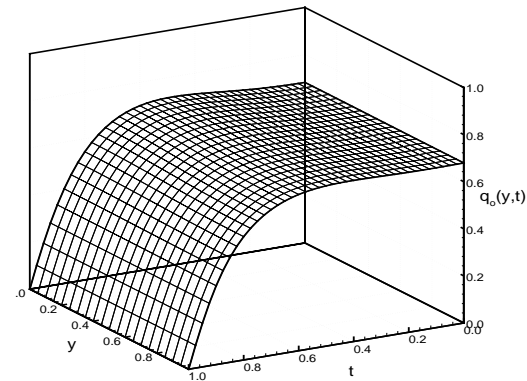
- Monotonic reduction of the cost functional
- Norm of the gradient decreases with CG iterations (but not monotonically)
- Maximum inaccuracy in the calculated solution is at  $t = t_{\max}$

## EFFECTS OF THE INITIAL GUESS HEAT FLUX

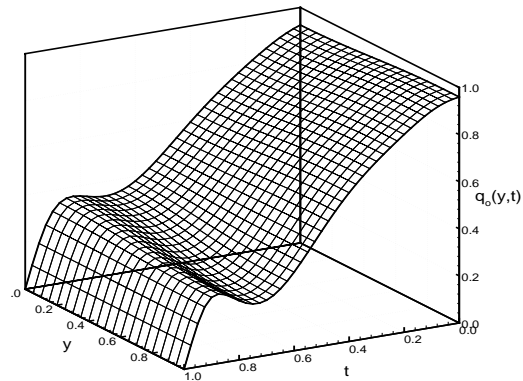
INITIAL GUESS  $q_0^0 = 1 - t^4$  AND INTERMEDIATE FLUXES  $q_0^k(y,t)$  AT ITERATIONS 1, 5, 20



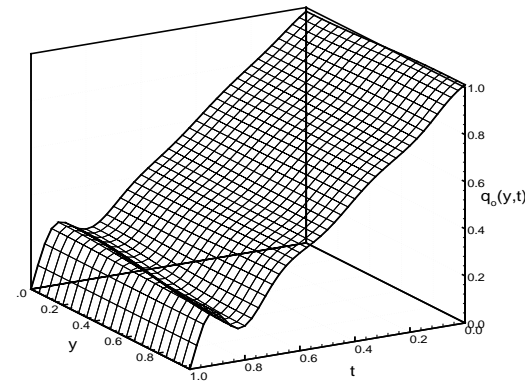
(a)



(b)



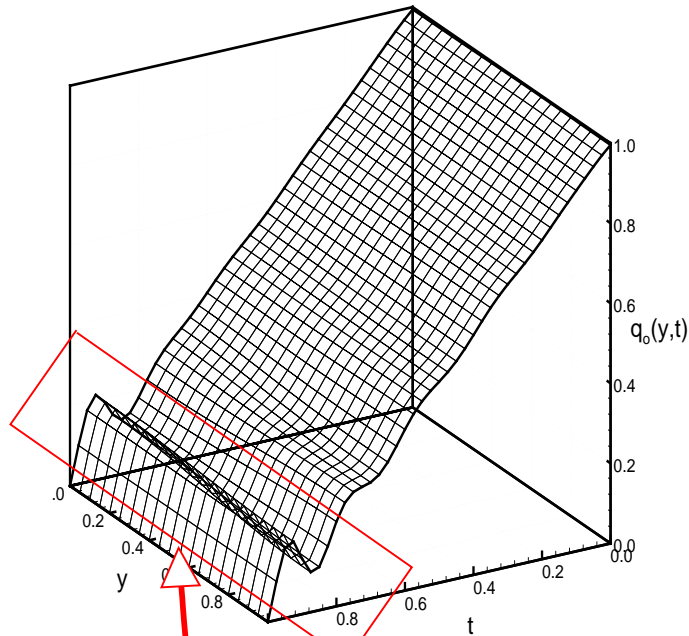
(c)



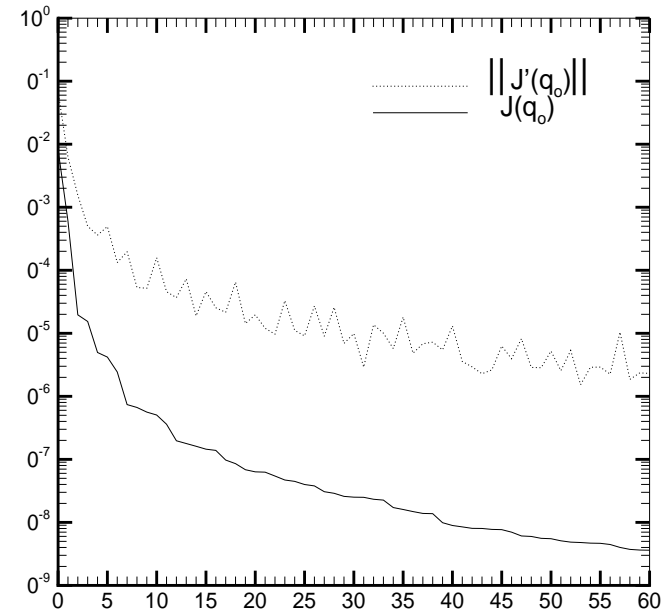
(d)

# CONVERGENCE OF THE CG METHOD FOR INITIAL GUESS

$$q_0^o(y,t) = 1 - t^4$$



OPTIMAL HEAT FLUX DISTRIBUTION CALCULATED AT THE 35th CONJUGATE-GRADIENT ITERATION

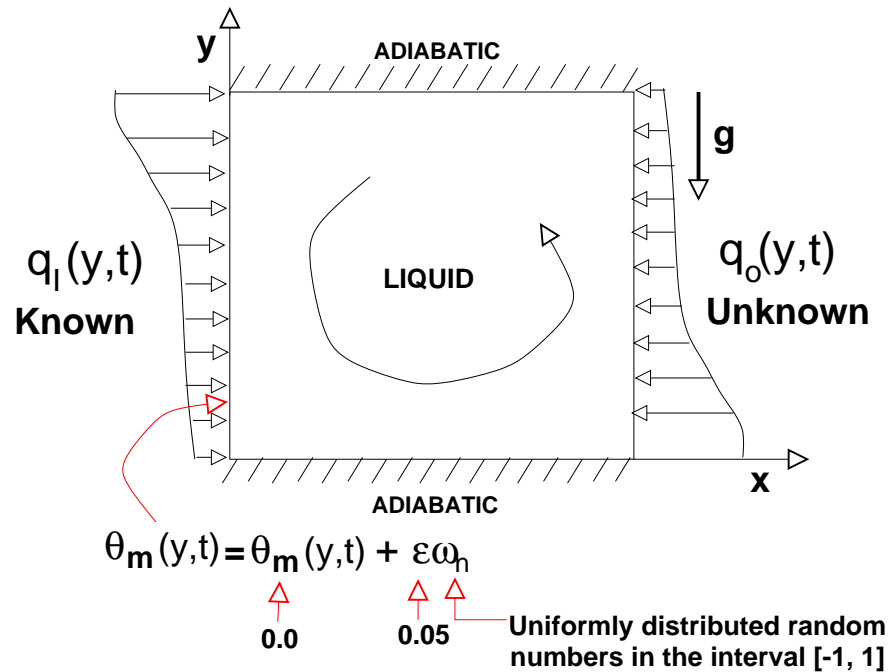


VARIATION OF THE COST FUNCTIONAL AND THE NORM OF THE GRADIENT WITH CG ITERATIONS

NOTICE THE PROMINENT DEVIATION OF THE CALCULATED SOLUTION FROM THE EXACT SOLUTION  $\bar{q}_0 = 1 - t$

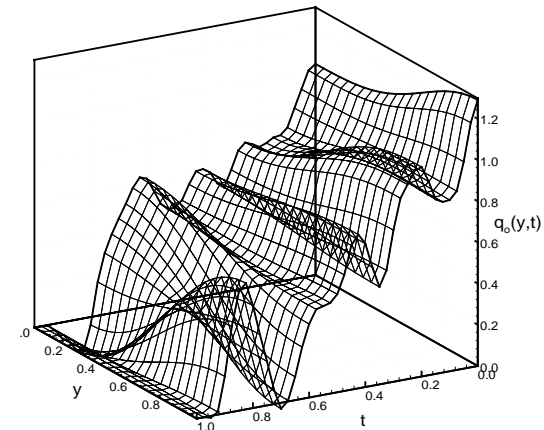
END-CONDITION PROBLEM ASSOCIATED WITH THE ADJOINT METHOD

## EFFECTS OF LARGE MEASUREMENT ERRORS

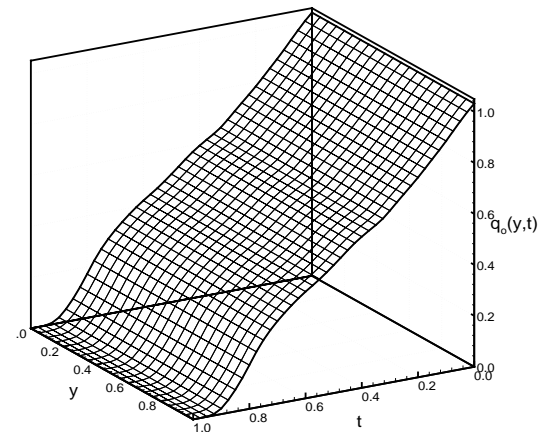


### OBJECTIVE OF THE INVERSE PROBLEM

Reconstruct a close approximation of the optimal solution  $q_o = 1 - t$  using the inexact temperature measurements and the given flux  $q_i(y,t)$ , starting from any arbitrary initial guess heat flux



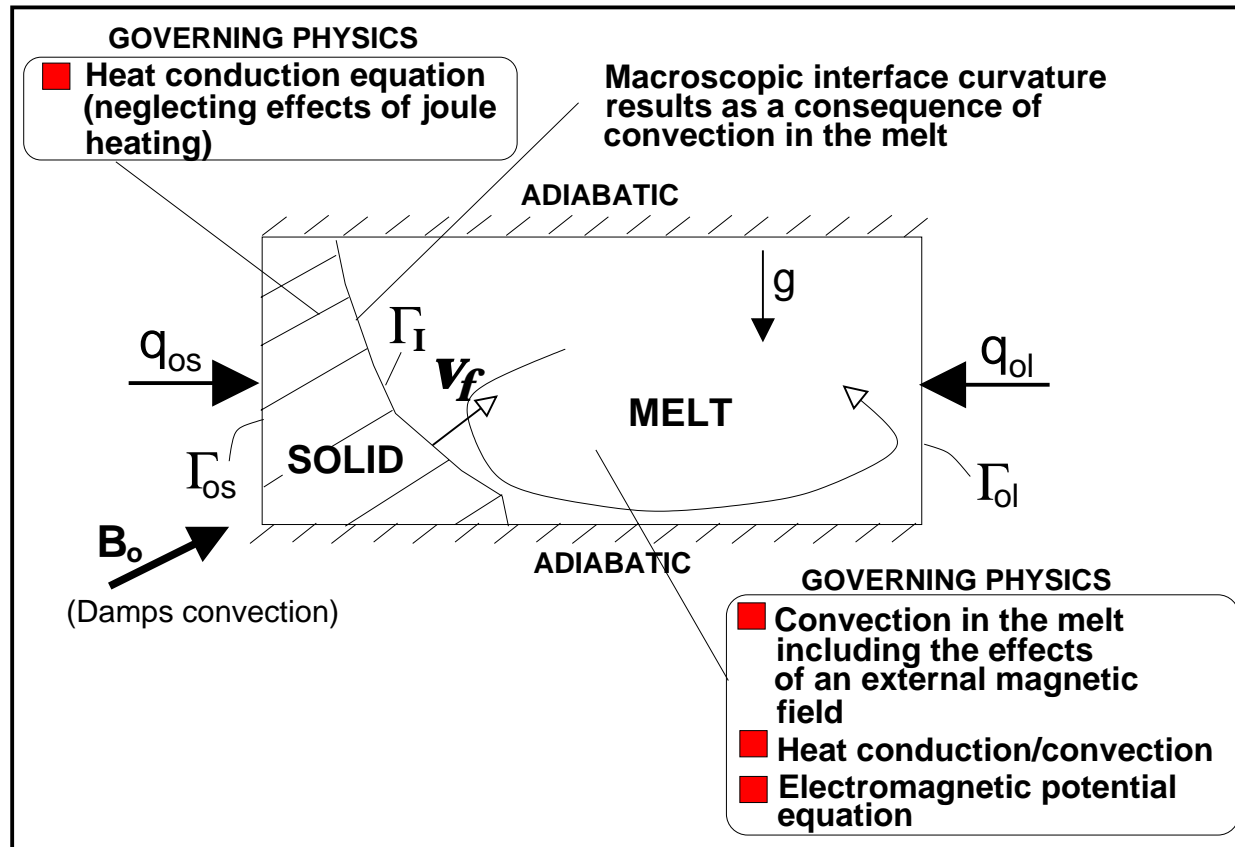
CALCULATED HEAT FLUX SOLUTION AT THE 30th ITERATION (NO REGULARIZATION)



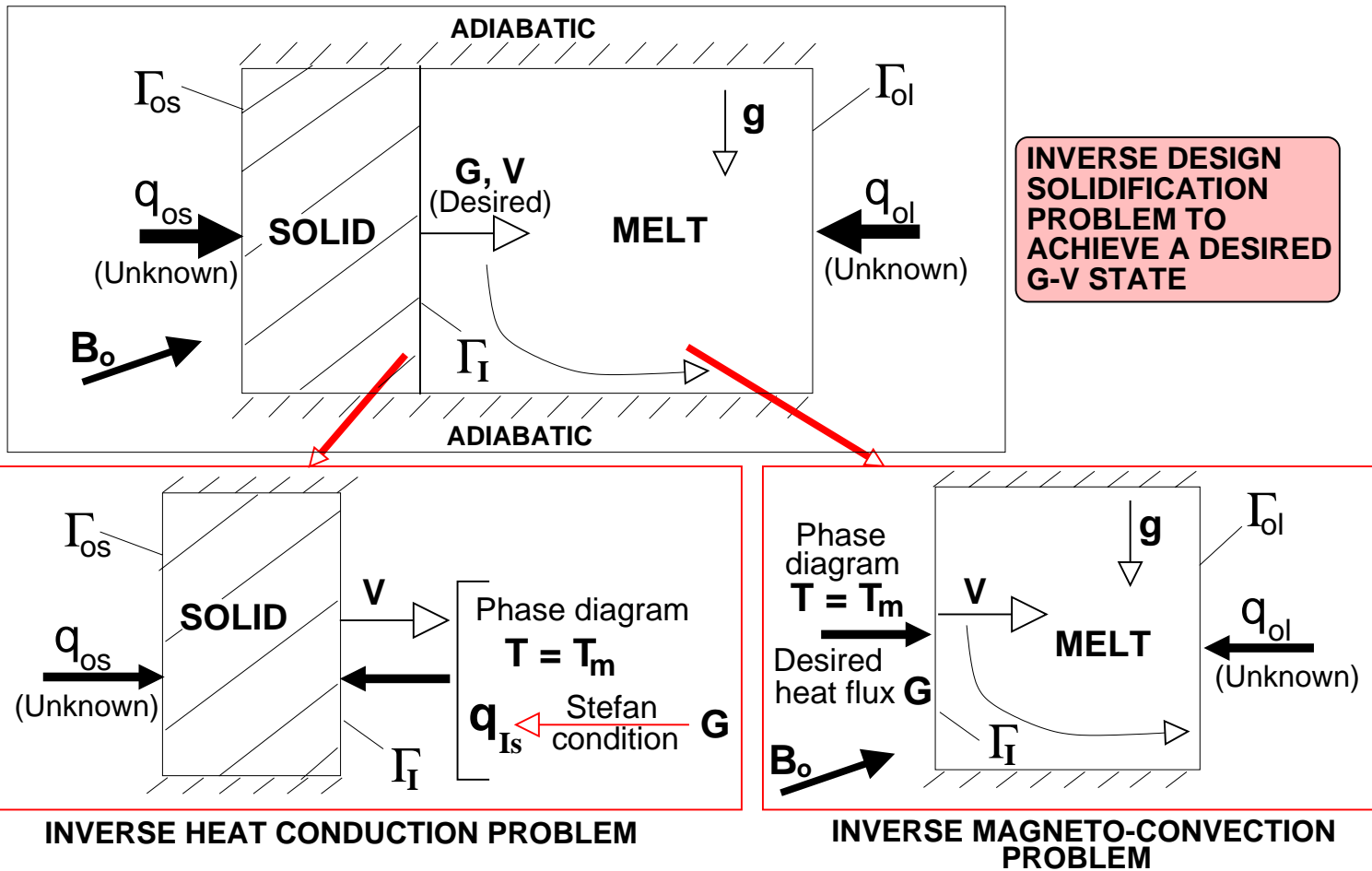
CALCULATED HEAT FLUX SOLUTION AT THE 30th ITERATION (WITH REGULARIZATION)

# APPLICATIONS TO DESIGN OF DIRECTIONAL SOLIDIFICATION PROCESSES

## PHYSICAL MODEL



# APPLICATIONS TO DESIGN OF DIRECTIONAL SOLIDIFICATION PROCESSES



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## SUMMARY

- **Systematic continuum adjoint formulation for the inverse design of convective systems under the influence of an external magnetic field**
- **Accurate reconstruction of heat fluxes for several example problems (including 3D systems) with exact measurement data**
- **Demonstration of the need for regularization for problems with large measurement errors**
- **$H^1$  regularized inverse design formulation for problems with large input errors**
- **Application of the developed methods to thermal design of directional solidification processes such that a desired G-V state is achieved**