



A functional optimization formulation of an inverse design magneto-convection problem

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1 INTRODUCTION

This report presents the preliminary studies conducted with respect to the inverse design optimization of binary alloys in the presence of an applied magnetic field. In particular, the functional optimization formulation of an inverse magneto-convection problem in a time invariant domain is considered here. The report is organized as follows: In section 2 the definition of the direct magneto-convection is addressed which is followed by section 3 in which the weak forms and the numerical formulation is presented. Next, in section 4 a sample numerical example of buoyancy driven convection in a horizontal Bridgman configuration under the action of a constant magnetic field is presented. The results are compared with published results and excellent comparison is shown to be obtained. The results demonstrate the distinct effects on the flow due to the application of the magnetic field. In section 5 we finally present the inverse formulation which includes the sensitivity equations and the derivation of the adjoint equations which provides us with the gradient we desire.

2 DEFINITION OF THE DIRECT MAGNETO-CONVECTION PROBLEM

Let Ω be a closed bounded region in $R^{n_{sd}}$, where n_{sd} is the number of space dimensions, with a piecewise smooth boundary Γ (Fig. 1). The region is occupied by an incompressible electrically conducting fluid and is subject to an external magnetic field in a nonisothermal environment. The motion of this fluid is initially driven by the temperature induced density gradients. Motion in the presence of a magnetic field will in turn give rise to a Lorentz or Laplace force, which acts on the fluid so that an extra body force term \mathbf{F} appears in the Navier-Stokes equation. The Lorentz force term \mathbf{F} in such a flow is given as follows:

$$\mathbf{F} = \rho_e \mathbf{E} + \mathbf{J} \times \mathbf{B} \quad (1)$$

where ρ_e is the electric charge density of the fluid, $\mathbf{E} = -\nabla\phi$ the electric field intensity, ϕ the electric field potential, \mathbf{J} the electric current density and \mathbf{B} the magnetic field. On the other hand, the electric current density is governed by Ohm's law for a moving medium:

$$\mathbf{J} = \rho_e \mathbf{v} + \sigma_e (-\nabla\phi + \mathbf{v} \times \mathbf{B}) \quad (2)$$

where σ_e is the electric conductivity and \mathbf{v} the fluid velocity vector. In addition to the applied magnetic field \mathbf{B}_o , there is an induced magnetic field produced by the electric currents in the liquid metal. We assume in the following that the walls of the cavity are electric insulators and the magnetic Reynolds number $Re_m = Pr_m Re_d$ is sufficiently small that the induced magnetic field is negligible with respect to the imposed constant magnetic field \mathbf{B}_o . (Note, since $\mathbf{B}_o Re_m$ is a good estimate for perturbation of the magnetic field by motion; if $Re_m \ll 1$, then we have the condition satisfied and this constraint usually holds for liquid metals which we are concerned with.) As ρ_e is very small in liquid metals, we can neglect the terms $\rho_e \mathbf{E}$ and $\rho_e \mathbf{v}$.

In addition to Ohm's law, the electric current density \mathbf{J} is governed by the conservation of electric current.

$$\nabla \cdot \mathbf{J} = 0 \quad (3)$$

This helps to get rid of the current density \mathbf{J} from the system of equations and we can write the governing equation for the scalar potential as:

$$\nabla^2 \phi = \nabla \cdot (\mathbf{v} \times \mathbf{e}_B) \quad \text{in } \Omega \times [0, t_{max}] \quad (4)$$

Thus, under the influence of any external magnetic field, Eq. 4 gives the potential function (if the velocity is known) and this function along with the magnetic field determines the Laplace force as given by Eq. 1.

We now introduce the governing equations to complete the definition of the problem.

Let L be a characteristic length of the domain, ρ the density, k the conductivity, α ($\alpha = k/\rho c$) the thermal diffusivity, σ the electrical conductivity and ν the kinematic viscosity. All the thermo-physical properties are assumed to be constant. The characteristic scale for time is taken as L^2/α and for velocity as α/L . The dimensionless temperature θ is taken as $\theta = (T - T_{ref})/(T_{in} - T_{ref})$ where T , T_{in} and T_{ref} are the temperature, initial temperature and reference temperature, respectively. The characteristic scale for the electric potential ϕ is taken as αB_o where \mathbf{B}_o is the externally applied magnetic field. Since we will be using only nondimensional quantities from here on, the same symbol ϕ is used for the nondimensional electric potential.

The key dimensionless quantities are the Prandtl number (Pr), Rayleigh number (Ra) and the Hartmann number (Ha). They are defined as $Pr = \nu/\alpha$, $Ra = g\beta(T_{in} - T_{ref})L^3/\nu\alpha$ and $Ha = \left[\left(\frac{\sigma}{\rho\nu} \right)^{1/2} B_o L \right]$ respectively, where β is the thermal expansion coefficient and g is the gravity constant.

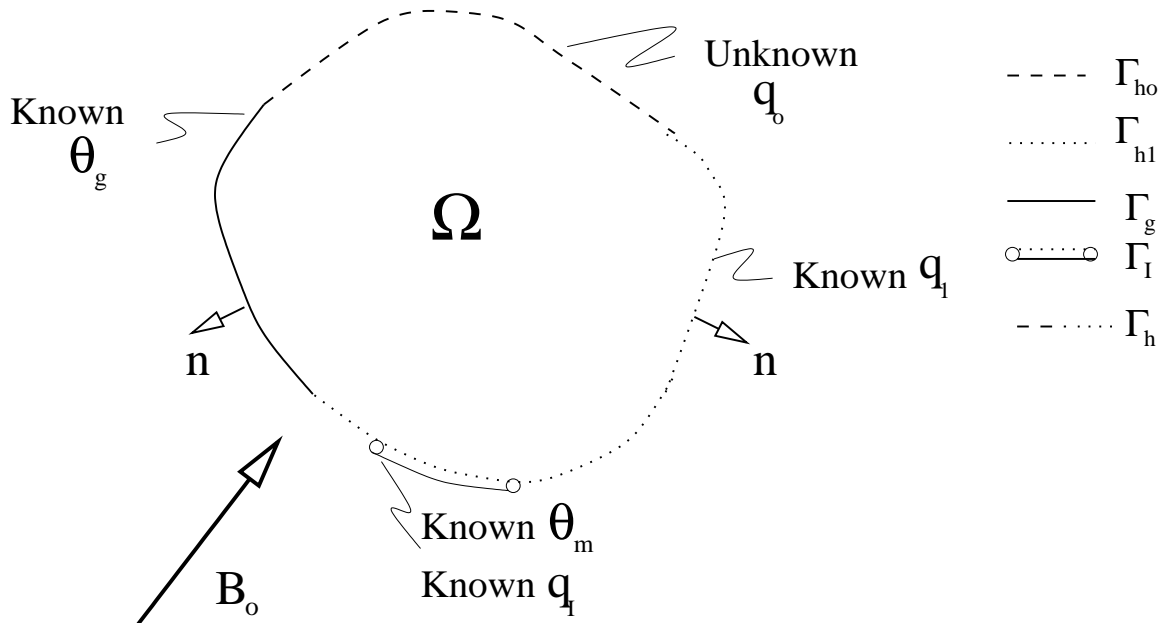


Figure 1: Schematic of the inverse magneto-convection problem

The incompressible NavierStokes equations are used for modeling the flow induced by both density variations and Laplace force. It is assumed that the flow is laminar and it has no viscous dissipation nor Joule heating effects. The conservation of momentum for the velocity field $\mathbf{v}(\mathbf{x}, t)$ in $(\mathbf{x}, t) \in \Omega \times [0, t_{max}]$ is given by

$$\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v}) \mathbf{v} = \nabla \cdot \boldsymbol{\sigma} - Pr Ra \theta \mathbf{e}_g + Ha^2 Pr [-\nabla \phi + \mathbf{v} \times \mathbf{e}_B] \times \mathbf{e}_B, \quad (5)$$

where the constitutive equation defining the stress tensor is given as

$$\boldsymbol{\sigma} = -p \mathbf{I} + Pr [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]. \quad (6)$$

The incompressibility condition takes the form

$$\nabla \cdot \mathbf{v}(\mathbf{x}, t) = 0, \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}]. \quad (7)$$

In the equations above, \mathbf{I} is a second order unit tensor, \mathbf{e}_g is a unit vector in the direction of gravity, \mathbf{e}_B is a unit vector in the direction of the externally applied magnetic field.

The temperature field in $\Omega \times [0, t_{max}]$ is governed by the following energy equation

$$\frac{\partial \theta}{\partial t} + \mathbf{v} \cdot \nabla \theta = \nabla \cdot \nabla \theta. \quad (8)$$

The electric potential field in $\Omega \times [0, t_{max}]$ is governed by the following poisson equation as described earlier

$$\nabla^2 \phi = \nabla \cdot (\mathbf{v} \times \mathbf{e}_B) \quad (9)$$

The known initial conditions are the following:

$$\mathbf{v}(\mathbf{x}, 0) = \mathbf{v}_i(\mathbf{x}), \quad \mathbf{x} \in \Omega \quad (10)$$

and

$$\theta(\mathbf{x}, 0) = \theta_i(\mathbf{x}), \quad \mathbf{x} \in \Omega. \quad (11)$$

The initial potential function can be easily solved for when the velocity field is known.

The fluid velocity, \mathbf{v} , is assumed known at the boundary Γ . The no-slip condition is used here, i.e.

$$\mathbf{v}(\mathbf{x}, t) = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}]. \quad (12)$$

In the part Γ_h of the boundary Γ , we assume that a heat flux boundary condition is applied, while in the remaining of the boundary, Γ_g a temperature boundary condition is considered, i.e. $\Gamma_h \cup \Gamma_g = \Gamma$ and $\Gamma_h \cap \Gamma_g = \emptyset$ (see Fig. 1).

The electric potential function $\phi(\mathbf{x}, t)$ is governed by insulating wall conditions on the boundary or,

$$\nabla \phi(\mathbf{x}, t) \cdot \mathbf{n} = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}] \quad (13)$$

The above partial differential equations along with initial and boundary conditions constitute a well-posed *direct problem* which can be solved to obtain the thermal, flow and potential fields. We next consider the numerical solution of the above direct problem using a Petrov-Galerkin finite element method.

3 Weighted residual formulation and numerical implementation

The classical streamline upwind/Petrov-Galerkin method of Brooks and Hughes is adopted here. Discontinuous scalar weighting functions of the form $\tilde{w} = w + q$ and vector weighting functions $\tilde{\mathbf{w}} = \hat{\mathbf{w}} + \hat{\mathbf{q}}$ are used for the thermal and fluid flow parts of the problem, respectively, where w and $\hat{\mathbf{w}}$ are continuous weighting functions and q and $\hat{\mathbf{q}}$ are the discontinuous streamline upwind contributions, with w , $\hat{\mathbf{w}}$, q and $\hat{\mathbf{q}}$ smooth in the element interiors. A continuous scalar weighting function \bar{w} is used for the potential equation. Now, the weighted residual formulation can be stated as: Find a velocity vector field \mathbf{v} , a temperature field θ and a potential field ϕ such that \mathbf{v} , θ , ϕ and their first partial derivatives with respect to the spatial coordinates and time are square integrable over Ω and satisfy the prescribed boundary conditions on Γ , and such that:

$$\int_{\Omega} w(\dot{\theta} + v_j \theta_{,j}) d\Omega + \int_{\Omega} w_{,j} \theta_{,j} d\Omega + \sum_{e=1}^{n_{el}} \int_{\Omega_e} q(\dot{\theta} + v_j \theta_{,j}) d\Omega = \int_{\Gamma_h} w q d\Gamma \quad (14)$$

$$\begin{aligned}
\int_{\Omega} \hat{w}_i (\dot{v}_i + v_j v_{i,j}) d\Omega &+ Pr \int_{\Omega} \hat{w}_{i,j} [v_{i,j} + v_{j,i}] d\Omega - Ha^2 Pr \int_{\Omega} v_i [e_{Bi} ((\hat{w}_k + \hat{q}_k) e_{Bk}) - (\hat{w}_i + \hat{q}_i)] d\Omega \\
&+ \mathbf{A} \int_{\Omega_e} \{ \hat{q}_i (\dot{v}_i + v_j v_{i,j} + Pr Ra e_{gi} \theta + Ha^2 Pr \epsilon_{ijk} \phi_{,j} e_{Bk}) \} - \int_{\Omega} p \hat{w}_{i,i} d\Omega \\
&+ Ha^2 Pr \int_{\Omega} \hat{w}_i \epsilon_{ijk} \phi_{,j} e_{Bk} d\Omega = -Pr Ra \int_{\Omega} \hat{w}_i e_{gi} \theta d\Omega, \tag{15}
\end{aligned}$$

$$\int_{\Omega} \bar{w}_{,k} \phi_{,k} d\Omega = - \int_{\Omega} v_k \epsilon_{ijk} \bar{w}_{,i} e_{Bj} d\Omega \tag{16}$$

where $i, j, k = 1, \dots, n_{sd}$ and the usual summation notation is implied for repeated indices.

A consistent penalty method using reduced integration for the penalty term is used to enforce incompressibility. This condition can be stated as:

$$p = -\lambda v_{j,j} \tag{17}$$

Now, the spatial interpolation of temperature, velocity and the potential function can now be represented as :

$$\theta(\mathbf{x}^e, t) = \sum_{\beta=1}^{n_{en}^e} \theta_{\beta}^e(t) N_{\beta}^e(\mathbf{x}^e), \quad v_j(\mathbf{x}^e, t) = \sum_{\beta=1}^{n_{en}^e} v_{j\beta}^e(t) N_{\beta}^e(\mathbf{x}^e) \tag{18}$$

$$\phi(\mathbf{x}^e, t) = \sum_{\beta=1}^{n_{en}^e} \phi_{\beta}^e(t) N_{\beta}^e(\mathbf{x}^e), \tag{19}$$

where $N_{\beta}^e(\mathbf{x}^e)$ are the elemental shape functions used to interpolate temperature, velocity and the potential function. The element contributions to the weighting functions w_i , \hat{w}_i and \bar{w}_i are selected as $N_{\alpha}^e(\mathbf{x}^e)$, whereas the discontinuous weighting functions corresponding to $N_{\alpha}^e(\mathbf{x}^e)$ are chosen as below:

$$q_{\alpha}^e = \tilde{k} v_j^e N_{\alpha,j}^e / \|\mathbf{v}^e\|, \tag{20}$$

where

$$\tilde{k} = (\hat{\xi} u_{\xi} h_{\xi} + \hat{\eta} u_{\eta} h_{\eta}) / (\gamma \|u\|). \tag{21}$$

For transient problems, we have selected $\gamma = \sqrt{15}$ and the rest of the notation above is standard.

Finally, with the incorporation of the incompressibility condition, we get the following matrix counterparts for the momentum, energy and electric potential equations:

Momentum equation

$$\mathbf{M} \mathbf{a} + \mathbf{C}' \mathbf{v} + \mathbf{C}'' \mathbf{v} + \mathbf{N}(\mathbf{v}) \mathbf{v} - \mathbf{B}(\mathbf{e}_B) \mathbf{v} + \mathbf{E}(\mathbf{T}) + \mathbf{H}(\phi) = 0 \tag{22}$$

where \mathbf{v} and \mathbf{a} are the vectors containing the velocity and acceleration degrees-of-freedom, respectively, \mathbf{T} is the vector containing the temperature degrees-of-freedom and ϕ is the vector containing the potential degrees-of-freedom. The matrices \mathbf{M} , \mathbf{C}' , \mathbf{C}'' , $\mathbf{N}(\mathbf{v})$, $\mathbf{B}(\mathbf{e}_B)$ and the vectors $\mathbf{E}(\mathbf{T})$ and $\mathbf{H}(\phi)$ are given as follows:

$$\mathbf{M}_{\hat{p}\hat{q}} = \mathbf{A} \left\{ \int_{\Omega_e} (N_{\alpha}^e + q_{\alpha}^e) N_{\beta}^e \delta_{ij} d\Omega \right\}, \tag{23}$$

$$\mathbf{C}''_{\hat{p}\hat{q}} = \lambda \mathbf{A} \left\{ \int_{\Omega_e} N_{\alpha,i}^e N_{\beta,j}^e d\Omega \right\}, \quad (24)$$

$$\mathbf{C}'_{\hat{p}\hat{q}} = Pr \mathbf{A} \left\{ \int_{\Omega_e} N_{\alpha,k}^e N_{\beta,k}^e \delta_{ij} d\Omega \right\}, \quad (25)$$

$$\mathbf{N}(\mathbf{v})_{\hat{p}\hat{q}} = \mathbf{A} \left\{ \int_{\Omega_e} (N_{\alpha}^e + q_{\alpha}^e) v_k^e N_{\beta,k}^e \delta_{ij} d\Omega \right\}, \quad (26)$$

$$\mathbf{B}(\mathbf{e}_B)_{\hat{p}\hat{q}} = Ha^2 Pr \mathbf{A} \left\{ \int_{\Omega_e} N_{\beta}^e \left[e_{Bi} (N_{\alpha}^e + q_{\alpha}^e) \left(\sum_{k=1}^{k=n_{sd}} e_{Bk} \right) - (N_{\alpha}^e + q_{\alpha}^e) \right] \delta_{ij} d\Omega \right\}, \quad (27)$$

$$\mathbf{E}(\mathbf{T})_{\hat{p}} = Pr Ra_T \mathbf{A} \left\{ \int_{\Omega_e} (N_{\alpha}^e + q_{\alpha}^e) \left(T - \frac{Ra_c}{Ra_T} c \right) \cos \gamma_i d\Omega \right\}, \quad (28)$$

$$\mathbf{H}(\phi)_{\hat{p}} = Ha^2 Pr \mathbf{A} \left\{ \int_{\Omega_e} (N_{\alpha}^e + q_{\alpha}^e) \epsilon_{ijk} \phi_{,j} e_{Bk} d\Omega \right\}, \quad (29)$$

where \hat{p} refers to the global velocity degree of freedom in the final system of equations that corresponds to the i^{th} velocity degree of freedom of the elemental node α ($i = 1, \dots, n_{sd}$) in the e^{th} element. Similarly, one can define \hat{q} . Here, q_{α}^e denotes the discontinuous contributions to the Petrov-Galerkin weights. Also, note that γ_j is the angle between the j^{th} coordinate axis and the gravity vector.

Energy equation

$$\mathbf{M}\dot{\mathbf{T}} + \mathbf{K}\mathbf{T} = -\mathbf{F}(\mathbf{v})\mathbf{T} \quad (30)$$

where the dot denotes time derivatives and \mathbf{T} are the temperature degrees of freedom. The same notation is used as in the discrete momentum equation in order to emphasize the similar structure of the two subproblems. The matrices \mathbf{M} , \mathbf{K} , $\mathbf{F}(\mathbf{v})$ are here defined as follows:

$$M_{pq} = \mathbf{A} \left\{ \int_{\Omega_e} (N_{\alpha}^e + q_{\alpha}^e) N_{\beta}^e d\Omega \right\}, \quad (31)$$

$$K_{pq} = \mathbf{A} \left\{ \int_{\Omega_e} N_{\alpha,k}^e N_{\beta,k}^e d\Omega \right\}, \quad (32)$$

$$\mathbf{F}(\mathbf{v})_{pq} = \mathbf{A} \left\{ \int_{\Omega_e} (N_{\alpha}^e + q_{\alpha}^e) v_k^e N_{\beta,k}^e d\Omega \right\}, \quad (33)$$

where p and q refer to the global degrees of freedom in equation (30).

$$\mathbf{K}\phi = -\mathbf{G}(\mathbf{v}) \quad (34)$$

where the dot denotes time derivatives and ϕ are the potential degrees of freedom. The matrix \mathbf{K} and the vector $\mathbf{G}(\mathbf{v})$ are here defined as follows:

$$K_{pq} = \mathbf{A}_{e=1}^{n_{el}} \left\{ \int_{\Omega_e} N_{\alpha,k}^e N_{\beta,k}^e d\Omega \right\}, \quad (35)$$

$$G(v)_p = \mathbf{A}_{e=1}^{n_{el}} \left\{ \int_{\Omega_e} \epsilon_{ijk} N_{\alpha,i}^e v_k e_{Bj} d\Omega \right\}, \quad (36)$$

3.1 Time stepping algorithm

The discretization of the governing equations is complete and the discrete equations listed in the previous section can be solved in a manner similar to that described in [3]. The time stepping is done in the following steps:

1. All dependent variables are known at time level t_n
2. Calculate the temperature values at time t_{n+1} from the energy discrete equation, using the velocity values at time level t_n .
3. Calculate the new velocity field at time t_{n+1} from the discretized Navier-Stokes equations using the updated values of the temperature field and the velocity and potential field at the previous time level t_n
4. Solve the potential equation to obtain the potential field at time t_{n+1} using the velocity field at time t_{n+1} .
5. Time step is completed, go to step 1.

3.2 Implementation

The development of the numerical software for this coupled system of partial differential equations is done using *diffpack* [4], which is a standard library of C++ routines. Sincere effort is made to make the code fully object-oriented. The details of the design and the development of class heirarchies follow next.

A buoyancy driven flow in the presence of a constant magnetic field is affected by three governing equations, in particular the NavierStokes equation, the energy equation and the electric potential equation. This mathematical structure of the problem involved automatically dictates the definition of a main class ‘MagnetoConvection’ and three sub classes ‘NavierStokes1’, ‘NIHeat1’ and ‘Potential’ each managing the data and solution process of the corresponding governing equations.

The structure of the code in the sense of the main classes involved is depicted in Fig. 2. The details of the main class ‘MagnetoConvection’ is shown in Box I.

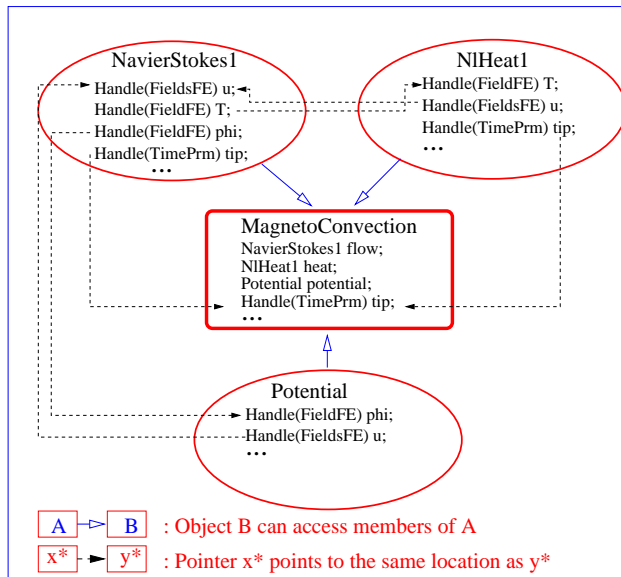


Figure 2: Details of the coupling of the various classes and fields

Box I

The definition of the class ‘MagnetoConvection’.

```

class MagnetoConvection : public HandleId {
protected:
    Handle(NIHeat1)      heat;           // pointer to heat transport problem
    Handle(NavierStokes1) flow;         // pointer to flow problem
    Handle(Potential)   potential;     // pointer to potential problem
    Handle(TimePrm)    tip;            // time integration parameters
    SetOfNo(real)      times_store;    // times to store simulations results
public:

    void define(MenuSystem& menu, int level = MAIN);
    void scan(MenuSystem& menu);
    void adm(MenuSystem& menu);
    void solveProblem();
    void storeResults();
    void solveAtThisTimeLevel();
    virtual void bindHandles()=0;
};

```

4 Numerical example

A test example of buoyancy driven convection under the action of a constant magnetic field was tried out for various values of hartmann numbers ranging from 0 to 200. The problem was obtained from [1]. The problem domain consists of a rectangular finite cavity of aspect ratio 4. The right and left hand side of the cavity are maintained at nondimensional temperature 1.0 and 0.0 respectively. The magnetic field is parallel to the

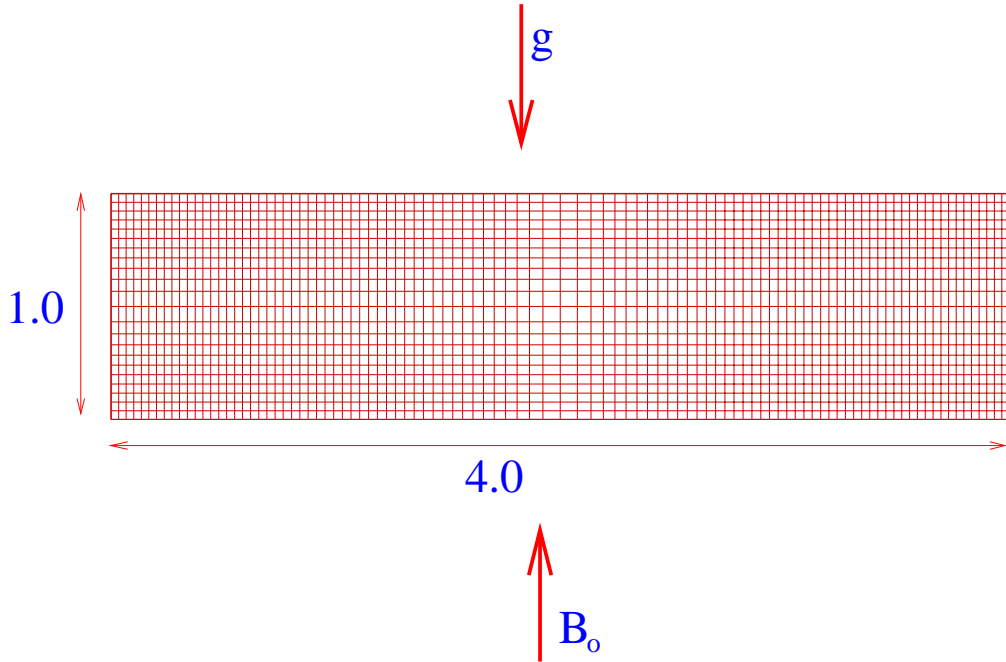


Figure 3: Finite element mesh and geometry.

Hartmann number	Ψ_{max}
0	0.55005
5	0.34475
50	0.00945
100	0.00246
200	0.00063

Table 1: Maximum stream function values versus the Hartmann number

positive y-axis and is assumed unaffected by the flow[2]. A grid of 23 by 101 was chosen to sufficiently capture the hartmann and also maintain the computational time at a low level (see Fig. 3). The Grashof number is chosen as 2×10^4 and the prandtl number to be 0.01, characteristic of semiconductor melts. The problem was run upto a nondimensional time of 10.0 at which the flow seemed to have reached a steady state. Due to stability restrictions a small nondimensional time step of 0.004 was chosen for the computation. The results show a distinct change in flow pattern with increasing magnetic field. At zero hartmann number the flow showed a intense central circulation loop and two weaker loops at the side. As the hartmann number was increased to 5 the weaker loops at the side disappeared. As the hartmann number is increased the streamlines accumulate near the walls of the cavity indicating a formation of a boundary layer. Also, a tremendous drop is seen in the flow intensity. This in turn leads to isotherms being parallel to the vertical walls and not being curved as for the zero hartmann number case. The streamlines and isotherms at the end of the simulation for a few hartmann numbers are shown in Fig. 5 and Fig. 4. Table 1. shows the maximum stream function values as a function of hartmann number. A comparison of normalized velocity profiles is shown in Fig. 6 and Fig. 7. A plot showing the variation of maximum of the horizontal and vertical velocity as a function of hartmann number is shown in Figs. 8 and 9. It is observed that high hartmann numbers the maximum horizontal velocity drops as Ha^{-2} whereas the maximum vertical velocity drops as $Ha^{-1.5}$.

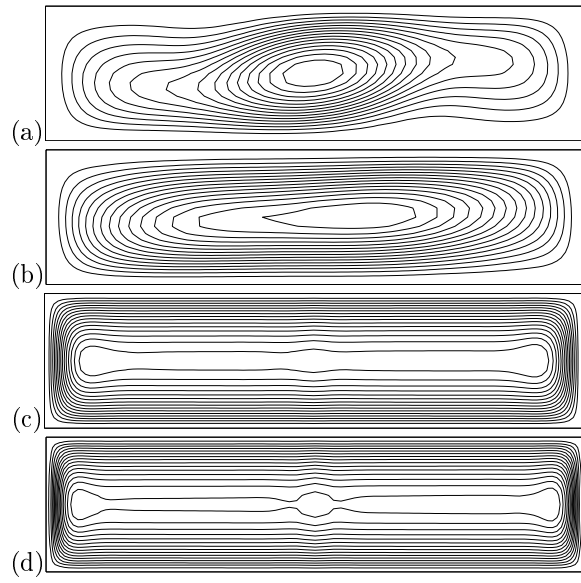


Figure 4: Streamlines giving the structure of the flow. Results shown for Hartmann numbers (a) 0 (b) 5 (c) 50 and (d) 100

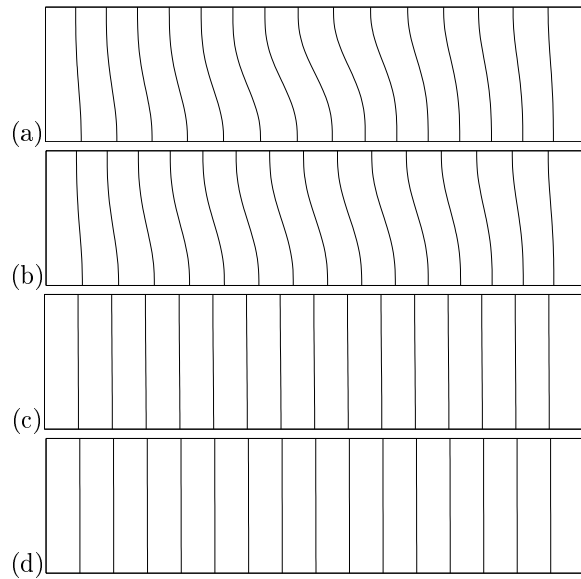


Figure 5: Isotherms giving the temperature distribution in the cavity. Results shown for Hartmann numbers (a) 0 (b) 5 (c) 50 and (d) 100

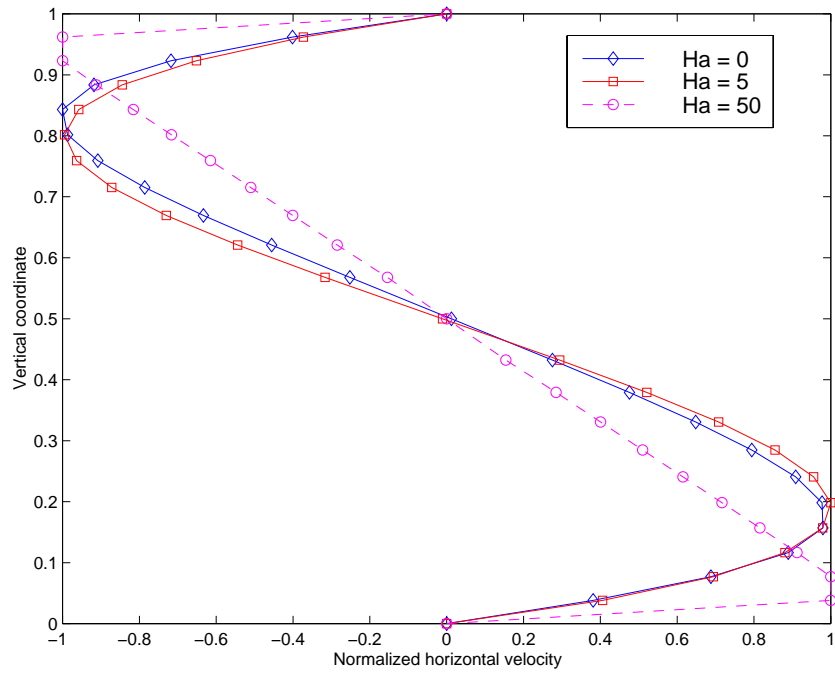


Figure 6: Vertical profile of the normalized horizontal velocity at midlength of the cavity

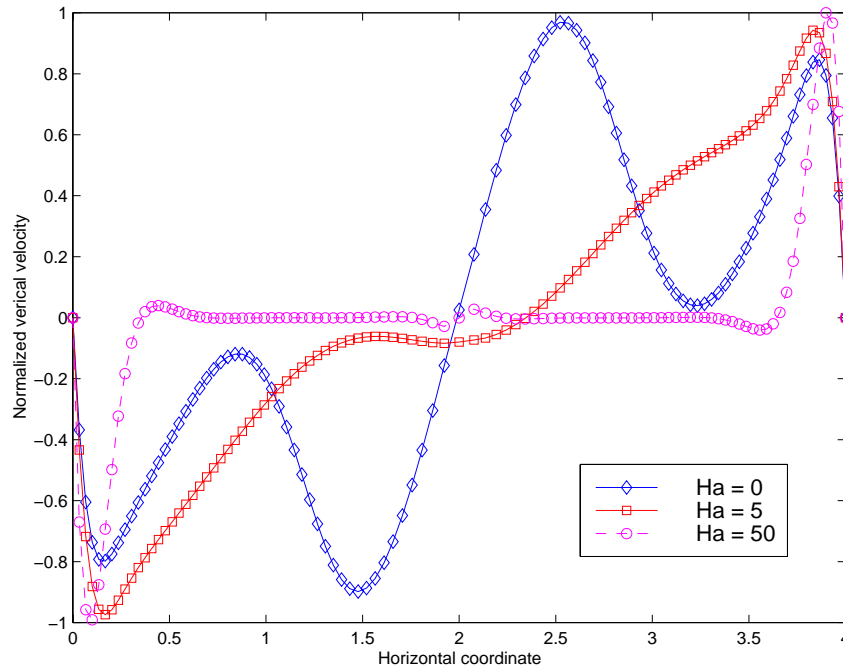


Figure 7: Horizontal profile of the normalized vertical velocity at midheight of the cavity

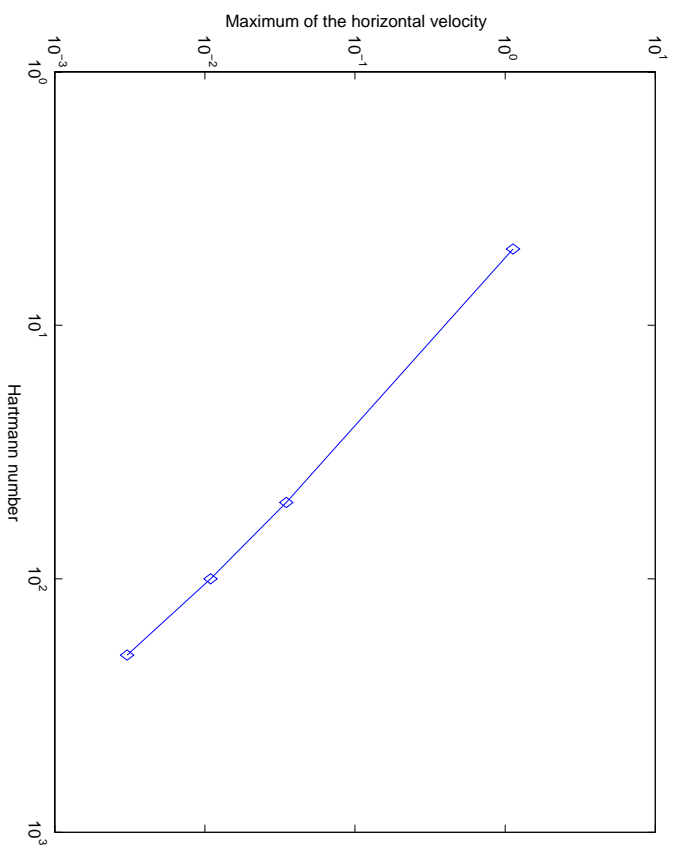


Figure 8: Plots of the maxima of the horizontal velocity versus Hartmann number

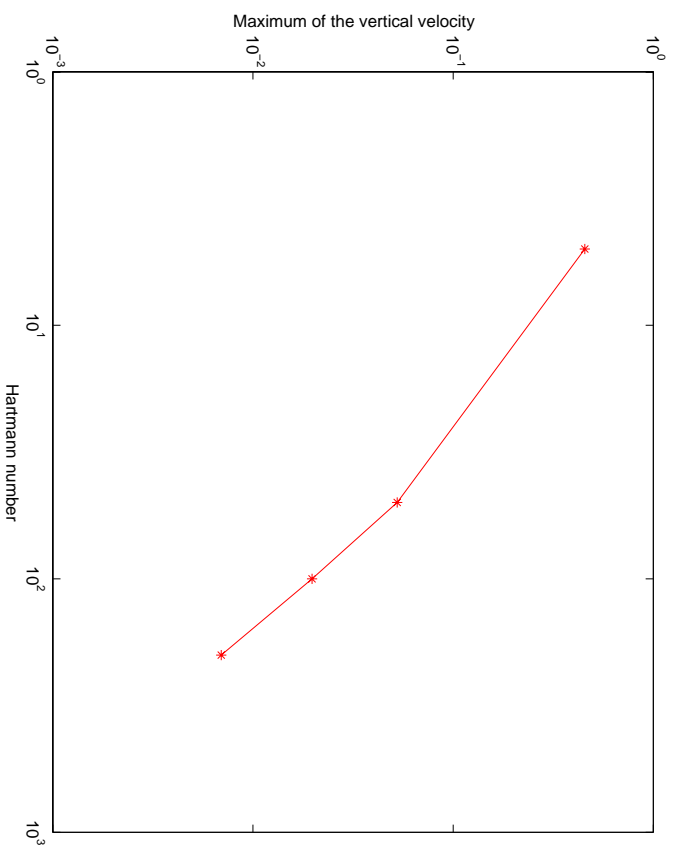


Figure 9: Plots of the maxima of the vertical velocity versus Hartmann number

5 Definition of the inverse magneto-convection problem

A well-posed direct magneto-convection problem is obtained only when all the boundary conditions are provided on the boundary. The inverse design is posed such that the boundary heat flux distribution at $\Gamma_{h0} \subset \Gamma_h$ is not known ($\Gamma_{h0} \cup \Gamma_{h1} = \Gamma_h$, $\Gamma_{h0} \cap \Gamma_{h1} = \emptyset$)

The known flux and temperature distributions are given below:

$$\theta(\mathbf{x}, t) = \theta_g(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_g \times [0, t_{max}] \quad (37)$$

$$q(\mathbf{x}, t) \equiv \nabla\theta(\mathbf{x}, t) \cdot \mathbf{n} = q_1(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_{h1} \times [0, t_{max}], \quad (38)$$

while the *unknown* flux distribution in Γ_{h0} is

$$q(\mathbf{x}, t) \equiv \nabla\theta(\mathbf{x}, t) \cdot \mathbf{n} = q_o(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_{h0} \times [0, t_{max}]. \quad (39)$$

The objective of the present work is to present a methodology for the calculation of the unknown heat flux $q_o(\mathbf{x}, t)$, $(\mathbf{x}, t) \in \Gamma_{h0} \times [0, t_{max}]$ given equations (5 – 13, 37 – 38) and some additional information about the temperature field.

In this work we assume that the temperature field is a-priori known in a subset Γ_I of the boundary Γ_{h1} where the flux $q_1(\mathbf{x}, t) \equiv q_I(\mathbf{x}, t)$ is known, i.e.

$$\theta(\mathbf{x}, t) = \theta_m(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_I \times [0, t_{max}], \quad (40)$$

where $\theta_m(\mathbf{x}, t)$ is known.

The over-specified thermal boundary condition on Γ_I together with equations (5 – 13, 37 – 38) define an *ill-posed inverse problem* that can be solved to calculate the unknown heat flux q_o on Γ_{h0} . Once this flux is calculated, equations (5 – 13, 37 – 39) can be used to solve a *direct magneto-convection problem* for the calculation of the temperature and velocity for each $(\mathbf{x}, t) \in \Omega \times [0, t_{max}]$.

In this work, we will assume that a solution to the inverse problem exists in the sense of Tichonov. In particular, we are looking for a (quasi-) solution $\bar{q}_o(\mathbf{x}, t) \in L_2(\Gamma_{h0} \times [0, t_{max}])$ such that:

$$S(\bar{q}_o) \leq S(q_o), \quad \forall q_o \in L_2(\Gamma_{h0} \times [0, t_{max}]), \quad (41)$$

where

$$\begin{aligned} S(q_o) &= \frac{1}{2} \|\theta(\mathbf{x}, t; q_o) - \theta_m(\mathbf{x}, t)\|_{L_2(\Gamma_I \times [0, t_{max}])}^2 \\ &= \frac{1}{2} \int_0^{t_{max}} \int_{\Gamma_I} [\theta(\mathbf{x}, t; q_o) - \theta_m(\mathbf{x}, t)]^2 d\Gamma dt. \end{aligned} \quad (42)$$

In the above equation, $\theta(\mathbf{x}, t; q_o)$, is defined as the solution of a direct magneto-convection problem with an applied magnetic field and with the thermal boundary conditions given by equations (37) and (38) and with the flux $q_o(\mathbf{x}, t)$ applied on Γ_{h0} . The direct problem that defines $\theta(\mathbf{x}, t; q_o)$, $\mathbf{v}(\mathbf{x}, t; q_o)$ and $\phi(\mathbf{x}, t; q_o)$ is summarized in Box II.

Box II

Direct problem to define $\theta(\mathbf{x}, t; q_o)$, $\mathbf{v}(\mathbf{x}, t; q_o)$ and $\phi(\mathbf{x}, t; q_o)$

$$\frac{\partial \theta(\mathbf{x}, t; q_o)}{\partial t} + \mathbf{v}(\mathbf{x}, t; q_o) \cdot \nabla \theta(\mathbf{x}, t; q_o) = \nabla^2 \theta(\mathbf{x}, t; q_o), \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (43)$$

$$\begin{aligned} \frac{\partial \mathbf{v}(\mathbf{x}, t; q_o)}{\partial t} + (\nabla \mathbf{v}(\mathbf{x}, t; q_o)) \mathbf{v}(\mathbf{x}, t; q_o) &= \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}, t; q_o) - RaPr\theta(\mathbf{x}, t; q_o)\mathbf{e}_g \\ + Ha^2Pr[-\nabla \phi(\mathbf{x}, t; q_o) + \mathbf{v}(\mathbf{x}, t; q_o) \times \mathbf{e}_B] \times \mathbf{e}_B & \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \end{aligned} \quad (44)$$

$$\boldsymbol{\sigma}(\mathbf{x}, t; q_o) = -p(\mathbf{x}, t; q_o)\mathbf{I} + Pr[\nabla \mathbf{v}(\mathbf{x}, t; q_o) + (\nabla \mathbf{v}(\mathbf{x}, t; q_o))^T], \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (45)$$

$$\nabla \cdot \mathbf{v}(\mathbf{x}, t; q_o) = 0, \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (46)$$

$$\theta(\mathbf{x}, 0; q_o) = \theta_{in}(\mathbf{x}), \quad \mathbf{x} \in \Omega \quad (47)$$

$$\mathbf{v}(\mathbf{x}, 0; q_o) = \mathbf{v}_{in}(\mathbf{x}), \quad \mathbf{x} \in \Omega \quad (48)$$

$$\mathbf{v}(\mathbf{x}, t; q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}] \quad (49)$$

$$\theta(\mathbf{x}, t; q_o) = \theta_g, \quad (\mathbf{x}, t) \in \Gamma_g \times [0, t_{max}] \quad (50)$$

$$\frac{\partial \theta}{\partial n}(\mathbf{x}, t; q_o) = q_1(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_{h1} \times [0, t_{max}] \quad (51)$$

$$\frac{\partial \theta}{\partial n}(\mathbf{x}, t; q_o) = q_o(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_{h0} \times [0, t_{max}] \quad (52)$$

$$\nabla^2 \phi(\mathbf{x}, t; q_o) = \nabla \cdot (\mathbf{v}(\mathbf{x}, t; q_o) \times \mathbf{e}_B), \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (53)$$

$$\frac{\partial \phi}{\partial n}(\mathbf{x}, t; q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}] \quad (54)$$

The main difficulty with the above optimization problem is the calculation of the gradient $S'(q_o(\mathbf{x}, t))$ of the cost functional in the $L_2(\Gamma_{h0} \times [0, t_{max}])$ space. Introducing the directional derivative $D_{\Delta q_o} S(q_o) \equiv (S'(q_o), \Delta q_o)_{L_2(\Gamma_{h0} \times [0, t_{max}])}$ of $S(q_o)$, and using eq. (42), we can write the following:

$$\begin{aligned} D_{\Delta q_o} S(q_o) &\equiv (S'(q_o), \Delta q_o)_{L_2(\Gamma_{h0} \times [0, t_{max}])} \\ &= (\theta(\mathbf{x}, t; q_o) - \theta_m, \Theta(\mathbf{x}, t; q_o, \Delta q_o))_{L_2(\Gamma_I \times [0, t_{max}])}, \end{aligned} \quad (55)$$

where the sensitivity temperature field $\Theta(\mathbf{x}, t; q_o, \Delta q_o) \equiv D_{\Delta q_o} \theta(\mathbf{x}, t; q_o)$, and the sensitivity velocity field and the sensitivity electric potential field written as $\mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o) \equiv D_{\Delta q_o} \mathbf{v}(\mathbf{x}, t; q_o)$ and $\Phi(\mathbf{x}, t; q_o, \Delta q_o) \equiv D_{\Delta q_o} \phi(\mathbf{x}, t; q_o)$ respectively, are defined as the linear Δq_o parts of $\theta(\mathbf{x}, t; q_o + \Delta q_o)$, $\mathbf{v}(\mathbf{x}, t; q_o + \Delta q_o)$ and $\phi(\mathbf{x}, t; q_o + \Delta q_o)$ calculated at q_o , i.e.

$$\theta(\mathbf{x}, t; q_o + \Delta q_o) = \theta(\mathbf{x}, t; q_o) + \Theta(\mathbf{x}, t; q_o, \Delta q_o) + O(\|\Delta q_o\|_{L_2(\Gamma_{h0} \times [0, t_{max}])}^2)$$

$$\mathbf{v}(\mathbf{x}, t; q_o + \Delta q_o) = \mathbf{v}(\mathbf{x}, t; q_o) + \mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o) + O(\|\Delta q_o\|_{L_2(\Gamma_{h0} \times [0, t_{max}])}^2)$$

$$\phi(\mathbf{x}, t; q_o + \Delta q_o) = \phi(\mathbf{x}, t; q_o) + \Phi(\mathbf{x}, t; q_o, \Delta q_o) + O(\|\Delta q_o\|_{L_2(\Gamma_{h0} \times [0, t_{max}])}^2)$$

As it becomes clear from eq. (55), the calculation of the gradient $S'(q_o)$ requires the evaluation of the adjoint to the sensitivity of the temperature operator. The definition of the thermal, fluid flow and electric potential sensitivity problems that define $\Theta(\mathbf{x}, t; q_o, \Delta q_o)$, $\mathbf{v}(\mathbf{x}, t; q_o, \Delta q_o)$ and $\Phi(\mathbf{x}, t; q_o, \Delta q_o)$ respectively, is undertaken next, while the calculation of the gradient $S'(q_o)$ is discussed after that.

5.1 A functional optimization formulation of the inverse magneto-convection problem

5.1.1 Governing equations for the sensitivity problem

Taking the directional derivatives of the governing equations of Box II, in the direction of Δq_o and calculated at the direct fields $\theta(\mathbf{x}, t; q_o)$, $\mathbf{v}(\mathbf{x}, t; q_o)$ and $\phi(\mathbf{x}, t; q_o)$ corresponding to the boundary flux q_o , results in a *linear sensitivity magneto-convection problem* that can be used to evaluate the fields $\Theta(\mathbf{x}, t; q_o, \Delta q_o)$, $\mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o)$ and $\Phi(\mathbf{x}, t; q_o, \Delta q_o)$. This sensitivity problem is summarized in Box III, where $\Sigma(\mathbf{x}, t; q_o, \Delta q_o)$ and $\Pi(\mathbf{x}, t; q_o, \Delta q_o)$ are used to denote the directional derivatives of $\sigma(\mathbf{x}, t; q_o)$ and $p(\mathbf{x}, t; q_o)$, respectively.

Box III

Sensitivity problem to define $\Theta(\mathbf{x}, t; q_o, \Delta q_o)$, $\mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o)$ and $\Phi(\mathbf{x}, t; q_o, \Delta q_o)$

$$\begin{aligned} \frac{\partial \Theta(\mathbf{x}, t; q_o, \Delta q_o)}{\partial t} + \mathbf{v}(\mathbf{x}, t; q_o) \cdot \nabla \Theta(\mathbf{x}, t; q_o, \Delta q_o) + \mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o) \cdot \nabla \theta(\mathbf{x}, t; q_o) \\ = \nabla^2 \Theta(\mathbf{x}, t; q_o, \Delta q_o), \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \end{aligned} \quad (56)$$

$$\begin{aligned} \frac{\partial \mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o)}{\partial t} + (\nabla \mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o)) \mathbf{v}(\mathbf{x}, t; q_o) + [\nabla \mathbf{v}(\mathbf{x}, t; q_o)] \mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o) = \\ \nabla \cdot \Sigma(\mathbf{x}, t; q_o, \Delta q_o) - Pr Ra \Theta(\mathbf{x}, t; q_o, \Delta q_o) \mathbf{e}_g + Ha^2 Pr [-\nabla \Phi + \mathbf{V} \times \mathbf{e}_B] \times \mathbf{e}_B, \\ (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \end{aligned} \quad (57)$$

$$\begin{aligned} \Sigma(\mathbf{x}, t; q_o, \Delta q_o) = -\Pi(\mathbf{x}, t; q_o, \Delta q_o) \mathbf{I} + Pr [\nabla \mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o) + (\nabla \mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o))^T], \\ (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \end{aligned} \quad (58)$$

$$\nabla \cdot \mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o) = 0, \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (59)$$

$$\Theta(\mathbf{x}, 0; q_o, \Delta q_o) = 0, \quad \mathbf{x} \in \Omega \quad (60)$$

$$\mathbf{V}(\mathbf{x}, 0; q_o, \Delta q_o) = 0, \quad \mathbf{x} \in \Omega \quad (61)$$

$$\mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}] \quad (62)$$

$$\Theta(\mathbf{x}, t; q_o, \Delta q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma_g \times [0, t_{max}] \quad (63)$$

$$\frac{\partial \Theta}{\partial n}(\mathbf{x}, t; q_o, \Delta q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma_{h1} \times [0, t_{max}] \quad (64)$$

$$\frac{\partial \Theta}{\partial n}(\mathbf{x}, t; q_o, \Delta q_o) = \Delta q_o(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_{ho} \times [0, t_{max}] \quad (65)$$

$$\nabla^2 \Phi(\mathbf{x}, t; q_o, \Delta q_o) = \nabla \cdot (\mathbf{V}(\mathbf{x}, t; q_o, \Delta q_o) \times \mathbf{e}_B), \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (66)$$

$$\frac{\partial \Phi}{\partial n}(\mathbf{x}, t; q_o, \Delta q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}] \quad (67)$$

5.1.2 Governing Equations for the Adjoint Problem

As we already mentioned, the calculation of the gradient of the objective function requires the appropriate evaluation of the adjoint operators to the sensitivity operators that are defined in II. We will derive the adjoint operator in this section. Let us use ψ to denote the adjoint temperature function, ϕ the adjoint velocity function and η to denote the adjoint potential function. Let us denote the sensitivity operators for the thermal, fluid flow and potential problems by \mathcal{F} , \mathcal{G} and \mathcal{H} respectively. The adjoint operators \mathcal{F}^* , \mathcal{G}^* , \mathcal{H}^* are defined from the following *Lagrange identities*:

$$(\mathcal{F}^* \psi, \Theta)_{L_2(\Omega \times [0, t_{max}])} = (\psi, \mathcal{F}(\Theta))_{L_2(\Omega \times [0, t_{max}])} \equiv 0, \quad (68)$$

$$(\mathcal{G}^* \phi, \mathbf{V})_{L_2(\Omega \times [0, t_{max}])} = (\phi, \mathcal{G}(\mathbf{V}))_{L_2(\Omega \times [0, t_{max}])} \equiv 0, \quad (69)$$

$$(\mathcal{H}^* \eta, \Phi)_{L_2(\Omega \times [0, t_{max}])} = (\eta, \mathcal{H}(\Phi))_{L_2(\Omega \times [0, t_{max}])} \equiv 0, \quad (70)$$

where $(f, g)_{L_2(\Omega \times [0, t_{max}])}$ is used to denote the dot product of any functions f and g in $L_2(\Omega \times [0, t_{max}])$. Let us first start from $(\phi, \mathcal{G}(\mathbf{V}))_{L_2(\Omega \times [0, t_{max}])} \equiv 0$ to calculate \mathcal{G}^* , i.e.

$$\int_0^{t_{max}} \int_{\Omega} \phi \cdot \left\{ \frac{\partial \mathbf{V}}{\partial t} + (\nabla \mathbf{V}) \mathbf{v} + (\nabla \mathbf{v}) \mathbf{V} + \nabla \Pi - Pr \nabla \cdot [\nabla \mathbf{V} + (\nabla \mathbf{V})^T] \right. \\ \left. + Pr Ra \Theta \mathbf{e}_g + Ha^2 Pr \nabla \Phi \times \mathbf{e}_B - Ha^2 Pr [V \times \mathbf{e}_B] \times \mathbf{e}_B \right\} d\Omega dt = 0. \quad (71)$$

Integration by parts of the first term of the above equation gives the following:

$$\int_0^{t_{max}} \int_{\Omega} \phi \cdot \frac{\partial \mathbf{V}}{\partial t} d\Omega dt = - \int_0^{t_{max}} \int_{\Omega} \mathbf{V} \cdot \frac{\partial \phi}{\partial t} d\Omega dt. \quad (72)$$

where we have introduced a final condition for the adjoint velocity ϕ as follows:

$$\phi(\mathbf{x}, t_{max}) = 0, \quad \mathbf{x} \in \Omega. \quad (73)$$

We can go on working on each term one by one and finally arrive at the following result(refer CMAME 144(1997)251-253 for exact details)

$$\int_0^{t_{max}} \int_{\Omega} \mathbf{V} \cdot \left\{ -\frac{\partial \phi}{\partial t} - (\nabla \phi) \mathbf{v} + (\nabla \mathbf{v})^T \phi - \nabla \cdot \zeta \right\} d\Omega dt + \int_0^{t_{max}} \int_{\Omega} Pr Ra (\phi \cdot \mathbf{e}_g) \Theta d\Omega dt \\ + \int_0^{t_{max}} \int_{\Omega} Ha^2 Pr (\phi \cdot (\nabla \Phi \times \mathbf{e}_B)) d\Omega dt - \int_0^{t_{max}} \int_{\Omega} Ha^2 Pr (\phi \cdot [V \times \mathbf{e}_B] \times \mathbf{e}_B) d\Omega dt = 0, \quad (74)$$

where we have restricted the adjoint velocity ϕ to satisfy the no-slip condition on the boundary Γ i.e.,

$$\phi(\mathbf{x}, t) = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}] \quad (75)$$

and also we have introduced the adjoint stress tensor $\zeta(\mathbf{x}, t)$ defined as follows:

$$\zeta(\mathbf{x}, t) = -\pi(\mathbf{x}, t) \mathbf{I} + Pr [\nabla \phi(\mathbf{x}, t) + (\nabla \phi(\mathbf{x}, t))^T], \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}]. \quad (76)$$

where $\pi(\mathbf{x}, t)$ is an adjoint pressure term defined to enforce incompressibility constraint for ϕ .

Having in mind the type of coupling that exists between the operators \mathcal{F} , \mathcal{G} and \mathcal{H} , we will show that similar type of coupling will be necessary for the operators \mathcal{F}^* , \mathcal{G}^* and \mathcal{H}^* .

Let us look at the last term in Eq. 74, i.e,

$$- \int_0^{t_{max}} \int_{\Omega} Ha^2 Pr (\phi \cdot [V \times \mathbf{e}_B] \times \mathbf{e}_B) d\Omega dt \quad (77)$$

Now consider $\phi \cdot [V \times \mathbf{e}_B] \times \mathbf{e}_B$,

$$\phi \cdot [V \times \mathbf{e}_B] \times \mathbf{e}_B = \phi_q [\epsilon_{ijk} V_i e_{Bj}] \epsilon_{kpq} e_{Bp} = \epsilon_{ijk} \epsilon_{kpq} [\phi_q V_i e_{Bj} e_{Bp}] = \\ \epsilon_{kij} \epsilon_{kpq} [\phi_q V_i e_{Bj} e_{Bp}] \quad (78)$$

Now $\epsilon_{kij} \epsilon_{kpq} = (\delta_{ip} \delta_{jq} - \delta_{iq} \delta_{jp})$

Therefore Eq. 78 becomes,

$$\phi \cdot [V \times \mathbf{e}_B] \times \mathbf{e}_B = (\delta_{ip} \delta_{jq} - \delta_{iq} \delta_{jp}) [\phi_q V_i e_{Bj} e_{Bp}] \\ = [\phi_j V_i e_{Bj} e_{Bi}] - [\phi_i V_i e_{Bj} e_{Bj}] = (\mathbf{V} \cdot \mathbf{e}_B) (\phi \cdot \mathbf{e}_B) - (\phi \cdot \mathbf{V}) (1) \\ = \mathbf{V} \cdot [\mathbf{e}_B (\phi \cdot \mathbf{e}_B) - \phi] \quad (79)$$

Hence, substituting Eq. 79 in Eq. 77, the last term in Eq. 74 becomes

$$-\int_0^{t_{max}} \int_{\Omega} Ha^2 Pr V \cdot [e_B(\phi \cdot e_B) - \phi] d\Omega dt \quad (80)$$

Now 74 becomes

$$\begin{aligned} & \int_0^{t_{max}} \int_{\Omega} \mathbf{V} \cdot \left\{ -\frac{\partial \phi}{\partial t} - (\nabla \phi) \mathbf{v} + (\nabla \mathbf{v})^T \phi - \nabla \cdot \zeta - Ha^2 Pr [e_B(\phi \cdot e_B) - \phi] \right\} d\Omega dt \\ & + \int_0^{t_{max}} \int_{\Omega} Pr Ra (\phi \cdot e_g) \Theta d\Omega dt + \int_0^{t_{max}} \int_{\Omega} Ha^2 Pr (\phi \cdot (\nabla \Phi \times e_B)) d\Omega dt = 0, \end{aligned} \quad (81)$$

Now lets us consider the last term in Eq. 81 i.e,

$$\int_0^{t_{max}} \int_{\Omega} Ha^2 Pr (\phi \cdot (\nabla \Phi \times e_B)) d\Omega dt \quad (82)$$

Now, $\phi \cdot (\nabla \Phi \times e_B) = -\nabla \Phi \cdot (\phi \times e_B)$, by the property of scalar triple products.

Now consider,

$$\begin{aligned} & \nabla \cdot ((\phi \times e_B) \Phi) = \Phi \nabla \cdot (\phi \times e_B) + \nabla \Phi \cdot (\phi \times e_B) \\ \Rightarrow & \nabla \cdot ((\phi \times e_B) \Phi) = \Phi \nabla \cdot (\phi \times e_B) - \phi \cdot (\nabla \Phi \times e_B) \end{aligned} \quad (83)$$

Integrating the left hand side of Eq. 83 we have,

$$\int_0^{t_{max}} \int_{\Omega} \nabla \cdot ((\phi \times e_B) \Phi) d\Omega dt = \int_0^{t_{max}} \int_{\Gamma} (\phi \times e_B) \Phi \cdot \mathbf{n} d\Gamma dt = 0 \quad (84)$$

because $\phi(\mathbf{x}, t) = 0$, $(\mathbf{x}, t) \in \Gamma$. This leads to,

$$\int_0^{t_{max}} \int_{\Omega} \Phi \nabla \cdot (\phi \times e_B) d\Omega dt = \int_0^{t_{max}} \int_{\Omega} \phi \cdot (\nabla \Phi \times e_B) d\Omega dt \quad (85)$$

Hence, Eq 81 can be rewritten as,

$$\begin{aligned} & \int_0^{t_{max}} \int_{\Omega} \mathbf{V} \cdot \left\{ -\frac{\partial \phi}{\partial t} - (\nabla \phi) \mathbf{v} + (\nabla \mathbf{v})^T \phi - \nabla \cdot \zeta - Ha^2 Pr [e_B(\phi \cdot e_B) - \phi] \right\} d\Omega dt \\ & + \int_0^{t_{max}} \int_{\Omega} Pr Ra (\phi \cdot e_g) \Theta d\Omega dt + \int_0^{t_{max}} \int_{\Omega} Ha^2 Pr \Phi \nabla \cdot (\phi \times e_B) d\Omega dt = 0, \end{aligned} \quad (86)$$

As already noted before we expect the operators \mathcal{F}^* , \mathcal{G}^* and \mathcal{H}^* to be coupled in a fashion similar to that of the coupling of the sensitivity operators. Keeping that in mind we rewrite Eq. 86 as follows:

$$\begin{aligned} & \int_0^{t_{max}} \int_{\Omega} \mathbf{V} \cdot \left\{ -\frac{\partial \phi}{\partial t} - (\nabla \phi) \mathbf{v} + (\nabla \mathbf{v})^T \phi - \nabla \cdot \zeta - Ha^2 Pr [e_B(\phi \cdot e_B) - \phi] \right. \\ & \quad \left. + Pr Ra \psi \nabla \theta + Ha^2 Pr [\nabla \eta \times e_B] \right\} d\Omega dt + \int_0^{t_{max}} \int_{\Omega} Pr Ra \{ (\phi \cdot e_g) \Theta \\ & - \psi \mathbf{V} \cdot \nabla \theta \} d\Omega dt + \int_0^{t_{max}} \int_{\Omega} Ha^2 Pr \{ \Phi \nabla \cdot (\phi \times e_B) - \mathbf{V} \cdot (\nabla \eta \times e_B) \} d\Omega dt = 0, \end{aligned} \quad (87)$$

and define the adjoint velocity operator \mathcal{G}^* such that

$$\begin{aligned} \mathcal{G}^*(\phi) \equiv & -\frac{\partial \phi}{\partial t} - (\nabla \phi) \mathbf{v} + (\nabla \mathbf{v})^T \phi - \nabla \cdot \zeta - Ha^2 Pr[\mathbf{e}_B(\phi \cdot \mathbf{e}_B) - \phi] \\ & + Pr Ra \psi \nabla \theta + Ha^2 Pr[\nabla \eta \times \mathbf{e}_B] = 0 \end{aligned} \quad (88)$$

With the above definition we have the following coupling criterion between the the adjoint fields ϕ , ψ and η ,

$$\int_0^{t_{max}} \int_{\Omega} \phi \cdot \mathbf{e}_g \Theta d\Omega dt = \int_0^{t_{max}} \int_{\Omega} \psi \mathbf{V} \cdot \nabla \theta d\Omega dt. \quad (89)$$

and

$$\int_0^{t_{max}} \int_{\Omega} \Phi \nabla \cdot (\phi \times \mathbf{e}_B) d\Omega dt = \int_0^{t_{max}} \int_{\Omega} \mathbf{V} \cdot (\nabla \eta \times \mathbf{e}_B) d\Omega dt \quad (90)$$

Remark 1: Note that the coupling criterion is as expected. We see that there is no direct coupling between the thermal and electromagnetic adjoint problems. The coupling is indirect through the fluid flow problem. The derivation of the operator \mathcal{H}^* is very similar to the fluid flow operator. We first start from $(\eta, \mathcal{H}(\Phi))_{L_2(\Omega \times [0, t_{max}])} \equiv 0$, i.e.

$$\int_0^{t_{max}} \int_{\Omega} \eta [\nabla^2 \Phi - \nabla \cdot (\mathbf{V} \times \mathbf{e}_B)] d\Omega dt = 0 \quad (91)$$

Consider the first term,

$$\int_0^{t_{max}} \int_{\Omega} \eta \nabla^2 \Phi d\Omega dt = \int_0^{t_{max}} \int_{\Omega} \Phi \nabla^2 \eta d\Omega dt + \int_0^{t_{max}} \int_{\Gamma} (\eta \nabla \Phi - \Phi \nabla \eta) \cdot \mathbf{n} d\Gamma dt \quad (92)$$

Introduce boundary conditions for the adjoint potential field η as

$$\nabla \eta(\mathbf{x}, t) \cdot \mathbf{n} = 0, \quad (\mathbf{x}, t) \in \Gamma \quad (93)$$

Using this and zero normal derivative condition for the sensitivity field Φ the last term in Eq. 92 vanishes and we have the following for the first term,

$$\int_0^{t_{max}} \int_{\Omega} \eta \nabla^2 \Phi d\Omega dt = \int_0^{t_{max}} \int_{\Omega} \Phi \nabla^2 \eta d\Omega dt \quad (94)$$

Now we consider the second term in Eq. 91, i.e.

$$- \int_0^{t_{max}} \int_{\Omega} \eta [\nabla \cdot (\mathbf{V} \times \mathbf{e}_B)] d\Omega dt \quad (95)$$

Now, consider the following identity,

$$\nabla \cdot [\eta(\mathbf{V} \times \mathbf{e}_B)] = \nabla \eta \cdot (\mathbf{V} \times \mathbf{e}_B) + \eta \nabla \cdot (\mathbf{V} \times \mathbf{e}_B) \quad (96)$$

Integrating Eq. 96 we have,

$$\begin{aligned} \int_0^{t_{max}} \int_{\Omega} \nabla \cdot [\eta(\mathbf{V} \times \mathbf{e}_B)] d\Omega dt &= \int_0^{t_{max}} \int_{\Gamma} \eta(\mathbf{V} \times \mathbf{e}_B) \cdot \mathbf{n} d\Gamma = 0 = \\ & \int_0^{t_{max}} \int_{\Omega} (\nabla \eta \cdot (\mathbf{V} \times \mathbf{e}_B)) d\Omega dt + \int_0^{t_{max}} \int_{\Omega} \eta (\nabla \cdot (\mathbf{V} \times \mathbf{e}_B)) d\Omega dt \end{aligned} \quad (97)$$

The boundary integral goes to zero because of the no-slip condition for the sensitivity velocity field \mathbf{V} . Now we have,

$$\begin{aligned} \int_0^{t_{max}} \int_{\Omega} \eta (\nabla \cdot (\mathbf{V} \times \mathbf{e}_B)) d\Omega dt &= - \int_0^{t_{max}} \int_{\Omega} (\nabla \eta \cdot (\mathbf{V} \times \mathbf{e}_B)) d\Omega dt = \\ &= \int_0^{t_{max}} \int_{\Omega} (\mathbf{V} \cdot (\nabla \eta \times \mathbf{e}_B)) d\Omega dt \end{aligned} \quad (98)$$

Now using Eq. 94 and Eq. 98 we can rewrite Eq. 91 as,

$$\begin{aligned} &\left\{ \int_0^{t_{max}} \int_{\Omega} \Phi \nabla^2 \eta d\Omega dt - \int_0^{t_{max}} \int_{\Omega} \Phi \nabla \cdot (\boldsymbol{\phi} \times \mathbf{e}_B) d\Omega dt \right\} + \\ &\left[\int_0^{t_{max}} \int_{\Omega} \Phi \nabla \cdot (\boldsymbol{\phi} \times \mathbf{e}_B) d\Omega dt - \int_0^{t_{max}} \int_{\Omega} (\mathbf{V} \cdot (\nabla \eta \times \mathbf{e}_B)) d\Omega dt \right] = 0 \end{aligned} \quad (99)$$

Note that the term in square brackets is zero because of the coupling condition Eq. 90, Hence we define the adjoint potential operator \mathcal{H}^* as,

$$\mathcal{H}^*(\eta) \equiv \nabla^2 \eta - \nabla \cdot (\boldsymbol{\phi} \times \mathbf{e}_B) = 0 \quad (100)$$

The derivation of the operator \mathcal{F}^* follows similar steps to those used to derive \mathcal{G}^* and \mathcal{H}^* . We start from $(\psi, \mathcal{F}(\Theta))_{L_2(\Omega \times [0, t_{max}])} \equiv 0$, i.e.

$$\int_0^{t_{max}} \int_{\Omega} \psi \left(\frac{\partial \Theta}{\partial t} + \mathbf{v} \cdot \nabla \Theta + \mathbf{V} \cdot \nabla \theta - \nabla^2 \Theta \right) d\Omega dt = 0. \quad (101)$$

Integration by parts of the first term of the above equation leads to the following:

$$\begin{aligned} \int_0^{t_{max}} \int_{\Omega} \psi \frac{\partial \Theta}{\partial t} d\Omega dt &= - \int_0^{t_{max}} \int_{\Omega} \Theta \frac{\partial \psi}{\partial t} d\Omega dt \\ &+ \int_{\Omega} \Theta(\mathbf{x}, t_{max}) \psi(\mathbf{x}, t_{max}) d\Omega - \int_{\Omega} \Theta(\mathbf{x}, 0) \psi(\mathbf{x}, 0) d\Omega. \end{aligned} \quad (102)$$

Recall that $\Theta(\mathbf{x}, 0) = 0$ (eq. 60) and let us introduce the following final condition for ψ :

$$\psi(\mathbf{x}, t_{max}) = 0, \quad \mathbf{x} \in \Omega. \quad (103)$$

Then eq. (102) is simplified as follows:

$$\int_0^{t_{max}} \int_{\Omega} \psi \frac{\partial \Theta}{\partial t} d\Omega dt = - \int_0^{t_{max}} \int_{\Omega} \Theta \frac{\partial \psi}{\partial t} d\Omega dt. \quad (104)$$

The second term in eq. (101) can be integrated by parts as follows:

$$\begin{aligned} \int_0^{t_{max}} \int_{\Omega} \psi \mathbf{v} \cdot \nabla \Theta d\Omega dt &= \int_0^{t_{max}} \int_{\Gamma} \psi \Theta \mathbf{v} \cdot \mathbf{n} d\Gamma dt \\ &- \int_0^{t_{max}} \int_{\Omega} \Theta [\mathbf{v} \cdot \nabla \psi + (\nabla \cdot \mathbf{v}) \psi] d\Omega dt. \end{aligned} \quad (105)$$

The above equation can be simplified substantially by using the incompressibility and non-slip conditions for \mathbf{v} . Its final form is as follows:

$$\int_0^{t_{max}} \int_{\Omega} \psi \mathbf{v} \cdot \nabla \Theta d\Omega dt = - \int_0^{t_{max}} \int_{\Omega} \Theta \mathbf{v} \cdot \nabla \psi d\Omega dt. \quad (106)$$

The fourth term of eq. (101) can also be simplified. Integration by parts results in the following equation:

$$\begin{aligned} \int_0^{t_{max}} \int_{\Omega} \psi \nabla^2 \Theta d\Omega dt &= \int_0^{t_{max}} \int_{\Omega} \Theta \nabla^2 \psi d\Omega dt \\ &+ \int_0^{t_{max}} \int_{\Gamma} (\psi \nabla \Theta - \Theta \nabla \psi) \cdot \mathbf{n} d\Gamma dt. \end{aligned} \quad (107)$$

Recall that $\Theta(\mathbf{x}, 0) = 0$ for $\mathbf{x} \in \Gamma_g$ (eq. 63), that $\nabla \Theta(\mathbf{x}, t) \cdot \mathbf{n} = 0$, $\mathbf{x} \in \Gamma_{h1}$ (eq. 64) and that $\nabla \Theta(\mathbf{x}, t) \cdot \mathbf{n} = \Delta q_o$, $\mathbf{x} \in \Gamma_{h0}$ (eq. 65). Let us also define the following boundary conditions for ψ :

$$\nabla \psi(\mathbf{x}, t) \cdot \mathbf{n} = 0, \quad (\mathbf{x}, t) \in (\Gamma_h - \Gamma_I) \times [0, t_{max}] \quad (108)$$

$$\psi(\mathbf{x}, t) = 0, \quad (\mathbf{x}, t) \in \Gamma_g \times [0, t_{max}]. \quad (109)$$

Then eq. (107) can be re-written as:

$$\begin{aligned} \int_0^{t_{max}} \int_{\Omega} \psi \nabla^2 \Theta d\Omega dt &= \int_0^{t_{max}} \int_{\Omega} \Theta \nabla^2 \psi d\Omega dt \\ &+ \int_0^{t_{max}} \int_{\Gamma_{h0}} \psi \Delta q_o d\Gamma dt - \int_0^{t_{max}} \int_{\Gamma_I} \Theta \nabla \psi \cdot \mathbf{n} d\Gamma dt \end{aligned} \quad (110)$$

Substitution of equations (104), (106) and (110) into (101) results in the following equation:

$$\begin{aligned} &\int_0^{t_{max}} \int_{\Omega} \Theta \left\{ -\frac{\partial \psi}{\partial t} - \mathbf{v} \cdot \nabla \psi - \nabla^2 \psi + \boldsymbol{\phi} \cdot \mathbf{e}_g \right\} d\Omega dt \\ &+ \int_0^{t_{max}} \int_{\Omega} (\psi \mathbf{V} \cdot \nabla \theta - \boldsymbol{\phi} \cdot \mathbf{e}_g \Theta) d\Omega dt \\ &+ \int_0^{t_{max}} \int_{\Gamma_I} \Theta \nabla \psi \cdot \mathbf{n} d\Gamma dt - \int_0^{t_{max}} \int_{\Gamma_{h0}} \psi \Delta q_o d\Gamma dt. \end{aligned} \quad (111)$$

Note that the term $\Theta \boldsymbol{\phi} \cdot \mathbf{e}_g$ was added in the first term of the above equation and then subtracted from the second term, in accordance to the coupling condition Eq. 89. Also, note that the second integral term in the above equation is identically zero from Eq. (89). Let us further define the operator \mathcal{F}^* as follows:

$$\mathcal{F}^*(\psi) \equiv -\frac{\partial \psi}{\partial t} - \mathbf{v} \cdot \nabla \psi - \nabla^2 \psi + \boldsymbol{\phi} \cdot \mathbf{e}_g = 0 \quad (112)$$

With the above definition and Eq. (89), eq. (111) takes the following form:

$$\int_0^{t_{max}} \int_{\Gamma_I} \Theta \nabla \psi \cdot \mathbf{n} d\Gamma dt - \int_0^{t_{max}} \int_{\Gamma_{h0}} \psi \Delta q_o d\Gamma dt = 0. \quad (113)$$

Let us define the last boundary condition for ψ as follows:

$$\nabla \psi(\mathbf{x}, t) \cdot \mathbf{n} = \theta(\mathbf{x}, t) - \theta_m(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_I \times [0, t_{max}]. \quad (114)$$

Then eq. (113) can be re-stated as follows:

$$\int_0^{t_{max}} \int_{\Gamma_I} \Theta (\theta - \theta_m) d\Gamma dt = \int_0^{t_{max}} \int_{\Gamma_{h0}} \psi \Delta q_o d\Gamma dt, \quad (115)$$

which according to eq. (55) implies that:

$$S'(q_o(\mathbf{x}, t)) = \psi(\mathbf{x}, t; q_o), \quad (\mathbf{x}, t) \in (\Gamma_{h0} \times [0, t_{max}]). \quad (116)$$

As such, the gradient of the cost functional is given by eq. (116), where the adjoint field ψ is defined via equations (103), (108), (109), (112) and (114). The well-posed problem defining the adjoint fields is summarized in Box IV, where the parametric dependencies of ψ and $\boldsymbol{\phi}$ on q_o are also shown.

Box IV

Adjoint problem to define $\psi(\mathbf{x}, t; q_o)$, $\phi(\mathbf{x}, t; q_o)$ and $\eta(\mathbf{x}, t; q_o)$

$$\begin{aligned} \frac{\partial \psi(\mathbf{x}, t; q_o)}{\partial t} + \mathbf{v}(\mathbf{x}, t; q_o) \cdot \nabla \psi(\mathbf{x}, t; q_o) &= -\nabla^2 \psi(\mathbf{x}, t; q_o) \\ &+ \phi(\mathbf{x}, t; q_o) \cdot \mathbf{e}_g, \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \end{aligned} \quad (117)$$

$$\begin{aligned} \frac{\partial \phi(\mathbf{x}, t; q_o)}{\partial t} + (\nabla \phi(\mathbf{x}, t; q_o)) \mathbf{v}(\mathbf{x}, t; q_o) - (\nabla \mathbf{v}(\mathbf{x}, t))^T \phi(\mathbf{x}, t; q_o) &= -\nabla \cdot \zeta \\ -Ha^2 Pr[\mathbf{e}_B(\phi \cdot \mathbf{e}_B) - \phi] + PrRa\psi\nabla\theta + Ha^2 Pr[\nabla\eta \times \mathbf{e}_B], &(\mathbf{x}, t) \in \Omega \times [0, t_{max}] \end{aligned} \quad (118)$$

$$\zeta(\mathbf{x}, t; q_o) = -\pi(\mathbf{x}, t; q_o)\mathbf{I} + Pr[\nabla\phi(\mathbf{x}, t; q_o) + (\nabla\phi(\mathbf{x}, t; q_o))^T], \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (119)$$

$$\nabla \cdot \phi(\mathbf{x}, t; q_o) = 0, \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (120)$$

$$\psi(\mathbf{x}, t_{max}; q_o) = 0, \quad \mathbf{x} \in \Omega \quad (121)$$

$$\phi(\mathbf{x}, t_{max}; q_o) = 0, \quad \mathbf{x} \in \Omega \quad (122)$$

$$\phi(\mathbf{x}, t; q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}] \quad (123)$$

$$\psi(\mathbf{x}, t; q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma_g \times [0, t_{max}] \quad (124)$$

$$\frac{\partial \psi}{\partial n}(\mathbf{x}, t; q_o) = 0, \quad (\mathbf{x}, t) \in (\Gamma_h - \Gamma_I) \times [0, t_{max}] \quad (125)$$

$$\frac{\partial \psi}{\partial n}(\mathbf{x}, t; q_o) = \theta(\mathbf{x}, t; q_o) - \theta_m(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_I \times [0, t_{max}] \quad (126)$$

$$\nabla^2 \eta(\mathbf{x}, t; q_o) = \nabla \cdot (\phi(\mathbf{x}, t; q_o) \times \mathbf{e}_B), \quad (\mathbf{x}, t) \in \Omega \times [0, t_{max}] \quad (127)$$

$$\frac{\partial \eta}{\partial n}(\mathbf{x}, t; q_o) = 0, \quad (\mathbf{x}, t) \in \Gamma \times [0, t_{max}] \quad (128)$$

6 Conclusion

A functional optimization formulation for an inverse magneto-convection problem is elaborated. The discussion first defines the direct magneto-convection problem and provides a numerical example to demonstrate the effects of a magnetic field on the flow pattern. This is followed by the development of a functional framework to define the optimization algorithm. A adjoint system is derived that provides an expression for the exact gradient of the objective or cost function. The developed formulation has numerous applications in solidification process control. The computational work done in this report has been obtained based on an object-oriented software developed for this purpose.

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