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Jeffrey Borggaard, John Burkardt,  
Max Gunzburger, and Janet Peterson  
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Editors:

Jeffrey Borggaard  
John Burkardt  
Max Gunzburger  
Janet Peterson  
Air Force Center for Optimal Design and Control  
Interdisciplinary Center for Applied Mathematics  
Virginia Tech  
Blacksburg, Virginia 24061-0531

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Contributors

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Multilevel A  
N. Alexa

Shape Optim  
E. Arian

Computation  
Nonlinear Pr  
J. Arora,

Optimal Con  
J. Berg, I

The Applicat  
J. Betts

Algorithms f  
J. Borgg  
H. Kim,

Generalized  
Trajectory O  
K. Brena

The Optimal  
M. Delfo

Uniformly S  
R. Fabia

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P. Gilmo

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## Optimal Control of Thermally Coupled Navier Stokes Equations

Kazufumi Ito, Jeffrey S. Scroggs, and Hien T. Tran  
Center for Research in Scientific Computation  
North Carolina State University  
Raleigh NC 27695-8205, USA

The optimal boundary temperature control of the stationary thermally coupled incompressible Navier-Stokes equation is considered. Well-posedness and existence of the optimal control and a necessary optimality condition are obtained. Optimization algorithms based on the augmented Lagrangian method with second order update are discussed. A test example motivated by control of transport process in the high pressure vapor transport (HPVT) reactor is presented to demonstrate the applicability of our theoretical results and proposed algorithm.

### 1. Introduction

In this paper we discuss the optimal control problem of the stationary thermally coupled incompressible Navier-Stokes equations. Consider the following optimal control problem

$$\text{minimize } J(g) = \varphi(u, T - T_0) + \frac{\beta}{2} \|g - T_0\|_{L^2(\Gamma_1)}^2, \quad g \in \mathcal{C} \quad (1)$$

subject to

$$\begin{aligned} u \cdot \nabla u + \nabla p &= \nu \Delta u + \gamma (T - T_0) e_d + f, \\ \nabla \cdot u &= 0, \quad u|_{\Gamma} = 0, \\ u \cdot \nabla T &= \nabla \cdot (\kappa \nabla T), \end{aligned} \quad (2)$$

$$T = T_0 \text{ on } \Gamma_0 \text{ and } n \cdot \nabla T = H(g - T) \text{ on } \Gamma_1,$$

where  $f \in L^2(\Omega)^d$  is a source field,  $u$ ,  $p$ ,  $T$  stand for the nondimensionalized velocity vector in  $R^d$  with  $d = 2, 3$ , pressure, and temperature, respectively and  $\mathcal{C}$  is the closed convex set in  $L^2(\Gamma_1)$  such that

$$\bar{T}_1 \leq g \leq \bar{T}_2 \text{ on } \Gamma_1 \quad (3)$$

Here,  $\bar{T}_1 \leq T_0 \leq \bar{T}_2$  and  $\Gamma_i$ ,  $i = 0, 1$  are disjoint open sets in  $\Gamma$  such that  $\Gamma = \bar{\Gamma}_0 \cup \bar{\Gamma}_1$ . The constant  $\gamma$  is given by  $\gamma = \frac{\bar{g}}{T_0}$  where  $T_0 > 0$  is a constant reference temperature and  $\bar{g}$  is the gravitational constant, and  $e_d$  denotes the  $d$ -th unit vector of  $R^d$ . Throughout this paper we assume that  $\Omega$  is sufficiently smooth and  $\nu$ ,  $\kappa$  and  $H$  are positive constants.

This control problem is motivated by control of transport and growth processes in the high pressure vapor transport (HPVT) reactor [13]. For example, we may

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consider the Scholz geometry (Figure 1 in [13]). The source material and the growing crystal are sealed in a fused silica ampoule that is heated by a furnace liner at its outer cylindrical surface. The substrate  $\Gamma_0$  (the single crystal) is located on a fused silica window (the bottom of the ampoule) which is cooled by a jet of helium gas from the outer surface. HPVT processes are based on physical vapor transport and can be described very roughly as proceeding via evaporation at the polycrystalline source and condensation at the surface of the cooler substrate. The system (1)-(2) is called the Boussinesq equations, where we assume that the flow is incompressible and the transport phenomena of a single (carrier) gas is modeled. At the wall we assume Newton's law of cooling holds.

The cost-functional can be of tracking type

$$\varphi(u, T - T_0) = \int_{\Omega} |u - u_d|^2 + |T - T_d|^2 dx$$

where  $(u_d, T_d)$  is the desired state, or minimization of friction force of flow in a subregion  $\Omega_1$  of  $\Omega$

$$\varphi(u, T - T_0) = \int_{\Omega_1} |\nabla \times u|^2 dx.$$

## 2. Well-posedness

In this section, we discuss existence and uniqueness of solutions to (2). Let  $U = L^2(\Gamma_1)$  be the control space,  $V = V_0 \times V_1$  where  $V_0$  is the divergence-free subspace of  $(H_0^1(\Omega))^d$  [7] and

$$V_1 = H_{\Gamma_0}^1 = \{\phi \in H^1(\Omega) : \phi|_{\Gamma_0} = 0\}$$

and set  $H = H_0 \times L^2(\Omega)$ .  $H_0$  is the closure of  $V_0$  with respect to the  $L^2(\Omega)^d$ -norm, and is defined by

$$H_0 = \{\phi \in L^2(\Omega)^d : \nabla \cdot \phi = 0 \text{ and } n \cdot \phi = 0 \text{ on } \Gamma\}.$$

$H$  is equipped with the natural  $L^2$ -norm and  $V$  is equipped with the norm

$$|(\phi, \chi)|_V^2 = |\phi|_{V_0}^2 + |\chi|_{V_1}^2$$

where

$$|\phi|_{V_0}^2 = |\nabla \phi|_{L^2(\Omega)}^2 \quad \text{and} \quad |\chi|_{V_1}^2 = |\nabla \chi|_{L^2(\Omega)}^2 + H |\chi|_{L^2(\Gamma_1)}^2$$

for  $\psi = (\phi, \chi) \in V$ . Define the trilinear form  $b$  on  $H^1(\Omega)^d$  by

$$b(\phi_1, \phi_2, \phi_3) = \langle \phi_1 \cdot \nabla \phi_2, \phi_3 \rangle \quad (4)$$

for  $\phi_i \in H^1(\Omega)^d$ ,  $i = 1, 2, 3$ . Then we have

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**Lemma 1** The trilinear form  $b$  satisfies

- (a)  $|b(\phi_1, \phi_2, \phi_3)| \leq |\phi_1|_{L^4} |\nabla \phi_2|_{L^2} |\phi_3|_{L^4} \leq M_1 |\phi_1|_{H^1} |\phi_2|_{H^1} |\phi_3|_{H^1}$
- (b)  $b(\phi_1, \phi_2, \phi_3) + b(\phi_1, \phi_3, \phi_2) = 0$   
provided that  $\nabla \cdot \phi_1 = 0$  and  $(n \cdot \phi_1)(\phi_2 \cdot \phi_3) = 0$  on  $\Gamma$
- (c)  $|b(\phi_1, \phi_2, \phi_3)| \leq M_2 |\phi_1|_{L^2}^{1/2} |\phi_1|_{H^1}^{1/2} |\phi_3|_{L^2}^{1/2} |\phi_3|_{H^1}^{1/2} |\phi_2|_{H^1}$  for  $d = 2$
- (d)  $|b(\phi_1, \phi_2, \phi_3)| \leq M_2 |\phi_1|_{L^2}^{1/4} |\phi_1|_{H^1}^{3/4} |\phi_3|_{L^2}^{3/4} |\phi_3|_{H^1}^{1/4} |\phi_2|_{H^1}$  for  $d = 3$

for  $\phi_i \in H^1(\Omega)^d$ ,  $i = 1, 2, 3$

*Proof:* By Green's formula

$$b(\phi_1, \phi_2, \phi_3) + b(\phi_1, \phi_3, \phi_2) = (\phi_1, \nabla(\phi_2 \cdot \phi_3)) = (n \cdot \phi_1, \phi_1 \cdot \phi_3)_\Gamma$$

for  $\phi_2 \in C^1(\Omega)$  and  $\nabla \cdot \phi_1 = 0$ . Hence (b) follows from the continuity of  $b$ . The last two assertions follow from the fact that  $|\psi|_{L^4} \leq c |\psi|_{L^2}^{1/2} |\psi|_{H^1}^{1/2}$  for  $d = 2$  and  $|\psi|_{L^4} \leq c |\psi|_{L^2}^{3/4} |\psi|_{H^1}^{1/4}$  for  $\psi \in H^1(\Omega)$  and some constant  $c$ .  $\square$

In particular, Lemma 1 implies that

$$b(u, \phi, \phi) = 0 \quad \text{for } u, \phi \in V_0. \quad (5)$$

The weak or variational form of (2) is given by

$$\nu (\nabla u, \nabla \phi) + b(u, u, \phi) = (f + \gamma (T - T_0) e_d, \phi) \quad (6)$$

for all  $\phi \in V_0$  and

$$\begin{aligned} \kappa (\nabla (T - T_0), \nabla \chi) + \langle u \cdot \nabla (T - T_0), \chi \rangle_{V_1^* \times V_1} \\ + \kappa (H (T - T_0), \chi)_{\Gamma_1} = \kappa (H (g - T_0), \chi)_{\Gamma_1}. \end{aligned} \quad (7)$$

for all  $\chi \in V_1$ . The pair  $(u, T - T_0) \in V$  is said to be a weak solution of (2) if (6), (7) holds for all  $\psi = (\phi, \chi) \in V$ . Then we have the following theorem.

**Theorem 2** Given  $g \in L^2(\Gamma_1)$  there exists a weak solution  $(u, T - T_0) \in V$  to (2) and

$$|(u, T - T_0)|_V \leq \text{const} (|f|_{L^2} + |g|_{L^2(\Gamma_1)}).$$

Moreover, if  $\bar{T}_1 \leq g(x) \leq \bar{T}_2$  a.e. in  $x \in \Gamma_1$  then  $\bar{T}_1 \leq T(x) \leq \bar{T}_2$  a.e. in  $\Omega$  for every solution  $(u, T - T_0) \in V$ .

*Step 1: (Existence)* We show that (6), (7) has a solution  $z = (u, T - T_0) \in V$ . Given  $\bar{u} \in V_0$ , we consider the linear equation

$$\nu (\nabla u, \nabla \phi) + b(\bar{u}, u, \phi) = (\gamma (T - T_0) e_d + f, \phi) \quad \text{for } \phi \in V_0 \quad (8)$$

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$$\begin{aligned} \kappa(\nabla(T - T_0), \nabla\chi) + \langle \bar{u} \cdot \nabla(T - T_0), \chi \rangle &+ \kappa(H(T - T_0), \chi) \\ &= \kappa(H(g - T_0), \chi)_{\Gamma_1}, \quad (9) \end{aligned}$$

for  $\chi \in V_1$ . First, we show that (8),(9) has the unique solution  $(u, T - T_0) \in V$ . Then, we show that the solution map  $S$  on  $V_0$  defined by  $S(\bar{u}) = u$  where  $(u, T - T_0) \in V$  is the unique solution to (8),(9) has a fixed point by Schauder fixed point theorem. The fixed point  $u \in V_0$  and the corresponding solution  $T - T_0 \in V_1$  define a solution to (6), (7). By Green's formula

$$\langle \bar{u} \cdot \nabla\theta, \chi \rangle + \langle \bar{u} \cdot \nabla\chi, \theta \rangle = 0 \quad \text{and in particular} \quad \langle \bar{u} \cdot \chi, \chi \rangle = 0 \quad (10)$$

for  $\bar{u} \in V_0$ , and  $\theta, \chi \in H^1(\Omega)$ . Hence, from Lemma 1 the sesquilinear form

$$\kappa(\nabla\chi_1, \nabla\chi_2) + \langle \bar{u} \cdot \nabla\chi_1, \chi_2 \rangle + \kappa(H\chi_1, \chi_2)_{\Gamma_1} = 0$$

on  $V_1 \times V_1$  is bounded and  $V_1$ -coercive. It thus follows from the Lax-Milgram theorem that equation (9) has a unique solution  $T - T_0 \in V_1$ . Choosing  $\chi = T - T_0$  in (9), we have (independent of  $\bar{u} \in V_0$ )

$$|T - T_0|_{V_1}^2 \leq H |g - T_0|_{L^2(\Gamma_1)}^2. \quad (11)$$

Next, the sesquilinear form on  $V_0 \times V_0$  defined by

$$v(\nabla\phi_1, \nabla\phi_2) + b(\bar{u}, \phi_1, \phi_2)$$

is bounded and  $V_0$ -coercive from Lemma 1 and (5). Thus, by the Lax-Milgram theorem, equation (8) has a unique solution  $u \in V_0$ , and we have

$$|u|_{V_0} \leq \frac{M_3}{v} (|f|_{L^2} + \gamma |T - T_0|_{L^2}) \quad (12)$$

where  $|\phi|_{H_0} \leq M_3 |\phi|_{V_0}$ ,  $\phi \in V_0$ . Let  $C$  be a closed convex subspace of  $V_0$ , defined by

$$C = \{\phi \in V_0 : |\phi|_{V_0} \leq \frac{M_3}{v} (|f|_{L^2} + \gamma M_4 H |g - T_0|_{L^2(\Gamma_1)})\},$$

where  $|\chi|_{L^2} \leq M_4 |\chi|_{V_1}$  for  $\chi \in V_1$ . Then it follows from (11)-(12) that  $S$  maps from  $C$  into  $C$ . Moreover, the solution map  $S$  is compact. In fact, if  $\bar{u}_k$  converges weakly to  $\bar{u}$  in  $V_0$  then  $|\bar{u}_k - \bar{u}|_{L^4} \rightarrow 0$  since  $H^1(\Omega)$  is compactly embedded into  $L^4(\Omega)$ . Let  $(u_k, T_k - T_0) \in V$  and  $(u, T - T_0) \in V$  be the corresponding solution of (8),(9), respectively to  $\bar{u}_k \in V_0$  and  $\bar{u} \in V_0$ . Then we have

$$\kappa(T_k - T, \chi)_{V_1} + \langle (\bar{u}_k - \bar{u}) \cdot \nabla(T - T_0) + \bar{u}_k \cdot \nabla(T_k - T), \chi \rangle = 0$$

for  $\chi \in V_1$  from Lemma 1 and (10)

$$\kappa |T_k - T|_{V_1} \leq M_1 |\bar{u}_k - \bar{u}|_{L^4} |T - T_0|_{V_1}$$

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which implies  $|T_k - T|_{V_1} \rightarrow 0$ . Similarly, we have

$$\nu |u_k - u|_{V_0} \leq M_1 |\bar{u}_k - \bar{u}|_{L^4} |u|_{V_0} + \gamma M_3 |T_k - T|_{L^2}$$

and thus  $|u_k - u|_{V_0} \rightarrow 0$ . Now, by the Schauder fixed point theorem (e.g, see [19]) there exists at least one solution to (6), (7).

Step 2: ( $L^\infty$  estimate) We show that if  $\bar{T}_1 \leq g \leq \bar{T}_2$  then

$$\bar{T}_1 \leq T \leq \bar{T}_2 \quad \text{a.e. } x \in \Omega.$$

for all solutions  $(u, T - T_0) \in V$  to (6), (7). In fact, let  $\chi = \inf(T, \bar{T}_1)$ . Then  $\chi \in V_1$  [19] and we have from (6), (7)

$$\kappa (\nabla T, \nabla \chi) + \langle u \cdot \nabla T, \chi \rangle + (\kappa H (T - g), \chi)_{\Gamma_1} = 0.$$

Since from (10)  $\langle u \cdot \nabla T, \chi \rangle = 0$  we have

$$\kappa (\nabla \chi, \nabla \chi) + (\kappa H (T - g), \chi)_{\Gamma_1} = 0$$

where

$$(T - g)\chi = (T - \bar{T}_1 - (g - \bar{T}_1))\chi \geq |\chi|^2 \quad \text{on } \Gamma_1.$$

Thus, we obtain  $|\chi|_{V_1}^2 = 0$  which implies  $\chi = 0$  and hence  $T \geq \bar{T}_1$ . Similarly, one can prove that  $T \leq \bar{T}_2$ , choosing the test function  $\chi = \sup(T, \bar{T}_2)$ .

We have also the uniqueness of solutions under the smallness assumption on  $f$  and  $g - T_0$ .

**Theorem 3** If  $|f|_{L^2}$  and  $\frac{1}{T_0}|g - T_0|_{L^2(\Gamma_1)}$  are sufficiently small then (6), (7) has a unique solution in  $V$ .

*Proof:* Suppose  $(u_i, T_i - T_0) \in V$ ,  $i = 1, 2$  are two solutions to (6), (7). Then we have

$$\begin{aligned} \nu (\nabla \bar{u}, \nabla \phi) + \langle u_1 \cdot \nabla \bar{u} + \bar{u} \cdot \nabla u_2, \phi \rangle &= \gamma (\bar{T} e_d, \phi) \\ \kappa (\nabla \bar{T}, \nabla \chi) + \langle u_1 \cdot \nabla \bar{T} + \bar{u} \cdot \nabla (T_2 - T_0), \chi \rangle &+ (\kappa H \bar{T}, \chi)_{\Gamma_1} = 0 \end{aligned}$$

for  $\phi \in V_0$  and  $\chi \in V_1$ , where  $\bar{u} = u_1 - u_2 \in V_0$  and  $\bar{T} = T_1 - T_2 \in V_1$ . Setting  $\phi = \bar{u}$  and  $\chi = \bar{T}$  we obtain from (5) and (10)

$$\begin{aligned} \nu |\bar{u}|_{V_0}^2 &\leq M_1 |u_2|_{V_0} |\bar{u}|_{V_0}^2 + \gamma M_3 M_4 |\bar{T}|_{V_1} |\bar{u}|_{V_0} \\ \kappa (|\nabla \bar{T}|^2 + H |\bar{T}|_{\Gamma_1}^2) &\leq M_1 |T_2 - T_0|_{V_1} |\bar{u}|_{V_0} |\bar{T}|_{V_1}. \end{aligned}$$

If we set  $X = |\bar{u}|_{V_0}$  and  $Y = |\bar{T}|_{V_1}$  then this implies

$$(\nu - M_1 |u_2|_{V_0}) X^2 \leq \gamma M_3 M_4 X Y \quad \text{and} \quad \kappa Y^2 \leq M_1 |T_2 - T_0|_{V_1} X Y.$$

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Hence if  $\kappa(v - M_1 |u_2|_{V_0}) - \gamma M_1 M_3 M_4 |T_2 - T_0|_{V_1} > 0$  then  $X = Y = 0$  and thus  $(u_1, T_1) = (u_2, T_2)$ . From (11)-(12) we have

$$\begin{aligned} |T_2 - T_0|_{V_1} &\leq H |g - T_0|_{L^2(\Gamma_1)} \\ |u_2|_{V_0} &\leq \frac{M_3}{v} (|f|_{L_2} + \gamma M_4 H |g - T_0|_{L^2(\Gamma_1)}). \end{aligned} \quad (13)$$

Thus, if  $|f|_{L^2}$  and  $\frac{1}{T_0} |g - T_0|_{L^2(\Gamma_1)}$  are sufficiently small then (6), (7) has a unique solution.  $\square$

Moreover, we can make the following demonstration of the regularity of the solution  $(u, T - T_0) \in V$ . Define the Stokes operator  $A$  on  $H_0$  by

$$(Au, \phi)_{H_0} = (\nabla u, \nabla \phi) \quad \text{for } \phi \in V_0 \quad (14)$$

with domain

$$\text{dom}(A) = \{u \in V_0 : |(\nabla u, \nabla \phi)| \leq c |\phi|_{H_0} \text{ for all } \phi \in V_0\}. \quad (15)$$

Then it is known [18] that  $A$  is a positive self-adjoint operator on  $H_0$ ,  $\text{dom}(A) \subset H^2(\Omega)^3$  and  $V_0 = \text{dom}(A^{1/2}) = [H_0, \text{dom}(A)]_{1/2}$ . Let  $d = 3$ . Since

$$|(u \cdot \nabla u, \phi)| \leq |u|_{L^6} |\nabla u|_{L^2} |\phi|_{L^3}$$

for  $u, \phi \in V_0$  and

$$H^1(\Omega) \subset L^6(\Omega) \quad \text{and} \quad V_{1/2} \subset L^3(\Omega),$$

where  $V_{1/2} = [V_0, H_0]_{1/2}$ ,  $u \nabla u \in V_{-1/2} = \text{dom}(A^{-1/4})$  for  $u \in V_0$ . Thus,

$$u = A^{-1}(\rho(T - T_0) e_3 + f - u \cdot \nabla u) \in \text{dom}(A^{3/4}) = [V, \text{dom}(A)]_{1/2} \subset H^{3/2}(\Omega)^3.$$

Hence,  $u \cdot \nabla u \in L^2(\Omega)^d$  and  $u \in \text{dom}(A) \subset H^2(\Omega)^3$ .

### 3. Necessary optimality condition

We now show the existence of solutions to the optimal control problem (1)-(2). Let us denote by  $S(g)$ , the solution set of (6), (7) for  $g \in L^2(\Gamma_1)$ .

**Theorem 4** Consider the minimization problem (1)-(2):

$$\begin{aligned} \text{minimize} \quad J(g) &= \varphi(u, T - T_0) + \frac{\beta}{2} |g - T_0|_{L^2(\Gamma_1)}^2 \\ \text{over } (u, T - T_0) &\in S(g) \text{ and } g \in C. \end{aligned} \quad (16)$$

Assume that  $\varphi$  satisfies

$$\begin{aligned} \varphi(z) : z = (u, T - T_0) \in V &\rightarrow R^+ \text{ is convex and lower semicontinuous} \\ \text{and } \varphi(z) &\leq b_1 |z|_V^2 + b_2 \text{ for } b_1, b_2 \in R^+. \end{aligned}$$

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*Proof:* Let  $\beta > 0$ ,  $|g_k|$ ,  $|(u_k, T_k - T_0)|$  by the same  $V \times C$  since trilinear form

for  $z_i = (u_i, T_i - T_0)$  bedded into  $\psi \in V$ , where the limit  $(z, T - T_0)$  lower semic

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*Proof:* It fo multiplier  $\lambda^*$

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= 0 and thus

Then Problem (1)-(2) has a solution.

*Proof:* Let  $((u_k, T_k - T_0), g_k) \in S(g_k) \times \mathcal{C}$  be a minimizing sequence. Since  $\beta > 0$ ,  $\|g_k - T_0\|_{L^2(\Gamma_1)}$  is uniformly bounded in  $k$  and thus from (11)-(12) so is  $\|(u_k, T_k - T_0)\|_V$ . Hence there exists a subsequence of  $\{k\}$ , which will be denoted by the same index, such that  $(u_k, T_k - T_0, g_k)$  converges weakly to  $(u, T - T_0, g) \in V \times \mathcal{C}$  since  $V \times L^2(\Gamma_1)$  is a Hilbert space and  $\mathcal{C}$  is closed and convex. Define the trilinear form  $\tilde{b}$  on  $V^3$  by

$$\tilde{b}(z_1, z_2, \psi) = b(u_1, u_2, \phi) + (u_1 \cdot \nabla \theta_2, \chi)$$

for  $z_i = (u_i, \theta_i)$ ,  $i = 1, 2$ ,  $\psi = (\phi, \chi) \in V$ . Since  $H^1(\Omega)$  is compactly embedded into  $L^4(\Omega)$  it follows from Lemma 1 that  $\tilde{b}(z_k, z_k, \psi) \rightarrow \tilde{b}(z, z, \psi)$  for  $\psi \in V$ , where  $z_k = (u_k, T_k - T_0)$  and  $z = (u, T - T_0)$ . Hence, for  $\psi = (\phi, \chi) \in V$  the limit  $(z, g)$  satisfies (6), (7) and thus  $z \in S(g)$ . Now, since  $\varphi$  is convex and lower semicontinuous, it follows from [5] that  $(z, g)$  minimizes (16).  $\square$

Problem (16) is equivalently written as a constrained minimization on  $x = ((u, T - T_0), g) \in X = V \times L^2(\Gamma_1)$  with

$$\begin{aligned} \text{minimize } J(x) &= \varphi(u, T - T_0) + \frac{\beta}{2} \|g - T_0\|_{L^2(\Gamma_1)}^2 \quad \text{over } x \in X \\ \text{subject to } e(x) &= 0 \text{ and } g \in \mathcal{C} \end{aligned} \quad (17)$$

where the equality constraint  $e : X \rightarrow Y = V^*$  is defined by (6), (7); i.e.,

$$\langle e(x), \psi \rangle = a(z, \psi) + \tilde{b}(z, z, \psi) - \kappa (H(g - T_0), \chi)_{\Gamma_1} - (f, \phi) \quad (18)$$

for  $\psi = (\phi, \chi) \in V$ , where

$$a(z, \psi) = \nu (\nabla u, \nabla \phi) - \gamma ((T - T_0) e_d, \phi) + \kappa (\nabla(T - T_0), \nabla \chi) + \kappa H(T - T_0, \chi)_{\Gamma_1}$$

for  $z = (u, T - T_0)$ ,  $\psi = (\phi, \chi) \in V$ . Assume that  $x^* = (z^* = (u^*, T^* - T_0), g^*)$  denotes the optimal pair of (16). Then we have

**Theorem 5** Assume that  $x^*$  is a regular point in the sense [14] that

$$0 \in \text{int} \{e'(x^*)(v, h - g^*) : v \in V \text{ and } h \in \mathcal{C}\}. \quad (19)$$

Then there exists a Lagrange multiplier  $\lambda^* \in V$  such that

$$a(\lambda^*, \psi) + \tilde{b}(\psi, z^*, \lambda^*) + \tilde{b}(z^*, \psi, \lambda^*) + \langle \varphi'(z^*), \psi \rangle = 0 \quad (20)$$

for  $\psi \in V$  and

$$(\beta g^* - \kappa H \lambda_2^*, h - g^*)_{\Gamma_1} \geq 0 \quad \text{for all } h \in \mathcal{C}. \quad \square \quad (21)$$

*Proof:* It follows from [14] that if (19) is satisfied, then there exists a Lagrange multiplier  $\lambda^* = (\lambda_1^*, \lambda_2^*) \in V$  such that

$$\langle \varphi'(z^*), \psi \rangle + \beta (g^*, h - g^*)_{\Gamma_1} + e'(x^*)(\psi, h - g^*) \geq 0$$

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for all  $\psi \in V$  and  $h \in \mathcal{C}$ , that is

$$\begin{aligned} & \langle \varphi'(z^*), \psi \rangle + \beta (g^*, h - g^*)_{\Gamma_1} + a(\lambda^*, \psi) \\ & + \tilde{b}(\psi, z^*, \lambda^*) + \tilde{b}(z^*, \psi, \lambda^*) - \kappa H(h - g^*, \lambda^*)_{\Gamma_1} \geq 0 \end{aligned} \quad (22)$$

for all  $\psi \in V$  and  $h \in K$ . Setting  $\psi = 0$ , we obtain (21). Next, setting  $h = g^*$  in (22), we obtain (20).  $\square$

Concerning the regular point condition (19), we have

**Lemma 6** *If  $g^* \in \text{int}(\mathcal{C})$  then the regular point condition (19) is equivalent to the condition that for  $v = (v_1, v_2) \in V$*

$$\begin{aligned} & a(v, \psi) + \tilde{b}(\psi, z^*, v) + \tilde{b}(z^*, \psi, v) = 0 \\ & \text{for all } \psi \in V \text{ and } v_2 = 0 \text{ on } \Gamma_1 \end{aligned} \quad (23)$$

implies  $v = 0$ .

*Proof:* If  $g^* \in \text{int}(\mathcal{C})$  then (19) is equivalent to the condition that  $G = e'(x^*)$  is surjective. Define the linear map  $C \in \mathcal{L}(X, V)$  by  $C(v, h) = \xi$  where  $\xi \in V$  is the unique solution to

$$a(\xi, \psi) + \tilde{b}(v, z^*, \psi) + \tilde{b}(z^*, v, \psi) - \kappa H(h, \chi)_{\Gamma_1} = 0 \quad \text{for } \psi = (\phi, \chi) \in V.$$

Then, since  $H^1(\Omega)$  is embedded compactly to  $L^4(\Omega)$ , Lemma 1 implies that  $C$  is compact. Thus, by the Banach closed range theorem and the Riesz-Schauder theorem,  $e'(x^*)(v, h)$  is surjective if and only if  $\ker(G^*) = \{0\}$  [4], which is equivalent to (21).  $\square$

#### 4. Augmented Lagrangian method

In this section we discuss applications of the augmented Lagrangian method for the constrained minimization problem (17). The augmented Lagrangian method [8], [15] is based on an equivalent formulation of (17):

$$\text{minimize } J(x) + \frac{c}{2} |e(x)|_Y^2 \quad \text{over } x \in X \text{ and } g \in \mathcal{C}. \quad (24)$$

subject to  $e(x) = 0$ , where  $x = ((u, T - T_0), g) \in X = V \times L^2(\Gamma_1)$  and  $c > 0$  is the penalty parameter. The augmented Lagrangian algorithm [8], [15] is the multiplier method applied to (17), i.e., it involves a sequence of minimizations of the functional

$$\begin{aligned} & L_{c_k}(x; \lambda^k) = J(x) + \langle \lambda^k, e(x) \rangle + \frac{c}{2} |e(x)|_Y^2 \\ & \text{subject to } g \in \mathcal{C}, \end{aligned} \quad (25)$$

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where the multiplier sequence  $\{\lambda^k\}$  in  $Y^*$  is generated by the first order update

$$(22) \quad \lambda^{k+1} = \lambda^k + c_k e(x_k), \quad (26)$$

for  $k \geq 1$ , where  $x_k$  is a minimizer of  $L_{c_k}(\cdot, \lambda^k)$  and we assumed that  $Y^* = Y$ , otherwise each element in  $Y^*$  has its Riesz representation. To carry out this iteration, a sequence of monotonically nondecreasing, positive real numbers  $\{c_k\}$ ,  $c_1 > c_0 \geq 0$  and a start up value  $\lambda^1$  for the Lagrange multiplier for the equality constraint  $e(x) = 0$  need to be chosen. The convergence results of the augmented Lagrangian method for the infinite dimensional optimization problem are established, for example, in [9], [16]. The augmented Lagrangian method is a hybrid of the penalty method (i.e.,  $\lambda^k = 0$ ) and the Lagrange multiplier method (i.e.,  $c_k = 0$ ) and combines good properties of both. It overcomes the difficulty of the penalty method which requires a large value of  $c_k$ . The augmented functional  $L_{c_k}(x, \lambda^k)$  is locally strictly convex provided that  $\lambda^k$  is sufficiently close to  $\lambda^*$  and the second order optimality condition

$$(23) \quad L''_0(x^*, \lambda^*)((v, h), (v, h)) \geq \sigma (|v|_V^2 + |h|_U^2) \quad (27)$$

for all  $(v, h) \in X$  satisfying  $e'(x^*)(v, h) = 0$ .

for some  $\sigma > 0$ , is satisfied. Here,  $L''_0(x^*, \lambda^*)$  denotes the bilinear form that characterizes the second derivative of  $L_0(x, \lambda) = J(x) + \langle \lambda, e(x) \rangle$  with respect to  $x$  at  $x^*$ . That is, it is not necessary that the cost functional  $J$  be (locally) convex, which is required for convergence of the multiplier method. The algorithm (25)-(26) has been successfully applied to parameter estimation problems in elliptic PDEs [10], [12] and optimal control problems for 2-D incompressible Navier-Stokes [4]. The first order update (26) provides Q-linear convergence of the iterates  $x_k$  in  $X$ . In [11] we have investigated a second order update scheme for the augmented Lagrangian method. In what follows we assume that  $g^* \in \text{int}(\mathcal{U})$ . Thus, (19) reduces to  $e'(x^*)$  is surjective (see Lemma 6). Hence the necessary condition implies that

$$(24) \quad L'_c(x^*, \lambda^*) = 0 \quad \text{and} \quad e(x^*) = 0, \quad (28)$$

for all  $c \geq 0$ . An algorithm proposed in [11] applies Newton's method to (28). The resulting algorithm is stated as: given a current iterate  $(x, \lambda)$  the next iterate  $(x_+, \lambda_+)$  satisfies

$$(25) \quad \begin{pmatrix} L''_c(x, \lambda) & e'(x)^* \\ e'(x) & 0 \end{pmatrix} \begin{pmatrix} x_+ - x \\ \lambda_+ - \lambda \end{pmatrix} = - \begin{pmatrix} L'_c(x, \lambda) \\ e(x) \end{pmatrix}. \quad (29)$$

Note that

$$(26) \quad L'_c(x, \lambda) = L'_0(x, \lambda + c e(x))$$

and

$$(27) \quad L''_c(x, \lambda) = L''_0(x, \lambda + c e(x)) + c \langle e'(x)(\cdot), e'(x)(\cdot) \rangle. \quad (30)$$

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Consequently, suppose  $|(x, \lambda) - (x^*, \lambda^*)|$  is sufficiently small. Then it follows from (27) [11] that  $L_c''(x, \lambda)$  is coercive on  $X \times Y$ . Thus equation (29) can be regarded as a general Stokes equation. Following an argument due to Bertsekas [2], we can avoid forming  $L_c''$  during the iteration. From the second equation of (29) we have  $e'(x)(x_+ - x) = -e(x)$ . Thus the first equation can be written as

$$L_0''(x, \lambda + c e(x))(x_+ - x) + e'(x)^*(\lambda_+ - (\lambda + c e(x))) = -L_0'(x, \lambda + c e(x))$$

and hence (29) is equivalent to

$$\begin{pmatrix} L_0''(x, \hat{\lambda}) & e'(x)^* \\ e'(x) & 0 \end{pmatrix} \begin{pmatrix} x_+ - x \\ \lambda_+ - \hat{\lambda} \end{pmatrix} = - \begin{pmatrix} L_0'(x, \hat{\lambda}) \\ e(x) \end{pmatrix} \quad (31)$$

where  $\hat{\lambda} = \lambda + c e(x)$ .

Note that  $\hat{\lambda}$  is nothing but the first order update of the Lagrange multiplier if the current iterate  $x$  minimizes  $L_c(x, \lambda)$ . Equation (31) is more advantageous than (29) since the squaring term  $c e'(x)^* e'(x)$  is absorbed and less calculation is involved. If we define a matrix operator  $S$  on  $X \times Y$  by

$$S(x, \lambda) = \begin{pmatrix} L_0''(x, \lambda) & e'(x)^* \\ e'(x) & 0 \end{pmatrix},$$

then it follows from (27) that  $S(x^*, \lambda^*)$  is boundedly invertible. Thus, if  $(x, \lambda)$  is sufficiently close to  $(x^*, \lambda^*)$ , then equation (31) has a unique solution. We summarize our discussions as

#### Algorithm 1

(1) Choose  $\lambda^1 \in Y$ ,  $c > \bar{c} \geq 0$ , and set  $\hat{c} = c - \bar{c}$ ,  $k = 1$ .

(2) Determine  $x = ((u, T - T_0), g) \in V \times C$  such that

$$L_c(x, \lambda^k) \leq L_c(x^*, \lambda^k) = f(x^*).$$

(3) Set  $\hat{\lambda} = \lambda^k + \hat{c} e(x)$ .

(4) Solve for  $(\tilde{x}_+, \lambda_+) \in X \times Y$ :

$$S(x, \hat{\lambda}) \begin{pmatrix} x_+ - x \\ \lambda_+ - \hat{\lambda} \end{pmatrix} = - \begin{pmatrix} L_0'(x, \hat{\lambda}) \\ e(x) \end{pmatrix}.$$

(5) Set  $x_{k+1} = x_+$  and  $\lambda^{k+1} = \lambda_+$ . If the convergence criterion is not satisfied then set  $k = k + 1$  and go to (2).

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*Remark.* A variant of Algorithm 1 is obtained by skipping step (2). Then it is reduced to the Newton method applied to equation (28). Step (2) implies a sufficient reduction of the merit functional (the augmented Lagrange functional). For example, if  $x = (z, g)$  minimizes  $L_c(\cdot, \lambda^k)$  over  $V \times \mathcal{C}$  then step (2) is completed. Assume that (19) and (27) hold. It is proved in [11] that if  $|\lambda^1 - \lambda^*|_Y$  is sufficiently small, then Algorithm 1 is well-posed and  $(x^k, \lambda^k)$  converges to  $(x^*, \lambda^*)$  Q-quadratically.

### 5. Hybrid method and test example

In this section we present an example to demonstrate the applicability of our theoretical results and proposed algorithm. We consider the optimal control of the two dimensional stationary thermally driven cavity flow

$$\begin{aligned} \text{minimize } J(g) &= \frac{1}{2} \int_{\Omega} |u - u_d|^2 + |T - T_d|^2 dx + \frac{\beta}{2} \|g - T_0\|_{L^2(\Gamma_1)}^2 \\ &\text{over } g \in L^2(\Gamma_1) \end{aligned} \quad (32)$$

subject to (2), where  $\Omega = (0, L)^2$ ,  $\Gamma_1 = (x_1, 1)$ ,  $0 < x_1 < L$  and  $\Gamma_0$  is the relative interior of  $\Gamma - \Gamma_1$ . On  $\Gamma_0$  we have the Dirichlet boundary condition:

$$\begin{aligned} T(0, x_2) &= T(L, x_2) = T_0, \quad 0 < x_2 < L \\ T(x_1, 0) &= T_0 - 50 \min(1, \frac{2}{3} (2.5 - |\frac{5}{L}x_1 - 2.5|)), \quad 0 < x_1 < L. \end{aligned} \quad (33)$$

with a reference temperature  $T_0 = 1350^\circ K$ , and the temperature on the substrate  $(x_1, 0)$ ,  $\frac{1.5}{5}L \leq x_1 \leq \frac{3.5}{5}L$  is  $1300^\circ K$ . The desired state  $(u_d, T_d)$  appearing in (32) is chosen as follows.  $u_d = L u^0$  where  $(u^0, T^0)$  is the solution pair for the flow with  $L = 1$  and  $g = T_0$  and  $T_d = T^1$  where  $(u^1, T^1)$  is the solution pair for the flow with  $L = 5$  and  $g = T_0$ . Here, our numerical calculation strongly indicates that the solution to (2) is unique and (dynamically) stable for the range of physical parameters that we chosen for our calculation.

The problem is scaled so that the velocity field  $u$  has dimension  $cm/sec$  and  $T$  has dimension  $K^\circ$ . The constants  $\nu$ ,  $\kappa$  are chosen for  $P_2$  at  $3atm$  pressure and are given by  $\nu = .155$  and  $\kappa = .110$ .  $H$ ,  $\beta$  and  $L$  are set to be  $H = 100$ ,  $\beta = \frac{1000}{1350^2} = 5.5 \times 10^{-5}$  and  $L = 5$  respectively. Figures 1 and 2 show the vector field of  $u^0$  and  $u^1$ , respectively. It can be observed that  $u^0$  has more vertical transport than  $u^1$  does and  $u^1$  is confined in the two bottom corners. Hence the cost-functional (24) is formulated so that the thermal control  $g$  on the top  $\Gamma_1$  increases the vertical transport of flow with  $L = 5$  while retaining the temperature distribution  $T^1$  at the reference temperature  $g = T_0$ .

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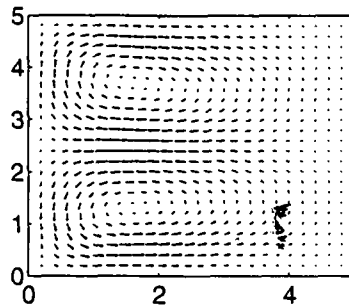


Figure 1. The desired flow.

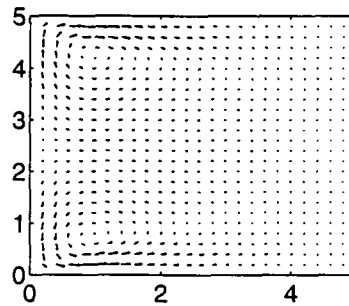


Figure 2. The uncontrolled flow.

The second order augmented Lagrangian method (Algorithm 1) described in Section 4 is used to solve problem (32). To obtain a good starting value  $\lambda^1$  for the Lagrange multiplier in Algorithm 1, we employed a few steps of the gradient method. The gradient of the cost functional can be calculated by the adjoint equation as follows. Consider the cost functional  $J(z, g)$  subject to  $E(z, g) = 0$  where  $z \in V$  and  $g \in U$ . Assume that  $V$  and  $U$  are Hilbert spaces,  $J(z, g) : X = V \times U \rightarrow R$  is Fréchet differentiable and  $E(z, g) : X \rightarrow Y$  is continuously Fréchet differentiable in a neighborhood of  $x_0 = (z_0, g_0)$ . Suppose that  $E_z(x_0) \in \mathcal{L}(V, Y)$ , the  $F$ -derivative of  $E$  with respect to  $z$  at  $x_0$ , has a bounded inverse. Then by the implicit function theorem, there exists a unique  $C^1$  mapping  $\Psi$  defined in a neighborhood  $N$  of  $g_0$  in  $U$ ,  $\Psi : U \rightarrow V$  such that  $\Psi(g_0) = z_0$  and  $E(\Psi(g), g) = 0$  for  $g \in N$ . Then the  $F$ -derivative  $d$  of  $J(\Psi(g), g)$  with respect to  $g$  in  $N$  exists and is given by

$$d = J_g + E_g^* \psi \quad (34)$$

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where  $\psi \in Y$  satisfies the adjoint equation

$$E_z^* \psi + J_z = 0. \quad (35)$$

Here we assume that  $V$ ,  $U$  and  $Y$  are identified with their dual spaces. In fact, if  $v = \Psi'(h)$ ,  $h \in U$  then

$$(d, h)_U = (J_g, h)_U + (J_z, v)_V$$

and  $v \in V$  satisfies

$$E_z v + E_g h = 0.$$

Hence, for  $h \in U$

$$(d, h)_U = (J_g, h)_U - (E_z^* \psi, v)_V = (J_g, h)_U + (\lambda, E_z h)_V = (J_g + E_z^* \psi, h)$$

which implies (34). The projected gradient method can be written as:

### Algorithm 2

- (1) Choose  $g_1 \in U$  and set  $k = 1$ .
- (2) Let  $z_k$  be a solution of  $E(z, g_k) = 0$ ,  $\psi_k$  be the solution of  $E_z(z_k, g_k)^* \psi_k + J_z(z_k, g_k) = 0$  and set  $d_k = J_g(z_k, g_k) + E_g(z_k, g_k)^* \psi_k$ .
- (3) Set  $\hat{d}_k = J_g(z_k, g_k)$  and determine  $\alpha_k \geq 0$  such that  $J(\Psi(g_\alpha), g_\alpha)$  is minimized where  $g_\alpha = \text{Proj}(g_k - \alpha d_k)$ .
- (4) Set  $g_{k+1} = g_k - \alpha_k d_k$ . If the convergence criterion is not satisfied, then set  $k = k + 1$  and go to Step (2).

In our specific example equation (35) is written as

$$\begin{aligned} -v \Delta \lambda - u \cdot \nabla \lambda + \lambda' \nabla u - (T - T_0) \nabla \mu + \nabla q + u - u_d &= 0 \\ \nabla \cdot \lambda &= 0 \quad \text{and} \quad \lambda|_\Gamma = 0 \\ -\kappa \Delta \mu - u \cdot \nabla \mu - \frac{g}{T_0} \lambda_2 + T - T_d &= 0 \\ \mu &= 0 \text{ on } \Gamma_0 \quad \text{and} \quad n \cdot \nabla \mu + \kappa H \mu = 0 \text{ on } \Gamma_1, \end{aligned} \quad (36)$$

where  $\psi = (\lambda, \mu) \in V = V_0 \times V_1$ ,  $q \in L^2(\Omega)$  and

$$E_z^* \psi = -\kappa H \mu \quad \text{on } \Gamma_1. \quad (37)$$

We used the mixed-finite element method [7] based on the Legendre polynomials to approximate problem (1)-(2) numerically. Detailed discussions about the method are given in [13]. In our implementation we calculated the adjoint system for the approximated problem and solved equations (2) and (36) using GMRES [3]. The specific implementation of GMRES applied to our example is described in [13] in detail. Concerning the divergence-free constraint  $\nabla \cdot u = 0$ , we employed

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the feasible method, projecting the first equation onto the divergence-free space  $V_0$  as in [4], [6], [13]. The line search in Step 3 of Algorithm 2 was performed by the linearization of the constraint  $E(z, g) = 0$  at  $(z_k, g_k)$  since the cost functional is quadratic. That is, if  $v_k$  is the solution to  $E_z(z_k, g_k)v_k + E_g(z_k, g_k)d_k = 0$  then  $\alpha > 0$  is chosen so that  $J(z_k - \alpha v_k, g_k - \alpha d_k)$  is minimized.

For this specific example, three steps of Algorithm 2 were performed. We then set  $x^1$  and  $\lambda^1$  as  $x^1 = (z_4, g_4)$  and  $\lambda^1 = \psi_3$  for Algorithm 1 without Step 2. The matrix operator  $S(x, \lambda)$  was calculated for the approximated system and the resulting linear equation (31) was again solved by GMRES.

The calculations were performed using a  $20 \times 20$  Cartesian product of Legendre polynomials, choosing  $c = 1$  and  $g_1 = 0$ . Algorithm 1 was terminated after three iterates, since the necessary and sufficient optimality condition (28) was satisfied within a residual norm of  $1 \times 10^{-7}$ .

We may compare this rapid convergence of the hybrid method with the results of using either algorithm by itself. Algorithm 2 did not fully converge after 50 iterates. Algorithm 1, with the start-up  $x^1 = ((u^1, T^1), 0) \in X$  and  $\lambda^1 = 0$ , also failed to converge. Thus, the use of the hybrid method combining the gradient method and the second-order augmented Lagrangian was essential for the success of our numerical calculations. Figure 3 shows the iterates  $g_k$  (the first three curves from top to middle) for Algorithm 1 and the (calculated) optimal control  $g^*$  (the lowest curve). The iterates for Algorithm 1 are not shown because they coincide with  $g^*$  within the accuracy of the plotting. Figure 4 shows the resulting vector field  $u^*$  which corresponds to  $g^*$ . It shows clearly that the vertical transport of flow is increased.

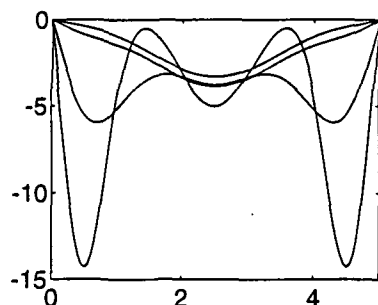


Figure 3. Optimal control iterates.

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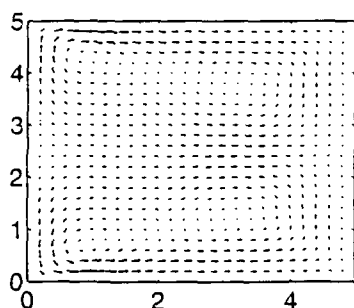


Figure 4. The controlled flow.

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