

# Optimal Spatial Field Control of Distributed Parameter Systems

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**Abstract**—Optimal control problems are formulated and solved in which the manipulation is distributed over a three-dimensional (3D) spatial field with constraints on the spatial variation. These spatial field control problems that arise in applications in acoustics, structures, epidemiology, cancer treatment, and tissue engineering have much higher controllability than boundary control problems, but have vastly higher degrees of freedom. Efficient algorithms are developed for computing optimal manipulated fields by combination of modal analysis and least-squares optimization over a basis function space. Small minimum control error is observed in applications to distributed parameter systems with reaction, diffusion, and convection.

## I. INTRODUCTION

*Spatial field control* is a class of control problems for distributed parameter systems (DPS) in which manipulation occurs as a spatial field, in contrast to the more commonly studied problem of boundary control (e.g., [15]) in which manipulation only occurs at the boundaries. The interior of a spatial domain provides much more controllability than the boundary, which can be quite limited depending on the shape of the desired spatial field and the spatiodynamics of the DPS. At the same time, spatial field control problems have much more degrees of freedom than the corresponding boundary control problem. The manipulated variable for 3D spatial field control is  $u(x, y, z, t)$ , compared to boundary control which is only defined on the 2D external surface. While the brute-force application of control vector parameterization [14] may be applied to boundary control and most other optimal control problems, spatial field control problems need to be formulated with care to arrive at a computationally feasible solution. Below is the formal definition of a prototypical problem.

*Definition 1:* The *optimal spatial field control problem* is the minimization of the quadratic cost

$$\min_{u(x,y,z,t) \in \mathcal{U}(x,y,z,t)} \int_0^{t_f} \int_V (R(x,y,z,t) - C(x,y,z,t))^2 dV dt, \quad (1)$$

where  $V$  is the spatial domain of interest,  $R(x, y, z, t)$  is the reference (desired) field,  $C(x, y, z, t)$  is the controlled field which is related to the manipulated field  $u(x, y, z, t)$  by a known partial differential equation (PDE), and  $\mathcal{U}(x, y, z, t)$  is the set of allowable manipulated fields, which can be continuous or discrete in space or time.

Spatial field control problems arise in a variety of applications including

- 1) minimization of vibration throughout a structure by using internally placed piezo-actuators [11],
- 2) minimization of noise in acoustic enclosures using internally placed loudspeakers and/or microphones [12],
- 3) control of the spread of disease by placement of insecticide-treated targets or by insecticide spraying to reduce the disease carrier population to zero over large tracts of land [5],
- 4) control of the differentiation of stem cell populations by internal release of growth factors to produce biological tissues for clinical use [6], and
- 5) the controlled release of drug cocktails for optimized cancer treatment therapies [16].

The spatial field control literature includes many theoretical results on controllability and the structure of the optimal control for certain classes of PDEs when the spatial field is continuous or consists of a finite number of point sources (e.g., see [2], [8], [9] and citations therein) but has relatively few contributions that compute the optimal control for specific applications. An exception is [11] that computes  $H_2$ - and  $H_\infty$ -optimal vibration controllers for the case in which the manipulation is restricted to discrete positions in the spatial domain.  $H_2$ - and  $H_\infty$ -control for the spatially distributed formulation of the problem results in better performance than the lumped-parameter representation.

This paper presents a computationally efficient solution to the optimal spatial field control problem for the reaction-diffusion and reaction-diffusion-convection equations in which the manipulation  $u(x, y, z, t)$  is continuously distributed throughout the spatial domain with constraints on the spatial variation. These particular control problems are motivated by biomedical control problems [6], [16], in which molecules are released within a biological tissue from fixed embedded polymer nano- and microparticles designed to provide controlled release. The transport of these molecules is described by 3D reaction-diffusion or reaction-diffusion-convection equations, and the control problem is to provide a desired spatial and temporal uptake of these molecules throughout the biological tissue. More details on the biological motivation for the optimal control problem, including numerous references to the biomedical literature, was provided in a previous paper [6].

The approach taken in this paper is based on modal analysis and least-squares optimization over a basis function space [10]. This approach does not involve the discretizations of the spatial variables or problem-independent basic function expansions (e.g., proper orthogonal decomposition) that have

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become popular in the applied PDE control literature (e.g., [7]) but are much more computational expensive when applied to spatial field control problems. Also, this paper considers 3D optimal nonlinear control problems, in contrast to the literature that primarily considers 1D linear problems, and the paper also considers coupled systems of PDEs. The algorithmic discussions are followed by two numerical examples and the conclusions.

## II. SPATIAL FIELD CONTROL OF THE REACTION-DIFFUSION EQUATION

The following descriptions of the system and control problem hold throughout the paper unless stated otherwise.

Consider the reaction-diffusion equation, which is the parabolic PDE

$$\frac{\partial C}{\partial t} = D\nabla^2 C - g(C) + u(x, y, z, t), \quad \forall t > 0, \quad (x, y, z) \in \Omega \quad (2)$$

where  $C(x, y, z, t)$  is the concentration field,  $D > 0$  is an effective diffusion coefficient,  $g(C)$  is a sublinear algebraic function that characterizes the net consumption of species by chemical reactions, and the spatial domain  $\Omega$  is the unit cube. To simplify the presentation, suppose the Dirichlet boundary condition

$$C(x, y, z, t) = 0, \quad \text{on } \partial\Omega, \quad (3)$$

and zero initial condition,

$$C(x, y, z, 0) = 0. \quad (4)$$

The control objective is to determine a smooth manipulated field  $u(x, y, z, t)$  of constrained spatial variation that minimizes the control error<sup>1</sup>

$$E = \int_0^{t_f} \int_{\Omega} (R(x, y, z, t) - C(x, y, z, t))^2 dV dt, \quad (5)$$

where  $R(x, y, z, t)$  is the reference concentration field with  $R(x, y, z, 0) = 0$ . For solving this problem, first define  $\bar{u}(x, y, z, t) = u(x, y, z, t) - g(C)$ , then

$$\frac{\partial C}{\partial t} = D\nabla^2 C + \bar{u}(x, y, z, t), \quad \forall t > 0, \quad (x, y, z) \in \Omega. \quad (6)$$

For this PDE, it can be verified that the manipulated field

$$\bar{u}(x, y, z, t) = \bar{u}_{mnl}(t) \sin m\pi x \sin n\pi y \sin l\pi z, \quad (7)$$

excites only the modes  $\sin m\pi x$ ,  $\sin n\pi y$ ,  $\sin l\pi z$ , that is, the solution to the PDE for that manipulated field is of the form

$$C(x, y, z, t) = c_{mnl}(t) \sin m\pi x \sin n\pi y \sin l\pi z. \quad (8)$$

Additionally,  $\bar{u}_{mnl}(t)$  and  $c_{mnl}(t)$  are related by

$$\bar{u}_{mnl}(t) = \frac{dc_{mnl}}{dt} + D(m^2 + n^2 + l^2)\pi^2 c_{mnl}. \quad (9)$$

<sup>1</sup> $\int_{\Omega} dV = \int_0^1 \int_0^1 \int_0^1 dx dy dz$

With the manipulated field  $\bar{u}(x, y, z, t)$  parameterized in terms of the eigenfunctions,<sup>2</sup>

$$\begin{aligned} \bar{u}(x, y, z, t) &= \sum \bar{u}_{mnl}(t) \sin m\pi x \sin n\pi y \sin l\pi z \\ &\equiv \bar{u}_{MNL}(x, y, z, t), \end{aligned} \quad (10)$$

the spatial variation constraint is specified by selection of finite values of  $M$ ,  $N$ , and  $L$ .

By linearity of (6), the solution to the PDE (6) is

$$\begin{aligned} C(x, y, z, t) &= \sum c_{mnl}(t) \sin m\pi x \sin n\pi y \sin l\pi z \\ &\equiv C_{MNL}(x, y, z, t), \end{aligned} \quad (11)$$

and it is useful to expand the reference field as

$$R(x, y, z, t) = R_{MNL}(x, y, z, t) + \epsilon(x, y, z, t), \quad (12)$$

where

$$R_{MNL}(x, y, z, t) \equiv \sum r_{mnl}(t) \sin m\pi x \sin n\pi y \sin l\pi z, \quad (13)$$

and

$$r_{mnl}(t) = 8 \int_{\Omega} R(x, y, z, t) \sin m\pi x \sin n\pi y \sin l\pi z dV. \quad (14)$$

When the reference field  $R(x, y, z, t)$  is continuously differentiable, Dirichlet's theorem [1] implies that the series expansion converges pointwise in the domain  $\Omega$ , and  $\epsilon$  can be written as a linear combination of the eigenmodes not included in the summation.

With the above definitions and parameterization of the manipulated field, the control error (5) can be written as

$$\begin{aligned} E &= \int_0^{t_f} \int_{\Omega} \left[ \left( \sum (r_{mnl}(t) - c_{mnl}(t)) \sin m\pi x \sin n\pi y \sin l\pi z \right)^2 \right. \\ &\quad \left. + \epsilon^2(x, y, z, t) \right] dV dt, \end{aligned} \quad (15)$$

which follows from orthogonality of the eigenfunctions. The control error is minimized for  $r_{mnl}(t) = c_{mnl}(t)$  for all  $m, n, l$ , which is obtained by setting

$$\bar{u}_{mnl}(t) = \frac{dr_{mnl}}{dt} + D(m^2 + n^2 + l^2)\pi^2 r_{mnl}. \quad (16)$$

Once  $\bar{u}(x, y, z, t) = \sum \bar{u}_{mnl}(t) \sin m\pi x \sin n\pi y \sin l\pi z$  is determined, the manipulated field for the original PDE (2) for this basis function expansion can be determined from

$$u(x, y, z, t) = \bar{u}(x, y, z, t) + g(C), \quad (17)$$

where  $C$  is inserted from (11). If the reaction term  $g(C)$  is linear in  $C$ , then

$$\begin{aligned} u(x, y, z, t) &= \\ &= \sum (\bar{u}_{mnl}(t) + g_{mnl}(t)) \sin m\pi x \sin n\pi y \sin l\pi z, \end{aligned} \quad (18)$$

<sup>2</sup>The summations are over every integer from  $(m, n, l) = (1, 1, 1)$  to  $(M, N, L)$  unless otherwise stated.

for some  $g_{mnl}(t)$ , and the concentration field  $C(x, y, z, t)$  and manipulated field  $u(x, y, z, t)$  share the same spatial modes. Whether the reaction term  $g(C)$  is linear or nonlinear, the optimization for determining  $\bar{u}_{mnl}$  for each  $(m, n, l)$  is independent. If the integral (14) can be solved analytically, then (10) can be determined analytically from (16) and the computational cost of computing the optimal manipulated field is negligible. If the integral (14) cannot be solved analytically, then the  $r_{mnl}(t)$  can be computed efficiently by sampling with a uniform mesh and applying available numerical software for computing multidimensional fast Fourier transforms [4]. This solution of the optimal control problem is very closely related to *spectral methods* [3] for the numerical simulation of PDEs.

The behavior of the minimum control error as  $(M, N, L)$  increases can be derived from well-known properties of Fourier series [1]. The minimum control error obtained using the finite Fourier sine series expansion (10) is

$$E = \int_0^{t_f} \int_{\Omega} \epsilon^2(x, y, z, t) dV dt, \quad (19)$$

which is independent of the diffusion coefficient and reaction rate, and is only a function of the portion of the reference field not described by the selected eigenfunctions. Relaxing the spatial variation constraint increases the number of terms in the series and decreases the minimum control error.

By the Riesz-Fischer theorem, a Fourier series expansion converges in the space  $l^2$  if the corresponding function is square integrable [1]. This result can be applied to show the above manipulated field converges in  $l^2$  at each time  $t$  as the number of eigenmodes approaches infinity. Define

$$\bar{E}(t) = \int_{\Omega} \epsilon^2(x, y, z, t) dV, \quad (20)$$

then

$$\lim_{M, N, L \rightarrow \infty} \bar{E}(t) = 0, \quad \forall t > 0, \quad (21)$$

if  $R(x, y, z, t)$  is square integrable.<sup>3</sup> Although the Fourier series of a continuous function need not converge pointwise in general [13], it can be shown that if

$$\sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \sum_{l=1}^{\infty} |c_{mnl}| < \infty, \quad (22)$$

then

$$C(x, y, z, t) \equiv \lim_{M, N, L \rightarrow \infty} C_{MNL}(x, y, z, t) \quad (23)$$

and

$$\lim_{M, N, L \rightarrow \infty} \left| R(x, y, z, t) - C_{MNL}(x, y, z, t) \right| = 0. \quad (24)$$

<sup>3</sup>This result generalizes to any problem in which  $R(x, y, z, t)$  is odd or the spatial domain  $\Omega$  is a box in the positive quadrant bordered on three sides by the  $x = 0$ ,  $y = 0$ , and  $z = 0$  planes, so that the Fourier series collapses to a Fourier sine series. The spatial coordinates can always be rotated and shifted so that the latter condition holds. Other boundary conditions may involve the other Fourier series expansions.

Equations (21) and (23) can be used to show that the minimum control error approaches zero as the number of terms approaches infinity:

$$\lim_{M, N, L \rightarrow \infty} \left| \int_{\Omega} (R(x, y, z, t) - C_{MNL}(x, y, z, t))^2 dV - \int_{\Omega} (R(x, y, z, t) - C(x, y, z, t))^2 dV \right| = 0 \quad (25)$$

by application of the triangular inequality. By a similar argument, if

$$\sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \sum_{l=1}^{\infty} |u_{mnl}| < \infty, \quad (26)$$

then

$$u(x, y, z, t) \equiv \lim_{M, N, L \rightarrow \infty} u_{MNL}(x, y, z, t), \quad (27)$$

and, if  $u(x, y, z, t)$  is square integrable,

$$\lim_{M, N, L \rightarrow \infty} \int_{\Omega} (u(x, y, z, t) - u_{MNL}(x, y, z, t))^2 dV = 0. \quad (28)$$

### III. SPATIAL FIELD CONTROL OF THE REACTION-DIFFUSION-CONVECTION EQUATION I

Consider the same control problem as in the previous section except with the PDE replaced by the reaction-diffusion-convection equation

$$\frac{\partial C}{\partial t} = D\nabla^2 C - v \cdot \nabla C - g(C) + u(x, y, z, t), \quad (29)$$

where  $v \neq 0$  is the vector velocity field assumed to be spatially uniform. By using a standard transformation method,

$$\bar{C}(x, y, z, t) \equiv C(x, y, z, t) e^{-\alpha x - \beta y - \gamma z + \theta t}, \quad (30)$$

$$\bar{u}(x, y, z, t) \equiv \hat{u}(x, y, z, t) e^{-\alpha x - \beta y - \gamma z + \theta t}, \quad (31)$$

with

$$\hat{u}(x, y, z, t) = u(x, y, z, t) - g(C), \quad (32)$$

$$\alpha = \frac{v_x}{2D}, \quad \beta = \frac{v_y}{2D}, \quad \gamma = \frac{v_z}{2D}, \quad \theta = \frac{v_x^2 + v_y^2 + v_z^2}{4D}, \quad (33)$$

the PDE (29) is reduced a forced diffusion equation

$$\frac{\partial \bar{C}}{\partial t} = D\nabla^2 \bar{C} + \bar{u}(x, y, z, t), \quad (34)$$

with the boundary condition (3) and initial condition (4) remaining in the same form, respectively:

$$\bar{C}(x, y, z, t) = 0, \quad \text{on } \partial\Omega, \quad (35)$$

$$\bar{C}(x, y, z, 0) = 0. \quad (36)$$

Then  $\bar{u}$  is related to  $\bar{C}$  in the same way that  $\bar{u}$  is related to  $C$  in the previous section. The cost function is

$$E = \int_0^{t_f} \int_{\Omega} \left( R(x, y, z, t) e^{-(\alpha x + \beta y + \gamma z - \theta t)} - \bar{C}(x, y, z, t) \right)^2 dV dt$$

$$e^{2(\alpha x + \beta y + \gamma z - \theta t)} dV dt. \quad (37)$$

The optimal control problem can be solved as a least-squares optimization over a Hilbert space. First write

$$\begin{aligned} \bar{C}(x, y, z, t) &= \sum \bar{c}_{mnl}(t) \sin m\pi x \sin n\pi y \sin l\pi z \\ &= \sum_{i=1}^{MNL} \bar{c}_i(t) s_i(x, y, z) \\ &= s^T \bar{c}(t), \end{aligned} \quad (38)$$

where  $s_i(x, y, z) \equiv \sin m\pi x \sin n\pi y \sin l\pi z$  and the vectors  $s$  and  $\bar{c}(t)$  have  $s_i(x, y, z)$  and  $\bar{c}_i(t)$  as their elements, respectively. Define inner products by

$$\begin{aligned} \langle a(x, y, z, t) | b(x, y, z, t) \rangle &= \\ &= \int_{\Omega} e^{2(\alpha x + \beta y + \gamma z - \theta t)} a(x, y, z, t) b(x, y, z, t) dV, \end{aligned} \quad (39)$$

the Gram matrix by

$$\begin{aligned} G(t) &= \begin{bmatrix} \langle s_1 | s_1 \rangle & \cdots & \langle s_1 | s_{MNL} \rangle \\ \langle s_1 | s_2 \rangle & \cdots & \vdots \\ \vdots & \vdots & \vdots \\ \langle s_1 | s_{MNL} \rangle & \cdots & \langle s_{MNL} | s_{MNL} \rangle \end{bmatrix} \\ &\equiv H e^{-2\theta t}, \end{aligned} \quad (40)$$

and

$$r(t) = \begin{bmatrix} \langle R e^{-(\alpha x + \beta y + \gamma z - \theta t)} | s_1 \rangle \\ \langle R e^{-(\alpha x + \beta y + \gamma z - \theta t)} | s_2 \rangle \\ \vdots \\ \langle R e^{-(\alpha x + \beta y + \gamma z - \theta t)} | s_{MNL} \rangle \end{bmatrix}. \quad (41)$$

The solution to the optimal control problem for the manipulated field is given by  $\bar{c}(t)$  that satisfies

$$G(t) \bar{c}(t) = r(t) \iff H e^{-2\theta t} \bar{c}(t) = r(t). \quad (42)$$

For reference fields whose inner product with each eigenmode can be determined analytically, the main computational cost is the inversion of the scaled Gram matrix.

The scaled Gram matrix  $H$  is dense, which implies that the optimal control solution is not decoupled into separate optimal control problems for each eigenmode, as it was for the convection-free case. The expression for the minimum control error, which is substantially more complicated than (19), depends on all of the model parameters  $D$  and  $v$ .

The solution to the optimal control problem is simplified when the reference is separable in space and time:

$$R(x, y, z, t) = R_{xyz}(x, y, z) R_t(t), \quad (43)$$

in which case

$$r(t) = q e^{-\theta t} R_t(t), \quad (44)$$

where  $q$  is a constant vector, and

$$\begin{aligned} R(x, y, z, t) &= \sum q_{mnl} R_t(t) \sin m\pi x \sin n\pi y \sin l\pi z e^{-(\alpha x + \beta y + \gamma z)} \\ &\quad + \epsilon(x, y, z, t). \end{aligned} \quad (45)$$

The remainder of this section assumes (43) to simplify the presentation (the general expressions are somewhat more complicated). From (42), the optimal concentration field is

$$\begin{aligned} C(x, y, z, t) &= \sum_{i=1}^{MNL} s_i(x, y, z) \bar{c}_i(t) e^{\alpha x + \beta y + \gamma z - \theta t} \\ &= \sum \sin m\pi x \sin n\pi y \sin l\pi z \\ &\quad (H^{-1} q e^{\theta t})_{mnl} R_t(t) e^{\alpha x + \beta y + \gamma z - \theta t}, \end{aligned} \quad (46)$$

and the optimal manipulated field

$$\begin{aligned} u(x, y, z, t) &= g(C) + e^{\alpha x + \beta y + \gamma z} \sum \sin m\pi x \sin n\pi y \sin l\pi z \\ &\quad (H^{-1} q)_{mnl} \left( \frac{dR_t}{dt} + (D(m^2 + n^2 + l^2)\pi^2 + \theta) R_t(t) \right) \end{aligned} \quad (47)$$

where  $(H^{-1} q)_{mnl}$  is the  $(mnl)^{th}$  element of the product of the inverse of a scaled  $(mnl) \times (mnl)$  Gram matrix  $H$  of the eigenmodes and  $q$  is a scaled vector of inner products of the eigenmodes and the reference field. Again, if  $g(C)$  is linear in  $C$ , then the concentration field  $C(x, y, z, t)$  and manipulated field  $u(x, y, z, t)$  share the same spatial modes. With this optimal control, the optimal control objective is

$$\begin{aligned} E &= \int_0^{t_f} \int_{\Omega} \left( \sum R_t(t) \sin m\pi x \sin n\pi y \sin l\pi z e^{-(\alpha x + \beta y + \gamma z)} \right. \\ &\quad \left. (q_{mnl} - (H^{-1} q)_{mnl}) e^{2(\alpha x + \beta y + \gamma z)} + \epsilon \right)^2 dV dt. \end{aligned} \quad (48)$$

While the minimum control error decreases as more terms are taken, its further characterization is more complicated than for the convection-free case. Provided that the effects of diffusion are significant (that is, the parameters in (33) are less than 1), low values of  $(M, N, L)$  in  $\bar{u}(x, y, z, t)$  directly translate into low spatial variation on  $u(x, y, z, t)$ .

#### IV. SPATIAL FIELD CONTROL OF THE REACTION-DIFFUSION-CONVECTION EQUATION II

Consider the same system as the previous section. With the definition

$$\bar{u}(x, y, z, t) = u(x, y, z, t) - v \cdot \nabla C - g(C), \quad (49)$$

$\bar{u}(x, y, z, t)$  can be determined in the same way as in Section II and used to compute  $C(x, y, z, t)$  and the optimal manipulated field from  $u(x, y, z, t) = \bar{u}(x, y, z, t) + v \cdot \nabla C + g(C)$ . With this approach, the optimal solution is

$$u(x, y, z, t) = g(C) + \sum u_{1,mnl}(t) \sin m\pi x \sin n\pi y \sin l\pi z$$

$$\begin{aligned}
& + \sum u_{2,mnl}(t) \cos m\pi x \sin n\pi y \sin l\pi z, \\
& + \sum u_{3,mnl}(t) \sin m\pi x \cos n\pi y \sin l\pi z, \\
& + \sum u_{4,mnl}(t) \sin m\pi x \sin n\pi y \cos l\pi z, \quad (50)
\end{aligned}$$

where

$$u_{1,mnl}(t) = \frac{dr_{mnl}}{dt} + D(m^2 + n^2 + l^2)\pi^2 r_{mnl}, \quad (51)$$

$$u_{2,mnl}(t) = m\pi v_x r_{mnl}(t), \quad (52)$$

$$u_{3,mnl}(t) = n\pi v_y r_{mnl}(t), \quad (53)$$

$$u_{4,mnl}(t) = l\pi v_z r_{mnl}(t). \quad (54)$$

These equations can be easily verified by inserting the manipulated field into the PDE (29). As in the previous sections, superposition can be used to construct a solution to the optimal control problem. With the form of the manipulated field being the same as in the reaction-diffusion case, the minimum control error, the computational cost of the optimal control problem, and the other analyses are the same.

## V. SPATIAL FIELD CONTROL OF COUPLED REACTION-DIFFUSION-CONVECTION EQUATIONS

Consider the optimal spatial field control of coupled reaction-diffusion-convection equations:

$$\begin{aligned}
\min_{\substack{u_i(x,y,z,t) \\ \in \mathcal{U}_i(x,y,z,t)}} \sum_i \int_0^{t_f} \int_V (R_i(x,y,z,t) - C_i(x,y,z,t))^2 dV dt, \quad (55)
\end{aligned}$$

where

$$\frac{\partial C_i}{\partial t} = D_i \nabla^2 C_i - v \cdot \nabla C_i - g_i(C_1, \dots, C_N) + u_i(x,y,z,t), \quad (56)$$

$$C_i(x,y,z,t) = 0, \quad \text{on } \partial\Omega, \quad (57)$$

and

$$C_i(x,y,z,0) = 0. \quad (58)$$

With the definitions

$$\bar{u}_i = u_i(x,y,z,t) - g_i(C_1, \dots, C_N), \quad i = 1, \dots, N, \quad (59)$$

or

$$\bar{u}_i = u_i(x,y,z,t) - v \cdot \nabla C_i - g_i(C_1, \dots, C_N), \quad (60)$$

$$i = 1, \dots, N,$$

the determination of the optimal  $\bar{u}_i$  are decoupled. Once the optimal  $\bar{u}_i$  have been determined, the species concentration fields  $C_i$  and untransformed optimal manipulated fields  $u_i$  are determined in the same way as in the previous section.

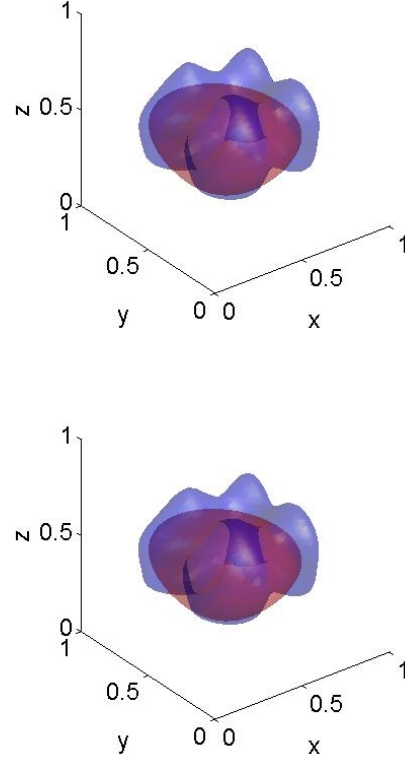


Fig. 1. The concentration isosurface  $C(x,y,z,t) = 0.009$  for the reference (convex) and controlled (lumpy) concentration fields for  $N = M = L = 5$ ,  $t = 0.5$ , and a spatial grid size of 0.025 used for plotting. The top plot is the case of no convection ( $v_x = v_y = v_z = 0$ ) and for the case with convection ( $v_x = 0.8, v_y = 0.5, v_z = 0.3$ ) obtained using the approach described in Section IV (both cases result in the same figure). The bottom plot is for the same problem with convection obtained using the approach described in Section III.

## VI. NUMERICAL EXAMPLES

Consider the optimal spatial field control of the reaction-diffusion and reaction-diffusion-convection equations for the reference concentration field

$$\begin{aligned}
R(x,y,z,t) = & (e^{-x} - e^{-3x})(e^{-y} - e^{-4y})(e^{-2z} - e^{-4z})(e^{-t} - e^{-2t}), \quad (61)
\end{aligned}$$

for linear chemical reaction kinetics  $g(C) = kC$  with dimensionless rate constant  $k = 0.1$  and dimensionless effective diffusion coefficient  $D = 1$ . In a stem tissue engineering application, this reference field corresponds to 3D spatial region and time in which a cellular uptake of growth factor is desired to cause the stem cells in that region to differentiate to form a specific type of cell (such as an islet cell in the generation of a pancreas for treatment of a diabetic patient). The reader is referred to a previous paper for a more detailed discussion of these applications [6].

The isosurfaces for the reference and controlled concentration fields show good correspondence for 5 terms in each of

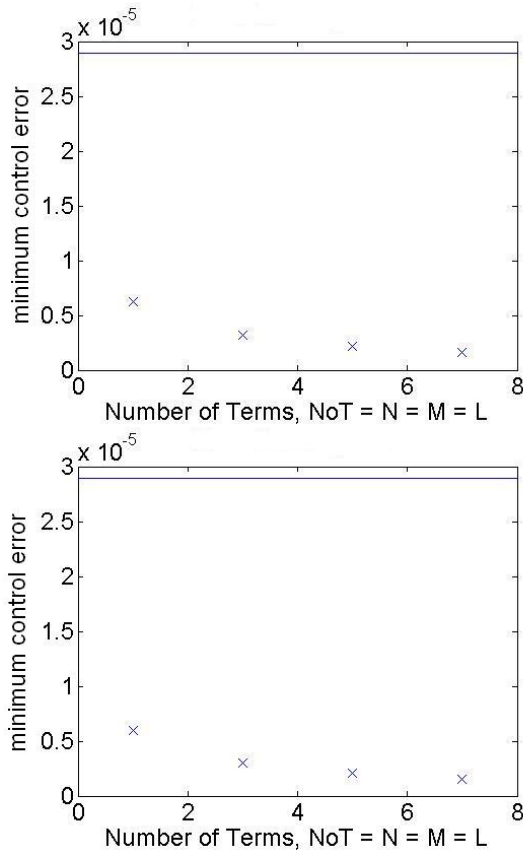


Fig. 2. The value of the minimum control error  $E$ . The horizontal line shows the control error when the manipulated field is zero. The plots have the corresponding parameter values as in Fig. 1.

the three spatial directions, both for the cases with and without convection and with application of several of the proposed approaches (see Fig. 1). The controlled concentration fields and the minimum control errors are very similar for both PDEs and all three approaches. Most of the reduction in the minimum control error occurs with only 1 term (see Fig. 2), with a 90% reduction with 3 terms in each spatial direction ( $3^3 = 27$  total terms). The minimum control error decreases monotonically as the number of terms in each spatial direction increases, which is consistent with the theoretical analysis.

## VII. CONCLUSIONS

A modal control approach is investigated for optimal control problems in which the manipulation is distributed over a 3D spatial field with constraints on its spatial variation. Application to reaction-diffusion and reaction-diffusion-convection equations demonstrated small minimum control error for a 3D time-varying reference field with modest spatial variation. In the convection-free case, the minimum control error is independent of the values of the model parameters and all eigenmodes are decoupled. In the case with convection, two approaches were proposed. The first approach produces a manipulated field in terms of eigenmodes, which requires a dense matrix inversion but has fewer summation terms for the

same  $(M, N, L)$  than the second approach. Depending on the reference field, either approach could require higher values of  $(M, N, L)$  to achieve a certain control error. The extension of the proposed approach to coupled PDEs was also briefly described.

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