OPTIMAL CONTROL OF ADVECTION-DIFFUSION EQUATION

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1 Introduction

Advection-diffusion equation is certainly a frequently studied PDE with important applications such as, e.g., modeling the dispersion of pollutants in air or water. Moreover, the goal could be not only to simulate dispersion processes but also to control emissions with an active device and maximum efficiency [1, 2]. The present paper concerns with the solution of such kind of issues, which involve an optimization problem with the following features: derivation of optimality system, numerical resolution of governing PDEs and definition of a suitable algorithm to implement the optimization. Each step of the general procedure is explained in section 2, while some numerical tests are presented in section 3.

In the present study the following assumptions are made: monodimensional and unbounded domain, unsteady state. Moreover, the particular case of source and control concentrated at single points is considered.

2 Method

2.1 Theoretical framework

2.1.1 State equation

The governing PDE of the model, which acts like a constraint in the optimization problem written as the state equation, is:

$$F(C,q) = \frac{\partial C}{\partial t} + \frac{\partial (U \cdot C)}{\partial x} - D\frac{\partial^2 C}{\partial x^2} - g - q = 0 \tag{2.1}$$

with $0 < x < L$ and $0 < t < T$ and where $C = C(x,t)$ is the concentration rate of a scalar quantity of interest, $U = U(x,t)$ is the velocity of the advective flow, D is the diffusivity coefficient, $g = g(x,t)$ is the source term and $q = q(x,t)$ is the control one. U and g are known distributions, while C is obtained by solving the PDE; optimal q (which minimizes the objective function, defined later) is computed with an iterative optimization procedure. Boundary conditions are $C(0,t) = C(L,t) = 0$ in order to simulate an unbounded domain, while initial condition is $C(x,0) = C_0(x)$.

2.1.2 Objective function

In the present study the goal is chosen to minimize the concentration rate at a point P while minimizing the cost of the control, which is located at a point C. Hence, the objective function, using Dirac deltas, is defined as:

$$J(C,q) = \gamma_1 \int_{-\infty}^{\infty} C(x,T)\delta(x - x_P)\mathrm{d}x + \frac{1}{2}\gamma_2 \int_0^T \int_{-\infty}^{\infty} [q(x,t)]^2 \mathrm{d}x\,\mathrm{d}t$$

with the choice of $q(x,t) = Q(t)\delta(x - x_C)$, as mentioned in the introduction, and where $\delta(x-\bar{x}) = \begin{cases} 1 & x = \bar{x} \\ 0 & x \neq \bar{x} \end{cases}$, $\int_{-\infty}^{\infty} f(x)\delta(x-\bar{x})\mathrm{d}x = f(\bar{x})$; thus we can rewrite the expression above as:

$$J(C,q) = \gamma_1 C(x_P,T) + \frac{1}{2}\gamma_2 \int_0^T [Q(t)]^2 \mathrm{d}t$$

2.1.3 Optimality System

The Lagrangian is defined as:

$$\begin{aligned}
\mathcal{L}(C,q,a) &= J \quad - \langle a, F\rangle - \langle b, C(x,0) - C_0\rangle - \langle c, C(0,t)\rangle - \langle d, C(L,t)\rangle \\
&= \quad \gamma_1 C(x_P,T) + \frac{1}{2}\gamma_2 \int_0^T [Q(t)]^2\mathrm{d}t - \int_0^T \int_{-\infty}^{\infty} a\left(\frac{\partial C}{\partial t} + \frac{\partial (U\cdot C)}{\partial x} - D\frac{\partial^2 C}{\partial x^2} - g - q\right)\mathrm{d}x\,\mathrm{d}t + \\
&\quad - \int_{-\infty}^{\infty} b(C(x,0) - C_0)\mathrm{d}x - \int_0^T c\,C(0,t)\mathrm{d}t - \int_0^T d\,C(L,t)\mathrm{d}t
\end{aligned}$$

where $a = a(x,t)$, $b = b(x)$,$c = c(t)$,$d = d(t)$ are the Lagrange multipliers.

Next step is to apply the stationarity condition on $\mathcal{L}$. Thus, the following system is obtained:

$$\begin{cases}
\frac{\delta\mathcal{L}}{\delta a} = 0 & \Rightarrow & F = 0 & \text{(state equation)} \\
\frac{\delta\mathcal{L}}{\delta b} = 0 & \Rightarrow & C(x,0) = C_0 & \text{(initial condition)} \\
\frac{\delta\mathcal{L}}{\delta c} = 0 & \Rightarrow & C(0,t) = 0 & \text{(boundary conditions)} \\
\frac{\delta\mathcal{L}}{\delta d} = 0 & \Rightarrow & C(L,t) = 0 & \\
\frac{\delta\mathcal{L}}{\delta C} = 0 & \Rightarrow & \frac{\partial a}{\partial t} + U\frac{\partial a}{\partial x} + D\frac{\partial^2 a}{\partial x^2} = 0 & \text{(adjoint equation)} \\
 & & a(x,T) = \gamma_1 & \text{(terminal condition)} \\
\frac{\delta\mathcal{L}}{\delta q} = 0 & \Rightarrow & q(x_C,t) = -\gamma_2\, a(x_C,t) & \text{(optimality condition)}
\end{cases}$$

2.2 Numerical methods and implementation

2.2.1 Discretization

State and adjoint equations are solved by discretization with finite difference method using an explicit, first order in time and second order in space scheme (using central difference for advection term). Hence, for the state equation it turns: $\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}$,$\frac{\partial^2 C}{\partial x^2} \approx \frac{C_{i+1} - 2C_i + C_{i-1}}{(\Delta x)^2}$, $\frac{\partial (U\cdot C)}{\partial x} \approx \frac{(U\cdot C)_{i+1} - (U\cdot C)_{i-1}}{2\Delta x}$. Approximation of 2.1 is then:

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{(U\cdot C)_{i+1}^n - (U\cdot C)_{i-1}^n}{2\Delta x} - D\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} = g_i^n + q_i^n$$

Hence, the scheme is:

$$
\begin{aligned}
C_i^{n+1} &= C_i^n - \Delta t\, \frac{(U\cdot C)_{i+1}^n - (U\cdot C)_{i-1}^n}{2\Delta x} + D\Delta t\, \frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{(\Delta x)^2} + \Delta t\, g_i^n + \Delta t\, q_i^n \\
&= (\beta - \frac{\lambda}{2} U_{i+1}^n)\, C_{i+1}^n + (1-2\beta)\, C_i^n + (\beta + \frac{\lambda}{2} U_{i-1}^n)\, C_{i-1}^n + \Delta t\, g_i^n + \Delta t\, q_i^n
\end{aligned} \tag{2.2}
$$

where $\lambda = \frac{\Delta t}{\Delta x}$, $\beta = D\frac{\Delta t}{(\Delta x)^2}$, and for $i = 2, \ldots, M-1$, $n = 1, \ldots, N$, where M is the number of nodes in space and N is the number of nodes in time.

Equation 2.2 has to satisfy two conditions in order to have numerical stability, according to [3]:

$$
\sigma^2 \leq 2\beta \leq 1 \tag{2.3}
$$

where $\sigma = max(U) \cdot \lambda$.

2.3 involves a limitation on the time step:

$$
\Delta t \leq min\left(\frac{2D}{U_{max}^2}, \frac{(\Delta x)^2}{2D} \right)
$$

Furthermore, stability check by calculation of eigenvalues is performed.

Each time step is solved looking at a vectorial form of 2.2, introducing the matrix $\boldsymbol{V}$:

$$
\boldsymbol{C}^{n+1} = \boldsymbol{V}\, \boldsymbol{C}^n + \Delta t\, \boldsymbol{g}^n + \Delta t\, \boldsymbol{q}^n
$$

$$
\boldsymbol{V} = \begin{pmatrix}
1-2\beta & \beta - \frac{\lambda}{2} U_{i+1}^n & 0 & 0 & 0 \\
\beta + \frac{\lambda}{2} U_{i-1}^n & \ddots & \ddots & 0 & 0 \\
0 & \ddots & \ddots & \ddots & 0 \\
0 & 0 & \ddots & \ddots & \beta - \frac{\lambda}{2} U_{i+1}^n \\
0 & 0 & 0 & \beta + \frac{\lambda}{2} U_{i-1}^n & 1-2\beta
\end{pmatrix}
$$

The same approach has been chosen for solving the adjoint equation and the resulting scheme is similar:

$$
\boldsymbol{a}^n = \boldsymbol{V}^\dagger\, \boldsymbol{a}^{n+1}
$$

$$
\boldsymbol{V}^\dagger = \begin{pmatrix}
1-2\beta & \beta + \frac{\lambda}{2} U_i^n & 0 & 0 & 0 \\
\beta - \frac{\lambda}{2} U_i^n & \ddots & \ddots & 0 & 0 \\
0 & \ddots & \ddots & \ddots & 0 \\
0 & 0 & \ddots & \ddots & \beta + \frac{\lambda}{2} U_i^n \\
0 & 0 & 0 & \beta - \frac{\lambda}{2} U_i^n & 1-2\beta
\end{pmatrix}
$$

2.2.2 Accuracy of the adjoint

Implementation is checked with the computation of the following error:

$$
\epsilon_{adj} = |\boldsymbol{a}^N \cdot \boldsymbol{C}^N - \boldsymbol{a}^1 \cdot \boldsymbol{C}^1 - \sum_{n=1}^{N-1} \Delta t\, \boldsymbol{a}^{n+1} (\boldsymbol{g}^n + \boldsymbol{q}^n)| \tag{2.4}
$$

Comforting values of ϵ_{adj} (less than about 10^{-15}) are found during computations.

2.2.3 Iterative algorithm

The optimization technique is implemented with the following iterative scheme:

1. Initialization of all variables
2. Solution of state equation
3. Computation of objective function and relative error
4. Solution of adjoint equation and accuracy check of the adjoint
5. Computation of control (optimality condition)
6. If the desired tolerance has not been reached, repetition from step 2 with updated variables.

3 Numerical tests

Two examples are presented to test the developed method and to view at significant results.
It has to be recalled that for advection-diffusion model, the Peclét number has great importance, being defined as $Pe = \frac{UL}{D}$. Large Pe indicates dominant advection.
For both cases, the assumed domain is $x \in [0, 1]$ and $D = 0.005$, $\gamma_2 = 1$ and a parametrization of the weight coefficient γ_1 is done. For simplicity, a constant advective field $U(x, t) = U_0$, with $U_0 = 0.5$ (and $Pe = 100$), is assumed, even if the method works with any velocity distribution. Firstly, initial situation and stability check are presented, then results of optimization are given.
Computations are made using *Gnu Octave* [4].

3.1 Dispersion of a spot

This case could be representative of the accidental dumping of a certain substance into air or water and a consequent operating procedure aimed to minimize the concentration rate of the dispersed substance at a specific point (e.g. a point that must be particularly preserved). For simulating this situation, $g = 0$ and an initial profile of concentration is defined (see at fig. 3.1(a)).

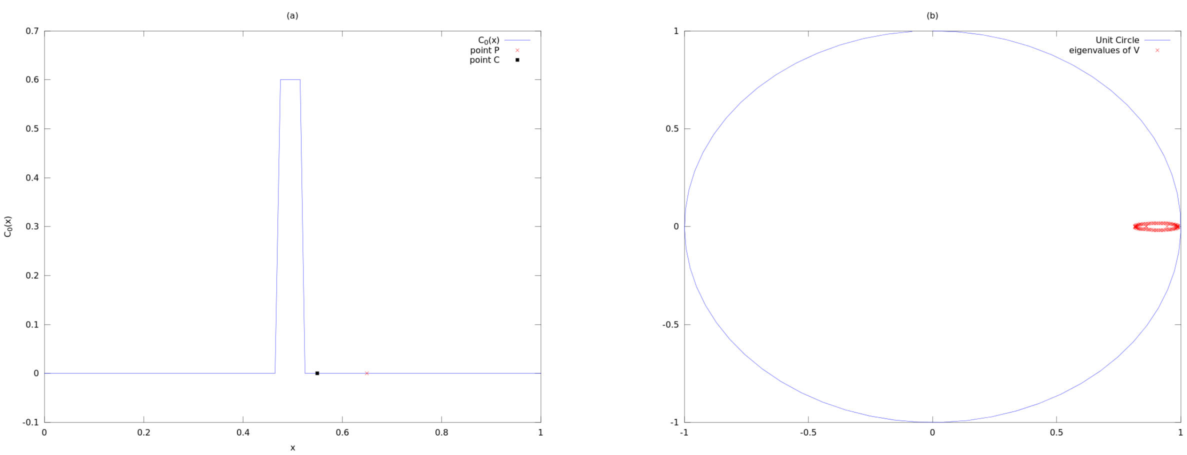

Figure 3.1: *Case 1 - dispersion of a spot: (a)Initial situation and location of points P and C. (b)Plot of eigenvalues of companion matrix for stability check.*

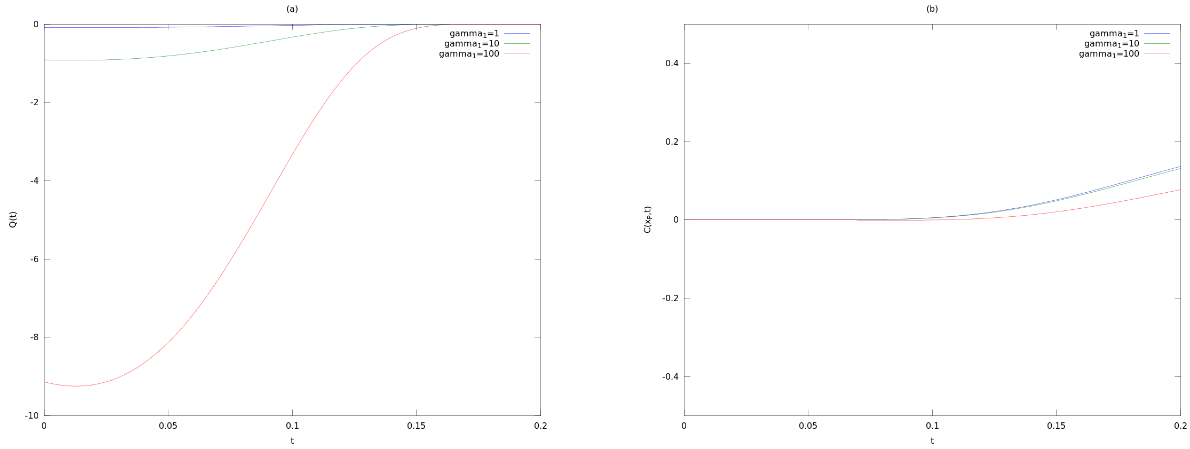

Figure 3.2: *Case 1 - dispersion of a spot: (a)Optimal control laws. (b)Concentration at point P.*

3.2 Constant point source

In the second case we consider a point source ($g(x,t) = G(t)\delta(x - x_S)$), e.g. an industrial chimney, starting to blow at the initial time and at a constant rate. Optimal control could be needed to limit the emissions of the plant. Point C and point S are set as coincident. Actually, this case deals with a transient situation. No initial concentration and constant advective field (with $U_0 = 0.5$ and $Pe = 100$) are assumed for the test.

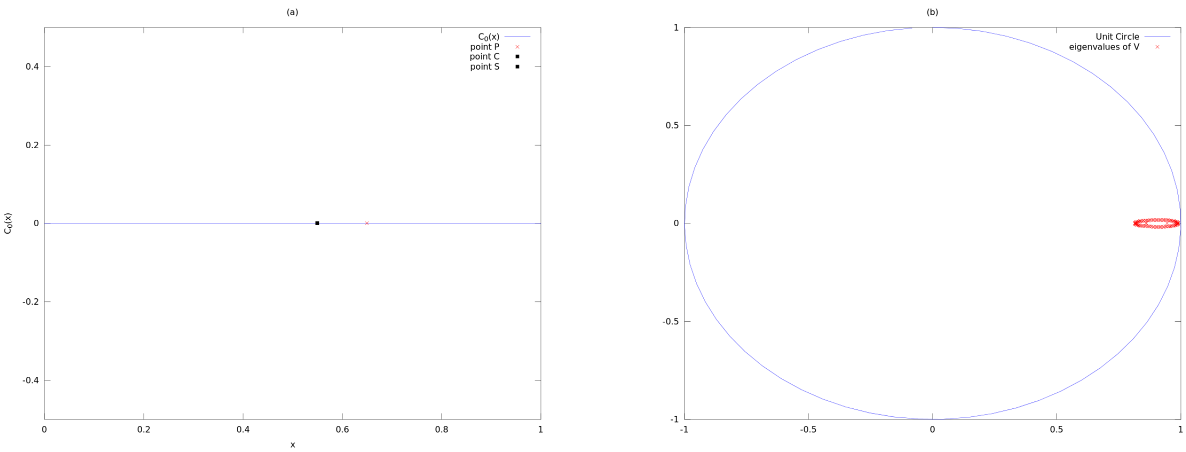

Figure 3.3: *Case 2 - point source: (a)Initial situation and location of points P,C and S. (b)Plot of eigenvalues of companion matrix for stability check.*

4 Discussion

Optimality system for monodimensional unsteady advection-diffusion control problem, in the case of point source and point control, has been derived and a suitable algorithm, numerical methods and relative stability test have been presented. Computations have been also verified by checking errors on the adjoint identity 2.4. Two numerical examples have been presented, besides applicability is certainly wider. The resulting method could be useful for forecasting particular situations in environmental scenarios like dispersion of pollutants.
A remark must be done on the convergence of iterations, which has been seen, in some not presented cases, not always successful; further analyses could be therefore developed for this particular issue. Anyway, the

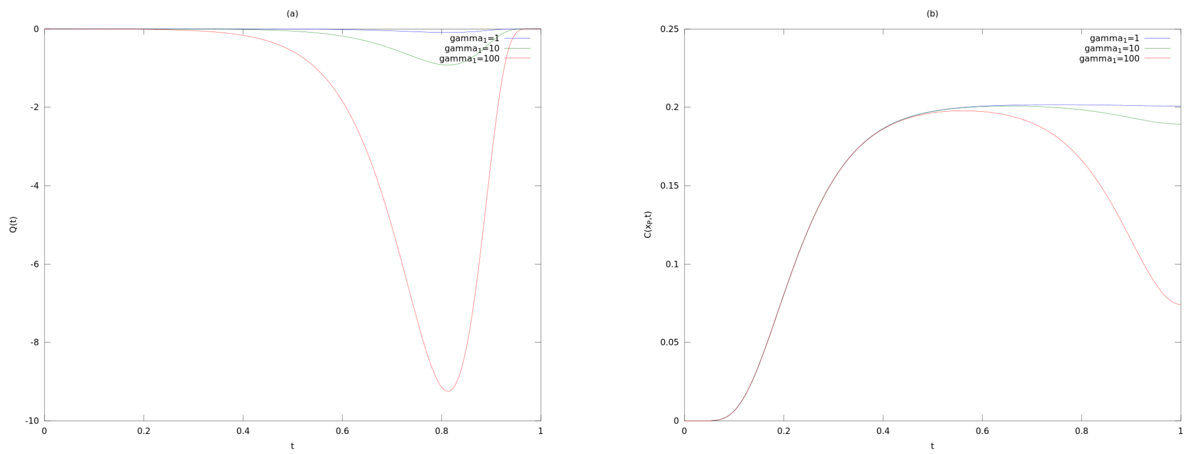

Figure 3.4: *Case 2 - point source: (a)Optimal control laws. (b)Concentration at point P.*

developed code can be applied to different situations by adjusting variables, especially the weight coefficients in the objective function.

References

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[3] C. Hirsch, 2007. *Numerical Computation of Internal and External Flows: The Fundamentals of Computational Fluid Dynamics, Second Edition*, Butterworth-Heinemann, p. 357

[4] *GNU Octave.* http://www.gnu.org/software/octave/