Handbook for Advanced Mathematical Methods for Engineering

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Conjugate Gradient Algorithm for Solving an Optimal Multiple Control Problem on a System of Partial Differential Equations

1 Introduction

Given the partial differential system:

$$\begin{cases} \frac{\partial y}{\partial t} - \mu\frac{\partial^2 y}{\partial x^2} + \epsilon\frac{\partial y}{\partial x} - y = 0 & \text{in } Q = (0,L)\times(0,T) \\ y(x,0) = y_0, & t = 0, \\ -\mu\frac{\partial y(0,t)}{\partial x} = 0, & x = 0, \\ \mu\frac{\partial y(L,t)}{\partial x} = 0, & x = L. \end{cases} \tag{S}$$

A conjugate gradient algorithm with several control on $(0,L)$ is developed for it.

2 Several Control for S

With an appropriate function $v(x,t)$, the system can be controlled, by example on $x = 0$ or $x = L$, and also, let be controls in $x_k = \frac{k}{M}L, k = 1,\ldots,M-1$ (see figure 1).

$$\begin{cases} \frac{\partial y}{\partial t} - \mu\frac{\partial^2 y}{\partial x^2} + \epsilon\frac{\partial y}{\partial x} - y = \chi_{x_k}v & \text{in } Q = (0,L)\times(0,T), i = 1,\ldots,M-1 \\ y(x,0) = y_0, & t = 0, \\ -\mu\frac{\partial y(0,t)}{\partial x} = \chi_0 v(t) = v_0(t), & x = 0, \\ \mu\frac{\partial y(L,t)}{\partial x} = \chi_M v(t) = v_M(t), & x = L. \end{cases} \tag{SE}$$

In this case, the corresponding control problem is

$$\begin{cases} \text{Find } u^* \in \mathcal{U}, \\ J(u^*) \le J(v), \forall v \in \mathcal{U} \end{cases} \tag{CP}$$

where

$$\begin{aligned} J(v) & = \frac{k_0}{2}\iint_Q \chi_i v^2 \mathrm{d}x\mathrm{d}t + \frac{k_1}{2}\iint_Q y^2 \mathrm{d}x\mathrm{d}t + \frac{k_2}{2}\int_0^L (y(x,T) - z(x))^2\,\mathrm{d}x, \\ & \quad \frac{k_0}{2}\sum_{k=0}^M \int_0^T v_i^2 \mathrm{d}t + \frac{k_1}{2}\iint_Q y^2 \mathrm{d}x\mathrm{d}t + \frac{k_2}{2}\int_0^L (y(x,T) - z(x))^2\,\mathrm{d}x, \end{aligned}$$

$v_k = \chi_{x_k}v(x,t)$, $z(x)$ is a given function to reach at $t = T$, and y is the solution of (SE) for each v_k (see figure 1).
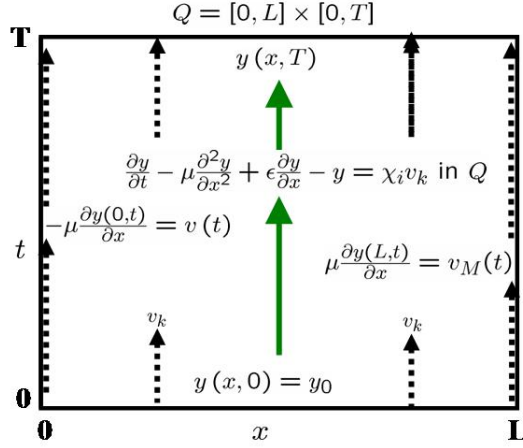
Figure 1: System (SE).

The equivalent form as an optimization problem is:

$$\min_{v \in \mathcal{U}} J(v) = \frac{k_0}{2} \sum_{k=0}^{M} \int_0^T v_k^2 \mathrm{d}t + \frac{k_1}{2} \iint_Q y^2 \mathrm{d}x \mathrm{d}t + \frac{k_2}{2} \int_0^L \left(y(x,T) - z(x) \right)^2 \mathrm{d}x,$$

where y is the solution of (SE) given v.

In this case, the objective of the optimization problem is to reduce the cost or weight of control variable v, keep lower the cost of the evolution of the system $y(x,t)$, and reduce the cost of final state of the system $y(x,T)$.

3 The continuous case

The continuous case is computing by a perturbation of (CP) and (SE) and using the optimally condition $\delta J(v) = 0$.

$$\delta J(v) = k_0 \sum_{k=0}^{M} \int_0^T v_i \delta v_i \mathrm{d}t + k_1 \iint_Q y \delta y \mathrm{d}x \mathrm{d}t + k_2 \int_0^L \left(y(x,T) - z(x) \right) \delta y(x,T) \mathrm{d}x.$$

The perturbation system of the equation (SE) is

$$\begin{cases} \frac{\partial \delta y}{\partial t} - \mu \frac{\partial^2 \delta y}{\partial x^2} + \epsilon \frac{\partial \delta y}{\partial x} - \delta y = \chi_{x_i} \delta v_k & \text{in } Q = (0,L) \times (0,T), i, k = 1, \ldots, M-1 \\ \delta y(x,0) = 0, & t = 0, \\ -\mu \frac{\partial \delta y(0,t)}{\partial x} = \delta v_0(t), & x = 0, \\ \mu \frac{\partial \delta y(L,t)}{\partial x} = \delta v_M(t), & x = L. \end{cases} \quad (\delta\text{SE})$$

Let $p(x,t)$ a sufficiently smooth function that allow to integrate (δSE) in Q

$$\begin{aligned} 0 &= \iint_Q p \left(\frac{\partial \delta y}{\partial t} - \mu \frac{\partial^2 \delta y}{\partial x^2} + \epsilon \frac{\partial \delta y}{\partial x} - \delta y - \chi_{x_i} \delta v \right) \mathrm{d}x \mathrm{d}t \\ &= \iint_Q p \frac{\partial \delta y}{\partial t} \mathrm{d}x \mathrm{d}t - \mu \iint_Q p \frac{\partial^2 \delta y}{\partial x^2} \mathrm{d}x \mathrm{d}t + \epsilon \iint_Q p \frac{\partial \delta y}{\partial x} \mathrm{d}x \mathrm{d}t - \iint_Q p \delta y \mathrm{d}x \mathrm{d}t - \iint_Q p \chi_{x_i} \delta v \mathrm{d}x \mathrm{d}t. \end{aligned}$$

The integration of (δSE) is achieved by the formula of integration by parts:

2

$$\int_a^b v\,\mathrm{d}u = vu\big|_a^b - \int_a^b u\,\mathrm{d}v.$$

Therefore

$$
\begin{aligned}
\iint_Q p\frac{\partial \delta y}{\partial t}\mathrm{d}x\mathrm{d}t &= \int_0^L \left[\int_0^T p\frac{\partial \delta y}{\partial t}\mathrm{d}t\right]\mathrm{d}x \\
v &= p,\ \mathrm{d}u = \frac{\partial \delta y}{\partial t}\mathrm{d}t \\
&= \int_0^L \left[p\left(x,T\right)\delta y\left(x,T\right)\right]_0^T \mathrm{d}x - \iint_Q \frac{\partial p}{\partial t}\delta y\,\mathrm{d}x\mathrm{d}t \\
&= \int_0^L p\left(x,T\right)\delta y\left(x,T\right)\mathrm{d}x - \int_0^L p\left(x,0\right)\delta y\left(x,0\right)\mathrm{d}x - \iint_Q \frac{\partial p}{\partial t}\delta y\,\mathrm{d}x\mathrm{d}t \\
&\quad \left(\delta y\left(x,0\right)=0\right) \\
&= \int_0^L p\left(x,T\right)\delta y\left(x,T\right)\mathrm{d}x + \iint_Q \left(-\frac{\partial p}{\partial t}\right)\delta y\,\mathrm{d}x\mathrm{d}t
\end{aligned}
\tag{1}
$$

$$
\begin{aligned}
-\mu\iint_Q p\frac{\partial^2 \delta y}{\partial x^2}\mathrm{d}x\mathrm{d}t &= -\mu\int_0^T \left[\int_0^L p\frac{\partial^2 \delta y}{\partial x^2}\mathrm{d}x\right]\mathrm{d}t \\
v &= p,\ \mathrm{d}u = \frac{\partial^2 \delta y}{\partial x^2}\mathrm{d}x \\
&= -\mu\int_0^T \left[p\left(x,t\right)\frac{\partial \delta y\left(x,t\right)}{\partial x}\right]_0^L \mathrm{d}t + \mu\iint_Q \left[\frac{\partial p}{\partial x}\frac{\partial \delta y}{\partial x}\mathrm{d}x\right]\mathrm{d}t \\
v &= \frac{\partial p}{\partial x},\ \mathrm{d}u = \frac{\partial \delta y}{\partial x}\mathrm{d}x \\
&= \int_0^T p\left(L,t\right)\left(-\mu\frac{\partial \delta y\left(L,t\right)}{\partial x}\right)\mathrm{d}t - \int_0^T p\left(0,t\right)\left(-\mu\frac{\partial \delta y\left(0,t\right)}{\partial x}\right)\mathrm{d}t \\
&\quad +\mu\int_0^T \left[\frac{\partial p\left(x,t\right)}{\partial x}\delta y\left(x,t\right)\right]_0^L \mathrm{d}t - \mu\iint_Q \frac{\partial^2 p}{\partial x^2}\delta y\,\mathrm{d}x\mathrm{d}t.
\end{aligned}
\tag{2}
$$

$$\left(\mu\frac{\partial\delta y\left(L,t\right)}{\partial x}=\delta v_M\left(t\right),-\mu\frac{\partial\delta y\left(0,t\right)}{\partial x}=\delta v_0\left(t\right)\right)$$

$$=\quad -\int_0^T p\left(L,t\right)\delta v_M\left(t\right)\mathrm{dt}-\int_0^T p\left(0,t\right)\delta v_0\left(t\right)\mathrm{dt}+\mu\int_0^T\left[\frac{\partial p\left(x,t\right)}{\partial x}\delta y\left(x,t\right)\right]_0^L\mathrm{dt}$$

$$-\mu\iint_Q\frac{\partial^2 p}{\partial x^2}\delta y\mathrm{dxdt}$$

$$=\quad \int_0^T p\left(L,t\right)\left(-\delta v_M\left(t\right)\right)\mathrm{dt}-\int_0^T p\left(0,t\right)\delta v_0\left(t\right)\mathrm{dt}+\mu\int_0^T\frac{\partial p\left(L,t\right)}{\partial x}\delta y\left(L,t\right)\mathrm{dt}$$

$$-\mu\int_0^T\frac{\partial p\left(0,t\right)}{\partial x}\delta y\left(0,t\right)\mathrm{dt}-\mu\iint_Q\frac{\partial^2 p}{\partial x^2}\delta y\mathrm{dxdt}$$

$$=\quad \int_0^T\left(-p\left(L,t\right)\right)\left(\delta v_M\left(t\right)\right)\mathrm{dt}+\int_0^T\left(-p\left(0,t\right)\right)\delta v_0\left(t\right)\mathrm{dt}+\int_0^T\mu\frac{\partial p\left(L,t\right)}{\partial x}\delta y\left(L,t\right)\mathrm{dt}$$

$$+\int_0^T\left(-\mu\frac{\partial p\left(0,t\right)}{\partial x}\right)\delta y\left(0,t\right)\mathrm{dt}-\mu\iint_Q\frac{\partial^2 p}{\partial x^2}\delta y\mathrm{dxdt}$$

$$=\quad \int_0^T\left(-p\left(L,t\right)\right)\left(\delta v_M\left(t\right)\right)\mathrm{dt}+\int_0^T\left(-p\left(0,t\right)\right)\delta v_0\left(t\right)\mathrm{dt}+\int_0^T\mu\frac{\partial p\left(L,t\right)}{\partial x}\delta y\left(L,t\right)\mathrm{dt}$$

$$+\int_0^T\left(-\mu\frac{\partial p\left(0,t\right)}{\partial x}\right)\delta y\left(0,t\right)\mathrm{dt}+\iint_Q\left(-\mu\frac{\partial^2 p}{\partial x^2}\right)\delta y\mathrm{dxdt}$$

$$\epsilon\iint_Q p\frac{\partial\delta y}{\partial x}\mathrm{dxdt}\quad=\quad \epsilon\int_0^T\left[\int_0^L p\frac{\partial\delta y}{\partial x}\mathrm{dx}\right]\mathrm{dt}\tag{3}$$

$$v\quad=\quad p,\ \mathrm{d}u=\frac{\partial\delta y}{\partial x}\mathrm{dx}$$

$$=\quad \epsilon\int_0^T\left[p\left(x,t\right)\delta y\left(x,t\right)\right]_0^L\mathrm{dt}-\epsilon\iint_Q\frac{\partial p}{\partial x}\delta y\mathrm{dxdt}$$

$$=\quad \epsilon\int_0^T p\left(L,t\right)\delta y\left(L,t\right)\mathrm{dt}-\in\int_0^T p\left(0,t\right)\delta y\left(0,t\right)\mathrm{dt}-\epsilon\iint_Q\frac{\partial p}{\partial x}\delta y\mathrm{dxdt}$$

$$=\quad \int_0^T\epsilon p\left(L,t\right)\delta y\left(L,t\right)\mathrm{dt}+\int_0^T\left(-\in p\left(0,t\right)\right)\delta y\left(0,t\right)\mathrm{dt}-\epsilon\iint_Q\frac{\partial p}{\partial x}\delta y\mathrm{dxdt}$$

$$-\iint_Q p\delta y\mathrm{dxdt}=\iint_Q\left(-p\right)\delta y\mathrm{dxdt}.\tag{4}$$

$$-\iint_Q p\chi_{x_i}\delta v\mathrm{dxdt}\quad=\quad \sum_{i=1}^{M-1}\int_0^T\left(-p_i\right)\delta v_i\mathrm{dt}\tag{5}$$

$$\text{where }\chi_{x_i}p\quad=\quad p_i.$$

$$
\begin{aligned}
0 \;=\; & (1)+(2)+(3)+(4)+(5) \\
=\; & \int_0^L p\left(x,T\right)\delta y\left(x,T\right)\mathrm{d}x + \iint_Q \left(-\frac{\partial p}{\partial t}\right)\delta y\mathrm{d}x\mathrm{d}t \\
& + \int_0^T \left(-p\left(L,t\right)\right)\left(\delta v_M\left(t\right)\right)\mathrm{d}t + \int_0^T \left(-p\left(0,t\right)\right)\delta v_0\left(t\right)\mathrm{d}t + \int_0^T \mu\frac{\partial p\left(L,t\right)}{\partial x}\delta y\left(L,t\right)\mathrm{d}t \\
& + \int_0^T \left(-\mu\frac{\partial p\left(0,t\right)}{\partial x}\right)\delta y\left(0,t\right)\mathrm{d}t + \iint_Q \left(-\mu\frac{\partial^2 p}{\partial x^2}\right)\delta y\mathrm{d}x\mathrm{d}t \\
& + \int_0^T \epsilon p\left(L,t\right)\delta y\left(L,t\right)\mathrm{d}t + \int_0^T \left(- \in p\left(0,t\right)\right)\delta y\left(0,t\right)\mathrm{d}t - \epsilon \iint_Q \frac{\partial p}{\partial x}\delta y\mathrm{d}x\mathrm{d}t \\
& + \iint_Q \left(-p\right)\delta y\mathrm{d}x\mathrm{d}t \\
& + \sum_{i=1}^{M-1}\int_0^T \left(-p_i\right)\delta v_i\mathrm{d}t \\
=\; & \sum_{i=0}^{M}\int_0^T \left(-p_i\right)\delta v_i\mathrm{d}t \\
& + \iint_Q \left(-\frac{\partial p}{\partial t} - \mu\frac{\partial^2 p}{\partial x^2} - \epsilon\frac{\partial p}{\partial x} - p\right)\delta y\mathrm{d}x\mathrm{d}t \\
& + \int_0^L p\left(x,T\right)\delta y\left(x,T\right)\mathrm{d}x \\
& + \int_0^T \left(\mu\frac{\partial p\left(L,t\right)}{\partial x} + \epsilon p\left(L,t\right)\right)\delta y\left(L,t\right)\mathrm{d}t + \int_0^T \left(-\mu\frac{\partial p\left(0,t\right)}{\partial x} - \epsilon p\left(0,t\right)\right)\delta y\left(0,t\right)\mathrm{d}t
\end{aligned}
$$

Adjusting terms with

$$
\delta J\left(v\right) = k_0\sum_{k=0}^{M}\int_0^T v_i\delta v_i\mathrm{d}t + k_1\iint_Q y\delta y\mathrm{d}x\mathrm{d}t + k_2\int_0^L \left(y\left(x,T\right) - z\left(x\right)\right)\delta y\left(x,T\right)\mathrm{d}x,
$$

the adjoint system is

$$
\begin{cases}
p\left(x,T\right) = k_2\left(y\left(x,T\right) - z\left(x\right)\right), & x \in [0,L] \\
\mu\frac{\partial p}{\partial x}\left(L,t\right) + \epsilon p\left(L,t\right) = 0, & t \in [0,T] \\
\mu\frac{\partial p}{\partial x}\left(0,t\right) + \epsilon p\left(0,t\right) = 0 & t \in [0,T] \\
\frac{\partial p}{\partial t} + \mu\frac{\partial^2 p}{\partial x^2} + \epsilon\frac{\partial p}{\partial x} + p = -k_1 y, & \text{in } Q
\end{cases}
\tag{δASE}
$$

also

$$
\nabla J\left(v\right) = k_0\sum_{k=0}^{M}\left(v_i - p_i\left(x,t\right)\right).
$$

4 Discretization on Time

The discretization on time of $J^{\Delta t}\left(v\right)$ is

$$
J^{\Delta t}\left(v\right) = \frac{\Delta t}{2}\sum_{k=0}^{M}\sum_{n=0}^{N}\left\|v^n\right\|^2 + \frac{k_1\Delta t}{2}\sum_{n=0}^{N}\int_0^L \left\|y^n\right\|^2\mathrm{d}x + \frac{k_2}{2}\int_0^L \left\|y^{N+1}\left(x\right)\right\|^2\mathrm{d}x
$$

where $N > 0$, and $\Delta t = \frac{T}{N}$.
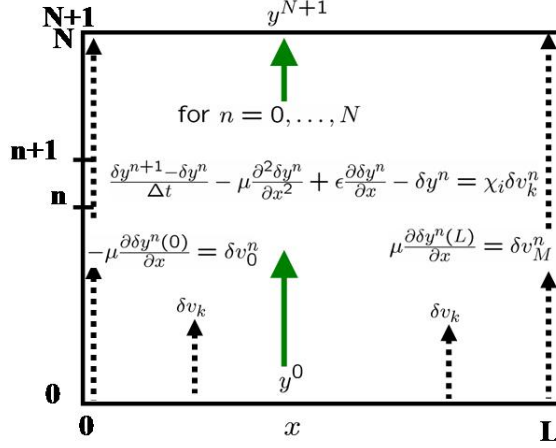Now, the forward discretization on time of (SE) is

Figure 2: Discretization on time of (SE).

$$\begin{cases} y^0 = y_0. \\ \text{for } n = 0, \ldots, N \\ \frac{y^{n+1} - y^n}{\Delta t} - \mu \frac{\partial^2 y^n}{\partial x^2} + \epsilon \frac{\partial y^n}{\partial x} - y^n = \chi_{x_i} \delta v_k^n, \\ -\mu \frac{\partial y^n(0)}{\partial x} = v_0^n, \\ \mu \frac{\partial y^n(L)}{\partial x} = v_M^n. \end{cases} \tag{SE$^{\triangle t}$}$$

Figure 2 depicts (SE$^{\triangle t}$).
The optimal condition is

$$\delta J^{\Delta t}(v) = \left(\nabla J^{\Delta t}(v), \delta v \right)_{\mathcal{U}^{\Delta t}} = 0.$$

And

$$\delta J^{\Delta t}(v) = \Delta t \sum_{n=0}^{N} v^n \delta v^n + k_1 \Delta t \sum_{n=0}^{N} \int_0^L y^n \delta y^n \mathrm{d}x + k_2 \int_0^L y^{N+1} \delta y^{N+1} \mathrm{d}x.$$

By the other hand, the perturbation of (SE$^{\triangle t}$) is

$$\begin{cases} \delta y^0 = 0. \\ \text{for } n = 0, \ldots, N \\ \frac{\delta y^{n+1} - \delta y^n}{\Delta t} - \mu \frac{\partial^2 \delta y^n}{\partial x^2} + \epsilon \frac{\partial \delta y^n}{\partial x} - \delta y^n = \chi_{x_i} \delta v_k^n, \\ -\mu \frac{\partial \delta y^n(0)}{\partial x} = \delta v_0^n, \\ \mu \frac{\partial \delta y^n(L)}{\partial x} = \delta v_M^n. \end{cases} \tag{δSE$^{\triangle t}$}$$

Now, multiplying these by appropriate functions p^n for integrating:

$$\Delta t \sum_{n=0}^{N} \int_0^L p^n \left(\frac{\delta y^{n+1} - \delta y^n}{\Delta t} - \mu \frac{\partial^2 \delta y^n}{\partial x^2} + \epsilon \frac{\partial \delta y^n}{\partial x} - \delta y^n - \chi_{x_i} \delta v_k^n \right) \mathrm{d}x = 0.$$
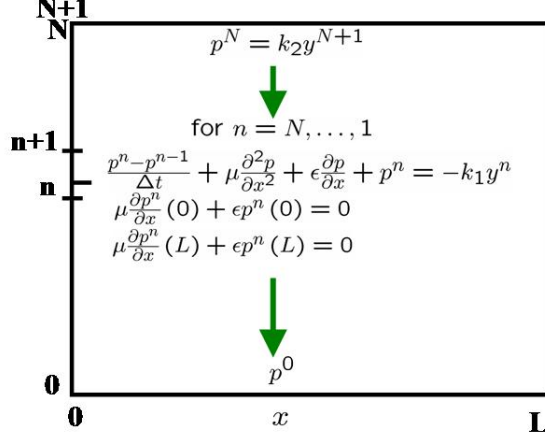
Figure 3: Discretization on time of adjoint system of (SE).

$$\Delta t \sum_{n=0}^{N} \int_0^L p^n \left(\frac{\delta y^{n+1} - \delta y^n}{\Delta t} \right) \mathrm{d}x \quad = \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (6)$$

$$= \quad -\int_0^L p^0 \frac{\delta y^0}{\Delta t} \mathrm{d}x - \Delta t \sum_{n=1}^{N} \int_0^L \left(\frac{p^n - p^{n-1}}{\Delta t} \right) \delta y^n \mathrm{d}x + \int_0^L p^N \delta y^{N+1} \mathrm{d}x$$

$$-\Delta t \sum_{n=1}^{N} \int_0^L \left(\frac{p^n - p^{n-1}}{\Delta t} \right) \delta y^n \mathrm{d}x + \int_0^L p^N \delta y^{N+1} \mathrm{d}x.$$

$$\Delta t \sum_{n=0}^{N} \int_0^L p^n \left(-\mu \frac{\partial^2 \delta y^n}{\partial x^2} \right) \mathrm{d}x \quad = \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (7)$$

$$= \quad \Delta t \sum_{n=0}^{N} p \left[-\mu \frac{\partial \delta y}{\partial x} \right]_0^L + \mu \Delta t \sum_{n=0}^{N} \frac{\partial p}{\partial x} \left[\delta y \right]_0^L - \mu \Delta t \sum_{n=0}^{N} \int_0^L \frac{\partial^2 p}{\partial x^2} \delta y \mathrm{d}x$$

$$= \quad -\Delta t \sum_{n=0}^{N} p^n (0) (\delta v^n) + \mu \Delta t \sum_{n=0}^{N} \frac{\partial p^n (L)}{\partial x} \delta y (L)$$

$$-\mu \Delta t \sum_{n=0}^{N} \int_0^L \frac{\partial^2 p}{\partial x^2} \delta y \mathrm{d}x.$$

$$\Delta t \sum_{n=0}^{N} \int_0^L p^n \left(\epsilon \frac{\partial \delta y^n}{\partial x} \right) \mathrm{d}x = \epsilon \sum_{n=0}^{N} p^n (L) \delta y (L) - \epsilon \sum_{n=0}^{N} \int_0^L \frac{\partial p}{\partial x} \delta y \mathrm{d}x. \qquad (8)$$

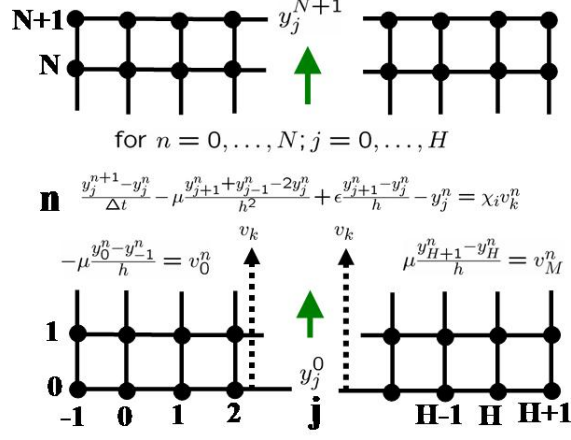$$\Delta t \sum_{n=0}^{N} \int_0^L p^n \left(-\delta y^n \right) \mathrm{d}x. \qquad\qquad\qquad\qquad\qquad (9)$$

Figure 4: Fully discretization of (SE).

$$0 = (5) + (6) + (7) + (8) \quad +(8) = \quad \Delta t \sum_{n=1}^{N} \int_0^L \left(-\frac{p^n - p^{n-1}}{\Delta t} - \mu \frac{\partial^2 p}{\partial x^2} - \epsilon \frac{\partial p}{\partial x} - p^n \right) \delta y^n \mathrm{d}x + \int_0^L p^N \delta y^{N+1} \mathrm{d}x$$

$$-\Delta t \sum_{n=0}^{N} p(0)(\delta v^n) + \mu \Delta t \sum_{n=0}^{N} \frac{\partial p^n}{\partial x}(L) \delta y(L) + \epsilon \sum_{n=0}^{N} p(L) \delta y(L).$$

Therefore the discritization on time of the adjoint system (see figure 3) is

$$\begin{cases} p^N = k_2 y^{N+1}. \\ \text{for } n = N, \ldots, 1 \\ \frac{p^n - p^{n-1}}{\Delta t} + \mu \frac{\partial^2 p}{\partial x^2} + \epsilon \frac{\partial p}{\partial x} + p^n = -k_1 y^n, \\ \mu \frac{\partial p^n}{\partial x_n}(0) + \epsilon p^n(0) = 0 \\ \mu \frac{\partial p^n}{\partial x}(L) + \epsilon p^n(L) = 0. \end{cases} \tag{ASE$^{\Delta t}$}$$

And

$$\nabla J^{\Delta t}(v) = \{v^n - p^n(0)\}_{n=0}^N.$$

4.1   Fully discretization

Let $H > 0$ an integer, and $\triangle x = h = \frac{L}{H}$. The indices for axis x are $-1 \le j \le H + 1$. Note that two sets of points are added on $j = -1$, and $j = H + 1$, this is convenient because the frontier conditions on $x = 0$ $\left(-\mu \frac{\partial y(0,t)}{\partial x} = v(t),\right)$ and $x = L$ $\left(\mu \frac{\partial y(L,t)}{\partial x} = 0\right)$ can be inserted before and after the points of interest 0 to H on x. The corresponding fully discrete steady equations (see figure 4)are

$$\begin{cases} y_j^0 = y_{0,j}, \, j = 0, \ldots, H \\ \text{for } n = 0, \ldots, N, \, j = 0, \ldots, H \\ \frac{y_j^{n+1} - y_j^n}{\Delta t} - \mu \frac{y_{j+1}^n + y_{j-1}^n - 2y_j^n}{h^2} + \epsilon \frac{y_{j+1}^n - y_j^n}{h} - y_j^n = \chi_j v_k \\ -\mu \frac{y_0^n - y_{-1}^n}{h} = v_0^n \\ \mu \frac{y_{H+1}^n - y_H^n}{h} = v_M^n. \end{cases} \tag{SE$_{\triangle x}^{\Delta t}$}$$

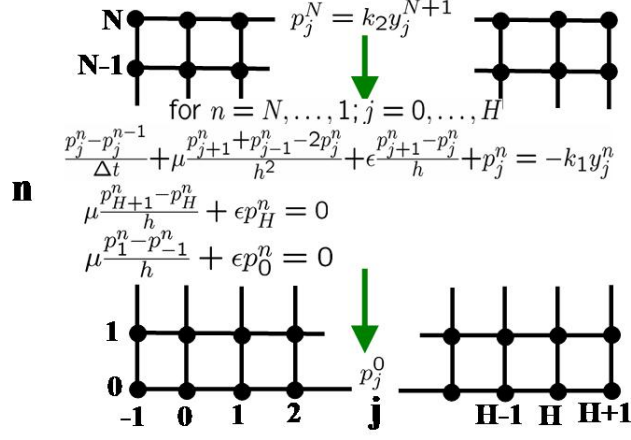$-\mu \frac{y_0^n - y_{-1}^n}{h} = v_0^n$

$-\mu y_0^n + \mu y_{-1}^n = h v_0^n$

Figure 5: Fully discretization of adjoint system of (SE).

$+y_{-1}^n = \left(hv_0^n + \mu y_0^n\right)/\mu$

$+y_{-1}^n = \frac{h}{\mu}v_0^n + y_0^n$

$\mu\frac{y_{H+1}^n - y_H^n}{h} = v_M^n$

$\mu\left(y_{H+1}^n - y_H^n\right) = hv_M^n$

$\mu y_{H+1}^n - \mu y_H^n = hv_M^n$

$\mu y_{H+1}^n = \mu y_H^n + hv_M^n$

$y_{H+1}^n = y_H^n + \frac{h}{\mu}v_M^n$

The adjoint equations (see figure 5) are

$$\begin{cases} p_j^N = k_2 y_j^{N+1},\ j = 0,\ldots,H \\ \text{for } n = N,\ldots,1,\ j = 0,\ldots,H \\ \frac{p_j^n - p_j^{n-1}}{\Delta t} + \mu\frac{p_{j+1}^n + p_{j-1}^n - 2p_j^n}{h^2} + \epsilon\frac{p_{j+1}^n - p_j^n}{h} + p_j^n = -k_1 y_j^n \\ \mu\frac{p_{H+1}^n - p_H^n}{h} + \epsilon p_H^n = 0. \\ \mu\frac{p_0^n - p_{-1}^n}{h} + \epsilon p_{-1}^n = 0 \end{cases} \qquad (\text{ASE}_{\triangle x}^{\triangle t})$$

$\frac{p_j^n - p_j^{n-1}}{\Delta t} + \mu\frac{p_{j+1}^n + p_{j-1}^n - 2p_j^n}{h^2} + \epsilon\frac{p_{j+1}^n - p_j^n}{h} + p_j^n = -k_1 y_j^n$, Solution is : $p_j^{n-1} = \frac{h^2 p_j^n + \mu\Delta t p_{j+1}^n + \mu\Delta t p_{j-1}^n - 2\mu\Delta t p_j^n + \epsilon\Delta t h p_{j+1}^n - \epsilon\Delta t h p_j^n + p_j^n \Delta t h^2}{h^2}$

$p_j^{n-1} = p_j^n + \frac{\mu\Delta t p_{j+1}^n + \mu\Delta t p_{j-1}^n - 2\mu\Delta t p_j^n + \epsilon\Delta t h p_{j+1}^n - \epsilon\Delta t h p_j^n + p_j^n \Delta t h^2}{h^2} + k_1 y_j^n \Delta t =$

$p_j^{n-1} = p_j^n + \frac{\mu\Delta t\left(p_{j+1}^n + p_{j-1}^n - 2p_j^n\right)}{h^2} + \frac{\epsilon\Delta t\left(p_{j+1}^n - hp_j^n\right)}{h} + p_j^n \Delta t + k_1 y_j^n \Delta t =$

$\mu\frac{p_0^n - p_{-1}^n}{h} + \epsilon p_{-1}^n = 0$

$\frac{\mu}{h}p_0^n - \frac{\mu}{h}p_{-1}^n + \epsilon p_{-1}^n = 0$

$\mu p_0^n - \mu p_{-1}^n + \epsilon h p_{-1}^n = 0$

$p_{-1}^n = \mu p_0^n/\left(\mu - \epsilon h\right)$

$\mu\frac{p_{H+1}^n - p_H^n}{h} + \epsilon p_H^n = 0$

$\mu p_{H+1}^n - \mu p_H^n = -\epsilon h p_H^n$

$\mu p_{H+1}^n = \left(\mu - \epsilon\right)p_H^n/\mu$

And the corresponding perturbation equations are

$$\begin{cases} \delta y_j^0 = 0, \ j = 0, \ldots, H \\ \text{for } n = 0, \ldots, N, \ j = 0, \ldots, H \\ \frac{\delta y_j^{n+1} - \delta y_j^n}{\Delta t} - \mu \frac{\delta y_{j+1}^n + \delta y_{j-1}^n - 2\delta y_j^n}{h^2} + \epsilon \frac{\delta y_{j+1}^n - \delta y_j^n}{h} - \delta y_j^n = \chi_j \delta v_k^n \\ -\mu \frac{\delta y_0^n - \delta y_{-1}^n}{h} = \delta v_0^n, \\ \mu \frac{\delta y_{H+1}^n - \delta y_H^n}{h} = \delta v_M^n. \end{cases} \qquad (\delta\mathrm{SE}_{\triangle x}^{\triangle t})$$

The corresponding control problem is

$$\begin{cases} u = \{u^n\} \in \mathcal{V} = \mathcal{U}_{\triangle x}^{\triangle t} = \mathbf{R}^N \\ J_{\triangle x}^{\triangle t}(u) \le J_{\triangle x}^{\triangle t}(v), \ \forall \underline{v} \in \mathcal{V} \end{cases} \qquad (\mathrm{CP}_{\triangle x}^{\triangle t})$$

where

$$J_{\triangle x}^{\triangle t}(v) = \frac{\Delta t}{2} \sum_{k=0}^{M} \sum_{n=0}^{N} [v_k^n]^2 + \frac{k_1 \Delta t h}{2} \sum_{n=0}^{N} \sum_{j=0}^{H} [y_j^n]^2 + \frac{k_2 h}{2} \sum_{j=0}^{H} [y_j^{N+1}]^2,$$

and $y = \{y_j^n\}_{-1 \le j \le H+1}^{0 \le n \le N+1}$ is the solution of $(\mathrm{SE}_{\triangle x}^{\triangle t})$ with v.

5 The Conjugate Gradient Algorithm

The CG algorithm for the fully discrete control problem $(\mathrm{CP}_{\triangle x}^{\triangle t})$ is:

1. Given ε (the tolerance to stop the algorithm), $0 < \varepsilon \ll 1$, and $\{u^{n,0}\} \in \mathcal{V}$.

2. Solve the equation $(\mathrm{SE}_{\triangle x}^{\triangle t})$, and

   with the solution $\{y_j^{n,0}\}_{-1 \le j \le H+1}^{0 \le n \le N+1}$ solve $(\mathrm{ASE}_{\triangle x}^{\triangle t})$ to get $\{p_j^{n,0}\}_{-1 \le j \le H+1}^{0 \le n \le N}$.

3. Compute $g^0 = \{u_{j_k}^{n,0} + p_{j_k}^{n,0}\}_{0 \le j_k \le H}^{0 \le n \le N}$, and set $w^0 = g^0$.

   Now, we have u^m, g^m, and w^m.

4. If $\frac{(g^{m+1}, g^{m+1})_{\mathcal{V}}}{(g^0, g^0)_{\mathcal{V}}} < \epsilon^2$ take u^{m+1} as the solution and stop.

5. Compute $m = m + 1$.

6. Solve the equation $(\delta\mathrm{SE}_{\triangle x}^{\triangle t})$, and

   with the solution $\bar{y} = \{\delta y_j^{n,m}\}_{-1 \le j \le H+1}^{0 \le n \le N+1}$ solve $(\mathrm{ASE}_{\triangle x}^{\triangle t})$ to get $\bar{p} = \{p_j^{n,m}\}_{-1 \le j \le H+1}^{0 \le n \le N}$.

7. Compute $\bar{g}^m = \{w_{j_k}^{n,m} + \bar{p}_{j_k}^{n,m}\}_{0 \le j_k \le H}^{0 \le n \le N}$, $\rho^m = (g^m, g^m)_{\mathcal{V}}$, $u^{m+1} = u^m - \rho^m w^m$, and $g^{m+1} = g^m - \rho^m \bar{g}^m$.

8. If $\frac{(g^{m+1}, g^{m+1})_{\mathcal{V}}}{(g^0, g^0)_{\mathcal{V}}} < \epsilon^2$ take u^{m+1} as the solution and stop.

9. Compute $\gamma^m = \frac{(g^{m+1}, g^{m+1})_{\mathcal{V}}}{(g^m, g^m)_{\mathcal{V}}}$, and $w^{m+1} = g^{m+1} + \gamma^m w^m$

10. Go to step 5.

6   Motivation

We preferred to leave this section at the end, because these notes are principally aimed for graduate students, which could be interested in developing their own simulators. It is possibly, that they already know the importance of the Theory of Control on Systems over Partial Differential Equations.

From the abundant literature, we mention the book of partial differential equations [4], and for Control the books [1, 3]. These notes were developed from the talk in [2].

The following problem depicts a classical problem for a parabolic equation with three physical-chemical components.

1. Advection. It is the scalar variation at each point of a vector field, by example, the contaminant entrainment in a medium.

2. Reaction. It is the response or reaction of the system, by example, the heat exchanges in a system.

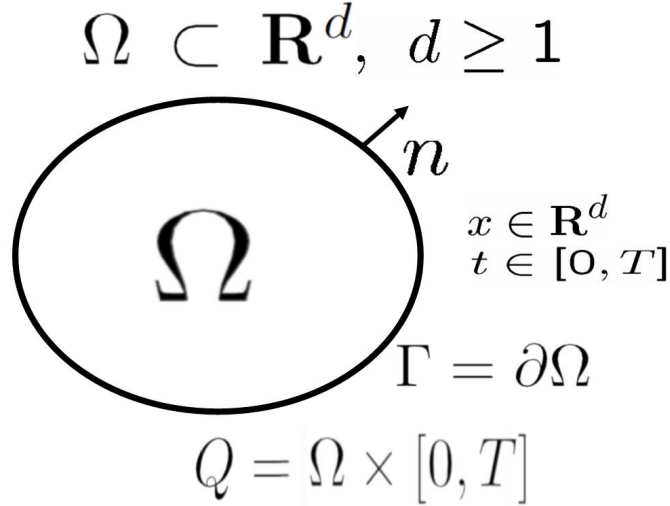3. Diffusion. It is the gradient (change or transport) of system components.

$$\Omega \subset \mathbf{R}^d, \ d \geq 1$$

$$n$$

$$\Omega$$

$$x \in \mathbf{R}^d$$
$$t \in [0, T]$$

$$\Gamma = \partial\Omega$$

$$Q = \Omega \times [0, T]$$

Figure 6: Sistem's domain

Let be the following parabolic equation where the advection is $V \cdot \nabla\varphi$, the reaction is $f(\varphi)$, and the diffusion is $\nabla \cdot (A\nabla\varphi)$ acting over the time. It is Equation of the State System.

$$
\begin{array}{l}
\frac{\partial\varphi}{\partial t} - \nabla \cdot (A\nabla\varphi) + V \cdot \nabla\varphi + f(\varphi) = 0 \text{ en } Q = \Omega \times [0, T], \\
A\nabla\varphi \cdot n = 0 \text{ en } \Sigma = \Gamma \times [0, T], \\
\varphi(x, 0) = \varphi_0(x) \ \ x \in \Omega
\end{array}
\tag{SEE}
$$

where $\Omega \subset \mathbf{R}^d$ ($d \geq 1$, dimension) it is a smooth region, with orientated boundary $\Gamma = \partial\Omega$, n represents a normal unit vector on Γ (pointing outside of Ω), $T > 0$ is the time (including the possiblity $T = \infty$). Figure 6 depicts (SEE).

The intern product $\cdot$ is the usual, $a, b \in \mathbf{R}^d, a \cdot b = \sum\limits_{i=1}^{d} a_i b_i$, A is a real tensor function (diffusion matrix), $V : \Omega \to \mathbf{R}^d$ is a vectorial function, $f : \mathbf{R} \to \mathbf{R}$ is a real function, and $\varphi(x, t)$ is the phenomena function that occurs in Q.

In addition we assume that:

$$A(x)\xi \cdot \xi \geq \alpha |\xi|^2, \forall \xi \in \mathbf{R}^d \text{ for almost all } x \in \Omega$$

which means that A is uniformly positive definite for almost all x in Ω.
For the vector function V, we assume:

$$
\begin{aligned}
\nabla \cdot V &= 0 \text{ (divergence free)} \\
\frac{\partial V}{\partial t} &= 0 \text{ (it is constant over time)} \\
V \cdot n &= 0 \text{ on } \Gamma
\end{aligned}
$$

Control is necessary for this System, let be a reaction function given by

$$
f(\varphi) = C - \lambda e^{\varphi}
$$

where $C, \lambda > 0$ are real positive constants.
Then the steady state solution for such f fulfill:

$$
\frac{\partial \varphi}{\partial t} + f(\varphi) = 0 \tag{10}
$$

and it is given by

$$
\varphi_s = \frac{\ln C}{\lambda}
$$

Note that φ_s is constant, so that the equation (10), substituting φ_s is fulfill (because $f(\varphi_s) = C - \lambda e^{\varphi_s} = C - \lambda e^{\frac{\ln C}{\lambda}} = 0$).
Assuming that for some $t > 0$, the system was its stable steady state solution $\varphi = \varphi_s$.
Now, $\varphi = \varphi_s$ at some time $t_0 = 0$ has a small constant perturbation $\delta\varphi$, independent from x y t (with $\nabla \delta\varphi = 0$ y $\frac{\partial \delta\varphi}{\partial t} = 0$).
For this perturbation, the system evolves under the following ordinary differential equation:

$$
\begin{aligned}
\frac{\mathrm{d}\varphi}{\mathrm{d}t} &= \lambda e^{\varphi} - C, \ \lambda, C > 0, \text{ real constants} \\
\varphi(0) &= \varphi_s + \delta\varphi
\end{aligned}
$$

This model behaves with a constant positive perturbation, $\delta\varphi > 0$, such that $\varphi \to +\infty$. By other hand, if the perturbation is a constant negative, $\delta\varphi < 0$, then $\varphi_{t\to\infty} \to -\infty$. In the following paragraphs, it is showed that in the former the deviation from the stable state grows fast to $+\infty$, and in the second case the deviation of the stable state is slow and steady toward $-\infty$ as the time progress.
This means that around a stable steady state solution, the introduction a small constant perturbation makes the system unstable. To verify the above statement, we proceed by the Euler Method to numerically integrate the above equation:

$$
\begin{aligned}
\frac{\mathrm{d}\varphi}{\mathrm{d}t} &= \lambda e^{\varphi} - C, \ \lambda, C > 0, \text{ real constants} \\
\varphi(0) &= \frac{\ln C}{\lambda} + \delta\varphi
\end{aligned}
$$

Without loss of generality we take $\triangle t = 1$, $C = 1, \lambda = 1, \delta\varphi = 0.1 > 0$, and approach $\frac{d\varphi}{dt}$ by a time difference between n and $n-1$.
The resulting approximation difference equation is
$\varphi_n = \exp(\varphi_{n-1}) + \varphi_{n-1} - 1$.
From the initial condition:
$\varphi_0 = \frac{\ln C}{\lambda} + \delta\varphi = 0.1$
The numerical estimations are
$\varphi_1 = \exp(0.1) + 0.1 - 1 = 0.205\,17$

$\varphi_2 = \exp(0.205\,17) + 0.205\,17 - 1 = 0.432\,9$
$\varphi_3 = \exp(0.432\,9) + 0.432\,9 - 1 = 0.974\,64$
$\varphi_4 = \exp(0.974\,64) + 0.974\,64 - 1 = 2.\,624\,8$
$\varphi_5 = \exp(2.\,624\,8) + 2.\,624\,8 - 1 = 15.\,427$
$\varphi_6 = \exp(15.\,427) + 15.\,427 - 1 = 5.\,010\,3 \times 10^6$
$\varphi_7 = \exp(5.\,010\,3 \times 10^6) + 5.\,010\,3 \times 10^6 - 1 = 4.\,392\,2 \times 10^{2175945}$
$\varphi(t)$ in a finite time grows very quickly, it tends accelerated to ∞.

By other hand, assuming that $\delta\varphi = -0.1 < 0$, and using the same constants C y λ, the numerical estimations for this case are

$\varphi_0 = -0.1$
$\varphi_1 = \exp(-0.1) + (-0.1) - 1 = -0.195\,16$
$\varphi_2 = \exp(-0.195\,16) + (-0.195\,16) - 1 = -0.372\,46$
$\varphi_3 = \exp(-0.372\,46) + (-0.372\,46) - 1 = -0.683\,42$
$\varphi_4 = \exp(-0.683\,42) + (-0.683\,42) - 1 = -1.\,178\,5$
$\varphi_5 = \exp(-1.\,178\,5) + (-1.\,178\,5) - 1 = -1.\,870\,8$
$\varphi_6 = \exp(-1.\,870\,8) + (-1.\,870\,8) - 1 = -2.\,716\,8$
$\varphi_7 = \exp(-2.\,716\,8) + (-2.\,716\,8) - 1 = -3.\,650\,7$
$\varphi_8 = \exp(-3.\,650\,7) + (-3.\,650\,7) - 1 = -4.\,624\,7$
$\varphi_9 = \exp(-4.\,624\,7) + (-4.\,624\,7) - 1 = -5.\,614\,9$
$\varphi_{10} = \exp(-5.\,614\,9) + -5.\,614\,9 - 1 = -6.\,611\,3$
$\varphi_{11} = \exp(-6.\,611\,3) + -6.\,611\,3 - 1 = -7.\,610\,0$
$\varphi(t)$ is decreasing slowly to $-\infty$.

The previous numerical results clearly depicts that a control is necessary to prevent such behavior and to return the system to the steady state solution φ_s.

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