Handbook for Advanced Mathematical Methods for Engineering

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

1 Introduction

Given the partial differential system:

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

With an appropriate function $v(t, x)$, the system can be controlled, by example on $x = 0$ or $x = L$. Let choice one control in $x_i = \frac{i}{M} L, i = 0, 1, \ldots, M$ (see figure 1).

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

In this case, the corresponding control problem is

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

where

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

$v_i = \chi_i v(x, t)$, $z(x)$ is a given function to reach at $t = T$, and y is the solution of (SE) for v (see figure 1).
The equivalent form as an optimization problem is:

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

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 $y(x, T)$.

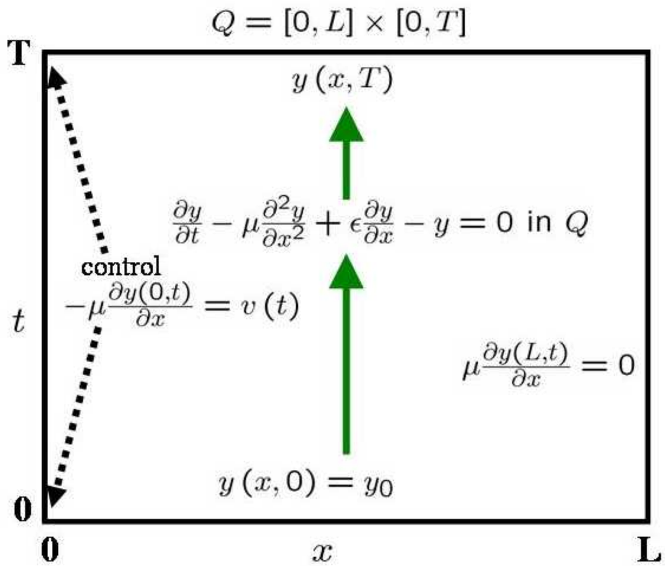

Figure 1: System (SE).

2 The continuous case

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

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

The perturbation system of the equation (SE) is

$$\begin{cases} \frac{\partial \delta y}{\partial t} - \mu \frac{\partial^2 \delta y}{\partial x^2} + \epsilon \frac{\partial \delta y}{\partial x} - \delta y - \chi_i \delta v = 0 & \text{in } Q = (0, L) \times (0, T)\; i = 1, \ldots, M-1 \\ \delta y(x, 0) = 0, & t = 0, \\ -\mu \frac{\partial \delta y(0,t)}{\partial x} = \delta v_0(t), & x = 0, \\ \mu \frac{\partial \delta y(L,t)}{\partial x} = \delta v_M(t), & x = L. \end{cases} \tag{δSE}$$

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

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

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

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

Therefore

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

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

$$
\begin{aligned}
&\left(\mu\frac{\partial \delta y\left(L,t\right)}{\partial x} = \delta v_M\left(t\right), -\mu\frac{\partial \delta y\left(0,t\right)}{\partial x} = \delta v_0\left(t\right)\right) \\
=\ & -\int_0^T p\left(L,t\right)\delta v_M\left(t\right)\mathrm{d}t - \int_0^T p\left(0,t\right)\delta v_0\left(t\right)\mathrm{d}t + \mu\int_0^T \left[\frac{\partial p\left(x,t\right)}{\partial x}\delta y\left(x,t\right)\right]_0^L \mathrm{d}t \\
& -\mu\iint_Q \frac{\partial^2 p}{\partial x^2}\delta y\mathrm{d}x\mathrm{d}t \\
=\ & \int_0^T p\left(L,t\right)\left(-\delta v_M\left(t\right)\right)\mathrm{d}t - \int_0^T p\left(0,t\right)\delta v_0\left(t\right)\mathrm{d}t + \mu\int_0^T \frac{\partial p\left(L,t\right)}{\partial x}\delta y\left(L,t\right)\mathrm{d}t \\
& -\mu\int_0^T \frac{\partial p\left(0,t\right)}{\partial x}\delta y\left(0,t\right)\mathrm{d}t - \mu\iint_Q \frac{\partial^2 p}{\partial x^2}\delta y\mathrm{d}x\mathrm{d}t \\
=\ & \int_0^T \left(-p\left(L,t\right)\right)\left(\delta v_M\left(t\right)\right)\mathrm{d}t + \int_0^T \left(-p\left(0,t\right)\right)\delta v_0\left(t\right)\mathrm{d}t + \int_0^T \mu\frac{\partial p\left(L,t\right)}{\partial x}\delta y\left(L,t\right)\mathrm{d}t \\
& +\int_0^T \left(-\mu\frac{\partial p\left(0,t\right)}{\partial x}\right)\delta y\left(0,t\right)\mathrm{d}t - \mu\iint_Q \frac{\partial^2 p}{\partial x^2}\delta y\mathrm{d}x\mathrm{d}t \\
=\ & \int_0^T \left(-p\left(L,t\right)\right)\left(\delta v_M\left(t\right)\right)\mathrm{d}t + \int_0^T \left(-p\left(0,t\right)\right)\delta v_0\left(t\right)\mathrm{d}t + \int_0^T \mu\frac{\partial p\left(L,t\right)}{\partial x}\delta y\left(L,t\right)\mathrm{d}t \\
& +\int_0^T \left(-\mu\frac{\partial p\left(0,t\right)}{\partial x}\right)\delta y\left(0,t\right)\mathrm{d}t + \iint_Q \left(-\mu\frac{\partial^2 p}{\partial x^2}\right)\delta y\mathrm{d}x\mathrm{d}t
\end{aligned}
$$

$$
\begin{aligned}
\epsilon \iint_Q p \frac{\partial \delta y}{\partial x} \mathrm{d}x\mathrm{d}t &= \epsilon \int_0^T \left[\int_0^L p \frac{\partial \delta y}{\partial x} \mathrm{d}x \right] \mathrm{d}t && (3)\\
v &= p,\ \mathrm{d}u = \frac{\partial \delta y}{\partial x} \mathrm{d}x \\
&= \epsilon \int_0^T \left[p\left(x,t\right) \delta y \left(x,t\right) \right]_0^L \mathrm{d}t - \epsilon \iint_Q \frac{\partial p}{\partial x} \delta y \mathrm{d}x\mathrm{d}t \\
&= \epsilon \int_0^T p\left(L,t\right) \delta y \left(L,t\right) \mathrm{d}t - \in \int_0^T p\left(0,t\right) \delta y\left(0,t\right) \mathrm{d}t - \epsilon \iint_Q \frac{\partial p}{\partial x} \delta y \mathrm{d}x\mathrm{d}t && (4)\\
&= \int_0^T \epsilon p\left(L,t\right) \delta y\left(L,t\right) \mathrm{d}t + \int_0^T \left(- \in p\left(0,t\right)\right) \delta y\left(0,t\right) \mathrm{d}t - \epsilon \iint_Q \frac{\partial p}{\partial x} \delta y \mathrm{d}x\mathrm{d}t
\end{aligned}
$$

$$
- \iint_Q p \delta y \mathrm{d}x\mathrm{d}t = \iint_Q \left(-p\right) \delta y \mathrm{d}x\mathrm{d}t. \tag{5}
$$

$$
\begin{aligned}
- \iint_Q p \chi_i \delta v \mathrm{d}x\mathrm{d}t &= \sum_{i=1}^{M-1} \int_0^T \left(-p_i\right) \delta v_i \mathrm{d}t && (6)\\
\text{where } \chi_i p &= p_i.
\end{aligned}
$$

$$
\begin{aligned}
0 &= (1) + (2) + (3) + (5) + (7) \\
&= \int_0^L p\left(x,T\right) \delta y\left(x,T\right) \mathrm{d}x + \iint_Q \left(-\frac{\partial p}{\partial t}\right) \delta y \mathrm{d}x\mathrm{d}t \\
&\quad + \int_0^T \left(-p\left(L,t\right)\right) \left(\delta v_M\left(t\right)\right) \mathrm{d}t + \int_0^T \left(-p\left(0,t\right)\right) \delta v_0\left(t\right) \mathrm{d}t + \int_0^T \mu \frac{\partial p\left(L,t\right)}{\partial x} \delta y\left(L,t\right) \mathrm{d}t \\
&\quad + \int_0^T \left(-\mu \frac{\partial p\left(0,t\right)}{\partial x}\right) \delta y\left(0,t\right) \mathrm{d}t + \iint_Q \left(-\mu \frac{\partial^2 p}{\partial x^2}\right) \delta y \mathrm{d}x\mathrm{d}t \\
&\quad + \int_0^T \epsilon p\left(L,t\right) \delta y\left(L,t\right) \mathrm{d}t + \int_0^T \left(- \in p\left(0,t\right)\right) \delta y\left(0,t\right) \mathrm{d}t - \epsilon \iint_Q \frac{\partial p}{\partial x} \delta y \mathrm{d}x\mathrm{d}t \\
&\quad + \iint_Q \left(-p\right) \delta y \mathrm{d}x\mathrm{d}t \\
&\quad + \sum_{i=1}^{M-1} \int_0^T \left(-p_i\right) \delta v_i \mathrm{d}t \\
&= \sum_{i=0}^{M} \int_0^T \left(-p_i\right) \delta v_i \mathrm{d}t \\
&\quad + \iint_Q \left(-\frac{\partial p}{\partial t} - \mu \frac{\partial^2 p}{\partial x^2} - \epsilon \frac{\partial p}{\partial x} - p\right) \delta y \mathrm{d}x\mathrm{d}t \\
&\quad + \int_0^L p\left(x,T\right) \delta y\left(x,T\right) \mathrm{d}x \\
&\quad + \int_0^T \left(\mu \frac{\partial p\left(L,t\right)}{\partial x} + \epsilon p\left(L,t\right)\right) \delta y\left(L,t\right) \mathrm{d}t + \int_0^T \left(-\mu \frac{\partial p\left(0,t\right)}{\partial x} - \epsilon p\left(0,t\right)\right) \delta y\left(0,t\right) \mathrm{d}t
\end{aligned}
$$

Adjusting terms with

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

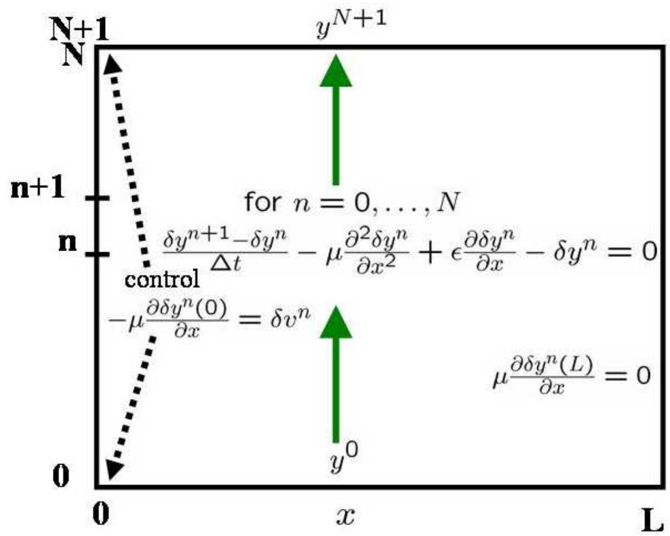

Figure 2: Discretization on time of (SE).

the adjoint system is

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

also

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

3 Discretization on Time

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

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

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

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

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

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

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

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

$$\begin{aligned} \Delta t \sum_{n=0}^{N} \int_0^L p^n \left(\frac{\delta y^{n+1} - \delta y^n}{\Delta t} \right) \mathrm{d}x &= \\ &= -\int_0^L p^0 \frac{\delta y^0}{\Delta t} \mathrm{d}x - \Delta t \sum_{n=1}^{N} \int_0^L \left(\frac{p^n - p^{n-1}}{\Delta t} \right) \delta y^n \mathrm{d}x + \int_0^L p^N \delta y^{N+1} \mathrm{d}x \\ &\quad -\Delta t \sum_{n=1}^{N} \int_0^L \left(\frac{p^n - p^{n-1}}{\Delta t} \right) \delta y^n \mathrm{d}x + \int_0^L p^N \delta y^{N+1} \mathrm{d}x. \end{aligned} \tag{7}$$

$$\begin{aligned} \Delta t \sum_{n=0}^{N} \int_0^L p^n \left(-\mu \frac{\partial^2 \delta y^n}{\partial x^2} \right) \mathrm{d}x &= \\ &= \Delta t \sum_{n=0}^{N} p \left[-\mu \frac{\partial \delta y}{\partial x} \right]_0^L + \mu \Delta t \sum_{n=0}^{N} \frac{\partial p}{\partial x} \left[\delta y \right]_0^L - \mu \Delta t \sum_{n=0}^{N} \int_0^L \frac{\partial^2 p}{\partial x^2} \delta y \mathrm{d}x \\ &= -\Delta t \sum_{n=0}^{N} p^n(0) \left(\delta v^n \right) + \mu \Delta t \sum_{n=0}^{N} \frac{\partial p^n(L)}{\partial x} \delta y(L) \\ &\quad -\mu \Delta t \sum_{n=0}^{N} \int_0^L \frac{\partial^2 p}{\partial x^2} \delta y \mathrm{d}x. \end{aligned} \tag{8, 9}$$

$$\Delta t \sum_{n=0}^{N} \int_0^L p^n \left(\epsilon \frac{\partial \delta y^n}{\partial x} \right) \mathrm{d}x = \epsilon \sum_{n=0}^{N} p^n(L) \delta y(L) - \epsilon \sum_{n=0}^{N} \int_0^L \frac{\partial p}{\partial x} \delta y \mathrm{d}x. \tag{10}$$

$$\Delta t \sum_{n=0}^{N} \int_0^L p^n \left(-\delta y^n \right) \mathrm{d}x. \tag{11}$$

$$\begin{aligned} 0 = (7) + (8) + (10) + (11) &= \Delta t \sum_{n=1}^{N} \int_0^L \left(-\frac{p^n - p^{n-1}}{\Delta t} - \mu \frac{\partial^2 p}{\partial x^2} - \epsilon \frac{\partial p}{\partial x} - p^n \right) \delta y^n \mathrm{d}x + \int_0^L p^N \delta y^{N+1} \mathrm{d}x \\ &\quad -\Delta t \sum_{n=0}^{N} p(0) \left(\delta v^n \right) + \mu \Delta t \sum_{n=0}^{N} \frac{\partial p^n}{\partial x}(L) \delta y(L) + \epsilon \sum_{n=0}^{N} p(L) \delta y(L). \end{aligned}$$

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

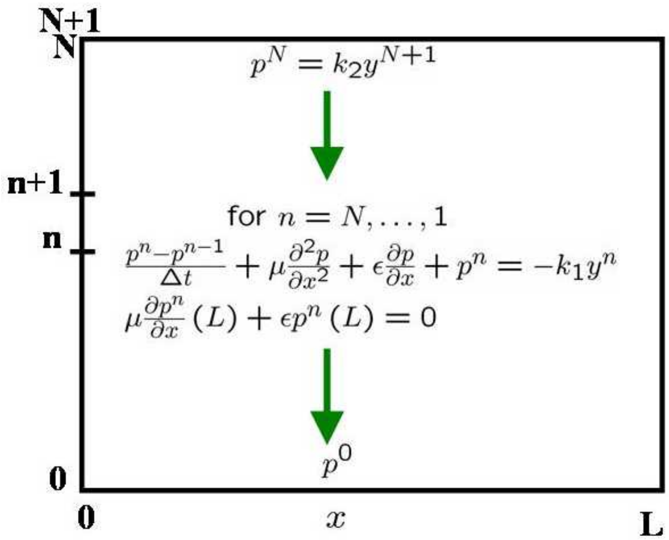

Figure 3: Discretization on time of adjoint system of (SE).

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

And

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

3.1 Fully discretization

Let $H > 0$ an integer, and $\triangle x = h = \frac{L}{H}$. The indices for axis x are $-1 \leq j \leq H+1$. Note that two sets of points are added on $j = -1$, and $j = H+1$, this is convenient because the frontier conditions on $x = 0$ $(-\mu \frac{\partial y(0,t)}{\partial x} = v(t),)$ and $x = L$ $(\mu \frac{\partial y(L,t)}{\partial x} = 0)$ 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

$$\left\{\begin{array}{l} y_j^0 = y_{0,j},\ j = 0, \dots, H \\ \text{for } n = 0, \dots, N,\ j = 0, \dots, H \\ \frac{y_j^{n+1} - y_j^n}{\Delta t} - \mu \frac{y_{j+1}^n + y_{j-1}^n - 2y_j^n}{h^2} + \epsilon \frac{y_{j+1}^n - y_j^n}{h} - y_j^n - \chi_j v_i = 0 \\ -\mu \frac{y_0^n - y_{-1}^n}{h} = v_0^n \\ \mu \frac{y_{H+1}^n - y_H^n}{h} = v_M^n. \end{array}\right. \tag{SE$^{\Delta t}_{\Delta x}$}$$

$-\mu \frac{y_0^n - y_{-1}^n}{h} = v_0^n$
$-\mu y_0^n + \mu y_{-1}^n = h v_0^n$
$+y_{-1}^n = (h v_0^n + \mu y_0^n)/\mu$
$+y_{-1}^n = \frac{h}{\mu} v_0^n + y_0^n$
$\mu \frac{y_{H+1}^n - y_H^n}{h} = v_M^n$
$\mu\left(y_{H+1}^n - y_H^n\right) = h v_M^n$
$\mu y_{H+1}^n - \mu y_H^n = h v_M^n$
$\mu y_{H+1}^n = \mu y_H^n + h v_M^n$
$y_{H+1}^n = y_H^n + \frac{h}{\mu} v_M^n$
The adjoint equations (see figure 5) are

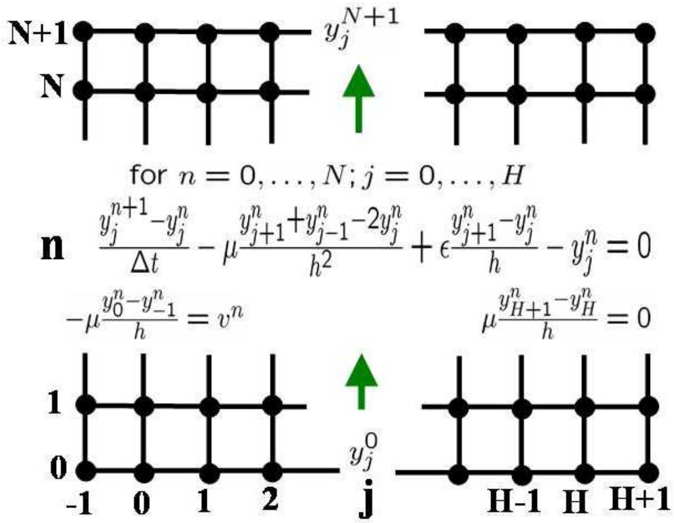

Figure 4: Fully discretization of (SE).

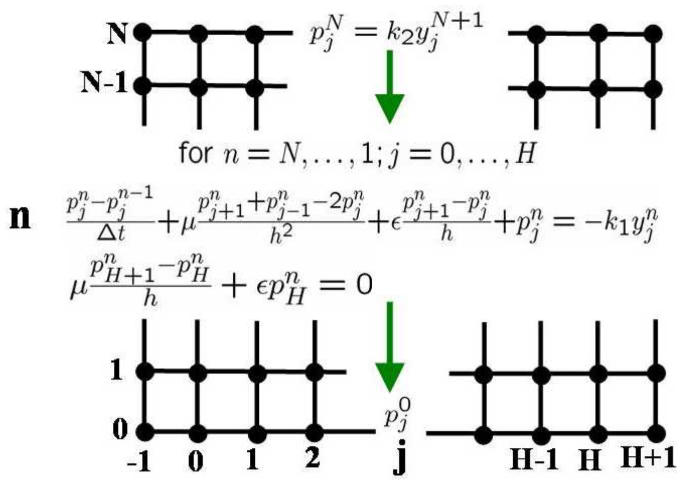

Figure 5: Fully discretization of adjoint system of (SE).

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

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

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

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

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

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

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

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

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

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

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

And the corresponding perturbation equations are

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

The corresponding control problem is

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

where

$$
J^{\triangle t}_{\triangle x}(v) = \frac{\Delta t}{2} \sum_{n=0}^{N} [v^n]^2 + \frac{k_1 \Delta t h}{2} \sum_{n=0}^{N} \sum_{j=0}^{H} \left[y_j^n\right]^2 + \frac{k_2 h}{2} \sum_{j=0}^{H} \left[y_j^{N+1}\right]^2,
$$

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

4 The Conjugate Gradient Algorithm

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

1. Given ε (the tolerance to stop the algorithm), $0 < \varepsilon \ll 1$, and $\left\{u^{n,0}\right\} \in \mathcal{V}$.
2. Solve the equation (SE$^{\triangle t}_{\triangle x}$), and

   with the solution $\left\{y_j^{n,0}\right\}_{-1 \leq j \leq H+1}^{0 \leq n \leq N+1}$ solve (ASE$^{\triangle t}_{\triangle x}$) to get $\left\{p_j^{n,0}\right\}_{-1 \leq j \leq H+1}^{0 \leq n \leq N}$.
3. Compute $g^0 = \left\{u^{n,0} + p_0^{n,0}\right\}^{0 \leq n \leq N}$, and set $w^0 = g^0$.

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

4. If $\frac{(g^{k+1},g^{k+1})_{\mathcal{V}}}{(g^0,g^0)_{\mathcal{V}}} < \epsilon^2$ take u^{k+1} as the solution and stop.
5. Compute $k = k + 1$.
6. Solve the equation ($\delta\mathrm{SE}_{\triangle x}^{\triangle t}$), and

   with the solution $\overline{y} = \left\{\delta y_j^{n,k}\right\}_{-1\leq j\leq H+1}^{0\leq n\leq N+1}$ solve ($\mathrm{ASE}_{\triangle x}^{\triangle t}$) to get $\overline{p} = \left\{p_j^{n,k}\right\}_{-1\leq j\leq H+1}^{0\leq n\leq N}$.
7. Compute $\overline{g}^k = \left\{w^{n,k} + \overline{p}_0^{n,k}\right\}^{0\leq n\leq N}$, $\rho^k = \left(g^k, g^k\right)_{\mathcal{V}}$, $u^{k+1} = u^k - \rho^k w^k$, and $g^{k+1} = g^k - \rho^k \overline{g}^k$.
8. If $\frac{(g^{k+1},g^{k+1})_{\mathcal{V}}}{(g^0,g^0)_{\mathcal{V}}} < \epsilon^2$ take u^{k+1} as the solution and stop.
9. Compute $\gamma^k = \frac{(g^{k+1},g^{k+1})_{\mathcal{V}}}{(g^k,g^k)_{\mathcal{V}}}$, and $w^{k+1} = g^{k+1} + \gamma^k w^k$
10. Go to step 5.

Motivación

Se ha preferido dejar esta seccin al final, ya que las notas estn dirigigas principalmente a estudiantes de posgrado interesados en desarrollar sus propios simuladores y que posiblemente saben de la importancia de la Teora de Control sobre Sistemas de Ecuaciones Diferenciales Parciales.
De la abundante literatura, sólo mencionamos para ecuaciones diferenciales parciales el libro [4] y de Control los libros [1, 3]. Las notas se elaboraron a partir de las pláticas [2].
El siguiente problema es un caso de una ecuación parabólica con tres componentes de fenómenos físico-químicos.

1. Advección. Es la variación escalar en cada punto de un campo vectorial, por ejemplo el arrastre de contaminante en un medio.
2. Reacción. Es la respuesta o reacción del sistema, por ejemplo el proceso de cambio de calor de un sistema.
3. Difusión. Es el gradiente (cambio o transporte) de los componentes del sistema.

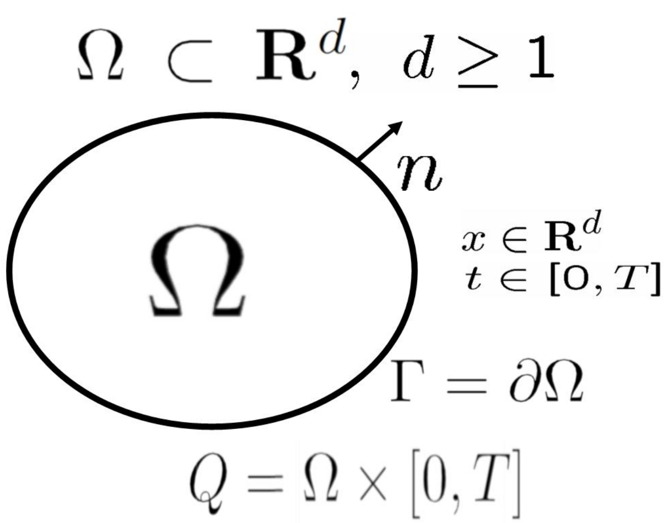

Figure 6: Dominio del Sistema ??

Ecuación parabólica de advección ($V \cdot \nabla\varphi$), reacción($f(\varphi)$) y difusión ($\nabla \cdot (A\nabla\varphi)$) en el tiempo que llamaremos Sistema de la Ecuación de Estado

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

donde $\Omega \subset \mathbf{R}^d$ ($d \geq 1$, dimensión) es el dominio, una región suave, con frontera $\Gamma = \partial\Omega$ suave, n representa un vector unitario normal en Γ (apuntando hacia fuera de Ω), $T > 0$ es el tiempo (incluso $T = \infty$).
La figura 6 muestra el dominio de (SEE). El producto interno $\cdot$ es el usual ($a, b \in \mathbf{R}^d, a \cdot b = \sum_{i=1}^{d} a_i b_i$), A es una función tensor real (matriz de difusión), $V : \Omega \to \mathbf{R}^d$ es una función vectorial, $f : \mathbf{R} \to \mathbf{R}$ es una función real y $\varphi(x,t)$ es la función del fenómeno que ocurre en Q.
Además se asume que:

$$A(x)\xi \cdot \xi \geq \alpha |\xi|^2, \forall \xi \in \mathbf{R}^d \text{ para casi todo } x \in \Omega$$

lo que significa que A es uniformemente definida positiva para casi todo x en Ω.
Para la función vectorial V se tiene:

$$\begin{aligned} \nabla \cdot V &= 0 \text{ (libre de divergencia)} \\ \frac{\partial V}{\partial t} &= 0 \text{ (constante en el tiempo)} \\ V \cdot n &= 0 \text{ on } \Gamma \end{aligned}$$

Veamos las razones por lo que un control es necesario.
Sea una función reacción dada por

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

donde $C, \lambda > 0$ son constantes reales positivas.
Entonces la solución de estado estable para tal f de

$$\frac{\partial \varphi}{\partial t} + f(\varphi) = 0 \tag{12}$$

está dada por

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

Note que φ_s es constante por lo que la ecuación (12), sustituyendo φ_s se cumple (ya que $f(\varphi_s) = C - \lambda e^{\varphi_s} = C - \lambda e^{\frac{\ln C}{\lambda}} = 0$).
Se supone que para $t < 0$, el sistema estuvo en su solución estacionaria estable $\varphi = \varphi_s$.
Ahora con $\varphi = \varphi_s$ en $t = 0$ se introduce una perturbación constante en $\delta\varphi$, independiente de x y t (o sea con $\nabla\delta\varphi = 0$ y $\frac{\partial \delta\varphi}{\partial t} = 0$).
Dado que se trata de una perturbación constante en el tiempo y el espacio, el sistema evoluciona bajo el siguiente modelo de una ecuación diferencial ordinaria:

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

Este modelo se comporta con una perturbación constante y positiva, $\delta\varphi > 0$, de forma que $\varphi \to +\infty$ (pero además en un tiempo finito crece muy rápidamente), o bien si la perturbación es negativa, $\delta\varphi < 0$, se tiene que $\varphi_{t\to\infty} \to -\infty$ o sea tiende a menos infinito conforme avanza el tiempo.

Lo anterior significa que alrededor de una solución de estado estable, la introducción de una pequeña perturbación constante hace al sistema inestable.
Para verificar lo anterior se procede mediante el Método de Euler para integrar numéricamente a la ecuación anterior:

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

Sin perdida de generalidad tomamos $\triangle t = 1$, $C = 1, \lambda = 1, \delta\varphi = 0.1 > 0$ y aproximamos $\frac{d\varphi}{dt}$ por una a diferencia entre el tiempo n y el tiempo $n-1$. De donde resulta
$\varphi_n = \exp\left(\varphi_{n-1}\right) + \varphi_{n-1} - 1.$
La condición inicial es
$\varphi_0 = \frac{\ln C}{\lambda} + \delta\varphi = 0.1$
Por tanto
$\varphi_1 = \exp(0.1) + 0.1 - 1 = 0.20517$
$\varphi_2 = \exp(0.20517) + 0.20517 - 1 = 0.4329$
$\varphi_3 = \exp(0.4329) + 0.4329 - 1 = 0.97464$
$\varphi_4 = \exp(0.97464) + 0.97464 - 1 = 2.6248$
$\varphi_5 = \exp(2.6248) + 2.6248 - 1 = 15.427$
$\varphi_6 = \exp(15.427) + 15.427 - 1 = 5.0103 \times 10^6$
$\varphi_7 = \exp\left(5.0103 \times 10^6\right) + 5.0103 \times 10^6 - 1 = 4.3922 \times 10^{2175945}$
Note que $\varphi(t)$ crece muy rápidamente en tiempo finito, o sea tiende aceleradamente a ∞.
Suponiendo que $\delta\varphi = -0.1 < 0$, con las mismas constantes C y λ, se tiene
$\varphi_0 = -0.1$
$\varphi_1 = \exp(-0.1) + (-0.1) - 1 = -0.19516$
$\varphi_2 = \exp(-0.19516) + (-0.19516) - 1 = -0.37246$
$\varphi_3 = \exp(-0.37246) + (-0.37246) - 1 = -0.68342$
$\varphi_4 = \exp(-0.68342) + (-0.68342) - 1 = -1.1785$
$\varphi_5 = \exp(-1.1785) + (-1.1785) - 1 = -1.8708$
$\varphi_6 = \exp(-1.8708) + (-1.8708) - 1 = -2.7168$
$\varphi_7 = \exp(-2.7168) + (-2.7168) - 1 = -3.6507$
$\varphi_8 = \exp(-3.6507) + (-3.6507) - 1 = -4.6247$
$\varphi_9 = \exp(-4.6247) + (-4.6247) - 1 = -5.6149$
$\varphi_{10} = \exp(-5.6149) + -5.6149 - 1 = -6.6113$
$\varphi_{11} = \exp(-6.6113) + -6.6113 - 1 = -7.6100$
En este caso $\varphi(t)$ es decreciente y lentamente tiende a $-\infty$.
En cualquier caso es claro que se necesita un control para evitar tales comportamientos y regresar al sistema a la solución de estado estable φ_s.

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