Numerics and Control of PDEs

Lecture 4

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The 1D Heat equation with non homogeneous boundary conditions

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1. The Heat equation with Homogeneous Boundary Conditions

We consider the equation

$$(HHE) \qquad \begin{aligned} &\frac{\partial z}{\partial t} - \frac{\partial^2 z}{\partial x^2} = 0 \quad \text{in } (0,1)\times(0,\infty), \\ &z(0,t) = 0 \quad \text{and} \quad z(1,t) = 0 \quad \text{for } t \in (0,\infty), \\ &z(x,0) = z_0(x) \quad \text{in } (0,1). \end{aligned}$$

We assume that $z_0 \in L^2(0,1)$. The eigenvalues of $A = d^2/dx^2$, with Dirichlet boundary conditions, and the corresponding eigenfunctions are

$$\lambda_k = -\pi^2 k^2, \quad \xi_k(x) = \sqrt{2}\sin(k\,\pi\,x).$$

The family $(\xi_k)_{k\in\mathbb{N}^*}$ is a Hilbertian basis in $L^2(0,1)$. We can decompose the intial condition z_0 in this basis:

$$z_0 = \sum_{k=1}^{\infty} \zeta_{0,k}\xi_k, \quad \text{with} \quad \zeta_{0,k} = (z_0, \xi_k)_{L^2(0,1)}.$$

If we look for a solution z to the heat equation in the form

$$z(x,t) = \sum_{k=1}^{\infty} \zeta_k(t)\, \xi_k(x),$$

we can show that ζ_k satisfies the differential equation

$$\zeta_k' = \lambda_k\, \zeta_k, \quad \zeta_k(0) = \zeta_{0,k}.$$

Thus $\zeta_k(t) = e^{\lambda_k t}\zeta_{0,k}$, and

$$z(x,t) = \sum_{k=1}^{\infty} e^{\lambda_k\, t}\big(z_0, \xi_k\big)_{L^2(0,1)}\xi_k,$$

is a candidate to be a solution to (HHE).
We can show that, if $z_0 \in L^2(0,1)$, the above series converges in $C([0,T];L^2(0,1))$, while it converges in $C([0,T];H_0^1(0,1))$ if $z_0 \in H_0^1(0,1)$.

The semigroup of the heat operator

For all $t \geq 0$, we define the operator $e^{tA} \in \mathcal{L}(L^2(0,1))$ as follows

$$e^{tA} z_0 = \sum_{k=1}^{\infty} e^{\lambda_k t} \big(z_0, \xi_k\big)_{L^2(0,1)} \xi_k.$$

We can check that the family of operators $(e^{tA})_{t \geq 0}$ obeys the following properties

- $e^{0A} = I$,
- For $t \geq 0$, $s \geq 0$, $e^{tA} e^{sA} = e^{sA} e^{tA} = e^{(t+s)A}$,
- $\lim_{t \searrow 0} \|e^{tA} z_0 - z_0\|_{L^2(0,1)} = 0$, for all $z_0 \in L^2(0,1)$.

Thus, this family of operators has properties similar to those of the exponential of a matrix. It is called a strongly continuous semigroup on $L^2(0,1)$.

In addition we have

$$\frac{d}{dt}e^{tA} = Ae^{tA} \quad \textit{for } t > 0,$$

where

$$Az = \frac{d^2 z}{dx^2} \quad \textit{if } z \in H^2(0,1) \cap H_0^1(0,1).$$

Notice that

$$e^{tA}z_0 \in H^2(0,1) \cap H_0^1(0,1) \textit{ for } t > 0,$$

even if $z_0 \in L^2(0,1)$. Indeed

$$\frac{d^2}{dx^2}e^{tA}z_0 = \sum_{k=1}^{\infty} \lambda_k e^{\lambda_k t}\big(z_0, \xi_k\big)_{L^2(0,1)}\xi_k,$$

and the series converges in $L^2(0,1)$ because

$$\sum_{k=1}^{\infty} \left|\lambda_k e^{\lambda_k t}\big(z_0, \xi_k\big)_{L^2(0,1)}\right|^2 < \infty.$$

The nonhomogeneous heat equation

We consider the equation

$$
(NHHE) \qquad
\begin{aligned}
&\frac{\partial z}{\partial t} - \frac{\partial^2 z}{\partial x^2} = f \quad \text{in } (0,1)\times(0,\infty),\\
&z(0,t) = 0 \quad \text{and} \quad z(1,t) = 0 \quad \text{for } t \in (0,\infty),\\
&z(x,0) = z_0(x) \quad \text{in } (0,1).
\end{aligned}
$$

We assume that $z_0 \in L^2(0,1)$ and $f \in L^2(0,T;L^2(0,1))$.
Arguing as above, and with the variation of constant formula, we can show that the solution to $(NHHE)$ is

$$
z(t) = e^{tA}z_0 + \int_0^t e^{(t-s)A} f(s)\, ds.
$$

We shall call it 'the Duhamel formula'.

2. The heat equation with a nonhomogeneous boundary condition

We consider the equation

$$
(NHBC) \qquad
\begin{aligned}
&\frac{\partial z}{\partial t} - \frac{\partial^2 z}{\partial x^2} = 0 \quad \text{in } (0,1)\times(0,T),\\
&z(0,t) = 0 \quad \text{and} \quad z(1,t) = u(t) \quad \text{for } t \in (0,T),\\
&z(x,0) = z_0(x) \quad \text{in } (0,1).
\end{aligned}
$$

We assume that $z_0 \in L^2(0,1)$ and $u \in L^2(0,T)$.

Weak formulation (WF) for (*NHBC*)

In order to take into account the non homogeneous B.C., the most usual weak formulation is

$$(WF) \qquad \begin{aligned} &\text{Find } z \in L^2(0,T;H^1_{\{0\}}(0,1)) \text{ such that} \\ &\frac{d}{dt}(z(t),\phi)_{L^2} = -\int_0^1 \frac{\partial z}{\partial x}(x,t)\,\frac{d\phi}{dx}\,dx \quad \forall \phi \in H^1_0(0,1), \\ &z(1,t) = u(t), \\ &(z(0),\phi)_{L^2} = (z_0,\phi)_{L^2} \quad \forall \phi \in H^1_0(0,1). \end{aligned}$$

We shall use that formulation for the numerical approximation of the equation. But we cannot use that formulation to obtain a controlled system of the form

$$z' = Az + Bu \quad \text{in } (0,\infty), \quad z(0) = z_0.$$

Solutions defined by transposition in the case of $(NHBC)$

We say that $z \in L^2(0,T;L^2(0,1))$ is a weak solution to equation $(NHBC)$ if and only if for all test functions $\phi \in H^2(0,1) \cap H_0^1(0,1)$, the function $t \longmapsto (z(t),\phi)_{L^2}$ belongs to $H^1(0,T)$, and

$$\frac{d}{dt}(z(t),\phi)_{L^2} = \int_0^1 z(x,t)\,\phi_{xx}(x)\,dx - u(t)\phi_x(1),$$
$$(z(0),\phi)_{L^2} = (z_0,\phi)_{L^2}.$$

Thus

$$\langle Bu(t),\phi\rangle = (u(t),B^*\phi)_{\mathbb{R}} = -u(t)\phi_x(1),$$

that is

$$B^*\phi = -\phi_x(1).$$

Lifting of the boundary condition

We look for a solution to $(NHBC)$ in the form

$$z = y + w,$$

where

$$w(x,t) = x\,u(t).$$

We decompose z, y and w in the basis $(\xi_k)_{j\in\mathbb{N}^*}$

$$z(x,t) = \sum_{k=1}^{\infty} \zeta_k(t)\xi_k(x), \quad y = \sum_{k=1}^{\infty} y_k(t)\xi_k, \quad w = \sum_{k=1}^{\infty} w_k\xi_k.$$

We have

$$w_k(t) = u(t)(x,\xi_k)_{L^2} = u(t)\,\sqrt{2}\int_0^1 x\sin(k\pi x)dx = -u(t)\,\frac{\sqrt{2}}{k\pi}(-1)^k.$$

The equation satisfied by y is

$$\frac{\partial y}{\partial t} - \frac{\partial^2 y}{\partial x^2} = -x\, u'(t) \quad \text{in } (0,1) \times (0,T),$$
$$y(0,t) = 0 \quad \text{and} \quad y(1,t) = 0 \quad \text{for } t \in (0,T),$$
$$y(x,0) = z_0(x) - x\, u(0) \quad \text{in } (0,1).$$

Thus we have

$$y(t) = e^{tA}(z_0(x) - x\, u(0)) + \int_0^t e^{(t-s)A}(-x\, u'(s))\, ds.$$

We use the decomposition of y in the Duhamel formula

$$y(x,t) = \sum_{k=1}^{\infty} y_k(t)\,\xi_k(x).$$

Each component y_k obeys the Duhamel formula

$$y_k(t) = e^{\lambda_k t}(\zeta_{0,k} - (x,\xi_k)_{L^2}\,u(0)) + \int_0^t e^{(t-s)\lambda_k}(-x,\xi_k)_{L^2}\,u'(s)\,ds.$$

In order to find the controlled system satisfied by z, we integrate by part

$$y_k(t) = e^{\lambda_k t}\zeta_{0,k} + \lambda_k \int_0^t e^{(t-s)\lambda_k}(-x,\xi_k)_{L^2}\,u(s))\,ds + (-x,\xi_k)_{L^2}\,u(t).$$

Thus

$$\zeta_k(t) = y_k(t) + (x,\xi_k)_{L^2}\,u(t) = e^{\lambda_k t}\zeta_{0,k} + \lambda_k \int_0^t e^{(t-s)\lambda_k}(-x,\xi_k)_{L^2}\,u(s)\,ds.$$

This means that ζ_k is the solution to the following differential equation

$$\zeta_k' = \lambda_k\zeta_k + (-\lambda_k)w_k(t), \quad \zeta_k(0) = \zeta_{0,k}.$$

By summing

$$\zeta_k(t)\xi_k = e^{\lambda_k t}\zeta_{0,k}\xi_k + \lambda_k \int_0^t e^{(t-s)\lambda_k}(-x,\xi_k)_{L^2}\, u(s)\,\xi_k\, ds,$$

we obtain

$$z(t) = e^{tA}z_0 + (-A)\int_0^t e^{(t-s)A}w(s)\,ds.$$

Thus, we formally have

$$z'(t) = Az + (-A)w, \quad z(0) = z_0.$$

This is formal as long as we have not precisely defined $(-A)w$. We can say that

$$(-A)w = \sum_{k=1}^{\infty} w_k(-A)\xi_k = \sum_{k=1}^{\infty} w_k(-\lambda_k)\xi_k,$$

but the series does not converge in $L^2(0,1)$. It converges in a weaker norm.

Comparison between the variational-transposition method and the lifting method

By choosing $\phi = \xi_k$ as test function in the variational method, we get

$$\frac{d}{dt}(z(t), \xi_k)_{L^2} = \int_0^1 z(x,t)\,\lambda_k \xi_k\, dx - u(t)\xi_{k,x}(1),$$
$$(z(0), \xi_k)_{L^2} = (z_0, \xi_k)_{L^2},$$

where $\xi_{1,x}(1) = \frac{d\xi_k}{dx}(1)$, and

$$\xi_{k,x}(1) = k\pi\sqrt{2}\,(-1)^k.$$

That is

$$\zeta_k' = \lambda_k \zeta_k - u(t)\,\pi\, k\,(-1)^k\sqrt{2}, \quad \zeta_k(0) = \zeta_{0,k}.$$

We have to compare with

$$\zeta_k' = \lambda_k \zeta_k + (-\lambda_k) w_k(t), \quad \zeta_k(0) = \zeta_{0,k}.$$

Since

$$w_k = -u(t)\,\frac{\sqrt{2}}{k\pi}(-1)^k \quad \text{and} \quad -\lambda_k = k^2\pi^2,$$

we have

$$\zeta_k' = \lambda_k \zeta_k - u(t)\,\pi\, k\,(-1)^k\sqrt{2}, \quad \zeta_k(0) = \zeta_{0,k}.$$

We fortunately recover the same result.

When $u \in H^1(0,T)$ and $z_0 \in L^2(0,1)$, the solution z to $(NHBC)$ belongs to $C([0,T]; L^2(0,1))$. If we only have $u \in L^2(0,T)$, the solution z to $(NHBC)$ belongs to $L^2(0,T; L^2(0,1))$.

We introduce the operator $D \ : \ \mathbb{R} \longmapsto L^2(0,1)$, defined by $Du = w = u\,x$. We have

$$z'(t) = Az + (-A)w = Az + (-A)Du = Az + Bu, \quad z(0) = z_0.$$

As mentioned above the meaning of Bu is clear for each component of z in the basis $(\xi_k)_{k\in\mathbb{N}^*}$, that is

$$\langle Bu, \xi_k \rangle = -u(t)\xi_{k,x}(1).$$

Since we have written the PDE as a controlled system, we may adapt the results from control theory in the finite dimensional case to this infinite dimensional model.

We also have

$$B^*\xi_k = -\xi_{k,x}(1) \quad \text{for all } k \in \mathbb{N}^*.$$

3. F.E. approximation of the 1D heat equation

For the numerical approximation of the heat equation with NHBC, we use the following weak formulation.

$$(WF) \qquad \begin{aligned} &\text{Find } z \in L^2(0,T;H^1_{\{0\}}(0,1)) \text{ such that} \\ &\frac{d}{dt}(z(t),\phi)_{L^2} = -\int_0^1 \frac{\partial z}{\partial x}(x,t)\,\frac{d\phi}{dx}\,dx \quad \forall \phi \in H^1_0(0,1), \\ &z(1,t) = u(t), \\ &(z(0),\phi)_{L^2} = (z_0,\phi)_{L^2} \quad \forall \phi \in H^1_0(0,1). \end{aligned}$$

We choose a regular subdivision of $[0,1]$:

$$0 = x_0 < x_1 < \cdots < x_N = 1, \quad h = \frac{1}{N}, \quad x_k = kh \quad \forall k \in \{0,\cdots,N\}.$$

We introduce two finite dimensional subspaces of $H^1(0,1)$:

$$Z_h = \{\phi \in C([0,1]) \mid \phi|_{[x_{i-1},x_i]} \in P_1, \quad \phi(0) = 0\}$$

$$Z_{h,0} = \{\phi \in C([0,1]) \mid \phi|_{[x_{i-1},x_i]} \in P_1, \quad \phi(0) = 0, \quad \phi(1) = 0\}.$$

We notice that

$$\dim Z_h = N \quad \text{and} \quad \dim Z_{h,0} = N-1.$$

A very useful basis of $Z_{h,0}$ is

$$\{\phi_1, \cdots, \phi_{N-1}\}, \quad \text{with} \quad \phi_j(x_k) = \delta_{j,k}.$$

The corresponding basis for Z_h is

$$\{\phi_1, \cdots, \phi_N\}, \quad \text{with} \quad \phi_j(x_k) = \delta_{j,k}.$$

Any function $z \in Z_h$ is decomposed as follows

$$z = \sum_{j=1}^{N} z_j \, \phi_j \quad \text{with} \quad z_j = z(x_j).$$

We approximate the weak formulation by

$$(DWF) \qquad \begin{aligned} & \text{Find } z \in L^2(0, T; Z_h) \text{ such that} \\ & \frac{d}{dt}(z(t), \phi)_{L^2} = -\int_0^1 \frac{\partial z}{\partial x}(x, t) \, \frac{d\phi}{dx} \, dx \quad \forall \phi \in Z_{h,0}, \\ & z(1, t) = u(t), \\ & (z(0), \phi)_{L^2} = (z_0, \phi)_{L^2} \quad \forall \phi \in Z_{h,0}. \end{aligned}$$

This approximate weak formulation is equivalent to

$$\text{Find } z = \sum_{j=1}^{N} z_j \, \phi_j, \text{ with } z_j \in L^2(0, T), \text{ such that}$$

$$\frac{d}{dt}(z(t), \phi_k)_{L^2} = -\int_0^1 \frac{\partial z}{\partial x}(x, t) \, \frac{d\phi_k}{dx} \, dx \quad \forall k \in \{1, \cdots, N-1\},$$

$$z_N(t) = u(t),$$

$$(z(0), \phi_k)_{L^2} = (z_0, \phi_k)_{L^2} \quad \forall k \in \{1, \cdots, N-1\}.$$

Since $z_N(t) = u(t)$ is known, the above system is a differential system in $\mathbb{R}^{N-1}$ satisfied by $\mathbf{z} = (z_1, \cdots, z_{N-1})^T$. To write this differential system we introduce the 'mass matrix' $\mathbf{E} \in \mathbb{R}^{(N-1)\times(N-1)}$ and the rigidity matrix $\mathbf{A} \in \mathbb{R}^{(N-1)\times(N-1)}$:

$$\mathbf{E} = (E_{i,j})_{1 \le i, j \le N-1} \quad \text{with} \quad E_{i,j} = \int_0^1 \phi_i \, \phi_j \, dx,$$

$$\mathbf{A} = (A_{i,j})_{1 \le i, j \le N-1} \quad \text{with} \quad A_{i,j} = -\int_0^1 \frac{d\phi_i}{dx} \, \frac{d\phi_j}{dx} \, dx.$$

If we choose an exact integration formula, we have

$$\mathbf{E} = h \begin{bmatrix} \frac{2}{3} & \frac{1}{6} & 0 & & & & \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & \ddots & & \ddots & \\ 0 & \frac{1}{6} & \frac{2}{3} & & & & \\ & \ddots & & \ddots & & \ddots & \\ & & & & \frac{2}{3} & \frac{1}{6} & 0 \\ & \ddots & & \ddots & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ & & & & 0 & \frac{1}{6} & \frac{2}{3} \end{bmatrix}$$

$$\mathbf{A} = \frac{1}{h} \begin{bmatrix} -2 & 1 & 0 & & & & \\ 1 & -2 & 1 & \ddots & & \ddots & \\ 0 & 1 & -2 & & & & \\ & \ddots & & \ddots & & \ddots & \\ & & & & -2 & 1 & 0 \\ & \ddots & & \ddots & 1 & -2 & 1 \\ & & & & 0 & 1 & -2 \end{bmatrix}$$

The differential system is

$$
\begin{aligned}
E_{1,1}z_1'(t) + E_{1,2}z_2'(t) &= A_{1,1}z_1(t) + A_{1,2}z_2(t),\\
E_{1,1}z_1(0) + E_{1,2}z_2(0) &= (z_0, \phi_1)_{L^2},\\
E_{2,1}z_1'(t) + E_{2,2}z_2'(t) + E_{2,3}z_3'(t) &= A_{2,1}z_1(t) + A_{2,2}z_2(t) + A_{2,3}z_3(t),\\
E_{2,1}z_1(0) + E_{2,2}z_2(0) + E_{2,3}z_3(0) &= (z_0, \phi_2)_{L^2},
\end{aligned}
$$

$$\vdots$$

$$
\begin{aligned}
&E_{N-2,N-3}z_{N-3}'(t) + E_{N-2,N-2}z_{N-2}'(t) + E_{N-2,N-1}z_{N-1}'(t)\\
&= A_{N-2,N-3}z_{N-3}'(t) + A_{N-2,N-2}z_{N-2}(t) + A_{N-2,N-1}z_{N-1}(t),\\
&\quad E_{N-2,N-3}z_{N-3}(0) + E_{N-2,N-2}z_{N-2}(0) + E_{N-2,N-1}z_{N-1}(0) = (z_0, \phi_{N-2})_{L^2},\\
&E_{N-1,N-2}z_{N-2}'(t) + E_{N-1,N-1}z_{N-1}'(t) + u'(t)\int_0^1 \phi_N\,\phi_{N-1}\\
&= A_{N-1,N-2}z_{N-2}(t) + A_{N-1,N-1}z_{N-1}(t) - u(t)\int_0^1 \frac{d\phi_N}{dx}\,\frac{d\phi_{N-1}}{dx},\\
&\qquad E_{N-1,N-2}z_{N-2}(0) + E_{N-1,N-1}z_{N-1}(0) = (z_0, \phi_{N-1})_{L^2}.
\end{aligned}
$$

For simplicity, we do not choose an exact integration formula, but the trapezoidal formula for the term $u'(t)\int_0^1 \phi_N\,\phi_{N-1}$. Thus we approximate this term by zero since in the trapezoidal formula

$$\int_0^1 \phi_N\,\phi_{N-1} \quad \text{is approximated by}$$
$$\frac{h}{2}\left((\phi_N\,\phi_{N-1})(x_{N-1}) + (\phi_N\,\phi_{N-1})(x_N)\right) = 0.$$

The term $-u(t)\int_0^1 \frac{d\phi_N}{dx}\,\frac{d\phi_{N-1}}{dx}$ is

$$-u(t)\int_0^1 \frac{d\phi_N}{dx}\,\frac{d\phi_{N-1}}{dx} = -u(t)\int_{x_{N-1}}^{x_N} \frac{1}{h}\left(\frac{-1}{h}\right)\,dx = \frac{u(t)}{h}.$$

We introduce the matrix

$$\mathbf{B} = \frac{1}{h}\begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \in \mathbb{R}^{N-1}.$$

The approximation of the coefficients of the rigidity matrix by the trapezoidal formula is exact, while the approximation of the mass matrix by the trapezoidal formula gives

$$\mathbf{E} = h \begin{bmatrix} 1 & 0 & 0 & & & & \\ 0 & 1 & 0 & \ddots & & \ddots & \\ 0 & 0 & 1 & & & & \\ & \ddots & & \ddots & & \ddots & \\ & & & & 1 & 0 & 0 \\ & \ddots & & \ddots & 0 & 1 & 0 \\ & & & & 0 & 0 & 1 \end{bmatrix} = h\, I_{\mathbb{R}^{N-1}}.$$

Using the the trapezoidal formula for the term $\int_0^1 \phi_N\, \phi_{N-1}$, the term u' disappears and the differential system is

$$\mathbf{E}\mathbf{z}'(t) = \mathbf{A}\mathbf{z}(t) + \mathbf{B}u(t), \quad \mathbf{E}\mathbf{z}(0) = \left((z_0, \phi_i)_{L^2}\right)_{1 \le i \le N-1}.$$

Here $\mathbf{E}$ can be either the exact mass matrix, or $h\, I_{\mathbb{R}^{N-1}}$.

4. Time integration scheme

A Backward Differentiation Formule (BDF) is used to solve the initial value problem

$$\mathbf{E}\mathbf{z}'(t) = \mathbf{A}\mathbf{z}(t) + \mathbf{B}u(t), \quad \mathbf{E}\mathbf{z}(0) = ((z_0, \phi_i)_{L^2})_{1 \le i \le N-1} \,.$$

The general BDF for a nonlinear differential equation $z' = f(z, t)$, $z(0) = z_0 = z^{(0)}$, can be written as

$$\sum_{k=0}^{s} a_k z^{(n+k)} = \Delta t \beta f(z^{(n+s)}, t^{n+s}), \quad a_s = 1,$$

where Δt denotes the step size and $t^n = n\Delta t$. The coefficients a_k and β are chosen so that the method achieves order s , which is the maximum possible. BDF methods are implicit and, as such, require the solution of nonlinear equations at each step (in our case the equation is linear).

Here we use the BDF of order 2

$$\mathbf{E}\left(\mathbf{z}^{n+2} - \frac{4}{3}\mathbf{z}^{n+1} + \frac{1}{3}\mathbf{z}^{n}\right) = \frac{2}{3}\Delta t \left(\mathbf{A}\mathbf{z}^{n+2} + \mathbf{B}u^{n+2}\right).$$

For $t^1 = \Delta t$, the solution can be calculated with an implicit Euler scheme

$$\mathbf{E}\left(\mathbf{z}^1 - \mathbf{z}^0\right) = \Delta t\left(\mathbf{A}\mathbf{z}^1 + \mathbf{B}u^1\right).$$

We solve

$$\left(\mathbf{E} - \Delta t\,\mathbf{A}\right)\mathbf{z}^1 = \mathbf{E}\,\mathbf{z}^0 + \Delta t\,\mathbf{z}^1 + \Delta t\,\mathbf{B}u^1,$$

by using a *LU* decomposition and with $\mathbf{z}^0$ as the FEM approximation of z_0.
For $t^2 = 2\Delta t$, we solve the system

$$\mathbf{E}\left(\mathbf{z}^2 - \frac{4}{3}\mathbf{z}^1 + \frac{1}{3}\mathbf{z}^0\right) = \frac{2}{3}\Delta t\left(\mathbf{A}\mathbf{z}^2 + \mathbf{B}u^2\right).$$

that is

$$\left(\mathbf{E} - \frac{2}{3}\Delta t\mathbf{A}\right)\mathbf{z}^2 = \mathbf{E}\left(\frac{4}{3}\mathbf{z}^1 - \frac{1}{3}\mathbf{z}^0\right) + \frac{2}{3}\Delta t\,\mathbf{B}u^2,$$

and so on.

5. Approximation of the normal derivative

In the estimation problem, if we measure the flux $\frac{\partial z}{\partial x}$ at the extremity $x = 0$ of the domain $[0, 1]$, we have to approximate it in the numerical experiments. We denote by $\partial_n^h z(0)$, or by $-\partial_x^h z(0)$, an approximation of $-\frac{\partial z}{\partial x}(0)$. The notation ∂_n^h refers to an approximate normal derivative (see the 2D case). The idea is to use the equation satisfied by z. When $z \in L^2(0, T; H^2(0, 1))$, we can write

$$\int_0^1 \frac{\partial^2 z}{\partial x^2}(x,t)\,\phi = -\frac{\partial z}{\partial x}(0)\,\phi(0) - \int_0^1 \frac{\partial z}{\partial x}(x,t)\,\frac{d\phi}{dx}\,dx \quad \forall \phi \in H^1_{\{1\}}(0,1).$$

Using the equation satisfied by z, we replace $\frac{\partial^2 z}{\partial x^2}(x,t)$ by $\frac{\partial z}{\partial t}(x,t)$. Thus we have

$$-\frac{\partial z}{\partial x}(0,t)\,\phi(0) = \frac{d}{dt}\,(z(t),\phi)_{L^2} + \int_0^1 \frac{\partial z}{\partial x}(x,t)\,\frac{d\phi}{dx}\,dx \quad \forall \phi \in H^1_{\{1\}}(0,1).$$

In particular, choosing $\phi = \phi_0$, we have

$$-\frac{\partial z}{\partial x}(0,t) = -\frac{\partial z}{\partial x}(0)\,\phi_0(0) = \frac{d}{dt}\,(z(t),\phi_0)_{L^2} + \int_0^1 \frac{\partial z}{\partial x}(x,t)\,\frac{d\phi_0}{dx}\,dx.$$

The approximation of the integral $(z(t),\phi_0)_{L^2}$ by a trapezoidal formula is zero. We set

$$-\partial_x^h z(0,t) = \int_0^1 \frac{\partial z}{\partial x}(x,t)\,\frac{d\phi_0}{dx}\,dx,$$

for the solution z to the (DWF).
Thus the variational approximation of $\frac{\partial z}{\partial x}(0,t)$ is

$$\frac{z(h,t) - z(0,t)}{h}.$$

But in 2D or even in 1D if we use another type of finite element method, the variational approximation of $\frac{\partial z}{\partial x}(0,t)$ may be different from the finite difference quotient.