Fokker-Plank equation

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Contents

Notation

This list is part of the notation we use throughout the text:

- $\langle X \rangle = \mathbb{E}[X]$ is the expected value of the random variable X.
- For $f, g \in H^1(\Omega)$, we define $\langle f, g \rangle = \int_\Omega f(x)g(x)\,dx$
- $\|f\|_{L^2}^2 = \int_\Omega \|f(x)\|^2\,dx$.

1 Introduction

Consider a particle of mass m immersed in a fluid [6]. The fluid applies a friction force on the particle which can be described by Stokes' law. In this simple model, the velocity of the equation can be modelled through the following Ordinary Differential Equation (ODE)

$$m\dot{v} + \alpha v = 0 \implies v(t) = v(0)\exp\left\{-\frac{\alpha}{m}t\right\} \overset{t\to\infty}{\to} 0. \tag{1}$$

However, for small values of m, thermal fluctuations may have a relevant effect on the particle's velocity. To simulate this effect, we include a random fluctuation force $F_f(t)$ in equation (1), leading to

$$m\dot{v} + \alpha v = F_f(t). \tag{2}$$

The randomness simplifies the modelling of all particle interactions. The *Langevin force* is given by the fluctuating force per unit of mass $\Gamma(t) = F_f(t)/m$. In average, we expect that the velocity is determined by (1). By this reason, we consider $\langle\Gamma(t)\rangle = 0$. Moreover, $\langle\Gamma(t)\Gamma(t')\rangle = q\delta(t - t')$.

The Stochastic Differential Equation (SDE) in (2) induces a distribution on the velocity, since it is a random variable. The corresponding probability density function (PDF) W is given by a Partial Differential Equation (PDF), called *Fokker-Planck* equation. Its simple form is given by

$$\frac{\partial W}{\partial t} = \frac{\alpha}{m}\frac{\partial(vW)}{\partial v} + \frac{\alpha}{m}\frac{kT}{m}\frac{\partial^2 W}{\partial v^2},$$

where $W(v, t)$ is the PDF of v at time t.

The general form of Fokker-Planck equation in one dimension is given by

$$\frac{\partial W}{\partial t}(x,t) = \left[-\sum_{i=1}^{N}\frac{\partial}{\partial x_i}D_i^{(1)}(x) + \sum_{i,j=1}^{N}\frac{\partial^2}{\partial x_i \partial x_j}D_{ij}^{(2)}(x)\right]W(x,t), \tag{3}$$

where $D^{(1)}$ is the drift coefficient and $D^{(2)}$ is the diffusion coefficient. Consider the SDE

$$dX_t = -\nabla G(x)\,dt + \sqrt{2\nu}dB_t.$$

The PDF ρ of the process $\{X_t\}_{t\in\mathbb{R}_+}$ defined for $(x,t) \in \Omega \times \mathbb{R}_+$ is the solution to

$$\rho_t(x,t) = \nabla \cdot J(x,t),$$

where

$$J(x,t) = \nu \nabla \rho(x,t) + \rho(x,t)\nabla G(x)$$

is the probability current. To guarantee that for all $t \geq 0$,

$$\int_\Omega \rho(x,t)\,dx = \int_\Omega \rho_0(x)\,dx,$$

where $\rho_0(x) = \rho(x,0)$, the probability current is subject to the boundary condition

$$J(x,t) \cdot \vec{n} = 0 \text{ on } \partial\Omega \times \mathbb{R}_+.$$

This corresponds to a particle being reflected after hitting the boundary of Ω.

The steady state of this equation is the solution to

$$\nabla \cdot J(x,t) = 0 \text{ in } \Omega \times \mathbb{R}_+,$$

subject to $J(x,t) = 0$ on $\partial\Omega \times \mathbb{R}_+$, when it does not depend on time. Let $\rho(x,t) = ce^{-G(x)/\nu}$, where c is a normalising constant given by the initial condition. Therefore,

$$J(x,t) = \nu\left(-\frac{\nabla G(x)}{\nu}\rho(x,t)\right) + \rho(x,t)\nabla G(x) = 0,$$

independent of t, which implies that the steady state ρ_∞ is

$$\rho_\infty(x) \propto e^{-G(x)/\nu}.$$

2 Well-posedness

We search for a solution $\rho \in W(0,T) = L^2(0,T;H^1(\Omega)) \cap H^1(0,t;(H^1(\Omega))^*)$ and

$$\langle \rho_t, \phi\rangle + \langle \nu\nabla\rho(t) + \rho(t)\nabla G, \nabla\phi\rangle + u(t)\langle \rho(t)\nabla\alpha, \nabla\phi\rangle = 0, \forall \phi \in H^1(\Omega),$$

where integration by parts was applied. It is assumed that

$$G, \alpha \in W^{1,\infty}(\Omega) \cap W^{2,\max(2,n)}(\Omega).$$

With that in mind, is possible to prove that for every $u \in L^2(0,T)$ and $\rho_0 \in L^2(\Omega)$, there exists an unique solution to Fokker-Planck equation.

Moreover the solution satisfies

(i) For every $t \in [0,T]$, we have that $\langle \rho(t) - \rho_0, 1_\Omega \rangle = 0$.

(ii) If $\rho_0 \geq 0$ almost everywhere on Ω, then $\rho(x,t) \geq 0$ for all $t > 0$ and almost all $x \in \Omega$.

Some additional references:

- [3]: covers the existence and the uniqueness of a class of Fokker-Planck equations with coefficients in Sobolov spaces $W^{1,p}$.
- [5]: existence of steady state of Fokker-Planck equation in $\Omega \subseteq \mathbb{R}^n$.

3 Optimal control problem

To accelerate the convergence to the steady state as $t \to \infty$ [2], we include a control function $u : \mathbb{R}_+ \to \mathbb{R}$ which acts in the space according to the control shape function $\alpha : \Omega \to \mathbb{R}$, which satisfies $\nabla\alpha \cdot \vec{n} = 0$ on $\partial\Omega$. Therefore, we substitute the potential G to

$$V(x,t) = G(x) + u(t)\alpha(x),$$

Notice that with the format of α, the boundary condition is unchangeable

$$0 = (\nu\nabla\rho + \rho\nabla V) \cdot \vec{n} = (\nu\nabla\rho + \rho\nabla G) \cdot \vec{n} + \cancel{u\, \rho(\nabla\alpha) \cdot \vec{n}}.$$

Define $y = \rho - \rho_\infty$. We want that $\|y\|_{L^2}$ converges to 0 the faster as possible. With the change of variables, the problem turns to

$$\begin{aligned} y_t &= \nabla \cdot [\nu\nabla(y + \rho_\infty) + (y + \rho_\infty)\nabla V] \\ &= \nabla \cdot (\nu\nabla y + y\nabla V + u\nabla\alpha\rho_\infty) + \cancel{\nabla \cdot (\nu\nabla\rho_\infty + \rho_\infty\nabla G)} \\ &= \nabla \cdot (\nu\nabla y + y\nabla G) + u\nabla \cdot (y\nabla\alpha) + u\nabla \cdot (\rho_\infty\nabla\alpha), \end{aligned}$$

in $\Omega \times \mathbb{R}_+$ subject to

$$0 = (\nu\nabla(y + \rho_\infty) + (y + \rho_\infty)\nabla G) \cdot \vec{n} = (\nu\nabla y + y\nabla G) \cdot \vec{n} \text{ on } \partial\Omega \times \mathbb{R}_+$$

and $y(x, 0) = \rho_0(x) - \rho_\infty(x)$ in Ω. We can write the above problem as a bilinear abstract control system

$$\dot{y} = \mathcal{A}y + u\mathcal{N}y + \mathcal{B}u, \quad y(0) = y_0,$$

where we define the operators

$$\begin{aligned} \mathcal{A} : \mathcal{D}(\mathcal{A}) \to L^2(\Omega), \quad & \mathcal{D}(\mathcal{A}) = \{\phi \in H^2(\Omega) : (\nu\nabla\phi + \phi\nabla G) \cdot \vec{n} = 0 \text{ on } \partial\Omega\} \\ \mathcal{A}\phi = \nu\Delta\phi + \nabla \cdot (\phi\nabla G), & \end{aligned}$$

and

$$\mathcal{N} : H^1(\Omega) \to L^2(\Omega), \quad \mathcal{N}\rho = \nabla \cdot (\rho\nabla\alpha).$$

The adjoint operators are well-defined and given by

$$\mathcal{A}^*\varphi = \nu\Delta\varphi - \nabla G \cdot \nabla\varphi, (\nu\nabla\varphi) \cdot \vec{n} = 0 \text{ on } \partial\Omega$$

and

$$\mathcal{N}^*\varphi = -\nabla\varphi \cdot \nabla\alpha.$$

We look at the functional cost

$$\mathcal{J}(y, u) = \frac{1}{2}\int_0^\infty \langle y, \mathcal{M}y\rangle + |u|^2 \, dt.$$

Disregarding the bilinear expression $\mathcal{N}$, we get to the linear optimal control problem

$$\min \; J(y, u) \tag{4}$$
$$\text{s.t. } \dot{y} = \mathcal{A}y + \mathcal{B}u, \tag{5}$$
$$y(0) = y_0, \tag{6}$$

where $\mathcal{A}$ incorporates the boundary condition $\nabla \cdot (\nu\nabla y + y\nabla G) = 0$.

4 Ricatti-based feedback control

The Ricatti equation associated to the optimal control problem in (4), that is, the linearised version of the system with the term uNy dropped is

$$\mathcal{A}^*\Pi + \Pi\mathcal{A} - \Pi\mathcal{B}\mathcal{B}^*\Pi + \mathcal{M} = 0.$$

The feedback optimal control is given by $u = -\mathcal{B}^*\Pi y$.

Another strategy is based on the solution Γ to a Lyapunov equation

$$\mathcal{A}^*\Upsilon + \Upsilon\mathcal{A} + 2\mu I = 0,$$

for a properly chosen parameter $\mu > 0$.

5 Methods for solving Fokker-Planck equation

The equation we want to solve is

$$y_t = \nabla \cdot (\nu\nabla y + y\nabla G + uy\nabla\alpha + u\rho_\infty\nabla\alpha),$$

subject to $(\nu\nabla y + y\nabla G) \cdot \vec{n} = 0$ on the boundary and $y = \rho_0 - \rho_\infty$ as initial condition. In the weak formulation, for every $\phi \in H^1(\Omega)$, we have

$$\langle y_t, \phi\rangle = -\langle \nu\nabla y + y\nabla G, \nabla\phi\rangle - u(t)\langle\nabla\alpha y, \nabla\phi\rangle - u(t)\langle\nabla\alpha\rho_\infty, \nabla\phi\rangle.$$

(a) Spectral-Legendre method

(b) Finite elements

(c) Finite differences: [4] build a scheme where positivity and conservation of mass are maintained.

(d) Collocation methods, which is a spectral method in the strong sense

5.1 Spectral-Legendre method

Let us consider the one-dimensional case $\Omega = [a, b]$. To simplify future calculations, we consider the variable

$$\tilde{y}(x,t) = y\left(\left(\frac{b-a}{2}\right)x + \left(\frac{a+b}{2}\right), t\right), \forall x \in [-1,1], t > 0.$$

We do the same for G, α and ρ_∞. For sake of conciseness, we drop the $\sim$ for now. The weak formulation turns to

$$\langle y_t, \phi \rangle = -\left(\frac{2}{b-a}\right)^2 \langle \nu y_x + y\dot{G} + uy\dot{\alpha} + u\rho_\infty\dot{\alpha}, \dot{\phi} \rangle.$$

Consider the space

$$X_n = \{\phi \in P_n : \nu\dot{\phi}(\pm 1) + \phi(\pm 1)\dot{G}(\pm 1) = 0\},$$

where P_n is the space of polynomials with degree up to n. Notice that $\dim(X_n) = n-1$. Let $\{\phi_i\}_{i=0}^{n-2}$ be a basis for X_n and write

$$y(x,t) \approx \sum_{j=0}^{n-2} y_j(t)\phi_j(x).$$

Considering the set of test equal to the trial functions, we get in the following formulation

$$\sum_{j=0}^{n-2} \dot{y}_j(t)\langle \phi_j, \phi_i \rangle = -\left(\frac{2}{b-a}\right)^2 \sum_{j=0}^{n-2} y_j(t)\left(\nu\langle \dot{\phi}_j, \dot{\phi}_i \rangle + \langle \dot{G}\phi_j, \dot{\phi}_i \rangle + u(t)\langle \dot{\alpha}\phi_j, \dot{\phi}_i \rangle\right)$$
$$+ u(t)\langle \dot{\alpha}\rho_\infty, \dot{\phi}_i \rangle,$$

which can be rewritten as a system of ODEs

$$\Phi\dot{y}(t) = -\left(\frac{2}{b-a}\right)^2 (\Lambda + \Theta^1 + u(t)\Theta^2)y(t) - \left(\frac{2}{b-a}\right)^2 u(t)v.$$

Following the suggestion from $[7, p.7]$, we consider

$$\phi_k(x) = L_k(x) + \alpha_k L_{k+1}(x) + \beta_k L_{k+2}(x),$$

where L_k is the Legendre polynomial of degree k and the coefficients are chosen to satisfy the boundary conditions. Therefore, we want that

$$\begin{aligned}&\nu(\dot{L}_k(\pm 1) + \alpha_k \dot{L}_{k+1}(\pm 1) + \beta_k \dot{L}_{k+2}(\pm 1))\\ &+ \dot{G}(\pm 1)(L_k(\pm 1) + \alpha_k L_{k+1}(\pm 1) + \beta_k L_{k+2}(\pm 1)) = 0.\end{aligned}$$

which can be written in matrix formulation

$$\begin{bmatrix} \nu(k+1)(k+2) - 2g_- & -\nu(k+2)(k+3) + 2g_- \\ \nu(k+1)(k+2) + 2g_+ & \nu(k+2)(k+3) + 2g_+ \end{bmatrix} \begin{bmatrix} \alpha_k \\ \beta_k \end{bmatrix} = \begin{bmatrix} \nu k(k+1) - 2g_- \\ -\nu k(k+1) - 2g_+ \end{bmatrix},$$

where $g_\pm = \dot{G}(\pm 1)$ and the system is numerically solved.

Let's now pre-calculate the matrices in terms of the legendre polynomials.

$$\begin{aligned}\Phi_{ij} = \langle \phi_i, \phi_j \rangle &= \langle L_i, L_j \rangle + \alpha_i \langle L_{i+1}, L_j \rangle + \beta_i \langle L_{i+2}, L_j \rangle \\ &+ \alpha_j \langle L_i, L_{j+1} \rangle + \alpha_i \alpha_j \langle L_{i+1}, L_{j+1} \rangle + \beta_i \alpha_j \langle L_{i+2}, L_{j+1} \rangle \\ &+ \beta_j \langle L_i, L_{j+2} \rangle + \alpha_i \beta_j \langle L_{i+1}, L_{j+2} \rangle + \beta_i \beta_j \langle L_{i+2}, L_{j+2} \rangle \\ &= 2\frac{\delta_{ij}}{2i+1} + 2\alpha_i \frac{\delta_{i+1,j}}{2(i+1)+1} + \beta_i \frac{\delta_{i+2,j}}{2(i+2)+1} \\ &= 2\alpha_j \frac{\delta_{i,j+1}}{2i+1} + 2\alpha_i \alpha_j \frac{\delta_{ij}}{2(i+1)+1} + 2\beta_i \alpha_j \frac{\delta_{i+1,j}}{2(i+2)+1} \\ &= 2\beta_j \frac{\delta_{i,j+2}}{2i+1} + 2\alpha_i \beta_j \frac{\delta_{i,j+1}}{2(i+1)+1} + 2\beta_i \beta_j \frac{\delta_{ij}}{2(i+2)+1}\end{aligned}$$

$$\begin{aligned}\Lambda_{ij} = \nu \langle \dot{\phi}_i, \dot{\phi}_j \rangle &= \nu [\langle \dot{L}_i, \dot{L}_j \rangle + \alpha_i \langle \dot{L}_{i+1}, \dot{L}_j \rangle + \beta_i \langle \dot{L}_{i+2}, \dot{L}_j \rangle \\ &+ \alpha_j \langle \dot{L}_i, \dot{L}_{j+1} \rangle + \alpha_i \alpha_j \langle \dot{L}_{i+1}, \dot{L}_{j+1} \rangle + \beta_i \alpha_j \langle \dot{L}_{i+2}, \dot{L}_{j+1} \rangle \\ &+ \beta_j \langle \dot{L}_i, \dot{L}_{j+2} \rangle + \alpha_i \beta_j \langle \dot{L}_{i+1}, \dot{L}_{j+2} \rangle + \beta_i \beta_j \langle \dot{L}_{i+2}, \dot{L}_{j+2} \rangle],\end{aligned}$$

where $\langle \dot{L}_i, \dot{L}_j \rangle = L_{\max(i,j)}(1)\dot{L}_{\min(i,j)}(1) - L_{\max(i,j)}(-1)\dot{L}_{\min(i,j)}(-1)$, integrating by parts and observing that Legendre polynomials are orthogonal to other polynomials with smaller degree. Therefore,

$$\langle \dot{L}_i, \dot{L}_j \rangle = \frac{1}{2} \min(i,j)(\min(i,j)+1) \left(1 + (-1)^{i+j}\right).$$

Finally, we calculate

$$\Theta^1_{ij} = \langle \dot{G}\phi_j, \dot{\phi}_i\rangle, \Theta^2_{ij} = \langle \dot{\alpha}\phi_j, \dot{\phi}_i\rangle \text{ and } v_i = \langle \dot{\alpha}\rho_\infty, \dot{\phi}_i\rangle$$

This is the method of solving the PDE. Before solving it, we need to compute the optimal control. For that, we have to discretise the operators $\mathcal{A}, \mathcal{B}$ and $\mathcal{M}$:

The discretised versions are

$$A_{ij} = \langle \mathcal{A}\phi_j, \phi_i\rangle = -\left(\frac{2}{b-a}\right)^2 \langle \nu\dot{\phi}_j + \dot{G}\phi_j, \dot{\phi}_i\rangle \implies A = -\left(\frac{2}{b-a}\right)^2 (\Lambda + \Theta^1)$$

and

$$B_i = \langle \mathcal{B}\cdot 1, \phi_i\rangle = -\left(\frac{2}{b-a}\right)^2 \langle \rho_\infty \dot{\alpha}, \dot{\phi}_i\rangle \implies B = -\left(\frac{2}{b-a}\right)^2 v.$$

With that in mind, we have to solve the discrete Ricatti equation

$$A^T\Pi + \Pi A + \Pi B B^T \Pi + M = 0.$$

with $u(t) = -B^T\Pi y(t)$. With this feedback, we solve

$$\begin{aligned}\Phi\dot{y} &= \left(A + \left(\frac{2}{b-a}\right)^2 B^T\Pi y(t)\Theta^2\right) y(t) - BB^T\Pi y(t) \\ &= \left(A - BB^T\Pi + \left(\frac{2}{b-a}\right)^2 B^T\Pi y(t)\Theta^2\right) y(t).\end{aligned}$$

After solving this system, we have to come back to the original coordinate system.

Remark 5.1.1. *Notice that $M_{ij} = \langle \mathcal{M}\phi_j, \phi_i\rangle$. For instance, if $\mathcal{M}$ is the identity operator, we have $M = \Phi$.*

5.2 Finite elements

The second method we consider is the finite elements method. In this case, we also consider the weak formulation and look for a basis $\{\phi_i\}_{i=0}^n$. In the interval $[a, b]$, set the *node points* $a = x_0 < \cdots < x_n = b$. The *elements* are the sub-intervals $[x_i, x_{i+1}]$ with $x_{i+1} - x_i = h$, for $i = 0, \ldots, n-1$. We set the values $\phi_k(x_i) = \delta_{ik}$ and for each element a linear function. D efine the function

$$\phi(x) = \begin{cases} x/h, & \text{if } x \in [0,h] \\ 2 - x/h, & \text{if } x \in [h,2h] \\ 0, & \text{otherwise} \end{cases}$$

and $\phi_k(x) = \phi(x - x_{k-1})$, for $k = 0, \ldots, n$ and $x \in [a,b]$, setting $x_{-1} = a - h$. With that in mind, it remain to calculate the same matrices as the previous method. Here, it is not necessary to rescale the function to the interval $[-1,1]$. Then, if $i \geq j$,

$$\begin{aligned} \Phi_{ij} = \langle \phi_i, \phi_j \rangle &= \int_a^b \phi(x - x_{i-1})\phi(x - x_{j-1})\,dx \\ &= \int_0^{2h} \phi(y)\phi(y + x_{i-1} - x_{j-1})\,dy \\ &= \int_0^h \frac{y}{h}\phi(y + (i-j)h)\,dy + \int_h^{2h} \left(2 - \frac{y}{h}\right)\phi(y + (i-j)h)\,dy \end{aligned}$$

Notice that for $i - j \geq 2$, both integrals are 0, since $\phi(y + 2h) = 0$ for $y \geq 0$. If $i = j+1$, the second integral is zero, while the first is

$$\int_0^h \frac{y}{h}\left(2 - \frac{y+h}{h}\right)\,dy = h\int_0^1 z\,(1-z)\,dz = \frac{h}{6}.$$

If $n > i = j > 0$, the integrals are

$$\int_0^h \frac{y^2}{h^2}\,dy = \frac{h}{3}, \quad \int_h^{2h} \left(2 - \frac{y}{h}\right)^2 dy = h\int_0^1 z^2\,dz = \frac{h}{3},$$

which implies $\Phi_{ii} = 2h/3$ and, finally, $\Phi_{00} = \Phi_{nn} = h/3$. For $i < j$, $\Phi_{ij} = \Phi_{ji}$. For calculating Λ, for $i \geq j$,

$$\begin{aligned} \Lambda_{ij} = \nu\langle \dot{\phi}_i, \dot{\phi}_j \rangle &= \int_a^b \dot{\phi}(x - x_{i-1})\dot{\phi}(x - x_{j-1})\,dx \\ &= \int_0^{2h} \dot{\phi}(y)\dot{\phi}(y + x_{i-1} - x_{j-1})\,dx \\ &= \frac{1}{h}\int_0^h \dot{\phi}(y + (i-j)h)\,dy - \frac{1}{h}\int_h^{2h} \dot{\phi}(y + (i-j)h)\,dy. \end{aligned}$$

If $i-j \geq 2$, both integrals are 0. If $i=j+1$, the second integral vanishes, while the first is

$$\int_0^h -\frac{1}{h}\,dx = -1 \implies \Lambda_{ij} = -\frac{\nu}{h}.$$

If $i=j$, the first integral is 1, while the second is -1, implying that $\Lambda_{ii} = 2\nu/h$. Finally, if $i<j$, then $\Lambda_{ij} = \Lambda_{ji}$.

The other three matrices have some simplification, but need numerical integration.

$$\begin{aligned}
\Theta^1_{i,i+1} = \langle \dot{G}\phi_{i+1}, \dot{\phi}_i\rangle &= \int_h^{2h} \dot{G}(y+x_{i-1})\phi(y-h)\dot{\phi}(y)\,dy \\
&= -\frac{1}{h}\int_h^{2h} \dot{G}(y+(a+(i-1)h))\left(\frac{y-h}{h}\right)\,dy \\
&= -\frac{1}{h}\left[\int_h^{2h} \dot{G}(y+a+ih-h)\frac{y}{h}\,dy - G(a+ih+h) + G(a+ih)\right] \\
&= -\frac{1}{h}\left[G(a+(i+1)h) - \frac{1}{h}\int_h^{2h} G(y+a+ih-h)\,dy\right] \\
&= -\frac{1}{h}\left[G(a+(i+1)h) - \frac{1}{h}\int_{a+ih}^{a+(i+1)h} G(y)\,dy\right],
\end{aligned}$$

for $i=0,\ldots,n-1$.

$$\begin{aligned}
\Theta^1_{i,i-1} = \langle \dot{G}\phi_{i-1}, \dot{\phi}_i\rangle &= \int_0^{h} \dot{G}(y+x_{i-1})\phi(y+h)\dot{\phi}(y)\,dy \\
&= \frac{1}{h}\int_0^{h} \dot{G}(y+(a+(i-1)h))\left(2-\frac{y+h}{h}\right)\,dy \\
&= -\frac{1}{h}\left[\int_0^{h} \dot{G}(y+a+ih-h)\frac{y}{h}\,dy - G(a+ih) + G(a+(i-1)h)\right] \\
&= -\frac{1}{h}\left[G(a+(i-1)h) - \frac{1}{h}\int_0^{h} G(y+a+ih-h)\,dy\right] \\
&= -\frac{1}{h}\left[G(a+(i-1)h) - \frac{1}{h}\int_{a+(i-1)h}^{a+ih} G(y)\,dy\right],
\end{aligned}$$

for $i = 1, \ldots, n$

$$\begin{aligned}
\Theta^1_{i,i} = \langle \dot{G}\phi_i, \dot{\phi}_i \rangle &= \int_0^{2h} \dot{G}(y + x_{i-1})\phi(y)\dot{\phi}(y)\,dy \\
&= \frac{1}{h}\left[\int_0^h \dot{G}(y + x_{i-1})\left(\frac{y}{h}\right)\,dy - \int_h^{2h} \dot{G}(y + x_{i-1})\left(2 - \frac{y}{h}\right)\,dy\right] \\
&= \frac{1}{h}\left[\int_0^{2h} \dot{G}(y + x_{i-1})\left(\frac{y}{h}\right)\,dy - 2(G(x_{i+1}) - G(x_i))\right] \\
&= \frac{1}{h}\left[2G(a + ih) - \frac{1}{h}\int_{a+(i-1)h}^{a+(i+1)h} G(y)\,dy\right],
\end{aligned}$$

for $i = 1, \ldots, n-1$. For $i = 0$, we only have the decreasing part.

$$\Theta^1_{00} = -\frac{1}{h}\int_h^{2h} \dot{G}(y + (a-h))\left(2 - \frac{y}{h}\right)\,dy = \frac{1}{h}\left[G(a) - \frac{1}{h}\int_a^{a+h} G(y)\,dy\right].$$

On the other hand, for $i = n$, we only have the increasing part.

$$\Theta^1_{nn} = \frac{1}{h}\int_0^h \dot{G}(y + (b-h))\left(\frac{y}{h}\right)\,dy = \frac{1}{h}\left[G(b) - \frac{1}{h}\int_{b-h}^{b} G(y)\,dy\right].$$

On the other hand, for $i = n$, we only have the increasing part. If $i - j \geq 2$, we have $\Theta^1_{ij} = 0$. Notice that Θ^2 has similar calculations substituting G by α.

Finally, we calculate the vector v. For $i = 1, \ldots, n-1$,

$$v_i = \langle \dot{\alpha}\rho_\infty, \dot{\phi}_i \rangle = \frac{1}{h}\left[\int_{a+(i-1)h}^{a+ih} \dot{\alpha}(y)\rho_\infty(y)\,dy - \int_{a+ih}^{a+(i+1)h} \dot{\alpha}(y)\rho_\infty(y)\,dy\right]$$

and

$$v_0 = -\frac{1}{h}\int_a^{a+h} \dot{\alpha}(y)\rho_\infty(y)\,dy, v_n = \frac{1}{h}\int_{b-h}^{b} \dot{\alpha}(y)\rho_\infty(y)\,dy.$$

The discrete matrices A, B can be obtained from the same manner. Besides that, we need to consider the boundary condition $\nu y_x + yG_x = 0$. Therefore,

$$\sum_{j=0}^{n} y_j(t)\left[\nu\dot{\phi}_j(x) + \dot{G}(x)\phi_j(x)\right] = 0, x = a, b, t \geq 0,$$

which defines to linear conditions,

$$y_0(t)\left[-\nu/h+\dot{G}(a)\right]+y_1(t)\left[\nu/h\right]=0$$
$$y_{n-1}(t)\left[-\nu/h\right]+y_n(t)\left[\nu/h+\dot{G}(b)\right]=0.$$

So we can write $y_0(t)=\nu y_1(t)/(\nu-h\dot{G}(a))$ and $y_n(t)=\nu y_{n-1}(t)/(\nu+h\dot{G}(b))$. This tells us that we can decrease the system of EDOs in two variables.

6 Optimality conditions

From now on, we consider the following optimal control problem:

$$\min_u J(\rho,u):=\frac{1}{2}\int_0^T \alpha_Q\|\rho-\rho_Q\|^2_{L^2(\Omega)}+\gamma|u(t)|^2+2\beta u(t)\,dt+\alpha_\Omega\|\rho(\cdot,T)-\rho_\Omega\|^2_{L^2(\Omega)} \tag{7}$$

$$\text{s.t. } \partial_t\rho(x,t)-\nabla\cdot(\nu\nabla\rho(x,t)+\rho(x,t)W[u(t)]),(x,t)\in\Omega\times(0,T), \tag{8}$$
$$\rho(x,0)=\rho_0(x),x\in\Omega \tag{9}$$
$$(\nu\nabla\rho(x,t)+\rho(x,t)W[u(t)])\cdot\vec{n}=0,(x,t)\in\partial\Omega\times(0,T), \tag{10}$$

for a fixed time T, a bounded set $\Omega\subseteq\mathbb{R}^n$ and $W[u(t)]=c(x)+u(t)b(x)$, where $b,c\in L^\infty(\Omega;\mathbb{R}^n)$ such that $\nabla b\cdot\vec{n}=0$ on the boundary and $u\in L^\infty(0,T)$. Moreover, we assume that $\rho_0\in L^1(\Omega)$. The weak formulation of the PDE is given by

$$\int_\Omega \partial_t\rho(x,t)\phi(x)\,dx=-\int_\Omega(\nu\nabla\rho(x,t)+\rho(x,t)W[u(t)])\cdot\nabla\phi(x)\,dx, \tag{11}$$

after integrating by parts.

We first discretise the PDE through the spectral method. Therefore, we set

$$\rho(x,t)=\sum_{i=0}^{N-2}\rho_j(t)\phi_j(x), \tag{12}$$

where $\{\phi_j\}_{j=0}^{N-2}$ is a basis of functions for a pre-specified set of functions.

Substituting the approximation in (12) to the weak formulation in (12) we get

$$\sum_{j=0}^{N-2} \rho_j(t) \int_\Omega \phi_j(x)\phi(x)\,dx = -\sum_{j=0}^{N-2} \rho_j(t) \int_\Omega (\nu \nabla \phi_j(x) + W[u(t)]\phi_j(x)) \cdot \nabla \phi(x)\,dx.$$

The Spectral Galerkin method chooses the test functions to be the sabe as the trials, leading to, for $i = 0, \ldots, N-2$.

$$\sum_{j=0}^{N-2} \rho_j(t) \int_\Omega \phi_j(x)\phi_i(x)\,dx = -\sum_{j=0}^{N-2} \rho_j(t) \int_\Omega (\nu \nabla \phi_j(x) + W[u(t)]\phi_j(x)) \cdot \nabla \phi_i(x)\,dx.$$

Define the matrices

$$\begin{aligned} \Phi_{ij} &= \int_\Omega \phi_j(x)\phi_i(x)\,dx \\ \Lambda_{ij} &= \int_\Omega \nu \nabla \phi_j(x) \cdot \nabla \phi_i(x)\,dx \\ B_{ij} &= \int_\Omega \phi_j(x) b(x) \cdot \nabla \phi_i(x)\,dx \\ C_{ij} &= \int_\Omega \phi_j(x) c(x) \cdot \nabla \phi_i(x)\,dx, \end{aligned}$$

which allows us to rewrite the discrete version of the PDE in a system of ODEs as

$$\Phi \dot{\underline{\rho}}(t) = -(\Lambda + C + u(t)B)\underline{\rho}(t), t \in (0, T)$$

where $\underline{\rho} = (\rho_0(t), \rho_1(t), \ldots, \rho_{n-2}(t)) \in W^{1,\infty}([0,T]; \mathbb{R}^{N-1})$. The next step is to consider the discrete version of the cost functional:

$$\begin{aligned} &\frac{1}{2} \int_0^T \gamma |u(t)|^2 + 2\beta u(t) \\ &\qquad + \alpha_Q \sum_{i=0}^{N-2} \sum_{j=0}^{N-2} (\rho_i(t) - \rho_{Q,i}(t))(\rho_j(t) - \rho_{Q,j}(t)) \int_\Omega \phi_i(x)\phi_j(x)\,dx\,dt \\ &\qquad + \alpha_\Omega \sum_{i=0}^{N-2} \sum_{j=0}^{N-2} (\rho_i(T) - \rho_{\Omega,i})(\rho_j(T) - \rho_{\Omega,j}) \int_\Omega \phi_i(x)\phi_j(x)\,dx \\ = &\frac{1}{2} \int_0^T \gamma |u(t)|^2 + 2\beta u(t) \\ &\qquad + \alpha_Q (\underline{\rho}(t) - \underline{\rho}_Q(t))^T \Phi (\underline{\rho}(t) - \underline{\rho}_Q(t))\,dt + \alpha_\Omega (\underline{\rho}(T) - \underline{\rho}_\Omega)^T \Phi (\underline{\rho}(T) - \underline{\rho}_\Omega), \end{aligned}$$

where $\underline{\rho}_Q$ and $\underline{\rho}_\Omega$ are the coefficients of the spectral representation of ρ_Q and ρ_Ω. We also define $\underline{\rho}_0$ as the coefficients of the spectral representation of ρ_0. Just as a reminder, they are calculated through the system of equations

$$\sum_{j=0}^{N-2} \rho_j(0) \int_\Omega \phi_j(x)\phi_i(x)\, dx = \int_\Omega \rho_0(x)\phi_i(x), i = 0, \dots, N-2.$$

Therefore, the finite-dimension optimal control problem is given by

$$\min_u \frac{1}{2} \int_0^T \gamma |u(t)|^2 + 2\beta u(t) + \alpha_Q (\underline{\rho}(t) - \underline{\rho}_Q(t))^T \Phi (\underline{\rho}(t) - \underline{\rho}_Q(t))\, dt \tag{13}$$

$$+ \alpha_\Omega (\underline{\rho}(T) - \underline{\rho}_\Omega)^T \Phi (\underline{\rho}(T) - \underline{\rho}_\Omega), \tag{14}$$

$$\text{s.t. } \dot{\underline{\rho}}(t) = -\Phi^{-1}(\Lambda + C + u(t)B)\underline{\rho}(t), t \in (0,T), \tag{15}$$

$$\underline{\rho}(0) = \underline{\rho}_0, \tag{16}$$

where the basis of functions are chosen to satisfy the boundary conditions.

Let $q \in W^{1,\infty}([0,T]; R^{N-2})$. The Hamiltonian of the above problem is given by

$$H(\rho, q, t) = -\underline{q}^T(t)\Phi^{-1}(\Lambda + C + u(t)B)\underline{\rho}(t) + \frac{1}{2}\alpha_Q \|\underline{\rho}(t) - \underline{\rho}_Q(t)\|_\Phi + \frac{1}{2}\gamma u(t)^2 + \beta u(t),$$

where q satisfies the adjoint equation

$$\dot{q} = -H_{\underline{\rho}} = (\Lambda + C + uB)^T \Phi^{-1} \underline{q} - \alpha_Q \Phi (\underline{\rho}(t) - \underline{\rho}_Q(t))$$
$$q(T) = \alpha_\Omega \Phi (\underline{\rho}(T) - \underline{\rho}_\Omega).$$

Finally, the optimal solution solves for each $t \in (0,T)$,

$$u^*(t) = \arg\min \left\{ -u(t) q^T(t) \Phi^{-1} B \underline{\rho} + \gamma u(t)^2/2 + \beta u(t) \right\},$$

which is given by

$$u^*(t) = (q^T \Phi^{-1} B \underline{\rho} - \beta)/\gamma.$$

Going back to the infinite dimensional optimal control problem in (7), [1] derives the adjoint equation for the *adjoint state* p associated with (ρ, u), which in the weak formulation is written as

$$\int_\Omega (-\partial_t p\phi + \nu\nabla p\cdot\nabla\phi + (W[u]\cdot\nabla p)\phi)\; dx = \alpha_Q \int_\Omega (\rho-\rho_Q)\phi\, dx,$$

with final time $p(x,T)=\alpha_\Omega(\rho(x,T)-\rho_\Omega)$ in Ω and $\partial_N p = 0$ on $\partial\Omega$.

The optimal solution is given by

$$u^*(t) = \left(\int_\Omega \rho(x,t)b(x)\nabla p(x,t)\, dx - \beta\right)/\gamma$$

Using the spectral approximation, we get

$$p(x,t) = \sum_{j=0}^{N-2} p_j(t)\phi_j(x),$$

and testing against the same basis of functions, we get

$$-\Phi\dot{\overline{p}} + (\Lambda + C^T + u(t)B^T)\overline{p} = \alpha_Q\Phi(\underline{\rho}-\underline{\rho}_Q),$$

with boundary condition $\Phi\underline{p}(T) = \alpha_\Omega\Phi(\underline{\rho}(T)-\underline{\rho}_\Omega)$. Notice that with $q=\Phi\underline{p}$, both adjoint equation derived from the discretised system and the discretisation of the adjoint equation from the infinite dimensional system agree. Moreover, the optimal control solution is also the same

$$u^*(t) = (\underline{p}^T B\underline{\rho}-\beta)/\gamma.$$

From now on we consider the problem in one dimension. Let ϕ_i be the Legendre polynomial of degree e rescaled so as to

$$\int_\Omega \phi_i^2(x)\, dx = 1,$$

then Φ is the $N+1$ identity matrix. Therefore, $\phi_i = \sqrt{j+1/2}L_i$ for each i, where L_i is the Legendre polynomial. Moreover,

$$\Lambda_{ij} = \nu\int_\Omega \phi_i'(x)\phi_j'(x)\, dx = \frac{\nu}{2}\sqrt{(i+1/2)(j+1/2)}\,\min(i,j)(\min(i,j)+1)\left(1+(-1)^{i+j}\right).$$

The matrices B and C are computed numerically. With respect of that, we solve the system for $\underline{\rho}$, and its respective adjoint state q. By the previous calculation, we now that $q = \underline{p}$ such that $\underline{p}$ is the coefficients of $p(x,t)$ in the Legendre basis. Finally, we make a change of variables to

$$\rho(x,t) = \sum_{j=0}^{N-2} \tilde{\rho}_j(t)\varphi_j(x),$$

such that $\varphi_j(x) = \phi_j(x) + \alpha_j \phi_{j+1}(x) + \beta_j \phi_{j+2}(x)$ is a polynomial that satisfies

$$\nu \nabla \varphi(\pm 1) + \varphi(\pm 1) c(\pm 1) = 0.$$

Notice we could do it with the same for $p(x,t)$ with

$$p(x,t) = \sum_{j=0}^{N-2} \tilde{p}_j(t)\psi_j(x),$$

such that $\psi_j(x) = \phi_j(x) + \alpha_{j,2}\phi_{j+1}(x) + \beta_{j,2}\phi_{j+2}(x)$ is a polynomial that satisfies

$$\psi_j'(\pm 1) = 0.$$

Let us calculate the coefficients for the basis satisfy the boundary conditions. For each k, the coefficients $D_{k,k+1} = \alpha_k$ and $D_{k,k+2} = \beta_k$ are determined through

$$\begin{bmatrix} \sqrt{k+3/2}(\nu(k+1)(k+2) - 2c_-) & \sqrt{k+5/2}(-\nu(k+2)(k+3) + 2c_-) \\ \sqrt{k+3/2}(\nu(k+1)(k+2) + 2c_+) & \sqrt{k+5/2}(\nu(k+2)(k+3) + 2c_+) \end{bmatrix} \begin{bmatrix} \alpha_k \\ \beta_k \end{bmatrix}$$
$$= \begin{bmatrix} \sqrt{k+1/2}(\nu k(k+1) - 2c_-) \\ \sqrt{k+1/2}(-\nu k(k+1) - 2c_+) \end{bmatrix}.$$

Then $\underline{\rho} = D^T \underline{\tilde{\rho}}$. Moreover we calculate the E matrix similarly with

$$\begin{bmatrix} -\sqrt{k+3/2}(k+1)(k+2) & \sqrt{k+5/2}(k+2)(k+3) \\ \sqrt{k+3/2}(k+1)(k+2) & \sqrt{k+5/2}(k+2)(k+3) \end{bmatrix} \begin{bmatrix} \alpha_{k,2} \\ \beta_{k,2} \end{bmatrix}$$
$$= \begin{bmatrix} -\sqrt{k+1/2}k(k+1) \\ -\sqrt{k+1/2}k(k+1) \end{bmatrix}.$$

Let $G(u)$ the trajectory associated with the control u and $F(G(u), u)$ for the finite dimensional optimal control problem in (13). The Gateaux derivative of F with respect to u in the direction of v is

$$F'(u)v = \int_0^T \left(\gamma u(t) + \beta - q^T(t)\Phi^{-1}B\underline{\rho}(t)\right) v(t)\, dt.$$

Consider a partition $\{t_i\}_{i=0}^m$ for the interval $[-1, 1]$. Denoting the vector of values of u at these points by $\underline{u} \in \mathbb{R}^{m+1}$, we can verify that, for every vector $v \in \mathbb{R}^{m+1}$,

$$F'(\underline{u})v = \frac{T}{m}\left[\sum_{i=0}^{m-1} \left(\gamma u(t_i) + \beta - q(t_i)^T B\underline{\rho}(t_i)\right)\frac{v_i}{2} + \left(\gamma u(t_{i+1}) + \beta - q(t_{i+1})^T B\underline{\rho}(t_{i+1})\right)\frac{v_{i+1}}{2}\right].$$

What remains to be seen is that we cannot use the same basis of functions for approximating ρ and p since they have different boundary conditions.

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