Semidiscrete finite element approximation of a fractional Fokker–Planck equation

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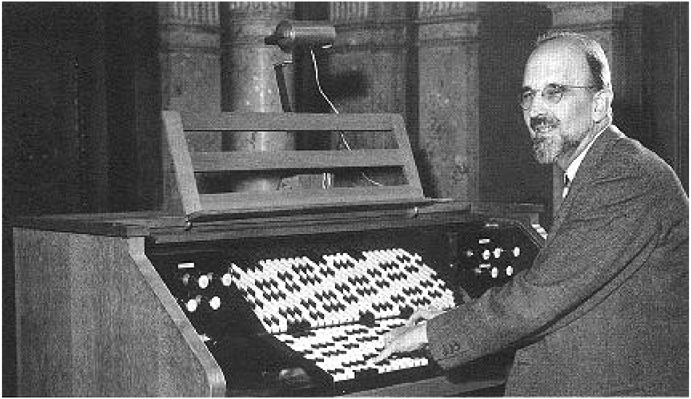
Adriaan Fokker 1887–1972

A. D. Fokker, Die mittlere Energie rotierender elektrischer Dipole im Strahlungsfeld, *Annalen der Physik* **348**, 810–820, 1914.



Max Karl Ernst Ludwig Planck 1858–1947

Über einen Satz der statistischen Dynamik und seine Erweiterung in der Quantentheorie, *Sitzungsber. Preuss. Akad. Wiss.* **24**, 1917.

Andrey Kolmogorov 1903–1987

Über die analytischen Methoden in der Wahrscheinlichkeitstheorie
Mathematische Annalen **104**, 1931. 448–451].

450 A. Kolmogoroff.

(132)
$$\int_a^b \frac{\partial}{\partial t} f(s, x, t, y)\, R(y)\, dy$$
$$= \int_a^b \left\{ -\frac{\partial}{\partial y}[A(t,y) f(s,x,t,y)] + \frac{\partial^2}{\partial y^2}[B^2(t,y) f(s,x,t,y)] \right\} R(y)\, dy;$$

da $R(y)$ bis auf die oben erwähnten Bedingungen willkürlich ist, schließt man leicht, daß für die (t, y)-Punkte mit nicht identisch verschwindender Determinante $D(t, y, u', z', u'', z'')$ auch *die zweite fundamentale Differentialgleichung*

(133)
$$\boxed{\frac{\partial}{\partial t} f(s,x,t,y) = -\frac{\partial}{\partial y}[A(t,y) f(s,x,t,y)] + \frac{\partial^2}{\partial y^2}[B^2(t,y) f(s,x,t,y)]}$$

gilt.

Fractional Fokker–Planck equation

$$\frac{\partial P}{\partial t} = \partial_t^{1-\alpha}\left(\kappa_\alpha \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\alpha}\frac{\partial}{\partial x}F(x)\right)P(x,t).$$

- Metzler, Klafter, Barkai, *Europhys. Lett.* **46**, 1999.
- Metzler, Barkai, Klafter, *Phys. Rev. Lett.* **82**, 1999.

$$\frac{\partial P}{\partial t} = \left(\kappa_\alpha \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\alpha}\frac{\partial}{\partial x}F(x,t)\right)\partial_t^{1-\alpha}P(x,t).$$

- Heinsalu, Patriarca, Goychuk, Hänggi, *Phys. Rev. Lett.* **99**, 2007.
- Henry, Langlands and Straka, *Phys. Rev. Lett.* **105**, 2010.

Outline

Lattice model

Initial-boundary value problem

Semidiscrete finite element method

Error estimate

Numerical experiments

Lattice model

Consider particles diffusing in 2D under the influence of a spatially-varying and time-dependent force.

Model using a continuous-time random walk on a lattice

$$\mathbf{r}_{jk} = (j\,\Delta x, k\,\Delta y).$$

Particle at $\mathbf{r}_{jk}$ waits a random time and then jumps to one of its four nearest neighbours with probabilities

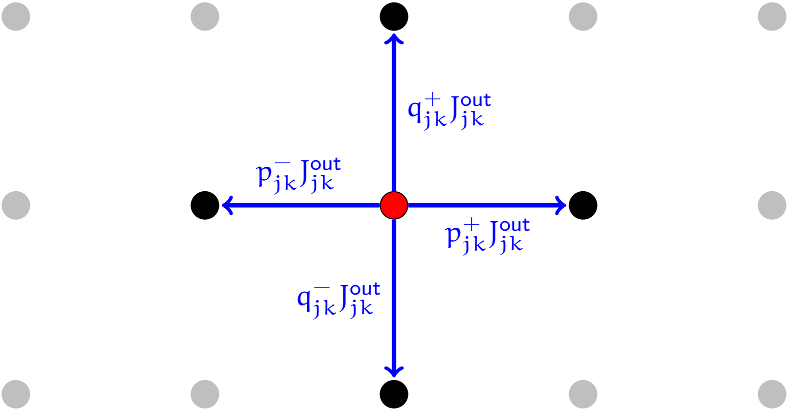
$$p^{\pm}_{jk}(t) = \mathcal{P}(\text{jump to } \mathbf{r}_{j\pm1,k} \text{ at time } t),$$
$$q^{\pm}_{jk}(t) = \mathcal{P}(\text{jump to } \mathbf{r}_{j,k\pm1} \text{ at time } t),$$

satisfying

$$p^{+}_{jk}(t) + p^{-}_{jk}(t) + q^{+}_{jk}(t) + q^{-}_{jk}(t) = 1.$$

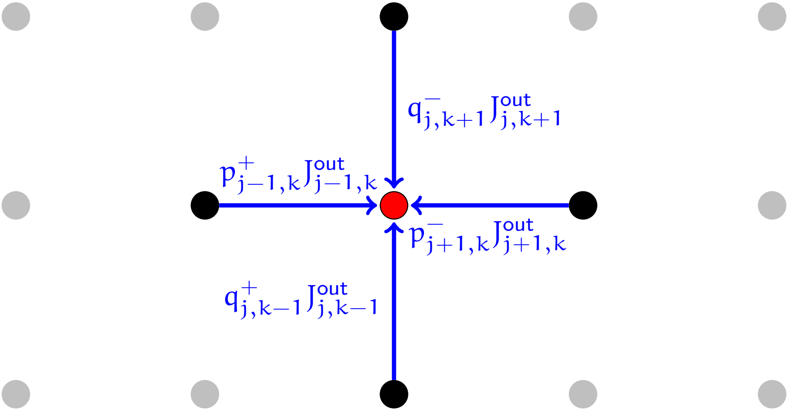
Loss flux

$J^{out}_{jk}(t)$ = total flux of particles leaving $\mathbf{r}_{jk}$



Gain flux

$J^{in}_{jk}(t)$ = total flux of particles arriving at $\mathbf{r}_{jk}$



Conservation of mass

Let

$$u_{jk}(t) = \text{concentration of particles at } \mathbf{r}_{jk},$$

then

$$\frac{du_{jk}}{dt} = J^{\text{in}}_{jk}(t) - J^{\text{out}}_{jk}(t)$$

with

$$J^{\text{in}}_{jk}(t) = p^{+}_{j-1,k}(t)\, J^{\text{out}}_{j-1,k}(t) + p^{-}_{j+1,k}(t)\, J^{\text{out}}_{j+1,k}(t) \\ + q^{+}_{j,k-1}(t)\, J^{\text{out}}_{j,k-1}(t) + q^{-}_{j,k+1}(t)\, J^{\text{out}}_{j,k+1}(t).$$

Waiting times

Let $\psi(t)$ denote the waiting-time probability density function:

$$\int_a^b \psi(t)\,dt$$

equals the probability that a particle jumps after waiting a time t in the range $a \leqslant t \leqslant b$.

Loss flux at time t due to

- particles originally at $\mathbf{r}_{jk}$ that waited time t to leave, plus
- particles that arrived at $\mathbf{r}_{jk}$ at an intervening time s and waited a time $t - s$ to leave.

Thus,

$$J_{jk}^{\mathrm{out}}(t) = \psi(t)u_{jk}(0) + \int_0^t \psi(t-s)J_{jk}^{\mathrm{in}}(s)\,ds.$$

Laplace transform

Notation:

$$\hat{f}(z) = (\mathcal{L}f)(z) = \int_0^\infty e^{-zt} f(t)\, dt, \quad \Re z > 0.$$

Since

$$\frac{du_{jk}}{dt} = J_{jk}^{\text{in}}(t) - J_{jk}^{\text{out}}(t).$$

we have

$$z\hat{u}_{jk}(z) - u_{jk}(0) = \widehat{J_{jk}^{\text{in}}}(t) - \widehat{J_{jk}^{\text{out}}}(z),$$

and since

$$J_{jk}^{\text{out}}(t) = \psi(t) u_{jk}(0) + \int_0^t \psi(t-s)\, J_{jk}^{\text{in}}(s)\, ds$$

we have

$$\widehat{J_{jk}^{\text{out}}}(z) = \hat{\psi}(z) u_{jk}(0) + \hat{\psi}(z)\, \widehat{J_{jk}^{\text{in}}}(z).$$

Eliminating $\widehat{J^{in}_{jk}}(z)$, we find

$$\widehat{J^{out}_{jk}}(z) = \hat{\psi}(z)u_{jk}(0) + \hat{\psi}(z)\left[\widehat{J^{out}_{jk}}(z) + z\hat{u}_{jk}(z) - u_{jk}(0)\right],$$

and thus

$$\frac{1-\hat{\psi}(z)}{z}\,\widehat{J^{out}_{jk}}(z) = \hat{\psi}(z)\hat{u}_{jk}(z).$$

The survival probability

$$\Phi(t) = \int_t^\infty \psi(s)\,ds = 1 - \int_0^t \psi(s)\,ds$$

satisfies $\Phi(0) = 1$ and $\Phi'(t) = -\psi(t)$, so

$$\widehat{\Phi}(z) = \frac{1-\hat{\psi}(z)}{z}.$$

Express fluxes in terms of concentration

Thus, if we define $M(t)$ via its Laplace transform,

$$\widehat{M}(z) = \frac{\hat{\psi}(z)}{\widehat{\Phi}(z)} = \frac{z\psi(z)}{1-\psi(z)},$$

then $\widehat{J^{\text{out}}_{jk}}(z) = \widehat{M}(z)\hat{u}_{jk}$ so

$$J^{\text{out}}_{jk}(t) = (M * u_{jk})(t) = \int_0^t M(t-s)u_{jk}(s)\,ds.$$

Put

$$f^{\pm}_{jk}(t) = p^{\pm}_{jk}(t)\,J^{\text{out}}_{jk}(t) \quad \text{and} \quad g^{\pm}_{jk}(t) = q^{\pm}_{jk}(t)\,J^{\text{out}}_{jk}(t)$$

so that

$$J^{\text{in}}_{jk}(t) = f^{+}_{j-1,k} + f^{-}_{j+1,k} + g^{+}_{j,k-1} + g^{-}_{j,k-1}.$$

Taylor expansion

Recall $f^{\pm}_{jk}(t) = p^{\pm}_{jk}(t)\, J^{out}_{jk}(t)$, and assume

$$p^{\pm}_{jk}(t) = \tfrac{1}{4} \pm \tfrac{1}{2} G(r_{jk}, t)\, \Delta x + O(\Delta x^2 + \Delta y^2)$$

then

$$\begin{aligned} f^{+}_{j-1,k} + f^{-}_{j+1,k} = (f^{+} + f^{-})_{jk} - (f^{+}_{x} - f^{-}_{x})_{jk}\, \Delta x \\ + \tfrac{1}{2}(f^{+}_{xx} + f^{-}_{xx})_{jk}\, \Delta x^2 + O(\Delta x^3) \end{aligned}$$

and

$$\begin{aligned} f^{+} + f^{-} &= (p^{+} + p^{-})\, J^{out}, \\ (f^{+}_{x} - f^{-}_{x})\, \Delta x &= \left(G\, J^{out}\right)_{x} \Delta x^2 + O(\Delta x^3 + \Delta x\, \Delta y^2), \\ \tfrac{1}{2}(f^{+}_{xx} + f^{-}_{xx})\, \Delta x^2 &= \tfrac{1}{4} J^{out}_{xx}\, \Delta x^2 + O(\Delta x^4 + \Delta x^2\, \Delta y^2). \end{aligned}$$

Likewise assume

$$q^{\pm}_{jk}(t) = \tfrac{1}{4} \pm \tfrac{1}{2}H(\mathbf{r}_{jk}, t)\,\Delta y + O(\Delta x^2 + \Delta y^2)$$

then

$$\begin{aligned} J^{in} = \left(p^{+} + p^{-} + q^{+} + q^{-}\right) J^{out} - \left[(G\,J^{out})_x\,\Delta x^2 + (H\,J^{out})_y\,\Delta y^2\right] \\ + \tfrac{1}{4}\left(J^{out}_{xx}\,\Delta x^2 + J^{out}_{yy}\,\Delta y^2\right) + O(\Delta x^3 + \Delta y^3). \end{aligned}$$

Since $p^{+} + p^{-} + q^{+} + q^{-} = 1$, we have

$$\begin{aligned} \frac{du}{dt} = J^{in} - J^{out} = \frac{\Delta x^2}{4}\left(-4G\,J^{out} + J^{out}_x\right)_x \\ + \frac{\Delta y^2}{4}\left(-4H\,J^{out} + J^{out}_y\right)_y + O(\Delta x^3 + \Delta y^3). \end{aligned}$$

Microscopic time scale

Compared to macroscopically observable changes, random jumps occur on a very small time scale τ over very small spatial scales Δx and Δy.

Rescale the waiting-time distribution by replacing ψ with

$$\psi_\tau(t) = \frac{1}{\tau}\,\psi\left(\frac{t}{\tau}\right)$$

then the survival probability becomes $\Phi_\tau(t) = \int_t^\infty \psi_\tau(s)\,ds$, with

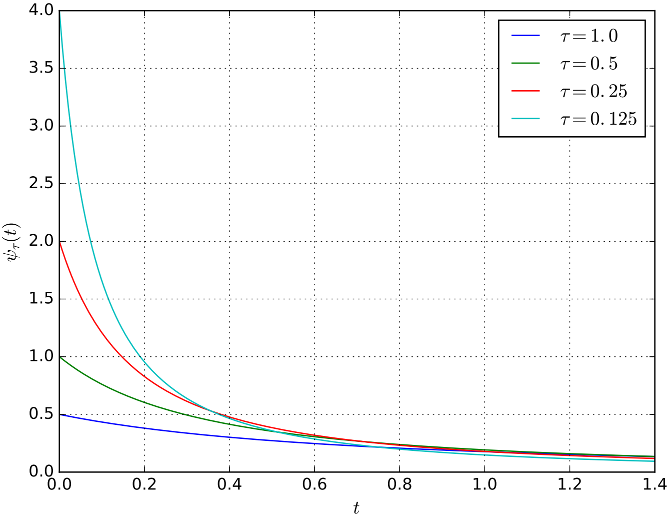
$$\hat{\psi}_\tau(z) = \hat{\psi}(\tau z) \quad \text{and} \quad \widehat{\Phi}_\tau(z) = \frac{1 - \hat{\psi}(\tau z)}{z}.$$

Note that $\psi_\tau(t)$ is again a probability distribution with

$$\int_0^\infty \psi_\tau(t)\,dt = \hat{\psi}_\tau(0) = \hat{\psi}(0) = 1.$$

Example

Rescaling $\psi(t) = \alpha/(1+t)^{1+\alpha}$ with $\alpha = 1/2$.



General power law

Let $0 < \alpha < 1$ and assume that

$$\psi(t) = \frac{A}{t^{1+\alpha}} + O\left(\frac{1}{t^{2+\alpha}}\right) \quad \text{as } t \to \infty.$$

Due to the "Fat tail", the expected waiting time is infinite, and the motion is subdiffusive.

Rescaled distribution is again a power law: $\psi_\tau(t) \sim \tau^\alpha A/t^{1+\alpha}$.

Theorem

Fix $\delta > 0$. If $z \to 0$ with $\arg z \leqslant \pi/2 - \delta$, then

$$\hat{\psi}(z) = 1 - \frac{z^\alpha}{B_\alpha} + O(z)$$

where

$$B_\alpha = \frac{\alpha}{A\Gamma(1-\alpha)}.$$

Riemann–Liouville fractional derivative

Thus, when ψ is a power law,

$$\begin{aligned}
\hat{\psi}_\tau(z) &= 1 + O(\tau^\alpha z^\alpha), \\
\widehat{\Phi}_\tau(z) &= \frac{\tau^\alpha z^{\alpha-1}}{B_\alpha}\big(1 + O(\tau^{1-\alpha} z^{1-\alpha})\big), \\
\widehat{M}(z) &= \frac{\hat{\psi}_\tau(z)}{\widehat{\Phi}_\tau(z)} = \frac{B_\alpha z^{1-\alpha}}{\tau^\alpha}\,\frac{1 + O(\tau^\alpha z^\alpha)}{1 + O(\tau^{1-\alpha} z^{1-\alpha})},
\end{aligned}$$

and so

$$\tau^\alpha \widehat{M}(z)\hat{u}(z) \to B_\alpha z^{1-\alpha}\hat{u}(z) \quad \text{as } \tau \to 0.$$

It follows that

$$\tau^\alpha J^{\mathrm{out}}(t) = \tau^\alpha (M * u)(t) \to B_\alpha \partial_t^{1-\alpha} u \quad \text{as } \tau \to 0,$$

where

$$\partial_t^{1-\alpha} u(\mathbf{r}, t) = \partial_t \mathcal{J}^\alpha u(\mathbf{r}, t) = \frac{\partial}{\partial t}\int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}\, u(\mathbf{r}, s)\, ds.$$

Scaling limit

Since

$$\frac{du}{dt} = \frac{\Delta x^2}{4\tau^\alpha}\left(-4G\tau^\alpha J^{out} + \tau^\alpha J^{out}_x\right)_x + \frac{\Delta y^2}{4\tau^\alpha}\left(-4H\tau^\alpha J^{out} + \tau^\alpha J^{out}_y\right)_y + O(\Delta x^3 + \Delta y^3),$$

we send τ, Δx and Δy to zero with limiting ratios

$$B_\alpha \frac{\Delta x^2}{4\tau^\alpha} \to \kappa_{\alpha,1} \quad \text{and} \quad B_\alpha \frac{\Delta y^2}{4\tau^\alpha} \to \kappa_{\alpha,2},$$

and obtain the fractional PDE

$$\frac{\partial u}{\partial t} = \kappa_{\alpha,1}\left(-4G\partial_t^{1-\alpha}u + \partial_t^{1-\alpha}u_x\right)_x + \kappa_{\alpha,2}\left(-4H\partial_t^{1-\alpha}u + \partial_t^{1-\alpha}u_y\right)_y.$$

Fractional Fokker–Planck equation

Put

$$\mathbf{F}(\mathbf{r},t) = 4\begin{bmatrix}\kappa_{\alpha,1}G(\mathbf{r},t)\\ \kappa_{\alpha,2}H(\mathbf{r},t)\end{bmatrix} \quad \text{and} \quad \boldsymbol{\kappa}_\alpha = \begin{bmatrix}\kappa_{\alpha,1} & 0\\ 0 & \kappa_{\alpha,2}\end{bmatrix}$$

to write the fractional Fokker–Planck equation as a conservation law

$$\frac{\partial u}{\partial t} + \nabla\cdot\mathbf{Q}_\alpha = 0,$$

where the generalised flux vector is

$$\mathbf{Q}_\alpha = \mathbf{F}\,\partial_t^{1-\alpha}u - \boldsymbol{\kappa}_\alpha\nabla\partial_t^{1-\alpha}u.$$

At each point $\mathbf{r}$, the fractional derivatives mean that $\mathbf{Q}_\alpha(\mathbf{r},t)$ depends on the complete history since time 0 of the concentration u and its spacial gradient ∇u.

A 1D example

Let

$$\Omega = (-4, 4), \quad F(x,t) = -\frac{\partial V}{\partial x}, \quad \alpha = \frac{3}{4}, \quad T = 20$$

where the potential is given by

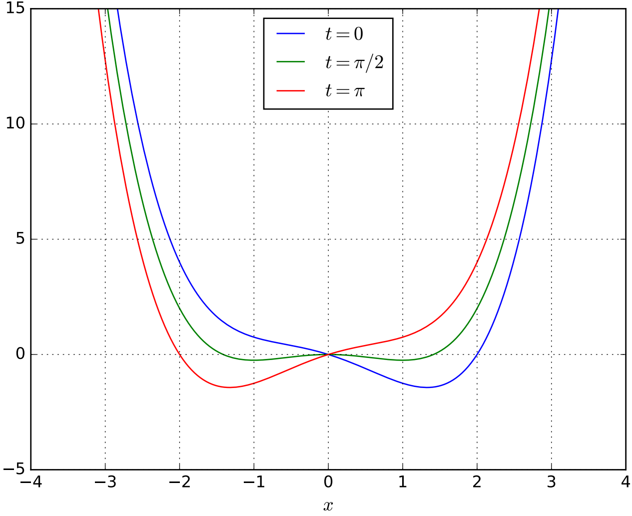
$$V(x,t) = \tfrac{1}{4}x^4 - \tfrac{1}{2}x^2 - x\cos t;$$

(Gammaitoni et al., *Reviews of Modern Physics*, 1998.)

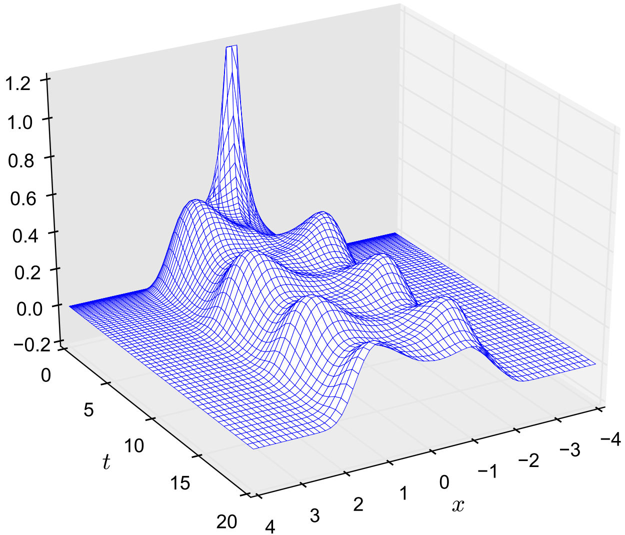
Initial data $u_0(x) = \delta(x)$.

Zero-flux boundary condition at $x = \pm 4$.

Wobbling double-well potential $V(x, t)$



Numerical solution



Finite mean waiting time

If, instead of a power law, we assume that

$$\int_0^\infty t\psi(t)\,dt = 1 \quad \text{and} \quad \int_0^\infty t^2\psi(t)\,dt < \infty,$$

then $\hat\psi$ is twice differentiable with $\hat\psi(0) = 1$ and $\hat\psi'(0) = -1$, so Taylor expansion gives

$$\hat\psi(z) = 1 - z + O(z^2) \quad \text{as } z \to 0.$$

Thus,

$$\hat\psi_\tau(z) = 1 + O(\tau z) \quad \text{and} \quad \widehat\Phi_\tau(z) = \tau\big(1 + O(\tau z)\big),$$

and so

$$\widehat{M}(z) = \frac{\hat\psi_\tau(z)}{\widehat\Phi_\tau(z)} = \tau^{-1}\big(1 + O(\tau z)\big).$$

Hence, if $\tau \to 0$ then

$$\tau\widehat{M}(z)\hat u(z) \to \hat u(z) \quad \text{and} \quad \tau J^{\mathrm{out}}(t) \to u(t).$$

Classical Fokker–Planck equation ($\alpha = 1$)

Since

$$\frac{du}{dt} = \frac{\Delta x^2}{4\tau}\left(-4G\tau J^{out} + \tau J_x^{out}\right)_x + \frac{\Delta y^2}{4\tau}\left(-4H\tau J^{out} + \tau J_y^{out}\right)_y + O(\Delta x^3 + \Delta y^3),$$

we now send τ, Δx and Δy to zero with limiting ratios

$$\frac{\Delta x^2}{4\tau} \to \kappa_1 \quad \text{and} \quad \frac{\Delta y^2}{4\tau} \to \kappa_2,$$

and obtain the PDE

$$\frac{\partial u}{\partial t} = \kappa_1\left(-4Gu + u_x\right)_x + \kappa_2\left(-4Hu + u_y\right)_y.$$

Classical flux

Put

$$\mathbf{F} = 4\begin{bmatrix}\kappa_1 G(\mathbf{r},t)\\ \kappa_2 H(\mathbf{r},t)\end{bmatrix} \quad \text{and} \quad \boldsymbol{\kappa} = \begin{bmatrix}\kappa_1 & 0\\ 0 & \kappa_2\end{bmatrix}$$

to obtain

$$\frac{\partial u}{\partial t} + \nabla\cdot\mathbf{Q}_{\mathrm{cl}} = 0 \quad \text{where} \quad \mathbf{Q}_{\mathrm{cl}} = \mathbf{F}u - \boldsymbol{\kappa}\nabla u.$$

The classical flux $\mathbf{Q}_{\mathrm{cl}}$ depends only on the instantaneous values of the concentration u and its spatial gradient ∇u at a given point.

Fractional Fokker–Planck equation with a steady force

Again consider $0 < \alpha < 1$, but assume $\mathbf{F} = \mathbf{F}(\mathbf{r})$ is independent of t. The generalised flux can then be written as

$$\mathbf{Q}_\alpha = \partial_t^{1-\alpha}\big[\mathbf{F}(\mathbf{r})u - \kappa_\alpha \nabla u\big] = \partial_t^{1-\alpha}\widetilde{\mathbf{Q}},$$

where

$$\widetilde{\mathbf{Q}} = \mathbf{F}(\mathbf{r})u - \kappa_\alpha \nabla u.$$

Thus,

$$\partial_t u + \partial_t^{1-\alpha}\nabla \cdot \widetilde{\mathbf{Q}} = 0.$$

We can reformulate this equation using the Caputo fractional derivative of order α,

$$\tilde{\partial}_t^\alpha u = \mathcal{J}^{1-\alpha}\partial_t u = \int_0^t \frac{(t-s)^{-\alpha}}{\Gamma(1-\alpha)}\, u'(s)\, ds.$$

Alternative form of the fractional Fokker–Planck equation

We have

$$\mathcal{J}^1 \partial_t u = \mathcal{J}^\alpha \mathcal{J}^{1-\alpha} \partial_t u = \mathcal{J}^\alpha \tilde{\partial}_t^\alpha u,$$

and, assuming $(\mathcal{J}^\alpha f)(0) = 0$,

$$(\mathcal{J}^1 \partial_t^{1-\alpha} f)(t) = (\mathcal{J}^1 \partial_t \mathcal{J}^\alpha f)(t) = \int_0^t (\mathcal{J}^\alpha f)'(s)\, ds = (\mathcal{J}^\alpha f)(t).$$

Thus,

$$\mathcal{J}^\alpha \big(\tilde{\partial}_t^\alpha u + \nabla \cdot \widetilde{\mathbf{Q}}\big) = \mathcal{J}^1 \big(\partial_t u + \partial_t^{1-\alpha} \nabla \cdot \widetilde{\mathbf{Q}}\big) = 0,$$

giving

$$\tilde{\partial}_t^\alpha u + \nabla \cdot \widetilde{\mathbf{Q}} = 0 \qquad \text{(if } F \text{ is independent of } t).$$

Initial-boundary value problem

Assume $\Omega \subseteq \mathbb{R}^d$ is an interval $(d = 1)$, a polygon $(d = 2)$ or a polyhedron $(d = 3)$. We impose the initial condition

$$u(x, t) = u_0(x) \quad \text{for } x \in \Omega \text{ when } t = 0,$$

and enforce either a homogeneous Dirichlet (essential) boundary condition,

$$u(x, t) = 0 \quad \text{for } x \in \partial\Omega \text{ and } t > 0,$$

or else a zero-flux (natural) boundary condition,

$$\mathbf{n} \cdot \mathbf{Q}_\alpha = \mathbf{n} \cdot \left(\mathbf{F}\partial_t^{1-\alpha} - \kappa_\alpha \nabla \partial_t^{1-\alpha} u\right) = 0 \quad \text{for } x \in \partial\Omega \text{ and } t > 0.$$

In the latter case, the total mass is conserved:

$$\int_\Omega u = \int_\Omega u_0.$$

Integration by parts

Write

$$\langle u, v\rangle = \int_\Omega uv \quad \text{and} \quad \langle \mathbf{F}, \mathbf{G}\rangle = \int_\Omega \mathbf{F}\cdot\mathbf{G},$$

with

$$\|u\|^2 = \langle u, u\rangle \quad \text{and} \quad \|\mathbf{F}\|^2 = \langle \mathbf{F}, \mathbf{F}\rangle.$$

Since

$$\nabla\cdot(\mathbf{Q}_\alpha v) = (\nabla\cdot\mathbf{Q}_\alpha)v + \mathbf{Q}_\alpha\cdot\nabla v,$$

the divergence theorem implies that

$$\int_{\partial\Omega} \mathbf{n}\cdot\mathbf{Q}_\alpha v = \int_\Omega (\nabla\cdot\mathbf{Q}_\alpha)v + \int_\Omega \mathbf{Q}_\alpha\cdot\nabla v.$$

Thus, if $v = 0$ on $\partial\Omega$, or if $\mathbf{n}\cdot\mathbf{Q}_\alpha = 0$ on $\partial\Omega$, then LHS $= 0$ so

$$\langle \nabla\cdot\mathbf{Q}_\alpha, v\rangle = -\langle \mathbf{Q}_\alpha, \nabla v\rangle.$$

Weak formulation

Dirichlet boundary condition: weak solution $u : (0, T] \to H_0^1(\Omega)$ satisfies

$$\langle \partial_t u, v \rangle - \langle \mathbf{Q}_\alpha, \nabla v \rangle = 0 \quad \text{for all } v \in H_0^1(\Omega).$$

Neumann boundary condition: weak solution $u : (0, T] \to H^1(\Omega)$ satisfies

$$\langle \partial_t u, v \rangle - \langle \mathbf{Q}_\alpha, \nabla v \rangle = 0 \quad \text{for all } v \in H^1(\Omega).$$

In both cases, $u(x, 0) = u_0(x)$ and

$$\langle \partial_t u, v \rangle + \langle \kappa_\alpha \partial_t^{1-\alpha} \nabla u, \nabla v \rangle - \langle F \partial_t^{1-\alpha} u, \nabla v \rangle = 0.$$

Stability in $L_2(\Omega)$ when $\alpha = 1$

A simple energy argument shows that the classical Fokker–Planck equation is well-posed. Taking $v = u$ in the weak formulation gives

$$\langle \partial_t u, u \rangle + \langle \boldsymbol{\kappa} \nabla u, \nabla u \rangle - \langle \mathbf{F} u, \nabla u \rangle = 0,$$

and since

$$\langle \boldsymbol{\kappa} \nabla u, \nabla u \rangle \geqslant c \|\nabla u\|^2, \qquad c = \min(\kappa_1, \kappa_2),$$

we have

$$\frac{d}{dt} \frac{\|u\|^2}{2} + \cancel{c\|\nabla u\|^2} \leqslant \langle \mathbf{F} u, \nabla u \rangle \leqslant \frac{1}{4c} \|\mathbf{F} u\|_\infty^2 + \cancel{c\|\nabla u\|^2}.$$

$$\frac{d}{dt}\|u\|^2 \leqslant \frac{\|Fu\|_\infty^2}{2c}.$$

Assuming F is bounded,

$$\|u(t)\|^2 \leqslant \|u_0\|^2 + \frac{\|F\|_\infty^2}{2c}\int_0^t \|u(s)\|^2\,ds,$$

so Gronwall's lemma implies that

$$\|u(t)\| \leqslant \|u_0\| \exp\left(\frac{\|F\|_\infty^2 T}{4c}\right) \quad \text{for } 0 \leqslant t \leqslant T,$$

Semidiscrete finite element method

Triangulate Ω and write $h =$ maximum element diameter.

Dirichlet boundary condition: $\mathbb{S}_h \subseteq H_0^1(\Omega)$ denotes the space of continuous, piecewise-linear functions that vanish on $\partial\Omega$. Finite element solution $u_h : [0, \infty) \to \mathbb{S}_h$ defined by

$$\langle \partial_t u_h, \chi \rangle + \langle \kappa_\alpha \partial_t^{1-\alpha} \nabla u_h, \nabla \chi \rangle - \langle \mathbf{F} \partial_t^{1-\alpha} u_h, \nabla \chi \rangle = 0$$

for all $\chi \in \mathbb{S}_h$, with $u_h(0) = u_{0h} \approx u_0$ where $u_{0h} \in \mathbb{S}_h$.

Neumann (zero-flux) boundary condition: $\mathbb{S}_h \subseteq H^1(\Omega)$ now includes *all* continuous piecewise-linear functions. Aside: choosing $\chi = 1$ shows $\int_\Omega u_h = \int_\Omega u_{0h}$, that is, total mass is conserved exactly.

Method of lines

Number of degrees of freedom $\mathsf{DoF} = \dim \mathbb{S}_h$.

Free nodes $\mathbf{r}_m$ for $1 \leqslant m \leqslant \mathsf{DoF}$.

Nodal basis functions $\phi_m \in \mathbb{S}_h$ satisfy $\phi_m(\mathbf{r}_k) = \delta_{mk}$.

Semidiscrete solution

$$u_h(\mathbf{r}, t) = \sum_{m=1}^{\mathsf{DoF}} U_m(t)\phi_m(\mathbf{r})$$

with nodal values

$$U_m(t) = u_h(\mathbf{r}_m, t) \approx u(\mathbf{r}_m, t).$$

Matrix formulation

Define DoF $\times$ DoF matrices $\mathbf{M}$ and $\mathbf{G}(t)$ with entries

$$M_{km} = \langle \phi_m, \phi_k \rangle$$

and

$$G_{km}(t) = \langle \kappa_\alpha \nabla \phi_m, \nabla \phi_k \rangle - \langle \mathbf{F}(\cdot, t)\phi_m, \nabla \phi_k \rangle.$$

Vector of nodal values $\mathbf{U}(t) = [U_m(t)]$ satisfies a system of fractional ODEs:

$$\mathbf{M}\,\frac{d\mathbf{U}}{dt} + \partial_t^{1-\alpha}\mathbf{G}(t)\mathbf{U} = \mathbf{0} \quad \text{for } t > 0, \quad \text{with } \mathbf{U}(0) = \mathbf{U}_0.$$

Equivalent system of Volterra integral equations:

$$\mathbf{M}\mathbf{U}(t) = \mathbf{M}\mathbf{U}_0 + \int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}\,\mathbf{G}(s)\mathbf{U}(s)\,ds.$$

Steady forcing

When $\mathbf{F} = \mathbf{F}(x)$ is independent of t, we have the alternative formulation

$$\langle \tilde{\partial}_t^\alpha u_h, \chi \rangle + \langle \kappa_\alpha \nabla u_h, \nabla \chi \rangle - \langle \mathbf{F} u_h, \nabla \chi \rangle = 0,$$

or, in matrix notation,

$$\mathbf{M} \tilde{\partial}_t^\alpha \mathbf{U} + \mathbf{G}(t) \mathbf{U} = 0.$$

Literature:

- finite differences Weihua Deng, *J. Comput. Phys.*, 2007,
- finite elements Weihua Deng, *SIAM J. Numer. Anal.*, 2008.
- orthogonal collocation Fairweather, Zhang, Yang & Xu *Numer. Meth. PDEs* 2015,
- spectral method Zheng, Liu, Turner & Anh *SISC* 2015.

Stability in $L_2(\Omega)$

Theorem

Assume that $\mathbf{F}$, $\partial_t \mathbf{F} \in L_\infty\big(\Omega \times (0,T), \mathbb{R}^d\big)$. *There is a constant* C, *depending on* α, T, $\|\mathbf{F}\|_\infty$ *and* $\|\partial_t \mathbf{F}\|_\infty$, *such that*

$$\|u_h(t)\| \leqslant C\|u_{0h}\| \quad \text{for } 0 \leqslant t \leqslant T.$$

Remark

For the classical Fokker–Planck equation ($\alpha = 1$), *result follows by repeating the energy argument for the continuous problem, with* C *depending on* T *and* $\|\mathbf{F}\|_\infty$.

Remark

For $0 < \alpha < 1$, *if* $\mathbf{F} = 0$ *then we can show* $C = 1$ *using the positivity property*

$$\int_0^T \big\langle \kappa_\alpha \nabla \partial_t^{1-\alpha} v, \nabla v \big\rangle \, dt \geqslant 0.$$

Fractional Gronwall lemma

Mittag–Leffler function

$$E_\beta(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+n\beta)}.$$

The following result is one key ingredient in the stability proof.

Theorem (Dixon and McKee, *ZAMM Z. Angew. Math. Mech.* **66**, 1986)

Let $\beta > 0$ *and* $T > 0$. *Assume that* $a(t)$ *and* $b(t)$ *are non-negative and non-decreasing functions for* $0 \leqslant t \leqslant T$. *If* $y : [0,T] \to \mathbb{R}$ *is an integrable function satisfying*

$$0 \leqslant y(t) \leqslant a(t) + b(t)(\mathcal{J}^\beta y)(t) \quad \text{for } 0 \leqslant t \leqslant T,$$

then

$$y(t) \leqslant a(t) E_\beta\left(b(t)t^\beta\right) \quad \text{for } 0 \leqslant t \leqslant T.$$

First step in the stability proof

Integrate finite element equation in time, choose $\chi = \mathcal{J}^\alpha u_h(t)$, integrate a second time, use technical estimates involving fractional integrals, and apply fractional Gronwall lemma.

Find that

$$\int_0^t \left(\langle u_h, \mathcal{J}^\alpha u_h\rangle + \|\mathcal{J}^\alpha \nabla u_h\|^2\right) ds \leqslant Ct^{1+\alpha}\|u_{0h}\|^2$$

and

$$\int_0^t \|\mathcal{J}^\alpha u_h\|^2 \, ds \leqslant Ct^{1+2\alpha}\|u_{0h}\|^2$$

for $0 \leqslant t \leqslant T$.

Second step

Multiplication operator:

$$\mathcal{M}u_h(t) = tu_h(t).$$

Integrate finite element equation, choose $\chi = \mathcal{I}^\alpha u_h(t)$, multiply both sides by t, integrate again, ...

Find that

$$\int_0^t \left(\langle \mathcal{M}u_h, \mathcal{I}^\alpha \mathcal{M}u_h\rangle + \|\mathcal{I}^\alpha \mathcal{M}\nabla u_h\|^2\right) ds \leqslant Ct^{3+\alpha}\|u_{0h}\|^2$$

and

$$\int_0^t \|\mathcal{I}^\alpha \mathcal{M}u_h\|^2 \, ds \leqslant Ct^{3+2\alpha}\|u_{0h}\|^2$$

for $0 \leqslant t \leqslant T$.

Third step

Multiply finite element equation by t, differentiate with respect to t, choose $\chi = \partial_t^{1-\alpha}\mathcal{M}u_h$, ...

Find that

$$\int_0^t \left(\langle(\mathcal{M}u_h)', \mathcal{J}^\alpha(\mathcal{M}u_h)'\rangle + \|\mathcal{J}^\alpha(\mathcal{M}\nabla u_h)'\|^2\right) ds \leqslant Ct^{1+\alpha}\|u_{0h}\|^2$$

for $0 \leqslant t \leqslant T$. Then put $\phi = \mathcal{M}u_h(t)$ in the inequality

$$\|\phi(t) - \phi(0)\|^2 \leqslant \frac{t^{1-\alpha}}{(1-\alpha)^2}\int_0^t \langle\phi'(s), (\mathcal{J}^\alpha\phi')(s)\rangle\, ds.$$

Error estimate

Introduce the Ritz (elliptic) projection $R_h v \in \mathbb{S}_h$ of $v \in H^1(\Omega)$ defined by

$$\langle \nabla R_h v, \nabla \chi \rangle + \langle R_h v, \chi \rangle = \langle \nabla v, \nabla \chi \rangle + \langle v, \chi \rangle \quad \text{for all } \chi \in \mathbb{S}_h.$$

Quasi-optimality in $H^1(\Omega)$:

$$\|v - R_h v\|_1 \leqslant C \min_{w \in \mathbb{S}_h} \|v - w\|_1 \leqslant Ch\|v\|_2.$$

Aubin–Nitsche (duality) estimate:

$$\|v - R_h v\| \leqslant Ch^2 \|v\|_2.$$

Need to assume the polyhedron Ω is convex so that the Poisson problem is H^2-regular.

Error equation

Decompose the FE error $e_h = u_h - u$ as

$$e_h = \theta_h - \rho_h \quad \text{where} \quad \theta_h = u_h - R_h u \quad \text{and} \quad \rho_h = u - R_h u.$$

Preceding estimates for R_h immediately give

$$\|\rho_h(t)\| \leqslant Ch^2 \|u(t)\|_2.$$

Using the definition of R_h, find that θ_h satisfies

$$\begin{aligned}\langle \partial_t \theta_h, \chi \rangle + \langle \partial_t^{1-\alpha} \nabla \theta_h, \nabla \chi \rangle - \langle \mathbf{F} \partial_t^{1-\alpha} \theta_h, \nabla \chi \rangle \\ = \langle \partial_t \rho_h - \partial_t^{1-\alpha} \rho_h, \chi \rangle - \langle \mathbf{F} \partial_t^{1-\alpha} \rho_h, \nabla \chi \rangle.\end{aligned}$$

Repeat arguments in stability proof.

Regularity assumption and error bound

We assume that, for some r in the range $0 \leqslant r \leqslant 2$, there is a constant K_r such that

$$\|u(t)\|_2 + t\|\partial_t u(t)\|_2 \leqslant K_r t^{\alpha(r-2)/2} \quad \text{for } 0 < t \leqslant T.$$

Such a bound is known to hold with $K_r = C\|u_0\|_r$ if $F = 0$.

Let $P_h v \in \mathbb{S}_h$ denote the L_2-projection, that is,

$$\langle P_h v, \chi \rangle = \langle v, \chi \rangle \quad \text{for } v \in L_2(\Omega) \text{ and } \chi \in \mathbb{S}_h.$$

Theorem

If u satisfies the above regularity assumption with $0 \leqslant r \leqslant 2$, then

$$\|u_h(t) - u(t)\| \leqslant C\|u_{0h} - P_h u_0\| + Ct^{\alpha(r-2)/2}h^2 K_r$$

for $0 < t \leqslant T$. The constant C depends on α, T and F.

Numerical experiments

We let

$$\Omega = (0, \pi), \quad F(x,t) = -x + \sin t, \quad T = 1,$$

with homogeneous Dirichlet boundary conditions $u(0,t) = 0 = u(\pi, t)$ and discontinuous initial data

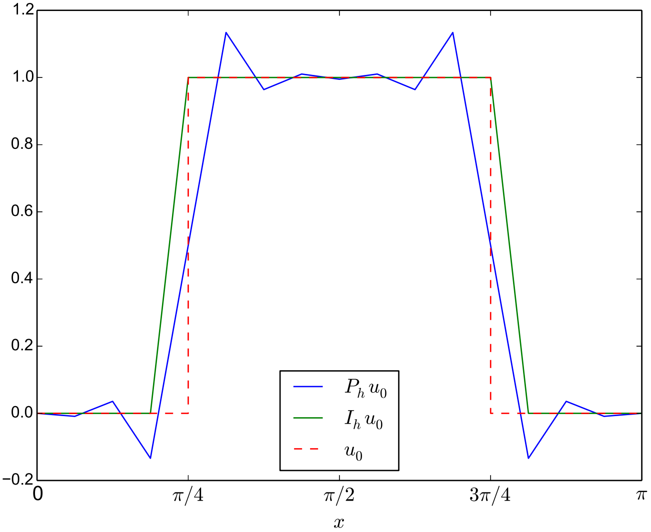
$$u_0(x) = \begin{cases} 1, & \pi/4 \leqslant x \leqslant 3\pi/4, \\ 0, & \text{otherwise.} \end{cases}$$

Find that $u_0 \in H_0^r(\Omega)$ for $0 \leqslant r < 1/2$ with $\|u_0\|_r \leqslant C/\sqrt{1-2r}$. Putting $r = \frac{1}{2} - \epsilon$ where $\epsilon^{-1} = \log(e^2 + t^{-1})$ so that $t^{-\epsilon} \leqslant e$ and $0 < \epsilon < 1/2$, we expect

$$\|u_h(t) - u(t)\| \leqslant C\|u_{0h} - P_h u_0\| + C t^{-3\alpha/4} h^2 \sqrt{\log(e^2 + t^{-1})}$$

for $0 < t \leqslant 1$.

Gibbs phenomenon



Weighted error with respect to a reference solution

We computed a reference solution U_{ref} using a fine mesh with $N = 10{,}000$ time steps and $Q_h = 255$ degrees of freedom. The mesh was uniform in space but graded in time:

$$t_n = (n/N)^\gamma T \quad \text{for } 0 \leqslant n \leqslant N \text{ with } \gamma = 1/\alpha.$$

With $u_{0h} = P_h u_0$, we then computed

$$E^n_{h,k} = \|U^n_h - U_{\text{ref}}(t_n)\| \quad \text{for } 1 \leqslant n \leqslant N,$$

and estimated the convergence rate $\sigma_{h,k}$ such that

$$E^*_{h,k} = \max_{0 \leqslant n \leqslant N} \frac{t_n^{3\alpha/4} E^n_{h,k}}{\sqrt{\log(e^2 + t_n^{-1})}} \approx C h^{\sigma_{h,k}}$$

from the relation $\sigma_{h,k} \approx \log_2(E^*_{2h,k}/E^*_{h,k})$. Expect $\sigma_{h,k} \approx 2$.

Behaviour of the weighted error $E^*_{h,k}$

Q_h	$\alpha = 0.25$		$\alpha = 0.50$		$\alpha = 0.75$	
7	7.98e-03		7.77e-03		7.84e-03	
15	1.96e-03	2.024	1.91e-03	2.024	1.94e-03	2.017
31	4.88e-04	2.008	4.75e-04	2.008	4.82e-04	2.007
63	1.21e-04	2.014	1.18e-04	2.014	1.19e-04	2.015

Expect only first-order convergence using the nodal interpolant $u_{0h} = I_h u_0$, since

$$\langle u_{0h} - P_h u_0, \chi \rangle = \langle u_{0h} - u_0, \chi \rangle \leqslant \|u_{0h} - u_0\| \|\chi\|,$$

and by letting $\chi = u_{0h} - P_h u_0$ we have

$$\|u_{0h} - P_h u_0\| \leqslant \|u_{0h} - u_0\| = \sqrt{\frac{2}{3}}\, h.$$

Error in $L_2(\Omega)$ behaves like $t^{-3\alpha/4}h^2$