Superdiffusion in the presence of a reflecting boundary

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Abstract

We study the effect of having a reflecting boundary condition in a superdiffusive model. Firstly it is described how the problem formulation is affected by this type of physical boundary and then it is shown how to implement an implicit numerical method to compute the numerical solutions. The consistency and stability analysis of the numerical method are discussed. In the end numerical experiments are presented to show the performance of the scheme and to visualize the consequences of having a reflecting wall.

Keywords: Lévy flights, reflecting boundary, fractional differential equations, finite difference methods

1. Introduction

Anomalous diffusive transport, in particular superdiffusion, arises in a large variety of physical problems. One of the models that describes superdiffusion is related to Lévy flights and formulated via a fractional differential equation [16, 19]. Boundary value problems for Lévy flights are not easily formulated since the long jumps pose certain difficulties when non-trivial boundary conditions are involved. In fact, the presence of boundaries may modify the nonlocal spatial operator since they cannot be uncoupled from the fractional partial differential equation as it happens when the order of the space derivative is an integer. In literature, when discussing Lévy flights in the one dimensional half-space the boundary conditions mainly considered have been absorbing or reflecting boundaries. Absorbing boundary conditions have been imposed by assuming zero outside the problem domain. However, regarding reflecting boundary conditions several formulations have been proposed [2, 3, 5, 7, 8, 9, 12, 13].

We present how to formulate the superdiffusive problem with a left reflecting wall and how to determine its numerical solutions. The formulation of the boundary is according to [13], where a symmetric diffusive problem on a semi-infinite domain is considered. Physically, when considering a trajectory of the particle in $[0,\infty)$ with the reflecting boundary condition at $x=0$, the jumps that end at $x<0$ are reflected, then $-x$ is defined as a starting point to the next jump.

The superdiffusive model associated with Lévy flights is defined in the whole real line and the governing equation involves Riemann-Liouville fractional derivatives [16]. The left and right Riemann-Liouville fractional derivatives of order α, for $x \in \mathbb{R}$, are given respectively by

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{-\infty}^{x} u(\xi,t)(x-\xi)^{1-\alpha}d\xi, \quad (1<\alpha<2), \tag{1}$$

$$\frac{\partial^\alpha u}{\partial(-x)^\alpha}(x,t) = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{x}^{\infty} u(\xi,t)(\xi-x)^{1-\alpha}d\xi, \quad (1<\alpha<2). \tag{2}$$

The fractional differential equation describing the superdiffusive model in the open domain, for $1<\alpha<2$ and $-1\le\beta\le 1$, can be stated as

$$\frac{\partial u(x,t)}{\partial t} = D\left(\frac{1+\beta}{2}\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) + \frac{1-\beta}{2}\frac{\partial^\alpha u}{\partial(-x)^\alpha}(x,t)\right) + p(x,t), \tag{3}$$

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where D is the diffusive parameter and $p(x,t)$ is a source term. The parameter α describes the tail of the solution and the parameter $-1 \leq \beta \leq 1$ is the skewness and specifies if the solution is skewed to the left ($\beta < 0$), right ($\beta > 0$) of if it is symmetric ($\beta = 0$).

The model under study consists of a reflecting wall restraining the diffusing particles to a semi-infinite domain. This barrier can be viewed as a force field applied to the particles. It is assumed that the particles arriving at the boundary are bounced back as in elastic collisions, that is, if they reach the position $x = -a$ with $a > 0$, then they will end at $x = a$, describing the mirror trajectory with respect to the wall. In a porous medium such a boundary may represent a wall permeable to the fluid, but impermeable to the tracer. Mathematically, we have a problem defined in $x > 0$ by equation (3) and subjected to the wall condition, suggested in [13], $u(x,t) = u(-x,t)$, for $x < 0$ and illustrated in Figure 1.

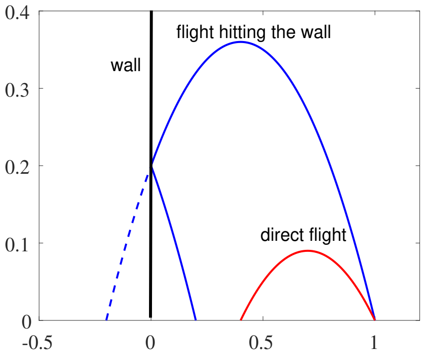

Figure 1: Illustration of the reflecting boundary condition at $x = 0$.

If we take in consideration that $u(x,t) = u(-x,t)$, for $x < 0$, the left Riemann-Liouville fractional derivative is affected by this condition and we have, for $x > 0$,

$$\begin{aligned}\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) &= \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{-\infty}^{0} u(\xi,t)(x-\xi)^{1-\alpha}d\xi + \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{0}^{x} u(\xi,t)(x-\xi)^{1-\alpha}d\xi \\ &= \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{-\infty}^{0} u(-\xi,t)(x-\xi)^{1-\alpha}d\xi + \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{0}^{x} u(\xi,t)(x-\xi)^{1-\alpha}d\xi.\end{aligned}$$

By doing a change of variables we obtain what we will define as the reflecting left Riemann-Liouville fractional derivative, for $x > 0$,

$$\frac{\partial^\alpha_{ref} u}{\partial x^\alpha}(x,t) := \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{0}^{\infty} u(\xi,t)(x+\xi)^{1-\alpha}d\xi + \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{0}^{x} u(\xi,t)(x-\xi)^{1-\alpha}d\xi. \quad (4)$$

The right Riemann-Liouville derivative is not affected by the reflecting wall and therefore it is still defined by (2), for $x > 0$.

Formally when subjected to a reflecting wall we have the following problem

$$\frac{\partial u}{\partial t}(x,t) = D\left(\frac{1+\beta}{2}\frac{\partial^\alpha_{ref} u}{\partial x^\alpha}(x,t) + \frac{1-\beta}{2}\frac{\partial^\alpha u}{\partial(-x)^\alpha}(x,t)\right) + p(x,t), \quad x > 0, \quad (5)$$

$$u(x,t) = u(-x,t), \quad \text{for all} \quad x < 0, \quad (6)$$

with an initial condition $u(x,0) = u_0(x)$, $x \geq 0$.

2. The numerical method

Recently, a great number of numerical methods for space fractional differential equations have been appearing in literature [1, 4, 10, 11, 15, 18, 20, 21]. The problem under discussion can be solved following the ideas presented in [6, 14, 17] and explained succinctly in what follows.

Consider the problem defined in the whole real line and denote the integrals in definitions (1) and (2) respectively by

$$\mathcal{I}^l u(x,t) = \frac{1}{\Gamma(2-\alpha)} \int_{-\infty}^{x} u(\xi,t)(x-\xi)^{1-\alpha} d\xi \quad \text{and} \quad \mathcal{I}^r u(x,t) = \frac{1}{\Gamma(2-\alpha)} \int_{x}^{\infty} u(\xi,t)(\xi-x)^{1-\alpha} d\xi. \tag{7}$$

The domain discretisation is given by $x_k = x_{k-1} + \Delta x,\ k \in \mathbb{Z}$. If we approximate the function inside the integrals in (7) by a linear spline [6, 14, 17] we arrive at the following approximations for the left and right integrals respectively

$$I^l u(x_j,t) = \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{m=0}^{\infty} a_m u(x_{j-m},t), \quad I^r u(x_j,t) = \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{m=0}^{\infty} a_m u(x_{j+m},t), \tag{8}$$

with

$$a_0 = 1, \qquad a_m = (m+1)^{3-\alpha} - 2m^{3-\alpha} + (m-1)^{3-\alpha}.$$

When we have a reflecting boundary condition at $x = 0$, since the left fractional derivative is modified to (4), the modified left fractional integral is now defined by

$$\mathcal{I}^l_{ref} u(x_j,t) = \frac{1}{\Gamma(2-\alpha)} \int_0^{\infty} u(\xi,t)(x+\xi)^{1-\alpha} d\xi + \frac{1}{\Gamma(2-\alpha)} \int_0^{x} u(\xi,t)(x-\xi)^{1-\alpha} d\xi. \tag{9}$$

The right fractional integral is still defined by (7) and therefore can be approximated by (8). Following a similar approach as in the open domain, where u inside the integral is approximated by a linear spline, we obtain the following approximation for the left fractional integral (9),

$$I^l_{ref} u(x_j,t) = \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{m=0}^{j} a_m u(x_{j-m},t) + \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{m=j+1}^{\infty} a_m u(x_{m-j},t). \tag{10}$$

To discretize the modified left Riemann-Liouville derivative $\frac{\partial^2}{\partial x^2}\mathcal{I}^l_{ref} u(x,t)$ and the right Riemann-Liouville derivative $\frac{\partial^2}{\partial x^2}\mathcal{I}^r u(x,t)$, we approximate the second order derivative by a second order central approximation and take in consideration (8) and (10). For the right Riemann-Liouville derivative, by taking in consideration (8), we obtain, as explained in detail in [17], the approximation

$$\frac{\partial^2}{\partial x^2}\mathcal{I}^r u(x_j,t) \approx \frac{1}{\Delta x^{\alpha}\Gamma(4-\alpha)} \sum_{m=-1}^{\infty} b_m u(x_{j+m},t) =: \frac{\delta^{\alpha}_r u(x_j,t)}{\Delta x^{\alpha}},$$

with

$$b_{-1} = a_0, \quad b_0 = -2a_0 + a_1, \quad b_m = a_{m+1} - 2a_m + a_{m-1}, \quad m \geq 1. \tag{11}$$

Proceeding in a similar manner, for the modified left Riemann-Liouville derivative, it follows

$$\frac{\partial^2}{\partial x^2}\mathcal{I}^l_{ref} u(x_j,t) \approx \frac{1}{\Delta x^{\alpha}\Gamma(4-\alpha)} \sum_{m=-1}^{j} b_m u(x_{j-m},t) + \frac{1}{\Delta x^{\alpha}\Gamma(4-\alpha)} \sum_{m=j+1}^{\infty} b_m u(x_{m-j},t) =: \frac{\delta^{\alpha}_{ref,l} u(x_j,t)}{\Delta x^{\alpha}}. \tag{12}$$

We assume a uniform mesh in time and space with $t_{n+1} = t_n + \Delta t,\ n \geq 0,\ x_j = x_{j-1} + \Delta x,\ j \in \mathbb{N}$. Let U_j^n be the approximated solution of $u(x_j, t_n)$ and define $\mu_\alpha = \frac{D\Delta t}{\Delta x^{\alpha}}$. Consider the Crank-Nicolson scheme to approximate equation (3) given by

$$\left(1 - \frac{1}{2}\mu_\alpha \delta^{\alpha}_{\beta,ref}\right) U_j^{n+1} = \left(1 + \frac{1}{2}\mu_\alpha \delta^{\alpha}_{\beta,ref}\right) U_j^{n} + p_j^{n+1/2} \tag{13}$$

where $p_j^{n+1/2} = (p_j^{n+1} + p_j^n)/2$ and

$$\delta^{\alpha}_{\beta,ref} u(x_j,t) = \frac{1+\beta}{2}\delta^{\alpha}_{ref,l} u(x_j,t) + \frac{1-\beta}{2}\delta^{\alpha}_r u(x_j,t). \tag{14}$$

3. Convergence of the numerical method: consistency and stability

We start to present a known result in the open domain. The dependency of the solution u on t is omitted in the following results for the sake of clarity and simplicity.

Theorem 1 ([17]). *Let $u \in C^{(4)}(\mathbb{R})$ and such that the spatial derivatives vanish at infinity in an appropriate manner. Then*

$$\frac{\partial^\alpha u}{\partial(-x)^\alpha}(x_j) - \frac{\delta_r^\alpha u}{\Delta x^\alpha}(x_j) = \epsilon_r(x_j),$$

with $\epsilon_r(x_j) \leq C_r \Delta x^2$, where C_r does not depend on Δx.

The next result determines the truncation error for the approximation (12) of the modified left Riemann-Liouville derivative.

Theorem 2. *Let $u \in C^{(4)}(\mathbb{R})$ and such that verifies (6). Additionally the spatial derivatives vanish at infinity in an appropriate manner. Then*

$$\frac{\partial_{ref}^\alpha u}{\partial x^\alpha}(x_j) - \frac{\delta_{ref,l}^\alpha u}{\Delta x^\alpha}(x_j) = \epsilon_{ref,l}(x_j),$$

with $\epsilon_{ref,l}(x_j) \leq C_{ref,l} \Delta x^2$, where $C_{ref,l}$ does not depend on Δx.

Proof. We have that

$$I_{ref}^l u(x_j) = \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{m=0}^{j} a_m u(x_{j-m}) + \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{m=j+1}^{\infty} a_m u(x_{m-j}).$$

Taking in consideration (6)

$$\begin{aligned} I_{ref}^l u(x_j) &= \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{m=0}^{j} a_m u(x_{j-m}) + \frac{\Delta x^{2-\alpha}}{\Gamma(4-\alpha)} \sum_{m=j+1}^{\infty} a_m u(x_{j-m}) \\ &= \frac{1}{\Gamma(4-\alpha)} \sum_{k=-\infty}^{j} \int_{x_{k-1}}^{x_k} s_k(\xi)(x_j-\xi)^{1-\alpha} d\xi, \end{aligned}$$

where

$$s_k(\xi) = \frac{x_k - \xi}{\Delta x} u(x_{k-1}) + \frac{\xi - x_{k-1}}{\Delta x} u(x_k).$$

Additionally, by doing a change of variable and taking in consideration the reflecting condition (6), we have for the exact value of the integral the following equalities

$$\begin{aligned} &\mathcal{I}_{ref}^l u(x_j) = \int_0^{x_j} u(\xi)(x_j-\xi)^{1-\alpha} d\xi + \int_0^{\infty} u(\xi)(x_j+\xi)^{1-\alpha} d\xi \\ &= \int_0^{x_j} u(\xi)(x_j-\xi)^{1-\alpha} d\xi - \int_0^{-\infty} u(-\xi)(x_j-\xi)^{1-\alpha} d\xi = \frac{1}{\Gamma(4-\alpha)} \sum_{k=-\infty}^{j} \int_{x_{k-1}}^{x_k} u(\xi)(x_j-\xi)^{1-\alpha} d\xi. \end{aligned}$$

Therefore

$$\mathcal{I}_{ref}^l u(x_j) - I_{ref}^l u(x_j) = \frac{1}{\Gamma(4-\alpha)} \sum_{k=-\infty}^{j} \int_{x_{k-1}}^{x_k} (u(\xi) - s_k(\xi))(x_j-\xi)^{1-\alpha} d\xi.$$

From this point on the proof can follow the same steps as the proof of Theorem 2 in [17]. □

We introduce a lemma that is necessary to prove the stability of the numerical method based on Fourier analysis.

Lemma 1 ([17]). *The coefficients b_m, defined by (11), verify:*

$$|b_{m+1}| < |b_m|,\ m \geq 1;\ \lim_{m\to\infty} b_m = 0;\ \sum_{m=-1}^{\infty} b_m = 0;\ \sum_{m=-1}^{\infty} b_m \cos(m\phi) \leq 0.$$

Theorem 3. *The numerical method (13) is unconditionally stable.*

Proof. The difference operator defined in (14) can be rewritten as

$$\begin{aligned}
\delta^{\alpha}_{\beta,ref} U^n_j &= \frac{1+\beta}{2}\left[\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{j} b_m U^n_{j-m} + \frac{1}{\Gamma(4-\alpha)}\sum_{m=j+1}^{\infty} b_m U^n_{m-j}\right] + \frac{1-\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m U^n_{j+m}\\
&= \frac{1+\beta}{2}\left[\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{j} b_m U^n_{j-m} + \frac{1}{\Gamma(4-\alpha)}\sum_{m=j+1}^{\infty} b_m U^n_{j-m}\right] + \frac{1-\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m U^n_{j+m}.
\end{aligned}$$

The proof of the stability using Fourier analysis consists on inserting a single mode $\kappa^n \mathrm{e}^{ij\phi}$ into the numerical scheme (13), neglecting the source term, and to verify if the amplification factor κ is not larger than 1, for all $\phi \in [0, \pi]$.

Inserting a single mode $\kappa^n \mathrm{e}^{ij\phi}$ into the numerical scheme (13), neglecting the source term, and taking in consideration the previous equality for the reflecting operator, then

$$\begin{aligned}
&\kappa^{n+1}\mathrm{e}^{ij\phi} - \frac{1}{2}\mu_\alpha \kappa^{n+1}\left[\frac{1+\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{i(j-m)\phi} + \frac{1-\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{i(j+m)\phi}\right]\\
&= \kappa^{n}\mathrm{e}^{ij\phi} + \frac{1}{2}\mu_\alpha \kappa^{n}\left[\frac{1+\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{i(j-m)\phi} + \frac{1-\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{i(j+m)\phi}\right].
\end{aligned}$$

Simplifying $\kappa^n \mathrm{e}^{ij\phi}$ on both sides we obtain

$$\begin{aligned}
&\kappa\left\{1 - \frac{1}{2}\mu_\alpha\left[\frac{1+\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{-im\phi} + \frac{1-\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{im\phi}\right]\right\}\\
&= 1 + \frac{1}{2}\mu_\alpha\left[\frac{1+\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{-im\phi} + \frac{1-\beta}{2}\frac{1}{\Gamma(4-\alpha)}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{im\phi}\right].
\end{aligned}$$

If the real part of

$$\left[\frac{1+\beta}{2}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{-im\phi} + \frac{1-\beta}{2}\sum_{m=-1}^{\infty} b_m \mathrm{e}^{im\phi}\right]$$

is negative or zero then $|\kappa(\phi)| \leq 1$. The real part is given by

$$\left[\frac{1+\beta}{2}\sum_{m=-1}^{\infty} b_m \cos(m\phi) + \frac{1-\beta}{2}\sum_{m=-1}^{\infty} b_m \cos(m\phi)\right]$$

and by the previous lemma we can conclude that is non positive. □

4. Numerical experiments

Let U_j^n and u_j^n be the approximate solution and the exact solution respectively at $x_j = j\Delta x$ and $t_n = n\Delta t$, $j \in \mathbb{N}_0$, $n \in \mathbb{N}$. The error and the rate of convergence, at a specific time t_n, are defined respectively by

$$E(\Delta x) = \left(\Delta x \sum_{j=0}^{M} (u_j^n - U_j^n)^2 \right)^{1/2}, \quad \text{Rate} = \frac{\log(E(\Delta x_{\text{new}})/E(\Delta x_{\text{old}}))}{\log(\Delta x_{\text{new}}/\Delta x_{\text{old}})}.$$

Consider the problem with a reflecting wall at $x = 0$ and with a source term defined such that the solution $u(x,t) = 4e^{-t}(2+x)^2(2-x)^2$ is an exact solution of equation (5) with $D = 1$, for $0 < x < 2$. We display the rate of convergence at $t_n = 1$ for $\beta = -0.8, 0, 0.8$ in Figure 2, where for each β the rate is plotted for $\alpha = 1.2, 1.5, 1.8$. We note the expected spatial second order convergence.

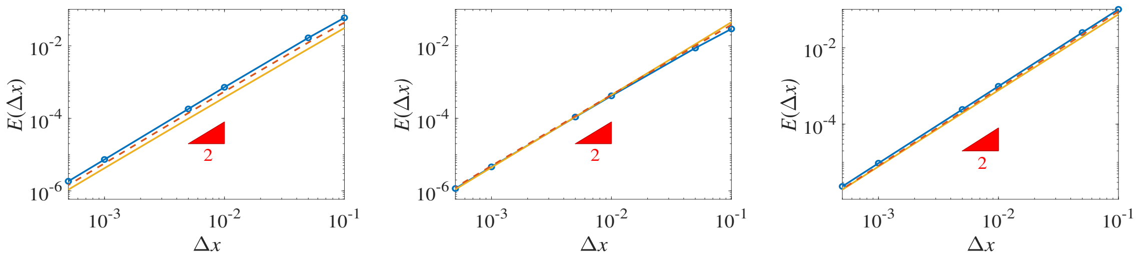

Figure 2: Log-log plot of the error as a function of the space step Δx when $\alpha = 1.2(-\circ-)$, $\alpha = 1.5(--)$, $\alpha = 1.8(-)$. Left to right: $\beta = -0.8, 0, 0.8$. The solid (red) triangle is the reference of second order.

To observe the effect of having a reflecting wall we present the solutions of the problem (5)-(6) with the initial condition $\delta_\epsilon(x) = \frac{1}{\sqrt{\pi}\epsilon} e^{-(x-x_0)^2/\epsilon^2}$, $x_0 = 0.5$, $\epsilon = 0.1$. This initial condition is an approximation of the Dirac delta function since as ϵ goes to zero this function approaches the Dirac delta function.

In Figure 3 we plot, for $t_n = 0.5$, the numerical solutions for the problem with a reflecting wall at $x = 0$ versus the numerical solutions for the problem defined in the open domain to see the differences between both solutions. The solutions are plotted for two values of α, $\alpha = 1.4, 1.8$ and three values of β, $\beta = -0.8, 0, 0.8$. In all cases the solution of the problem with a reflecting wall is above the solution of the problem defined in the open domain. For smaller values of α, the effect of the wall is highly visible between the boundary and the support of the initial condition $x_0 = 0.5$. For larger values of α the effect of the wall is also significant beyond the value $x_0 = 0.5$. In general, we can say that the area that is under the solution in the interval $(-\infty, 0)$, for the problem defined in the open domain, it accumulates under the solution of the problem with the reflecting wall in the positive semi-infinite domain, specially near the boundary.

5. Conclusion

We have shown how to formulate a superdiffusion model with a reflecting wall and presented a second order implicit numerical method unconditionally stable to determine its numerical solutions. The influence of the boundary condition in the final solution has been illustrated by displaying the solution of the same model without boundaries versus the model with a reflecting boundary.

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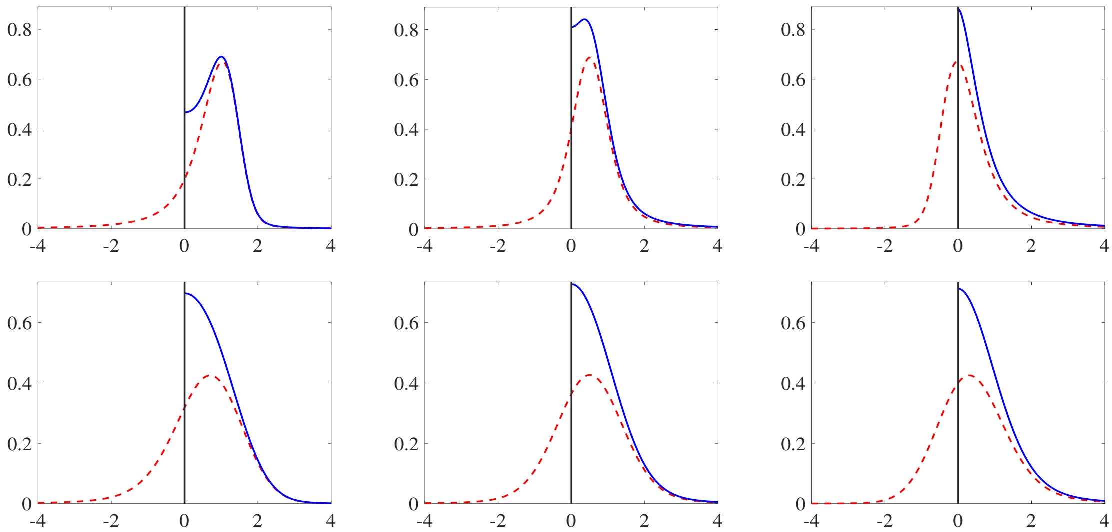

Figure 3: Plot of the numerical solutions for $D = 1$ and $t_n = 0.5$ in the infinite domain $(--)$ versus in the semi-infinite domain with a reflecting wall at $x = 0$ $(-)$. Left to right: $\beta = -0.8, 0, 0.8$; Top: $\alpha = 1.4$; Bottom: $\alpha = 1.8$.

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