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Evaluation of Fractional Dispersion Models

by

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Abstract

The usual second order advection-diffusion equation is known to under predict dispersion in turbulent flows. It is thought we can replace the diffusion term with a fractional diffusion term to better predict the dispersion.

The main concern of this work will be the numerical methods used for solving the fractional diffusion equation. Before we are able to begin with the derivation of the numerical schemes, an understanding of some fractional calculus is needed, we will therefore give a disscusion on this and detail the definitions and derivatives which are needed for our numerical methods.

We notice in the literature that it is mainly finite difference methods that have been proposed. We shall see that this is perhaps the most obvious and straight forward numerical method to develop given the definitions for fractional derivatives. Due to the non-local nature of the fractional derivative the finite difference approach is computationally expensive as it usually requires a large number of degrees of freedom to obtain an accurate solution. We will therefore be interested in developing other numerical schemes in particular schemes based on non-local methods such as the spectral method.

Acknowledgments

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Declaration

I confirm that this is my own work and the use of all material from

Chapter 1

Introduction

1.1 Why Fractional Dispersion

The second order advection-dispersion equation is usually used to model dispersion in flows. However in complex flows such as turbulent flows this model is no longer adequate, in fact it under predicts dispersion.

In non turbulent flows the dispersion of a contaminant is driven by the mean flow velocity and local interactions between particles i.e. particles push each other. This results in a series of small amplitude, random displacements of the contaminant particles and is known as Brownian motion. However, in complex flows such as flow through porous medium or turbulent flows it is now possible to have large variations from the mean velocity in the flow. This results in particles of the contaminant being dispersed large distances in the flow. Brownian motion is no longer an adequate description for this type of dispersion, we wish to model a butions. Unlike the Gaussian distribution, which is the PDF of Brownian motion, Lévy distributions have heavier tails and an infinite variance which implies they allow contaminant particles to be dispersed or jump large distances. Where the second order advection-dispersion equation is describing Brownian motion, Lévy motion can be described by a fractional order advection-diffusion equation. Therefore we wish to use the fractional advection-diffusion equation to model dispersion in these complex flows, with the purpose that this will give us a more realistic model of the dispersion.

The fractional advection-dispersion equation only uses a fractional derivative on the diffusion term therefore it is the diffusion term that will be which take into account extreme market volatility. Here instead of modelling particle jumps price jumps are modelled see [8].

One example from [14] talks about anomalous diffusion in fluids which are partitioned into convective cells e.g a steady state atmosphere. Diffusion here is characterised by two types of motion, one is the fast convective motion within a convective cell and the other is the random walk behaviour for the crossing of the convective cells, this type of motion leads to the diffusion behaviour at large scales.

There are also many papers on diffusion through porous media in aquifers see [2, 13] the ideas developed in this area will be of particular use to us. A specific

Chapter 2

Ordinary Diffusion and Fractional Diffusion

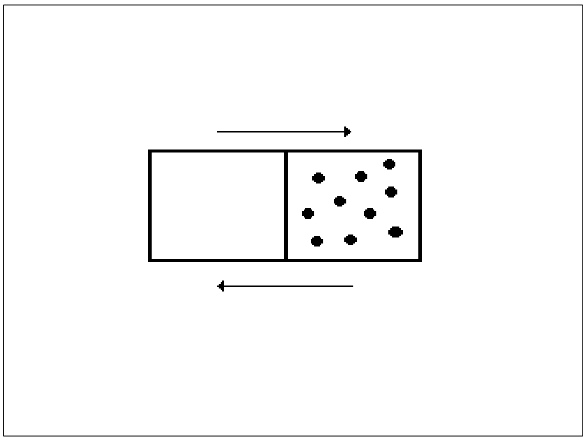


Figure 2.1: Particles diffusing between two volumes

This idea leads us to Fick's Law,

$$F = -K\frac{\partial c}{\partial x}, \tag{2.1}$$

which states that the particle flux is proportional to the concentration gradient acting towards the area of lower concentration [4]. The diffusion equation can then be obtained by taking changes of the concentration in the volume with respect to time, this is equal to the negative of the rate of change of the flux from the volume giving,

$$\frac{\partial c}{\partial t} = -\frac{\partial F}{\partial x} = \frac{\partial}{\partial x}\left(K\frac{\partial c}{\partial x}\right). \tag{2.2}$$

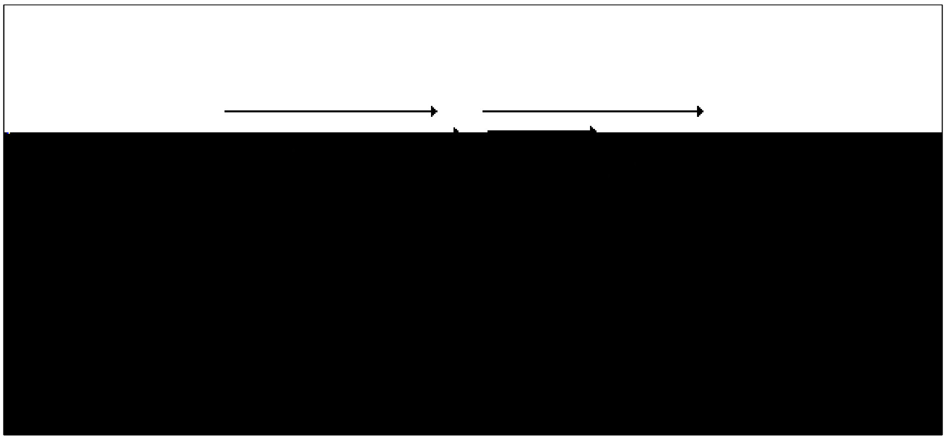
The diffusion equation. K is known as the diffusion coefficient.

It is important to see that Fick's law is a local process, Fig. 2.1, particles are only transported to other volumes next to their current volume in the flow, which is caused by the gradient of the concentration between the two volumes. 'Again from Crank [4] it is stated that Fick's law is only consistent for an isotropic medium which is a flow in which its structure and diffusion proper neighbourhood of any point'. This presents a problem when considering diffusion in turbulent flows.

In turbulent flows diffusion is due to the random fluctuations in the velocity, this can randomly transport particles of the contaminant over larger distances i.e beyond the local volumes. This is easy to imagine if we consider the analogy of rotating eddies in a flow, here the velocities in the flow varies greatly. Therefore we want a method for modelling diffusion that provides a more global process. [13] provides a discussion on this for the case where velocity variations are produced by flow through porous medium rather than eddies. To develop this new method of modelling diffusion we first need to look at Brownian motion which will lead us on to Lévy motion and the global process.

2.2 Brownian Motion

To introduce the idea of Brownian motion we first find the solution of the second order diffusion Eq. (2.2) using Fourier transforms, see [8]. To do t



Chapter 3

Fractional Calculus

Before we begin to develop any sort of numerical scheme we need to become familiar with fractional derivatives and how they are defined. If we consult [12] we see that there are many definitions for the fractional derivative and ways of defining the derivatives of standard functions.

3.1 Main Definition

Perhaps the easiest way to see where one of these definitions comes from is to first

Here we are using the notation,

$$D_-^\alpha = \frac{d^\alpha c}{d(-x)^\alpha}$$

and

$$D_+^\alpha = \frac{d^\alpha c}{dx^\alpha}.$$

$\frac{1}{2}(1-\beta)$ and $\frac{1}{2}(1+\beta)$ gives the probability of whether a particle will jump backwards or forwards respectively, with $-1 \leq \beta \leq 1$. The use of the β value allows us to select whether a particle will di�use more to the left or to the right. If $\beta = 1$ we just get Eq. (3.2) and if $\beta = -1$ we just get Eq. (3.3). We can see from these definitions that the fractional derivative uses a sum of all values over the domain.

which is defined over the domain [x, ∞]. Eqs. (3.5).(3.6) can then be shortened to the following

$$D^{\alpha}_{\pm} f(x) = \frac{(\pm 1)^{n}}{\Gamma(n-\alpha)} \frac{d^{n}}{dx^{n}} \int_{0}^{\infty} \xi^{n-\alpha-1} f(x \mp \xi) d\xi, \tag{3.7}$$

in these cases n is the smallest integer larger than the real number α see [1] for these definitions.

We can see some equivalence in these definitions as under certain conditions we can obtain the Grunwald sum from the Riemann-Louiville definition. These certain as a series expansion if exponentials [12]. If

$$f = \sum c_j e^{b_j x}, \tag{3.9}$$

the derivative can then be expressed as,

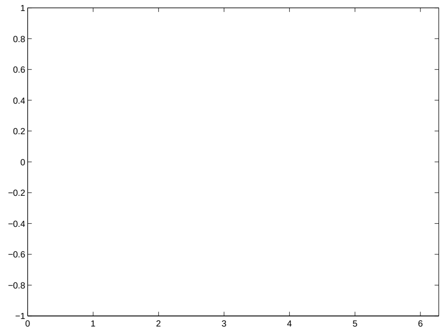
$$\frac{d^\alpha f}{dx^\alpha} \equiv \sum_{j=0}^{\infty} c_j b_j^\alpha e^{b_j x}. \tag{3.10}$$

3.3 Standard Derivatives

If we are to develop a spectral method to numerically model the fractional diffusion equation then we need derivatives for functions such as cos(x), sin(x) and e^x. Firstly we shall look at the fractional derivative for cos(x), [12] gives the derivative as,

$$\frac{d^\alpha}{dx^\alpha}\cos(x) = \cos\left(x + \frac{\pi\alpha}{2}\right) + \frac{x^{-2-\alpha}}{\Gamma(-\alpha-1)} - \frac{x^{-4-\alpha}}{\Gamma(-\alpha-3)} + \cdots \tag{3.11}$$

however,


1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
0
1
2
3
4
5
6

transport of particles further than the immediate points. These weights indicate that using fractional diffusion could be a good model for diffusion in turbulent flows.

When it comes to developing our finite difference scheme it is beneficial to use the same definition of the weights for both fractional and regular diffusion. However, this presents a problem if we use Eq. (3.16) since the Gamma function is not defined for negative integers, see Fig. 3.5.

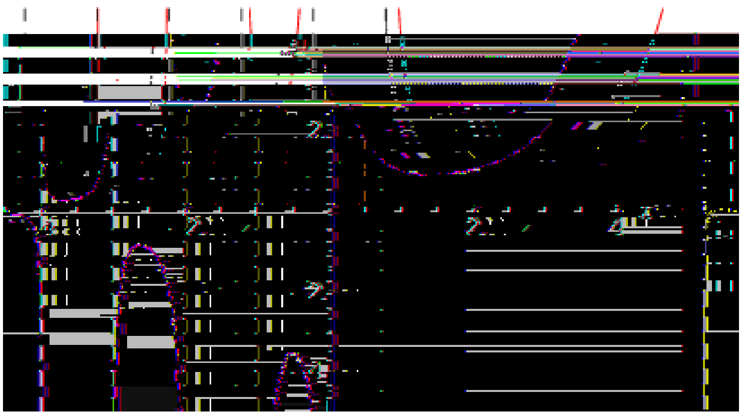


Figure 3.5: Plot of Gamma functions, [16]

To allow us to use the same definition for both cases we use Eq. (3.17) for the weights as given by Meerschaert and Tadjeran [10].

$$\begin{aligned} w_0 &= 1 \\ w_1 &= -\alpha \\ w_k &= \frac{(-\alpha)(-\alpha+1).....(-\alpha+k-1)}{k!} \text{ for all } k \geq 2, \end{aligned} \tag{3.17}$$

This can be derivived from Eq. (3.16) to do this we use the gamma function recursion relationship,

$$\Gamma(x+1) = x\Gamma(x), \tag{3.18}$$

and its reflection identity,

$$\Gamma(-x) = \frac{-\pi \mathrm{cosec}(\pi x)}{\Gamma(x+1)}. \tag{3.19}$$

To show how this works we will look at a select few cases for $k = 0, 1$. Taking $k = 0$ we get the weight as,

$$w_0 = \frac{\Gamma(-\alpha)}{\Gamma(-\alpha)\Gamma(1)}$$

for an integer we have,

$$\Gamma(n) = \frac{n!}{n}$$

and so we get $w_0 = 1$.

Moving on to $k = 1$ we have the weight as,

$$w_1 = \frac{\Gamma(1-\alpha)}{\Gamma(-\alpha)\Gamma(2)},$$

using the reflection identity Eq. (3.19) we get,

$$w_1 = \frac{\Gamma(1-\alpha)\Gamma(\alpha+1)}{-\pi \mathrm{cosec}(\pi x)},$$

then using the recursion relationship Eq. (3.18) and the reflection identity again we get,

$$w_1 = \frac{-\alpha\Gamma(\alpha+1)(-\pi \mathrm{cosec}(\pi x))}{\Gamma(\alpha+1)(-\pi \mathrm{cosec}(\pi x))},$$

Chapter 4

Finite Difference Approximations

The majority of methods to solve the fractional diffusion equation use a finite difference approach see [10, 9, 15].

4.1 Numerical Approximation

Although the definitions for fractional derviatives suggest a finite difference scheme should be straight forward to develop, it is important to take make sure the scheme becomes the usual central difference scheme for a second order derivative

$$\frac{\partial^2 c}{\partial x^2} \approx c_{i-1}$$

Our new shifted definitions for the fractional derivative are,

$$\frac{d^{\alpha} f}{dx^{\alpha}} \equiv \lim_{\Delta x \to 0} \frac{1}{\Delta x^{\alpha}} \left[\sum_{k=0}^{\infty} \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} f\left(x-(k-1)\Delta x\right) \right] \tag{4.1}$$

and

$$\frac{d^{\alpha} f}{d(-x)^{\alpha}} \equiv \lim_{\Delta x \to 0} \frac{1}{\Delta x^{\alpha}} \left[\sum_{k=0}^{\infty} \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} f\left(x+(k-1)\Delta x\right) \right] . \tag{4.2}$$

the concentrate for the next time step. We then be repeate for however many time steps we require, with the chosen boundary conditions being applied at each stage. Meerschaert, Tadjeran and Scheffler [10, 15] look at implicit and semi implicit methods and the stability regions for the methods. Developed in [15] is an equivalent Crank-Nicolson method for the fractional diffusion term. We however will only consider the explicit case for ease of implementation and to allow us to move on to other methods.

This method is easily extended to two dimensions. Schemes for doing this are explored by Meerschaert, Tadjeran and Scheffler [9]. The basic way to extend the scheme we already have is to just use another summation for the y derivative. Using this fractional approach does not limit us to using the same value for α for both x and y derivatives, we can use different values that allow us to have a more variable model for diffusion. Therefore we now want to approximate the equation,

$$\frac{\partial c}{\partial t} = K_\alpha \frac{\partial^\alpha c}{\partial x^\alpha} + D_\eta \frac{\partial^\eta c}{\partial x^\eta} \tag{4.6}$$

where $1 \le \alpha \le 2$ and $1 \le \eta \le 2$ and K_α, D_η are the diffusivity constants for either the x or y dimension. This is easily done by using the ideas developed in the previous section giving us our numerical scheme as,

$$\begin{aligned} c_{i,j}^{n+1} = c_{i,j}^{n} &+ \frac{K_\alpha \Delta t}{\Delta x^\alpha}\left(\frac{1}{2}\sum_{k=0}^{i} w_k c^n_{i-(k-1),j} + \frac{1}{2}\sum_{k=0}^{N-i} w_k c^n_{i+(k-1),j}\right) \\ &+ \frac{D_\eta \Delta t}{\Delta x^\eta}\left(\frac{1}{2}\sum_{k=0}^{j} w_k c^n_{i,j-(k-1)} + \frac{1}{2}\sum_{k=0}^{N-j} w_k c^n_{i,j+(k-1)}\right). \end{aligned} \tag{4.7}$$

Here i denotes the x position, j denotes the y position and n denotes the time we can choose the required set of summations to model that particular di�usion. Further to this, we could also use a modification of our symmetric scheme in one dimension where we can pick the value of

This has the exact solution

$$u(x,t) = e^{-t}x^3.$$

4.2.2 Right Scheme Test

To check the right sided derivative we can modify this example by replacing the x with $1-x$. This gives us a suitable function that the right sided derivative will work for. The example we use now becomes,

$$\frac{\partial u(x,t)}{\partial t} = d(x)\frac{\partial^{1.8}u(x,t)}{\partial x^{1.8}} + q(x,t)$$

at each point squared. This is perhaps best given in the following expression,

$$\text{error} = \left(\frac{\int (e_a - e_n)^2 dx}{\int e_a{}^2 dx} \right)^{\frac{1}{2}}. \tag{4.8}$$

This is known as the L_2 error.

We then fix the time step at 0.0001, change the space step and the calculate the error Eq. (4.8) for each space step. The results for spaces steps between 1/10 and 1/100 are given in Tab. 4.1.

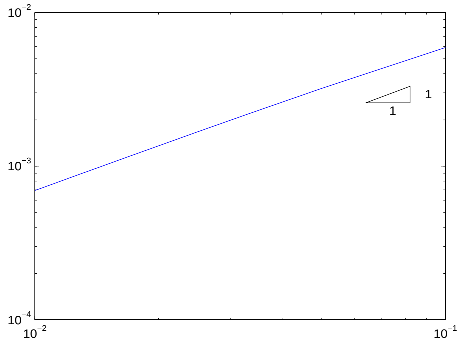
Δx	left error	right error
1/10	0.0059	0.0059
1/20	0.0032	0.0032
1/30	0.0022	0.0022
1/40	0.0017	0.0017
1/50	0.0014	0.0014
1/60	0.0011	0.0011
1/70	0.001	0.001
1/80	0.0009	0.0009
1/90	0.0008	0.0008
1/100	0.0007	0.0007

Table 4.1: Error for left and right sided schemes

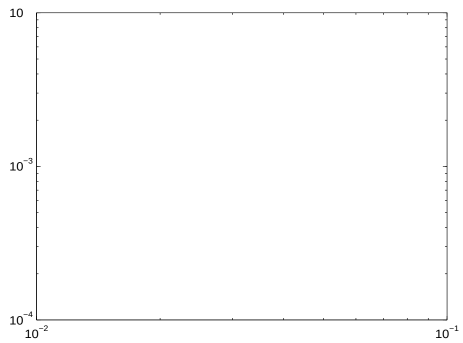
We only have an analytical solution for one sided problems and so the errors are calculated using either the left or right sided derivative, however we can see that both schemes give the same error. If we then plot these results on a log log scale we can get the convergence rate that is almost linear, see Fig. 4.2.

4.2.4 Stability

We now consider the stability of the schemes, notice that for the error analysis we used a time step of 0.0001. This allows us to obtain a stable solution for all sizes



(a) Left sided scheme



4.3.1 Test of 2D Scheme

The example we use to test our numerical scheme as given in [9] is a follows, the fractional differential equation we wish to solve is,

$$\frac{\partial u(x,y,t)}{\partial t} = d(x,y)\frac{\partial^{1.8} u(x,y,t)}{\partial x^{1.8}} + e(x,y)\frac{\partial^{1.6} u(x,y,t)}{\partial y^{1.6}} + q(x,y,t).$$

This is defined on a rectangular domain $0 < x < 1$, $0 < y < 1$ for time $0 \le t \le 1$. The diffusion coefficients $d(x,y)$ and $e(x,y)$ are given as,

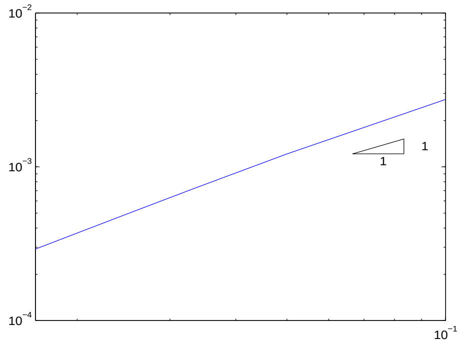
$$d(x,y) = \Gamma(2.2)x^{2.8}y/6 = 0.18363375x^{2.8}y,$$

$$e(x,y) = 2xy^{2.6}/\Gamma(4.6) = 0.1494624672xy^{2.6}.$$

We set the time step $\Delta t = 0.001$ and the space steps $\Delta x = \Delta y = 0.1$ and run up to a final time of one second. Fig. 4.3 and Fig. 4.4 show the numerical and analytical solutions to the example.

4.3.2 Accuracy

To assess the accuracy of the scheme, we use the same method as for one dimension


10^−2
10^−3
10^−4
10^−1
1
1

space step for the next time step.

$$\begin{aligned} c^{n+1}_{i,j} &= c^{n}_{i,j} + \Delta t \left(-\frac{u}{\Delta x}\left(c^{n}_{i,j} - c^{n+1}_{i,j} \right) \right. \\ &+ \left. \frac{K_\eta}{\Delta y^\eta} \left(\frac{1}{2}\sum_{k=0}^{j} w_k c^{n}_{i,j-(k-1)} + \frac{1}{2}\sum_{k=0}^{N-j} w_k c^{n}_{i,j+(k-1)} \right) \right) \end{aligned} \tag{4.11}$$

To get our numerical result we use the domain $0 \le x \le 10$, $0 \le y \le 10$ with the initial condition of a small section in the middle of the $x = 0$ axis equal to one and everywhere else equal to zero. To simulate a dye being continuously introduced into the tank we set our boundary condition so that it is one for a small section in the middle of the $x = 0$ axis and zero elsewhere. What we are doing is setting the boundary back to its initial value each time step. We do not want to allow to pass through the horizontal walls of the tank so the boundary conditions for both y axis are set to zero. To simulate fluid begin able to flow through the far boundary we use a Neumann boundary condition so $\frac{\partial}{\partial x}c(10,t) = 0$. In the solutions obtained $\Delta x = \Delta y = 0.2$, $\Delta t = 0.002$, the final time is 10 seconds, $u = 2$ and $K_\eta = 1$. See Fig. 4.17.

These are only preliminary results, further investigation needs to go into checking there validity. A start would be to calculate the width of the plume for the various values of η. Although from these we can see that as η decreases we get a result that looks more linear.

Chapter 5

A numerical scheme using Spectral Methods

We now wish to develop a spectral method to numerically calculate our solution. Our idea is that because spectral methods use global data rather than data from immediate surrounding points, they should be better suited to fractional diffusion.

5.1 A spectral method for fractional diffusion

scheme gives us the following system of ODEs,

$$\int_0^2 \phi_l(x)\phi_l(x)dx \left(\frac{a_l^n - a_l^{n+1}}{\Delta t}\right) = K \sum_{k=0}^{N} \int_0^2 \frac{d^\alpha \phi_k(x)}{dx^\alpha}\phi_l(x)dx a_l^{n+1}.$$

Like the finite element method we can define a mass matrix M as,

$$M_{kl} = \left(\int_0^2 \phi_l(x)\phi_l(x)dx\right)\delta_{kl}$$

and a stiffness or diffusivity matrix D as,

$$D_{kl} = \int_0^2 \frac{d^\alpha \phi_k(x)}{dx^\alpha}\phi_l(x)dx.$$

This leaves us with a matrix system in the form of,

$$(M - D\Delta t)a_l^{n+1} = M a_l^n \tag{5.3}$$

that needs to be solved over time. Then for time steps where the actual solution is required we substitute the $a_k(t)$ into Eq. (3.9). Here we have discritized the time step implicitly but it can just as easily be solved explicity or using any other integration scheme.

One other thing to consider is obtaining the initial condition for the $a_k(t)$ this can formulated as so,

$$\int_0^2 \sum_{k=0}^{N} a_k(0)\phi$$

and again using the orthogonality condition there is only a non zero solution when

5.2.1 Cosine Expansion Function

For the cosine expansion function we take $\phi_k(x) = \cos(kx)$ and $\phi_l(x) = \cos(lx)$ this gives the mass matrix as,

$$M_{kl} = \int_0^2 \cos(kx)\cos(lx)dx.$$

For cosine we have the orthogonality condition,

$$\int_0^2 \cos(mx)\cos(nx)dx = \begin{cases} 2\pi & \text{if } m = n \\ 0 & \text{if } m \neq n, \end{cases}$$

this means that the mass matrix only has diagonal entries. The stiffness matrix can be defined as,

$$D_{kl} = \int_0^2 \frac{d^\alpha \cos(kx)}{dx^\alpha} \cos(lx)dx.$$

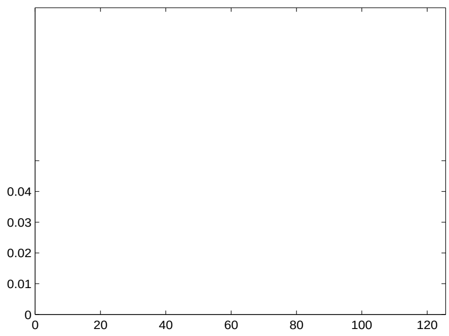
Using the definitions for the fractional derivative of cosine we see that the orthogonality condition is no longer valid so the derivative involves a shifted cosine wave. Therefore [illegible]

function is not the best choice.

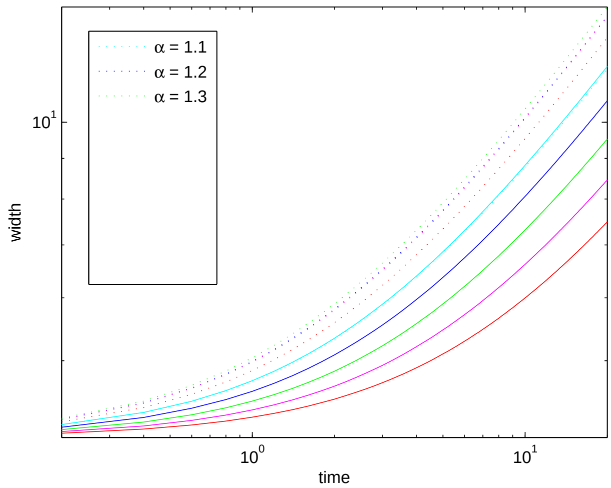
On the positive side we also find that the complex exponential case is valid on any domain.

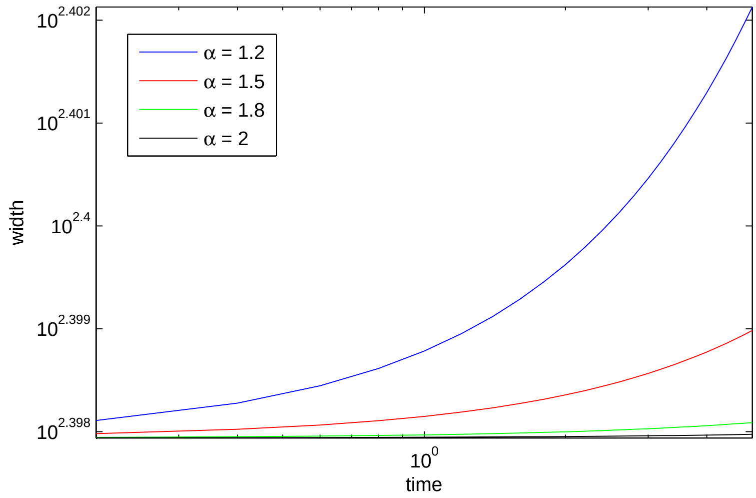
5.3 Results and Comparison with Finite Difference Scheme

To look at a range of results and compare to our finite difference scheme we shall use the spectral method that uses complex exponential expansion functions. This

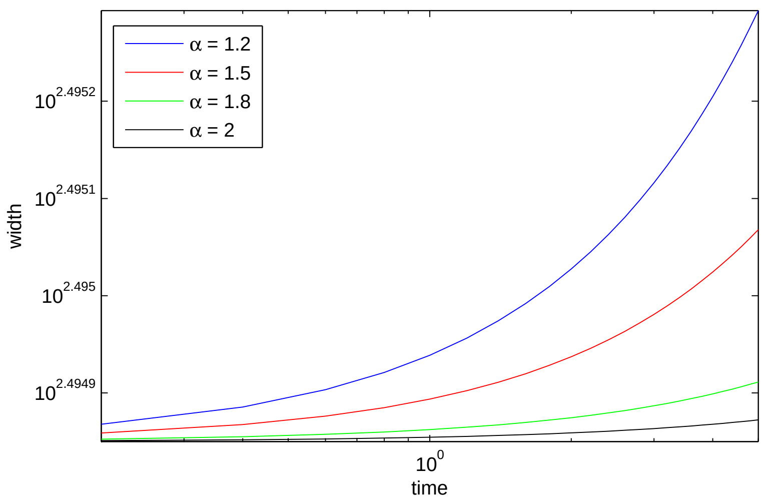

0.04
0.03
0.02
0.01
0
0
20
40
60
80
100
120

We then evaluate the standard deviation at various times and calculate its evolution see Fig. 5.4 this gives a very similar result to that displayed in Fig. 4.10.





(a) Spectral method



(b) Finite difference method

Figure 5.5: Comparision of Plume Widths

Chapter 6

Conclusions and Future Work

6.1 Fractional Diffusion

We have determined that Levy distributions are a solution to the fractional diffus-

Further work can be done to fit the fractional diffusion equation to a real world example and assess the how well it fits the data over using the ordinary second order diffusion equation.

6.2ta.

modelling an advecting plume. Again only a few results have been produced here. Further investigation would allow us to determine whether using the fractional diffusion term allows a better fit for real life diffusing f

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