NEW NUMERICAL ALGORITHM TO COMPUTE $E_\alpha(-z^\alpha)$

Botomanovatsara[1], S.H. Rakotonasy[2], N.M.V.Ravonimanantsoa[3], A.Ratiarison[4]
[1, 4]Université d'Antananarivo, Laboratoire DYACO Département de Physique, Faculté des Sciences BP 906, Madagascar
[2]Université d'Antananarivo, Département Mathématiques et Informatique, Faculté des Sciences BP 906, Madagascar
[3]Université d'Antananarivo, ESPA, Département Télécommunication BP 1500, Madagascar

ABSTRACT
The present paper deals with a new method to compute the Mittag-Leffler function $E_\alpha(-z^\alpha)$ for arbitrary complex argument $z \in \mathbb{C}$ and parameter $\alpha \in \mathbb{R}^+$. Such function is known to play a fundamental role in fractional differential equations with various applications in physics given the fact that Mittag-Leffler function interpolates smoothly between exponential and algebraic functional behaviour. The method is based on calculation of the inverse of the mapping $Id + \Lambda I^\alpha$ where Id, $I^\alpha$are respectively the identity and Riemann-Liouville integral operator of order. Numerical implementation of the present method is found to be fast and easy. In the other hand, its comparison with existing methods as the Pade algorithm and the integral representation shows good accuracy. Thus, the present method appears to be a useful alternative way to compute Mittag-Leffler function $E_\alpha(-z^\alpha)$.Finally, an application to anomalous transport in porous media is carried out to illustrate the interest of the method.

KEYWORDS: *Algorithm, Mittag-Leffler function, fractional partial differential equation, anomalous transport.*

I. INTRODUCTION

Recently, scientists have focused on the Mittag-Leffler function for several reasons. In particular, MittagLeffler functions are building blocks of fundamental solutions of many ordinary differential equations involving derivatives of non-integer order, thus extending the role of exponentials. Such equations arise in various domains of physics, including generalized fractional kinetic equations, diffusive transport and coupled systems [15], [16], [27] [19], [20],[21], [22]. It motivated addressing mathematical property of Mittag-Leffler functions [23], [24], [25], [26], [28], [29],.Mittag-Leffler functions also appear in the solution of boundary value problems with integro-differential equations of Volterra [18].The function of Mittag-Leffler is used in other domains, such as fluid flow, rheology, electrical networks, probability theory and statistical distribution. Furthermore, characteristics and applications of this function can be found in the following works [19], [20], [21], [22], [23], [24], [25], [26], [28], [29], [30]. In the present paper, we introduce and validate a new method to calculate Mittag-Leffler functions $E_\alpha(-z^\alpha)$ for α between 0 and 1 with z been a complex number. The method is based on triangular matrix inversion at each step. With only the last elements of the matrix need to be re-actualized at each time steps. Hence, the method is fast and its generalization is easy. Comparisons with other existing methods show a good accuracy of our method. Note that a numerical evaluation of $E_{\alpha,\beta}(-x)$ is treated by J.W. hanneken and Al. in [33]. The paper is written in five parts. In next section we will detail the basis of the method. Comparison with other existing methods is given in the section 3. The fourth section will be devoted to an application related to $\boldsymbol{E_{\alpha}(-z^{\alpha})}$. We end the paper with some concluding remarks about the present work.

II. Description Of The Calculation Method

2.1. Definition of generalized Mittag-Leffler function

Function ez that plays an essential role in ordinary differential equations, was generalized by G.M. Mittag-Leffler in [1] and [2] also studied by A. Wimam [34], [35].This basic function that generalize the exponential can be defined as.

$$E_{\alpha}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+\alpha k)} \alpha \in \mathbb{R}_+, \mathcal{Z} \in \mathbb{C}, \quad (1)$$

Where Γ() is the gamma function defined as

$$\Gamma(z) = \int_0^{+\infty} t^{z-1} e^{-t} dt$$

The function $E_{\alpha}(z)$ satisfies ordinary differential equations: differently from that happens for $= 1$. Two-parameter functions $E_{\alpha,\beta}(z)$ of the Mittag-Leffler type introduced by Agarwal [3], according to

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta+\alpha k)} \ \alpha \in \mathbb{R}_+, \beta \in \mathbb{R}, z \in \mathbb{C}, \ (2)$$

The link between the $E_{\alpha,\beta}(z)$(with $E_{\alpha}(z) = E_{\alpha,1}(z)$) and their derivatives are detailed in [46].
The operator $(Id + \Lambda I^{\alpha})^{-1}$ is present in the expression which calculates the density of mobiles particles and the flux in fractal MIM model (f-MIM).
This model was used to represent the anomalous transport. As we shall see in the following that this operator applied to the function 1 is not other than $E_{\alpha}(-z^{\alpha})$.
Analytic solutions to fractional-order differential equations are often expressed in terms of the Mittag-Leffler function, and so we need to know the best scheme that computes this special function, which is the topic of this section.

2.2. Method to estimate $E_{\alpha}(-z^{\alpha})$

-Riemann-Liouville fractional integral

In the classical calculus of Newton and Leibniz, Cauchy reduced the calculation of an n-flod integration of the function $f(x)$ into a single convolution integral possessing an Abel (power law) kernel,

$$I^n = \int_0^x \int_0^{x_n-1} \dots \int_0^{x_1} f(x_0) d_{x_0} \dots d_{x_{n-2}} d_{x_{n-1}}$$
$$= \frac{1}{(n-1)!} \int_0^x \frac{1}{(x-x')^{1-n}} f(x') dx' \ n \in \mathbb{N}, x \in \mathbb{R}_+, \quad (3)$$

Where I^n is the n-flod integral operator with $I^0 f(x) = f(x)$. Liouville and Riemann analytically continued Cauchy's result, replacing the discrete factorial $(n-1)!$ with Euler's continuous gamma function $\Gamma(n)$, noting that $(n-1)! = \alpha(n)$,

$$I^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_0^x \frac{1}{(x-x\prime)^{1-\alpha}} f(x') dx' \alpha, x \ \in \mathbb{R}_+, \qquad (4)$$

Where $I^{\alpha}$is the Riemann-Liouville integral operator of order α , which commutes (i.e $I^{\alpha} I^{\beta} f(x) = I^{\beta} I^{\alpha} f(x) = I^{\alpha+\beta} f(x), \forall \alpha, \beta \in \mathbb{R}_+$)
A brief history of the development of fractional calculus can be found in Ross [49] and Miller and Ross (C h a p t e r 1) [50]. A survey of many emerging applications of the fractional calculus in areas of science and engineering can be found in the recent text by Podlubny (Chapter 10) [51].

-Inverting $Id + \Lambda I^{\alpha}$

The Mittag-Leffler function $E_{\alpha}(-\Lambda t^{\alpha})$ can also be obtained by integring a fractional operator. We see it for real values of Λ and t and pass to complex arguments upon rescaling. A numerical approximation of $E_{\alpha}(-\Lambda t^{\alpha})$will than be deduced.

A look at the Laplace transform $\frac{1}{\lambda(1+\Lambda\lambda^{-\alpha})}$ of $E_\alpha(-\Lambda t^\alpha)$ suggest doing $E_\alpha(-\Lambda t^\alpha) = (Id + \Lambda I_0^\alpha)^{-1}\, for\ t \in \mathbb{R}^+$, provided the inverse makes sense.
In fact, its exist and can be expanded in Neumann series, in spaces where fractional integrals are small, whatever the value of _ that even can be complex.
Such spaces are, for instance, the $X_{x,T} = \{f/\|e_{-x}f\|_{L^P[0,T]} < \infty\}$, with $e_{-x}(t) = e^{-x^t}$.
The lemma 3 of [45] states that $\|e_{-x}I_0^\alpha, +f\|_{L^P[0,T]} \leq X^{-\alpha}\|e_{-x}f\|_{L^P[0,T]}$ for every f in $X_{x,T}$
For each $T > 0$ and each complex number Λ choosing$X_n > 0$ such that $|\Lambda|X^{-\alpha} < 1$ yelds that the Neumann serie $\sum_{n\geq 0}(-\Lambda I_{0,+}^\alpha)^n$ converges and we have:

$$E_\alpha(-\Lambda t^\alpha) = (Id + \Lambda I_{0,+}^\alpha)^{-1}$$

For $t > 0$ and $\Lambda\ in\ \mathbb{C}$

III. COMPARATIVE STUDY

3.1. Integral representations of the Mittag-Leffler function

Integral representations play a prominent role in the analysis of entire functions. For the Mittag-Leffler function such representations in form of an improper integral along the Hankel loop have been treated in the case $\beta = 1$ and in the general case with arbitrary β.
They use contours $\alpha(\rho;\varphi)$ of the complex plan indexed by $\rho > 0$ and$0 < \varphi' \leq \pi, \alpha(\rho;\varphi) = S_{-\varphi} \cup C_\varphi(0,\rho) \cup S_\varphi$consisting three parts representedon figure (3.1). Elements $S_{\pm\varphi}$are defined by• arrays $S_{\pm\varphi} = \{\lambda/\arg\lambda = \pm\varphi, |\lambda| \geq \rho\}$;

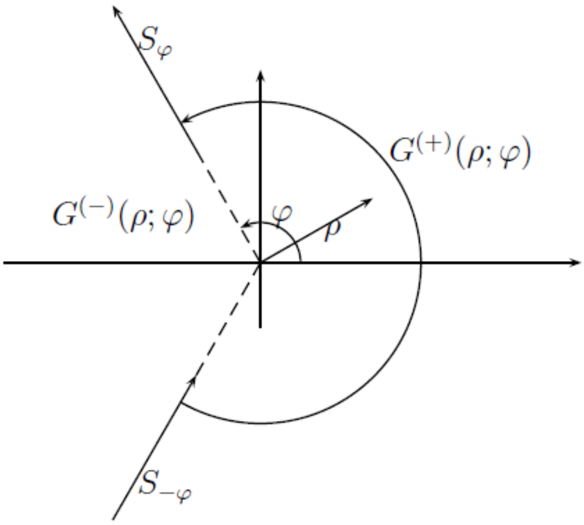

Figure 1: The contourα(ρ; φ)[47]

circular arcs $C_\varphi(0{:}\rho)$ are defined by $C_\varphi(0{:}\rho) = \{-\varphi \leq arg\lambda \leq \varphi\}$ofcircumference.
In the general case $0 < \varphi < \pi$, the complex plane is divided into two partsby $\alpha(\rho;\varphi)$domain $G^{(-)}(\rho;\varphi)$ is at the left of the contour, while domain$G^{(+)}(\rho;\varphi)$ stays on his right.
For $\varphi = \pi$ the contour $\alpha(\rho;\varphi)$is composed of the circle $|\lambda| = \rho$and $-\infty < \lambda \leq -\varphi$. In this case, domain $G^{(-)}(\rho;\varphi)$ becomes a disk of radius $|\lambda| < \rho$,while $G^{(+)}(\rho;\varphi)$ becomes the area $\{\lambda : |arg\lambda| < \pi, |\lambda| > \rho\}$. let$0 < \alpha < 2$, β_ an arbitrary number and ' a positive number such that:

$$\frac{\alpha\pi}{2} < \varphi \leq min\{\pi, \alpha\pi\} \quad (5)$$

So we have the integral representation of the Mittag-Leffler function:

$$E_{\alpha,\beta}(z) = \frac{1}{2i\pi\alpha}\int_{\alpha(\rho;\varphi)} \frac{e^{\lambda^{1/\alpha}}\lambda^{(1-\beta)/\alpha}}{\lambda - z} d\lambda\,, z \in G^{(-)}(\rho;\varphi) \qquad (6)$$

and

$$E_{\alpha,\beta}(z) = \frac{z^{(1-\beta)/\alpha} e^{z^{1/\alpha}}}{\alpha} \frac{1}{2i\pi\alpha} \int_{\alpha(\rho;\varphi)} \frac{e^{\lambda^{1/\alpha}} \lambda^{(1-\beta)/\alpha}}{\lambda - z} d\lambda, z \in G^{(+)}(\rho;\varphi). \quad (7)$$

If β is a real number, then the equations (6) and (7) can be written in forms more appropriate to the numerical approach. In particular, if $0 < \alpha \le 1, \beta \in \mathbb{R}, |\arg \lambda| > \alpha\pi, z \neq 0$, then:

$$E_{\alpha,\beta}(z) = \int_{\rho}^{\infty} K(\alpha,\beta,\chi,z) d\chi + \int_{-\alpha\pi}^{\alpha\pi} P(\alpha,\beta,\varphi,z) d\varphi, \ \rho > 0 \quad (8)$$

$$E_{\alpha,\beta}(z) = \int_{\rho}^{\infty} K(\alpha,\beta,\chi,z) d\chi, \ if \ \beta < 1 + \alpha \quad (9)$$

$$E_{\alpha,\beta}(z) = -\frac{1}{z} - \frac{\sin(\alpha\pi)}{\alpha\pi} \int_{\rho}^{\infty} \frac{e^{-\chi^{1/\alpha}}}{\chi^2 - 2\chi z \cos(\alpha\pi) + z^2} d\chi, \ if \ \beta = 1 + \alpha \quad (10)$$

in which:

$$K(\alpha,\beta,\chi,z) = \frac{\chi^{(1-\beta)/\alpha} e^{-\chi^{1/\alpha}}}{\alpha\pi} \frac{\chi \sin[\pi(1-\beta)] - z \sin[\pi(1-\beta) + \alpha)]}{\chi^2 - 2\chi z \cos(\alpha\pi) + z^2}$$

$$P(\alpha,\beta,\varphi,z) = \frac{\rho^{1+(1-\beta)/\alpha}}{2\alpha\pi} \frac{e^{\rho^{1/\alpha} \cos(1/\alpha)} [\cos(\omega) + i \sin\omega]}{\rho^{e^{i\varphi}} - z}$$

$$\omega = \rho^{1/\alpha} \sin(\varphi/\alpha) + \varphi[1 + (1-\beta)/\alpha]$$

Using this integral representation in (6) and (7), it is easier to get an asymptotic extension of the Mittag-Leffler function in the complex plane [48]. Let$\alpha < 2, \beta$ an arbitrary number and φsatisfies the condition selected in (5).
Then, for all $p \in \mathbb{N}$ and $|z| \to \infty$:

1. if $|argz| \le \varphi$,

$$E_{\alpha,\beta}(z) = \frac{z^{(1-\beta)/\alpha} e^{z^{1/\alpha}}}{\alpha} - \sum_{k=1}^{p} \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + O(|z|^{-1-p}) \quad (11)$$

2. if $\varphi \le |argz| \le \pi$,

$$E_{\alpha,\beta}(z) = -\sum_{k=1}^{p} \frac{z^{-k}}{\Gamma(\beta - \alpha k)} + O(|z|^{-1-p}) \quad (12)$$

Table 1: Table showing the difference between the three approaches where f, g, h represent respectively the Padé algorithm, the inverse of the mappy $(\mathrm{Id} - \mathrm{I}^{\alpha})$ and the integral formulation

	$\alpha = 0.25$	$\alpha = 0.45$	$\alpha = 0.50$	$\alpha = 0.60$	$\alpha = 0.75$	$\alpha = 0.99$
$\| f - g \|_2$	0.000057539	0.00007051	0.0006851	0.000065982	0.000067651	0.000640797
$\| f - h \|_2$	0.00125627	0.000067079	0.00003165	0.000010414	0.000136774	0.00067857
$\| g - h \|_2$	0.00131381	0.000137589	0.00010016	0.000076396	0.000069123	0.000037773

3.2. The Pade algorithm for Mittag-Leffler function

The Pade algorithm is start from the series (2) to estimate the Mittag-Leffler functions [9].This method presents a scheme for fast computations of:

$$E_{\alpha,1}(-x^{\alpha}), 0 < \alpha < , x \in \mathbb{R}_+$$

It uses, equation (2), on interval $0 < x < 0.1$. Instead it uses asymptotic series, equation (12), is for $x > 15$. Pade approximations (or rational polynomials)
are used for $0.1 < x < 15$, according to:

$$E_{\alpha,1}(-x^{\alpha}) \approx \begin{cases} \sum_{k=0}^{4} \frac{(-x)^{\alpha k}}{\Gamma(1+\alpha k)}, & 0 < x < 0.1 \\ \frac{a_0+a_1x+a_2x^2}{1+b_1x+b_2x^2+b_3x^3}, & 0.1 < x < 15 \\ \sum_{k=0}^{4} \frac{(-x)^{-\alpha k}}{\Gamma(1-\alpha k)}, & x \geq 15, \end{cases} \quad (13)$$

where coefficients $a_0, a_1, a_2, b_1, b_2, b_3$are listed in Table 2 of [14] for values of αbetween 0.01 et 0.99.

3.3. Comparison of the methods

In this section we present the results obtained on the different methods that we have used to calculate$E_{1-\alpha}(-x^{1-\alpha})$,with $0 < \alpha < 1$. The table1 show the differences between the three approaches calculated within theeuclideannorm .
In the case where $\alpha = 0,5$,the three methods coincide perfectly even if wesee a small shift in the curve obtained by the integral formulation (figure(3)).
But in cases where $\alpha < 0,5$ ($here\ \alpha = 0,25\ and\ \alpha = 0,45$ (figure2), Thetable above shows that the approach obtained by the integral method differsfrom the results obtained with other two methods, but this difference is very obvious when the value of αincrease down, in our case ,we can see very clearly when $\alpha = 0.25$.
However, when the value of αclose 1, we see that the curve obtained by themethod of Pad deviates from the curve obtained by the integral formulationand that calculated by the Neumann series, this differences increases with the value of α (figure 4). We also note that the curves obtained by the Neumannseries and the integral formulation coincides.

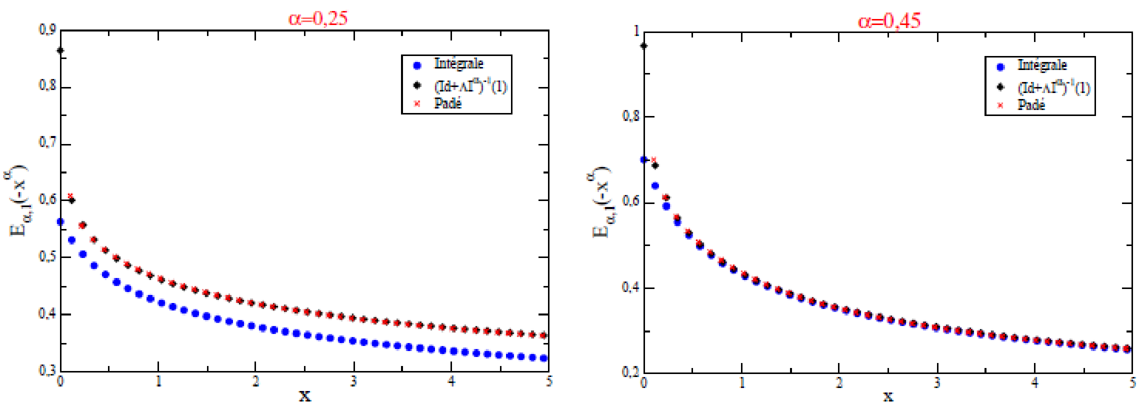

Figure 2: $E_{\alpha\_}(-x^{\alpha})$ with different value of $\alpha < 0.5$

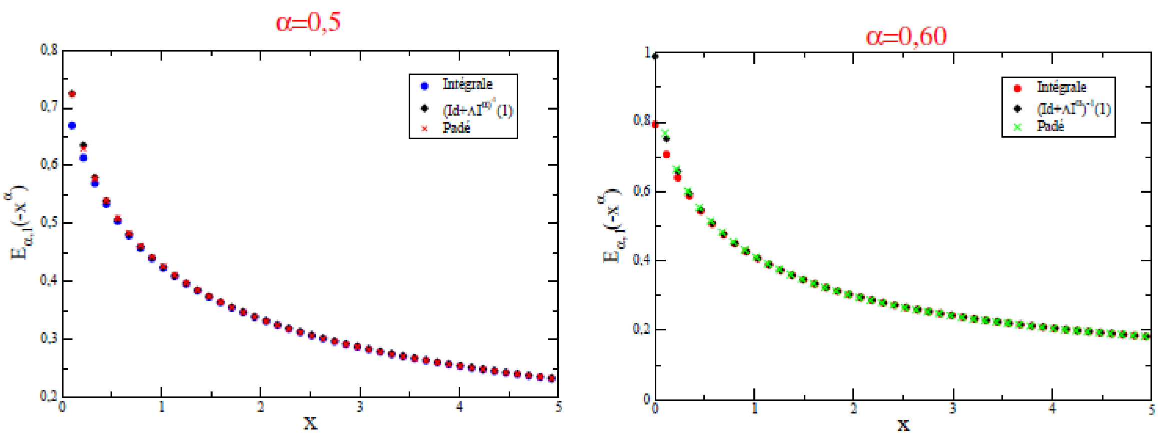

Figure 3: $E_{\alpha\_}(-x^{\alpha})$ with different value of α close 0.5

We can conclude that compared to the other two approaches, the computation of the Mittag-Leffler function by inverting the mappy $(Id - I^{\alpha})$ ismore stable for all value of αbetween 0 to 1.

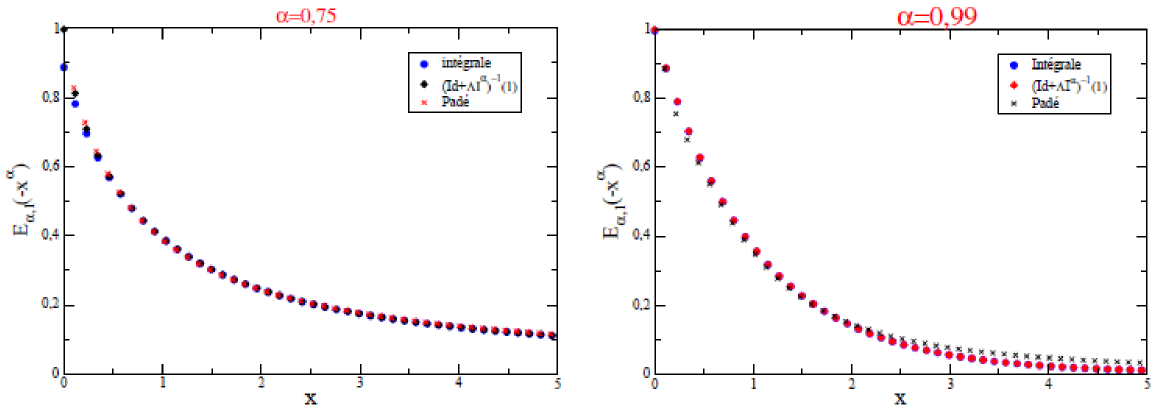

Figure 4:$E_{\alpha\_}(-x^{\alpha})$ with different value of α close 1

IV. APPLICATION IN THE CASE OF ANOMALOUS TRANSPORT

The process of dispersion of solutes in porous media may not be follow theusual laws of diffusion, especially in unsaturated regime. As an example, data from simple laboratory column filled of unsaturated (though not especially heterogeneous) porous media, show a breakthrough curves (BTC) with a heavy-tailed [4],[5],[8].
In particular, the long tails a behavior characteristics in the large time of the BTC follows a power law decay of time, reflecting some property of the medium to retain long time abnormally a fraction of the solute. This characteristic constitutes a memory effect that is beyond the scope of traditional models of diffusion based on the properties of Markovian in small scale.
In roughly the power law distribution of waiting times led to the use of the time fractional derivative in the diffusion equation [12].

4.1. The microscopic scale model

On the scale of fluid particles, the model where we use is described by a random walk. This is true for fluid particles and the solute particles. For a random walk, the idea to produce effects of stagnation is to impose of stopping times that can be drawn randomly. It is therefore to make a distinction between the time for which the walker makes a motion (operational time)and immobility time that could be abnormally large [42]. For the fractal MIM model, the evolution of the position of a particle of the random walk is given by:

$$\begin{cases} x_{n+1} = x_n + v\tau + \sqrt{2D_{\tau}}N_n \\ t_{n+1} = t_n + \tau + \tau^{1/\alpha}W_n \end{cases} \quad (14)$$

The Nn represent a Gaussian random variables independent and identicallydistributed, theWn forming a sequence of random variables with positivevalue, according to a stable Levy law [43] of exponent α between 0 and 1,and positive scale factor Λ. This means that the asymptotic behavior of the density of w_n is $\frac{\Lambda t^{-\alpha-1}}{|\Gamma(-\alpha)|}$. The parameters $v, \tau$and D are respectively avelocity of advection, the time step of the walk and the diffusion coefficientof the medium.
If $\tau \to 0$, the random walk described by equation (14) converges in law [42]to a stochastic process $x(t)$ given by:

$$x(t) = x_0 + vZ(t) + \sqrt{2D}B(Z(t)) \quad (15)$$

For solute particles in a tracer experiment, x_0 represents the position wherethey are injected, but for the fluid particles, x0 is a random variable uniformlydistributed. Moreover B is the standard Brownian motion and $Z(t)$is a stochastic process giving the operational time of the random walk. Theproperties of the process Z are determined by the parameters Λ and αdefiningthe probability distribution of W_n.

They have been studied in [42]. The relation (15) shows that the model is a time subordinated Brownian motion (physical time has been replaced by the operational time $Z(t)$).

4.2. Macroscopic version

Through a procedure of transition to the macroscopic limit, the fractal MIM model is given by the following differential equation [10]:

$$\partial_t P = \partial_x[\partial_x D\left(Id + \Lambda I_{0,+}^{1-\alpha}\right)^{-1} P - v\left(Id + \Lambda I_{0,+}^{1-\alpha}\right)^{-1} P] \quad (16)$$

where$I_{0,+}^{1-\alpha}$the fractional integral of order $1-\alpha$, Id the identity andΛtherate of stationary particles. Note that here $(Id + \Lambda I_{0,+}^{1-\alpha})^{-1} P(x,t)$ representsthe density of the mobile phase of the solute at position x in time t. Thisequation describes correctly the BTC evolving according to a power law[5],[31], because its solution $P(x,t)$ decreases such as $t^{-\alpha}$at large value of$t$. This behavior is incompatible with the classic MIM version [7], whichcorresponds to the case$\alpha = 1$, and is equivalent to the advection dispersionequation (ADE) which represents the dispersion in a homogeneous medium.

To solve this equation is equivalent to invert the operator$(Id + \Lambda I_{0,+}^{1-\alpha})$

Indeed, the equation (16) is identical to:

$$\partial_t P(x,t) = -\nabla F(x,t) \quad (17)$$

where F(x, t) represents the propagation flux of the solute at position at time t defined by [10].

$$F(x,t) = -D\nabla\left(Id + \Lambda I_{0,+}^{1-\alpha}\right)^{-1} P(x,t) + v\left(Id + \Lambda I_{0,+}^{1-\alpha}\right)^{-1} P(x,t) \qquad (18)$$

It is also interesting to note that the solution (16) presents an asymptotic decay in power law of time similar to observations reported in experiments in unsaturated porous media [11][13].

V. CONCLUSION

In this work, different numerical methods were used to compute $E_{1-\alpha,1}(-x^{1-\alpha})$.A comparative study of results are carried. We notice a good coincidence of Pad method and the inversion$(Id + I_{0,+}^{1-\alpha})$when $\alpha < 0.5$, through against when $\alpha < 0.5$ and even close to 1, the methodthat uses the integral formulation and inversion of the operator $(Id + I_{0,+}^{1-\alpha})$coincide perfectly. Note that greater the value of α approach 1, the Pad method differs from the other two methods. Note that the difference between the three methods is not very significant.

However, even if the Pad algorithm is fast Pad when the value of x is between 0.1 and 15, the method that inverse the operator $(Id + I_{0,+}^{1-\alpha})$remains fastest at the execution of thecomputation.

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AUTHORS

Botomanovatsara have a Master Degree in Physics Atmospheric engineering machinery, He prepare Ph.D. in physical domain, modeling, applied computer science (comparison between stochastic model and the fractional Fokker-Planck equation for the mass transport in porous media)

Rakotonasy have Mathematics Ph.D., his specialty is the mechanical and he has many papers on stockastic models, he is a teacher researcher at science faculty at the University of Antananarivo

Ratiarison is Professor of atmospheric physics in University of Antananarivo , Adolphe lead Laboratoire DYACO Laboratory in Science faculty and his specialization in oceans Mechanical

Ravonimanantsoa Manda VY have a PhD in telecommunications, he is a specialist in applied computing, VoIP, networks, computer science, he is a teacher researcher at ESPAat the University of Antananarivo