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A FINITE DIFFERENCE SCHEME FOR FRACTIONAL PARTIAL DIFFERENTIAL EQUATION

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ABSTRACT

Fractional derivative is a new promising field of mathematics. Nowadays many researchers are interested in defining fractional derivatives that generalize the conventional derivatives. In this paper we are interested in approximating the Caputo derivative, a classical fractional derivative. The discretization of this derivative is not an easy thing and the whole works on its discretization imply heavy memory cost and large time of computations. We present in this paper a fast scheme to discretize the Caputo derivative, and apply it in solving a fractional heat equation via a finite element method. The problem statement that this work solves is the large cost of time to discretize fractional derivative by existing methods in the literacy of numerical method. Several tests cases prove the efficiency and accuracy of our proposed scheme.

Keywords: *Caputo Derivative; Fractional Heat Equation; Finite Difference Scheme*.

1. INTRODUCTION

This document treats a fractional heat equation defined bellow:

$$\begin{cases} \frac{\partial^\alpha u}{\partial t} &= -\mu\Delta u + f(x) \; On\;\Omega \\ u(0,x) &= h(x) \; On\;\Omega \\ u &= g \; On\;\partial\Omega \end{cases} \quad (1)$$

Ω is a bounded domain in the space. In this article we are interested in discretizing the fractional derivative defined as the Caputo derivative

$$\frac{\partial^\alpha u}{\partial t} = \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-x)^{n-\alpha-1} u^{(n)}(x)dx$$

There are many reasons to study and define fractional derivatives. One reason is it possible use in modeling physics phenomena as the Superconductivity phenomenon [1,2]. Noticing that the modeling of wave's functions or operator are better described and estimated by fractional relationships rather than using integer parameters. Fractional derivative is then a better way to define models in spite of the incompleteness of a promising definition. Another reasons to use fractional derivative is implication in fast resolution of non-linear equation, and its applications in data analysis [3,4].Also, we can use fractional calculus to accelerate domain decomposition and splitting methods [3,4]. Finally, the memory effect of fractional derivative is under consideration [7,8] and we notice that the finite difference we apply in this article could be used to any memory operator in the form of the bellowing [9,10]:

$$\int_a^t F(t-x)u^{(n)}(x)dx$$

Where F is a regular and increasing function.

There are many numerical methods to discretize the Caputo derivative. The classical one is the Grünwald scheme. This method has good accuracy but it cost a lot of time to be executed and need a lot of requirement in memory storage because the computation of the solution need the storage of all its history values per time. Eventually for 3D partial differential equations, the cost is enormous. So, as an alternative, the most proposed method in this context is the spectral methods [11, 12]. These methods are efficient in some basic problems, but the choice of the basis and the collocation points make them hard to use for complex geometries and problems which make them instable and inaccurate. Finally, by analogy to solving conventional partial differential equations, the finite difference and the finite element methods, will be suitable to discretize the problems of fractional derivative equations. The classical Grunewald, or high order in time methods [17,18,19] costs large time computations and saturates the memory because we need to stock the entire solutions to compute the next state of the solution.

In this paper we first present a new finite difference method to approximate the Caputo derivative and other memory operators. We give then, some drawbacks of the Caputo definition and propose new definitions and some solutions to avoid these drawbacks. We then, present the proposed finite difference method to solve the fractional heat equation (1). The consistence and stability of the scheme could be proved by analogy to scheme of the classical heat equation. Finally, we presents some numerical results on some test-cases implemented the Freefem software. Several test cases, Show the efficiency and accuracy of our proposed method.

2. DRAWBACKS OF THE CAPUTO DERIVATIVE

The classical and most used fractional derivative are the Riemann-Liouvile derivative, The Grünwlad derivative and the Caputo derivative. We prefer to use the Caputo derivative because the Caputo derivative of a constant function is zero. Another derivative used in the literacy of fractional derivative is the fractal derivative defined as:

$$\frac{D^\alpha f}{D t} = \lim_{x \to t} \frac{f(x) - f(t)}{x^\alpha - t^\alpha}$$

This derivative and other conformal derivatives have the advantageous proprieties of Leibeneiz and chain rule which make its use easy but, it doesn't verify the Fourier assertion:

$$\mathfrak{F} D^\alpha u(k) = (ik)^\alpha \mathfrak{F}(u)$$

The Caputo and the Riemann-Liouville derivative support this formula. There is a Leibeniz and Chain rule formula for this derivative but it's an infinite sum and is hard to use in practice eventually in finite element methods or in space of distributions. The Caputo derivative is

$$\frac{D_a^\alpha u}{D t^\alpha} = \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-x)^{n-\alpha-1} u^{(n)}(x) dx$$

This derivative has the property to be linear, it cancel constant functions and satisfy the proposition:

Proposition: If u is continuous function in the neighborhood of a and has a derivative in a then,

$$\lim_{x \to a} D^\alpha u(x) = 0$$

Proof: We have:

$$\begin{aligned} \Gamma(\alpha) D_a^\alpha u(x) &= \int_a^x \frac{u'(t)}{\sqrt{x-t}} dt \\ &= u'(\zeta_x) \int_a^x \frac{1}{\sqrt{x-t}} dt \quad \text{(by the mean theorem)} \\ &= u'(\zeta_x)[-2\sqrt{x-t}]_a^x \\ &= u'(\zeta_x) 2\sqrt{x-a} \end{aligned}$$

$\zeta_x \in [a, x]$

Since u is derivable in a, $\lim_{x \to a} u'(x) = u'(a)$ and then

$$\lim_{x \to a} D_a^\alpha u(x) = 0$$

Remark1:

If $D_a^\alpha u(a) = Cte \neq 0$ then f is not derivable in a and

$$f'(x) \underset{a}{\sim} \frac{Cte}{\sqrt{x-a}}$$

Thus, when we use the Caputo derivative in partial differential equation, we have to ensure that $D_a^\alpha u(a) \neq 0$. Eventually the second member of the initial condition in our problem (1) should be zero in a. If not, the solution will be not regular and unbounded in the Hilbert space. This issue could be solved by well posing problem (1) or modifying the partial differential equation to verify the necessary condition $D_a^\alpha u(a) = 0$.

Remark2:

Another drawback of the Caputo definition: Considering the function of figure (1), this function is constant over the interval [a, +∞[(zone 1). By intuition the fractional derivative should be zero in this area but, the Caputo derivative is not zero and if the function is constant over the entire interval the Caputo derivative will be large. To solve this issue we present by the next a new definition to the fractional derivative which we can prove its link to the Caputo definition.

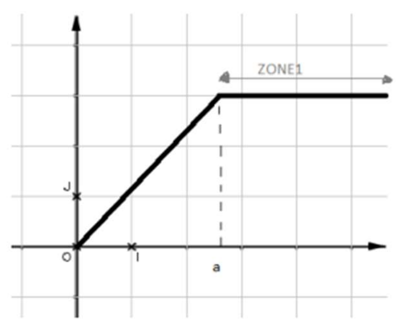

Figure1: A Continuous Function

The definition that we give next for the fractional derivative is done by construction:

Definition: We call D^α the local fractional derivative that verifies the bellowing properties:

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- If f is a constant function in the neighborhood of x then $D^\alpha f(x) = 0$.
- $D^\alpha t^k = \frac{\Gamma(k+1)}{\Gamma(k+1-\alpha)} t^{k-\alpha}$ for any real k
- D^α is a linear operator
- If f is a continuous function in the neighborhood of a point x then there exist a polynomial sequence (P_n) that converge uniformly to f in this neighborhood. We say that $D^\alpha f(x)$ exists or f has a derivative of order α if the limit $\lim_{n\to\infty} D^\alpha P_n(x)$ exists and the convergence is uniform in the neighborhood of x. In this case $D^\alpha f(x)$ is this limit. We can prove that this local fractional derivative support the whole properties of a simple derivative and then generalize it. We will not show these properties in this article but we will treat it in another.

Remark:
In the definition we have used the assertion"...there exist a polynomial sequence (P_n) that converge uniformly to f in this neighborhood". The polynomials can be constructed by the Weistrass theorem or Bernouili formula and we can prove that he limit is independent of the polynomial's choice.

3. FINITE DIFFERENCE SCHEME FOR THE FRACTIONAL DERIVATIVE

In all this section we take $0 < \alpha < 1$ (The same work could be done for other case of α).
We are next interested in discretizing the fractional derivative over time:
Let u defined on [0, T], $\Delta t = \frac{T}{N}$, $t_i = i\Delta t$ and $u(t_i) = u_i$. We have:

$$\begin{aligned}
\Gamma(1-\alpha)(D_a^\alpha u(t_n)) &= \int_a^{t_n} \frac{u'(x)}{(t_n-x)^\alpha}dx \\
&= \frac{1}{1-\alpha}\left(\int_a^{t_n} \frac{u''(x)}{(t_n-x)^{\alpha-1}}dx + t_n^{1-\alpha}u'(0)\right) \\
\int_a^{t_n} \frac{u''(x)}{(t_n-x)^{\alpha-1}}dx &= \sum_{i=0}^{n-1}\int_{t_i}^{t_{i+1}} \frac{u''(x)}{(t_n-x)^{\alpha-1}}dx
\end{aligned} \tag{2}$$

Using a trapezoidal approximation of regular integrals we have

$$\begin{aligned}
\int_a^{t_n} \frac{u''(x)}{(t_n-x)^{\alpha-1}}dx &= \sum_{i=0}^{n-1} u''(t_i)(t_n - t_{i+0.5})^{1-\alpha} + \circ(\Delta t) \\
&= \sum_{i=1}^{n-1} \frac{u_{i+1}-2u_i+u_{i-1}}{2\Delta t}(\Delta t)^{1-\alpha}(n-2i+1)^{1-\alpha} + \circ(\Delta t)
\end{aligned} \tag{3}$$

So we have a first scheme for the Caputo derivative. We can improve scheme (3) by using the Simpson formula and high finite difference scheme. This scheme is accurate but need reserving huge memory amount to compute the term u_N because, we need to stock all its past values u_i. It's the same drawback for the Grünwald approximation.

Now, we present the scheme we used to solve the fractional heat equation (1):

$$\begin{aligned}
\Gamma(1-\alpha)(D_a^\alpha u(t_{n+1} - D_a^\alpha)u(t_n)) &= \int_a^{t_{n+1}} \frac{u'(x)}{(t_{n+1}-x)^\alpha}dx - \int_a^{t_n} \frac{u'(x)}{(t_n-x)^\alpha}dx \\
&= \int_{t_n}^{t_{n+1}} \frac{u'(x)}{(t_{n+1}-x)^\alpha}dx + \int_a^{t_n} \frac{u'(x)}{(t_{n+1}-x)^\alpha}dx - \int_a^{t_n} \frac{u'(x)}{(t_n-x)^\alpha}dx \\
&= \int_{t_n}^{t_{n+1}} \frac{u'(x)}{(t_{n+1}-x)^\alpha}dx + \int_a^{t_n} u'(x)\left(\frac{1}{(t_{n+1}-x)^\alpha} - \frac{1}{(t_n-x)^\alpha}\right)dx
\end{aligned}$$

Using integration by parts

$$\begin{aligned}
\int_a^{t_n} u'(x)\left(\frac{1}{(t_{n+1}-x)^\alpha} - \frac{1}{(t_n-x)^\alpha}\right)dx &= \frac{1}{1-\alpha}\int_a^{t_n} u''(x)\left(\frac{1}{(t_{n+1}-x)^{\alpha-1}} - \frac{1}{(t_n-x)^{\alpha-1}}\right)dx \\
&+ \frac{1}{1-\alpha}(u'(a)(t_{n+1}^{1-\alpha} - t_n^{1-\alpha}) + u'(t_n)(\Delta t)^{1-\alpha})
\end{aligned}$$

By the mean formula

$$\begin{aligned}
\frac{1}{1-\alpha}\int_a^{t_n} u''(x)\left(\frac{1}{(t_{n+1}-x)^{\alpha-1}} - \frac{1}{(t_n-x)^{\alpha-1}}\right)dx &= \frac{1}{1-\alpha}((t_{n+1}-x)^{1-\alpha} - (t_n-x)^{1-\alpha})\int_a^{t_n} u''(x)dx \\
&= \frac{1}{1-\alpha}\lambda_n \Delta t(u'(t_n) - u'(a)) + \circ(\Delta t) = \circ(\Delta t)
\end{aligned}$$

Thus,

$$\begin{aligned}
\Gamma(1-\alpha)(D_a^\alpha u(t_{n+1} - D_a^\alpha)u(t_n)) &= \frac{1}{1-\alpha}(u'(a)(t_{n+1}^{1-\alpha} - t_n^{1-\alpha}) + u'(t_n)(\Delta t)^{1-\alpha}) + \circ(\Delta t) \\
&= \frac{1}{1-\alpha}\left(\left(\frac{u_1-u_0}{2\delta t}\right)(t_{n+1}^{1-\alpha} - t_n^{1-\alpha}) + \left(\frac{u_{n+1}-u_n}{2\Delta t}\right)(\Delta t)^{1-\alpha}\right) + \circ(\Delta t)
\end{aligned} \tag{4}$$

The term $t_{n+1}^{1-\alpha} - t_n^{1-\alpha}$ should be not neglected for small values of t_n.
Next we apply this scheme to the partial differential equation

$$\begin{cases}
\frac{\partial^\alpha u}{\partial t^\alpha} = -\mu\Delta u + f(x) \ \ On\ \Omega \\
u(0,x) = h(x) \ \ On\ \Omega \\
u = g \ \ On\ \partial\Omega
\end{cases} \tag{5}$$

The finite difference scheme for this equation is:

$$\begin{cases}
\frac{1}{1-\alpha}\left(\left(\frac{u_1-u_0}{2\delta t}\right)(t_{n+1}^{1-\alpha} - t_n^{1-\alpha}) + \left(\frac{u_{n+1}-u_n}{2\delta t}\right)(\Delta t)^{1-\alpha}\right) = \Gamma(1-\alpha)(-\mu\Delta u_{n+1} - \Delta u_n + f_{n+1}(x) - f_n(x)) \ \ On\ \Omega \\
u_0(x) = h(x) \ \ On\ \Omega \\
u_n = g \ \ On\ \partial\Omega
\end{cases} \tag{6}$$

The spatial resolution could be done by finite difference or finite element. The stability and consistency of the last scheme is the same things we do as for discretizing the heat equation without a fractional derivative.

4. NUMERICAL SIMULATION

We used the Freefem software to test the numerical simulation of the scheme (6) and compared it to the exact solution u_{exact}. Given a function u_{exact}, we build a partial differential equation that u_{exact} is the solution.

The PDE equation is:

$$\begin{cases}
\frac{\partial^\alpha u}{\partial t^\alpha} = -\mu\Delta u + f(x,t) \ \ On\ \Omega \\
u(0,x) = h(x) \ \ On\ \Omega \\
u = 0 \ \ On\ \partial\Omega
\end{cases} \tag{7}$$

Where $f(x,t) = \frac{\partial^\alpha u_{exact}}{\partial t^\alpha} + \mu\Delta u_{exact}$act and $h(x) = u_{exact}(0, x)$. For the next numerical simulation, we took $= \frac{1}{2}$.
The exact solutions we considered are:

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Test case1: $u_{exact}(t,x,y) = t^2(1-y^2-(x-2)^2)(x^2-4x)(y^2-4)$ see figure 2

Test case2: $u_{exact}(t,x,y) = (1+t)^2x^2y^2(x-1.)(y-1.)$ see figure 3

Test case3: $u_{exact}(t,x,y) = (1+t)^2 = x(x-1.)(2x-1.)y(y-1.)(2y-1)$ see figure 4

Test case4: $u_{exact}(t,x,y) = (e^t - \frac{1}{1+t})x^2y^2(1.-x-y)$ figure 5

These figures present the results of simulation of different partial differential equations associated to the exact solution for test1, test2, … test4 at the end time T and for given meshes.

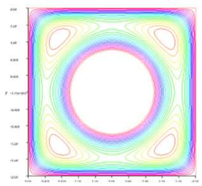

Figure 2: case1.

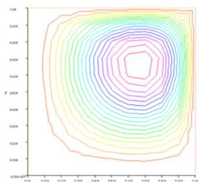

Figure 3: case2.

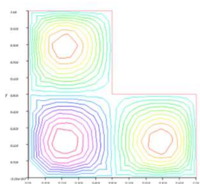

Figure 4: case3

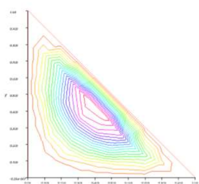

Figure 5: case4

The next tables present the $L^\infty(\Omega)$ error between the exact solution of the problem (7) and the approximated solution of this problem by scheme 4. The norm is computed at time T=1 for each test, h is the spatial mesh and Δt is the temporal mesh and μ = 1. We also give time execution to each simulation. The Freefem code is executed with the P_1 space.

Table 1: Test case1

	$\Delta t = 0.1$ & h=0.1	$\Delta t = 0.1$ & h=0.05	$\Delta t = 0.05$ & h=0.1	$\Delta t = 0.05$ & h=0.05
$\|u-u_{exact}\|_{L^\infty}$	1.20	0.3018	0.938	0.23
Time execution	0.094s	0.313s	0.172s	0.578s

For test 1 the geometry is complex so it's used that the finite element is not accurate for this problem which explain that the results are not accurate in this case.

Table 2: Test case2

	$\Delta t = 0.1$ & h=0.1	$\Delta t = 0.1$ & h=0.05	$\Delta t = 0.05$ & h=0.1	$\Delta t = 0.05$ & h=0.05
$\|u-u_{exact}\|_{L^\infty}$	4.e-004	1.05e-005	7.e-006	1.e-006
Time execution	0.016s	0.327s	0.13s	0.46s

Table 3: Test case3

	$\Delta t = 0.1$ & h=0.1	$\Delta t = 0.1$ & h=0.05	$\Delta t = 0.05$ & h=0.1	$\Delta t = 0.05$ & h=0.05
$\|u-u_{exact}\|_{L^\infty}$	0.0049	0.0015	0.0001	3.46e-004
Time execution	0.02s	0.35s	0.21s	0.76s

Table 4: Test case4

	$\Delta t = 0.1$ & h=0.1	$\Delta t = 0.1$ & h=0.05	$\Delta t = 0.05$ & h=0.1	$\Delta t = 0.01$ & h=0.05
$\|u-u_{exact}\|_{L^\infty}$	0.00013	1.84725e-005	0.00001	1.04e-005
Time execution	0.016s	0.2s	0.24s	0.67s

As a comparison of different results, we conclude that we have a good accuracy. The results of the scheme we have proposed for the heat equation are accurate and are executed in a convenient time execution. Also, the results could be considered similar to those of the conventional heat equation. We notice that the accuracy of our scheme is dependent on the geometry of the domain Ω. Also we did notice the same remarks for $\alpha \neq \frac{1}{2}$: The accuracy is good and not affected if we took another α even if it is close to 0.

In the next we give a comparison between our iterative method DF and two new spectral methods, the first is cited in [13] and based on the Laguerre spectral collocation method LCSM and the second one is an iterative new method INM cited in [16]. The table 3 present the $L^2(\Omega)$ error between the exact solution of the problem (7) and the approximated solutions of this problem by our scheme, the LCSM method and INM method. We take $\alpha = \frac{1}{3}$ and h=0.1 and Δt=0.01 and consider the test case 2.

Table3: $L^2(\Omega)$ Error for some T

Method	LCSM	INM	DF
T=0.1	2.410^{-4}	9.110^{-5}	10^{-6}
T=10	1.3	4.510^{-3}	1.0110^{-6}
T=100	17.5	0.345	4.0310^{-5}

Analyzing the results, we observe that the error increases after large time computation T(final execution time) and our finite difference is better accurate in time and that's is explained by the fact that our method doesn't do a lot of computations, we need just the last value of the history in the opposite of the other methods that consider all the history values to proceed . In addition, the time's cost is high enough for the other methods compared to our method.

5. CONCLUSION

We have first treated the drawback of the Caputo derivative definition and proposed some solution to it. We will treat this issue in another article and give the necessary theory and properties. We next presented a finite difference scheme to discretize the Caputo derivative. We applied this scheme to solve the fractional heat equation. We finally gave some tests of our proposition by numerical simulation and show the accuracy and efficiency of

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our model. We confirm that several tests show the efficiency and accuracy of our proposition.

We notice that the cost in time and accuracy is better than any other methods, because the computation of the solution need only the last value of the solution in the iterative computations in the contrary of the other known methods. We observed this result when comparing some test of our method and two spectral methods.

For the next work, we propose to apply our scheme to other nonlinear equations like turbulent models.

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