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# NEW ASPECTS OF THE MOTION OF A PARTICLE IN A CIRCULAR CAVITY

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**Abstract.** In this work, we consider the free motion of a particle in a circular cavity. For this model, we obtain the classical and fractional Lagrangian as well as the fractional Hamilton's equations (FHEs) of motion. The fractional equations are formulated in the sense of Caputo and a new fractional derivative with Mittag-Leffler nonsingular kernel. Numerical simulations of the FHEs within these two fractional operators are presented and discussed for some fractional derivative orders. Numerical results are based on a discretization scheme using the Euler convolution quadrature rule for the discretization of the convolution integral. Simulation results show that the fractional calculus provides more flexible models demonstrating new aspects of the real-world phenomena.

***Key words***: Fractional calculus, Caputo derivative, Mittag-Leffler kernel, particle, circular cavity, Euler method.

## 1. INTRODUCTION

Molecular Dynamics (MD) is a computational approach, which is used to predict the time dependent behaviour of a molecular system. The MD simulations have provided full information on fluctuations and conformational changes of proteins and nucleic acids. This method is now generally used to investigate the structure, dynamics, and thermodynamics of biological molecules as well as their complexes. The theoretical basis of MD incarnates many of important results produced by great names of analytical mechanics – Euler, Hamilton, Lagrange, and Newton. Their contributions are now to be found in introductory mechanics texts.

A material point, or the mass point called particle, is a mathematical model of a body with nonzero mass whose motion can be described by neglecting its dimension. The classical dynamic equations of motion are valid for slow and heavy particles. On the other hand, the MD is used for numerical solution of Lagrange equations [1].

Fractional calculus has been widely used in many branches of science and engineering [2–6]. Many efforts have been paid to the formulation of fractional Lagrangian and Hamiltonian mechanics [7–11]. Hence, the properties of these equations should be deeper investigated and numerical methods should be continuously developed in order to analyze better the advantages of models within this calculus. In many applications, the fractional differential equations (FDEs) appear and can be treated numerically and analytically [12–17]. The decomposition method has been introduced for solving such equations [18–21]. This method has also been used to study the fractional Lagrange and Hamilton's equations of motion for a number of physical models (see for example [22] and the references therein).

The rest of this work is designated as follows. In Section 2, we discuss briefly the fundamental definitions of fractional derivatives. In Section 3, we introduce the investigated model and study it. Section 4 studies the numerical simulations of fractional Hamilton's equation (FHEs). Finally, we finish the manuscript by concluding remarks.

## 2. PRELIMINARLIES

In this Section, we give in brief some preliminaries concerning the fractional derivatives. There are some definitions of the fractional derivatives including Riemann-Liouville, Weyl, Caputo, Marchaud, and Riesz [23]. Moreover, a new fractional derivative with Mittag-Leffler nonsingular kernel (ABC) was proposed recently and applied to some real-world models [24]. Below, we define the fractional derivatives in terms of classic Caputo and ABC. Starting with the classic Caputo, we present the following definitions.

*Definition* 2.1 [23]. Let $x:[a,b]\to R$ be a time dependent function. Then, the left and right Caputo fractional derivatives are defined as

$$ {}_{a}^{C}D_{t}^{\alpha}x \triangleq \frac{1}{\Gamma(n-\alpha)}\int_{a}^{t}\frac{x^{(n)}(\xi)}{(t-\xi)^{1+\alpha-n}}\mathrm{d}\xi, \quad {}_{t}^{C}D_{b}^{\alpha}x \triangleq \frac{1}{\Gamma(n-\alpha)}\int_{t}^{b}\frac{(-1)^{n}x^{(n)}(\xi)}{(t-\xi)^{1+\alpha-n}}\mathrm{d}\xi, \tag{1}$$

respectively, where $\Gamma(\cdot)$ denotes the Euler's Gamma function and $\alpha$ represents the fractional derivative order such that $n-1<\alpha<n$.

*Definition* 2.2 [24]. For $g\in H^{1}(a,b)$ and $0<\alpha<1$, the left and right ABC fractional derivatives are defined as

$$ {}_{a}^{ABC}D_{t}^{\alpha}g \triangleq \frac{B(\alpha)}{1-\alpha}\int_{a}^{t}E_{\alpha}\left(-\alpha\frac{(t-\xi)^{\alpha}}{1-\alpha}\right)\dot{g}(\xi)\mathrm{d}\xi, \quad {}_{t}^{ABC}D_{b}^{\alpha}g \triangleq -\frac{B(\alpha)}{1-\alpha}\int_{t}^{b}E_{\alpha}\left(-\alpha\frac{(\xi-t)^{\alpha}}{1-\alpha}\right)\dot{g}(\xi)\mathrm{d}\xi, \tag{2}$$

respectively, where $B(\alpha)$ is a normalization function obeying $B(0)=B(1)=1$ and the symbol $E_{\alpha}$ denotes the generalized Mittag-Leffler function

$$E_{\alpha}(t)=\sum_{k=0}^{\infty}\frac{t^{k}}{\Gamma(\alpha k+1)}. \tag{3}$$

For more details on the new ABC fractional operator and its properties, the interested reader can refer to [25, 26].

## 3. PHYSICAL DESCRIPTION OF THE MODEL

The investigated model in this work consists of a particle in a circular cavity as shown below in Fig. 1.

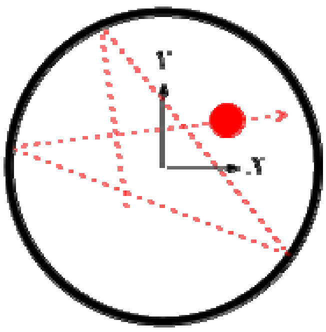



Fig. 1 – A particle of mass ($m$) in a circular cavity.

The particle of mass ($m$) moves randomly in all directions within the circular cavity. Using the Cartesian coordinates, we can express the kinetic and potential energies respectively as

$$T=\frac{m}{2}(\dot{x}^{2}+\dot{y}^{2}), \quad V=\gamma e^{-\delta(R-r)}=\gamma e^{-\delta\left(R-\sqrt{x^{2}+y^{2}}\right)}, \tag{4}$$

where the parameter $R$ is the radius of the circular cavity, $r$ is the distance between the particle and centre of circular cavity ($r=\sqrt{x^2+y^2}$), $\delta$ is a relative scaling factor, and $\gamma$ is a scalar constant. For the physical model under consideration, the classical Lagrangian takes the from

$$L=\frac{m}{2}(\dot{x}^2+\dot{y}^2)-\gamma e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}, \tag{5}$$

which results the classical Euler-Lagrange equations (CELEs)

$$m\ddot{x}=-\frac{\gamma\delta x}{r}e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}, \qquad m\ddot{y}=-\frac{\gamma\delta y}{r}e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}. \tag{6}$$

In the following, we investigate the fractional form of classical Lagrangian (5), which reveals new aspects of the physical system under consideration. The classical Lagrangian (5) can be fractionalized as

$$L^F=\frac{m}{2}[({}_aD_t^\alpha x)^2+({}_aD_t^\alpha y)^2]-\gamma e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}, \tag{7}$$

where ${}_aD_t^\alpha$ denotes the left Caputo or ABC fractional operator. Using

$$\frac{\partial L^F}{\partial q}+{}_tD_b^\alpha\frac{\partial L^F}{\partial\,{}_aD_t^\alpha q}+{}_aD_t^\beta\frac{\partial L^F}{\partial\,{}_tD_b^\beta q}=0, \tag{8}$$

in which ${}_tD_b^\alpha$ denotes the right fractional operator in the Caputo or ABC sense, the fractional Euler-Lagrange equations (FELEs) read

$$m\,{}_tD_b^\alpha\,{}_aD_t^\alpha x=\frac{\gamma\delta x}{r}e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}, \qquad m\,{}_tD_b^\alpha\,{}_aD_t^\alpha y=\frac{\gamma\delta y}{r}e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}. \tag{9}$$

As $\alpha\to1$, the FELEs (9) reduce to the CELEs given by Eq. (6).

Below, we are going to obtain the fractional Hamilton's equation (FHEs) of motion. For this purpose, we have to introduce the following generalized momenta

$$P_{\alpha,x}=\frac{\partial L^F}{\partial\,{}_aD_t^\alpha x}=m\,{}_aD_t^\alpha x,\; P_{\beta,x}=\frac{\partial L^F}{\partial\,{}_tD_b^\beta x}=0,\; P_{\alpha,y}=\frac{\partial L^F}{\partial\,{}_aD_t^\alpha y}=m\,{}_aD_t^\alpha y,\; P_{\beta,y}=\frac{\partial L^F}{\partial\,{}_tD_b^\beta y}=0. \tag{10}$$

As a result, the fractional Hamiltonian function can be obtained from

$$H^F=P_{\alpha,x}\,{}_aD_t^\alpha x+P_{\beta,x}\,{}_tD_b^\beta x+P_{\alpha,y}\,{}_aD_t^\alpha y+P_{\beta,x}\,{}_tD_b^\beta y-L^F. \tag{11}$$

Substituting Eqs. (7) and (10) into Eq. (11), we derive

$$H^F=\frac{m}{2}[({}_aD_t^\alpha x)^2+({}_aD_t^\alpha y)^2]+\gamma e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}. \tag{12}$$

Now, the FHEs of motion are obtained as

$$\frac{\partial H^F}{\partial x}={}_tD_b^\alpha P_{\alpha,x}+{}_aD_t^\beta P_{\beta,x}\Rightarrow m\,{}_tD_b^\alpha\,{}_aD_t^\alpha x=\frac{\gamma\delta x}{r}e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}, \tag{13}$$

$$\frac{\partial H^F}{\partial y}={}_tD_b^\alpha P_{\alpha,y}+{}_aD_t^\beta P_{\beta,y}\Rightarrow m\,{}_tD_b^\alpha\,{}_aD_t^\alpha y=\frac{\gamma\delta y}{r}e^{-\delta\left(R-\sqrt{x^2+y^2}\right)}. \tag{14}$$

We notice that, the above coupled FHEs of motion are the same as the corresponding FELEs in Eq. (9). Again, as $\alpha \to 1$, Eqs. (13–14) reduce to the CELEs (6). Our aim now is to obtain the numerical solution of Eqs. (13–14) for different values of $\alpha$ while considering two different fractional operators namely the Caputo and ABC.

## 4. NUMERICAL ANALYSIS

In this Section, we develop an approximation scheme for the numerical solution of FHEs (13–14) within the Caputo and ABC fractional operators. Starting with the ABC fractional derivative, we first reformulate Eqs. (13–14) in the following way. Let us define the new state variables $x_1 \triangleq x$, $x_2 \triangleq {}^{ABC}_{a}D^{\alpha}_{t} x_1$, $y_1 \triangleq y$ and $y_2 \triangleq {}^{ABC}_{a}D^{\alpha}_{t} y_1$. Then, Eqs. (13–14) can be rewritten in the form of the following system of FDEs

$$\begin{cases} {}^{ABC}_{a}D^{\alpha}_{t} x_1 = x_2, \quad {}^{ABC}_{t}D^{\alpha}_{b} x_2 = \dfrac{\gamma\delta}{m}\dfrac{x_1}{\sqrt{x_1^2+y_1^2}} e^{-\delta\left(R-\sqrt{x_1^2+y_1^2}\right)}, \\ {}^{ABC}_{a}D^{\alpha}_{t} y_1 = y_2, \quad {}^{ABC}_{t}D^{\alpha}_{b} y_2 = \dfrac{\gamma\delta}{m}\dfrac{y_1}{\sqrt{x_1^2+y_1^2}} e^{-\delta\left(R-\sqrt{x_1^2+y_1^2}\right)}. \end{cases} \tag{15}$$

Using the definition of ABC fractional integral [24], Eq. (15) can be rewritten as the following system of fractional integral equations

$$\begin{cases} x_1(t) = x_1(a) + \dfrac{1-\alpha}{B(\alpha)} x_2(t) + \dfrac{\alpha}{B(\alpha)\Gamma(\alpha)} \displaystyle\int_a^t (t-\xi)^{\alpha-1} x_2(\xi)\mathrm{d}\xi, \\ x_2(t) = x_2(b) + \dfrac{1-\alpha}{B(\alpha)} f(x_1(t), y_1(t)) + \dfrac{\alpha}{B(\alpha)\Gamma(\alpha)} \displaystyle\int_t^b (\xi-t)^{\alpha-1} f(x_1(\xi), y_1(\xi))\mathrm{d}\xi, \\ y_1(t) = y_1(a) + \dfrac{1-\alpha}{B(\alpha)} y_2(t) + \dfrac{\alpha}{B(\alpha)\Gamma(\alpha)} \displaystyle\int_a^t (t-\xi)^{\alpha-1} y_2(\xi)\mathrm{d}\xi, \\ y_2(t) = y_2(b) + \dfrac{1-\alpha}{B(\alpha)} g(x_1(t), y_1(t)) + \dfrac{\alpha}{B(\alpha)\Gamma(\alpha)} \displaystyle\int_t^b (\xi-t)^{\alpha-1} g(x_1(\xi), y_1(\xi))\mathrm{d}\xi. \end{cases} \tag{16}$$

Now, we consider a uniform mesh on [$a$, $b$] and label the nodes 0, 1, …, $N$, where $N$ is an arbitrary positive integer and $h_N = \dfrac{b-a}{N}$ is the time step size. We denote $x_{i,j}$ and $y_{i,j}$ as the numerical approximations of $x_i(t_j)$ and $y_i(t_j)$, respectively, where $i = 1$, 2 and $t_j = a + jh_N$ is the time at node $j$ for $0 \le j \le N$. Using the Euler convolution quadrature rule for the discretization of the convolution integral in the right-hand side of Eq. (16), we deduce the following fractional Euler method

$$\begin{cases} X_1 - \dfrac{1-\alpha}{B(\alpha)} X_2(t) - \dfrac{\alpha}{B(\alpha)} B_N^{(\alpha)} X_2 = X_{1,0}, \\ X_2(t) - \dfrac{1-\alpha}{B(\alpha)} F\left(X_1, Y_1\right) - \dfrac{\alpha}{B(\alpha)} F_N^{(\alpha)} F\left(X_1, Y_1\right) = X_{2,N}, \\ Y_1 - \dfrac{1-\alpha}{B(\alpha)} Y_2 - \dfrac{\alpha}{B(\alpha)} B_N^{(\alpha)} Y_2 = Y_{1,0}, \\ Y_2(t) - \dfrac{1-\alpha}{B(\alpha)} G\left(X_1, Y_1\right) - \dfrac{\alpha}{B(\alpha)} F_N^{(\alpha)} G\left(X_1, Y_1\right) = Y_{2,N}, \end{cases} \tag{17}$$

where

$$X_i = \begin{bmatrix} x_{i,0} \\ \vdots \\ x_{i,N} \end{bmatrix}, \ Y_i = \begin{bmatrix} y_{i,0} \\ \vdots \\ y_{i,N} \end{bmatrix}, \quad i = 1, 2, \tag{18}$$

$$X_{1,0} = \begin{bmatrix} x_{1,0} \\ \vdots \\ x_{1,0} \end{bmatrix}, \ Y_{1,0} = \begin{bmatrix} y_{1,0} \\ \vdots \\ y_{1,0} \end{bmatrix}, \ X_{2,N} = \begin{bmatrix} x_{2,N} \\ \vdots \\ x_{2,N} \end{bmatrix}, \ Y_{2,N} = \begin{bmatrix} y_{2,N} \\ \vdots \\ y_{2,N} \end{bmatrix}, \tag{19}$$

$$B_N^{(\alpha)} = h_N^{\alpha} \begin{bmatrix} \omega_0^{(\alpha)} & 0 & \dots & 0 \\ \omega_1^{(\alpha)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \omega_N^{(\alpha)} & \dots & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} \end{bmatrix}, \ F_N^{(\alpha)} = \left(B_N^{(\alpha)}\right)^T, \tag{20}$$

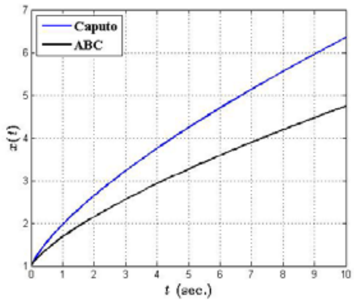
$$F(X_1, Y_1) = \begin{bmatrix} f(x_{1,0}, y_{1,0}) \\ \vdots \\ f(x_{1,N}, y_{1,N}) \end{bmatrix}, \ G(X_1, Y_1) = \begin{bmatrix} g(x_{1,0}, y_{1,0}) \\ \vdots \\ g(x_{1,N}, y_{1,N}) \end{bmatrix}, \tag{21}$$

$$f(x, y) = \frac{\gamma\delta}{m} \frac{x}{\sqrt{x^2 + y^2}} e^{-\delta\left(R - \sqrt{x^2 + y^2}\right)}, \ g(x, y) = \frac{\gamma\delta}{m} \frac{y}{\sqrt{x^2 + y^2}} e^{-\delta\left(R - \sqrt{x^2 + y^2}\right)}, \tag{22}$$

and the binomial coefficient $\omega_j^{(\alpha)}$ can be calculated by using the recursive formula $\omega_0^{(\alpha)} = 1$ and $\omega_j^{(\alpha)} = (\frac{\alpha + j - 1}{j})\omega_{j-1}^{(\alpha)}$, $j = 1, 2, \dots$. Note that, the aforementioned results can be used in the Caputo sense by using the Caputo fractional integral [23] instead of its ABC counterpart in Eq. (16) and following the same discretizing procedure as above.

### 4.1. Simulation results

In the following simulations we choose $\gamma = 10^{-27}\,\text{J}$, $\delta = 4\ \text{nm}^{-1}$, $R = 10\ \text{nm}$ and $m = 10^{-9}\,\text{kg}$. In Figs. 2–4, the graphs of $x(t) = x_1(t)$ and $y(t) = y_1(t)$ are plotted for $\alpha = 0.7, 0.8, 0.9, 1$, $x(0) = 1\ \text{nm}$, ${}_0D_t^{\alpha} x(t)\big|_{t=10} = 1\ \text{nm/s}$, $y(0) = -2.552\ \text{nm}$ and ${}_0D_t^{\alpha} y(t)\big|_{t=10} = 0.5\ \text{nm/s}$. In these figures, we also consider the Caputo and ABC fractional operators for the FHEs (13–14). These figures indicate that the numerical solution of FHEs (13–14) exhibits complex behaviours for different fractional operators. Thus, taking into account the new fractional derivatives provides more flexible models, which help us to adjust better the dynamical behaviours of the real-world phenomena.



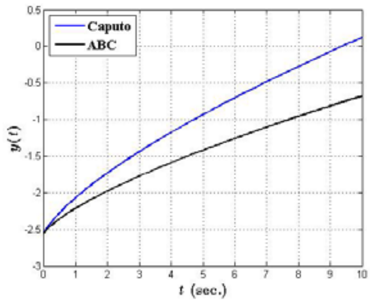




Fig. 2 – Simulation curves of $x(t)$ and $y(t)$ within the Caputo and ABC fractional operators for α = 0.7..

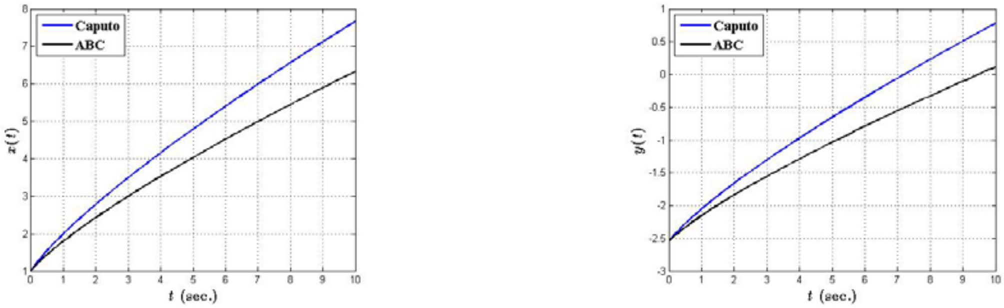



Fig. 3 – Simulation curves of $x(t)$ and $y(t)$ within the Caputo and ABC fractional operators for $\alpha = 0.8$.

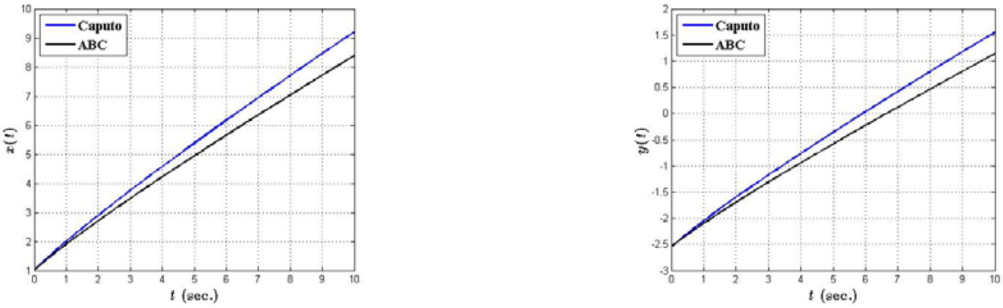



Fig. 4 – Simulation curves of $x(t)$ and $y(t)$ within the Caputo and ABC fractional operators for $\alpha = 0.9$.

## 5. CONCLUSION

Fractional calculus is an efficient tool to describe the complex behaviours of many real world systems. The numerical analysis of FDEs is a very important issue to be considered by researchers. In this study, we discussed the motion of a particle moving in a circular cavity by using the fractional calculus. We obtained the classical and fractional Lagrangian of the model together with the FHEs of motion. The fractional equations were formulated by using two approaches. The first approach used the Caputo fractional derivative while the second one employed a new formulation with nonsingular kernel. Finally, we investigated numerically the solution of FHEs within these two fractional operators. The numerical scheme for both operators was based on a discretization technique using the Euler convolution quadrature rule for the discretization of the convolution integral. The results shown in Figs. 2–4 indicate that the behaviours of the FHEs depend on the fractional operators. Thus, the new aspects of the fractional calculus provide more flexible models that help us to adjust better the dynamical behaviours of many real-world phenomena.

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