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ARTIGO ORIGINAL

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The Monte Carlo method applied to the fractional SIR model

O Método de Monte Carlo aplicado ao modelo SIR fracionário

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ABSTRACT

In the present work, we propose an algorithm based on the Monte Carlo Method for solving fractional dynamical systems. As an example of application, we use the proposed method in the fractional SIR model. In order to investigate the statistical convergence of the method, we compare the results obtained with the solution obtained by the Finite Differences Method.

Keywords: Monte Carlo method. Fractional Calculus. SIR.

RESUMO

No presente trabalho propomos um algoritmo baseado no Método de Monte Carlo para a resolução de sistemas dinâmicos fracionários. Como exemplo de aplicação, utilizamos o método proposto no modelo SIR fracionário. Para investigar a convergência estatística do método, comparamos os resultados obtidos com a solução obtida pelo Método das Diferenças Finitas.

Palavras-chave: Método de Monte Carlo. Cálculo Fracionário. SIR

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1. INTRODUCTION

When Leibniz proposed a derivation of the order $\frac{1}{2}$ in a letter to l'Hôpital in 1695, the study of fractional calculus began (see (OLDHAM and SPANIER, 1974; SAMKO et al., 1993) for a historical review). Currently, all generalizations of ordinary calculus for derivatives and integrals of non-integer order are called fractional calculus. Other great mathematicians in history have also contributed to the development of fractional calculus, including names such as Euler, Laplace, Liouville, Grunwald, Letnikov, Riemann, and many others. Although almost as old as the usual Calculus of derivatives and integrals of integers, fractional calculus has attracted greater attention only in recent decades because of its applications in various fields of science and engineering and in the solution and study of complex systems. according to (SABATIER et al., 2007) and (Hilfer 2000). Fractional derivatives are, in general, nonlocal operators. Consequently, the complex systems in which we use Fractional Calculus are systems with nonlocal behavior or with memory-dependent dynamics.

Applications include several areas of science and engineering, including fluid flow, viscous media, rheology, diffusive transport, electrical networks, electromagnetic theory, field theory, probability, etc., according to (SABATIER et al, 2007; HILFER, 2000; KILBAS, 2006). In this sense, the construction of efficient methods for solving differential equations, especially nonlinear cases, is a great challenge for mathematical modeling, especially when working with fractional calculus, since there are still few theories of numerical and analytical solutions. With the aim of overcoming these difficulties and obtaining a numerical method that can be used to solve fractional differential equations with different formulations of derivatives, we propose in the present work the construction of an algorithm based on the Monte Carlo method (MCM) for systems of ordinary fractional differential equations. It is important to point out that the use of MCM in solving ordinary differential equations (with whole-order derivatives of integer order) is a topic that, according to (KALOS and WHITLOCK, 2009), is very little studied in the literature. The reason it is rarely used is that the finite difference method (FDM) and its variants generally have a lower computational cost than MCM for well-behaved ordinary differential equations, as described in (AKHTAR et al., 2015). However, MCM is traditionally used to solve partial differential equations and integral equations, where it has several advantages over other methods when the problem boundary is very complicated, as (AKHTAR et al., 2015) and (KALOS and WHITLOCK, 2009). In this context, and taking into account that fractional differential equations are actually integral equations, it is curious to observe that MCM is still not very little studied in the context of fractional calculus, as pointed out by (FERREIRA and LAZO, 2022).

With this in mind, the main goal of this work is to show that MCM can be used to solve systems of fractional differential equations, even when the integrands of these equations are singular. The algorithm proposed in this paper for solving systems of fractional differential equations is adapted from the recent work of (FERREIRA and LAZO, 2022), who proposed an MCM for solving ordinary fractional differential equations according to the formulation of Caputo and Riemann-Liouville.

As an application example, in this paper, we apply the proposed method to a model that is already widely used in the literature, namely the fractional SIR model. The SIR model and its various generalizations are widely used in systems modeling aimed at understanding the dynamics of a particular disease in a population. As a recent application example, we can cite the modeling of the COVID -19 pandemic to explain the spread and define vaccination strategies, as we did in (BARROS et al., 2021) and (TAVARES and LAZO, 2022). To analyze the statistical convergence of the proposed MCM, we compare the results found with the solution of the FDM variant used in (TAVARES and LAZO, 2022).

2. PRELIMINARY

In this section, we present some definitions and basic results of Caputo's fractional calculus, the Monte Carlo method, and the fractional model SIR, which will be used throughout the article.

2.1 Fractional calculus

A brief introduction to the mathematical theory of fractional calculus is presented with the definition of fractional integral proposed by Riemann-Liouville (RL) and the most famous definitions of fractional calculus used in this article.

Definition 2.11 (Riemann-Liouville Fractional Integral)

Let $\alpha \in \mathbb{R}_+$ be the operator ${}_aJ_x^\alpha$ which in is given by $L_1([a,b])$ is given by

$$ {}_aJ_x^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-u)^{\alpha-1} f(u)du, \tag{1} $$

called the left-hand Riemann-Liouville fractional integral, where $\Gamma(\cdot)$ is the gamma function and $a, b \in \mathbb{R}$ with $a < b$.

For $\alpha = n$ integer, the fractional integral of RL (1) coincides with the usual Riemann integral repeated n times, according to (DIETHELM 2004). It follows from the definition 2.11 that the integral of RL exists for any integrable function f if $\alpha > 1$. Moreover, it is possible to prove the existence of the integral of RL (1) for f in $L_1([a,b])$ even if $0 < \alpha < 1$, according to (DIETHELM 2004).

The fractional integral of RL (1) plays a central role in defining Caputo's fractional derivatives. Before we define Caputo's derivative, it is important to mention that for positive integers $n > m$ the identity $D_x^m f(x) = D_x^n {}_aJ_x^{n-m} f(x)$ holds, where D_x^m is a derivative $\frac{d^m}{dx^m}$ of order m. By reversing the order between integral and derivative in this relation and replacing the integer m by a positive real value α, we obtain Caputo's definition of the derivative (see (DIETHELM 2004) for more details).

Definition 2.12 (Caputo's fractional derivative)

The left fractional derivative of Caputo of order $\alpha \in \mathbb{R}_+$ is defined by ${}_a^C D_x^\alpha f(x) := {}_aJ_x^{n-\alpha} D_x^n f(x)$ with $n = [\alpha] + 1$, that is:

$$ {}_a^C D_x^\alpha f(x) := \frac{1}{\Gamma(n-\alpha)} \int_a^x \frac{f^{(n)}(u)}{(x-u)^{1+\alpha-n}} du, \tag{2}$$

where $a \le x \le b$ and $f^{(n)}(u) = \frac{d^n f(u)}{du^n} \in L_1([a,b])$.

An important consequence of the definition 2.12 is that Caputo's fractional derivatives are non-local operators. These left derivatives depend on the values of the left function of x, i.e., $a \le u \le x$. On the other hand, it is important to note that when $\alpha = n$ an integer, Caputo's fractional derivatives reduce to integer derivatives n according to (DIETHELM 2004).

Finally, the RL integrals and the fractional derivatives of Caputo satisfy the following fractional generalization of the fundamental theorem of the infinitesimal calculus:

Theorem 2.13 (Caputo's Fundamental Theorem of Calculus)

Let $0 < \alpha < 1$, and let f be a differentiable function on $[a,b]$. The following equality is satisfied:

$$ {}_aJ_b^\alpha {}_a^C D_x^\alpha f(x) = f(b) - f(a). \tag{3}$$

The proof of the theorem 2.13 can be read for example in (DIETHELM 2004).

2.2 Monte Carlo method

The Monte Carlo Method (MCM) is a powerful tool for solving many problems in physics, biology, engineering, finance, and other fields (see (MORDECHAI, 2011) for an overview). According to (MORDECHAI, 2011), its origin dates back to the pioneering work of Comte de Buffon, who in 1777 proposed a statistical method for calculating the value of the number π based on the throwing of a needle. The MCM became popular during World War II when it was used to design the atomic bomb, as (MORDECHAI, 2011). Currently, the MCM represents a large class of statistical methods that use random number sampling to obtain numerical solutions to various types of problems.

One of the simplest and most interesting applications of MCM is the computation of π, as shown in (WILLIAMSON, 2013).

Another important application is the computation of definite integrals. A simple MCM for computing integrals involves applying the mean value theorem for integrals. Let $f(x)$ be a Riemann integrable function on the interval $[a, b]$. Then let

$$\int_a^b f(x)dx = (b-a)\langle f\rangle, \tag{4}$$

where $\langle f\rangle$ is the average value of the function in $[a, b]$. At this point, a sample of random numbers can be used to approximate $\langle f\rangle$. Given a set of N uniformly distributed random numbers ($x_1, x_2, ..., x_N$) in $[a, b]$, we obtain an approximation $\langle f\rangle_N$ for $\langle f\rangle$ by simply computing $f(x)$ for each random number selected. We have:

$$\langle f\rangle_N = \frac{1}{N}\sum_{i=1}^{N} f(x_i), \tag{5}$$

where $\langle f\rangle_N$ statistically converges to $\langle f\rangle$ in the limit $N \to \infty$ (see (DUNN and SHULTIS, 2022)), i.e. $\langle f\rangle = \lim_{N\to\infty}\langle f\rangle_N$. Therefore, (5) gives us an approximation to the integral (4):

$$\int_a^b f(x)dx \approx \frac{b-a}{N}\sum_{i=1}^{N} f(x_i), \tag{6}$$

which statistically converges against the exact value of the integral when $N \to \infty$. The variance σ^2 for f, according to (DUNN and SHULTIS, 2022), is given by:

$$\sigma^2 = \frac{b-a}{N}\sum_{i=1}^{N} f^2(x_i) - \left(\frac{b-a}{N}\sum_{i=1}^{N} f(x_i)\right)^2, \tag{7}$$

and the standard error Err is:

$$Err = \frac{\sqrt{\sigma^2}}{\sqrt{N}}. \tag{8}$$

The approximation (6) yields a result for the integral that differs from the exact value by up to one standard error with probability 68.3% (and differs from the exact value by up to two standard errors with probability 95.4%). Since the estimated error is proportional to the variance and inversely proportional to the square root of N, there are two ways to reduce the error. The first is to increase N and the second is to decrease the variance using N random numbers ($x_1, x_2, ..., x_N$) that are not uniformly distributed in $[a, b]$, as in (KALOS and WHITLOCK, 2009; DUNN and SHULTIS, 2022; NIEDERREITER, 1992).

On the other hand, if $\int_a^b f(x)^2 dx$ diverges, the convergence will be slower than for (8) (NIEDERREITER, 1992). Finally, it is important to note that MCM converges for fractional derivatives and integrals, since the Riemann-Liouville fractional calculus is defined for $L^1[a, b]$ functions and the Caputo derivatives are defined for differentiable functions.

2.3 Fractional SIR model

With the work of (KERMACK and MCKENDRICK, 1927) began the study of epidemiological models known as SIR model. The model they proposed describes the spread of infectious diseases in a population divided into subgroups of susceptible individuals (with a proportion of $0 \le S \le 1$), infected (with a proportion of $0 \le I \le 1$), and recovered (with a proportion of $0 \le R \le 1$), with the dynamics of each of these groups described by an ordinary differential equation (ODE). In (TAVARES and LAZO, 2022) we analyzed the fractional model SIR (Susceptible-Infectious-Recovered) with two interacting populations, in this work we will analyze the case of only one population. The model we will analyze is given by:

$$\begin{cases} {}_0^C D^\alpha S(t) = -\beta SI - \mu(S-1) \\ {}_0^C D^\alpha I(t) = \beta SI - (\mu+\gamma)I \\ {}_0^C D^\alpha R(t) = \gamma I - \mu R, \end{cases} \tag{9}$$

where $0 < \alpha \le 1$ is the order of the derivative, β is the fractional transmission rate of the disease (proportional to the average contact rate within the population and within the population), γ is the fractional reciprocal of the mean infection period. It is also assumed that the fractional death rate μ is equal to the birth rate, so that the total number N of the population is constant during the disease. Therefore, $S(t) + I(t) + R(t)$ must be equal to 1. Regarding the size of the parameters in the model, it is also important to note that since S,

I, and R are dimensionless, the fractional derivative operator ${}_0^C D_t^\alpha$ has the time $\text{dimension}^{-\alpha}$ (as the integer derivative $\frac{d}{dt}$ has time dimension^{-1}), the fractional rates β, γ and μ must have time $\text{dimension}^{-\alpha}$.

The equilibrium points $P(S^*, I^*, R^*)$ of the system (9), i.e. ${}_0^C D^\alpha S(t) = 0$, ${}_0^C D^\alpha I(t) = 0$ and considering $R = 1 - S - I$ are given by (see (TAVARES and LAZO, 2022)):

$$\mathrm{P}_0 = P_0(1,0,0); \qquad P_1 = P_1\left(\frac{\mu+\gamma}{\beta}, \frac{\mu(\mu+\gamma-\beta)}{\beta(\mu+\gamma)}, \frac{2\beta\mu+\beta\gamma-\gamma\mu-\gamma^2}{\beta(\mu+\gamma)}\right).$$

Where P_0 is the infection-free break-even point and P_1 is the endemic break-even point.

3. RESULTS

In this section, an MCM is proposed to obtain the numerical solution of the system (9) considering the Caputo derivatives.

The first step to obtain the solution of the system (9) is to use Caputo's Fundamental Theorem of Infinitesimal Calculus (2.13). Thus, assuming that $S(t),\ R(t)$ and $I(t)$ are differentiable in the domain, and integrating both sides of (9) with a fractional integral of RL (1) given by ${}_0J_t^\alpha$, we obtain:

$$\begin{cases} S(t) = S(0) - \beta_0 J_t^\alpha SI - \mu_0 J_t^\alpha (S-1) \\ I(t) = I(0) + \beta_0 J_t^\alpha SI - (\mu+\gamma)_0 J_t^\alpha I \\ R(t) = R(0) + \gamma_0 J_t^\alpha I - \mu_0 J_t^\alpha R, \end{cases} \tag{10}$$

The second step is to use the MCM to obtain the solution of the integrals in (9). However, since $S(t),\ R(t)$, and $I(t)$ are not known, MCM cannot be directly applied to the computation of these integrals. Therefore, we first define a discretization of these functions. For a positive integer L, we have $t_n = t_0 + nh$ ($n = 0, 1, ..., L$), where $h = \frac{t_L - t_0}{L}$ and $t_0 = 0$. Let then $X^{(n)} = X(t_n)$ (where X represents each of the functions $S,\ I$ and R), the discretization of the functions is defined by:

$$X^L(t) = X^{(n)} \quad \text{if} \quad t_n \le t < t_{n+1}. \tag{11}$$

Since it was assumed that $X(t)$ is differentiable, we have $\lim_{L\to\infty} X^L(t) = X(t)$. Therefore, the discretized function $X^L(t)$ is a good approximation to the function $X(t)$ for a sufficiently large L. You can then determine the values $X(t_n)$ from the following recursion relation:

$$\begin{cases} S^{(n)} = S(0) - \beta \frac{1}{\Gamma(\alpha)} \int_0^{t^n} \frac{S^L I^L}{(t_n - t)^{1-\alpha}} dt - \mu \frac{1}{\Gamma(\alpha)} \int_0^{t^n} \frac{S^L - 1}{(t_n - t)^{1-\alpha}} dt \\ I^{(n)} = I(0) + \beta \frac{1}{\Gamma(\alpha)} \int_0^{t^n} \frac{S^L I^L}{(t_n - t)^{1-\alpha}} dt - (\mu + \gamma) \frac{1}{\Gamma(\alpha)} \int_0^{t^n} \frac{I^L}{(t_n - t)^{1-\alpha}} dt \\ R^{(n)} = R(0) + \gamma \frac{1}{\Gamma(\alpha)} \int_0^{t^n} \frac{I^L}{(t_n - t)^{1-\alpha}} dt - \mu \frac{1}{\Gamma(\alpha)} \int_0^{t^n} \frac{R^L}{(t_n - t)^{1-\alpha}} dt, \end{cases} \quad (12)$$

Finally, if we compute the integrals in (12) using the MCM (as in (6)), we obtain the approximate solution of the fractional system SIR (9):

$$\begin{cases} S^{(n)} = S(0) - \frac{\beta t_n}{\Gamma(\alpha) N} \sum_{i=1}^{N} (t_n - t_i^*)^{\alpha-1} S^L(t_i^*) I^L(t_i^*) - \frac{\mu t_n}{\Gamma(\alpha) N} \sum_{i=1}^{N} (t_n - t_i^*)^{\alpha-1} (S^L(t_i^*) - 1) \\ I^{(n)} = I(0) + \frac{\beta t_n}{\Gamma(\alpha) N} \sum_{i=1}^{N} (t_n - t_i^*)^{\alpha-1} S^L(t_i^*) I^L(t_i^*) - \frac{(\mu + \gamma) t_n}{\Gamma(\alpha) N} \sum_{i=1}^{N} (t_n - t_i^*)^{\alpha-1} I^L(t_i^*) \\ R^{(n)} = R(0) + \frac{\gamma t_n}{\Gamma(\alpha) N} \sum_{i=1}^{N} (t_n - t_i^*)^{\alpha-1} I^L(t_i^*) - \frac{\mu t_n}{\Gamma(\alpha) N} \sum_{i=1}^{N} (t_n - t_i^*)^{\alpha-1} R^L(t_i^*), \end{cases} \quad (13)$$

where N is a positive integer and ($t_1^*, ..., t_N^*$) are random numbers uniformly distributed in $[0, t_n]$. Finally, it is important to emphasize that the proposed MCM can also be used to obtain the solution of the SIR system with integer derivative by substituting $\alpha = 1$ into (13).

4. DISCUSSION

In this section, we will obtain the numerical solution of the fractional SIR model (9) by the proposed MCM, for this purpose we implement the equations (13) in the Python language. To generate uniformly distributed random numbers ($t_1^*, ..., t_N^*$), we use a Python module called random, which is a pseudo-random number generator.

For the numerical simulation, the domain was divided into $L = 300$ parts, and samples of $i = 5,\ i = 10,\ i = 100,$ and $i = 1000$ random points were made in each of these parts ($N_x = in,$ for $a + (n-1)\Delta x \leq x < a + n\Delta x$ where n is the $n - th$ part of the domain and $\Delta x = \frac{b-a}{L}$). Also, for simplicity, we choose $h = \Delta x = \frac{b-a}{L}$.

The solutions were obtained considering $\alpha = 0.75$ and using the following values for the initial conditions: $S(0) = 1 - \frac{1}{N_p}$, $I(0) = \frac{2}{N_p}$ and $R(0) = 0 \text{ with } N_p = 100000$, for the other parameters $\beta = 0.7$, $\gamma = 0.1$ and $\mu = 0$ were considered. To compare the solution found with the Monte Carlo method (MCM), the solution of the system (13) was used with the finite difference method (FDM) as used in the work of (TAVARES and LAZO, 2022).

In Figure 1 we see the system solution (9) using MCM and FDM. In this solution, a step $h = t_n - t_{n-1} = 0.5$ days, and $i = 5$ was used to show the statistical fluctuations generated by the MCM. The value of i gives us the number of random numbers generated at each sample for time t_n.

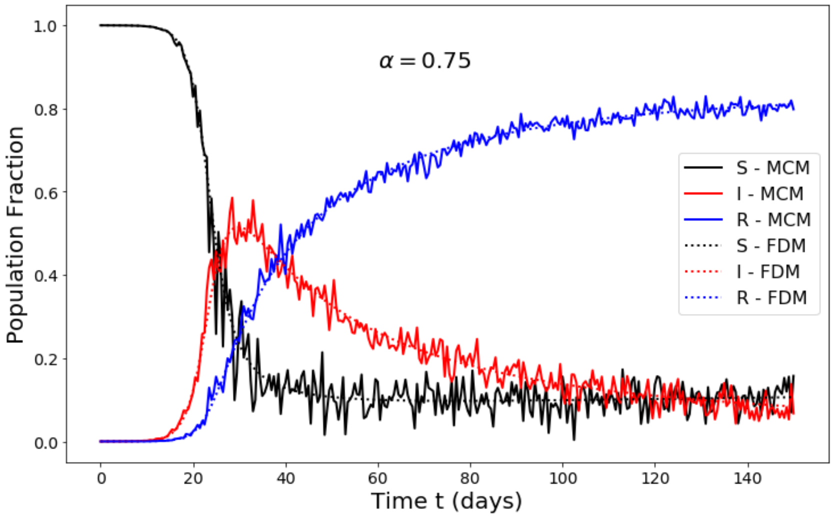

Figure 1. Comparison of the SIR -fractional system solution by FDM and by MCM with $L = 300$, $h = 0.5$ and $i = 5$.

To check how the statistical convergence of the solution occurs, the value of i was doubled in Figure 2. In this case, despite a small change in i, better convergence can be seen compared to the previously obtained solution.

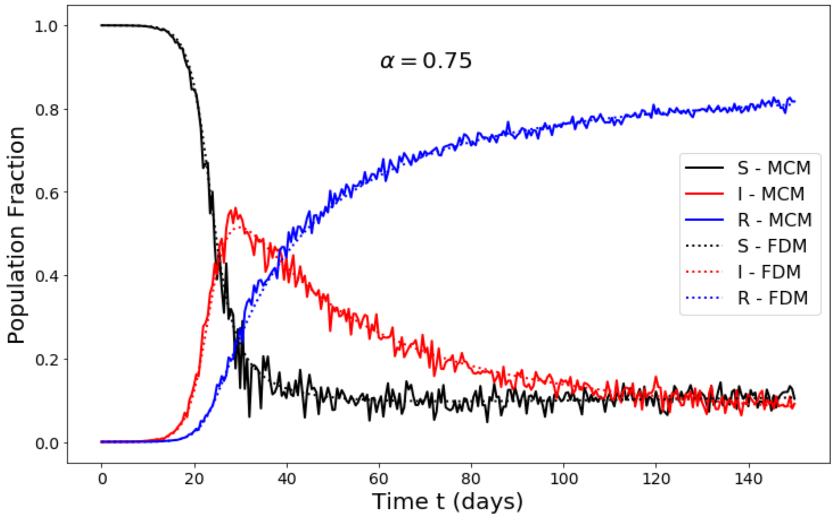

Figure 2. Comparison of the SIR -fractional system solution by FDM and by MCM with $L = 300$, $h = 0.5$ and $i = 10$.

Using $i = 100$ and $i = 1000$, we obtain in figures 3 and 4 MCM solutions that are much closer to those of FDM.

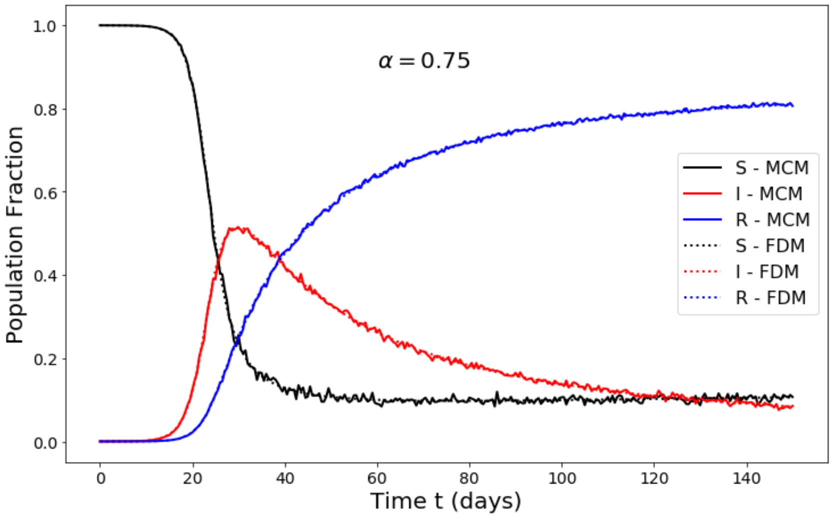

Figure 3. Comparison of the SIR -fractional system solution by FDM and by MCM with $L = 300$, $h = 0.5$ and $i = 100$.

These results illustrate how statistical convergence of the system solution occurs by increasing the value of i. This is due, as we saw in (8), to the reduction of the standard error.

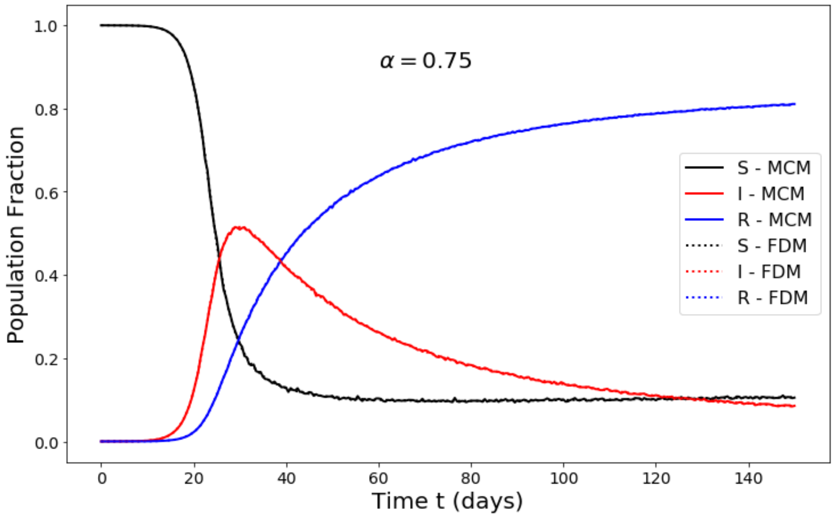

Figure 4. Comparison of the SIR -fractional system solution by FDM and by MCM with $L = 300$, $h = 0.5$ and $i = 1000$.

5. CONCLUSIONS

Fractional calculus is a mathematical tool used to study problems involving nonlocality and memory effects in various fields of knowledge. An example is the study of the effects of memory in an epidemic (see (BARROS et al., 2021) and (TAVARES and LAZO, 2022)). In this context, it becomes necessary to develop efficient numerical methods to solve fractional differential equations. The method proposed in this article is the MCM. As an example, we apply the MCM to obtain the solution of the fractional SIR model. To study the statistical convergence, we compare the solution obtained with MCM with the solution obtained with the FDM proposed in (TAVARES and LAZO, 2022). It is important to emphasize that the goal of this work was to show that MCM can be used to solve systems of fractional differential equations, even when these equations contain singular integrands. For this reason, we have chosen as an example of application a well-known and well-performing system, the fractional SIR model. Given the complexity and computational cost, a study will be carried out in the future comparing the solution of more complicated systems by MCM with the solution by other numerical methods.

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