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**From Newton equation to fractional diffusion
and wave equations**

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From Newton equation to fractional diffusion and wave equations

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Abstract

Fractional Calculus represents a natural instrument to model nonlocal (or long-range dependence) phenomena either in space or time. The processes that involve different space and time scales appear in a wide range of contexts, from Physics and Chemistry to Biology and Engineering. In many of these problems, the dynamics of the system can be formulated in terms of fractional differential equations which include the nonlocal effects either in space or time. We give a brief, non exhaustive, panoramic view of the mathematical tools associated to the Fractional Calculus as well a description of some fields where either it is applied or could be potentially applied.

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1 Introduction

Fractional Calculus (see [40]) offers a very suggestive and stimulating scenario where we have the convergence of deep and fundamental mathematical questions, development of appropriate numerical algorithms, as well as the applications to modellizations in different frameworks. An illustration of the physical applications of Fractional Calculus is the recent following books and special issues on applications on nanotechnology and other important topics [12, 13, 3, 32, 46, 32], among many others.

From the mathematical point of view, the modellization of the long-range dependence is associated to integro-differential equations in a broad sense. On the other hand, in many cases such integro-differential equations can be understood as fractional differential equations and they can be studied in the Fractional Calculus framework.

Up to 1994 a very extensive review about the nonlinear nonlocal wave equations with applications in hydrodynamics, magnetohydrodynamics and plasma can be found in the book of Naumkin and Shishmarev [30]. The nonlocality in space is associated to the long range interactions (many space scales) while the nonlocality in time is related to the effects with memory / delay (many time scales). The corresponding nonlocal systems are described by general integral equations. We have a large spectrum of scenarios where the integral equations occur [24, 8, 2, 52, 54, 49, 1, 35]: Potential Theory, Signal processing, Problems in

Geophysics, Problems in Electricity and Magnetism, Hereditary Phenomena in Physics and Biology, Problems in Population Growth and Industrial Replacement, Radiation Problems, Optimization and Automatic Control Systems, Communication Theory, Stochastic Problems and Mathematical Economics and Financial Phenomena.

Prof. R.L. Magin in his recent book, *Fractional Calculus in Bioengineering* [26] establish clearly the underlying mathematical context of the Fractional Calculus:

The purpose of this book is to explore the behavior of biological systems from the perspective of fractional calculus. Fractional calculus, integration and differentiation of an arbitrary or fractional order, provides new tools that expand the descriptive power of calculus beyond the familiar integer-order concepts of rates of change and area under a curve... Fractional Calculus adds new functional relationships and new functions to the familiar family of exponentials and sinusoids that arise in the realm of ordinary linear differential equations. Among such functions that play an important role, we have the Euler Gamma function, the Euler Beta function, the Mittag-Leffler functions, the Wright and Fox functions, etc.

From the historical point of view, the origin of the Fractional Calculus coincides with that of Differential Calculus. In a letter [22] dated on September 9, 1695, and addressed to G. Leibniz, M. de L'Hopital raises the question of the possible meaning of $\frac{d^n f(x)}{dx^n}$ if $n = 1/2$. The answer of Leibniz was: "... $d^{1/2}x$ will be equal to $x\sqrt{dx} : x$. This is an apparent paradox from which, one day, useful consequences will be drawn". The Fractional Calculus arises to give a meaning to the non integer derivatives. This concept was also analyzed by E. Euler, J. Liouville, P.S. Laplace or Fourier. The generalization of this framework indicates that it is more appropriate to talk of *Integration and Differentiation of arbitrary order*. The book by Samko et alii [40] reflects the situation of the Fractional Calculus up to 1990 with a wide bibliography and many applications. Therefore we can think in the field of Fractional Calculus as an old topic, but from 20 years ago the real applications of the so-called fractional models in so many branches of Applied Sciences and Engineering have increased in a dramatic way, so we can consider the topic of Fractional differential Equations and their applications as a emergent field.

A non-exhaustive list of works that support the mentioned modern development of the Fractional Calculus and their Applications are the following: [31, 29, 33, 17, 36, 39, 5, 58]. From our point of view, the monographic work by Metzler nad Klafter in 2000 [28] could be consider as the last breakpoint in developing the field of the study of fractional differential equations and their applications. Some of the more important publications on the mentioned topic during last five years, among so many references, could be the the following books Kilbas [20], [59], [48], [21], [25], [7], [44] and [18].

There are different definitions of fractional derivatives and, as a consequence, of fractional integrals, since the fractional derivation is the inverse operation of the fractional integration. This a generalization of what happens in ordinary calculus with the standard integer derivatives and integrals according to the Fundamental Theorem of Calculus. The different fractional derivatives coincide in the integer case, up to a constant in some cases. We have the fractional derivatives and integrals of Riemann-Liouville, Liouville, Caputo, etc., and their general feature is the *nonlocal character* since they depend on the values of the function in an interval. As an illustration we have a derivative of order β of the function $f(t)$:

$$\frac{d^\beta f(t)}{dt^\beta} = \frac{1}{\Gamma(m-\beta)} \int_0^t \frac{f^{(m)}(\tau)}{(t-\tau)^{\beta+m-1}} d\tau \quad (1.1)$$

where $m = 1, 2, \dots$ and $0 \leq m-1 < \beta \leq m$. This definition requires the absolute integrability of the derivative of order m .

The nonlocal character makes the fractional derivatives suitable for the modellization of systems with long range interactions. On the other hand, the freedom in the definition of fractional derivatives allow us to incorporate different types of information. At the same time, the fractional derivatives with non-integer exponents stress which algebraic scale properties are relevant to the data analysis.

In this contribution, we present a standard approach to construct fractional differential equations from the basic equations of Classical and Quantum Mechanics (Section 2). In Section 3, we analyze the possible bridges between the Fractional Calculus and Fractals while in Section 4 , we consider the relation of the Fractional calculus with the modellization of relaxation processes.

2 Fractional Differential Equations

Following the models of Classical Mechanics ([11]) and Quantum Mechanics ([9]), let us consider a possible standard path among the basic equations of Physics that would allow us to interpret in a more wide context the level of *fractionarization* of the basic differential equations by analyzing the associated dynamics and solutions in the framework of the corresponding modellization [28, 41, 15, 20, 56].

For the sake of simplicity, let us consider systems in one space dimension. Newton's equation for a particle of mass m moving in a one-dimensional force field F , u being the displacement, is:

$$m \frac{d^2 u}{dt^2} = F. \quad (2.1)$$

Let us consider now a discrete system, formed by infinite point-like masses, m , spaced a distance L and connected by strings of the same constant k . If we name u_i the displacement of the particle i from the equilibrium, the equation of motion is given by

$$\frac{m}{L} \frac{d^2 u_i}{dt^2} = kL \frac{u_{i+1} - 2u_i + u_{i-1}}{L^2} \quad (2.2)$$

This equation is written in such a way as to interpret appropriately the continuous limit of the system when $L \rightarrow 0$:

$u_i \rightarrow u(x), \quad \frac{m}{L} \rightarrow \rho$ (linear mass density)
$kL \rightarrow Y$ (Young's modulus)
$\frac{u_{i+1} - 2u_i + u_{i-1}}{L^2} \rightarrow \frac{\partial^2 u}{\partial x^2}$

Thus we have the equation

$$\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0, \quad (2.3)$$

where $c^2 = Y/\rho$. With this mechanical approach, we get the wave equation which appears in many contexts according to the different meanings of u and c . If we assume a damping mechanism either in the discrete system or in the continuous limit we have the equation

$$\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} + \frac{1}{D} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0 \quad (2.4)$$

When the damping term, $\frac{1}{D} \frac{\partial u}{\partial t}$, dominates over the inertial one, $\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2}$, we have the standard diffusion equation

$$\frac{\partial u}{\partial t} - D \frac{\partial^2 u}{\partial x^2} = 0 \quad (2.5)$$

Other basic equations are obtained by considering extra linear terms. This the case of the *Klein-Gordon equation*:

$$\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + \mu^2 u = 0 \quad (2.6)$$

and the *Telegraph equation*:

$$\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} + \frac{1}{D} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + \mu^2 u = 0. \quad (2.7)$$

All this can be summarized in the following table, where we also include Dirac's equation to be discussed in the following paragraphs:

Newton's equation for one particle	→	Newton's equation for one-dimensional system of particles linearly coupled
System of particles linearly coupled	<u>Continuous limit</u> →	One-dimensional wave
Wave equation with damping Klein-Gordon equation	→	Diffusion equation → Fractional Dirac equation Dirac equation, Telegraph equation

According to the previous statements, we have a set of very important features

- The fractional calculus provide a natural interpolation between different equations. For instance, we have the fractional interpolation between the wave equation (hyperbolic) and the diffusion equation (parabolic). Thus, we have the family of fractional equations

$$\frac{\partial^\beta u}{\partial t^\beta} - D \frac{\partial^2 u}{\partial x^2} = 0. \quad (2.8)$$

When $\beta = 2$ we have the wave equation, while we have the diffusion equation for $\beta = 1$. The study of the such possible interpolations has not been fully exploited yet.

- The different equations above can be fractionalized by replacing the integer derivatives either in space or time by fractional derivatives. The range of fractional equations is very wide at the same time that the exploration of the associated dynamics and solutions is a task to be fulfilled. On the other hand, it is an open issue to analyze the relation of the different fractionalizations at the discrete and the continuous levels.
- **The Standard Diffusion Equation.** The diffusion equation (2.5) appears in very different physical contexts which leads to a better understanding and interpretation of the generalized diffusion equations. Such different applications allow a richer phenomenology to understand the possible meaning of the different possible fractionalizations. As an example, the equation is obtained by combining the following laws with the associated continuity equation
- *Darcy Law*

$$\vec{q} = -K \nabla h \quad (2.9)$$

where q is the flux of groundwater, K is the medium property: hydraulic conductivity and h is the potential related to the head.

- *Fourier Law*

$$\vec{Q} = -\kappa \nabla T \quad (2.10)$$

where Q is the flux of heat, κ is the medium property: thermal conductivity and T is the potential related to the temperature.

- *Fick Law*

$$\vec{f} = -D \nabla C \quad (2.11)$$

where f is the flux of solute, D is the medium property: diffusion coefficient and C is the potential related to the concentration.

- *Ohm Law*

$$\vec{j} = -\sigma \nabla V \quad (2.12)$$

where j is the flux of charge (electrical current), σ is the medium property: electrical conductivity and V is the potential related to the voltage.

- The Fractional Dirac equation (see [50],[51], [16], [52],[34]). The free Dirac equation ([9]) can be considered as the square root of the Klein-Gordon equation. This is also true for the case of $\mu = 0$ in Eq. (2.6) which corresponds to the wave equation. More precisely in this last case, we have the following diagram: where A and B are matrices satisfying

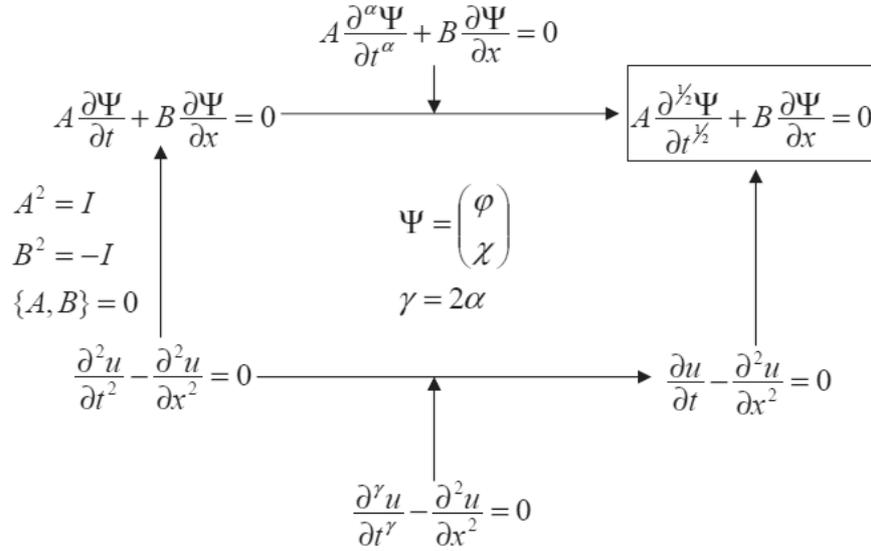


Figure 1: Fractional diffusion equation and Fractional Dirac-type equation

the indicated algebra. The function $u(x, t)$ is scalar while $\Psi(x, t)$ is a multicomponent function with, at least, two scalar space-time components.

$$\Psi = \begin{pmatrix} \varphi(x, t) \\ \chi(x, t) \end{pmatrix} \quad (2.13)$$

In the context of the diagram above, we can understand equation

$$A \frac{\partial^{1/2} \Psi}{\partial t^{1/2}} + B \frac{\partial \Psi}{\partial x} = 0 \quad (2.14)$$

as the square root of the standard diffusion equation (2.5). It is another way to view the possible interpolations between the hyperbolic operator of the wave equation and the parabolic one of the classical diffusion equation. Every scalar component of $\Psi(x, t)$ satisfies also the diffusion equation above. Such solutions can be interpreted as probability distributions with internal structure associated to internal degrees of freedom of the system. We could name them *diffunors* in analogy with the spinors of Quantum Mechanics.

According to the possible representations of the Pauli algebra for A and B, we have either an uncoupled system or a coupled system of equations. An example of the first case is the representation.

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (2.15)$$

The transition between the two limit behaviours indicated in the diagram is not well understood and it deserves a deep analysis. As an illustration of the possible rich phenomenology associated to the interpolating fractional wave and Dirac equations is their behaviour with respect the discrete symmetries: time T and space inversion P , ([34]).

This analysis of the fractional wave, diffusion and Dirac equations, fits in the general context of establish bridges between the Fractional Calculus and the Classical and Quatum Mechanics [53, 47]. This is also the approach of the works of D. Baleanu and coworkers ([37]).

3 Fractional Calculus and Fractals

The Fractals and the Fractional Calculus generate parameters of intermediate order: Arbitrary dimensions as well as arbitrary order of integration and differentiation [57], [27]. Let us consider the basic aspects associated to both conceptual blocks and we will remark possible bridges between them to be explored:

1. The Fractals show self-similar structures, being the same structure at all scale levels. Such structures are introduced by using the concept of a reference structure and repeating itself over many scales, telescoping both downward and upward in scale. In general, the fractals structures are defined by an iterative process instead of an explicit mathematical formula. A simple case is the *Cantor Set* which is a limiting set of points which results from discarding the middle third of each line segment in going from generation to generation, and starting from a line segment of unit length. The *fractal dimension* D is a measure of the irregularity of the fractal structure, and in the case of the Cantor set the fractal dimension is $D = \frac{\ln 2}{\ln 3} \approx 0.6309$.

The fractal property can be either in space or in time. In the first case we have the fractal geometric structures as the Cantor set while in the temporal context we have the structures of sequence of data generated for a system over an interval of time. A

special case is the *Weierstrass Function* which is an example of a function continuous everywhere but nowhere differentiable:

$$W(z) = \sum_{n=-\infty}^{\infty} \frac{(1 - e^{i\gamma^n z})e^{i\phi_n}}{\gamma^{(2-D)n}}, \quad (3.1)$$

where $\gamma > 1$, ϕ_n is an arbitrary phase and $1 < D < 2$, being D the fractal dimension of the self-similar structure defined by $W(z)$. The function can be interpreted as a superposition of harmonic terms: the first one with unit amplitude and unit frequency and the n -order term with amplitude $\gamma^{(2-D)(n-1)}$ and frequency γ^{n-1} .

The lack of differentiability of $W(z)$ is related to the integer derivatives. On the other hand, it has been established that the fractional derivative (fractional integral) of the Weierstrass function is another fractal function with a greater (lesser) fractal dimension [38]. At the same time, it has been proved that the Weierstrass function is a solution of a fractional differential stochastic equation of motion. In particular, we have the following relations for the Weierstrass function:

- The fractional Riemann-Liouville integral of order β , with $0 < \beta < 1$:

$$D_{RL}^{-\beta}W(z) = \frac{1}{\Gamma(\beta)} \int_{-\infty}^z \frac{W(u)du}{(z-u)^{1-\beta}} \quad (3.2)$$

- The fractional Riemann-Liouville derivative of order β , with $0 < \beta < 1$:

$$D_{RL}^{\beta}W(z) = \frac{1}{\Gamma(1-\beta)} \int_{-\infty}^z \frac{W(u)du}{(z-u)^{\beta}} \quad (3.3)$$

- The relation between the fractal dimensions of the fractional derivative and integral of the Weierstrass function

$$Dim[D_{RL}^{-\beta}W] = Dim[W] - \beta Dim[D_{RL}^{\beta}W] = Dim[W] + \beta \quad (3.4)$$

2. One of the possible experimental contexts to apply together the concepts of Fractals and Fractional Calculus is related to the propagation of waves [4], [14] and [19]. In the XIX Century, James Clerk Maxwell and Lord Rayleigh studied the interaction of electromagnetic waves with Euclidean regular structures (cylinders, spheres,). On the other hand, there are either non regular artificial structures or from Nature that show many length scales and they are no suitable to be studied in the Euclidean context. This is the case of non regular surfaces, disordered media, structures with specific properties of scattering,...etc. In this context, the fundamental issue of special technological impact is *the relation between the geometrical parameters (structure descriptors) and the physical quantities that characterize electromagnetically the system*. For instance, a relevant information is the relation between the fractal dimension of the scattering surface and the scattered wave. Related to that, we have that a recent field of research has been to explore the possible links between the fractional calculus and the electromagnetic theory ([10]). The fractionalization of certain linear operators in electromagnetic theory has led to relevant solutions in radiation and scattering problems.

As a simple illustration, let us consider the propagation of a wave in fractal media. The Geometrical Optics cannot be applied and the eikonal equation is not longer valid since it applies for wave lengths $\lambda \ll$ *Dimension of any change in the media*. This condition

cannot be satisfied for fractal media because in this case there is no a characteristic length of the system. We can consider the associated stationary eigenvalue problem that appear in two contexts: the wave equation in a fractal potential and the wave equation with fractal boundary conditions. In the last case, we have the general equation

$$Lu = \mu u \quad (3.5)$$

where, L is a linear differential operator on \mathbb{R}^n with boundary conditions $u_0(x)$ on a non-differentiable surface but which admits the fractional derivative D^β with $\beta < 1$. If we define $\Phi = D^{\beta-1}u$, we have the problem $L\Phi = \mu\Phi$ with the boundary condition $\Phi_0(x)$, being Φ differentiable. Thus with the help of the fractional derivative we transformed the original boundary problem into another one more suitable to be studied.

4 Fractional Calculus and Relaxation Processes

In the study of the behavior of the materials under applied forces, we have two ideal relations between such forces and the resultant displacements in the material which are represented by linear differential equations:

- *Linear Elastic Behavior* which is described by the Hooke's law (ideal solid):

$$\sigma(t) = E\varepsilon(t) \quad (4.1)$$

where E is Young's modulus, $\sigma = \frac{\text{force}}{\text{area}}$ is the stress and $\varepsilon = \frac{\text{elongation}}{\text{original length}}$ is the strain of the corresponding mechanical model, that in this case it is represented by a spring characterized by the constant E .

- *Ideal Viscous Fluid Behavior* which is described by Newton' fluid law (ideal fluid):

$$\sigma(t) = \eta \frac{d\varepsilon(t)}{dt} \quad (4.2)$$

where η is the viscosity coefficient, and in this case the phenomenological model is represented by a dashpot

In general, the real materials exhibit characteristics which combine the behaviors of the ideal solids and liquids and are named *viscoelastic materials*. The basic models of such materials are based on combinations of springs and dashpots [26], [12], [55]. As an illustration, let us consider the combination of a spring and a dashpot in series. In this case the stresses are equal for both structural parts while the strains add. This leads to the classical Maxwell model which is described by the following linear differential equation obtained from the above two equations:

$$E \frac{d\varepsilon(t)}{dt} = \frac{d\sigma(t)}{dt} + \frac{1}{\tau} \sigma(t) \quad (4.3)$$

where $\tau = \frac{\eta}{E}$. If we consider the Laplace transform of the above equation we obtain the *relaxation modulus* $g(s) = \frac{\sigma(s)}{\varepsilon(s)} = \frac{E}{s + 1/\tau}$. Finally the stress relaxation modulus for the Maxwell model is

$$G(t) = E \exp -t/\tau \quad (4.4)$$

which indicates that the Maxwell model shows an exponential stress decay, while different behaviors are observed in real materials. The fractional calculus allow us to introduce generalizations of the Maxwell model and the basic constitutive equation that lead to more general behaviors of the stress relaxation modulus:

- The fractional constitutive equation

$$\sigma(t) = E(\tau)^\alpha \frac{d^\alpha \varepsilon(t)}{dt^\alpha} \quad (4.5)$$

which is an interpolation between Hooke's law ($\alpha = 0$) and Newton's law ($\alpha = 1$). This fractional relation can be realized physically through hierarchical arrangements and in the limit of an infinite number of springs and dashpots [12].

- The general fractional Maxwell equation offers a wide range of possible behaviors

$$E\tau^\delta \frac{d^\delta \varepsilon(t)}{dt^\delta} = \tau^\rho \frac{d^\rho \sigma(t)}{dt^\rho} + \sigma(t) \quad (4.6)$$

the solutions are well analyzed in [12, 26] as well as in the references therein.

- In order to consider other, generalizations and approaches for possible different applications, we can interpret the *Relaxation Process* either as an initial value problem or a memory problem:

– *Initial Value Problem*

The relaxation (4.4) can be interpreted as the solution of the initial value problem

$$\tau \frac{dG(t)}{dt} = -G(t), \quad G(0) = G_0 \quad (4.7)$$

with solution $G(t) = G_0 e^{-t/\tau}$. From (4.7) we can write as starting point for the fractional generalization:

$$G(t) - G_0 = -\tau^{-1} \int_0^t du G(u) = -\tau^{-1} \frac{d^{-1}G(t)}{dt^{-1}} \quad (4.8)$$

from where, we get formally the fractional generalization

$$G(t) - G_0 = -\tau^{-\alpha} \frac{d^{-\alpha}G(t)}{dt^{-\alpha}}. \quad (4.9)$$

– *Memory Problem*

Another natural generalization of the equation (4.7) is the following

$$\frac{dG(t)}{dt} = \int_0^t K(t-u)G(u) du. \quad (4.10)$$

If $K(t) = K_0 \delta(t)$ we recover the exponential behavior of the Maxwell model (4.4). If we have constant memory, $K = K_0$, we have the periodic behavior: $K(t) = G_0 \cos \sqrt{K_0}t$. Finally, if $K(t) = K_0 t^{q-2}$ with $0 < q \leq 2$, the equation (4.10) can be written as a fractional derivative and the solution can be expressed in terms of the Fox functions.

One possible application field for the Fractional Calculus would be the modellization of the *Shape Memory Alloys (SMA)*. These are basically materials that change shape when energy is applied or extracted from them. They exhibit hardness and elasticity properties that change radically at distinct temperatures [42]. There is a high complexity in the relation between the microscopic and macroscopic behaviors. There are no reliable constitutive models, although some have been studied by Tanaka [43], Liang-Rogers [23] and Brinson [6]. The key feature of these materials, as the name indicates, is that their dynamics is memory dependent. Thus the possible realistic models should include the nonlocal effects in time through integrodifferential equations and, possibly fractional differential equations.

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UNIVERSIDAD COMPLUTENSE DE MADRID
MA-UCM 2010**

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