

A generalized Stefan model accounting for system memory and non-locality

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Abstract

The Stefan problem, involving the tracking of an evolving phase-change front, is the prototypical example of a moving boundary problem. In basic one-dimensional problems it is well known that the front advances as the square root of time. When memory or non-locality are introduced into the system however, this classic signal may be anomalous; replaced by a power-law advance with a time exponent that differs from $n = 1/2$. Up to now memory treatments in Stefan problem models have only been able to reproduce sub-diffusive front movements with exponents $n < 1/2$ and non-local treatments have only been able to reproduce super-diffusive behavior $n > 1/2$. In the present paper, using a generalized Caputo fractional derivative operator, we introduce new memory and non-local treatment for Stefan problems. On considering a limit case Stefan

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problem, related to the melting problem, we are able to show that, this general treatment can not only produce arbitrary power-law in time predictions for the front movement but, in the case of memory treatments, can also produce non-power-law anomalous behaviors. Further, also in the context of the limit problem, we are able to establish an equivalence between non-locality and a space varying conductivity and memory and a time varying conductivity.

Keywords: Stefan problems, fractional moving boundary problems, melting processes, anomalous diffusion.

1. Introduction

A classical free boundary problem, generally referred as the Stefan problem [1], concerns the study of the transient diffusion-controlled melting/solidification (phase change) of a solid/liquid adjacent to a heated/cooled surface. In the one-dimensional form of this problem, the time-dependent position of the liquid-solid interface $s(t)$, relative to the heated/cooled surface, advances as the square root of time, $s(t) \sim t^n$, $n = 1/2$ [1], which is the expected normal behavior for a diffusion process. Experimental observations of Stefan like and related phase-change problems, e.g., frost growth [2] and moisture infiltration [3], however, indicate that in some physical settings different time exponents, i.e., $n > 1/2$ (super-diffusive) or $n < 1/2$ (sub-diffusive), can manifest. These observations have motivated theoretical studies to investigate general Stefan models formulations that can produce anomalous behaviors [4, 5, 6, 7, 8, 9, 10]. We also refer to the recent discussion paper [11] and the references therein about fractional Stefan problems.

The recent work in [12] provides an extensive review on the theory and applications of anomalous behavior in heat transfer system. One method to treat anomalous behavior is by the introduction of a *memory* into the system of interest, requiring that the current state of the system depends on a weighting (usually decaying) of previous states in time; this can be achieved in Stefan models by replacing the transient terms in the governing equations

with a $0 < \nu \leq 1$ order time-fractional derivative, representing a convolution
 in time [4, 5, 6, 7, 8, 9]. An alternative approach is to invoke a *non-local* be-
 havior in which the operation of a process at a given space point in the system
 depends not just on the conditions at that point but also on a weighting of the
 current conditions throughout the whole domain; this can be achieved in Stefan
 models by replacing the temperature gradient in the heat flux definition with a
 $0 < \nu \leq 1$ order space-fractional derivative representing a convolution in space
 [4, 7, 8, 9]. Voller [8], working with a limit case Stefan problem related to melt-
 ing process, investigates how replacing the transient and gradient terms with
 Caputo fractional derivatives [13] of order $0 < \nu < 1$, representing, in turn, the
 effects of memory (time-fractional) and non-locality (space-fractional), produces
 predictions for the power-law advance of the phase front exhibiting a range of
 exponents i.e., $0 \leq n \leq 1$. Replacing the transient term with a time-fractional
 derivative (memory) results in a sub-diffusive power-law front advance $s = t^n$,
 $0 \leq n \leq 1/2$. In contrast, replacing the gradient term with a space-fractional
 derivative (non-local), produces a super-diffusive advance $s = t^n$, $1/2 \leq n \leq 1$.
 We stress the point that predictions from a Stefan model with a fractional time
 derivative are restricted to sub-diffusive anomalous behavior while predictions
 from models with a fractional gradient term are restricted to super-diffusive
 anomalous behavior.

Outside of using fractional calculus models, however, anomalous behaviors
 for the phase front movement from a Stefan problem can also be obtained by
 using a space and/or time dependent thermal conductivity in a conventional
 (integer derivative) Fourier heat transport equation. For example, on using
 a power-law in space definition of the conductivity (e.g., a graded material),
 Falcini and Voller [10] derive a closed analytical solution of a one-dimensional
 Stefan problem in which the phase front movement recovers the full range of
 power-law in time exponents, $0 \leq n \leq 1$. In more recent work, Falcini et al. [4],
 working with a generalized Fourier heat transport model that combines both
 Caputo space and time fractional derivatives with a power-law in space depen-
 dent conductivity, explore the connections between memory, non-locality, and

variable conductivity in setting the space-time scaling for diffusion controlled problems. While this work provides a theoretical underpinning for the anomalous behaviors associated with generalized Stefan models it also introduces some ambiguity related to matching a given model choice (memory, non-local, variable conductivity) to a given observation of the phase front movement; e.g., as shown in [4], with the appropriate choice of time derivative order or power-law spacial variation of conductivity, both memory and non-linear conductivity models can predict a power-law in time phase front movement $s = t^n$ with an identical sub-diffusive exponent $0 \leq n \leq 1/2$.

At this point, we should recognize that anomalous diffusion signals are not restricted to the form of a power-law in time but more correctly include any signals whose variance does not grow linearly in time. In this light, another interesting class of anomalous diffusion processes to consider is ultraslow scaled Brownian processes, where the variance grows logarithmically in time (see for example [14] and the references therein). Recovering such a behavior for the phase front movement, however, is out of the reach of the current memory, non-local and variable conductivity treatments that have been proposed for Stefan models.

The objective of this paper is to introduce a general, fractional based treatments for modeling memory and non-locality in a Stefan problem. The key step is to replace the standard Caputo fractional derivative of temperature with respect to time t or space x , used in previous general Stefan model treatments, with an integro-differential evolution operator that is essentially the Caputo fractional derivative of temperature with respect to a general function of time $f(t)$ or space $f(x)$. With appropriate settings, using these treatments in the Stefan problem, even in the absence of a space or time varying conductivity, can not only predict phase front movements with arbitrary positive power-law time exponents $0 \leq n \leq 1$ but can also predict front movements that exhibit non-power-law anomalous behaviors. Further, in the context of the limit melting Stefan problem introduced in Voller [8], we are able to mitigate some of the ambiguity in matching a suitable model treatment to given observations of

front movement and temperature profile. In particular, we show, in this limit
 85 problem, (i) that non-local treatments are essentially equivalent to treatments
 that use a spatially varying conductivity (representing a graded material), (ii)
 that memory treatments are essentially equivalent to treatments that use a time
 varying conductivity (representing an aging effect), and (iii) a clear delineation
 of anomalous behaviors resulting from memory and non-local treatments.

90 **2. A one-phase, one-dimensional Stefan model**

Without too much loss of generality we will carry our arguments in this work
 by considering a one-phase, one-dimensional Stefan problem. This involves the
 melting of a solid in a one-dimensional domain $x \geq 0$. Initially the solid is at
 the unique phase change temperature, $T = 0$ say, and melting is induced at
 95 time $t = 0$, by raising and fixing the temperature at $x = 0$ to a fixed value, e.g.,
 $T_0 > 0$. The governing equation representing the heat conduction in the liquid
 domain is (see [1])

$$\rho c \frac{\partial T}{\partial t} = -\frac{\partial q}{\partial x}, \quad 0 \leq x \leq s(t), \quad (1)$$

where q is the flux term, ρ is density and c is the specific heat (assumed constant
 in this work). The initial condition is $T(x > 0, t = 0) = 0$ and the boundary
 100 conditions are $T(0, t) = T_0$ at $x = 0$ and $T(s(t), t) = 0$. Since the problem
 is posed in an expanding domain, an extra condition is needed at the moving
 interface $s(t)$

$$q(s(t)) = \rho L \frac{ds}{dt}, \quad (2)$$

stating that the advance of the front depends on the rate at which heat arriving
 at the front can supply the latent heat L , required to melt the solid.

105 Simply proposing alternative phenomenological models for the flux term q
 will allow us to build from eqs. (1) and (2) alternative memory and non-local
 models.

3. Definitions and properties of operators

In order to provide a high degree of flexibility in the definitions of the flux q in eqs. (1) and (2), in this work we will use a number of convolution operators related to the fractional calculus. In the first place, following the monograph by Kilbas et al. [13] (Section 2.5) we consider the fractional $0 < \nu \leq 1$ order integral of a function $g(z)$ with respect to another function $f(z)$. Under the restrictions that $f(z)$ is a strictly monotonic increasing C^1 function in the interval $(0, z)$ with $f(0) = 0$, we can write this integral as

$${}_0I_z^{\nu, f} g(z) := \frac{1}{\Gamma(\nu)} \int_0^z (f(z) - f(\zeta))^{\nu-1} f'(\zeta) g(\zeta) d\zeta. \quad (3)$$

We note that, when $f(z) = z$, we recover the Riemann–Liouville fraction integral of order $0 < \nu \leq 1$ and, on associating z with time t , when $f(z) = z^{\alpha/\beta}$ we recover the definition of Erdélyi–Kober fractional integral recently applied in the studies on Generalized Grey Brownian Motion (see, e.g., [15, 16]). From this definition, appealing to the recent work of Almeida in [17], we can write down a Caputo-type regularization for an order $0 < \nu \leq 1$ fractional derivative of a function $g(z)$ with respect to $f(z)$ as

$${}_0\widehat{O}_z^{\nu, f} g(z) := {}_0I_z^{1-\nu, f} \left(\frac{1}{f'(z)} \frac{dg(z)}{dz} \right) := \frac{1}{\Gamma(1-\nu)} \int_0^z (f(z) - f(\zeta))^{-\nu} \frac{dg}{d\zeta} d\zeta. \quad (4)$$

We note the following properties of this derivative (see Theorem 5 in [17]),

$${}_0\widehat{O}_z^{\nu, f} {}_0I_z^{\nu, f} g(z) = g(z), \quad (5)$$

and (see Lemma 1 in [17])

$${}_0\widehat{O}_z^{\nu, f} f(z)^\beta \sim f(z)^{\beta-\nu}, \quad \beta > 0. \quad (6)$$

4. Particular Stefan Models

4.1. A conventional Stefan model

In the conventional treatment we assume that the flux can be represented by Fourier's first law

$$q = q^F = -K \frac{\partial T}{\partial x}, \quad (7)$$

giving rise to the following governing equation and front balance condition

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(K \frac{\partial T}{\partial x} \right), \quad 0 \leq x \leq s(t), \quad (8)$$

$$-K \frac{\partial T}{\partial x} \Big|_{x=s(t)} = \rho L \frac{ds}{dt}, \quad (9)$$

130 where, in a general setting, we can allow for both time and space variations in the conductivity K . The initial $T(x > 0, t = 0) = 0$ and boundary $T(0, t) = T_0$, $T(s(t), t) = 0$ conditions, remain as before.

4.2. A general Stefan model with memory

To introduce memory, we use the fractional order integral define in eq. (3)

135 to construct the following generalization of the Fourier law

$$q = q^{FM}(x, t) = -\frac{\kappa}{\Gamma(\nu)} \frac{\partial}{\partial t} \int_0^t (f(t) - f(\tau))^{\nu-1} \frac{\partial T}{\partial x} f'(\tau) d\tau = -\kappa \frac{\partial}{\partial t} {}_0I_t^{\nu, f} \left(\frac{\partial T}{\partial x} \right), \quad (10)$$

where $0 < \nu \leq 1$, and κ is a scaling constant. Note on setting $f(t) = t$ we recover the flux model introduced in the memory Stefan model proposed in [7].

By using eq. (10) in our base Stefan model eqs. (1) and (2), we arrive at the following memory model

$$\rho c \frac{\partial T}{\partial t} = \kappa \frac{\partial}{\partial x} \left(\frac{\partial}{\partial t} {}_0I_t^{\nu, f} \left(\frac{\partial T}{\partial x} \right) \right), \quad 0 \leq x \leq s(t), \quad (11)$$

140 with

$$-\kappa \frac{\partial}{\partial t} {}_0I_t^{\nu, f} \left(\frac{\partial T}{\partial x} \right) \Big|_{x=s(t)} = \rho L \frac{ds}{dt}. \quad (12)$$

Due to its conserved nature, this will be our preferred form for a memory model.

Note, however, that by dividing by $f'(t)$ and applying the fractional integral operator ${}_0I_t^{1-\nu, f}$ to both side of eqs. (11) and (12), we arrive, on using the properties of the general-Caputo definition in eqs. (4) and (5), the alternative

145 form of memory Stefan problem

$$\rho c {}_0\hat{O}_t^{\nu, f} T = \kappa \frac{\partial^2 T}{\partial x^2}, \quad 0 \leq x \leq s(t), \quad (13)$$

$$-\kappa \left(\frac{\partial T}{\partial x} \right) \Big|_{x=s(t)} = \rho L {}_0\widehat{O}_t^{\nu, f} s(t). \quad (14)$$

On setting $f(t) = t$, we recover the fractional derivative memory forms, found in the current literature (e.g., [4, 5, 6, 7, 8, 9]).

4.3. A general non-local Stefan model

A general non-local (GNL) model is constructed through using the general-
 150 Caputo fractional derivative definition in eq. (4) to replace the gradient term
 in the Fourier law (eq. (7)), i.e.,

$$q = q^{GNL}(x, t) = -\kappa_0 \left({}_0\widehat{O}_x^{\nu, f} T \right), \quad (15)$$

leading to the non-local Stefan model

$$\rho c \frac{\partial T}{\partial t} = \kappa_0 \frac{\partial}{\partial x} \left({}_0\widehat{O}_x^{\nu, f} T(x, t) \right), \quad 0 \leq x \leq s(t), \quad (16)$$

$$-\kappa_0 \widehat{O}_x^{\nu, f} T(s(t)) = \rho L \frac{ds}{dt}. \quad (17)$$

5. A limit case Stefan model

To arrive at analytical solutions that will expose the anomalous signals,
 155 associated with the various flux choices in the general Stefan model introduced
 in the previous section, we consider the limit Stefan problem, previously studied
 in [4, 8, 9]. This is obtained by setting the density ρ and latent heat L to unity
 and letting the specific heat $c \rightarrow 0$. In the context of the one-dimensional
 Stefan problem studied here, the physical interpretation of the limit problem is
 160 the moisture filling (infiltration) into an initially dry, horizontal, porous tube
 under the application of a fixed pressure head at $x = 0$.

5.1. The conventional limit Stefan model

Letting $c \rightarrow 0$ in the conventional Stefan problem, eqs. (8) and (9), leads to the following limit problem

$$\frac{\partial}{\partial x} \left(K \frac{\partial T}{\partial x} \right) = 0, \quad 0 \leq x \leq s(t), \quad (18)$$

$$-K \frac{\partial T}{\partial x} \Big|_{x=s(t)} = \frac{ds}{dt}. \quad (19)$$

165 The initial and boundary conditions, used here and in all alternative versions of this problem are, $T(x > 0, t = 0) = 0$ and boundary $T(0, t) = 1$, $T(s(t), t) = 0$ (see Fig. 1).

In a general setting, the conductivity K could be a function of space or time. For example we could imagine that the media is graded such that the
170 conductivity increases or decreases with space. Alternatively we might imagine a situation where the uniform ambient conditions are changing in such away to induce temporal changes in the conductivity. We will examine particular solutions for these two cases in detail below.

5.2. A limit Stefan model with memory

175 Letting $c \rightarrow 0$ in the memory Stefan problem, eqs. (11) and (12), leads to the following limit problem

$$\frac{\partial}{\partial x} (q^{FM}) = \frac{\partial}{\partial x} \left(\frac{\partial}{\partial t} {}_0 I_t^{\nu, f} \left(\frac{\partial T}{\partial x} \right) \right) = 0, \quad 0 \leq x \leq s(t), \quad (20)$$

with

$$q^{FM} = -\kappa \frac{\partial}{\partial t} {}_0 I_t^{\nu, f} \left(\frac{\partial T}{\partial x} \right) \Big|_{x=s(t)} = \frac{ds}{dt}. \quad (21)$$

From eq. (20) we can infer, for this problem, that the memory flux q^{FM} , defined in eq. (10), can only be a function of time. This in turn implies that
180 the gradient derivative, $\partial T / \partial x$, under the time fractional integration also has to be a function of time alone. Thus, the solution for the temperature profile that satisfies the equation and boundary conditions is linear in space, i.e.,

$$T = 1 - \frac{x}{s(t)}, \quad \frac{\partial T}{\partial x} = -\frac{1}{s(t)}. \quad (22)$$

To move forward we make the *ansatz* that, for any given monotonically function $f(t)$, with $f(0) = 0$, the front advance is given by $s(t) = f^{\frac{\nu}{2}}$. In this way, $f'/s \sim (f^{1-\frac{\nu}{2}})'$ and we can write the memory flux, define in eq. (10), as

$$q^{FM}(t) = \frac{\kappa}{\Gamma(\nu)} \frac{d}{dt} \int_0^t (f(t) - f(\tau))^{\nu-1} \frac{d}{d\tau} (f^{1-\frac{\nu}{2}}) d\tau \sim \frac{d}{dt} \hat{O}_t^{1-\nu, f} f^{1-\frac{\nu}{2}}. \quad (23)$$

Thus, by the general Caputo property in eq. (6), the memory flux in this limit case Stefan problem can be written as

$$q^{FM} \sim \frac{d}{dt} f^{\frac{\nu}{2}}. \quad (24)$$

On substituting this in the front condition of eq. (21) we do indeed see that $s(t) = f^{\frac{\nu}{2}}$.

The above result imparts a high degree of utility to the Stefan memory model. Effectively, whenever the observed temperature profile is linear, this model can be used to fit any observed monotonic advance of the phase front with time. For example a setting of $f(t) = t^m$, with $m > 0$, will fit any observed front movement with the general power-law form $s = t^n$, $n = (m\nu)/2 > 0$. Further, if $f(t) \sim \ln(1+t)$, our generalized Caputo derivative in eq. (4) has the form of the regularized Hadamard derivative [18] and we can match the observation of an ultraslow motion of the melting front where $s(t) \sim \ln^{\nu/2}(1+t)$.

Note, in the setting of this limit problem we can, using the second component of eq. (22), rearrange the memory flux term in eq. (24):

$$q^{FM} \sim \frac{d}{dt} f^{\frac{\nu}{2}} = f' f^{\frac{\nu}{2}-1} = \frac{f' f^{\nu-1}}{s} = f'(t) f(t)^{\nu-1} \frac{\partial T}{\partial x}. \quad (25)$$

From (25) we see that, this limit case Stefan problem based on the memory flux q^{FM} , defined in eq. (10), is equivalent to the flux in a conventional model $q^F = -K \partial T / \partial x$ with a time dependent conductivity $K(t) = f'(t) f(t)^{\nu-1}$.

5.3. A limit non-local Stefan model

Letting $c \rightarrow 0$ in the non-local Stefan problem, eqs. (16) and (17), leads to
 205 the following limit problem

$$\frac{\partial}{\partial x} (q^{GNL}) = \frac{\partial}{\partial x} \left({}_0\widehat{O}_x^{\nu, f} T(x, t) \right) = 0, \quad 0 \leq x \leq s(t), \quad (26)$$

$$q^{GNL} = -\kappa_0 \widehat{O}_x^{\nu, f} T(s(t)) = \frac{ds}{dt}. \quad (27)$$

Now we see that the non-local flux q^{GNL} can only be a function of time t . By the property eq. (5) of the general Caputo derivative, eq. (4), this requires, on accounting for the boundary conditions, that

$$T(x, t) = 1 - \frac{f(x)^\nu}{f(s)^\nu}, \quad {}_0\widehat{O}_x^{\nu, f} T(x, t) \sim \frac{1}{f(s)^\nu}. \quad (28)$$

In this way, if we restrict ourselves to power-law functions with the form $f(x) =$
 210 x^m , with $m > 0$, we can readily generate power-law in time predictions for the advance of the phase front as $s = t^n$, $0 \leq n = 1/(1 + m\nu) \leq 1$.

There are two point to make here. First, in contrast to the general-memory approach, the ability of the general non-local approach, to match a given monotonic advance of the phase front is restricted to power-laws in time, with exponents in the range $0 < n \leq 1$. Secondly, again in contrast to the general-memory
 215 approach, the general non-local approach will always generate a curved temperature profile, eq. (28). A linear profile is only recovered under normal-diffusion conditions, $\nu = 1$, $f(x) = x$.

Note further, in considering the limit case Stefan problem with $f(x) = x^m$,
 220 $m > 0$, if we set a non linear conductivity as $K(x) = f^{(1-\nu)}/f' = x^{1-m\nu}$ we see that our non-local flux is equivalent to a local flux with a non-linear conductivity, i.e., within an appropriate constant, $q^{GNL} \equiv K(x)(\partial T/\partial x)$.

6. Discussion

In this work our focus has been to study the influence of the flux definition
 225 on the prediction of the temperature profile $T(x, t)$ and phase front movement

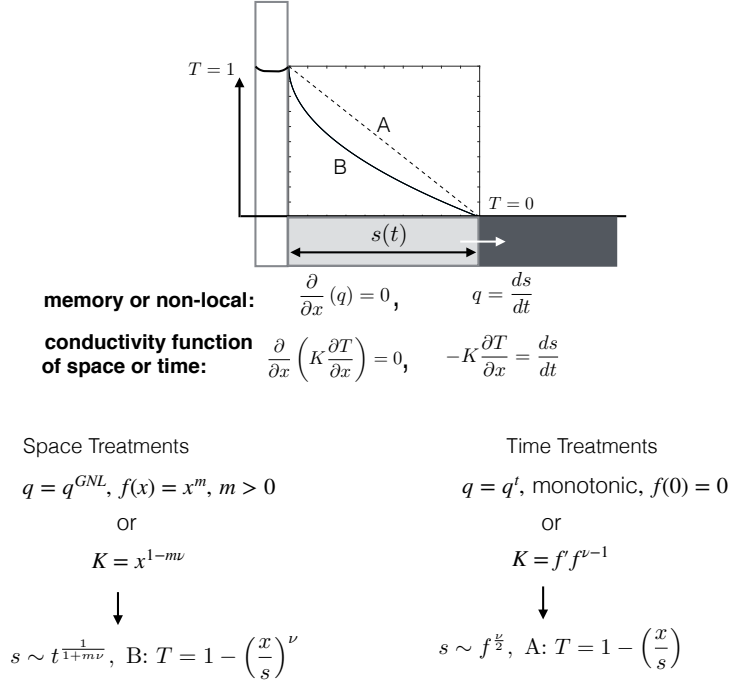


Figure 1: Model choices for limit case Stefan problem

$s(t)$ from a one-dimensional one-phase Stefan melting problem. We select three different flux definitions to investigate; (i) a conventional Fourier law (conductivity \times temperature gradient) with a conductivity as function of time (aging) or space (graded material), (ii) a flux that can account for system memory expressed in terms of an order $0 < \nu \leq 1$ fractional derivative of the temperature with respect to a general function of time $f(t)$, and (iii) a flux that can account for non-locality, expressed in terms of an order $0 < \nu \leq 1$ fractional derivative of the temperature with respect to a general function of space $f(x)$. All of these flux definitions can produce anomalous diffusion signals in which the monotonic advance of the melting front differs from the normally expected value of $1/2$.

As we have noted in our introduction, recent work on Stefan problems [4] has suggested that, in matching a given anomalous observation, there is some ambiguity in selecting an appropriate flux definition. For example, an observed anomalous front advance can be independently matched by two of the three

240 choices of flux model. Here, through investigating and solving a particular limit
case Stefan problem (a model of moisture infiltration into a porous tube), we
have mitigated some of the ambiguity. In particular, we have shown that when
we base the model choice on two physical observations, the front movement
and the temperature profile, we are able to distinguish between the predictions
245 from a memory and a non-local model. In addition, in the context of our
limit model, as summarized in Fig. 1, we have shown that the memory flux
is equivalent to a conventional flux with a time dependent conductivity and
that the non-local flux is equivalent to a conventional flux with a power-law
in space dependent conductivity. Hence, while this may not be the case for
250 more general Stefan problems, for the infiltration problem, it is reasonable to
separate our phenomenological flux models into two classes, *time* treatments
(memory or non-linear in time conductivity) and *space* treatments (non-locality
or space dependent conductivity). We can select the appropriate treatment from
observations of the temperature profile; an observed linear profile indicating a
255 time treatment and an observed non-linear profile indicating a space treatment.
Both time and space treatments are able to match power-law time exponents
(sub- $0 < n \leq 1/2$ and super- $1/2 < n \leq 1$) for front advances. Time treatments,
however, are more versatile, with the mathematical ability to match power-law
exponents beyond the ballistic range $n > 1$ and alternative time dependencies
260 for the front movement, e.g., ultra slow log laws.

Acknowledgments

This research is supported by the Basque Government through the BERC
2014–2017 and BERC 2018–2021 programs, and by the Spanish Ministry of
Economy and Competitiveness MINECO through BCAM Severo Ochoa excel-
265 lence accreditations SEV-2013-0323 and SEV-2017-0718. The research began
and was primarily developed at BCAM, Bilbao, during the visiting fellowship
of Roberto Garra in August–October 2017.

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