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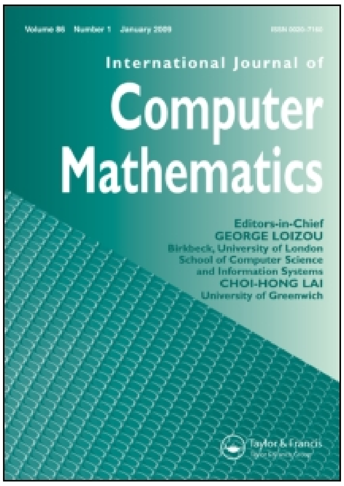

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On the moving boundary formulation for parabolic problems on unbounded domains

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On the moving boundary formulation for parabolic problems on unbounded domains

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The aim of this paper is to propose an original numerical approach for parabolic problems whose governing equations are defined on unbounded domains. We are interested in studying the class of problems admitting invariance property to Lie group of scalings. Thanks to similarity analysis the parabolic problem can be transformed into an equivalent boundary value problem governed by an ordinary differential equation and defined on an infinite interval. A free boundary formulation and a convergence theorem for this kind of transformed problems are available in [R. Fazio, *A novel approach to the numerical solution of boundary value problems on infinite intervals*, SIAM J. Numer. Anal. 33 (1996), pp. 1473–1483]. Depending on its scaling invariance properties, the free boundary problem is then solved numerically using either a noniterative, or an iterative method. Finally, the solution of the parabolic problem is retrieved by applying the inverse map of similarity.

Keywords: parabolic problems; unbounded domains; similarity analysis; iterative and noniterative transformation method

2000 AMS subject classification: 65L10; 35R35

CCS Category: G.1.8; G.1.7

1. Introduction

The main aim of this paper is to apply the similarity analysis in order to help us in understanding how a moving boundary formulation can be used for the numerical solution of parabolic problems defined on unbounded domains. The mathematical problem of interest here is, in its most general form, given by

$$\frac{\partial^2 u}{\partial x^2} = f\left(t, x, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t}\right) \quad \text{on } t > 0, \;\; 0 < x$$
$$\alpha(t)u(0,t) + \beta(t)\frac{\partial u}{\partial x}(0,t) = \gamma(t), \quad \alpha^2 + \beta^2 \neq 0, \;\; \gamma \neq 0$$

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$$u(x,0) = 0$$
$$u(x,t) \longrightarrow 0 \quad \text{as } x \longrightarrow \infty. \tag{1}$$

The direct search for analytical solutions to this class of problems is usually a very hard task whose difficulty is in general highly increased whenever the governing partial differential equation (PDE) is nonlinear.

On the other hand, standard numerical methods are not suitable to deal with problems where one or more boundary conditions are given at infinity. The most used approach to deal numerically with this kind of problem is to approximate them by introducing a finite truncated boundary (see [14, pp. 39–51] and the quoted references). However, even in the case of boundary value problems (BVPs) governed by ordinary differential equations (ODEs) defined on an infinite interval, the truncated boundary approach has been found to be a trial and error approach prone to relevant errors if the truncated boundary is not chosen sufficiently large (see [19]), so that any different strategy would be of interest. In this context, the so-called artificial boundary conditions to be imposed at a finite truncated boundary were introduced by Engquist and Majda [7] for hyperbolic problems, and by Keller and Givoli [17] for elliptic problems. Suitable artificial boundary conditions can be defined in several different ways and their construction is indeed a hard task (see [14, pp. 39–51]; [15,25,26]. In a different approach, introduced recently by Koleva [18], *ad hoc* finite difference methods, by using quasi-uniform meshes with a finite number of intervals, were used for solving parabolic problems on unbounded domains in the simplest case when the governing equation is the linear heat equation.

In this paper we investigate the extension of the free boundary formulation, introduced recently by Fazio [8], to parabolic problems defined on unbounded domains. In particular, we are interested in investigating the possibility to introduce a moving boundary formulation for the problem (1).

A moving boundary problem is a nonlinear initial-BVP where the position of the moving boundary is determined as part of the solution itself. Most of the existing bibliographies on this subject, such as that in the book by Crank [4], or the one by Tarzia [23], are essentially devoted to the solution of the well-known Stefan problem, which is governed by the linear heat equation. For the numerical solution of such a problem, several different approaches have been conceived over the years. Among the most famous are the front-tracking method, the front-fixing method, the domain-fixing method (see [4, pp. 217–281]) as well as other finite-difference or finite-element approaches (for instance, see [26]), or moving grid methods, level set methods, or phase field methods (see the review by [16]). Unfortunately, the proposed methods are introduced in the case of linear parabolic PDEs and they are not easily extended to nonlinear parabolic cases also belonging to the class of problem (1). In this paper we will propose a method to overtake these difficulties, provided that the problem is invariant with respect to a scaling group. To this end, we will use the similarity approach, described in full detail by Dresner [5], within Lie's invariance theory (see [2,3,6]). The application of the similarity theory to applied mathematics and numerical analysis has been a fruitful research field for at least a century. In fact, the first cited reference on the field is due to Töpfer [24] concerning the study of the celebrated Blasius problem within the boundary layer theory introduced by Prandtl [22]. Indeed, even classical theories have been revised according to similarity analysis (see for instance [1]). Na [21, Chapters 7–9] devoted three chapters of his book on computational methods for BVP to numerical methods derived from invariance properties. More recent accounts on the applications of the scaling invariance principle to numerical analysis are due to Fazio [10,11].

In this paper we show that problem (1), regardless of its linearity, provided that it is invariant with respect to a Lie group of scalings, can always be reduced into a similar BVP governed by an ODE (called principal ODE). Sometimes, it might be possible to find an analytical solution to the ODE governing equation. However, it is always a simpler task to look for a numerical solution to the reduced problem than to the original one. In our case the principal ODE is defined on an

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infinite interval, and, therefore, we formulate a free BVP so that its numerical solution can be achieved using either an iterative, or noniterative method, as shown by Fazio and Evans [13] and by Fazio [9,10].

The paper is organized as follows. In Section 2, we define the similarity analysis that can be used to transform the governing PDE into an ODE, we also investigate the existence of an associated group of scaling invariance for the latter equation. Moreover, the invariance of the initial-boundary conditions is investigated leading to a BVP for the ODE. Besides, since the transformed problem is defined on an infinite interval, an equivalent free boundary formulation for it is recalled. In Section 3, a practical nonlinear parabolic example is studied in detail and the results of a few numerical experiments are shown as well as the retrieval of the solution to the original problem. Section 4 is devoted to applying an iterative method to numerically solve a free boundary formulation for the linear heat equation defined on unbounded domains. Finally, in Section 5 we conclude focusing the advantages arising from the exploitation of similarity analysis in facing the approximating moving boundary problem.

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2. Similarity approach

2.1. *The principal governing equation*

A generic one-parameter Lie group of scalings is expressed by the following point transformation:

$$x^* = \mu x, \quad t^* = \mu^{\rho} t, \quad u^* = \mu^{\rho\sigma} u, \tag{2}$$

where μ is the group parameter, while ρ and σ are constants to be determined. The invariants on the (x, t, u) domain are the similarity variable η and the unknown function $F(\eta)$, given by

$$\eta = x t^{-1/\rho}, \quad F(\eta) = u(x, t) t^{-\sigma}, \tag{3}$$

with $\rho \neq 0$; by expressing the partial derivatives of $u(x, t)$ involved in the governing equation in terms of Equation (3), we get

$$\frac{\partial u}{\partial x} = t^{\sigma - 1/\rho} \frac{\mathrm{d}F}{\mathrm{d}\eta}, \quad \frac{\partial^2 u}{\partial x^2} = t^{\sigma - 2/\rho} \frac{\mathrm{d}^2 F}{\mathrm{d}\eta^2}, \quad \frac{\partial u}{\partial t} = t^{\sigma - 1} \left(\sigma F - \frac{\eta}{\rho} \frac{\mathrm{d}F}{\mathrm{d}\eta} \right), \tag{4}$$

and the original PDE, written in the similarity variables, reduces to

$$t^{\sigma - 2/\rho} \frac{\mathrm{d}^2 F}{\mathrm{d}\eta^2} = f\left(t, t^{1/\rho}\eta, t^{\sigma} F(\eta), t^{\sigma - 1/\rho} \frac{\mathrm{d}F}{\mathrm{d}\eta}, t^{\sigma - 1} \left(\sigma F - \frac{\eta}{\rho} \frac{\mathrm{d}F}{\mathrm{d}\eta} \right) \right)$$

so that, in order that the governing equation of (1) is invariant with respect to the point transformation (2), the function f must have the functional form

$$f(\cdot) = t^{\sigma - 2/\rho} \Phi \left(\eta, F, \frac{\mathrm{d}F(\eta)}{\mathrm{d}\eta}, \sigma F - \frac{\eta}{\rho} \frac{\mathrm{d}F}{\mathrm{d}\eta} \right);$$

in this particular case, the original PDE transforms into the following scalar principal second-order ODE

$$\frac{\mathrm{d}^2 F}{\mathrm{d}\eta^2} = \Phi \left(\eta, F, \frac{\mathrm{d}F}{\mathrm{d}\eta}, \sigma F - \frac{\eta}{\rho} \frac{\mathrm{d}F}{\mathrm{d}\eta} \right). \tag{5}$$

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In this case no bounds have been imposed on the values of exponents in Equation (2) and as a result they are both free. However, more often it happens that invariance is obtained provided that such exponents satisfy a bound equation. By referring to group (2), the bound equation assumes the following form

$$M\sigma\rho + N\rho = L,$$

where M, N, and L are constants fixed by the problem. In this case the other free exponent can be chosen in order to make invariant at least one out of the initial-boundary conditions. If ρ_0 and $\sigma_0\rho_0$ are these specific values, by introducing the new parameter $\lambda = \mu^{(\rho-\rho_0)/\rho_0}$, it can be proved that another scalings group remains defined, the so called associated group of Dresner [5, p. 31–33], which is of the form

$$\eta^* = \lambda\eta, \quad F^* = \lambda^{L/M} F, \tag{6}$$

leaving the principal ODE (5) invariant and, for instance, it may be used to reduce the ODE order by one. A further case exists when two bounds are needed for the invariance of the governing equation so that both the exponents are uniquely determined and no degree of freedom is left. This is the worst case since no initial-boundary conditions invariance properties can be exploited. Finally, there are problems where the governing equation or, at least, one of the boundary conditions is not invariant with respect to Equation (2), and reduction to an ODE problem is not possible.

2.2. *Boundary conditions for the ODE problem*

In terms of the similarity variable we can write

$$u(0,t) = t^\sigma F(0), \quad \frac{\partial u}{\partial x}(0,t) = t^{\sigma-1/\rho}\frac{\mathrm{d}F}{\mathrm{d}\eta}(0), \quad \left.\begin{matrix} u(x,0) \\ u(\infty,t) \end{matrix}\right\} = t^\sigma F(\infty),$$

and the boundary conditions for the similar problem become

$$\alpha(t)t^\sigma F(0) + \beta(t)t^{\sigma-1/\rho}\frac{\mathrm{d}F}{\mathrm{d}\eta}(0) = \gamma(t)$$
$$F(\infty) = 0,$$

with $\sigma \geq 0$, so that $F(\infty) = 0$ is well defined; $\rho > 0$, so that $u(x,0)$ and $u(\infty,t)$ reduce to the same boundary condition $F(\infty) = 0$, that is $\eta \to \infty$ for both $x \to \infty$ and $t = 0$. In order to study the invariance of the first boundary condition, we must assume that $\alpha(t)$, $\beta(t)$, and $\gamma(t)$ have the following monomial form

$$\alpha(t) = At^{\sigma_1}, \quad \beta(t) = Bt^{\sigma_2}, \quad \gamma(t) = Ct^{\sigma_3}.$$

In such a way that the boundary condition assumes the following form:

$$At^{\sigma_1+\sigma}F(0) + Bt^{\sigma_2+\sigma-1/\rho}\frac{\mathrm{d}F}{\mathrm{d}\eta}(0) = Ct^{\sigma_3},$$

and several cases are possible, depending on whether the values of the constants A, B, and C are different from zero or not. Table 1 summarizes all the possible cases. In particular, the left column reports the possible combinations of the coefficients, the central column lists the constraints to which the exponents σ, σ_1, σ_2, σ_3, and ρ must satisfy, and the right column shows the corresponding boundary condition for the principal ODE. As a result, through the similarity analysis we must obtain as boundary conditions for the principal ODE (5) one out of the three

Table 1. Classification of invariant boundary conditions.

$A \neq 0$ $B = 0$	$\sigma = \sigma_3 - \sigma_1$	$AF(0) = C$
$A = 0$ $B \neq 0$	$\sigma = \sigma_3 - \sigma_2 + 1/\rho$	$B\dfrac{\mathrm{d}F}{\mathrm{d}\eta}(0) = C$
$A \neq 0$ $B \neq 0$	$\sigma = \sigma_3 - \sigma_1$ $\sigma = \sigma_3 - \sigma_2 + 1/\rho$	$AF(0) + B\dfrac{\mathrm{d}F}{\mathrm{d}\eta}(0) = C$

possible ones reported above. In any case, at the end of this similarity analysis, we get a two-point BVP for a second-order ODE defined on an infinite interval. As far as the numerical solution of the ODE problem is concerned, in the next section we show how the exploitation of the similarity property may be helpful in solving it through a noniterative method. In case of lack of similarity, it can always be possible to provide a suitable similarity scaling through the introduction of an *ad hoc* dimensionless parameter for the activation of an iterative method.

In closing this section, it is worth pointing out that an essential condition for the similarity approach is the collapse of the initial and right boundary conditions for the original problem, as remarked by Dresner [5,6], into a unique boundary condition at infinity for the principal second-order ODE whose solution is the so-called similarity solution.

2.3. *Moving boundary formulation*

According to Fazio [8], provided that the solution of our BVP is regular enough to assume that $\mathrm{d}F/\mathrm{d}\eta(\infty) = 0$, we can introduce a free boundary η_ϵ as a new unknown to be determined by imposing the condition $\mathrm{d}F/\mathrm{d}\eta(\eta_\epsilon) = \epsilon$. Indeed, by assuming that η_ϵ is a differentiable function of ϵ on a nonempty interval including $\epsilon = 0$, and that $\lim_{\epsilon\to 0} \mathrm{d}\eta_\epsilon/\mathrm{d}\epsilon$ exists, we are under the hypotheses, given in [8, Lemma 1, Theorem 1], for the uniform convergence of free boundary problem solution to the one of the BVP defined on the infinite interval. In practice, our approach consists of introducing a free boundary unknown, η_ϵ, and in splitting the condition at infinity into the two others

$$F(\eta_\epsilon) = 0, \quad \frac{\mathrm{d}F}{\mathrm{d}\eta}(\eta_\epsilon) = \epsilon,$$

where $|\epsilon| << 1$. This is equivalent to approximate the original problem (1) through the replacement of the boundary condition at infinity

$$u(x,t) \longrightarrow 0 \quad x \longrightarrow \infty$$

with

$$u(x_\epsilon(t), t) = 0, \quad \frac{\partial u}{\partial x}(x_\epsilon(t), t) = \epsilon t^{\sigma - 1/\rho},$$

where $x_\epsilon(t)$ is an unknown moving boundary.

Finally, the solution to the original problem is retrieved by means of the inverse similarity map between the η axis and the (x,t) plane graphically depicted in Figure 1. For an application of this idea see Section 3.2.

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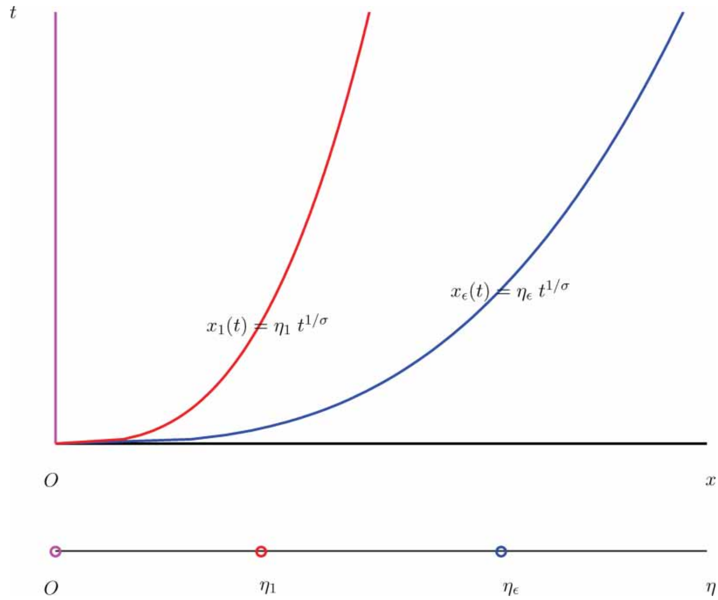

Figure 1. The similarity map. Note that the similarity lines $x = 0$ and $x_\epsilon(t)$ are mapped to $\eta = 0$ and η_ϵ, respectively.

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3. A practical example

As a practical example we refer to the following model

$$\begin{gathered}\frac{\partial^2 u}{\partial x^2} = u\frac{\partial u}{\partial t} \\ u(x,0) = 0 \quad x > 0 \\ u(x,t) \longrightarrow 0 \quad x \longrightarrow \infty \quad t > 0 \\ \frac{\partial u}{\partial x}(0,t) = -c \quad t > 0,\end{gathered} \tag{7}$$

describing thermal expulsion of fluid from a long slender heated tube, where u is flow velocity induced in the fluid by the heating of the tube wall (see [5, pp. 35–40]).

With regard to the scaling group (2), the governing equation results to be invariant provided that the bound equation is fulfilled

$$\sigma\rho - \rho = -2 \Longrightarrow \rho = \frac{2}{1-\sigma}.$$

The value for σ is determined from the boundary condition at $x = 0$ whose invariance is granted according to Table 1 in the case $\sigma_3 = 0$ (here $C = -c$), that is,

$$\begin{aligned}\sigma &= -\sigma_1 \\ \sigma &= -\sigma_2 + \frac{1}{\rho}.\end{aligned}$$

For the particular case considered by Dresner, $\sigma_2 = 0$ (and $A = 0$), we get $\sigma = 1/3$ and $\rho = 3$, and the two invariants for this problem are given by

$$\eta = xt^{-1/3}, \quad F(\eta) = u(x,t)t^{-1/3}.$$

By expressing the function $u(x, t)$ and its derivatives involved in the original equation in terms of the similarity variables, we obtain the principal ODE

$$\frac{\mathrm{d}^2 F}{\mathrm{d}\eta^2} = \frac{F}{3}\left(F - \eta\frac{\mathrm{d}F}{\mathrm{d}\eta}\right) \tag{8}$$

with the boundary conditions

$$\frac{\mathrm{d}F}{\mathrm{d}\eta}(0) = -c, \quad F(\infty) = 0. \tag{9}$$

According to what we have said about the associated group, we can identify its parameters as $M = 1$, $N = -1$, and $L = -2$, so that the associated group is given by

$$\eta^* = \lambda\eta, \quad F^* = \lambda^{-2}F. \tag{10}$$

From an analytical point of view, we could use such a result to reduce the principal ODE (8) into an equivalent first-order one, as it is done by Dresner [5], and then to carry out a qualitative analysis on the Lie plane. Nevertheless, it will be more helpful to use this scaling invariance to apply a noniterative numerical method.

3.1. *Numerical solution*

As mentioned above, one of the boundary conditions (9) is defined at infinity, so that we reformulate first the problems (8)–(9) as a free boundary problem, resulting to be

$$\begin{gathered}\frac{\mathrm{d}^2 F}{\mathrm{d}\eta^2} + \frac{\eta}{3}F\frac{\mathrm{d}F}{\mathrm{d}\eta} - \frac{F^2}{3} = 0,\\ \frac{\mathrm{d}F}{\mathrm{d}\eta}(0) = -c, \quad F(\eta_\epsilon) = 0, \quad \frac{\mathrm{d}F}{\mathrm{d}\eta}(\eta_\epsilon) = \epsilon.\end{gathered} \tag{11}$$

In this case we can use the noniterative method introduced by Fazio and Evans [13].

First, we fix $F^*(\eta^*_\epsilon) = 0$, $\mathrm{d}F^*/\mathrm{d}\eta^*(\eta^*_\epsilon) = -1$, that is $\epsilon^* = -1$. Then we choose a value for η^*_ϵ, and integrate the ODE in Equation (11) (written in the starred variables) backward from this value down to zero. In this way we compute the value of $\mathrm{d}F^*/\mathrm{d}\eta^*(0)$. From similarity relations (10) we can deduce the following relations

$$\frac{\mathrm{d}F^*}{\mathrm{d}\eta^*}(0) = \lambda^{-3}\frac{\mathrm{d}F}{\mathrm{d}\eta}(0), \quad \eta^*_\epsilon = \lambda\eta_\epsilon.$$

The first relation allows us to work out the value for the similarity parameter as

$$\lambda = \left(\frac{-c}{\mathrm{d}F^*/\mathrm{d}\eta^*(0)}\right)^{1/3},$$

whereas the second one can be used to find the values of the free boundary

$$\eta_\epsilon = \lambda^{-1}\eta^*_\epsilon.$$

In a similar way, we can work out the corresponding original (no-starred) value at the origin assumed by the function as well as the value of ϵ

$$F(0) = \lambda^2 F^*(0), \quad \epsilon = \lambda^3\epsilon^*.$$

A numerical experiment has been carried out and the results are summarized in Table 2 for the value of $c = 0.1$. The table caption shows the used boundary parameters. The convergence

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Table 2. Final condition and parameters used: $F^*(\eta_\epsilon^*) = 0$, $\mathrm{d}F^*/\mathrm{d}z^*(\eta_\epsilon^*) = -1$, $\mathrm{d}F/\mathrm{d}z(0) = -c = -0.1$.

η_ϵ^*	λ	η_ϵ	ϵ	$F(0)$
2.5	0.193356	12.929284	−7.2E−03	0.324044
2.6	0.167000	15.568807	−4.6E−03	0.324796
2.7	0.138673	19.470197	−2.7E−03	0.325240
2.8	0.107682	26.002384	−1.2E−03	0.325466
2.85	0.090787	31.392234	−7.5E−04	0.325523
2.9	0.072543	39.976513	−3.8E−04	0.325555
2.95	0.052287	56.418804	−1.4E−04	0.325569
3.0	0.028296	106.022609	−2.2E−05	0.325573
3.025	0.012804	236.248810	−2.1E−06	0.325573

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of the process is evident because, as the absolute value of ϵ decreases, it follows that the free boundary η_ϵ grows, thus proving the validity of the theoretical assumptions. All computations were performed by the ODE45 Runge–Kutta's routine available with MATLAB™, with a relative local error tolerance set equal to 10^{-6}.

Finally, we can notice that the scaling relations involving the function $F(\eta)$ and its derivative imply that the quantity

$$I = \frac{\mathrm{d}F/\mathrm{d}\eta(0)}{[F(0)]^{3/2}}$$

is an invariant that can be numerically deduced from the above table. As a result, for any other value of the parameter c, the missing initial condition is given by

$$F(0) = \left(\frac{-c}{I}\right)^{2/3}.$$

3.2. *Retrieval of the solution to the original problem*

Fixed a value of ϵ a corresponding surface $u_\epsilon(x, t)$ can be computed by using the relation linking the similarity variable η and the function $F(\eta)$ to the original independent and dependent variables. This $u_\epsilon(x, t)$ is an approximate solution to the original problem. In Figure 2 we show such a solution retrieved for the values of c, ϵ, and η_ϵ reported in the caption.

4. The linear heat equation

As reported by MacCluer [20], the linear heat equation defined on an infinite domain was used by Kelvin to model intersymbol distortion affecting pulse transmission in undersea cables. Indeed, transmitted pulses tend to smear spatially as they travel along the cable interfering with the previous and subsequent pulses and causing such a distortion. The mathematical model, in dimensionless variables, is given by

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}, \tag{12}$$

subjected to the initial-boundary conditions

$$u(x, 0) = 0, \quad u(0, t) = 1, \quad u(\infty, t) = 0, \tag{13}$$

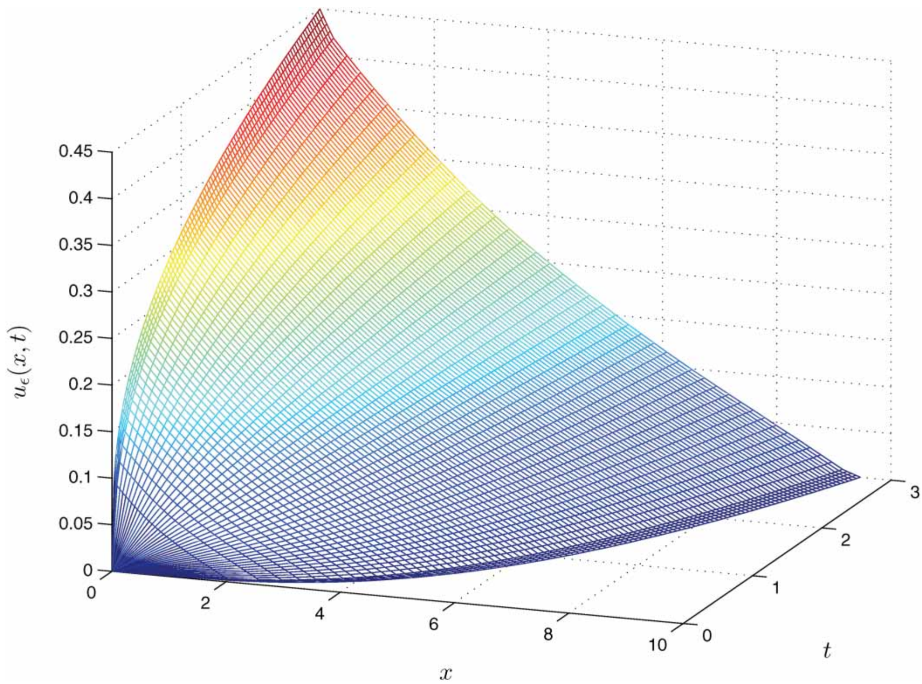

Figure 2. Solution obtained for $c = 0.1$, $\epsilon = 2.2 * 10^{-5}$, and $\eta_\epsilon \approx 106$.

where $u(x, t)$ represents the pulse voltage at location x and time t. By referring to the generic scaling group (2), we can reduce such a PDE to the corresponding principal ODE

$$\frac{\mathrm{d}^2 F}{\mathrm{d}\eta^2} = -\frac{\eta}{2}\frac{\mathrm{d}F}{\mathrm{d}\eta} + \sigma F,$$

with the boundary conditions

$$F(0) = 1, \quad F(\infty) = 0,$$

where, in order to grant the invariance for the principal equation and the boundary condition at the origin, the exponents must be such that $\rho = 2$ and $\sigma = 0$. As a consequence, the above principal ODE becomes

$$\frac{\mathrm{d}^2 F}{\mathrm{d}\eta^2} = -\frac{\eta}{2}\frac{\mathrm{d}F}{\mathrm{d}\eta},$$

with the same boundary conditions. By recalling what has already been said about the associate group, it is somehow surprising to find out that for the linear heat equation the associated group does not exist. This means that the resulting principal ODE is not invariant to any scaling group, and, as a consequence, we cannot apply a noniterative method to solve such a problem as we did in the previous section.

The only way to overcome this difficulty is to make use of an iterative method through the introduction of a dimensionless numerical parameter h subjected to a scaling relation $h^* = \lambda^\vartheta h$ inside the differential equation and/or its boundary conditions. In our case, for instance by assuming

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$\vartheta = 1$, the principal equation can be rewritten as

$$h^2 \frac{\mathrm{d}^2 F}{\mathrm{d}\eta^2} = -\frac{\eta}{2} \frac{\mathrm{d}F}{\mathrm{d}\eta},$$

and, by introducing a free boundary formulation, its boundary conditions become

$$F(0) = 1, \quad F(\eta_\epsilon) = 0, \quad \frac{\mathrm{d}F}{\mathrm{d}\eta}(\eta_\epsilon) = \epsilon.$$

As a result, the boundary condition for the function at the free boundary and the equation are invariant with respect to the scaling group

$$\eta^* = \lambda\eta, \quad F^* = \lambda^\delta F, \quad h^* = \lambda h,$$

where the exponent δ can be chosen freely; by fixing $\delta = 1$, also the boundary condition for the derivative at the free boundary is left invariant.

For the iterative transformation method we set values of h^*, η_ϵ^*, and ϵ, and integrate backward in $[0, \eta_\epsilon^*]$ to find $F^*(0)$ that can be used to compute

$$\lambda = F^*(0), \quad h = \lambda^{-1} h^*.$$

By fixing the values of η_ϵ^*, and ϵ, and considering h^* as variable, we can define the transformation function

$$\Gamma(h^*) = \lambda^{-1}\left(h^*\right)\, h^* - 1 \,.$$

Keeping in mind that for $h = 1$ we get the original problem, we can start an iterative process to be stopped when $|\Gamma| = |h - 1| < \mathrm{Tol}$, where Tol is a prescribed tolerance bound.

Let us carry out a numerical experiment mainly aimed to show how to implement the above iterative method. As a first step we try to isolate an interval containing at least one root of the function Γ. This is reported in Table 3.

The interval containing the sought zero is the one bounded by the values $h^* = 2^{-3}$ and $h^* = 2^{-2}$, that are used as starting points for an iterative method. To this end, because of the bad conditioning of the function Γ, we use the *regula falsi* method, whose main feature is the global convergence, despite its low order. The iteration is stopped when the condition $|\Gamma(h^*)| < 10^{-6}$ is fulfilled so as to get the numerical results shown in Table 4.

Finally, the theoretical implication concerning the free boundary formulation,

$$\epsilon \longrightarrow 0 \Longrightarrow \eta_\epsilon \longrightarrow \infty$$

can be numerically proved: to the progressive decreasing of the value of $|\epsilon|$ it corresponds to an increase of the free boundary η_ϵ as reported in Table 5.

Table 3. Results obtained for $\epsilon = -10^{-3}$.

h^*	$\Gamma(h^*)$
4.0	3957.506690
2.0	1917.047221
1.0	843.171744
0.5	245.295894
0.25	9.381854
0.125	−0.999937
0.0625	−1.000000

Table 4. Results obtained for $\eta^* = 1$ and $\epsilon = -10^{-3}$.

k	h^*	$\Gamma(h^*)$	η_ϵ	$\mathrm{d}F/\mathrm{d}\eta(0)$
1	0.250000	$\vdots$	$\vdots$	$\vdots$
2	0.125000	$\vdots$	$\vdots$	$\vdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
20	0.198642	$-5.1E-6$	5.034150	-0.564402
21	0.198642	$10.1E-6$	5.034220	-0.564393
22	0.198642	$2.5E-6$	5.034185	-0.564398
23	0.198642	$-1.3E-6$	5.034167	-0.564399
24	0.198642	$0.6E-6$	5.034176	-0.564399

Table 5. Values of η_ϵ and $\mathrm{d}F/\mathrm{d}\eta(0)$ obtained for decreasing ϵ.

ϵ	η_ϵ	$\mathrm{d}F/\mathrm{d}\eta(0)$
-10^{-2}	4.018603	-0.566734
-10^{-3}	5.034176	-0.564399
-10^{-4}	5.878291	-0.564208
-10^{-5}	6.616698	-0.564191
-10^{-6}	7.282442	-0.564190
-10^{-7}	7.896540	-0.564189

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As for problems (12) and (13) it exists the analytical solution expressed by $u(x,t) = erfc(x/2\sqrt{t})$ (see [20]); for the sake of completeness, it might be quite interesting to work out the amount of the error we make through the introduction of the free boundary formulation. By recalling that $u(x,t) = F(\eta)$, and referring to the value of the free boundary reported in Table 5 for $\epsilon = -10^{-7}$, we obtain the value $F(\eta_\epsilon) = 2.354588 \times 10^{-8}$ that represents the global (truncation + roundoff) error plus the error derived from the introduction of the free boundary formulation.

For the sake of brevity, we omit to reconstruct the approximate solution of the original problem as it was done at the end of the previous section.

Also in this case all computations were performed by the ODE45 Runge–Kutta's routine available with MATLAB, with a relative local error tolerance set equal to 10^{-6}.

5. Conclusions

In this paper we have shown how a similarity and numerical analysis can be used to solve the problems modelled by Equation (1) that are invariant with respect to a Lie scaling group. As a first step it was possible to characterize the class of invariant governing equation and side conditions. From a numerical viewpoint, a free boundary formulation is recalled for the transformed ODE problem which is defined on an infinite interval. Two problems, that have been defined in the applied sciences, were studied within the proposed framework. These problems were chosen to provide further details on the practical application of the free boundary formulation, i.e. the numerical solution of the corresponding similar problem via a noniterative or an iterative transformation method, as well as the retrieval of the solution to the original problem. The first problem, governed by a nonlinear parabolic PDE, can be solved by the noniterative method, but the second problem, governed by the linear heat equation, requires the application of the iterative method. In both cases, accurate numerical results were reported.

At the end of this study we can define a further topic of research which is more general than the one considered here. Our interest would be to investigate the possibility of approximating the parabolic problem (1) defined on unbounded domains by a related moving boundary problem. Generally speaking, we end up by replacing a boundary condition like

$$u(x,t) \longrightarrow 0 \quad x \longrightarrow \infty$$

with the moving boundary conditions

$$u(x_\epsilon(t),t) = 0, \quad \frac{\partial u}{\partial x}(x_\epsilon(t),t) = \epsilon t^\gamma,$$

where $x_\epsilon(t)$ is the unknown moving boundary and $\gamma \leq 0$.

Numerical techniques to solve moving boundary problems that are usually encountered operate directly dealing with all of the independent time-space variables involving a great deal of computational burden. The bibliography about this issue is very broad and we refer the interested reader to the book written by Crank [4]. An *ad hoc* application of the iterative transformation method, defined in detail by using the similarity properties of scaling invariance by Fazio [9], to a semi-discretization of moving boundary parabolic problem was already considered by Fazio [12]. On the contrary, the present similarity approach clearly represents a very good computational advantage as the solution is simply obtained by solving a BVP governed by a scalar ODE whose independent variable is the similarity one.

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