Construction of sequences of exact analytical solutions for heat diffusion in graded heterogeneous materials by the Darboux transformation method. Examples for half-space.

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Abstract. The Darboux transformation is a differential transformation which, like other related methods (supersymmetry quantum mechanics-SUSYQM, factorization method) allows generating sequences of solvable potentials for the stationary 1D Schrödinger equation. It was recently shown that the heat equation in graded heterogeneous media, after a Liouville transformation, reduces to a pair of Schrödinger equations sharing the same potential function, one for the transformed temperature and one for the square root of effusivity. Repeated joint PROperty and FIeld Darboux Transformations (PROFIDT method) then yield two sequences of solutions: one of new solvable effusivity profiles and one of the corresponding temperature fields. In this paper we present and discuss the outcome in the case of a graded half-space domain. The interest in this methodology is that it provides closed-form solutions based on elementary functions. They are thus easily amenable to an implementation in an inversion process aimed, for example, at retrieving a subsurface effusivity profile from a modulated or transient surface temperature measurement (photothermal characterization).

1. Introduction
The heat diffusion in heterogeneous media problem, i.e. where both volumetric heat capacity and conductivity are space-dependent, has no general closed-form solution when these parameters present arbitrary distributions, even in the one-dimensional (1D) case with respectively \( c(z) \) and \( \lambda(z) \) profiles. Until recently, exact analytical solutions were known only for a limited number of \( c(z) \) and \( \lambda(z) \) profiles or for diffusivity \( a(z) = \lambda/c \) and effusivity \( b(z) = \sqrt{\lambda c} \) profiles [1]-[9]. These solutions are available in closed-form in the Laplace or Fourier space (the corresponding property profiles will be called solvable profiles). In addition, series solutions were also proposed; they are either based on the use of the successive derivatives of conductivity [10], on the Generalized Integral Transform Technique (GITT) [11], or on the Spectral Parameter Power Series (SPPS) method [12]. Approximate methods were also developed which are restricted to the situations where the thermal properties variations are slow and/or of low amplitude ([2], [5], [13]-[15], just to name a few). Another type of approximate method consists in discretizing the domain and assuming that, in each interval, the property profile follows one of the solvable profiles mentioned before. The easiest way is of course to assume that the properties are constant in each interval. For reducing the model error one can either increase the number of intervals or select solvable profiles of higher order, e.g. linear profiles for conductivity or for effusivity. There is actually a need for solvable profiles that present a higher
flexibility: they should allow modelling heat diffusion in materials that possibly present steep profiles without requiring excessive discretization or even requiring no discretization at all.

A method was recently presented in [16] which allows building sequences of solvable effusivity profiles and their joint temperature/heat flux solutions, thereby involving an increasing number of parameters (up to two additional free parameters per step in each sequence). By increasing the number of parameters, it is expected that the solvable effusivity profiles obtained therefrom fit better and better to any real continuous profile (when the real profile presents a local jump, the procedure has to be performed separately on both sides of the discontinuity; the global solution is then obtained by quadrupole multiplication). The proposed method consists of a series of three transformations: first a Fourier/Laplace transformation, then a Liouville transformation [17] and finally a Darboux transformation [18] which is carried out jointly on the equation satisfied by a thermal property (the effusivity profile at power +/-1/2) and on the equation satisfied by a thermal field (either the transformed temperature or the transformed heat flux). This procedure amounts to the so-called PROFIDT method (joint PROperty and FIeld Darboux-Transformations).

The Darboux transformation is a differential transformation which allows generating sequences of solvable 2nd order ordinary differential equations (ODE) in Liouville-normal form [18] (now so-called stationary 1D Schrödinger equations). Like other related methods (supersymmetry quantum mechanics-SUSYQM, the factorization method) it found, since the 70', numerous applications in quantum mechanics and in the realm of nonlinear evolutionary equations (solitons) [19]. Surprisingly, no application of the Darboux transformation to the problem of heat diffusion in heterogeneous media could be found before the work presented in [16]. The only application related to thermal science we have found is in [20]. It deals with the heat equation expressed in the time domain, not in the Laplace-Fourier domain as we did in [16]. We actually found it more convenient to work in the Laplace-Fourier domain: the advantage is that the obtained solutions can be easily combined together through the quadrupole method in order to get solutions for more complex materials, i.e. heterogeneous multilayers with possibly discontinuous profiles. An alternative to the Darboux transformation method is the Bäcklund transformation method [21]. As illustrated in [16] the PROFIDT method allows building sequences of effusivity profiles and the corresponding thermal solutions in a more simple and systematic way.

Several examples of solvable effusivity profiles were provided in [16]. Some of them are not defined over the entire half-line $z \geq 0$. Others are unbounded, i.e. $b \to +\infty$ for $z \to +\infty$. They represent the case of a progressively more inertial material; this means that temperature is more and more “stable” at progressively higher distance from the surface $z = 0$, approaching asymptotically the case of a boundary condition of first type. In this paper we will focus on (simple) solvable effusivity profiles that are bounded and non-vanishing on the half-line $z \geq 0$.

We will first briefly recall the analytical tools that are involved in the PROFIDT method [16]. Then, we will describe the main properties of a simple solution based on merely three parameters which was already illustrated in [16]. Additional results as obtained by assuming heat losses at the free surface of the heterogeneous material will be presented. This will complement the illustrative examples in [16] aimed at demonstrating the interest in the PROFIDT method for constructing exact analytical solutions for heat diffusion in heterogeneous materials (actually for any linear transfer process – by diffusion or by wave propagation – provided that the transfer equation may be transformed into a stationary Schrödinger-type equation). The proposed solution sequences present the additional advantage that, in the Laplace-Fourier space, they are in closed-form and they involve only elementary functions.

2. Successive transformations of the heat equation

2.1. Liouville transformation
Let us consider the 1D linear heat equation in a continuously heterogeneous half space without heat sources in the Laplace-Fourier domain as obtained after a Laplace transformation (for modelling
transient phenomena) or a Fourier transformation (for modelling periodic phenomena), which changes
the temperature \( T(z, t) \) into \( \theta(z, p) \) and the heat flux \( \phi(z, t) \) into \( \phi(z, p) \):

\[
p\theta = \frac{1}{c(z)} \frac{d}{dz} \left( \lambda(z) \frac{d\theta}{dz} \right), \quad 0 \leq z < +\infty
\]

where \( p \) is respectively the Laplace variable or the Fourier variable \( i\omega \) where \( \omega \) is the angular
frequency \( 2\pi f \). The boundary condition at \( z = 0 \) will be considered later. The next step is a Liouville
transformation \[17\] which first consists in an independent variable change \( z \rightarrow \xi \) where \( \xi = \xi(z) \) is
the square root of the diffusion time (SRDT) along the \([0, z]\) interval, taking into account the possible
diffusivity variations therein: \( \xi = \sqrt{a^{-2}(u)du} \). It also involves a dependent variable change
\( \theta(\xi, p) \rightarrow \psi(\xi, p) \equiv \theta(\xi, p)\sqrt{b(\xi)} \). The equation for the new variable \( \psi(\xi, p) \) is a 2nd ODE that can be
cast in a system of two homologous Schrödinger-type equations (i.e. with same potential function
\( V(\xi) \)):

\[
\begin{align*}
\psi' &= (V(\xi) + p)\psi \\
n s' &= V(\xi)s
\end{align*}
\]

where primes denote derivatives with respect to the SRDT \( \xi \) and \( s(\xi) \) is a thermal-property
profile, namely \( s(\xi) = b^{-\xi^2}(\xi) \), the profile of the square root of effusivity. Let us mention that when
starting with the heat equation expressed for the heat flux instead of the temperature, we get the same
pair of equations as before, except \( \psi(\xi, p) \) is now the Liouville-transformed heat flux and \( s(\xi) \)
represents \( b^{-\xi^2}(\xi) \) \[16\]. A direct consequence is that when a solvable effusivity profile is found, one
has at hand a second solvable profile, namely its reciprocal.

2.2. Joint Darboux transformations (PROFIDT method)
The Darboux transformation \[18\], \[19\] allows generating a sequence of solvable potentials \( V_{[n]}(\xi) \),
starting from a given one, \( V_{[0]}(\xi) \). It is essentially based on two differential relations: the first one
relates a given potential \( V_{[n]}(\xi) \) with the next one in the sequence, \( V_{[n+1]}(\xi) \); the second relation
describes how getting a solution of the Schrödinger equation \( (2a) \) with the potential \( V_{[n]}(\xi) \) and
the parameter value \( p \) from a solution of the same equation but with the potential \( V_{[n]}(\xi) \). Both relations
are based on the choice of a particular solution of equation \( (2a) \) with the potential \( V_{[n]}(\xi) \) and a
particular (transformation) parameter value \( p = p_{n+1} \), which we write \( \bar{\psi}_{[n]}(\xi, p_{n+1}) \). They also involve
its logarithmic derivative \( \sigma_{[n, p_{n+1}]} = \bar{\psi}_{[n]}'/\bar{\psi}_{[n]} \) (it is called “superpotential” in the SUSY vocabulary).
The potentials are related by (other equivalent relations are presented in \[16\]):

\[
V_{[n+1]} = -V_{[n]} + 2\sigma_{[n, p_{n+1}]} - 2p_{n+1}
\]

We give now a transcription of the Darboux transformation aimed at relating the general solutions
corresponding to the potential \( V_{[n]}(\xi) \) and \( V_{[n+1]}(\xi) \). If the general solution at level \( n \) and for the
parameter value \( p \) is given by the linear combination (LC) of two independent solutions \( K_{[n]}(\xi, p) \)
and \( P_{[n]}(\xi, p) \), which we write \( \psi_{[n]}(\xi, p) \propto [K_{[n]}(\xi, p), P_{[n]}(\xi, p)] \), the general solution at level \( n+1 \) is
given by:
\[
\psi_{[n+1]}(\xi, p) \propto \left[ K_{[n+1]}(\xi, p) \right]^{\frac{K_{[n]} - \sigma_{[0, p_{n}]} K_{[n]} \!}{P_{[n]} - \sigma_{[0, p_{n}]} P_{[n]}}} \quad \text{for } p \neq p_{n+1}
\]

\[
\psi_{[n+1]}(\xi, p) \propto \left[ \tilde{\psi}_{[n+1]} \right]^{\frac{1}{2} \int \tilde{\psi}_{[n+1]}^{\prime} d\xi^*} \quad \text{for } p = p_{n+1}
\]

We refer the reader to [16] for an alternative expression for the one involving the primitive of \(\tilde{\psi}_{[n+1]}^{\prime} \). It allows avoiding this quadrature; it is however based on the derivative of \(\tilde{\psi}_{[n]}(\xi, p_{n+1}) \) vs. \(p \) at \(p_{n+1} \), which involves some differentiability/continuity constraints.

In reference to the fact that solutions \(s_{[n]}(\xi) \) in equation (2b) simply correspond to those of \(\psi_{[n]}(\xi, p) \) in equation (2a) for \(p = 0\), the PROFIDT method is nothing more nor less than a repetition of the procedure described in equation (4) for \(p = 0\). So, when the general solution of equation (2b) at level \(n \) (e.g. the thermal property profile \(s_{[n]}(\xi) \)) is given by the linear combination (LC) of two independent solutions \(B_{[n]}(\xi) \) and \(D_{[n]}(\xi) \), i.e. \(s_{[n]}(\xi) \propto [B_{[n]}(\xi), D_{[n]}(\xi)] \), the general solution at level \(n+1 \) is given by:

\[
s_{[n+1]}(\xi) \propto [B_{[n+1]}(\xi), D_{[n+1]}(\xi)] \quad \text{if } p_{n+1} \neq 0
\]

\[
s_{[n+1]}(\xi) \propto [\tilde{\psi}_{[n]} \left[ \int \tilde{\psi}_{[n]}^{\prime} d\xi^* \right] \quad \text{if } p_{n+1} = 0
\]

Interestingly, as previously announced, this new LC provides not only one, but two effusivity profiles families. As a matter of fact this LC describes either \(b_{[n]}^{-1/2}(\xi) \) or \(b_{[n]}^{-1/2}(\xi) \). Evidently, one must carefully select the constant parameters in the LC (as well as those defining the particular solution \(\tilde{\psi}_{[n]}(\xi, p_{n+1}) \)) so that \(s_{[n]}(\xi) \) is defined and positive on the considered \(\xi\)-domain (for retrieving \(b^{-1/2}(\xi) \), \(s_{[n]}(\xi) \) should also be node-free). One can find in [16] a discussion on how to relax this constraint when the objective is to retain only the results at a given final level \(n+1 = N \); all intermediate results can in fact be considered as non-physical entities: in particular the intermediate “effusivity” profiles could be negative or even complex-valued; the positivity constraint should apply only to the final \(s_{[n]}(\xi) \) profile in the sequence.

When repeating the Joint Property & Field Darboux Transformation one obtains progressively more sophisticated profiles together with the corresponding temperature/heat flux solutions. At each step, when the transformation parameter \(p_{n+1} \) is chosen different of \(0\), two additional free parameters are introduced in the definition of the new effusivity profile: the first one is \(p_{n+1} \) and the second one comes from the constant parameters in the LC defining the particular solution \(\tilde{\psi}_{[n]}(\xi, p_{n+1}) \) (the two constant parameters actually collapse into a single one when passing to the logarithmic derivative \(\sigma_{[0, p_{n}]} \)). When choosing \(p_{n+1} = 0 \), there is of course only one additional free parameter.

3. Example of a first order PROFIDT solution

The sequence is initiated with the simplest (trivial) potential function \(V_{[0]}(\xi) = 0 \). For getting effusivity profiles defined over a semi-infinite interval, we have to choose a positive transformation parameter: \(p_1 > 0 \) [16] A particular solution of equation (2a) is then \(\tilde{\psi}_{[0, p_{1}]}(\xi) \propto \left[ \cosh(\xi / \xi_1), \sinh(\xi / \xi_1) \right] \) where \(\xi_1 \equiv p_1^{-1/2} \) corresponds to a characteristic diffusion time of the material heterogeneity distribution. The
superpotential may then take two forms: \( \sigma_{[n,n]} = \xi^{-1} \tanh(\xi) \) or \( \sigma_{[0,n]} = \xi^{-1} \coth(\xi) \), where we introduced the modified SRDT \( \xi = \xi/\xi + \tau \); \( \tau \) is a free parameter in \( -\infty, +\infty \]. Applying the potential transformation in equation (3), we get two forms for the new potential: \( V_{[n]} = -2\xi^{-2} \cosh^{-2}(\xi) \) and \( V_{[0]} = -2\xi^{-2} \sinh^{-2}(\xi) \), where the first one is known as the one-soliton potential [19]. The solutions of equation (2a) with these new potentials, are obtained according to equation (4); those leading to bounded temperature and heat flux for \( \xi \to +\infty \) are defined by: 
\( \psi_{[n]}(\xi) \propto \exp\left(-\sqrt{p\xi}\left(\sqrt{p} + \sigma_{[n,n]}\right)\right) \). Two admissible classes for \( s_{[n]}(\xi) \) are found when applying equation (5): \( s_{[n]}(\xi) \propto \left[ \tanh(\xi) 1 - \xi \tanh(\xi) \right] \) and \( s_{[n]}(\xi) \propto \left[ \coth(\xi) 1 - \xi \coth(\xi) \right] \). When the coefficient leading the second function of these LC is strictly positive, no solution can be found for \( s_{[n]}(\xi) \) that is positive for \( \xi \geq 0 \). When this coefficient is strictly negative, such solutions can be found, however the induced effusivity profiles are either unbounded and increasing as \( \xi^{-2} \) or vanishing and decreasing as \( \xi^{-2} \). Therefore, like in [16] we will restrict to the cases of bounded, non-vanishing profiles as given by \( b_{[n]}^{1/2}(\xi) \propto \tanh^{1/2}(\xi) \). These so-called \( \tanh^{1/2}(\xi) \)-type profiles were already mentioned in [21] as leading to exact (thermal) solutions. In [16] we presented the associated temperature solutions both in the Laplace-Fourier domain and in the time domain for an adiabatic half-space. We will complement the presentation by providing the analytical thermal response in the case of linear (convective and/or radiative) heat losses (i.e. 3rd type boundary condition – BC).

By adjusting the free parameter \( \tau \), the \( \tanh^{1/2}(\xi) \)-type profiles can be made positive and monotonically increasing or decreasing over the half-line \( \xi \geq 0 \). By specifying that at the position \( z = 0 \) effusivity takes the value \( b_0 \) and that bulk effusivity is \( b_\infty \) we get the following expression:

\[
\sqrt{b_{[n]}(\xi)} = \sqrt{b_0} \left[ 1 + \sqrt{b_0/b_n} \tanh(\xi/b_\infty) \right] \left[ \sqrt{b_n/b_0} + \tanh(\xi/b_\infty) \right] ^{-1} \tag{6}
\]

Expressing this profile as function of physical position \( z \) instead of the SRDT \( \xi \) requires implementing an inverse Liouville transformation as described in [16], § 2.4. It necessitates an additional information, as for example, a constitutive law relating (some of) the thermal parameters \( a \), \( b \), \( c \), \( \lambda \). In particular, in the case of the commonly observed situation of a constant volumetric heat capacity \( c(z) = c_\infty \), the previous effusivity profile expresses implicitly through:

\[
\frac{z(\xi)}{z_\infty} = \sqrt{b_\infty} \left[ \frac{b_n}{b_0} \left( \frac{b_0}{b_n} \right)^{1/2} \tanh^{1/2}(\xi/b_\infty) \right] ^{-1} \left[ \sqrt{b_0/b_n} + 1 \right], \quad j = \begin{cases} +1 & b_0 < b_{[n]} < b_\infty \\ 0 & b_0 \geq b_{[n]} \geq b_\infty \end{cases} \tag{7}
\]

where the characteristic (real) depth for the profile transition, \( z_\infty \), was defined from the characteristic SRDT \( \xi_\infty \), in the following way, which involves the geometric mean of the surface diffusivity \( a_n \) and the bulk diffusivity \( a_\infty \) \( z_\infty = \xi_\infty (a_n a_\infty)^{1/2} \). A set of solvable effusivity profiles corresponding to the present model is shown in figure 1, for different values of the ratio \( b_n/b_0 \) between 0.4 and 2. As clearly shown, this model allows generating smooth semi-sigmoidal profiles evolving from a surface value \( b_0 \) to a bulk value \( b_\infty \). The surface impedance (i.e. the ratio of the local temperature to the heat flux density) is easily obtained by completing the inverse Liouville transformation [16]. For the present profiles it takes a particularly simple expression:

\[
Z_{[n]}(\xi = 0) = \frac{1}{b_0 \sqrt{p} \xi_\infty} \sqrt{p + b_0/b_n} \tag{8}
\]
Assuming now a 3rd type BC with a thermal solicitation \( g \) and a heat transfer coefficient \( h \) ( \( g \) encompasses the externally imposed heat fluxes and the external contribution \( h \theta_a \) where \( \theta_a \) is the surrounding fluid temperature), the surface temperature then reads: 
\[
\theta_b(\xi=0) = g(h + Z_0^{-1}(\xi=0))^{-1}.
\]

The result of the analytical Laplace inversion was provided in [16] for the adiabatic case ( \( h = 0 \)).

When heat losses are present, the expressions for the transient temperature \( T_\perp \) induced by a Dirac pulse of energy density \( Q \) and for the transient temperature \( T_\gamma \) induced by a step heating of power density \( P \) are given thereafter in terms of the reduced time \( t' = t\xi^{-2} \):
\[
T_\perp(t') = \frac{Q}{b_0 \xi} \left[ \frac{1}{x'} - A_+ v_+ \text{erfcx}(v_+ \sqrt{x'}) - A_- v_- \text{erfcx}(v_- \sqrt{x'}) \right], \quad (9)
\]
\[
T_\gamma(t') = \frac{P\xi}{b_0} \left[ H^{-1} - A_+ v_+^{-1} \text{erfcx}(v_+ \sqrt{x'}) - A_- v_-^{-1} \text{erfcx}(v_- \sqrt{x'}) \right], \quad (10)
\]
\[
A_\pm = \frac{v_\pm - \beta^{-1}}{v_\pm - v_\mp}; \quad A_\pm = \frac{v_\pm - \beta^{-1}}{v_\pm - v_\mp}; \quad \beta = \sqrt{\frac{b_0}{b_\infty}}; \quad H = \frac{h\xi}{b_0}; \quad v_\pm = \frac{1}{\sqrt{2}} \left[ \beta + H \pm \sqrt{(\beta + H)^2 - 4H} \right]. \quad (11)
\]

In equations (9) and (10) \text{erfcx}(x) = \exp(x^2)\text{erfc}(x)\) is the scaled complementary error function (in the event that the argument is complex, one should refer to the Faddeeva function). The normalized temperature for the Dirac case and the step heating case (i.e. the terms in bracket in the equations (9) and (10)) is plotted, respectively in figure 2 and 3 for two values of the bulk-to-surface effusivity ratio \( b_\gamma/b_\infty \) (0.5 for dashed curves and 2 for plain curves) and for three values for the reduced heat coefficient \( H \) (from top to bottom: 0, 0.01, 0.03, 0.1). The short-time transient response approaches the one of a homogeneous material with effusivity \( b_0 \) (the same happens for the high frequency response), whereas the long-time response (or the low frequency response) approaches the one of a homogeneous material with effusivity \( b_\infty \). The transition is naturally smoother than the one observed with a bi-layer made of two homogeneous materials with effusivity \( b_0 \) and \( b_\infty \).

4. Conclusion

This paper gave us the opportunity to present a short glimpse of the huge possibilities offered by the PROFIDT method. Many other examples of solvable profiles and their joint temperature solutions were presented in [16]. The example presented in the previous section was obtained after a single
Darboux transformation. Although very simple (the recovered effusivity profiles are merely monotonous over the half-line \( z \geq 0 \)), this model presents a noticeable interest:

- the half-sigmoidal shape of the solvable profiles (see figure 1) can approximate many real effusivity profiles (e.g. profiles in case-hardened steel [5], [8], [9], [10], [14], [15], in soils, in living tissue like skin and teeth, in Functionally Graded Materials (FGMs) – see the cited references in [16]);
- the corresponding (Laplace-Fourier) surface impedance has a very simple (rational) expression (see equation 8) which allows calculating very easily the modulated or the transient surface temperature, even in the case of heat losses, as shown just before. This feature opens new prospects for building an efficient inversion method for processing photothermal data and identifying a subsurface effusivity profile from the transient or modulated surface temperature.

Many other perspectives are envisioned:
- by performing a second PROFIDT, one will have at hand a broader family of still more “sophisticated” solvable effusivity profiles; they will indeed be defined with five parameters instead of only three. These profiles present subtle undulations and possibly a local maximum or minimum. They could thus fit more complicated real profiles. They will be presented in a forthcoming paper.
- another approach, as shown in [16], consists in stitching a semi-infinite profile of \( \tanh^{4}(\xi) \)-type with one or a series of profiles of \( \text{sech}(\xi) \)-type. The latter profiles are defined on finite intervals. They involve the hyperbolic secant function \( (\text{sech} = 1/\cosh) \) and they are defined with four parameters. Their outstanding interest is in that they are perfectly “flexible”: they can accommodate any quadruplet formed by the four values reached by effusivity and its slope at the ends of the interval. In the same way as three-degree polynomials are used for interpolating splines, the former profiles can be used to build “solvable effusivity splines”. A preliminary illustration was provided in [16] where a \( \text{sech}(\xi) \)-type profile was joined to a \( \tanh^{4}(\xi) \)-type profile whilst ensuring continuity up to the second derivative at the node. The global solution was obtained by implementing a specific quadrupole method. More complex solvable (synthetic) profiles will be presented in a forthcoming paper.

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Figure 2. Normalized temperature as induced by a Dirac pulse (equation 9); see text.  

Figure 3. Same as in figure 2 for a step heating (equation 10).
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