Boundary value problems and medical imaging

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Abstract. The application of appropriate transform pairs, such as the Fourier, the Laplace, the sine, the cosine and the Mellin transforms, provides the most well known method for constructing analytical solutions to a large class of physically significant boundary value problems. However, this method has several limitations. In particular, it requires the given PDE, domain and boundary conditions to be separable, and also may *not* be applicable if the given boundary value problem is non-self-adjoint. Furthermore, it expresses the solution as either an integral or an infinite series, neither of which are uniformly convergent on the boundary of the domain (for nonvanishing boundary conditions), which renders such expressions unsuitable for numerical computations. Here, we review a method recently introduced by the first author which *can* be applied to certain nonseparable and non-self-adjoint problems. Furthermore, this method expresses the solution as an integral in the complex plane which is uniformly convergent on the boundary of the domain. This method, which also suggests new numerical techniques, is illustrated for both evolution and elliptic PDEs. Athough this method was first applied to certain *nonlinear* PDEs called *integrable* and was originally formulated in terms of the so-called *Lax pairs*, it can actually be applied to *linear* PDEs without the need to analyse the associated Lax pair. The existence of Lax pairs is used here in order to motivate a related development, namely the emergence of a novel formalism for analysing certain inverse problems arising in medical imaging. Examples include PET and SPECT.

1. Boundary Value Problems

1.1. Evolution PDEs of the Half-Line

In order to introduce the new method we consider the simplest possible initial-boundary value (IBV) problem for an evolution PDE, namely the heat equation on the half-line:

$$u_t = u_{xx}, \quad 0 < x < \infty, \quad 0 < t < T, \quad T > 0, \tag{1}$$

where

$$u(x,0) = u_0(x), \quad 0 < x < \infty, \quad u(0,t) = g_0(t), \quad 0 < t < T. \tag{2}$$

The functions $u_0(x)$ and $g_0(t)$ are given functions with appropriate smoothness and $u_0(x)$ decays as $x \to \infty$.

The above IBV problem can be solved by the sine-transform pair,

$$\hat{f}(\lambda) = \int_0^\infty sin(\lambda x)f(x)dx, \quad \lambda > 0; \quad f(x) = \frac{2}{\pi}\int_0^\infty sin(\lambda x)\widehat{f}(\lambda)d\lambda, x > 0. \tag{3}$$
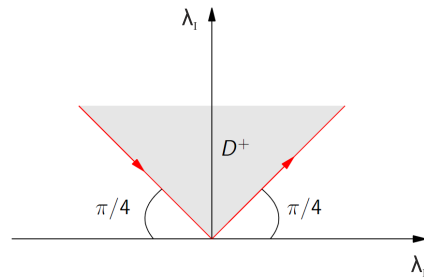
Figure 1. The domain D^+ for the heat equation.

Employing this transform we find

$$u(x,t) = \frac{2}{\pi} \int_0^\infty e^{-\lambda^2 t} \sin(\lambda x) \left[\int_0^\infty \sin(\lambda \xi) u_0(\xi) d\xi - \lambda \int_0^t e^{\lambda^2 s} g_0(s) ds \right] d\lambda. \qquad (4)$$

The above representation suffers from the generic disadvantage that is associated with *every* representation obtained via a classical transform, namely it is *not* uniformly convergent at the boundary. Indeed, if the right-hand-side of (4) converged uniformly at $x = 0$, then we could take the limit $x \to 0$ inside the integral and we would obtain $u(0,t) = 0$ instead of $u(0,t) = g_0(t)$.

The unified method yields

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^\infty e^{i\lambda x - \lambda^2 t} \hat{u}_0(\lambda) d\lambda - \frac{1}{2\pi} \int_{\partial D^+} e^{i\lambda x - \lambda^2 t} \left[\hat{u}_0(-\lambda) + 2i\lambda G_0(\lambda^2) \right] d\lambda, \qquad (5)$$

where the functions $\hat{u}_0(\lambda)$ and $G_0(\lambda)$ are defined by

$$\hat{u}_0(\lambda) = \int_0^\infty e^{-i\lambda x} u_0(x) dx, \quad \mathsf{Im}\,\lambda \leq 0, \quad G_0(\lambda) = \int_0^T e^{\lambda s} g_0(s) ds, \quad \lambda \in \mathbb{C}, \qquad (6)$$

and the contour ∂D^+ is the boundary of the domain D^+ shown in Fig. 1.

It is straightforward to show [1, 2] that the right-hand-side of (5) is indeed uniformly convergent at $x = 0$. Furthermore, the only (x,t) dependence of the right-hand-side of (5) is in the form $e^{i\lambda x - \lambda^2 t}$, thus it is immediately obvious that this representation satisfies the heat equation.

The experienced reader may worry about the dependence of $G_0(\lambda)$ on T, which contradicts causality (the solution of an evolution equation *cannot* depend on future data). However, using analyticity arguments, it can be shown [1, 2] that $G_0(\lambda)$ can be replaced by the function $G_0(\lambda, t)$, where

$$G_0(\lambda, t) = \int_0^t e^{\lambda s} g_0(s) ds, \quad \lambda \in \mathbb{C}. \qquad (7)$$

The limited applicability of the standard transforms becomes evident by considering the Stokes equation on the half-line:

$$u_t + u_{xxx} + u_x = 0, \quad 0 < x < \infty, \quad 0 < t < T, \quad T > 0, \qquad (8)$$

with the initial and boundary conditions defined in (2).

It can be rigorously established [3, 4] that there does *not* exist an appropriate x-transform for this problem, *i.e.* there does *not* exist the analogue of the sine transform for a linear evolution
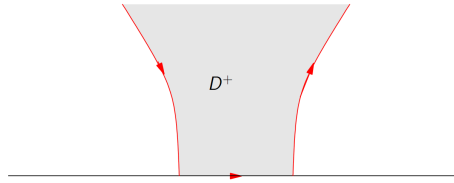
Figure 2. The domain D^+ for the Stokes equation.

PDF involving a third order derivative. One may attempt to solve the above IBV problem with the Laplace transform in t. But then one has to make the unnatural initial assumption of $T = \infty$, and furthermore one has to solve a cubic algebraic equation!

The unified method yields

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\lambda x - (i\lambda - i\lambda^3)t}\hat{u}_0(\lambda) - \frac{1}{2\pi}\int_{\partial D^+} e^{i\lambda x - (i\lambda - i\lambda^3)t}\tilde{g}(\lambda)d\lambda, \tag{9}$$

where the function $\hat{u}_0(\lambda)$ is defined in (6), $\tilde{g}(\lambda)$ is defined by

$$\tilde{g}(\lambda) = \frac{1}{\nu_1 - \nu_2}\left[(\nu_1 - \lambda)\hat{u}_0(\nu_2) + (\lambda - \nu_2)\hat{u}_0(\nu_1)\right] + (3\lambda^2 - 1)G_0(\omega(\lambda)), \tag{10}$$

with $G_0(\lambda)$ defined in (6) and $\omega(\lambda)$ given by $\omega(\lambda) = i\lambda - i\lambda^3$; the contour ∂D^+ is the boundary of the domain defined by

$$D^+ = \{\text{Re } \omega(\lambda) < 0\} \cap \mathbb{C}^+ \tag{11}$$

and shown in Fig. 2. The complex numbers ν_1 and ν_2 are the two nontrivial transformations $\lambda \to \nu_1(\lambda)$, $\lambda \to \nu_2(\lambda)$ which leave $\omega(\lambda)$ invariant, *i.e.* they are the two nontrivial roots of the equation $\omega(\lambda) = \omega(\nu(\lambda))$:

$$\nu_j^2 + \lambda\nu_j + \lambda^2 - 1 = 0, \quad j = 1, 2. \tag{12}$$

The unified method involves the following three steps:

Step 1: *Rewrite the given PDE in a divergence form, or equivalently in terms of a closed differential form.*

For the heat equation we find

$$(e^{-i\lambda x + \lambda^2 t}u)_t - (e^{-i\lambda x + \lambda^2 t}(u_x + i\lambda u))_x = 0, \quad \lambda \in \mathbb{C}. \tag{13}$$

Equivalently, the following differential one-form is closed:

$$W(x,t,\lambda) = e^{-i\lambda x + \lambda^2 t}[udx + (u_x + i\lambda u)dt]. \tag{14}$$

If the PDE is valid in a given domain Ω then Green's theorem immediately implies the following *global relation* (GR):

$$\oint_{\partial\Omega} W = 0. \tag{15}$$

For the heat equation on the half-line the GR becomes:

$$e^{\lambda^2 T}\hat{u}(\lambda, T) = \hat{u}_0(\lambda) - i\lambda G_0(\lambda^2) - G_1(\lambda^2), \quad \text{Im}\lambda \leq 0, \tag{16}$$
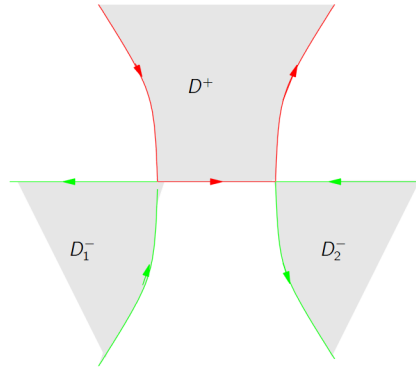
Figure 3. The analysis of the GR for the Stokes equation.

where $G_0(\lambda)$ is defined in (6) and the functions $G_1(\lambda)$ and $\hat{u}(\lambda, T)$ are defined by

$$G_1(\lambda) = \int_0^T e^{\lambda s} u_x(0,s) ds, \quad \lambda \in \mathbb{C}; \quad \hat{u}(\lambda, T) = \int_0^\infty e^{-i\lambda x} u(x,T) dx, \ \mathsf{Im}\lambda \le 0. \quad (17)$$

Step 2: *Integral representation of the solution.*
The representation can be obtained either using the Fourier transform on the half-line and then deforming the relevant integral from the real line to the complex λ-plane, or using the spectral analysis of the associated Lax pairs [2]. For the heat equation we find

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^\infty e^{i\lambda x - \lambda^2 t} \hat{u}_0(\lambda) d\lambda - \frac{1}{2\pi} \int_{\partial D^+} e^{i\lambda x - \lambda^2 t} [G_1(\lambda^2) + i\lambda G_0(\lambda^2)] d\lambda, \quad (18)$$

where ∂D^+ is shown in Fig. 1.
Step 3: *Elimination of the unknown boundary values.*
This can be achieved by using the GR and by employing all transformations in the complex λ-plane which leave the associated $\omega(\lambda)$ invariant. For the heat equation, $\omega(\lambda) = \lambda^2$, thus replacing in the GR λ with $-\lambda$, we find

$$e^{\lambda^2 T} \hat{u}(-\lambda, T) = \hat{u}_0(-\lambda) + i\lambda G_0(\lambda^2) - G_1(\lambda^2), \quad \mathsf{Im}\lambda \ge 0. \quad (19)$$

Solving this equation for G_1 and using the fact that $\hat{u}(-\lambda, T)$ does not contribute to the solution $u(x,t)$ [1, 2], we find that (18) becomes (5).

For the Stokes equation, the associated GR is

$$G_2 + i\lambda G_1 = (\lambda^2 - 1)G_0 - \hat{u}_0(\lambda) - e^{(i\lambda - i\lambda^3)T} \hat{u}(\lambda, T), \quad \mathsf{Im}\lambda \le 0. \quad (20)$$

Replacing in this equation λ by ν_1 and by ν_2 we find two equations, both of which are valid in D^+, see Fig. 3. Then, neglecting the contribution of $\hat{u}(\nu_1, T)$ and $\hat{u}(\nu_2, T)$, we find

$$G_1 \sim -i(\nu_1 + \nu_2)G_0 + i\frac{\hat{u}_0(\nu_1) - \hat{u}_0(\nu_2)}{\nu_1 - \nu_2}, \quad G_2 \sim -(1 + \nu_1\nu_2)G_0 + \frac{\nu_2\hat{u}_0(\nu_1) - \nu_1\hat{u}_0(\nu_2)}{\nu_1 - \nu_2}. \quad (21)$$

Numerical Implementation
For the case that $\hat{u}_0(\lambda)$ and $G_0(\lambda)$ can be computed explicitly, it is straightforward to compute
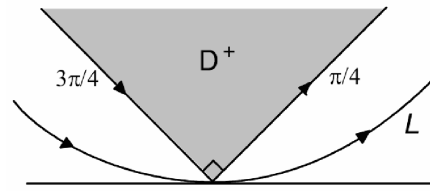
Figure 4. The contour L for the heat equation.

numerically the solution. Consider, for example, the heat equation with the following initial and boundary condition:

$$u_0(x) = x \exp(-a^2 x), \quad g_0(t) = \sin bt, \quad a, b > 0. \tag{22}$$

Then, (4) becomes

$$u(x,t) = \frac{1}{2\pi} \int_{\partial D^+} e^{i\lambda x - \lambda^2 t} \left[\frac{1}{(i\lambda + a)^2} - \frac{1}{(-i\lambda + a)^2} - \lambda \left(\frac{e^{(\lambda + ib)t} - 1}{\lambda + ib} - \frac{e^{(\lambda - ib)t} - 1}{\lambda - ib} \right) \right] d\lambda. \tag{23}$$

On the contour ∂D^+, $e^{i\lambda x}$ decays exponentially for large λ, whereas $e^{-i\lambda^2 t}$ oscillates. However, deforming ∂D^+ to the contour L, see Fig. 4, we achieve decay as $\lambda \to \infty$ in both $e^{i\lambda x}$ and $e^{-i\lambda^2 t}$. Thus, the deformed integral can be computed numerically most efficiently [5].

1.2. Evolution PDEs on the Interval
The heat and the Stokes equations with $\{0 < x < 1, 0 < x < T\}$ are analysed in [6]. For both these equations, the unified method yields $u(x,t)$ in terms of *integrals* in the complex λ-plane (as opposed to infinite series). It should be emphasized that it is *impossible* to express the solution of a typical IBV problem for the Stokes equation in terms of an infinite series. Therefore, the usual statement that a *finite* domain corresponds to a *discrete* spectrum is *not* valid in general (unless the associated problem is self-adjoint).

1.3. Elliptic PDEs in the Interior of a Polygon
For elliptic PDEs, including the Laplace, the modified Helmholtz and Helmholtz equations, formulated in the interior of a polygon, the unified method: (a) for certain simple domains, like the interior of an equilateral triangle, provides the analytical solution for a variety of boundary value problems, for which apparently the classical approaches fail. (b) For an arbitrary polygon, it provides a powerful approach for computing numerically the associated generalized *Dirichlet to Neumann map*, *i.e.* computing the unknown boundary value in terms of the given boundary data.

Consider for example the modified Helmholtz equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - \beta^2 u = 0, \quad \beta > 0, \quad x, y \in \mathbb{R}. \tag{24}$$

It is straightforward to verify that the following differential form W is closed:

$$W(x,y,\lambda) = e^{-i\frac{\beta}{2}\left(\lambda z - \frac{\bar{z}}{\lambda}\right)} \left\{ \left[-u_y + \frac{\beta}{2} \left(\lambda + \frac{1}{\lambda} \right) u \right] dx + \left[u_x + \frac{\beta}{2} \left(i\lambda + \frac{1}{i\lambda} \right) u \right] dy \right\},$$
$$\lambda \in \mathbb{C} \setminus \{0\}. \tag{25}$$

Hence, if $\partial\Omega$ denotes the boundary of Ω then the following GR is valid:

$$\int_{\partial\Omega} W(x, y, \lambda) = 0, \quad \lambda \in \mathbb{C} \setminus \{0\}. \tag{26}$$

In the particular case of a square with corners at (1,1), (1,-1),(-1,-1), (-1,1), (26) becomes

$$\sum_{j=1}^{4} \hat{u}_j(\lambda) = 0, \quad \lambda \in \mathbb{C} \setminus \{0\}, \tag{27}$$

where

$$\hat{u}_1(\lambda) = e^{\frac{\beta}{2}\left(i\lambda + \frac{1}{i\lambda}\right)} \int_{+1}^{-1} e^{\frac{\beta}{2}\left(\lambda + \frac{1}{\lambda}\right)y} \left[u_x^{(1)} + \frac{\beta}{2}\left(i\lambda + \frac{1}{i\lambda}\right) u^{(1)} \right] dy, \tag{28}$$

and similarly for $\{u_j(\lambda)\}_2^4$. Equation (27) involves four unknown functions, however (27) is valid for *all* $\lambda \in \mathbb{C} \setminus \{0\}$. By expanding the unknown functions in terms of Legandre polynomials and by choosing appropriate collocation points $\lambda = \lambda_j$, we can solve the GR in an efficient way with spectral accuracy [7, 8].

2. Medical Imaging

Equation (13) suggests the introduction of the "potential" $e^{-i\lambda x + \lambda^2 t}\mu$, satisfying

$$\left(e^{-i\lambda x + \lambda^2 t}\mu\right)_x = e^{-i\lambda x + \lambda^2 t}u, \quad \left(e^{-i\lambda x + \lambda^2 t}\mu\right)_t = e^{-i\lambda x + \lambda^2 t}(u_x + i\lambda u) \tag{29}$$

These equations provide a *Lax pair* formulation for the heat equation.

The initial value problem of the heat equation can be solved by the Fourier transform. The above Lax pair suggests that this transform can be constructed via the spectral analysis of the first of equations (29). Indeed, it was shown in [9] that the spectral analysis of the equation

$$\left(\partial_x - i\lambda\right)\mu(x, \lambda) = u(x), \tag{30}$$

yields the 1-D Fourier transform; similarly the spectral analysis of the equation

$$\left(\partial_{x_1} + i\partial_{x_1} - \lambda\right)\mu(x_1, x_2, \lambda) = u(x_1, x_2), \quad (x_1, x_2) \in \mathbb{R}^2, \tag{31}$$

yields the 2-D Fourier transform. This has lead to the emergence of a new method for deriving transforms, or equivalently for inverting certain integrals. The power of this new method was illustrated by R Novikov [10], who was able to invert the so-called *attenuated Radon transform*. This transform plays the same crucial role in SPECT that the Radon transform plays in CT and in PET [11, 12, 13, 14].

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