Time-dependent problems with the boundary integral equation method

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ABSTRACT

Time-dependent problems that are modeled by initial-boundary value problems for parabolic or hyperbolic partial differential equations can be treated with the boundary integral equation method. The ideal situation is when the right-hand side in the partial differential equation and the initial conditions vanish, the data are given only on the boundary of the domain, the equation has constant coefficients, and the domain does not depend on time. In this situation, the transformation of the problem to a boundary integral equation follows the same well-known lines as for the case of stationary or time-harmonic problems modeled by elliptic boundary value problems. The same main advantages of the reduction to the boundary prevail: Reduction of the dimension by one, and reduction of an unbounded exterior domain to a bounded boundary.

There are, however, specific difficulties due to the additional time dimension: Apart from the practical problems of increased complexity related to the higher dimension, there can appear new stability problems. In the stationary case, one often has unconditional stability for reasonable approximation methods, and this stability is closely related to variational formulations based on the ellipticity of the underlying boundary value problem. In the time-dependent case, instabilities have been observed in practice, but due to the absence of ellipticity, the stability analysis is more difficult and fewer theoretical results are available.

In this article, the mathematical principles governing the construction of boundary integral equation methods for time-dependent problems are presented. We describe some of the main algorithms that are used in practice and have been analyzed in the mathematical literature.

KEY WORDS: *Space-time boundary integral equations*; time domain; frequency domain; retarded potential; anisotropic Sobolev norms

1. INTRODUCTION

Like stationary or time-harmonic problems, transient problems can be solved by the boundary integral equation method. When the material coefficients are constant, a fundamental solution is known and the data are given on the boundary, the reduction to the boundary provides efficient numerical methods in particular for problems posed on unbounded domains.

Such methods are widely and successfully being used for numerically modeling problems in heat conduction and diffusion, in the propagation and scattering of acoustic, electromagnetic and elastic waves, and in fluid dynamics.

One can distinguish three approaches to the application of boundary integral methods on parabolic and hyperbolic initial-boundary value problems: Space-time integral equations, Laplace-transform methods, and time-stepping methods.

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1. *Space-time integral equations* use the fundamental solution of the parabolic or hyperbolic partial differential equations.

The construction of the boundary integral equations via representation formulas and jump relations, the appearance of single layer and double layer potentials, and the classification into first kind and second kind integral equations follow in a large part the formalism known for elliptic problems. Causality implies that the integral equations are of Volterra type in the time variable, and time-invariance implies that they are of convolution type in time.

Numerical methods constructed from these space-time boundary integral equations are global in time, i. e. they compute the solution in one step for the entire time interval. The boundary is the lateral boundary of the space-time cylinder and therefore has one dimension more than the boundary of the spatial domain. This increase in dimension at first means a substantial increase in complexity:
- To compute the solution for a certain time, one needs the solution for all the preceding times since the initial time.
- The system matrix is much larger.
- The integrals are higher-dimensional. For a problem with 3 space dimensions, the matrix elements in a Galerkin method can require 6-dimensional integrals.

While the increase in memory requirements for the storage of the solution for preceding times cannot completely be avoided, there are situations where the other two reasons for increased complexity are in part neutralized by special features of the problem:
- The system matrix has a special structure related to the Volterra structure (finite convolution in time) of the integral equations. When low order basis functions in time are used, the matrix is of block triangular Toeplitz form, and for its inversion only one block - which has the size of the system matrix for a corresponding time independent problem - needs to be inverted.
- When a strong Huyghens principle is valid for the partial differential equation, the integration in the integral representation is not extended over the whole lateral boundary of the space-time cylinder, but only over its intersection with the surface of the backward light cone. This means firstly that the integrals are of the same dimensionality as for time-independent problems, and secondly that the dependence is not extended arbitrarily far into the past, but only up to a time corresponding to the time of traversal of the boundary with the fixed finite propagation speed. These “retarded potential integral equations” are of importance for the scalar wave equation in three space dimensions and to a certain extent for equations derived from them, in electromagnetics and elastodynamics. On the other hand, such a Huyghens principle is not valid for the wave equation in two space dimension, nor for the heat equation nor for problems in elastodynamics nor in fluid dynamics.

2. *Laplace transform methods* solve frequency-domain problems, possibly for complex frequencies. For each fixed frequency, a standard boundary integral method for an elliptic problem is applied, and then the transformation back to the time domain employs special methods for the inversion of Fourier or Laplace transforms. The choice of a numerical method for the inverse Laplace transform can be guided by the choice of an approximation of the exponential function corresponding to a linear multistep method for ordinary differential equations. This idea is related to the *operational quadrature method* (Lubich, 1994).

Laplace or Fourier transform is also used the other way round, to pass from the time domain to the frequency domain. This can be done using FFT in order to simultaneously solve problems for many frequencies from one time-domain computation, or one can solve a time-domain problem with a time-harmonic right hand side to get the solution for one fixed frequency. It has been observed that this can be efficient, too (Sayah, 1998), due to less strict requirements for the spatial resolution.

3. *Time-stepping methods* start from a time discretization of the original initial-boundary value

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problem via an implicit scheme and then use boundary integral equations to solve the resulting elliptic problems for each time step. Here a difficulty lies in the form of the problem for one time step which has non-zero initial data and thus is not in the ideal form for an application of the boundary integral method, namely vanishing initial conditions and volume forces, and non-homogeneous boundary data. The solution after a time step, which defines the initial condition for the next time step, has no reason to vanish inside the domain. Various methods have been devised to overcome this problem:

Using volume potentials to incorporate the non-zero initial data often is not desirable, since it requires discretization of the domain and thus defies the advantage of the reduction to the boundary. Instead of a volume potential (Newton potential), another particular solution (or approximate particular solution) of the stationary problem can be used. This particular solution may be obtained by fast solution methods, for example FFT or a fast Poisson solver on a fictitious domain, or by meshless discretization of the domain using special basis functions, like thin-plate splines or other radial basis functions (so-called *dual reciprocity method*, see Aliabadi and Wrobel, 2002).

Another idea is to consider not a single time step, but all time steps up to the final time together as a discrete convolution equation for the sequence of solutions at the discrete time values. Such a discrete convolution operator whose (time-independent) coefficients are elliptic partial differential operators has a fundamental solution which can then be used to construct a pure boundary integral method for the solution of the time-discretized problem. A fundamental solution, which is also a discrete convolution operator, can be given explicitly for simple time discretization schemes like the backward Euler method ("Rothe method" Chapko and Kress, 1997). For a whole class of higher order onestep or multistep methods, it can be constructed using Laplace transforms via the *operational quadrature method* (Lubich and Schneider, 1992; Lubich, 1994).

These three approaches for the construction of boundary integral methods cannot be separated completely. There are many points of *overlap*:

The space-time integral equation method leads, after discretization, to a system that has the same finite time convolution structure one also gets from time-stepping schemes. The main difference is that the former needs the knowledge of a space-time fundamental solution. But this is simply the inverse Laplace transform of the fundamental solution of the corresponding time-harmonic problem.

The Laplace transform appears in several roles. It can be used to translate between the time domain and the frequency domain on the level of the formulation of the problem, but also on the level of the solution.

The stability analysis for all known algorithms, for the space-time integral equation methods as for the time-stepping methods, passes by the transformation to the frequency domain and corresponding estimates for the stability of boundary integral equations methods for elliptic problems. The difficult part in this analysis is to find estimates uniform with respect to the frequency.

For *parabolic* problems, some analysis of integral equation methods and their numerical realization has been known for a long time, and the classical results for second kind integral equations on smooth boundaries are summarized in the book by Pogorzelski (1966). All the standard numerical methods available for classical Fredholm integral equations of the second kind, like collocation methods or Nyström methods, can be used in this case. More recently, variational methods have been studied in a setting of anisotropic Sobolev spaces that allow the coverage of first kind integral equations and non-smooth boundaries. It has been found that, unlike the parabolic partial differential operator with its time-independent energy and no regularizing property in time direction, the first kind boundary integral operators have a kind of anisotropic space-time *ellipticity* (Costabel, 1990; Arnold and Noon, 1989; Brown, 1989; Brown and Shen, 1993).

This ellipticity leads to unconditionally stable and convergent *Galerkin methods* (Costabel, 1990;

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Arnold and Noon, 1989; Hsiao and Saranen, 1993; Hebeker and Hsiao, 1993). Because of their simplicity, *collocation methods* are frequently used in practice for the discretization of space-time boundary integral equations. An analysis of collocation methods for second-kind boundary integral equations for the heat equation was given by Costabel *et al.*, 1987. Fourier analysis techniques for the analysis of stability and convergence of collocation methods for parabolic boundary integral equations, including first kind integral equations, have been studied more recently by Hamina and Saranen (1994) and by Costabel and Saranen (2000; 2001; 2003).

The operational quadrature method for parabolic problems was introduced and analyzed by Lubich and Schneider (1992).

For *hyperbolic* problems, the mathematical analysis is mainly based on variational methods as well (Bamberger and Ha Duong, 1986; Ha-Duong, 1990; Ha-Duong, 1996). There is now a lack of ellipticity which on one hand leads to a loss of an order of regularity in the error estimates. On the other hand, most coercivity estimates are based on a passage to complex frequencies, which may lead to stability constants that grow exponentially in time. Instabilities (that are probably unrelated to this exponential growth) have been observed, but their analysis does not seem to be complete (Becache, 1991; Peirce and Siebrits, 1996; Peirce and Siebrits, 1997; Birgisson *et al.*, 1999). Analysis of variational methods exists for the main domains of application of space-time boundary integral equations: First of all for the scalar wave equation, where the boundary integrals are given by retarded potentials, but also for elastodynamics (Becache, 1993; Becache and Ha-Duong, 1994; Chudinovich, 1993c; Chudinovich, 1993b; Chudinovich, 1993a), piezoelectricity (Khutoryansky and Sosa, 1995), and for electrodynamics (Bachelot and Lange, 1995; Bachelot *et al.*, 2001; Rynne, 1999; Chudinovich, 1997). An extensive review of results on variational methods for the retarded potential integral equations is given by Ha-Duong (2003).

As in the parabolic case, collocation methods are practically important for the hyperbolic space-time integral equations. For the retarded potential integral equation, the stability and convergence of collocation methods has now been established (Davies, 1994; Davies, 1998; Davies and Duncan, 1997; Davies and Duncan, 2003).

Finally, let us mention that there have also been important developments in the field of *fast methods* for space-time boundary integral equations (Michielssen, 1998; Jiao *et al.*, 2002; Michielssen *et al.*, 2000; Greengard and Strain, 1990; Greengard and Lin, 2000).

2. SPACE-TIME INTEGRAL EQUATIONS

2.1. Notations

We will now study some of the above-mentioned ideas in closer detail. Let $\Omega \subset \mathbb{R}^n$, $(n \geq 2)$, be a domain with compact boundary Γ. The outer normal vector is denoted by $\mathbf{n}$ and the outer normal derivative by ∂_n.

Let $T > 0$ be fixed. We denote by Q the space-time cylinder over Ω and Σ its lateral boundary:

$$Q = (0,T) \times \Omega\,; \quad \Sigma = (0,T) \times \Gamma\,; \quad \partial Q = (\{0\} \times \overline{\Omega}) \cup \Sigma \cup (\{T\} \times \overline{\Omega})\,.$$

For the description of the general principles, we consider only the simplest model problem of each type. We also assume that the right hand sides have the right structure for the application of a "pure" boundary integral method: The volume sources and the initial conditions vanish, so that the whole system is driven by boundary sources.

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Elliptic problem (Helmholtz equation with frequency $\omega \in \mathbb{C}$):

$$\begin{aligned} &(\Delta + \omega^2)u = 0 \quad \text{in } \Omega \\ &u = g \ \text{(Dirichlet)} \quad \text{or } \partial_n u = h \ \text{(Neumann)} \quad \text{on } \Gamma \\ &\text{radiation condition at } \infty \end{aligned} \tag{$\mathcal{E}$}$$

Parabolic problem (heat equation):

$$\begin{aligned} &(\partial_t - \Delta)u = 0 \quad \text{in } Q \\ &u = g \ \text{(Dirichlet)} \quad \text{or } \partial_n u = h \ \text{(Neumann)} \quad \text{on } \Sigma \\ &u = 0 \quad \text{for } t \leq 0 \end{aligned} \tag{$\mathcal{P}$}$$

Hyperbolic problem (wave equation with velocity $c > 0$):

$$\begin{aligned} &(c^{-2}\partial_t^2 - \Delta)u = 0 \quad \text{in } Q \\ &u = g \ \text{(Dirichlet)} \quad \text{or } \partial_n u = h \ \text{(Neumann)} \quad \text{on } \Sigma \\ &u = 0 \quad \text{for } t \leq 0 \end{aligned} \tag{$\mathcal{H}$}$$

2.2. Space-time representation formulas

2.2.1. Representation formulas and jump relations The derivation of boundary integral equations follows from a general method that is valid (under suitable smoothness hypotheses on the data) in the same way for all 3 types of problems. In fact, what counts for ($\mathcal{P}$) and ($\mathcal{H}$) is the property that the lateral boundary Σ is non-characteristic.

The first ingredient for a BEM is a fundamental solution G. As an example, in 3 dimensions we have, respectively:

$$G_\omega(x) = \frac{e^{i\omega|x|}}{4\pi|x|} \tag{$\mathcal{E}$}$$

$$G(t,x) = \begin{cases} (4\pi t)^{-3/2} e^{-\frac{|x|^2}{4t}} & (t \geq 0) \\ 0 & (t \leq 0) \end{cases} \tag{$\mathcal{P}$}$$

$$G(t,x) = \frac{1}{4\pi|x|}\,\delta(t - \frac{|x|}{c}) \tag{$\mathcal{H}$}$$

Representation formulas for a solution u of the homogeneous partial differential equation and $x \notin \Gamma$ are obtained from Green's formula, applied with respect to the space variables in the interior and exterior domain. We assume that u is smooth in the interior and the exterior up to the boundary, but has a jump across the boundary. The jump of a function v across Γ is denoted by $[v]$:

$$u(x) = \int_\Gamma \{\partial_{n(y)} G(x-y)[u(y)] - G(x-y)[\partial_n u(y)]\}\, d\sigma(y) \tag{$\mathcal{E}$}$$

$$u(t,x) = \int_0^t \int_\Gamma \{\partial_{n(y)} G(t-s, x-y)[u(s,y)] - G(t-s,x-y)[\partial_n u(y)]\}\, d\sigma(y)\, ds \tag{$\mathcal{P}$}$$

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$$u(t,x) = \int_0^t \int_\Gamma \{\partial_{n(y)} G(t-s,x-y)[u(s,y)] - G(t-s,x-y)[\partial_n u(y)]\}\, d\sigma(y)\, ds \qquad (\mathcal{H})$$
$$= \int_\Gamma \{\partial_{n(y)} \frac{1}{4\pi|x-y|}[u(t-\frac{|x-y|}{c},y)] - \frac{\partial_{n(y)}|x-y|}{4\pi c|x-y|}[\partial_t u(t-\frac{|x-y|}{c},y)]$$
$$- \frac{1}{4\pi|x-y|}[\partial_n u(t-\frac{|x-y|}{c},y)]\, d\sigma(y)$$

Thus the representation in the parabolic case uses integration over the past portion of Σ in the form of a finite convolution over the interval $[0,t]$, whereas in the hyperbolic case, only the intersection of the interior of the backward light cone with Σ is involved. In 3D, where Huyghens' principle is valid for the wave equation, the integration extends only over the boundary of the backward light cone, and the last formula shows that the integration can be restricted to Γ, giving a very simple representation by "retarded potentials".

We note that in the representation by retarded potentials, all those space-time points (s,y) contribute to $u(t,x)$ from where the point (t,x) is reached with speed c by traveling through the space $\mathbb{R}^3$. In the case of waves propagating in the exterior of an obstacle this leads to the seemingly paradoxical situation that a perturbation at (s,y) can contribute to $u(t,x)$, although no signal from y has yet arrived in x, because in physical space it has to travel around the obstacle.

All 3 representation formulas can be written in a unified way by introducing the single layer potential $\mathcal{S}$ and the double layer potential $\mathcal{D}$:

$$u = \mathcal{D}([u]) - \mathcal{S}([\partial_n u])\,. \qquad (1)$$

In all cases, there hold the classical jump relations in the form

$$\begin{array}{rclcrcl} [\mathcal{D}v] &=& v &;& [\partial_n \mathcal{D}v] &=& 0 \\ [\mathcal{S}\varphi] &=& 0 &;& [\partial_n \mathcal{S}\varphi] &=& -\varphi \end{array}$$

It appears therefore natural to introduce the boundary operators from the sums and differences of the one-sided traces on the exterior (Γ^+) and interior (Γ^-) of Γ:

$$\begin{array}{rcll} V &:=& \mathcal{S}\big|_\Gamma & \text{(single layer potential)} \\ K &:=& \frac{1}{2}(\mathcal{D}\big|_{\Gamma^+} + \mathcal{D}\big|_{\Gamma^-}) & \text{(double layer potential)} \\ K' &:=& \frac{1}{2}(\partial_n\mathcal{S}\big|_{\Gamma^+} + \partial_n\mathcal{S}\big|_{\Gamma^-}) & \text{(normal derivative of single layer potential)} \\ W &:=& -\partial_n\mathcal{D}\big|_\Gamma & \text{(normal derivative of double layer potential)} \end{array}$$

2.2.2. Boundary integral equations In a standard way, the jump relations together with these definitions lead to boundary integral equations for the Dirichlet and Neumann problems. Typically one has a choice of at least 4 equations for each problem: The first 2 equations come from taking the traces in the representation formula (1) ("*direct method*"), the third one comes from a *single layer representation*

$$u = \mathcal{S}\psi \quad \text{with unknown } \psi$$

and the fourth one from a *double layer representation*

$$u = \mathcal{D}w \quad \text{with unknown } w\ :$$

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For the exterior Dirichlet problem ($u\big|_\Gamma = g$ given, $\partial_n u\big|_\Gamma = \varphi$ unknown):

$$\begin{array}{lll} (D1) & V\varphi & = & (-\frac{1}{2}+K)g \\ (D2) & (\frac{1}{2}+K')\varphi & = & -Wg \\ (D3) & V\psi & = & g \\ (D4) & (\frac{1}{2}+K)w & = & g \end{array}$$

For the exterior Neumann problem ($u\big|_\Gamma = g = v$ unknown, $\partial_n u\big|_\Gamma = h$ given):

$$\begin{array}{lll} (N1) & (\frac{1}{2}-K)v & = & -Vh \\ (N2) & Wv & = & -(\frac{1}{2}+K')h \\ (N3) & (\frac{1}{2}-K')\psi & = & -h \\ (N4) & Ww & = & -h \end{array}$$

Remember that this formal derivation is rigorously valid for all 3 types of problems. One notes that second-kind and first-kind integral equations alternate nicely. For open surfaces, however, only the first-kind integral equations exist. The reason is that a boundary value problem on an open surface fixes not only a one-sided trace but also the jump of the solution; and therefore the representation formula coincides with a single layer potential representation for the Dirichlet problem and with a double layer potential representation for the Neumann problem.

The same abstract form of space-time boundary integral equations (D1)–(D4) and (N1)–(N4) is obtained for more general classes of second order initial-boundary value problems. If a space-time fundamental solution is known, then Green's formulas for the spatial part of the partial differential operator are used to get the representation formulas and jump relations. The role of the normal derivative is played by the conormal derivative.

Since for time-independent boundaries the jumps across the lateral boundary Σ involve only jumps across the spatial boundary Γ at a fixed time t, the jump relations and representation formulas for a much wider class of higher order elliptic systems (Costabel and Dauge, 1997) could be used to obtain space-time boundary integral equations for parabolic and hyperbolic initial-boundary value problems associated to such partial differential operators. In the general case, this has yet to be studied.

2.2.3. Examples of fundamental solutions The essential requirement for the construction of a boundary integral equation method is the availability of a fundamental solution. This can be a serious restriction on the use of the space-time integral equation method, because explicitly given and sufficiently simple fundamental solutions are known for far less parabolic and hyperbolic equations than for their elliptic counterparts.

In principle, one can pass from the frequency domain to the time domain by a simple Laplace transform, and therefore the fundamental solution for the time-dependent problem always has a representation by a Laplace integral of the frequency-dependent fundamental solution of the corresponding elliptic problem. In practice, this representation can be rather complicated. An example where this higher level of complexity of the time-domain representation is visible, but possibly still acceptable, is the *dissipative wave equation* with a coefficient $\alpha > 0$ (and speed $c = 1$ for simplicity)

$$(\partial_t^2 + \alpha\partial_t - \Delta)u = 0$$

In the frequency domain, we obtain the same equation as for the wave equation with ω simply replaced by $\omega_\alpha = \sqrt{\omega^2 + i\alpha\omega}$. The time-harmonic fundamental solution in three dimensions is therefore simply

$$G_{\omega_\alpha}(x) = \frac{1}{4\pi|x|} e^{i|x|\sqrt{\omega^2+i\alpha\omega}}$$

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From this we obtain by inverse Laplace transformation

$$G(t,x) = \frac{e^{-\alpha t/2}}{4\pi|x|}\left(\delta(t-|x|) + \frac{\alpha|x|}{2\sqrt{t^2-|x|^2}}\, I_1(\frac{\alpha}{2}\sqrt{t^2-|x|^2})\,\theta(t-|x|)\right)$$

with the Dirac distribution δ, the Heaviside function θ and the modified Bessel function I_1. We see that there is no strong Huyghens principle, and the integrals in the corresponding space-time integral equations will be extended over the whole intersection of the boundary Σ with the solid backward light cone $\{(s,y) \mid t-s > |x-y|\}$.

For the case of *elastodynamics*, the corresponding space-time integral equations have not only been successfully used for a long time in practice (Mansur, 1983; Antes, 1985; Antes, 1988), but they have also been studied mathematically. Isotropic homogeneous materials are governed by the second-order hyperbolic system for the n-component vector field $\mathbf{u}$ of the displacement

$$\rho\partial_t^2\mathbf{u} - \operatorname{div}\sigma = 0 \quad \text{with } \sigma_{ij} = \mu(\partial_i u_j + \partial_j u_i) + \lambda\delta_{ij}\operatorname{div}\mathbf{u}$$

Here ρ is the density, and λ and μ are the Lamé constants. The role of the normal derivative ∂_n is played by the traction operator T_n where $T_n\mathbf{u} = \sigma\cdot\mathbf{n}$ is the normal stress. The role of the Dirichlet and Neumann boundary conditions are played by the displacement and traction boundary conditions, respectively:

$$\mathbf{u} = g \ \text{(displacement)} \quad \text{or } T_n\mathbf{u} = h \ \text{(traction)} \quad \text{on } \Sigma$$

In three dimensions, the space-time fundamental solution shows the longitudinal (pressure) and transversal (shear) waves that propagate with the two velocities

$$c_p = \sqrt{\frac{\lambda+2\mu}{\rho}} \quad \text{and } c_s = \sqrt{\frac{\mu}{\rho}}$$

But there is no strict Huyghens principle, the support of the fundamental solution is not contained in the union of the two conical surfaces determined by these two speeds but rather in the closure of the domain between these two surfaces. The fundamental solution is a (3×3) matrix G whose entries are given by

$$G_{jk}(t,x) = \frac{1}{4\pi\rho|x|^3}\left\{t^2\left(\frac{x_jx_k}{|x|^2}\delta(t-\frac{|x|}{c_p}) + (\delta_{jk}-\frac{x_jx_k}{|x|^2})\delta(t-\frac{|x|}{c_s})\right)\right.$$
$$\left. + t\left(3\frac{x_jx_k}{|x|^2}-\delta_{jk}\right)\left(\theta(t-\frac{|x|}{c_p}) - \theta(t-\frac{|x|}{c_s})\right)\right\}$$

Here δ_{jk} is the Kronecker symbol, δ is the Dirac distribution, and θ is the Heaviside function.

Detailed descriptions of the space-time boundary integral equations in elastodynamics corresponding to (D1)–(D4) and (N1)–(N4) above can be found in many places (Chudinovich, 1993b; Chudinovich, 1993a; Becache and Ha-Duong, 1994; Brebbia *et al.*, 1984; Antes, 1988; Aliabadi and Wrobel, 2002).

Whereas the frequency-domain fundamental solution is explicitly available for generalizations of elastodynamics such as certain models of anisotropic elasticity or thermoelasticity (Kupradze *et al.*, 1979) or viscoelasticity (Schanz, 2001b), the time-domain fundamental solution quickly becomes very complicated (for an example in two-dimensional piezoelectricity see Wang *et al.* (2003),), or completely unavailable.

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For the case of *electrodynamics*, space-time integral equations have been used and analyzed extensively, too, in the past dozen years (Pujols, 1991; Däschle, 1992; Terrasse, 1993; Bachelot and Lange, 1995; Chudinovich, 1997). An analysis of numerical methods based on variational formulations is available, and also the coupling of space-time integral equation methods with domain finite element methods has been studied (Sayah, 1998; Bachelot *et al.*, 2001).

Maxwell's equations being a first order system, the above formalism with its distinction between Dirichlet and Neumann conditions and between single and double layer potentials makes less sense here. There are, however, additional symmetries that allow to give a very "natural" form to the space-time boundary integral equations and their variational formulations. The close relationship between the Maxwell equations and the scalar wave equation in 3 dimensions implies the appearance of retarded potentials here, too.

The system of Maxwell's equations in a homogeneous and isotropic material with electric permittivity ε and magnetic permeability μ is

$$\mu\partial_t \mathbf{H} + \mathbf{curl}\,\mathbf{E} = 0$$
$$\varepsilon\partial_t \mathbf{E} - \mathbf{curl}\,\mathbf{H} = 0$$

The speed of light is $c = 1/\sqrt{\varepsilon\mu}$, and the corresponding retarded potential can be abbreviated as

$$\mathcal{S}(u)(t,x) = \frac{1}{4\pi}\int_\Gamma \frac{u(t-\frac{|x-y|}{c},y)}{|x-y|}\,d\sigma(y)$$

Then an analogue of representation formula (1) can be written in the following form:

$$\mathbf{E}(t,x) = -\mu\mathcal{S}(\partial_t[\mathbf{j}])(t,x) + \frac{1}{\varepsilon}\,\mathbf{grad}_x\,\mathcal{S}(\partial_t^{-1}\,\mathrm{div}_\Gamma[\mathbf{j}])(t,x) - \mathbf{curl}\,\mathcal{S}([\mathbf{m}])(t,x)$$
$$\mathbf{H}(t,x) = -\varepsilon\mathcal{S}(\partial_t[\mathbf{m}])(t,x) + \frac{1}{\mu}\,\mathbf{grad}_x\,\mathcal{S}(\partial_t^{-1}\,\mathrm{div}_\Gamma[\mathbf{m}])(t,x) + \mathbf{curl}\,\mathcal{S}([\mathbf{j}])(t,x)$$

where $[\mathbf{j}]$ and $[\mathbf{m}]$ are the surface currents and surface charge densities given by the jumps across Σ:

$$[\mathbf{j}] = [\mathbf{H}\wedge\mathbf{n}]\,;\quad [\mathbf{m}] = [\mathbf{n}\wedge\mathbf{E}]$$

and ∂_t^{-1} is the primitive defined by

$$\partial_t^{-1}\varphi(t,x) = \int_0^t \varphi(s,x)\,ds$$

Taking tangential traces on Σ, one then obtains systems of integral equations analogous to $(D1)$–$(N4)$ for the unknown surface current and charge densities. Due to special symmetries of the Maxwell equations, the set of four boundary integral operators V, K, K', W appearing in the boundary reduction of second-order problems is reduced to only two different boundary integral operators which we denote by $\mathbf{V}$ and $\mathbf{K}$, defined by

$$\mathbf{V}\boldsymbol{\varphi} = -\mathbf{n}\wedge\mathcal{S}(\frac{1}{c}\partial_t\boldsymbol{\varphi}) + \mathbf{curl}_\Gamma\,\mathcal{S}(c\partial_t^{-1}\boldsymbol{\varphi})$$
$$\mathbf{K}\boldsymbol{\varphi} = \frac{1}{2}(\gamma^+ + \gamma^-)\mathbf{n}\wedge\mathbf{curl}\,\mathcal{S}(\boldsymbol{\varphi})$$

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In the definition of $\mathbf{K}$, one takes the principal value which corresponds also to the mean value between the exterior trace γ^+ and the interior trace γ^-, analogous to the definition of the double layer potential operator K in section 2.2.1.

For the exterior initial value problem, the traces

$$\mathbf{v} = \mathbf{m} = \mathbf{n} \wedge \mathbf{E} \text{ and } \boldsymbol{\varphi} = \mu c \mathbf{j} = \sqrt{\frac{\mu}{\varepsilon}}\, \mathbf{H} \wedge \mathbf{n}$$

then satisfy the two relations corresponding to the four integral equations $(D1)$, $(D2)$, $(N1)$, $(N2)$ of the *direct method*

$$(\frac{1}{2} - \mathbf{K})\, \mathbf{v} = -\mathbf{V}\boldsymbol{\varphi} \quad \text{ and } (\frac{1}{2} - \mathbf{K})\, \boldsymbol{\varphi} = \mathbf{V}\mathbf{v}$$

From a *single layer representation*, i.e. $[\mathbf{m}] = 0$ in the representation formula for the electric field, one obtains the time-dependent *electric field integral equation* which now can be written as

$$\mathbf{V}\boldsymbol{\psi} = \mathbf{g}$$

where $\mathbf{g}$ is given by the tangential component of the incident field.

2.3. Space-time variational formulations and Galerkin methods

We will not treat the analysis of second-kind boundary integral equations in detail here. Suffice it to say that the key observation in the parabolic case is the fact that for smooth Γ, the operator norm in $L^p(\Sigma)$ of the weakly singular operator K tends to 0 as $T \to 0$. This implies that $\frac{1}{2} \pm K$ and $\frac{1}{2} \pm K'$ are isomorphisms in L^p (and also in C^m), first for small T and then by iteration for all T. The operators K and K' being compact, one can use all the well-known numerical methods for classical Fredholm integral equations of the second kind, including Galerkin, collocation, Nyström methods (Pogorzelski, 1966; Kress, 1989), with the additional benefit that the integral equations are always uniquely solvable. If Γ has corners, these arguments break down, and quite different methods, including also variational arguments, have to be used (Costabel, 1990; Dahlberg and Verchota, 1990; Brown, 1989; Brown and Shen, 1993; Adolfsson *et al.*, 1994).

2.3.1. Galerkin methods For the first kind integral equations, an analysis based on variational formulations is available. The corresponding numerical methods are space-time Galerkin methods. Their advantage is that they inherit directly the stability of the underlying variational method. In the elliptic case, this allows the well-known standard boundary element analysis of stability and errors, very similar to the standard finite element methods. In the parabolic case, the situation is still similar, but in the hyperbolic case, some price has to be paid for the application of "elliptic" techniques. In particular, one has then to work with two different norms.

Let X be some Hilbert space and let a be a bilinear form on $X \times X$. If we assume that a is bounded on X:

$$\exists M : \forall u, v \in X \ : \ |a(u,v)| \leq M \, \|u\| \|v\|$$

but that a is elliptic only with respect to a smaller norm $\| \cdot \|_0$, associated with a space X_0 into which X is continuously embedded:

$$\exists \alpha > 0 : \forall u \in X \ : \ |a(u,u)| \geq \alpha \, \|u\|_0^2$$

then for the variational problem: Find $u \in X$ such that

$$a(u,v) = <f, v> \quad \forall v \in X$$

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and its Galerkin approximation: Find $u_N \in X_N$ such that

$$a(u_N, v_N) = <f, v_N> \quad \forall v_N \in X_N$$

there are stability and error estimates with a loss:

$$\|u_N\|_0 \leq C \, \|u\| \quad \text{ and } \|u - u_N\|_0 \leq C \, \inf\{\|u - v_N\| \mid v_N \in X_N\}$$

The finite dimensional space X_N for the Galerkin approximation of space-time integral equations is usually constructed as a tensor product of a standard boundary element space for the spatial discretization and of a space of one-dimensional finite element or spline functions on the interval $[0, T]$ for the time discretization. Basis functions are then of the form

$$\varphi_{ij}(t, x) = \chi_i(t)\psi_j(x) \quad (i = 1, \ldots, I, j = 1, \ldots, J)$$

and the trial functions are of the form

$$u_N(t, x) = \sum_{i,j=1}^{I,J} \alpha_{ij}\varphi_{ij}(t, x)$$

The system of Galerkin equations for the unknown coefficients α_{ij} is

$$\sum_{i,j=1}^{I,J} a(\varphi_{ij}, \varphi_{kl})\alpha_{ij} = <f, \varphi_{kl}> \quad (k = 1, \ldots, I, l = 1, \ldots, J)$$

In the following, we restrict the presentation to the *single layer potential operator* V. We emphasize, however, that a completely analogous theory is available for the hypersingular operator W in all cases.

The variational methods for the first-kind integral operators are based on the first Green formula which gives, together with the jump relations, a formula valid again for all 3 types of equations: If φ and ψ are given on Γ or Σ, satisfy a finite number of conditions guaranteeing the convergence of the integrals on the right hand side of the formula (2) below, and

$$u = \mathcal{S}\varphi, \qquad v = \mathcal{S}\psi \, ,$$

then

$$\int_\Gamma \varphi V \psi \, d\sigma = \int_{\mathbb{R}^n \setminus \Gamma} \{\nabla u \cdot \nabla v + u \Delta v\} \, dx \, . \tag{2}$$

2.3.2. ($\mathcal{E}$) For the elliptic case, we obtain ($<\cdot, \cdot>_\Gamma$ denotes L^2 duality on Γ);

$$<\varphi, V\varphi>_\Gamma = \int_{\mathbb{R}^n \setminus \Gamma} (|\nabla u|^2 - \omega^2 |u|^2) \, dx \, .$$

This gives the following theorem that serves as a model for the other two types. I holds not only for the simple case of the Laplacian, but also, in particular its assertion (ii), for more general second order systems, including the Lamé system of linear elasticity (Costabel, 1988).

Theorem 2.1. *Let Γ be a bounded Lipschitz surface, open or closed. $H^{1/2}(\Gamma)$ and $H^{-1/2}(\Gamma)$ denote the usual Sobolev spaces, and $\widetilde{H}^{-1/2}(\Gamma)$ for an open surface is the dual of $H^{1/2}(\Gamma)$. Then*
(i) For $\omega = 0$, $n \geq 3$: $V : \widetilde{H}^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is an isomorphism, and there is an $\alpha > 0$ such that

$$<\varphi, V\varphi>_\Gamma \geq \alpha \|\varphi\|^2_{\widetilde{H}^{-1/2}(\Gamma)} \, .$$

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(ii) For any ω and n, there is an $\alpha > 0$ and a compact quadratic form k on $\widetilde{H}^{-1/2}(\Gamma)$ such that

$$\mathrm{Re} <\varphi, V\varphi>_\Gamma \geq \alpha \|\varphi\|^2_{\widetilde{H}^{-1/2}(\Gamma)} - k(\varphi)\,.$$

(iii) If ω is not an interior or exterior eigenfrequency, then V is an isomorphism, and every Galerkin method in $\widetilde{H}^{-1/2}(\Gamma)$ for the equation $V\psi = g$ is stable and convergent.

2.3.3. ($\mathcal{P}$) For the parabolic case of the heat equation, integration over t in the Green formula (2) gives

$$\begin{aligned} <\varphi, V\varphi>_\Sigma &= \int_0^T \int_{\mathbb{R}^n \setminus \Gamma} \{|\nabla_x u(t,x)|^2 + \partial_t u \overline{u}\}\, dx\, dt \\ &= \int\int |\nabla_x u(t,x)|^2\, dx\, dt + \frac{1}{2}\int_{\mathbb{R}^n} |u(T,x)|^2\, dx\,. \end{aligned}$$

From this, the positivity of the quadratic form associated with the operator V is evident. What is less evident is the nature of the energy norm for V, however. It turns out (Arnold and Noon, 1989; Costabel, 1990) that one has to consider anisotropic Sobolev spaces of the following form

$$\widetilde{H}_0^{r,s}(\Sigma) = L^2(0,T;\, \widetilde{H}^r(\Gamma)) \cap H_0^s(0,T;\, L^2(\Gamma))\,.$$

The index 0 indicates that zero initial conditions at $t = 0$ are incorporated. The optional $\widetilde{}$ means zero boundary values on the boundary of the (open) manifold Γ. One has the following theorem which is actually simpler than its elliptic counterpart, because the operators are always invertible, due to their Volterra nature.

Theorem 2.2. *Let Γ be a bounded Lipschitz surface, open or closed, $n \geq 2$.*
(i) $V : \widetilde{H}_0^{-\frac{1}{2},-\frac{1}{4}}(\Sigma) \to H_0^{\frac{1}{2},\frac{1}{4}}(\Sigma)$ is an isomorphism, and there is an $\alpha > 0$ such that

$$<\varphi, V\varphi>_\Sigma \geq \alpha \|\varphi\|^2_{-\frac{1}{2},-\frac{1}{4}}\,.$$

(ii) Every Galerkin method in $\widetilde{H}_0^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$ for the equation $V\psi = g$ converges. The Galerkin matrices have positive definite symmetric part. Typical error estimates are of the form

$$\|\varphi - \varphi_{h,k}\|_{-\frac{1}{2},-\frac{1}{4}} \leq C\,(h^{r+\frac{1}{2}} + k^{(r+\frac{1}{2})/2})\|\varphi\|_{r,\frac{r}{2}}\,,$$

if $\varphi_{h,k}$ is the Galerkin solution in a tensor product space of splines of mesh-size k in time and finite elements of mesh-size h in space.

2.3.4. ($\mathcal{H}$) For the wave equation, choosing $\varphi = \overline{\psi}$ in the Green formula (2) does not give a positive definite expression. Instead, one can choose $\varphi = \overline{\partial_t \psi}$. This corresponds to the usual procedure for getting energy estimates in the weak formulation of the wave equation itself where one uses $\partial_t u$ as a test function, and it gives

$$\begin{aligned} <\partial_t\varphi, V\varphi>_\Sigma &= \int_0^T \int_{\mathbb{R}^n \setminus \Gamma} \{\partial_t \nabla_x \overline{u} \cdot \nabla_x u + \partial_t \overline{u} \partial_t^2 u\}\, dx\, dt \\ &= \frac{1}{2}\int_{\mathbb{R}^n \setminus \Gamma} \{|\nabla_x u(T,x)|^2 + |\partial_t u(T,x)|^2\}\, dx\,. \end{aligned}$$

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Once again, as in the elliptic case, this shows the close relation of the operator V with the total energy of the system. In order to obtain a norm ($H^1(Q)$) on the right hand side, one can integrate a second time over t. But in any case, here the bilinear form $<\partial_t\varphi, V\varphi>_\Sigma$ will not be bounded in the same norm where its real part is positive. So there will be a loss of regularity, and any error estimate has to use two different norms. No "natural" energy space for the operator V presents itself.

2.4. Fourier-Laplace analysis and Galerkin methods

A closer view of what is going on can be obtained using space-time Fourier transformation. For this, one has to assume that Γ is flat, i. e. a subset of $\mathbb{R}^{n-1}$. Then all the operators are convolutions and as such are represented by multiplication operators in Fourier space. If Γ is not flat but smooth, then the results for the flat case describe the principal part of the operators. To construct a complete analysis, one has to consider lower order terms coming from coordinate transformations and localizations. Whereas this is a well-known technique in the elliptic and parabolic cases, namely part of the calculus of pseudodifferential operators, it has so far prevented the construction of a completely satisfactory theory for the hyperbolic case.

We denote the dual variables to (t, x) by (ω, ξ), and x' and ξ' are the variables related to $\Gamma \subset \mathbb{R}^{n-1}$. It is then easily seen that the form of the single layer potential is

$$\widehat{V\psi}(\xi') = \frac{1}{2}(|\xi'|^2 - \omega^2)^{-\frac{1}{2}}\hat{\psi}(\xi') \qquad (\mathcal{E})$$

$$\widehat{V\psi}(\omega, \xi') = \frac{1}{2}(|\xi'|^2 - i\omega)^{-\frac{1}{2}}\hat{\psi}(\omega, \xi') \qquad (\mathcal{P})$$

$$\widehat{V\psi}(\omega, \xi') = \frac{1}{2}(|\xi'|^2 - \omega^2)^{-\frac{1}{2}}\hat{\psi}(\omega, \xi') \qquad (\mathcal{H})$$

Note that ($\mathcal{E}$) and ($\mathcal{H}$) differ only in the role of ω: For ($\mathcal{E}$) it is a fixed parameter, for ($\mathcal{H}$) it is one of the variables, and this is crucial in the application of Parseval's formula for $<\varphi, V\varphi>$.

2.4.1. ($\mathcal{E}$) For the elliptic case, the preceding formula implies Theorem 2.1: If $\omega = 0$, then the function $\frac{1}{2}|\xi'|^{-1}$ is positive and for large $|\xi'|$ equivalent to $(1 + |\xi'|^2)^{-1/2}$, the Fourier weight defining the Sobolev space $H^{-1/2}(\Gamma)$. If $\omega \neq 0$, then the principal part (as $|\xi'| \to \infty$) is still $\frac{1}{2}|\xi'|^{-1}$, so only a compact perturbation is added. There is an additional observation by Ha-Duong (1990): If ω is real, then $\frac{1}{2}(|\xi'|^2 - \omega^2)^{-\frac{1}{2}}$ is either positive or imaginary, so its real part is positive except on the bounded set $|\xi'| \leq |\omega|$. This implies

Proposition 2.3. *Let $\omega^2 > 0$, Γ flat, $\operatorname{supp}\varphi$ compact. Then there is an $\alpha(\omega) > 0$ such that*

$$\operatorname{Re} <\varphi, V\varphi>_\Gamma \geq \alpha(\omega)\, \|\varphi\|^2_{\tilde{H}^{-1/2}}\,.$$

The work of transforming this estimate into error estimates for the BEM in the hyperbolic case is still incomplete. See Ha-Duong (2003) for a review of the state of the art on this question.

2.4.2. ($\mathcal{P}$) For the parabolic case, the symbol of the single layer potential,

$$\sigma_V(\omega, \xi') = \frac{1}{2}(|\xi'|^2 - i\omega)^{-\frac{1}{2}}$$

has again positive real part. In addition, it is sectorial:

$$|\arg \sigma_V(\omega, \xi')| \leq \frac{\pi}{4}\,.$$

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This has the consequence that its real part and absolute value are equivalent (an "elliptic" situation):

$$C_1 \left||\xi'|^2 - i\omega\right|^{-\frac{1}{2}} \leq \operatorname{Re} \sigma_V(\omega, \xi') \leq C_2 \left||\xi'|^2 - i\omega\right|^{-\frac{1}{2}} .$$

In addition, for large $|\xi'|^2 + |\omega|$, this is equivalent to $\left((1 + |\xi'|^2) + |\omega|\right)^{-1/2}$, the Fourier weight defining the space $H^{-\frac{1}{2},-\frac{1}{4}}(\Sigma)$. This explains Theorem 2.2. It also shows clearly the difference between the single layer heat potential operator on the boundary and the heat operator $\partial_t - \Delta$ itself: The symbol of the latter is $|\xi|^2 - i\omega$, and the real part $|\xi|^2$ and the absolute value $(|\xi|^4 + |\omega|^2)^{1/2}$ of this function are not equivalent uniformly in ξ and ω.

2.4.3. ($\mathcal{H}$) In the hyperbolic case, the symbol σ_V does not have positive real part. Instead, one has to multiply it by $i\overline{\omega}$ and to use a complex frequency $\omega = \omega_R + i\omega_I$ with $\omega_I > 0$ fixed. Then one gets

$$\operatorname{Re}\left(i\overline{\omega}(|\xi'|^2 - \omega^2)^{\frac{1}{2}}\right) \geq \frac{\omega_I}{2}(|\xi'|^2 + |\omega|^2)^{\frac{1}{2}}$$

and similar estimates given first by Bamberger and Ha Duong (1986). Note that with respect to $|\omega|$, one is losing an order of growth here. For fixed ω_I, the left hand side is bounded by $|\omega|^2$, whereas the right hand side is $\mathcal{O}(|\omega|)$. One introduces another class of anisotropic Sobolev spaces of the form

$$H^{s,r}(\mathbb{R} \times \Gamma) = \{u \mid u, \partial_t^r u \in H^s(\mathbb{R} \times \Gamma)\}$$

with the norm

$$\|u\|_{s,r,\omega_I} = \int\limits_{\operatorname{Im}\omega=\omega_I} \int_{\mathbb{R}^{n-1}} |\omega|^{2r}(|\xi'|^2 + |\omega|^2)^s |\hat{u}(\omega, \xi')|^2 \, d\xi' \, d\omega \, .$$

We give one example of a theorem obtained in this way.

Theorem 2.4. *Let Γ be bounded and smooth, $r, s \in \mathbb{R}$. Then*

(i) $V : \widetilde{H}_0^{s,r+1}(\Sigma) \to H_0^{s+1,r}(\Sigma)$ and $V^{-1} : H^{s+1,r+1}(\Sigma) \to \widetilde{H}_0^{s,r}(\Sigma)$ are continuous.

(ii) Let $\omega_I > 0$ and the bilinear form $a(\varphi, \psi)$ be defined by

$$a(\varphi, \psi) = \int_0^\infty e^{-2\omega_I t} \int_\Gamma (V\varphi)(t, x) \, \overline{\partial_t \psi}(t, x) \, d\sigma(x) \, dt \, .$$

Then there is an $\alpha > 0$ such that

$$\operatorname{Re} a(\varphi, \varphi) \geq \alpha \, \omega_I \, \|\varphi\|^2_{-\frac{1}{2},0,\omega_I} \, .$$

(iii) The Galerkin matrices for the scheme: Find $\varphi_N \in X_N$ such that

$$a(\varphi_N, \psi) = <g, \partial_t \psi>_\Sigma \quad \forall \psi \in X_N$$

have positive definite hermitian part, and there is an error estimate

$$\|\varphi - \varphi_N\|_{-\frac{1}{2},0,\omega_I} \leq C \, \omega_I^{-\frac{1}{2}} \inf_{\psi \in X_N} \|\varphi - \psi\|_{-\frac{1}{2},1,\omega_I} \, .$$

Thus one has unconditional stability and convergence for $\omega_I > 0$. In practical computations, one will use the bilinear form $a(\varphi, \psi)$ for $\omega_I = 0$ where the error estimate is no longer valid. Instabilities have been observed that are, however, probably unrelated to the omission of the exponential factor. They are also not caused by a too large CFL number (ratio between time step and spatial mesh width). In fact, too small and too large time steps have both been reported to lead to instabilities.

Corresponding results for elastodynamics and for electrodynamics can be found in the literature (besides the above-mentioned works, see the references given in Chudinovich (2001) and in Bachelot *et al.* (2001),).

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2.5. Collocation methods

In order to avoid the high-dimensional integrations necessary for the computation of the matrix elements in a Galerkin method such as the ones described in Theorems 2.2 and 2.4, one often uses collocation methods. Just like in the elliptic case, even for the classical first kind integral operators for the Laplace operator, the mathematical analysis lags seriously behind the practical experiences.

In more than two dimensions, only for very special geometries that are amenable to Fourier analysis, stability of collocation schemes can be shown. For time-dependent integral equations, even two space dimensions create problems that only recently have been overcome, and this only for special geometries, mainly flat boundaries or toroidal boundaries.

Collocation schemes for the single layer potential integral equation (D3) are easy to formulate. One usually takes basis functions of tensor product form, i. e.

$$\varphi_{ij}(t,x) = \chi_i(t)\psi_j(x)$$

where $\chi_i (i = 1, \ldots, M)$ is a basis of a space of finite elements (splines) of degree d_t on the interval $[0, T]$, and $\psi_j (j = 1, \ldots, N)$ is a basis of a space of finite elements of degree d_x on the boundary Γ. Then the trial functions are of the form

$$u_{kh}(t,x) = \sum_{i,j=1}^{M,N} \alpha_{ij}\varphi_{ij}(t,x)$$

Here the indices kh indicate the time step $k \sim T/M$ and the mesh width h of the discretization of the boundary Γ.

The linear system for the unknown coefficients is obtained from the equations

$$V u_{kh}(t_i, x_j) = g(t_i, x_j)$$

where $t_i \in [0, T] (i = 1, \ldots, M)$ are the time collocation points and $x_j \in \Gamma (j = 1, \ldots, N)$ are the space collocation points. The collocation points are usually chosen in the "natural" way, meaning midpoints for even degree splines in time, nodes for odd degree splines in time, barycenters for piecewise constants $d_x = 0$, nodes of the finite element mesh on Γ for $d_x = 1$, and more generally nodes of suitable quadrature rules for other values of d_x.

2.5.1. ($\mathcal{P}$) For the heat equation in a smooth domain in 2 space dimensions, it was shown in Costabel and Saranen (2000, 2003) that for $d_t = 0, 1$ one gets convergence in anisotropic Sobolev spaces of the "parabolic" class defined in subsection 2.3.3. There is a condition for optimality of the convergence which corresponds to a kind of anisotropic quasi-uniformity:

$$k \sim h^2$$

2.5.2. ($\mathcal{H}$) For the retarded potential integral equation, that is, the equation of the single layer potential for the wave equation in 3 space dimensions, Davies and Duncan (2003) prove rather complete stability and convergence results for the case of a flat boundary.

3. LAPLACE TRANSFORM METHODS

To pass from the time domain to the frequency domain, we define the (Fourier-) Laplace transform by

$$\widehat{u}(\omega) = \mathcal{L}u(\omega) = \int_0^\infty e^{i\omega t}\, u(t)\, dt \tag{3}$$

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If u is integrable with a polynomial weight or, more generally, a tempered distribution, and if, as we assume here throughout, $u(t) = 0$ for $t < 0$, then $\widehat{u}$ is holomorphic in the upper half-plane $\{\omega = \omega_R + i\omega_I \mid \omega_R \in \mathbb{R}, \omega_I > 0\}$. The inversion formula is

$$u(t) = \mathcal{L}^{-1}u(t) = \frac{1}{2\pi}\int_{-\infty+i\omega_I}^{\infty+i\omega_I} e^{-i\omega t}\,\widehat{u}(\omega)\,d\omega \tag{4}$$

Frequently, it is customary to define the Laplace integral by

$$\int_0^\infty e^{-st}\,u(t)\,dt$$

which is the same as (3) when s and ω are related by $s = -i\omega$. The upper half-plane $\omega_I > 0$ coincides with the right half-plane $\mathrm{Re}\, s > 0$.

The function $t \mapsto u(t)$ can take values in some Banach space (Arendt *et al.*, 2001), for example in a space of functions depending on x, in which case we write

$$\widehat{u}(\omega, x) = \mathcal{L}u(\omega, x) = \int_0^\infty e^{i\omega t}\,u(t, x)\,dt$$

By Laplace transformation, both the parabolic and the hyperbolic initial-boundary value problems are transformed into elliptic boundary value problems with an eigenvalue parameter λ depending on the frequency ω. Thus both the heat equation $(\partial_t - \Delta)u = 0$ and the wave equation $(c^{-2}\partial_t^2 - \Delta)u = 0$ are transformed into the Helmholtz equation $(\Delta - \lambda)\widehat{u}(\omega, x) = 0$, where

$$\lambda(\omega) = -i\omega \text{ for the heat equation, and}$$
$$\lambda(\omega) = -\frac{\omega^2}{c^2} \text{ for the wave equation}$$

The idea of the Laplace transform boundary integral equation method is to solve these elliptic boundary value problems for a finite number of frequencies with a standard boundary element method and then to insert the results into a numerical approximation of the Laplace inversion integral (4).

There exist various algorithms for numerical inverse Laplace transforms, see for example Davies and Martin (1979) or Abate and Whitt (1995). One will, in general, first replace the line of integration $\{\mathrm{Im}\,\omega = \omega_I\}$ by a suitable equivalent contour $\mathcal{C}$ and then choose some quadrature rule approximation of the integral. The end result will be of the form

$$u(t) = \frac{1}{2\pi}\int_{\mathcal{C}} e^{-i\omega t}\,\widehat{u}(\omega)\,d\omega \sim \sum_{\ell=1}^{L} w_\ell e^{-i\omega_\ell t}\,\widehat{u}(\omega_\ell) \tag{5}$$

with quadrature weights w_ℓ and a finite number of frequencies ω_ℓ.

One obvious candidate for such a quadrature formula is the trapezoidal rule on a large interval $[-R, R]$ where the line $\{\mathrm{Im}\,\omega = \omega_I\}$ is replaced by $[-R, R] + i\omega_I$. This can then be evaluated by Fast Fourier Transform which is clear when we write the Laplace inversion integral as inverse Fourier transform over the real line:

$$u(t) = \mathcal{L}^{-1}\widehat{u}(t) = e^{\omega_I t}\mathcal{F}^{-1}_{\omega_R \mapsto t}[\widehat{u}(\omega_r + i\omega_I)]$$

Let us describe the resulting procedure in more detail for the formulation with a single layer potential representation for the initial-Dirichlet problem, keeping in mind that any other type of boundary

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integral equation constructed in Section 2.2.2 would do as well and lead to a similar formalism. By Laplace transform we get the boundary value problem

$$(\Delta - \lambda(\omega))\widehat{u}(\omega, x) = 0 \text{ in } \Omega$$
$$\widehat{u}(\omega, x) = \widehat{g}(\omega, x) \text{ on } \Gamma$$

where the right hand side is the Laplace transform of the given boundary data g. For the unknown density ψ we get the first kind integral equation on Γ

$$V_{\lambda(\omega)}\widehat{\psi}(\omega) = \widehat{g}(\omega) \tag{6}$$

where $V_{\lambda(\omega)}$ is the weakly singular integral operator generated by convolution with the kernel (in three dimensions)

$$G_{\lambda(\omega)}(x) = \frac{e^{\sqrt{\lambda(\omega)}|x|}}{4\pi|x|}$$

Now let $V_{\lambda(\omega),h}$ be some finite dimensional boundary element approximation of $V_{\lambda(\omega)}$, so that

$$\widehat{\psi}_h(\omega) = V^{-1}_{\lambda(\omega),h}\widehat{g}(\omega)$$

is the corresponding approximate solution of equation (6). Inserting this into the numerical inversion formula (5) finally gives the following expression for the approximation of the unknown density $\psi(t, x)$ via the Laplace transform boundary element method

$$\psi_h(t, x) = \sum_{\ell=1}^{L} w_\ell e^{-i\omega_\ell t} \left(V^{-1}_{\lambda(\omega_\ell),h}\widehat{g}(\omega_\ell)\right)(x) \tag{7}$$

Note that on this level of abstraction, formula (7) *looks the same* for the parabolic case of the heat equation, the hyperbolic case of the wave equation, or even the dissipative wave equation. The only difference is the function $\lambda(\omega)$ which then determines, depending on the contour $\mathcal{C}$ and its discretization ω_ℓ, for which complex frequencies $\sqrt{-\lambda(\omega_\ell)}$ the single layer potential operator has to be numerically inverted.

For the practical computations, this difference can be essential: In a precise quadrature rule in (5) which is needed for high resolution in time, there will be some ω_ℓ with large absolute values. In the *hyperbolic* case (but not in the *parabolic* case!), this means large negative real parts for $\lambda(\omega_\ell)$, hence highly oscillating kernels, and some machinery for high-frequency boundary element methods has to be put in place (see, for example, Bruno (2003)).

Applications of the Laplace transform boundary integral equation methods in elastodynamics have a long history (Cruse and Rizzo, 1968; Cruse, 1968). For generalizations such as viscoelasticity, poroelasticity or piezoelectricity, these methods are more practical than the space-time boundary integral equation methods, because space-time fundamental solutions are not explicitly known or very complicated (Gaul and Schanz, 1999; Schanz, 1999; Schanz, 2001a; Wang *et al.*, 2003). Recently, Laplace domain methods related to the operational quadrature method (see subsection 4.4) have been used successfully in practice (Schanz and Antes, 1997b; Schanz and Antes, 1997a; Schanz, 2001b; Telles and Vera-Tudela, 2003).

A final remark on the Laplace transform boundary element method: Instead of, as described in this section, performing first the Laplace transform and then the reduction to the boundary, one can also first construct the space-time boundary integral equations as described in the previous section and then apply the Laplace transform. It is easy to see that the resulting frequency-domain boundary integral equations are exactly the same in both procedures.

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4. TIME-STEPPING METHODS

In the previous sections, the boundary reduction step was performed before any discretization had taken place. In particular, the description of the transient behavior of the solution by a finite number of degrees of freedom was introduced, via a Galerkin or collocation method for the space-time integral equation or via numerical Laplace inversion, only after the construction of the boundary integral equation.

It is possible to invert the order of these steps by first applying a time discretization scheme to the original initial-boundary value problem and then using a boundary integral equation method on the resulting problem that is discrete in time and continuous in space. One advantage of this idea is similar to the motivation of the Laplace transform method: The parabolic and hyperbolic problems are reduced to elliptic problems for which boundary element techniques are well known. Another attraction is the idea that once a procedure for one time-step is constructed, one can march arbitrarily far in time by simply repeating this same procedure.

In this section we will, for simplicity, only treat the parabolic case of the initial-Dirichlet problem for the heat equation. Quite analogous procedures are possible also for the hyperbolic case, and in particular the *operational quadrature method* has been analyzed for both the parabolic and the hyperbolic situation, see Lubich (1994). In the literature on applied boundary element methods, one can find many successful applications of similar time-stepping schemes to parabolic and hyperbolic problems of heat transfer, fluid dynamics, elastodynamics and various generalizations (Nardini and Brebbia, 1983; Partridge *et al.*, 1992; Gaul *et al.*, 2003).

4.1. Time discretization

We consider the initial-boundary value problem

$$\begin{aligned} &(\partial_t - \Delta)u(t,x) = 0 \quad \text{in } Q \\ &u = g \quad \text{on } \Sigma \\ &u(t,x) = 0 \quad \text{for } t \le 0 \end{aligned} \tag{8}$$

as an ordinary differential equation in time with operator coefficients. Consequently, we can employ any kind of one-step or multistep method known from the numerical analysis of ordinary differential equations. Only *implicit* schemes are of interest here, for two reasons: The first reason is the stability of the resulting scheme and secondly, explicit schemes would not really require a boundary integral equation method.

The solution $u(t,x)$ for $0 \le t \le T$ is approximated by a sequence $u^n(x)$, $n = 0, \ldots, N$, where

$$u^n \text{ is understood as an approximation of } u(t_n, \cdot),\ t_n = nk = nT/N$$

The simplest discretization of the derivative ∂_t with timestep k is the backward difference, which gives the *backward Euler* scheme for (8)

$$\begin{aligned} &\frac{u^n - u^{n-1}}{k} - \Delta u^n = 0 \quad \text{in } \Omega \quad (n = 1, \ldots, N) \\ &u^n(x) = g^n(x) = g(t_n, x) \quad \text{on } \Gamma \quad (n = 1, \ldots, N) \\ &u^0 = 0 \quad \text{for } t \le 0 \end{aligned} \tag{9}$$

The actual elliptic boundary value problem that one has to solve at each time step, $n = 1, \ldots, N$ is therefore

$$u^n - k\Delta u^n = u^{n-1} \text{ in } \Omega\,; \quad u^n = g^n \text{ on } \Gamma \tag{10}$$

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Higher order approximation in time can be achieved by multistep methods of the form

$$\sum_{j=0}^{r} \alpha_j u^{n-j} - k \sum_{j=0}^{r} \beta_j \Delta u^{n-j} = 0 \ \text{ in } \Omega \ ; \quad u^n = g^n \ \text{ on } \Gamma \tag{11}$$

The coefficients α_j and β_j define the characteristic function of the multistep scheme

$$\delta(\zeta) = \frac{\sum_{j=0}^{r} \alpha_j \zeta^j}{\sum_{j=0}^{r} \beta_j \zeta^j}$$

Consistency of the scheme (11) is characterized by $\delta(1) = 0$, $\delta'(1) = -1$, and the scheme is accurate of order p if $\delta(e^{-z})/z = 1 + \mathcal{O}(z^p)$ as $z \to 0$. One can assume that $\alpha_0 \beta_0 > 0$.

4.2. One step at a time

The problem to solve for one time step in both (10) and (11) is of the form

$$\eta^2 u - \Delta u = f \ \text{ in } \Omega \ ; \quad u = g \ \text{ on } \Gamma \tag{12}$$

Here $\eta^2 = 1/k$ for (10) and $\eta^2 = \alpha_0/(k\beta_0)$ for (11). The right hand side f is computed from the solution of the previous time step(s), and it has no reason to vanish except possibly for the very first time step. For the integral equation method, we therefore have to apply a representation formula that takes into account this inhomogeneous differential equation.

Let $u_p = Pf$ be a particular solution of the equation $\eta^2 u_p - \Delta u_p = f$ in Ω. Then $u_0 = u - u_p$ satisfies the homogeneous equation and can therefore be computed by a standard boundary integral equation method, for example by one of the methods from Section 2.2. For an exterior domain, we thus have the representation formula in Ω

$$\begin{aligned} u_0(x) &= \int_\Gamma \{\partial_{n(y)} G(x-y) u_0(y) - G(x-y) \partial_n u_0(y)\} \, d\sigma(y) \\ &= \mathcal{D}(\gamma_0 u_0)(x) - \mathcal{S}(\gamma_1 u_0)(x) \end{aligned}$$

Here G is the fundamental solution of the Helmholtz equation given in the three-dimensional case by

$$G(x) = \frac{e^{-\eta|x|}}{4\pi|x|}$$

Using our abbreviations for the single and double layer potentials and

$$\gamma_0 u = u\big|_\Gamma \ ; \quad \gamma_1 u = \partial_n u\big|_\Gamma$$

we have the representation for u

$$u = \mathcal{D}(\gamma_0 u) - \mathcal{S}(\gamma_1 u) + Pf - \mathcal{D}(\gamma_0 Pf) + \mathcal{S}(\gamma_1 Pf) \tag{13}$$

For the unknown $\varphi = \gamma_1 u$ in the direct method for the Dirichlet problem or for the unknown ψ in a single layer potential representation

$$u = \mathcal{S}\psi + Pf \tag{14}$$

or the unknown w in a double layer representation

$$u = \mathcal{D}w + Pf \tag{15}$$

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this leads to the choice of integral equations

$$\begin{array}{lll} (D1) & V\varphi & = (-\frac{1}{2}+K)g + (\frac{1}{2}-K)\gamma_0 Pf + V\gamma_1 Pf \\ (D2) & (\frac{1}{2}+K')\varphi & = -Wg + W\gamma_0 Pf + (-\frac{1}{2}+K')\gamma_1 Pf \\ (D3) & V\psi & = g - \gamma_0 Pf \\ (D4) & (\frac{1}{2}+K)w & = g - \gamma_0 Pf \end{array}$$

These are standard boundary integral equations that can be discretized and numerically solved in many ways. The one peculiarity is the appearance of the particular solution Pf in the representation formula (13) and in the integral equations $(D1)$–$(D4)$.

There are various possibilities for the construction of (an approximation of) Pf. Let us mention some of them that are being used in the boundary element literature and practice:

4.2.1. Newton potential In the standard representation formula for the inhomogeneous Helmholtz equation derived from Green's formula, Pf appears in the form

$$Pf(x) = \int_\Omega G(x-y)\, f(y)\, dy$$

This representation has the advantage that the last two terms in the representation formula (13) cancel, and therefore also the integral equations $(D1)$ and $(D2)$ simplify in that the integral operators acting on the traces of Pf are absent. For computing the Newton potential, the domain Ω has to be discretized, thus neutralizing one of the advantages of the boundary element method, namely the reduction of the dimension. Note, however, that this domain discretization is done only for purposes of numerical integration. No finite element grid has to be constructed. It is also to be noted that the domain discretization only enters into the computation of the right hand side; the size of the linear system to be solved is not affected.

4.2.2. Fourier series Another method to get an approximate particular solution Pf is to embed the domain Ω into a rectangular domain $\widehat{\Omega}$, then approximate an extension of f to $\widehat{\Omega}$ by trigonometric polynomials using Fast Fourier Transform, solve the Helmholtz equation in Fourier space, and go back by FFT again. Other fast Helmholtz solvers that exist for simple domains can be used in the same way.

4.2.3. Radial basis functions In the previous subsections, the right hand side f was approximated by a linear combination of special functions for which particular solutions of the Helmholtz equation are known: the Dirac distribution for the Newton potential method, and exponential functions for the FFT method. The particular solution Pf is then given by the corresponding linear combination of the individual particular solutions. Other special functions that can serve in the same way are radial basis functions, in the simplest case functions of the form $|x-x_j|$, where the x_j belong to some discretization of Ω by an unstructured grid. One advantage of the radial basis function technique is that there exist many practical and theoretical results about interpolation by such functions (Powell, 1992; Faul and Powell, 1999).

4.2.4. Higher fundamental solutions In the first time step, the solution $u = u^1$ is given, after solving the appropriate boundary integral equations, by the representation formula (13) with $f = 0$, i.e. by a combination of single and double layer potentials. This u^1 is then used as right hand side f in the next time step. A particular solution Pf can then be found, without any domain integral, by replacing the

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fundamental solution G of $(\eta^2 - \Delta)$ in the representation formula by a fundamental solution $G^{(1)}$ of $(\eta^2 - \Delta)^2$ satisfying

$$(\eta^2 - \Delta)G^{(1)}(x) = G(x)$$

Thus if

$$f(x) = \int_\Gamma \{\partial_{n(y)} G(x-y)w(y) - G(x-y)\varphi\}\, d\sigma(y)$$

then a particular solution Pf is given by

$$Pf(x) = \int_\Gamma \{\partial_{n(y)} G^{(1)}(x-y)w(y) - G^{(1)}(x-y)\varphi\}\, d\sigma(y)$$

In the next time step, the right hand side is then constructed from single and double layer potentials plus this Pf. Repeating the argument, one obtains a particular solution by using a fundamental solution $G^{(2)}$ of $(\eta^2 - \Delta)^3$. In the n-th time step, one then needs to use higher order fundamental solutions $G^{(j)}$, $(j < n)$ which satisfy the recurrence relations

$$(\eta^2 - \Delta)G^{(j+1)}(x) = G^{(j)}(x)$$

Such functions $G^{(j)}$ can be given explicitly in terms of Bessel functions. In this way, the whole time marching scheme can be performed purely on the boundary, without using domain integrals or any other algorithm requiring discretization of the domain Ω. Two other points of view that can lead, eventually, to an entirely equivalent algorithm for the time-discretized problem, are described in the following sections.

4.3. All time steps at once

Just as in the construction of the space-time integral equations the heat equation or wave equation was not considered as an evolution equations, i.e. an ordinary differential equation with operator coefficients, but as a translation invariant operator on $\mathbb{R}^{1+n}$ whose fundamental solution was used for integral representations, one can consider the time-discretized problem as a translation invariant problem on $\mathbb{Z} \times \mathbb{R}^n$ and construct a space-time fundamental solution for this semi-discretized problem. The role of the time derivative is then played by its one-step or multi-step discretization as in (10) or (11), and the role of the inverse of the time derivative and of other finite time convolutions appearing in the space-time integral operators is played by finite discrete convolutions.

In simple cases, such discrete convolution operators can be inverted explicitly. For a two-part recurrence relation such as the backward Euler method (9), the convolution operator can be represented by a triangular Toeplitz matrix with just one lower side diagonal. Let U denote the vector $u^1, \ldots, u^N$ and define G correspondingly. Then the backward Euler scheme (10) can be written as a system

$$AU = 0 \text{ in } \Omega\,; \quad U = G \text{ on } \Gamma \tag{16}$$

Here A is an elliptic system of second order, given by the matrix elements

$$a_{j,j} = 1 - k\Delta\,; \quad a_{j,j-1} = -1\,; \quad \text{all other } a_{i,j} = 0$$

Once a fundamental solution of this system is found, the system of equations (16) can be solved numerically by standard elliptic boundary element methods. Due to the simple form of A, such a fundamental solution can be written using the higher fundamental solutions $G^{(j)}$ of the Helmholtz equation defined in section 4.2.4. It is a lower triangular Toeplitz matrix $\mathfrak{G}$ with entries $(g_{i,j})$, where

$$g_{j,j}(x) = G(x)\,; \quad g_{i,j}(x) = G^{(i-j)} \text{ for } j < i\,; \quad g_{i,j}(x) = 0 \text{ for } j < i$$

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All boundary integral operators constructed from this fundamental solution will have the same lower triangular Toeplitz (finite convolution) structure, and their solutions can be found by inverting the single operator that generates the diagonal and by subsequent back substitution.

For a detailed description of the approximation of the two-dimensional initial-Dirichlet problem for the heat equation using such a method, including formulas for the kernels in $\mathfrak{G}$ and a complete error analysis of the resulting second kind integral equation as well as numerical results, see Chapko and Kress (1997).

4.4. The operational quadrature method

In the previous section, the simple structure of the backward Euler scheme was essential. The resulting numerical approximation is of only first order in time. If one wants to use schemes that are of higher order in time, one can employ multistep methods as described above. The resulting schemes still have the lower triangular Toeplitz structure of finite discrete convolutions in time. From the algebraic structure of these convolutions it is clear that also fundamental solutions, resulting boundary integral operators, and their solution operators all have this finite convolution structure.

Explicit constructions of kernels, however, will not be possible, in general. Just as for the original continuous-time problem the appropriate functional transform, the Laplace transform, allowed the reduction of the parabolic to elliptic problems, here for the discrete-time problem one can use the appropriate functional transform, namely the z-transform. In order to conserve the approximation order of the multistep method, one has to use a certain translation between continuous convolutions and discrete convolutions or equivalently, between Laplace transforms and z-transforms.

For the generators of the convolution algebras, namely the derivative ∂_t in the continuous case and its timestep k discretization ∂_t^k, this translation is given by the definition (11) of the multistep method, characterized by the rational function $\delta(z)$. For the whole convolution algebras, this translation leads to the discretization method described by Lubich's *operational quadrature* method, see Lubich and Schneider (1992); Lubich (1994). The general translation rule is the following (we use our notation for the (Fourier-)Laplace transform introduced above, not Lubich's notation):

Denote a finite convolution operator with operator-valued coefficients by

$$\widehat{K}(i\partial_t)u(t) = \mathcal{L}^{-1}_{\omega\mapsto t}(\widehat{K}(\omega)\widehat{u}(\omega))$$

If $\widehat{K}(\omega)$ decays sufficiently rapidly in the upper half plane, this operator is given by an integrable kernel K whose Laplace transform is $\widehat{K}(\omega)$:

$$\widehat{K}(i\partial_t)u(t) = \int_0^t K(s)\, u(t-s)\, ds$$

The corresponding discrete convolution operator is given by

$$(\widehat{K}(i\partial_t^k)u)_n = \sum_{j=0}^{n} K_j\, u_{n-j}$$

where the coefficients K_j are defined by their z-transform

$$\sum_{j=0}^{\infty} K_j\, z^j = \widehat{K}(i\frac{\delta(z)}{k})$$

Here k is the time step, and $\delta(z)$ is the characteristic function of the multistep method.

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The inverse of the z-transform is given by the Cauchy integral over some circle $|z| = \rho$

$$K_j = \frac{1}{2\pi i} \int_{|z|=\rho} \widehat{K}(i\frac{\delta(z)}{k})\, z^{-j-1}\, dz$$

It is not hard to see that this translation rule reduces, for the case of the derivative $\partial_t = \widehat{K}(i\partial_t)$ with $\widehat{K}(\omega) = -i\omega$, to the convolution defined by the characteristic function $\delta(z)$:

$$\partial_t^k\, u_n = \sum_{j=0}^{n} \delta_j\, u_{n-j} \quad \text{with } \delta(z) = \sum_{j=0}^{\infty} \delta_j\, z^j$$

In addition, this translation rule is an algebra homomorphism, i.e. it respects compositions of (operator-valued) convolution operators. This is easy to see, because

$$\widehat{K}_1(i\partial_t)\widehat{K}_2(i\partial_t) = (\widehat{K}_1\widehat{K}_2)(i\partial_t) \quad \text{ and also } \widehat{K}_1(i\partial_t^k)\widehat{K}_2(i\partial_t^k) = (\widehat{K}_1\widehat{K}_2)(i\partial_t^k)$$

By the relation $z = e^{i\omega k}$, one can see the analogy between the Cauchy integral over $|z| = \text{const}$ with measure $z^{-j-1}\, dz$ and the Laplace inversion integral for the time $t = t_j = jk$ over $\operatorname{Im}\omega = \text{const}$ with measure $e^{-it_j\omega}\, d\omega$.

This operational quadrature method can be applied at several different stages of an integral equation method for the time-discretized initial value problem:

It can be used to find a fundamental solution for the whole system in the form of a Cauchy integral over the frequency domain fundamental solutions G_ω. We get for the coefficients g_j of the semi-discrete space-time fundamental solution $\mathfrak{G}(i\partial_t^k)$ the formula

$$g_j(x) = \frac{1}{2\pi i} \int_{|z|=\rho} G_{\omega(z)}(x)\, z^{-j-1}\, dz \text{ with } \omega(z) = i\frac{\delta(z)}{k}$$

This integral over holomorphic functions can be evaluated numerically with high speed and high accuracy using the trapezoidal rule and FFT. In simple cases, it can be evaluated analytically, for example in the case of the backward Euler method, where we have the simple characteristic function

$$\delta(z) = 1 - z$$

The Cauchy integral then gives the higher order fundamental solutions $G^{(j)}$ of the previous section.

This fundamental solution $\mathfrak{G}(i\partial_t^k)$ can then be used in a standard boundary element method, keeping in mind that the time-discretized solution will be obtained by finite convolution.

The operational quadrature scheme can also (and equivalently) be introduced at a later stage in the integral equation method, after the frequency domain integral equations have been solved. Let us describe this at the example of the single layer representation method for the initial-Dirichlet problem of the heat equation.

The space-time single layer heat potential operator on Σ can be written as $V = \widehat{V}(i\partial_t)$, where $\widehat{V}(\omega)$ is the frequency-domain single layer potential operator on Γ whose kernel is the fundamental solution of the Helmholtz operator $(-i\omega - \Delta)$. Inverting V amounts to evaluating the Cauchy integral of the inverse z-transform where the frequency-domain single layer integral equations have been solved for those frequencies needed for the Cauchy integral. For the approximation ψ_n of the solution $\psi(t_n)$ at the time $t_n = nk$ with time step k and a space discretization $V_h(\omega)$ of $V(\omega)$ one obtains then

$$\psi_n = \frac{1}{2\pi} \int_{|z|=\rho} V_h(i\frac{\delta(z)}{k})^{-1} \left(\sum_{j=0}^{n} g_{n-j}\, z^{-j-1} \right) dz \tag{17}$$

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This can be compared to the Laplace inversion integral (5) where the contour $\mathcal{C}$ is the image of the circle $|z| = \rho$ under the mapping $z \mapsto \omega = i\frac{\delta(z)}{k}$. When the Cauchy integral in (17) is evaluated numerically by a quadrature formula, we obtain an end result that has a form very similar to what we got from the Laplace transform boundary element method in formula (7).

In the papers Lubich and Schneider (1992); Lubich (1994), the operational quadrature method has been analyzed for a large class of parabolic and hyperbolic initial-boundary value problems and multistep methods satisfying various stability conditions. Recent computational results show its efficiency in practice (Schanz and Antes, 1997b; Schanz and Antes, 1997a).

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