SOME APPLICATIONS OF INTEGRAL EQUATIONS TO THE SOLUTION OF TRANSIENT PARTIAL DIFFERENTIAL EQUATIONS

by

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ABSTRACT

This thesis studies boundary integral methods for solving time-dependent partial differential equations from continuum mechanics. The two models we analyze will be transient Stokes flow and scalar acoustic scattering by penetrable obstacles. We will see the two main flavors of analysis of Time Domain Boundary Integral Equations in these two problems: for analysis of the Stokes system we take a Laplace domain approach that dates to [7]. The analysis of the acoustic scattering and transmission problem will be carried out with the newer semigroup theory based analysis from [73] and [36].

We begin with a detailed exposition of a central tool, Convolution Quadrature, that we will use throughout the rest of the thesis for temporal discretization. We provide motivation for the method from various points of view and derive both multistep and Runge-Kutta Convolution Quadrature with an eye towards implementation of the method. From this foundation, we move on to the analysis of transient Stokes flow by way of the Laplace transform. This leads us to a detailed study the Brinkman equations. Analysis of the Brinkman Single Layer potential and operator is then used to derive stability and convergence results back in the time domain for the Stokes problem. We provide numerical experiments and simulations using various spatial discretization schemes. Finally, we study the scattering of acoustic waves by inhomogeneous penetrable obstacles. Chapter 4 presents a detailed stability and convergence analysis of a three-field boundary and finite element coupling scheme. By showing the underlying problem generates a C_0-group of isometries, we are able to prove stability and convergence of the scheme directly in the time domain. In a similar vein, Chapter 5 explores computationally two alternative coupling schemes.

Chapter 1

INTRODUCTION

In this work we present solutions of various time-dependent partial differential equations (PDEs) by way of time domain boundary integral equations (TDBIEs). Layer potentials give an explicit solution to PDEs through convolution with the fundamental solution of the problem at hand. Imposition of boundary conditions on layer potential representations leads to boundary integral equations. When considering discretization, integral equation methods deal better with unbounded domains, and are a natural choice for scattering problems. Boundary integral equations, as the name suggests, also reduce the problem of finding a solution in a volume to finding an unknown defined on the boundary of the obstacle of interest. The solution can then be reconstructed at points not on the boundary in a post-processing step. This reduction in dimension can be advantageous in the discretization of some problems, particularly in two spatial dimensions, when the solution to a boundary integral equation reduces to a one dimensional problem.

Integral equations are not immune from certain challenges. Integral equation solutions are suited to problems where the fundamental solution is known. This puts significant restrictions on the types of problems that can be handled: we are immediately relegated to linear, homogeneous, and constant coefficient problems. Any model that does not satisfy these constraints will generate volume integrals that need to be discretized, and might be less efficient than simply using another method from the start, although volume integral equations are a popular method of choice for some applications. We study a method to overcome some of these limitations by coupling boundary and finite elements in Chapters 5 and 6. From an implementation point of view, boundary elements are much more difficult to program than finite elements,

since they make use of singular integrals, which need special care. Upon discretization, integral solutions to PDEs generates dense matrices, which makes their storage and solution much more of a computational burden. There is much research aimed at ameliorating these challenges, including fast solvers based on the Fast Multipole Method [31] for matrix-vector multiplication and fast direct solvers [63]. To save on storage costs, there are tools like H-matrices [32] and H^2-matrices [33] for compressing the structured matrices of the boundary element method.

While this thesis makes exclusive use of Galerkin methods for spatial discretization, there is an alternative approach. A Nyström spatial discretization collocates the solution on chosen points, and applies a quadrature rule to the integral. While much simpler to implement, every new kernel requires potentially developing a new quadrature method. We will see the deltaBEM [26] tools in Chapter 3 that are Nyström flavored, but can still be understood as a non-conforming Petrov-Galerkin method.

The history of integral equations for the solution of PDEs goes back to potential theory for the Laplacian, which has been known for over a century. While well studied for steady state and time-harmonic problems, integral methods for transient problems took root in the mathematics community only in the 1980s, with the foundational papers of Bamberger and Ha-Duong [7, 8]. These early works focused on a Galerkin space-time approach for discretization of the time domain integral equations for acoustics. Around the same time, Christian Lubich developed the Convolution Quadrature method [58] for the stable and accurate discretization of Volterra-type convolution integrals. It took some time for CQ to become a key tool in the temporal discretization of TDBIEs, beginning with the heat equation [62] and other linear and semi-linear parabolic problems [61]. CQ-BEM discretizations of transient problems have also come to include problems from elasticity [77, 65] and electromagnetism [20, 21, 53]. The advantage of a CQ temporal discretization is that it makes use of the fundamental solution to the resolvent (Laplace-transformed) equations and time domain data to produce time domain output. This is advantageous compared with Galerkin-in-time discretizations, since the fundamental solution to the resolvent problem is generally

known and simpler, even when the fundamental solution to the transient problem is distributional. Until recently, analysis of CQ discretizations has made extensive use of the Laplace transform as well. This changed with the direct-in-time analysis of [73] that circumvents the Laplace transform method and provides sharper bounds in the case of L^∞ bounds for data with L^1 regularity in time. On the other hand, Laplace transform methods provide estimates based on weighted Sobolev norms in time with data in similar spaces. There are still open questions in the direct-in-time analysis of CQ discretizations. There is preliminary work on direct-in-time analysis for semi-linear and nonlinear problems [10], and the analysis is entirely missing for Runge-Kutta based CQ as well as high order backward difference formulae.

There has been much research on the CQ-BEM discretization of parabolic PDEs, but almost exclusively for the heat equation, including that of [4, 23] and [43]. There has also been interest in the use of fast methods by Tausch in [79, 80, 66]. The only references integral methods for transient Stokes flow we are aware of at present are [39] and [40]. In our work on transient Stokes flow, we will encounter the Laplace domain flavor of analysis mentioned earlier.

We then turn our attention to the scattering of acoustic waves by penetrable obstacles. This problem has applicability in the inverse problem, i.e., recovering properties of the (unknown) scatterer from the scattered wave. This is contrasted with the forward problem, where the obstacle and physical parameters are known, and we seek to compute the scattered wave. Developing fast, stable, and accurate methods for computing the scattering of acoustic waves by penetrable media can be used in geo-prospecting for oil, defect detection and non-destructive testing, sonar, and parameter estimation. Although the tools presented in this thesis are not applicable to this case, an application of boundary elements or coupled BEM-FEM would be interesting as well in the design and simulation of metamaterials, i.e. materials with a negative index of refraction.

Chapter 4 presents a complete direct-in-time analysis of a three-field symmetric BEM-FEM coupling scheme. We include a novel first-order formulation from [36] that

eliminates a number of technical difficulties that arise in the analysis of [73]. We derive stability and convergence results and provide a number of simulations to demonstrate the method. We also discuss a "reduction-to-the-boundary" algorithm that cuts the computation time significantly by allowing parallel time stepping. Chapter 5 presents a computational study of two different coupling schemes that eliminate one of the unknowns of the system. The first reduced coupling scheme, due to Costabel [22] and Han [35], can be shown to generate a C_0-group like its three-field cousin. The second coupling scheme, in the style of Johnson and Nédélec [44, 72], eliminates one of the constraints on the boundary integral representation, and as a result, we loose symmetry and cannot show that this method generates a C_0-group. We perform a number of experiments to test the stability of the method, since there is not a theoretical basis for its stability.

Chapter 2

AN ALGORITHMIC INTRODUCTION TO CONVOLUTION QUADRATURE

In this chapter we will explore in detail the algorithmic aspects of multistep and multistage Convolution Quadrature, following closely the introduction to CQ given in *Convolution Quadrature for Wave Simulations* (with F.–J. Sayas) [37]. Where appropriate, we have spent more time in developing the algorithms for CQ approximations to convolution equations and forsaken specific theoretical details. First we discuss the mathematical prerequisites for the types of functions and convolutions we will be handling. We then segue into CQ based on a linear multistep method. This includes derivation of the methods through various avenues, exposition of the algorithms, and a discussion of the convergence theory for linear multistep CQ. In the linear multistep case, we have two possible avenues for analysis of semi- and fully-discrete problems. The Laplace domain analysis dates to the original work of Lubich in [58], and is a standard method in the literature. More recently, there have been developments that circumvent the Laplace domain analysis through the application of finite-difference style analysis coupled with stability results from semigroup theory [11, 68, 38]. In particular, a direct-in-time analysis for BDF2-based CQ for scalar acoustics has run into technical challenges not experienced with trapezoidal rule and Backward Euler CQ, though current work aims to circumvent this [69]. There is also not yet a fully developed theory for direct-in-time analysis of Runge-Kutta CQ discretizations, though there is progress in the direction in [13].

Note that this chapter is purely expository and contains no novel material, although some approaches to the multistep and multistage CQ presented here are original.

2.1 Background

We now introduce the heart of the mathematics leading up to Convolution Quadrature: convolution of causal functions and distributions. Causal convolution operators will often be recognized through their Laplace transforms (which will be called their transfer functions). As a first step towards a precise determination of the kind of functions we will be dealing with, let us define the term causal. A function $f : \mathbb{R} \to X$ (where X is any vector space) is said to be an X-valued **causal** function when $f(t) = 0$ for all $t < 0$.

We will refer to the independent variable t as time. We make use of the notion of causality, rather than simply requiring functions to be defined only on $[0, \infty)$, because key results will require functions that vanish for negative times. We will consider functions with a nonzero value at $t = 0$ to be discontinuous at that point.

Causal Functions and Convolutions

The **convolution of two causal functions** $f : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$ is defined as

$$(f * g)(t) := \int_0^t f(t - \tau)g(\tau)d\tau. \tag{2.1}$$

This definition makes sense, for instance, if both functions are integrable. Note that this definition coincides with the more traditional form of the convolution of functions

$$(f * g)(t) = \int_{-\infty}^{\infty} f(t - \tau)g(\tau)d\tau,$$

when f and g are causal. The first extension we will need to consider is when $f : \mathbb{R} \to \mathbb{R}^{n\times m}$ and $g : \mathbb{R} \to \mathbb{R}^m$. In this case, (2.1) defines a causal function $f * g : \mathbb{R} \to \mathbb{R}^n$. In this more general definition (where the convolution integrals are easily defined component by component), it is clear that we cannot even discuss commutativity of the convolution operator (2.1). We can generalize further to two Hilbert spaces X and Y and the space $\mathcal{B}(X, Y) := \{A : X \to Y \ : \ A \text{ linear and bounded}\}$. We can then start with a causal continuous function $f : \mathbb{R} \to \mathcal{B}(X, Y)$ and a causal function $g : \mathbb{R} \to X$ and obtain through convolution (2.1) a causal function $f * g : \mathbb{R} \to Y$.

Because all functions involved have been assumed to be continuous, the integration in (2.1) can be understood in the sense of a Riemann integral for each value of t. A **causal convolution equation** is an equation of the form

$$(f * g)(t) = h(t) \qquad \forall t, \tag{2.2}$$

where $h : \mathbb{R} \to Y$ is causal, $f : \mathbb{R} \to \mathcal{B}(X, Y)$ is causal, and we look for a causal X-valued function g.

The simplest possible example of convolution is the causal antiderivative

$$\int_0^t g(\tau) d\tau,$$

corresponding to the convolution with the Heaviside function:

$$H(t) := \begin{cases} 1, & t \geq 0, \\ 0, & t < 0. \end{cases}$$

A slightly more general operator is given by the expression

$$\int_0^t e^{\lambda(t-\tau)} g(\tau) d\tau. \tag{2.3}$$

Note that if we define

$$y(t) = \int_0^t e^{\lambda(t-\tau)} g(\tau) d\tau, \tag{2.4}$$

then y is the only causal solution to the equation $\dot{y} - \lambda\, y = g$, or, in the more traditional language of ordinary differential equations, y satisfies

$$\dot{y} - \lambda\, y = g, \qquad \text{in } [0, \infty), \qquad y(0) = 0, \tag{2.5}$$

and has been extended by zero to the negative real axis. The formula (2.4) is the variation of parameters formula (or Duhamel's principle) for the initial value problem (2.5). Similarly

$$y(t) = \lambda^{-1} \int_0^t \sin(\lambda(t - \tau)) g(\tau) d\tau$$

is the operator that yields the unique causal solution to $\ddot{y} + \lambda^2 y = g$.

One example of causal convolution equation is the Abel integral equation

$$\int_0^t \frac{g(\tau)}{\sqrt{t-\tau}} d\tau = h(t) \qquad t \geq 0. \tag{2.6}$$

This singular integral equation can be solved, for example, as follows [49]:

$$\begin{aligned}\int_0^r \frac{h(t)}{\sqrt{r-t}} dt &= \int_0^r \frac{1}{\sqrt{r-t}} \int_0^t \frac{g(\tau)}{\sqrt{t-\tau}} d\tau dt \\ &= \int_0^t g(\tau) \int_\tau^r \frac{1}{\sqrt{(r-t)(t-\tau)}} dt d\tau = \pi \int_0^t g(\tau) d\tau,\end{aligned}$$

and therefore the solution to (2.6) is

$$g(t) = \frac{1}{\pi} \frac{d}{dt} \int_0^t \frac{h(\tau)}{\sqrt{t-\tau}} d\tau, \quad t \geq 0.$$

2.2 Transfer Functions and Convolution Operators

Suppose that f is a $\mathcal{B}(X,Y)$-valued causal Laplace transformable distribution and that g is an X-valued causal Laplace-transformable distribution. The **convolution** $f * g$ is defined as the Y-valued causal distribution whose Laplace transform satisfies

$$\mathcal{L}\{f * g\}(s) = \mathrm{F}(s)\mathrm{G}(s).$$

We can be more precise by using the notation and background of Appendix A. If $\mathrm{F} \in \mathcal{A}(\mu_1, \mathcal{B}(X,Y))$ and $\mathrm{G} \in \mathcal{A}(\mu_2, \mathcal{B}(X,Y))$, then $\mathrm{FG} \in \mathcal{A}(\mu_1+\mu_2, Y)$ and $\mathcal{L}^{-1}\{\mathrm{FG}\}$ exists. This means that if $f \in \mathrm{TD}(\mathcal{B}(X,Y))$ and $g \in \mathrm{TD}(\mathcal{B}(X))$, then $f * g \in \mathrm{TD}(Y)$ is well defined. We can similarly define a convolution of the form $f * g$ where $f \in \mathrm{TD}(\mathcal{B}(Y,Z))$ and $g \in \mathrm{TD}(\mathcal{B}(X,Y))$.

Having presented the appropriate tools to understand convolutions and convolution operators in a distributional setting, we now present a series of examples of increasing complexity.

If f is a differentiable function, then differentiation, given by

$$\dot{\delta}_0 * f = \dot{f} \quad \longleftrightarrow \quad s\mathrm{F}(s) = \mathcal{L}\{\dot{f}\}$$

is a convolution operator. If f takes values on a Banach space $\mathbb{X}$, then this still holds, but we must consider

$$\left(I_{\mathbb{X}} \otimes \dot{\delta}_0\right) * f = \dot{f}.$$

Backwards shifts (delays) are also causal convolution operators for $t_0 > 0$:

$$\delta_{t_0} * f = f(t - t_0) \quad \longleftrightarrow \quad e^{-st_0}\mathrm{F}(s).$$

We can combine derivatives and delays to form a convolution equation that seeks a causal function y such that given $t_0 > 0$

$$\dot{y} = g - g(\cdot - t_0).$$

By taking the Laplace transform, we see that this is equivalent to

$$\mathrm{Y}(s) = \frac{1 - e^{-st_0}}{s}\mathrm{G}(s).$$

If we assume $g \in \mathrm{TD}(\mathbb{R})$, then $\mathrm{G} \in \mathcal{A}(\mu, \mathbb{R})$ for some μ. It is clear that $\left|\frac{1-e^{-st_0}}{s}\right| \leq 2|s|^{-1}$. Therefore the product $\frac{1-e^{-st_0}}{s}\mathrm{G}(s) \in \mathcal{A}(\mu - 1, \mathbb{R})$, and so Y is the Laplace transform of a causal, polynomially bounded function y, which is the solution to the differential-delay equation.

Now we move to a more interesting example of a convolution operator. Suppose $\Omega \subset \mathbb{R}^d$ is an open and bounded set and $g \in L^2(\Omega)$. Consider the problem of looking for

$$u \in H_0^1(\Omega) \quad \text{s.t.} \quad (\nabla u, \nabla v)_\Omega + s^2(u, v)_\Omega = (g, v)_\Omega \quad \forall v \in H_0^1(\Omega).$$

The Lax-Milgram Lemma shows that there is a unique solution to this problem that depends continuously on g. However, we need a more precise bound in terms of s than what the Lax-Milgram Lemma gives us. To this end, we denote

$$a(u, v)_{s,\Omega} := (\nabla u, \nabla v)_\Omega + s^2(u, v)_\Omega \quad \text{and} \quad |\!|\!| u |\!|\!|_{|s|,\Omega}^2 := \|\nabla u\|_\Omega^2 + |s|^2\|u\|_\Omega^2.$$

We also have that if $\sigma := \operatorname{Re} s$ and $\underline{\sigma} := \min\{1, \sigma\}$, then

$$\underline{\sigma}\|u\|_{1,\Omega} \leq |\!|\!| u |\!|\!|_{|s|,\Omega} \leq \frac{|s|}{\underline{\sigma}}\|u\|_{1,\Omega}, \quad \forall u \in H^1(\Omega).$$

With this in hand we can show that

$$\|u\|_{1,\Omega} \leq C_\Omega \frac{|s|}{\underline{\sigma}}\|g\|_\Omega,$$

and therefore the solution operator $g \longmapsto u$ is a causal convolution operator. In particular, this variational problem corresponds to a distributional version of the wave equation

$$\ddot{u} = \Delta u + g$$

with homogeneous initial and boundary conditions.

Let us finally tackle Abel's equation. The kernel in Abel's equation is $f(t) = \frac{1}{\sqrt{t}}$, whose Laplace transform is $\mathcal{L}\{f(t)\}(s) = \frac{\sqrt{\pi}}{\sqrt{s}}$ for $s \in \mathbb{C}_+$. It is then clear that $s^{-1/2} \in \mathcal{A}(-1/2, \mathbb{C})$, and therefore if $g(t)$ and $h(t)$ have distributional Laplace transforms $\mathrm{G}(s)$ and $\mathrm{H}(s)$. The Laplace transform of Abel's equation is

$$\sqrt{\frac{\pi}{s}}\mathrm{G}(s) = \mathrm{H}(s),$$

which shows that Abel's equation and its solution operator are bona fide distributional convolution operators.

2.3 Multistep Convolution Quadrature.

Convolution Quadrature dates back to the work of Christian Lubich [58, 59] as a stable method to discretize causal convolution equations. A CQ discretization of a causal convolution or convolution equation possesses a number of desirable traits. The approximation can be made to high order for smooth enough data by changing the background ODE solver, which can be done quite easily. It also computes the convolution with time domain readings of the data and the Laplace transform of the convolution kernel. This is advantageous in cases where the convolution kernel in the time domain may be unknown or distributional. In the Laplace domain, however, convolution kernels are generally simpler than their Laplace domain counterparts, and are analytic in the complex Laplace parameter.

We now begin in earnest in the development of Convolution Quadrature. Our goal is the numerical approximation of forward convolutions

$$y(t) = \int_0^t f(t-\tau)g(\tau)d\tau, \quad t \geq 0,$$

and convolution equations

$$\int_0^t f(t-\tau)g(\tau)d\tau = h(t), \quad t \geq 0.$$

We will approximate the convolutions on a uniform grid of time step size $\kappa > 0$

$$t_n := n\kappa, \quad n \geq 0.$$

Data will be read in the time domain, leading to discrete forward convolutions

$$y(t_n) \approx y_n := \sum_{m=0}^{n} \omega_m^{\mathrm{F}}(\kappa) g(t_{n-m})$$

and discrete convolution equations

$$\sum_{m=0}^{n} \omega_m^{\mathrm{F}}(\kappa) g_{n-m} = h(t_{n-m}).$$

A very simple model problem

Let us now take some time to develop Backward Euler (BE) based CQ for a few simple problems to understand how CQ approximates convolutions. Suppose $g : \mathbb{R} \to \mathbb{R}$ is a causal function and $c > 0$. We seek a causal function y that satisfies the ODE

$$\dot{y} - cy = g. \tag{2.7}$$

Implicit in the causality of y is the use of a homogeneous initial condition. A non-homogeneous initial condition $y(0) = y_0$ can be handled by placing it on the right hand side:

$$\dot{y} - cy = g + y_0\delta_0.$$

This, however, requires modification of some of the CQ weights to retain the full order of convergence (at least for parabolic problems) [58, Corollary 4.2]. We will only consider the homogenous case. Applying a BE approximation to the time derivative in (2.7), we arrive at the approximation

$$\frac{1}{\kappa}(y_n - y_{n-1}) - cy_n = g(t_n). \tag{2.8}$$

We demand that $\{y_n\}$ be a causal sequence, so $y_n = 0$ for $n < 0$. Since BE looks one step into the past, we will have that $y_{-1} = 0$. We can show that $g(0) = g(t_0) = 0$ and therefore $y_0 = 0$. We can rearrange (2.8) into the time-stepping form

$$y_n = \frac{1}{1 - \kappa c} y_{n-1} + \frac{\kappa}{1 - \kappa c} g(t_n)$$

and work backwards until $n = 0$ to obtain

$$y_n = \kappa \sum_{m=0}^{n} \frac{1}{(1 - \kappa c)^{m+1}} g(t_{n-m}). \tag{2.9}$$

The exact solution to our ODE (2.7) is

$$y(t) = \int_0^t e^{c\tau} g(t - \tau) d\tau,$$

which, when we look at the point t_n, has the form

$$y(t_n) = \sum_{m=0}^{n} \int_{t_{m-1}}^{t_m} e^{c\tau} g(t_n - \tau) d\tau.$$

Therefore our BE ODE solver is making the approximation

$$\int_{t_{m-1}}^{t_m} e^{c\tau} g(t_n - \tau) d\tau \approx \frac{\kappa}{(1 - \kappa c)^{m+1}} g(t_n - t_m).$$

To better understand where this approximation is coming from, we need to introduce another tool, the ζ-transform. For a given causal sequence $\{y_n\}$ we can define its **ζ-transform** as the formal series

$$\mathrm{Y}(\zeta) := \sum_{n=0}^{\infty} y_n \zeta^n.$$

We do not concern ourselves with the convergence of the series and consider it as a formal transformation of causal sequences. The ζ-transform works well to solve recurrences such as those that arise from discretizing ODEs with a linear multistep method. We can displace the sequence to the right

$$(y_0, y_1, \dots) \longmapsto (0, y_0, y_1, \dots)$$

by multiplying its associated ζ-transform by ζ

$$\mathrm{Y}(\zeta) \longmapsto \zeta \mathrm{Y}(\zeta) = \sum_{n=1}^{\infty} y_{n-1} \zeta^n.$$

The second operation on ζ-transforms is convolution of two sequences $\{a_n\}$ and $\{b_n\}$, which in the discrete time domain corresponds to their Cauchy product,

$$\sum_{m=0}^{n} a_m b_{n-m},$$

or in ζ domain, is just the product of the ζ-transforms,

$$\mathrm{A}(\zeta)\mathrm{B}(\zeta) = \sum_{n=0}^{\infty} \left(\sum_{m=0}^{n} a_n b_{n-m} \right) \zeta^n.$$

If we encode our recurrence equation (2.8) using ζ-transforms, we get the equation

$$\left(\frac{1-\zeta}{\kappa} - c \right) \mathrm{Y}(\zeta) = \mathrm{G}(\zeta),$$

which yields

$$\mathrm{Y}(\zeta) = \frac{1}{\frac{1-\zeta}{\kappa} - c} \mathrm{G}(\zeta). \tag{2.10}$$

We can manipulate the right hand side of (2.10) algebraically or use Cauchy's Integral Formula to show that

$$\frac{1}{\frac{1-\zeta}{\kappa} - c} = \sum_{n=0}^{\infty} \frac{\kappa}{(1-\kappa c)^{n+1}} \zeta^n.$$

The above shows how we may use the Laplace transform of the convolution kernel (henceforth called the transfer function) and readings of data in the time domain to produce time domain output. We discretize continuous convolutions with discrete convolutions, where the coefficients of the discrete convolution are the coefficients in the ζ-transform of the transfer function. In a moment we will justify the use of Taylor series.

Some more examples and a general observation

If we want to instead discretize our basic ODE (2.7) with the Backward Differentiation Formula of order 2 (BDF2), our problem reads

$$\frac{1}{\kappa} \left(\frac{3}{2} y_n - 2 y_{n-1} + \frac{1}{2} y_{n-2} \right) - c y_n = g(t_n) \quad \forall n \geq 0.$$

We can take the ζ-transform of the recurrence to find

$$\mathrm{Y}(\zeta) = \left(\frac{3}{2\kappa} - 2\frac{\zeta}{\kappa} + \frac{\zeta^2}{2\kappa} - c \right)^{-1} \mathrm{G}(\zeta).$$

A last example involves discretization of (2.7) with the implicit trapezoid rule (TR). The recurrence reads

$$\frac{1}{\kappa}\left(y_n - y_{n-1}\right) - \frac{c}{2}(y_n - y_{n-1}) = \frac{1}{2}\left(g(t_n) + g(t_{n-1})\right),$$

which can be solved with the ζ-transform

$$\mathrm{Y}(\zeta) = \frac{1}{\frac{2}{\kappa}(\frac{1-\zeta}{1+\zeta}) - c}\mathrm{G}(\zeta).$$

All of these solutions have the general form of

$$\mathrm{Y}(\zeta) = \frac{1}{\frac{1}{\kappa}\delta(\zeta) - c}\mathrm{G}(\zeta), \tag{2.11}$$

where

$$\delta(\zeta) = \begin{cases} 1-\zeta & \text{BE}, \\ \frac{3}{2} - 2\zeta + \frac{1}{2}\zeta^2 & \text{BDF2}, \\ 2\frac{1-\zeta}{1+\zeta} & \text{TR}. \end{cases}$$

We notice that the unique causal solution to (2.7) is given in the Laplace domain by the expression

$$\mathrm{Y}(s) = \frac{1}{s-c}\mathrm{G}(s),$$

whereas the discrete versions have the form (2.11), or, in an implicit form,

$$\frac{1}{\kappa}\delta(\zeta)\mathrm{Y}(\zeta) - c\mathrm{Y}(\zeta) = \mathrm{G}(\zeta). \tag{2.12}$$

If we can expand the discretized transfer function as a power series

$$\left(\frac{1}{\kappa}\delta(\zeta) - c\right)^{-1} = \sum_{m=0}^{\infty} \omega_m^c(\kappa)\zeta^m$$

then the recurrence in (2.12) can be written as

$$y_n = \sum_{m=0}^{n} \omega_m^c(\kappa) g(t_{n-m}).$$

More general convolutions and Convolution Quadrature

We now consider the causal convolution

$$y = f * g, \tag{2.13}$$

where we assume $g : \mathbb{R} \to X$ and $f : \mathbb{R} \to \mathcal{B}(X, Y)$. We take g to be known and causal, and we only require that f have a known Laplace transform $\mathrm{F}(s)$. The Laplace transform of (2.13) is then

$$\mathrm{Y}(s) = \mathrm{F}(s)\mathrm{G}(s).$$

If we discretize this Laplace domain convolution, the equation becomes

$$\mathrm{Y}(\zeta) = \mathrm{F}\left(\tfrac{1}{\kappa}\delta(\zeta)\right)\mathrm{G}(\zeta), \quad \mathrm{G}(\zeta) := \sum_{n=0}^{\infty} g(t_n)\zeta^n. \tag{2.14}$$

If we can expand

$$\mathrm{F}\left(\tfrac{1}{\kappa}\delta(\zeta)\right) = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa)\zeta^m, \tag{2.15}$$

then the convolution (2.14) can be written explicitly

$$y_n = \sum_{m=0}^{n} \omega_m^{\mathrm{F}}(\kappa) g(t_{n-m}), \quad n \geq 0. \tag{2.16}$$

The discrete convolution (2.16) with coefficients given by (2.15) is said to be the Convolution Quadrature (CQ) approximation to the continuous convolution (2.13). Since we have assumed that F is analytic in $\mathbb{C}_+$, if $\delta(0) \in \mathbb{C}_+$ then the mapping $\zeta \longmapsto \mathrm{F}\left(\tfrac{1}{\kappa}\delta(\zeta)\right)$ is analytic in a neighborhood of $\zeta = 0$, and therefore the ζ series (2.15) is simply a Taylor series. This justifies our use of Cauchy's Integral formula for the computation of the convolution weights.

CQ approximation of convolution equations

Written in the Laplace domain, a convolution equation is

$$\mathrm{F}(s)\mathrm{G}(s) = \mathrm{H}(s) \quad \text{or} \quad \mathrm{G}(s) = \mathrm{F}(s)^{-1}\mathrm{H}(s),$$

with the caveat that on the right $\mathrm{F}(s)^{-1}$ may be unknown. Applying a CQ discretization to the convolution equation leads to the discrete convolution

$$\mathrm{F}\left(\tfrac{1}{\kappa}\delta(\zeta)\right)\mathrm{G}(\zeta) = \mathrm{H}(\zeta), \quad \mathrm{H}(\zeta) := \sum_{m=0}^{\infty} h(t_m)\zeta^m.$$

Written as a marching-on-in-time scheme, this becomes

$$\omega_0^{\mathrm{F}}(\kappa)g_n = h(t_n) - \sum_{m=1}^{n} \omega_m^{\mathrm{F}}(\kappa)g(t_{n-m}),$$

and so the CQ discretization is well-defined when $\omega_0^{\mathrm{F}}(\kappa)$ is invertible. We might wonder what happens if we know both $\mathrm{F}(s)$ and $\mathrm{F}(s)^{-1}$, and compute

$$\mathrm{F}\left(\tfrac{1}{\kappa}\delta(\zeta)\right) = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa)\zeta^m \quad \text{and} \quad \mathrm{F}\left(\tfrac{1}{\kappa}\delta(\zeta)\right)^{-1} = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}^{-1}}(\kappa)\zeta^m.$$

Then the convolution equation $\mathrm{F}(\frac{1}{\kappa}\delta(\zeta))\mathrm{G}(\zeta) = \mathrm{H}(\zeta)$ becomes simply

$$g_n = \sum_{m=0}^{n} \omega_m^{\mathrm{F}^{-1}}(\kappa)h(t_{n-m}).$$

Do these two methods produce the same solution? The answer is yes. We have assumed $\mathrm{F}(s)$ is a transfer function that is analytic in $\mathbb{C}_+$, and so is $\mathrm{F}(s)^{-1}$. Then

$$\mathrm{F}\left(\tfrac{1}{\kappa}\delta(\zeta)\right)\mathrm{F}\left(\tfrac{1}{\kappa}\delta(\zeta)\right)^{-1} = \mathrm{I}$$

for small enough ζ. Therefore

$$\omega_0^{\mathrm{F}}(\kappa)^{-1} = \omega_0^{\mathrm{F}^{-1}}(\kappa), \quad \sum_{m=0}^{n} \omega_m^{\mathrm{F}}(\kappa)\omega_{n-m}^{\mathrm{F}^{-1}}(\kappa) = 0 \quad n \geq 1.$$

This proves that

$$\mathrm{F}(\tfrac{1}{\kappa}\delta(\zeta))\mathrm{G}(\zeta) = \mathrm{H}(\zeta) \quad \text{and} \quad \mathrm{G}(\zeta) = \mathrm{F}(\tfrac{1}{\kappa}\delta(\zeta))^{-1}\mathrm{H}(\zeta)$$

produce the same sequence $\{g_n\}$.

2.4 A Discrete Differentiation Approach to CQ

We are interested in approximating the continuous causal convolution $y = f * g$, which reads in the Laplace domain $\mathrm{Y}(s) = \mathrm{F}(s)\mathrm{G}(s)$. We restrict ourselves for a moment to the case when $\mathrm{F}(s) = s$, which corresponds in the time domain to computing $y = \dot{g}$. We discretize this problem with Backward Euler with a fixed time step $\kappa > 0$:

$$y_\kappa := \tfrac{1}{\kappa}(g - g(\cdot - \kappa)).$$

The Laplace transform of this convolution is

$$\mathrm{Y}_\kappa(s) = \tfrac{1}{\kappa}(1 - e^{-s\kappa})\mathrm{G}(s),$$

which we can write as

$$\mathrm{Y}_\kappa(s) = s_\kappa \mathrm{G}(s), \tag{2.17}$$

where

$$s_\kappa = \tfrac{1}{\kappa}(1 - e^{-s\kappa}) = \tfrac{1}{\kappa}\delta(e^{-s\kappa}), \quad \delta(\zeta) = 1 - \zeta.$$

If we apply BDF2 to our toy ODE $y = \dot{g}$, we get

$$y \approx y_\kappa := \tfrac{1}{\kappa}(\tfrac{3}{2}g - 2g(\cdot - \kappa) + \tfrac{1}{2}g(\cdot - 2\kappa)),$$

which has the Laplace domain form

$$\mathrm{Y}_\kappa(s) = \tfrac{1}{\kappa}(\tfrac{3}{2} - 2e^{-s\kappa} + \tfrac{1}{2}e^{-2s\kappa})\mathrm{G}(s).$$

This has the same form as (2.17) with the discrete differentiation function

$$s_\kappa := \tfrac{1}{\kappa}\delta(e^{-s\kappa}),$$

$\delta(\zeta) = \frac{3}{2} - 2\zeta + \frac{1}{2}\zeta^2$. Finally, a trapezoidal rule discretization of the toy ODE reads

$$\tfrac{1}{2}(y_\kappa + y_\kappa(\cdot - \kappa)) = \tfrac{1}{\kappa}(g - g(\cdot - \kappa)),$$

which fits the form of (2.17) with the rational approximation

$$s_\kappa := \tfrac{2}{\kappa}\tfrac{1-e^{-s\kappa}}{1+e^{-s\kappa}} = \tfrac{1}{\kappa}\delta(e^{-s\kappa}).$$

As we did before, we can now consider approximating more general convolutions

$$\mathrm{Y}(s) = \mathrm{F}(s)\mathrm{G}(s) \quad \text{by} \quad \mathrm{Y}_\kappa(s) = \mathrm{F}(s_\kappa)\mathrm{G}(s).$$

To derive the method, we again expand the transfer function

$$\mathrm{F}(\tfrac{1}{\kappa}\delta(\zeta)) = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa)\zeta^m$$

and insert the discrete differentiation symbol

$$\mathrm{F}(s_\kappa) = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa)e^{-sm\kappa} = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa)e^{-t_m s}.$$

We recognize that $\mathrm{F}(s_\kappa)$ is the Laplace transform of the distribution

$$\sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa) \otimes \delta_{t_m},$$

and so $\mathrm{Y}_\kappa(s) = \mathrm{F}(s_\kappa)\mathrm{G}(s)$ is the Laplace transform of

$$y_\kappa(t) = \sum_{m=0}^{n} \omega_m^{\mathrm{F}}(\kappa)g(t - t_m), \quad t_n \le t < t_{n+1}.$$

If we sample at $t = t_n$, we recover our original CQ method:

$$y_n := y_\kappa(t_n) = \sum_{m=0}^{n} \omega_m^{\mathrm{F}}(\kappa)g(t_{n-m}).$$

An important observation is that there is a continuous-in-time convolution in the background of the CQ discretization. The previous two equations demonstrate that CQ produces a sampling at the time steps of this continuous convolution. However, we are only able to evaluate the solution at the prescribed time grid. If we wish to evaluate the solution at a point not on the time grid, we would have to start all over. There is a possibility of non-uniform time stepping which has been developed recently in [56, 57].

Operational notation

The original work of Lubich on CQ [58] made use of an operational notation to indicate causal convolutions and their CQ discretization. The idea is as follows.

In the Laplace domain, the multiply-by-s operator corresponds in the time domain to differentiation, so we write our toy ODE as $y = \dot{g} = \partial g$. We then use the notation

$$y = \mathrm{F}(\partial)g = f * g, \quad \text{where} \quad \mathrm{F}(s) = \mathcal{L}\{f\}(s).$$

In this way, the Laplace domain transfer function and time-dependent data are both clear. Upon discretizing with CQ, we make an approximation $\partial \approx \partial_\kappa$ for a fixed time step $\kappa > 0$. CQ replaces the continuous differentiation operator with a discrete one, $s_\kappa = \frac{1}{\kappa}\delta(e^{-s\kappa})$. The CQ method is written as

$$\mathrm{F}(\partial_\kappa)g = \sum_{m=0}^{n} \omega_m^{\mathrm{F}}(\kappa) g_\kappa(\cdot - t_m) = f_\kappa * g, \quad f_\kappa := \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa) \otimes \delta_{t_m}.$$

2.5 Lubich's Original Exposition

In this section we present the derivation of the CQ method as was originally presented in [58]. Note that the original presentation was for operators of negative order defined outside a sector

$$|\arg(s - c)| < \pi - \phi, \quad \phi < \pi/2, \quad c \in \mathbb{R}.$$

A negative order transfer function $\mathrm{F} : \mathbb{C}_+ \to \mathcal{B}(X, Y)$ satisfies

$$\|\mathrm{F}(s)\| \leq C(\operatorname{Re} s)|s|^\mu \qquad \mu < -1.$$

for all s outside of the sector. The constant $C(\cdot)$ is non-increasing and polynomially bounded (see Appendix A). This condition means that

$$f(t) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} e^{st} \mathrm{F}(s) ds = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{(\sigma + i\omega)t} \mathrm{F}(\sigma + i\omega) d\omega$$

defines a continuous and causal function whose Laplace transform is F, independent of the choice of σ. In addition, if $a > \sigma$, we have a non-standard Cauchy's integral formula

$$\frac{1}{n!}\mathrm{F}^{(n)}(a) = -\frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} \frac{1}{(s - a)^{n+1}} \mathrm{F}(s) ds, \tag{2.18}$$

derived by taking limits in a contour integral around a. We now proceed to compute

$$(f*g)(t) = \int_0^t f(\tau)g(t-\tau)d\tau = \int_0^t \left(\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} e^{s\tau}\mathrm{F}(s)ds\right) g(t-\tau)d\tau$$
$$= \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} \mathrm{F}(s)\left(\int_0^t e^{s\tau}g(t-\tau)d\tau\right)ds.$$

We denote the term

$$\int_0^t e^{s\tau}g(t-\tau)d\tau =: y(t;s)$$

and note that $y(t;s)$ satisfies the ODE $\dot{y} = sy + g$. The assumption of causality gives the initital condition as $y(0) = 0$. We can apply a Backward Euler discretization to $y(t;s)$ to get

$$\int_0^{t_n} e^{s\tau}g(t_n-\tau)d\tau \approx \kappa\sum_{m=0}^{n}\frac{1}{(1-\kappa s)^{m+1}}g(t_{n-m}).$$

Plugging back in, we obtain

$$(f*g)(t_n) \approx \sum_{m=0}^{n}\underbrace{\left(\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{\kappa}{(1-ks)^{m+1}}\mathrm{F}(s)ds\right)}_{\omega_m^{\mathrm{F}}(\kappa)}g(t_{n-m}).$$

To figure out the coefficients, we use the non-standard Cauchy integral formula (2.18) to show

$$\omega_m^{\mathrm{F}}(\kappa) = \frac{(-1)^m}{\kappa^m}\left(-\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{1}{(s-1/\kappa)^{m+1}}\mathrm{F}(s)ds\right)$$
$$= \frac{(-1)^m}{\kappa^m}\frac{1}{m!}\mathrm{F}^{(m)}(1/\kappa)$$
$$= \frac{1}{m!}\frac{d^m}{d\zeta^m}\left(\mathrm{F}\left(\frac{1-\zeta}{\kappa}\right)\right)\Big|_{\zeta=0}.$$

This is the same BE-CQ method as we derived before.

2.6 Convergence of Multistep CQ

We state here without proof the key convergence results for BDF-based and trapezoidal rule Convolution Quadrature. For proofs of the following convergence results for BDF-based CQ, we refer the reader to [58]. The results in [58] are valid for operators whose Laplace transform is of negative order and is defined outside a

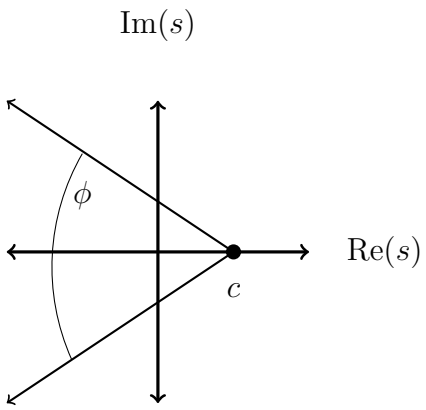

Figure 2.1: The sector $|\arg(s) - c| < \pi - \phi$. The domain of definition of F is the exterior of the sector.

sector. These were extended in [60] to operators whose transfer function is analytic in a half-plane and to transfer functions of positive or negative order. The trapezoidal rule convergence theory was completed later in [9] for transfer functions that take values in a half plane. To state the convergence results for BDF-CQ, we assume that the transfer function F is analytic in a sector $|\arg(s-c)| < \pi - \phi$ with $\phi < \frac{\pi}{2}$, $c \in \mathbb{R}$, and satisfies in the exterior of the sector

$$\|\mathrm{F}(s)\| \leq M|s|^{-\mu} \quad \text{for some } M > 0 \quad \text{and } \mu > 0.$$

We require that the linear multistep method be A(α) stable for $\alpha > \phi$. Geometrically, this means that the region of absolute stability for the multistep method must contain the domain of analyticity of F. We also require that it is stable in a neighborhood of infinity, strongly zero-stable, and consistent of order p. In terms of the generating function $\delta(\zeta)$, this corresponds to:

(1) $\delta(\zeta)$ is analytic and without zeros in a neighborhood of the closed unit disk $|\zeta| \leq 1$, with the exception of a simple root at $\zeta = 1$,

(2) $|\arg \delta(\zeta)| \leq \pi - \alpha$ for $|\zeta| < 1$, for some $\alpha > \phi$, and

(3) $\frac{1}{\kappa}\delta(e^{-\kappa}) = 1 + O(h^p)$ for some $p \geq 1$.

The backward difference family of ODE solvers of order $p \leq 6$, which corresponds to the choice

$$\delta(\zeta) = \sum_{i=1}^{p} \frac{1}{i}(1-\zeta)^i,$$

satisfy the hypotheses. The angles α for these methods are $\alpha = 90°, 90°, 88°, 73°, 51°, 18°$ for $p = 1, \ldots, 6$. The BDF-7 and higher methods are not zero-stable and are therefore unusable. Under these assumptions, Lubich states the following theorem.

Theorem 2.6.1 ([58, Theorem 3.1]). *Under the previous hypotheses on* F *and* δ*, there is a* $C > 0$ *such that if* $g \in \mathcal{C}^p([0,T])$

$$\begin{aligned}|\mathrm{F}(\partial_k)g(t) - \mathrm{F}(\partial)g(t)| \leq & Ct^{\mu-1}\left(\kappa|g(0)| + \cdots + \kappa^{p-1}|g^{(p-2)}(0)|\right. \\ & \left. + \kappa^p\left(|g^{(p-1)}(0)| + t\max_{0\leq\tau\leq t}|g^{(p)}(\tau)|\right)\right) \quad t \in [\kappa, T].\end{aligned}$$

The constant C *is independent of* κ *and* t *but depends on* T*.*

With this theorem we see that we recover the full order of the underlying time stepping method for smooth enough data with sufficiently many vanishing derivatives at $t = 0$. A second theorem extends Theorem 2.6.1 to the case of $\mu \leq 0$. The constant in its statement also depends on the final integration time T.

Theorem 2.6.2 ([58, Theorem 5.1]). *Under the previous assumptions on* δ *and* F*, we have for any positive integer* k

$$\begin{aligned}|s_\kappa^k \mathrm{F}(\partial_\kappa)g(t) - s^k\mathrm{F}(s)g(t)| \leq & Ct^{\mu-1-k}\left(\kappa|g(0)| + \cdots + \kappa^{(p-1)}|g^{(p-2)}(0)|\right. \\ & + \kappa^p\big(|g^{(p-1)}(0)| + t|g^{(p)}(0)| + \cdots + t^k|g^{(p+k-1)}(0)| \\ & \left. + t^{k+1}\max_{0\leq\tau\leq t}|g^{(p+k)}(\tau)|\big)\right).\end{aligned}$$

2.7 Algorithms for Multistep CQ

We now explain the implementation details for multistep CQ. We will use generic pseudocode for the actual algorithms, but implementation of the method follows closely. Another exposition of many of the CQ algorithms can be found in [16]. Before we proceed, we need to introduce some tools.

Given a vector $\mathbf{x} := (x_0, \ldots, x_M) \in \mathbb{C}^{M+1}$, we define its Discrete Fourier Transform (DFT), denoted as $\widehat{\mathbf{x}}$, by

$$\widehat{x}_\ell := \sum_{n=0}^{M} x_n \zeta_{M+1}^{-\ell n}, \quad \ell = 0, \ldots, M, \quad \text{where} \quad \zeta_{M+1} := e^{\frac{2\pi i}{M+1}}.$$

We can recover the original vector through the Inverse DFT (IDFT)

$$x_n := \frac{1}{M+1} \sum_{\ell=0}^{M} \widehat{x}_\ell \zeta_{M+1}^{\ell n}, \quad n = 0, \ldots, M.$$

Given $\mathbf{x}$, $\mathbf{y} \in \mathbb{C}^{M+1}$, we define their discrete periodic convolution $\mathbf{x} *_{\text{per}} \mathbf{y} \in \mathbb{C}^{M+1}$ by

$$(\mathbf{x} *_{\text{per}} \mathbf{y})_n := \sum_{m=0}^{n} x_m y_{n-m} + \sum_{m=n+1}^{M} x_m y_{M+1+n-m}, \quad n = 0, \ldots, M.$$

This definition of discrete periodic convolutions is somewhat complicated and does not reveal much of the structure of the result. Instead, we can consider the vectors as infinite sequences $\mathbf{x}, \mathbf{y} \in \ell^0(\mathbb{Z})$ that are $M+1$ periodic. Then the periodic sequence

$$(\mathbf{x} *_{\text{per}} \mathbf{y})_n = \sum_{m=0}^{M} x_m y_{n-m} \quad n \in \mathbb{Z},$$

which has a much more convolutional feel, coincides with the original definition of periodic convolution. The DFT diagonalizes discrete periodic convolutions as follows:

$$\widehat{(\mathbf{x} *_{\text{per}} \mathbf{y})}_\ell = \widehat{x}_\ell \widehat{y}_\ell.$$

In this way, we can compute discrete periodic convolutions quickly by taking the DFT of the two vectors, multiplying componentwise, and then taking the IDFT. Now, suppose that $\mathbf{x}$ and $\mathbf{y}$ are causal sequences. We need to compute the first N components of their discrete convolution

$$(\mathbf{x} * \mathbf{y})_n = \sum_{m=0}^{n} x_m y_{n-m}, \quad n = 0, \ldots, N. \tag{2.19}$$

We notice that we are really only using the vectors $(x_0, \ldots, x_N)$, $(y_0, \ldots, y_N) \in \mathbb{C}^{N+1}$. Define

$$\mathbf{x}^{\text{ext}} := (x_0, \ldots, x_N, \underbrace{0, \ldots, 0}_{N+1}), \quad \mathbf{y}^{\text{ext}} := (y_0, \ldots, y_N, \underbrace{0, \ldots, 0}_{N+1}) \in \mathbb{C}^{2N+2} \tag{2.20}$$

as the zero-extensions of the components of the sequences $\mathbf{x}$ and $\mathbf{y}$ that are relevant for the discrete convolution (2.19). Then it is easy to see that

$$(\mathbf{x} * \mathbf{y})_n = (\mathbf{x}^{\text{ext}} *_{\text{per}} \mathbf{y}^{\text{ext}})_n, \quad n = 0, \ldots, N. \tag{2.21}$$

Equations (2.20) and (2.21) provide an algorithm for computing the first terms of a discrete convolution of sequences (2.19).

Algorithm 2.7.1 (Computation of discrete convolutions)**.** *To compute the convolution*

$$(\mathbf{x} * \mathbf{y})_n = \sum_{m=0}^{n} x_m y_{n-m}, \quad n = 0, \ldots, N,$$

(1) keep $N+1$ components of the sequences $\mathbf{x}$ and $\mathbf{y}$ and extend them with $N+1$ zeros at the end,

(2) take the DFT of the extended vectors,

(3) multiply the resulting vectors component by component,

(4) take the IDFT of the result of (3), and

(5) keep the first $N+1$ components of (4).

Reducing computation by symmetry

Our data will be taken to be real-valued, and so we can reduce our computation by noticing that the DFT of real data exhibits a certain symmetry. Assume $\mathbb{X}$ is a Banach space with a conjugation operator and let $\mathbf{x} = (x_0, \ldots, x_N) \in \mathbb{X}^{N+1}$. If

$$x_{N+1-\ell} = \overline{x}_\ell \quad \ell = 1, \ldots, N,$$

we will say that the vector $\mathbf{x}$ is Hermitian. This is not a standard definition, but we will find it useful. It is precisely this type of symmetry that occurs when we take the DFT of real-valued data. In what follows, we will remark that an algorithm to compute a vector $\mathbf{x}$ can be symmetrized when we know in advance that $\mathbf{x}$ is Hermitian. In this case, we will:

(1) compute x_ℓ for $\ell = 0, \ldots, \lfloor \frac{N+1}{2} \rfloor$, and

(2) copy the missing components $x_{N+1-\ell}$ for $\ell = 1, \ldots, \lfloor \frac{N}{2} \rfloor$.

Computation of CQ weights

We will now work to compute the weights of the CQ method, given by

$$\omega_n^{\mathrm{F}}(\kappa) := \frac{1}{n!} \frac{d^n}{d\zeta^n} \left(\mathrm{F}\left(\frac{1}{\kappa} \delta(\zeta) \right) \right) \Big|_{\zeta=0}, \quad n = 0, \ldots, N. \tag{2.22}$$

The first coefficient is simply $\omega_0^{\mathrm{F}}(\kappa) = \mathrm{F}(\frac{1}{\kappa}\delta(0))$. Following the original works [58, 59], we will use Cauchy's integral formula to compute the remaining coefficients. We will take the integration contour to be a circle $C_R := \{\zeta \in \mathbb{C} \ : \ |\zeta| = R\}$ for a value of R to be determined. Because F is analytic (and therefore its derivatives are too), we will approximate Cauchy's integral formula with the composite trapezoidal rule. For simplicity, we will use the same number of quadrature points as CQ weights that we need. Studies on the impact of the number of quadrature nodes on the accuracy of the computation can be found in [18]. We now compute

$$\begin{aligned}
\omega_m^{\mathrm{F}}(\kappa) &= \frac{1}{2\pi i} \oint_{C_R} \zeta^{-m-1} \mathrm{F}(\tfrac{1}{\kappa}\delta(\zeta)) d\zeta \\
&= R^{-m} \int_0^1 e^{-2\pi i m\theta} \mathrm{F}(\tfrac{1}{\kappa}\delta(Re^{2\pi i\theta})) d\theta \\
&\approx \frac{R^{-m}}{N+1} \sum_{\ell=0}^{N} \zeta_{N+1}^{-m\ell} \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{\ell})) \\
&= \frac{R^{-m}}{N+1} \sum_{\ell=0}^{N} \zeta_{N+1}^{m\ell} \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{-\ell})).
\end{aligned}$$

Our approximate CQ weights are then given by

$$\omega_m^{\mathrm{F}}(\kappa) \approx \frac{R^{-m}}{N+1} \sum_{\ell=0}^{N} \zeta_{N+1}^{m\ell} \widehat{\mathrm{F}}_\ell, \qquad \widehat{\mathrm{F}}_\ell := \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{-\ell})).$$

One possible choice of radius is $R = \epsilon^{\frac{1}{2N+1}}$ where ϵ is machine epsilon. This choice strikes a balance between efficiency and accuracy, and allows about 8 digits of precision when computing the CQ coefficients [59]. If we have $\mathrm{F}(\overline{s}) = \overline{\mathrm{F}(s)}$ and $\delta(\overline{\zeta}) = \overline{\delta(\zeta)}$, then the sequence of evaluations of $\widehat{\mathrm{F}}_\ell$ is a Hermitian sequence, and its computation can be reduced by symmetry.

Algorithm 2.7.2 (Computation of CQ weights)**.** *In this algorithm and those that follow, we use the notation* **(Par + Sym)** *to denote steps that can be done in parallel and reduced by symmetry.*

(1) **(Par + Sym)** *Compute*

$$\widehat{\mathrm{F}}_\ell = \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{-\ell})), \quad \ell = 0, \ldots, N.$$

(2) Apply the IDFT

$$\mathrm{F}_m = \frac{1}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell \zeta_{N+1}^{n\ell}, \quad m = 0, \ldots, N.$$

When F *is matrix-valued, the IDFT must be done component-by-component.*

(3) Scale the weights

$$\omega_m^{\mathrm{F}}(\kappa) = R^{-m}\mathrm{F}_n, \quad m = 0, \ldots, N.$$

We can replace the approximation to the zeroth weight with its exact value

$$\omega_0^{\mathrm{F}}(\kappa) = \mathrm{F}(\tfrac{1}{\kappa}\delta(0)).$$

All-steps-at-once computation of convolutions

Our goal now is the computation of a forward convolution

$$\sum_{m=0}^{n} \omega_{n-m}^{\mathrm{F}}(\kappa) g_m, \qquad n = 0, \ldots, N,$$

where we assume that we are approximating the CQ weights by

$$\omega_n^{\mathrm{F}}(\kappa) \approx \frac{R^{-n}}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell \zeta_{N+1}^{\ell n}, \quad \widehat{\mathrm{F}}_\ell = \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{-\ell})).$$

Because of Cauchy's integral formula, all weights with negative index vanish:

$$\omega_n^{\mathrm{F}}(\kappa) = \frac{1}{2\pi i} \oint_{C_R} \zeta^{-n-1} \mathrm{F}(\zeta) d\zeta = 0 \qquad \forall n \leq -1.$$

We then compute

$$\begin{aligned} u_n &= \sum_{m=0}^{n} \omega_{n-m}^{\mathrm{F}}(\kappa) g_m = \sum_{m=0}^{N} \omega_{n-m}^{\mathrm{F}}(\kappa) g_m \\ &\approx \sum_{m=0}^{N} \left(\frac{R^{m-n}}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell \zeta_{N+1}^{\ell(n-m)} \right) g_m \\ &= R^{-n} \left(\frac{1}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell \left(\sum_{m=0}^{N} R^m g_m \zeta_{N+1}^{-m\ell} \right) \zeta_{N+1}^{\ell n} \right). \end{aligned}$$

This leads us to the following algorithm presented in [16] and based on algorithms developed in [34].

Algorithm 2.7.3 (All-steps-at-once forward convolution)**.** *We sample the input data at discrete times*

$$g_n = g(t_n), \qquad n = 0, \ldots, N$$

and approximate

$$u_n = \sum_{m=0}^{n} \omega_{n-m}^{\mathrm{F}}(\kappa) g_m, \qquad n = 0, \ldots, N.$$

(1) Scale the data

$$h_m := R^m g_m, \qquad m = 0, \ldots, N.$$

(2) Compute the DFT

$$\widehat{h}_\ell := \sum_{\ell=0}^{N} h_m \zeta_{N+1}^{-\ell m}, \qquad \ell = 0, \ldots, N.$$

(3) **(Par+Sym)** *Apply the discrete transfer functions in the Fourier domain*

$$\widehat{v}_\ell := \widehat{\mathrm{F}}_\ell \widehat{h}_\ell, \qquad \widehat{\mathrm{F}}_\ell := \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{-\ell})).$$

(4) Compute the IDFT

$$v_n := \frac{1}{N+1}\sum_{\ell=0}^{N} \widehat{v}_\ell \zeta_{N+1}^{\ell n}, \quad n = 0, \ldots, N.$$

(5) Rescale

$$u_n := R^{-n} v_n.$$

All-steps-at-once solution of convolution equations

We remarked earlier that solving a convolution equation $\mathrm{F}(\zeta)\mathrm{G}(\zeta) = \mathrm{H}(\zeta)$ is equivalent to computing the forward convolution $\mathrm{G}(\zeta) = \mathrm{F}^{-1}(\zeta)\mathrm{H}(\zeta)$ in the case that we know $\mathrm{F}^{-1}(\zeta)$. We can then modify the procedure for computing forward convolutions to handle convolution equations quite simply

$$\begin{aligned} g_n &= \sum_{m=0}^{n} \omega_m^{\mathrm{F}^{-1}}(\kappa) h(t_{n-m}), \qquad n = 0, \ldots, N \\ &= \sum_{m=0}^{N} \omega_m^{\mathrm{F}^{-1}}(\kappa) h(t_{n-m}) \\ &\approx \sum_{m=0}^{N} \left(\frac{R^{-n}}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell^{-1} \zeta_{N+1}^{-\ell n} \right) h(t_{n-m}), \quad \widehat{\mathrm{F}}_\ell^{-1} := \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{-\ell})^{-1}, \end{aligned}$$

which, upon re-arranging some terms, gives us the formula

$$g_n \approx R^{-n} \left(\frac{1}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell^{-1} \left(\sum_{m=0}^{N} R^m h_m \zeta_{N+1}^{-m\ell} \right) \zeta_{N+1}^{\ell n} \right).$$

We do not need to compute the inverses $\widehat{\mathrm{F}}_\ell^{-1}$, but instead we will solve linear systems.

Algorithm 2.7.4 (All-steps-at-once solution of convolution equations)**.** *We sample the data at discrete times*

$$h_n = h(t_n), \quad n = 0, \ldots, N$$

and seek to solve

$$\sum_{m=0}^{n} \omega_{n-m}^{\mathrm{F}} g_m = h_n, \quad n = 0, \ldots, N.$$

(1) Scale the data

$$v_m := R^m h_m, \quad m = 0, \ldots, N.$$

(2) Compute the DFT, $\widehat{v}_\ell$, for $\ell = 0, \ldots, N$.

(3) **(Par+Sym)** *Solve the linear systems in the Fourier domain*

$$\widehat{\mathrm{F}}_\ell \widehat{w}_\ell = \widehat{v}_\ell, \quad \widehat{\mathrm{F}}_\ell := \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{-\ell})).$$

(4) Compute the IDFT w_ℓ, for $\ell = 0, \ldots, N$.

(5) Scale

$$g_n := R^{-n} w_n, \quad n = 0, \ldots, N.$$

Computing convolutional tails

We focus now on computing

$$g_n := \sum_{m=0}^{Q} \widetilde{\omega}^{\mathrm{F}}_{n-m}(\kappa) u_m, \quad n = Q+1, \ldots, M, \tag{2.23}$$

where

$$\widetilde{\omega}^{\mathrm{F}}_n(\kappa) = \frac{R^{-n}}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell \zeta_{N+1}^{-n\ell}, \quad \widehat{\mathrm{F}}_\ell := \mathrm{F}(\tfrac{1}{\kappa}\delta(R\zeta_{N+1}^{-\ell})), \tag{2.24}$$

for a given $N \geq M$, which we will take to be $N = 2M$. We then proceed as follows:

$$\begin{aligned}
\widetilde{g}_k &:= g_{k+Q+1} \qquad (k = 0, \ldots, M-Q-1), \\
&= \sum_{m=0}^{Q} \left(\frac{R^{m-k-Q-1}}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell \zeta_{N+1}^{\ell(k+Q+1-m)} \right) u_m \\
&= R^{-k-Q-1} \left(\frac{1}{N+1} \sum_{\ell=0}^{N} \zeta_{N+1}^{\ell(Q+1)} \widehat{\mathrm{F}}_\ell \left(\sum_{m=0}^{Q} \zeta_{N+1}^{-\ell m} R^m u_m \right) \zeta_{N+1}^{\ell k} \right) \\
&= R^{-k-Q-1} \left(\frac{1}{N+1} \sum_{\ell=0}^{N} \zeta_{N+1}^{\ell(Q+1)} \widehat{\mathrm{F}}_\ell \left(\sum_{m=0}^{N} \zeta_{N+1}^{-\ell m} w_m \right) \zeta_{N+1}^{\ell k} \right),
\end{aligned}$$

where

$$w_m := \begin{cases} R^m u_m, & 0 \leq m \leq Q, \\ 0, & Q+1 \leq m \leq N. \end{cases} \tag{2.25}$$

Algorithm 2.7.5 (Computing convolutional tails)**.** *We now compute* (2.23)*. The value of* N *in* (2.24) *is a parameter. We assume the data* u_m*, for* $m = 0, \dots, Q$ *is already sampled.*

(1) Scale the data and append zeros according to (2.25)*.*

(2) Compute the DFT of the vector w_m *from the previous step,* $\widehat{w}_\ell$*,* $\ell = 0, \dots, N$*.*

(3) **(Par+Sym)** *Apply the operators*

$$\widehat{h}_\ell := \zeta_{N+1}^{\ell(Q+1)} \widehat{\mathrm{F}}_\ell \widehat{w}_\ell, \quad \ell = 0, \dots, N.$$

(4) Compute the IDFT h_k*, for* $k = 0, \dots, N$*.*

(5) Scale and cut the resulting vector

$$\widetilde{g}_k := R^{-k-Q-1} h_k, \quad k = 0, \dots, M - Q - 1.$$

(6) Re-index

$$g_n := \widetilde{g}_{n-Q-1}, \quad n = Q+1, \dots, M.$$

If we do not re-index in the last step, what we have computed is

$$\widetilde{g}_k := \sum_{m=0}^{Q} \widetilde{\omega}^{\mathrm{F}}_{k+Q+1-m}(\kappa) u_m, \qquad k = 0, \dots, M - Q - 1,$$

which can be understood as the formal product with a piece of a Toeplitz matrix

$$\begin{bmatrix} \widetilde{g}_0 \\ \widetilde{g}_1 \\ \vdots \\ \widetilde{g}_{M-Q-1} \end{bmatrix} = \begin{bmatrix} \widetilde{\omega}^{\mathrm{F}}_{Q+1}(\kappa) & \widetilde{\omega}^{\mathrm{F}}_{Q}(\kappa) & \dots & \widetilde{\omega}^{\mathrm{F}}_{1}(\kappa) \\ \widetilde{\omega}^{\mathrm{F}}_{Q+2}(\kappa) & \widetilde{\omega}^{\mathrm{F}}_{Q+1}(\kappa) & \dots & \widetilde{\omega}^{\mathrm{F}}_{2}(\kappa) \\ \widetilde{\omega}^{\mathrm{F}}_{Q+3}(\kappa) & \widetilde{\omega}^{\mathrm{F}}_{Q+2}(\kappa) & \dots & \widetilde{\omega}^{\mathrm{F}}_{3}(\kappa) \\ \vdots & \vdots & \ddots & \vdots \\ \widetilde{\omega}^{\mathrm{F}}_{M}(\kappa) & \widetilde{\omega}^{\mathrm{F}}_{M-1}(\kappa) & \dots & \widetilde{\omega}^{\mathrm{F}}_{M-Q}(\kappa) \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_Q \end{bmatrix}.$$

Solution of discrete convolution equations

We will now develop two strategies for the solution discrete convolution equations. First, we consider the solution of the block lower-triangular system arising from a CQ discretization using block forward substitution. We pick a block size $1 \leq J \leq N$ corresponding to the size of the lower triangular blocks we will invert directly. Taking the extreme $J = 1$ corresponds to simple marching-on-in-time scheme of the form

$$\omega_0^{\mathrm{F}}(\kappa) g_n = h_n - \sum_{m=1}^{n} \omega_m^{\mathrm{F}}(\kappa) g_{n-m}, \quad n = 0, \ldots, N,$$

and a choice of $J = N$ simply inverts the entire lower-triangular system in a single solve. Intermediate choices of J give the number of time steps we compute at once. In the case $J = 2$, a single step solves first the block system

$$\begin{bmatrix} \omega_0^{\mathrm{F}}(\kappa) & \\ \omega_1^{\mathrm{F}}(\kappa) & \omega_0^{\mathrm{F}}(\kappa) \end{bmatrix} \begin{bmatrix} g_0 \\ g_1 \end{bmatrix} = \begin{bmatrix} h(t_0) \\ h(t_1) \end{bmatrix},$$

and then updates the right-hand-side of the equation with the previously computed steps before solving for the next two time steps:

$$\begin{bmatrix} \omega_0^{\mathrm{F}}(\kappa) & \\ \omega_1^{\mathrm{F}}(\kappa) & \omega_0^{\mathrm{F}}(\kappa) \end{bmatrix} \begin{bmatrix} g_2 \\ g_3 \end{bmatrix} = \begin{bmatrix} h(t_2) \\ h(t_3) \end{bmatrix} - \begin{bmatrix} \omega_2^{\mathrm{F}}(\kappa) & \omega_1^{\mathrm{F}}(\kappa) \\ \omega_3^{\mathrm{F}}(\kappa) & \omega_2^{\mathrm{F}}(\kappa) \end{bmatrix} \begin{bmatrix} g_0 \\ g_1 \end{bmatrix}.$$

We denote a generic lower-triangular Toeplitz block by

$$\Omega_J = \begin{bmatrix} \omega_0^{\mathrm{F}}(\kappa) & & & \\ \omega_1^{\mathrm{F}}(\kappa) & \omega_0^{\mathrm{F}}(\kappa) & & \\ \vdots & \ddots & \ddots & \\ \omega_J^{\mathrm{F}}(\kappa) & \ldots & \omega_1^{\mathrm{F}}(\kappa) & \omega_0^{\mathrm{F}}(\kappa) \end{bmatrix}.$$

The algorithm is as follows.

Algorithm 2.7.6 (Lookahead solution of CQ convolution equations)**.** *We seek to solve a convolution equation*

$$\sum_{m=0}^{n} \omega_{n-m}^{\mathrm{F}}(\kappa) g_n = h_n, \quad n = 0, \ldots, N.$$

The parameter J breaks the list of indices into groups

$$\underbrace{0,\dots,J-1}_{b(1)},\underbrace{J,\dots,2J-1}_{b(2)},\dots,\underbrace{(k-1)J,\dots,kJ-1}_{b(k)},\underbrace{kn,\dots,N}_{remainder}.$$

where $b(i)=\{(i-1)J,\dots iJ-1\}$ is a generic block for $i=1,\dots,k$, where $k=\lfloor N/J\rfloor$. We then loop over the blocks $i=1,\dots,k$ and do the following:

(1) For a fixed i, solve the block system

$$\Omega_J\mathbf{g}=\mathbf{h}_{b(i)}.$$

(2) Compute the convolution tail with the formula

$$r_n=\sum_{m=0}^{J-1}\omega^{\mathrm{F}}_{n-m}(\kappa)h_m,\quad n=J,\dots,N-(i-1)J.$$

(3) Update the right hand side of the equations with

$$h_n=h_n-r_{n-(i-1)J},\quad n=iJ,\dots,N.$$

When we have looped over all of the blocks of size J, we may have remaining indices (when the number of time steps is not a multiple of J). Therefore, we have to solve for the last piece of the convolution directly:

$$(\mathbf{Par}+\mathbf{Sym})\quad \sum_{m=0}^{n}\omega^{\mathrm{F}}_{n-m}(\kappa)g_{kJ+m}=h_{kJ+m},\quad m=0,\dots,N-kJ.$$

A recursive approach is to again invert a lower triangular Toeplitz blocks of fixed size J, but instead of then calculating the contribution of the computed steps to the entire right hand side, we instead correct the right hand side with the square block that connects the two triangular blocks. This is illustrated in Figure (2.2). We now outline the fully recursive procedure, following the exposition of [17].

Algorithm 2.7.7 (Recursive solution of discrete convolution equations)**.** *We seek to solve the discrete convolutional system*

$$\sum_{m=0}^{n}\omega^{\mathrm{F}}_{m}(\kappa)g_{n-m}=h_n,\quad n=0,\dots,N.$$

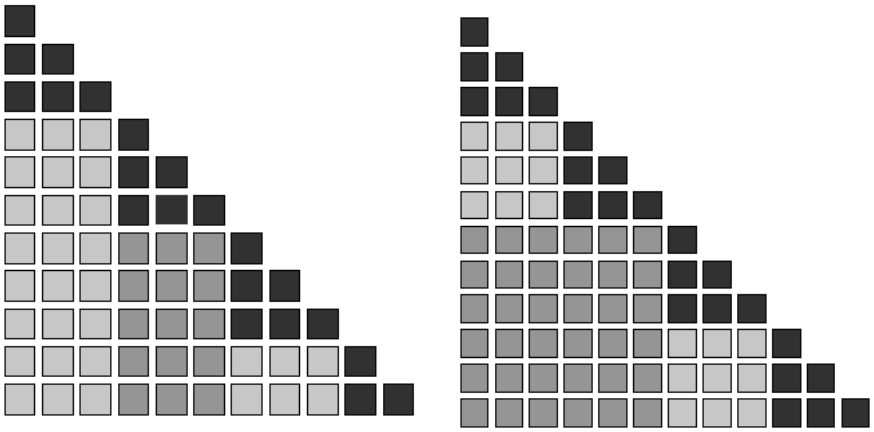

Figure 2.2: A graphical comparison of lookahead (left) and recursive (right) strategies for solving convolutional systems.

(1) If $N > J$, define $N_h = \lceil N/2 \rceil$ and solve recursively

$$\sum_{m=0}^{n} \omega_m^{\mathrm{F}}(\kappa) g_{n-m} = h_n \quad n = 0, \ldots, N_h,$$

i.e. if $N_h > J$, bisect again.

(2) Update the right hand side with

$$h_n = h_n - \sum_{m=0}^{N_h} \omega_m^{\mathrm{F}}(\kappa) g_{n-m}, \quad n = 0, \ldots, N_h.$$

(3) **(Par+Sym)** *Solve the remaining lower triangular block*

$$\sum_{N_h+1}^{n} \omega_m^{\mathrm{F}}(\kappa) g_{n-m} = h_n \quad n = N_h + 1, \ldots, N.$$

(4) **(Par+Sym)** *If $N \leq J$, solve directly the system*

$$\sum_{n=0}^{n} \omega_m^{\mathrm{F}}(\kappa) g_{n-m} = h_n, \quad n = 0, \ldots, N.$$

2.8 Multistage Convolution Quadrature

In the previous sections, we have developed the tools for multistep convolution quadrature. At a key moment, we discretized a linear ODE with an implicit multistep ODE solver to derive the method. A natural extension of the previous work is to the case of discretization of the underlying ODE by multistage time steppers. The mathematics is more complicated than in the linear multistep setup. We will take some time to introduce the necessary tools before proceeding with our study of Runge-Kutta Convolution Quadrature (RKCQ).

We will make use of non-standard vectorized notation for applying a scalar function to a vector. For a vector $\mathbf{c} \in \mathbb{R}^p$, we will write

$$\mathbf{c} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_p \end{bmatrix} \longmapsto g(t + \kappa \mathbf{c}) = \begin{bmatrix} g(t + \kappa c_1) \\ g(t + \kappa c_2) \\ \vdots \\ g(t + \kappa c_p) \end{bmatrix} \in \mathbb{R}^p.$$

Similarly, if $f = f(t, y)$, then we will write

$$\mathbf{c}, \mathbf{y} \in \mathbb{R}^p \longmapsto f(t + \kappa \mathbf{c}, \mathbf{y}) = \begin{bmatrix} f(t + \kappa c_1, y_1) \\ f(t + \kappa c_2, y_2) \\ \vdots \\ f(t + \kappa c_p, y_p) \end{bmatrix} \in \mathbb{R}^p.$$

An **implicit RK** scheme is given by its Butcher tableau

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^T \end{array} \qquad \mathbf{b}, \mathbf{c} \in \mathbb{R}^p, \qquad \mathbf{A} \in \mathbb{R}^{p \times p},$$

with the conditions

$$\mathbf{A1} = \mathbf{c}, \qquad \mathbf{b}^T \mathbf{1} = 1, \qquad \mathbf{1} = (1, \ldots, 1)^T. \tag{2.26}$$

The solution of an ODE

$$\dot{y} = f(t, y)$$

with an implicit Runge-Kutta method requires the solution of a system of (possibly non-linear) equations to find the stage values

$$\mathbf{y}_n = y_n \mathbf{1} + \kappa \mathbf{A} f(t_n + \kappa \mathbf{c}, \mathbf{y}_n), \tag{2.27}$$

followed by the computation of the next step

$$y_{n+1} = y_n + \kappa \mathbf{b}^T f(t_n + \kappa \mathbf{c}, \mathbf{y}_n). \tag{2.28}$$

The internal stages approximate

$$\mathbf{y}_n \approx y(t_n + \kappa \mathbf{c}), \quad y_n = y(t_n).$$

As in the multistep case, we are interested in the trivial ODE

$$\dot{y} = g$$

which is

$$s\mathrm{Y}(s) = \mathrm{G}(s)$$

in the Laplace domain. Applying (2.27) and (2.28) to this problem leads to

$$\mathbf{y}_n = y_n \mathbf{1} + \kappa \mathbf{A} \mathbf{g}_n, \quad y_{n+1} = y_n + \kappa \mathbf{b}^T \mathbf{g}_n, \quad \mathbf{g}_n := g(t_n + \kappa \mathbf{c}). \tag{2.29}$$

Written with the ζ transform, (2.29) becomes

$$\mathbf{Y}(\zeta) = \mathrm{Y}(\zeta)\mathbf{1} + \kappa \mathbf{A} \mathbf{G}(\zeta), \quad \zeta^{-1}\mathrm{Y}(\zeta) = \mathrm{Y}(\zeta) + \kappa \mathbf{b}^T \mathbf{G}(\zeta),$$

where

$$\mathrm{Y}(\zeta) := \sum_{m=0}^{\infty} y_m \zeta^m, \quad \mathbf{Y}(\zeta) := \sum_{m=0}^{\infty} \mathbf{y}_m \zeta^m, \quad \mathbf{G}(\zeta) := \sum_{m=0}^{\infty} \mathbf{g}_m \zeta^m.$$

We can solve the recurrence equations to find

$$\mathrm{Y}(\zeta) = \kappa \frac{\zeta}{1-\zeta} \mathbf{b}^T \mathbf{G}(\zeta) \quad \text{and} \quad \mathbf{Y}(\zeta) = \kappa \left(\frac{\zeta}{1-\zeta} \mathbf{1}\mathbf{b}^T + \mathbf{A} \right) \mathbf{G}(\zeta).$$

This corresponds to the RK discretization of

$$\mathrm{Y}(s) = s^{-1}\mathrm{G}(s),$$

and so our **discrete RK differentiation operator** will be given by the matrix

$$\Delta(\zeta) := \left(\frac{\zeta}{1-\zeta}\mathbf{1}\mathbf{b}^T + \mathbf{A}\right)^{-1}.$$

In other words,

$$s\mathrm{Y}(s) \quad \text{is discretized as} \quad \tfrac{1}{\kappa}\Delta(\zeta)\mathbf{Y}(\zeta).$$

A Runge-Kutta method is said to be **stiffly accurate** if the last row of $\mathbf{A}$ is the same as $\mathbf{b}^T$, i.e.

$$\mathbf{e}_p^T\mathbf{A} = \mathbf{b}^T, \quad \mathbf{e}_p^T = (0,\ldots,0,1).$$

For these types of methods, it is clear that $c_p = 1$. Going back to (2.29), we see

$$\mathbf{e}_p^T\mathbf{y}_n = y_n\mathbf{e}_p^T\mathbf{1} + \kappa\mathbf{e}_p^T\mathbf{A}f(t_n+\kappa\mathbf{c},\mathbf{y}_n) = y_n + \kappa\mathbf{b}^T f(t_n+\kappa\mathbf{c},\mathbf{y}_n) = y_{n+1}.$$

This shows that the last stages corresponds to the steps, and so we do not need to explicitly compute the steps. From here on, we will only focus on stiffly accurate RK methods and will no longer consider the steps independently from the stages.

2.9 Elementary Dunford Calculus

To continue with our exposition of RKCQ, we need to introduce some of the basics of Dunford Calculus. We will not try to justify any of these results, but they can be found in various sources, such as [25]. Suppose that $\mathrm{F} : \mathbb{C}_+ \to \mathbb{C}$ is analytic. Then, by Cauchy's integral formula, we have

$$\mathrm{F}(\lambda) = \frac{1}{2\pi i}\oint_C (z-\lambda)^{-1}\mathrm{F}(z)dz \qquad \lambda \in \mathbb{C}_+,$$

where C is some simple and positively oriented path surrounding λ. If $\mathbf{\Lambda}$ is a diagonal matrix with entries $\lambda_1,\ldots,\lambda_p \in \mathbb{C}_+$, then it is natural to define

$$\begin{aligned}\mathrm{F}(\mathbf{\Lambda}) &:= \frac{1}{2\pi i}\oint_C (z\mathbf{I}-\mathbf{\Lambda})^{-1}\mathrm{F}(z)dz \\ &= \mathrm{diag}\left(\frac{1}{2\pi i}\oint_C (z-\lambda_1)^{-1}\mathrm{F}(z)dz,\ldots,\frac{1}{2\pi i}\oint_C (z-\lambda_p)^{-1}\mathrm{F}(z)dz\right),\end{aligned}$$

where the curve C surrounds $\lambda_1, \ldots, \lambda_p$. Then it is clear we can extend this definition to diagonalizable matrices. If $\mathbf{B} = \mathbf{P}\mathbf{\Lambda}\mathbf{P}^{-1}$ is a spectral decomposition of $\mathbf{B}$, then

$$\begin{aligned}\mathrm{F}(\mathbf{B}) &= \frac{1}{2\pi i}\oint_C (z\mathbf{I} - \mathbf{B})^{-1}\mathrm{F}(z)dz = \frac{1}{2\pi i}\oint_C (z\mathbf{P}\mathbf{P}^{-1} - \mathbf{P}\mathbf{\Lambda}\mathbf{P}^{-1})^{-1}\mathrm{F}(z)dz \\ &= \frac{1}{2\pi i}\oint_C \mathbf{P}(z\mathbf{I} - \mathbf{\Lambda})^{-1}\mathbf{P}^{-1}\mathrm{F}(z)dz = \mathbf{P}\mathrm{F}(\mathbf{\Lambda})\mathbf{P}^{-1},\end{aligned}$$

as long as C surrounds the spectrum of $\mathbf{B}$. In the case of a defective matrix, things become a bit more complicated. The operator $\mathrm{F}(\mathbf{B})$ can be defined through the Jordan form of $\mathbf{B}$. We will focus on diagonalizable matrices for simplicity.

Products between matrices and operators and key properties

For a matrix $\mathbf{B} \in \mathbb{C}^{p\times q}$ and a $\mathrm{F} \in \mathcal{B}(X, Y)$ we define

$$\mathbf{B} \otimes \mathrm{F} := \begin{bmatrix} b_{11}\mathrm{F} & b_{12}\mathrm{F} & \ldots & b_{1q}\mathrm{F} \\ b_{21}\mathrm{F} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ b_{p1}\mathrm{F} & b_{p2}\mathrm{F} & \ldots & b_{pq}\mathrm{F} \end{bmatrix} \in \mathcal{B}(X^q, Y^p).$$

With this in hand, we can define the action of a bounded linear operator on a matrix. Suppose $\mathrm{F} : \mathbb{C}_+ \to \mathcal{B}(X, Y)$ is an analytic map, and $\mathbf{B} \in \mathbb{C}^{p\times q}$ with its spectrum in $\mathbb{C}_+$. We define

$$\mathrm{F}(\mathbf{B}) := \frac{1}{2\pi i}\oint_C (z\mathbf{I} - \mathbf{B})^{-1} \otimes \mathrm{F}(z)dz, \tag{2.30}$$

where C is a simple closed positively oriented curve that surrounds the spectrum of $\mathbf{B}$. With all of this defining out of the way, we will now work through the key properties of the Dunford calculus that we will use to develop RKCQ methods. First, for any matrix $\mathbf{B}$,

$$\frac{1}{2\pi i}\oint_C (z\mathbf{I} - \mathbf{B})^{-1} \otimes I_X dz = \left(\frac{1}{2\pi i}\oint_C (z\mathbf{I} - \mathbf{B})^{-1}dz\right) \otimes I_x = \mathbf{I} \otimes I_X = I_{X^p},$$

as long as C is a simple closed curve surrounding the spectrum of $\mathbf{B}$. If $\mathrm{F} : \mathbb{C}_+ \to \mathcal{B}(X, Y)$ and $\mathrm{G} : \mathbb{C}_+ \to \mathcal{B}(Z, X)$, then

$$\mathrm{FG}(\mathbf{B}) = \mathrm{F}(\mathbf{B})\mathrm{G}(\mathbf{B}).$$

For $\mathbf{B} \in \mathbb{C}^{p\times q}$ and $\mathbf{C} \in \mathbb{C}^{q\times r}$, we have

$$(\mathbf{BC}) \otimes \mathrm{F} = (\mathbf{B} \otimes I_Y)\,(\mathbf{C} \otimes \mathrm{F}). \tag{2.31}$$

If we specialize to the case when $\mathbf{\Lambda}$ is a $p \times p$ diagonal matrix, we can show

$$(\mathbf{\Lambda C}) \otimes \mathrm{F} = (\mathbf{\Lambda} \otimes I_Y)(\mathbf{C} \otimes \mathrm{F}) = \begin{bmatrix} \lambda_1 \mathrm{row}(\mathbf{C}, 1) \otimes \mathrm{F} \\ \vdots \\ \lambda_p \mathrm{row}(\mathbf{C}, p) \otimes \mathrm{F} \end{bmatrix}. \tag{2.32}$$

Combining (2.31) and (2.32), we have for $\mathbf{B} \in \mathbb{C}^{p\times q}$, $\Lambda \in \mathbb{C}^{q\times q}$ a diagonal matrix, and $\mathbf{C} \in \mathbb{C}^{q\times r}$

$$\begin{aligned}((\mathbf{B\Lambda C}) \otimes \mathrm{F})_{ij} &= (\mathbf{B} \otimes I_Y)_{i\ell}((\mathbf{\Lambda C}) \otimes \mathrm{F}))_{\ell j} = \mathbf{B}_{i\ell} I_Y (\mathbf{C\Lambda})_{\ell j} \mathrm{F} \\ &= \mathbf{B}_{i\ell}\delta_{\ell k}\lambda_\ell \mathbf{C}_{kj}\mathrm{F} = \lambda_\ell \mathbf{B}_{i\ell}\mathbf{C}_{\ell j}\mathrm{F}.\end{aligned}$$

Written less compactly, we have

$$(\mathbf{B\Lambda C}) \otimes \mathrm{F} = \sum_{j=1}^{p} \mathrm{col}(\mathbf{B}, j) \otimes (\lambda_j \mathrm{row}(\mathbf{C}, j) \otimes \mathrm{F}). \tag{2.33}$$

We are finally in a position to begin computing operator-valued functions of a diagonalizable matrix. Suppose that $\mathbf{B} = \mathbf{P\Lambda P}^{-1}$ is a spectral decomposition of $\mathbf{B}$. If $\mathrm{F} : \mathbb{C}_+ \to \mathcal{B}(X, Y)$ is an analytic operator-valued function and $z \notin \sigma(\mathbf{B}) = \{\lambda_j\}$,

$$\begin{aligned}(z\mathbf{I} - \mathbf{B})^{-1} &= \sum_{j=1}^{p} \mathrm{col}(\mathbf{P}, j) \otimes ((z - \lambda_j)^{-1}\mathrm{row}(\mathbf{P}^{-1}, j) \otimes \mathrm{F}(z)) \\ &= \sum_{j=1}^{p} \mathrm{col}(\mathbf{P}, j) \otimes (\mathrm{row}(\mathbf{P}^{-1}, j) \otimes (z - \lambda_j)^{-1}\mathrm{F}(z)).\end{aligned}$$

Integrating around a simple closed curve that surrounds $\sigma(\mathbf{B})$, we get

$$\mathrm{F}(\mathbf{B}) = \sum_{j=1}^{p} \mathrm{col}(\mathbf{P}, j) \otimes (\mathrm{row}(\mathbf{P}^{-1}, j) \otimes \mathrm{F}(\lambda_j)),$$

which is a simple way to compute the integral in (2.30).

2.10 Moving Towards RKCQ

As was done in the scalar case, we are interested in discretizing $y = f * g$ as

$$y(t_n + \kappa \mathbf{c}) \approx \mathbf{y}_n = \sum_{m=0}^{n} W_m^{\mathrm{F}}(\kappa)\mathbf{g}_{n-m}, \quad \mathbf{g}_n = g(t_n + \kappa \mathbf{c}),$$

where the convolution weights are the coefficients of the Taylor series

$$\mathrm{F}(\tfrac{1}{\kappa}\Delta(\zeta)) = \sum_{m=0}^{\infty} W_m^{\mathrm{F}}(\kappa)\zeta^m.$$

We can also use the ζ-transform

$$\mathbf{Y}(\zeta) = \mathrm{F}(\tfrac{1}{\kappa}\Delta(\zeta))\mathbf{G}(\zeta).$$

If we discretize a convolution equation $f * g = h$, we wind up with

$$\sum_{m=0}^{n} W_m^{\mathrm{F}}(\kappa)\mathbf{g}_{n-m} = \mathbf{h}_n,$$

which can be written as a marching-on-in-time scheme as

$$W_0^{\mathrm{F}}(\kappa)\mathbf{g}_n = \mathbf{h}_n - \sum_{m=1}^{n} W_m^{\mathrm{F}}(\kappa)\mathbf{g}_{n-m}.$$

Note that $W_0^{\mathrm{F}}(\kappa) = \mathrm{F}(\frac{1}{\kappa}\Delta(0)) = \mathrm{F}(\frac{1}{\kappa}\mathbf{A}^{-1})$, which is another way of showing that we are restricted to implicit RK methods for RKCQ. Actually, we require more of our RK method. We require that $\sigma(\mathbf{A}) \subset \mathbb{C}_+$, which is equivalent to the RK method being A-stable.

The convolution in continuous time

In the scalar CQ case we demonstrated that even though CQ produces output at discrete time steps, there is a continuous-in-time convolution in the background that we can study and use for theoretical purposes. Given an operator-valued distribution f and its Laplace transform F, we were able to understand

$$\mathrm{F}(\tfrac{1}{\kappa}\delta(\zeta)) = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa)\zeta^m, \quad \mathrm{F}(s_\kappa) = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa)e^{-st_n}, \quad s_\kappa = \tfrac{1}{\kappa}\delta(e^{-s\kappa})$$

as the Laplace domain version of

$$f_\kappa = \sum_{m=0}^{\infty} \omega_m^{\mathrm{F}}(\kappa) \otimes \delta_{t_m}, \quad \mathcal{L}\{f_\kappa\}(s) = \mathrm{F}(s_\kappa).$$

We can try to replicate this argument for RKCQ as follows. We define $\mathbf{S}_\kappa := \frac{1}{\kappa}\Delta(e^{-s\kappa})$ and compute

$$\mathrm{F}(\mathbf{S}_\kappa) = \sum_{m=0}^{\infty} W_m^{\mathrm{F}}(\kappa) e^{-st_m}.$$

This is the Laplace transform of the causal distribution

$$\mathbf{F}_\kappa := \sum_{m=0}^{\infty} W_m^{\mathrm{F}}(\kappa) \otimes \delta_{t_m}.$$

A difficulty arises because $W_m^{\mathrm{F}}(\kappa) \in \mathcal{B}(X^p, Y^p)$, and so these weights cannot act directly on a distribution $g \in X$. We must first modify g by

$$X \ni g \longmapsto \begin{bmatrix} g(\cdot + \kappa c_1) \\ \vdots \\ g(\cdot + \kappa c_p) \end{bmatrix} =: g(\cdot + \kappa \mathbf{c}) \in X^p.$$

Therefore, RKCQ is the sample at the level of stages of the continuous-in-time convolution

$$\mathbf{F}_\kappa * g(\cdot + \kappa \mathbf{c}) = \sum_{m=0}^{\infty} W_m^{\mathrm{F}}(\kappa) g(\cdot - t_m + \kappa \mathbf{c}).$$

RKCQ Algorithms

We will now present a summary of the algorithms for an implementation of RKCQ tools. We do not provide as many details as in the scalar case, since many of the steps are similar or the same. We take our integration contour to be $C_R := \{\zeta \in \mathbb{C} \ : \ |\zeta| = \epsilon^{1/(2N+2)}\}$ where we use $N+1$ points for the composite trapezoid rule quadrature of Cauchy's integral formula. We compute

$$\begin{aligned} W_m^{\mathrm{F}}(\kappa) &= \frac{1}{m!}\frac{d^m}{d\zeta^m}\,\mathrm{F}\left(\frac{1}{\kappa}\Delta(\zeta)\right)\Big|_{\zeta=0} = \frac{1}{2\pi i}\oint_{C_R} \zeta^{-n-1}\mathrm{F}(\tfrac{1}{\kappa}\Delta(\zeta))d\zeta \\ &\approx \frac{R^{-m}}{N+1}\sum_{\ell=0}^{N} \zeta_{N+1}^{n\ell}\mathrm{F}(\tfrac{1}{\kappa}\Delta(\zeta_{N+1}^{-\ell})), \quad n = 0, \ldots, N. \end{aligned}$$

Algorithm 2.10.1 (Computation of RKCQ coefficients)**.** *For a stiffly accurate method, we write* $\Delta(\zeta) = \mathbf{A}^{-1} + \zeta\mathbf{C}$ *where* $\mathbf{C} := \mathbf{A}^{-1}\mathbf{1}\mathbf{e}_p^T$*. We then proceed as follows:*

(1) For $\ell = 0, \dots N$ *find the spectral decomposition*

$$\mathbf{P}_\ell \mathbf{\Lambda}_\ell \mathbf{P}_\ell^{-1} = \frac{1}{\kappa}\Delta(R\zeta_{N+1}^{-\ell})$$

and loop over stages to compute

$$\widehat{\mathrm{F}}_\ell := \mathrm{F}(\tfrac{1}{\kappa}\Delta(R\zeta_{N+1}^{-\ell})).$$

(2) Apply the IDFT and scale

$$W_m^{\mathrm{F}}(\kappa) := R^{-m}\left(\frac{1}{N+1}\sum_{\ell=0}^{N}\widehat{\mathrm{F}}_\ell\zeta_{N+1}^{m\ell}\right).$$

Note that this algorithm assumes $\Delta(\zeta)$ *is diagonalizable for all* ζ *in the integration contour.*

All-steps-at-once computation of forward convolutions

Our goal is to compute $y = f * g$, where $\mathrm{F}(s) = \mathcal{L}\{f\}(s)$ and g are known. We begin by sampling the data g on the stages

$$\mathbf{g}_n := g(t_n + \kappa\mathbf{c}), \quad n = 0, \dots, N$$

and we aim to compute

$$\mathbf{y}_n = \sum_{m=0}^{n} W_{n-m}^{\mathrm{F}}(\kappa)\mathbf{g}(t_m) = \sum_{m=0}^{N} W_{n-m}^{\mathrm{F}}(\kappa)\mathbf{g}(t_m), \quad n = 0, \dots, N$$

where we have used that the convolution weights $W_m^{\mathrm{F}}(\kappa)$ are zero for $m < 0$. Using the approximation developed earlier, we have

$$W_m^{\mathrm{F}}(\kappa) \approx \frac{R^{-m}}{N+1}\sum_{\ell=0}^{N}\widehat{\mathrm{F}}_\ell\zeta_{N+1}^{m\ell}, \quad \widehat{\mathrm{F}} = \mathrm{F}(\tfrac{1}{\kappa}\Delta(R\zeta_{N+1}^{-\ell})),$$

and so our approximation to $y = f * g$ takes the form

$$\mathbf{y}_n \approx R^{-n}\left(\frac{1}{N+1}\sum_{\ell=0}^{N}\widehat{\mathrm{F}}_\ell\left(\sum_{m=0}^{N}R^m\mathbf{g}_m\zeta_{N+1}^{-m\ell}\right)\zeta_{N+1}^{\ell}\right).$$

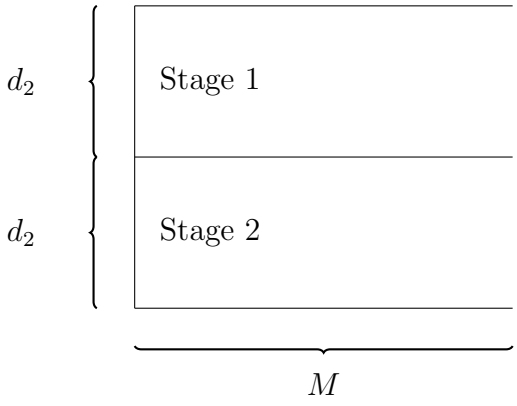

Figure 2.3: Organization of data for RKCQ in the finite dimensional case.

Let us now take a moment to consider the case when we are working with finite-dimensional data, $g : \mathbb{R} \to \mathbb{R}^{d_2}$ and $f : \mathbb{R} \to \mathbb{R}^{d_1 \times d_2}$. It is most natural to work with the sampled data $\mathbf{g}_n \in \mathbb{R}^{pd_2}$ organized in p blocks of d_2 components. This is illustrated in Figure (2.3) for $p = 2$. The key step is the multiplication $\widehat{\mathrm{F}}_\ell \widehat{\mathbf{h}}_\ell$ for a given vector $\mathbf{h}_n \in \mathbb{C}^{pd_2}$. When we have the eigendecomposition $\frac{1}{\kappa}\Delta(R\zeta_{N+1}^{-\ell}) = \mathbf{P}_\ell \mathbf{\Lambda}_\ell \mathbf{P}_\ell^{-1}$, then we can use our earlier results from the Dunford calculus to show

$$\widehat{\mathrm{F}}_\ell \widehat{\mathbf{h}}_\ell = (\mathbf{P}_\ell \otimes \mathbf{I}_{d_1})\mathrm{diag}(\mathrm{F}(\lambda_1), \ldots, \mathrm{F}(\lambda_p))(\mathbf{P}_\ell^{-1} \otimes \mathbf{I}_{d_2})\widehat{\mathbf{h}}_\ell. \tag{2.34}$$

We can now proceed to describe the algorithm.

Algorithm 2.10.2 (All steps at once forward convolutions)**.** *We assume data has been sampled at the discrete times*

$$\mathbf{g}_n = g(t_n + \kappa \mathbf{c}) \in X^p, \quad n = 0, \ldots, N.$$

(1) Scale the data: $\mathbf{h}_m := R^m \mathbf{g}_m, \quad m = 0, \ldots, N.$

(2) Compute the DFT

$$\widehat{\mathbf{h}}_\ell := \sum_{m=0}^{N} \mathbf{h}_m \zeta_{N+1}^{-m\ell}, \quad \ell = 0, \ldots, N.$$

These are formal DFTs, componenwise in X^p. When $X = \mathbb{R}^d$, these can be broken into pd separate scalar DFTs.

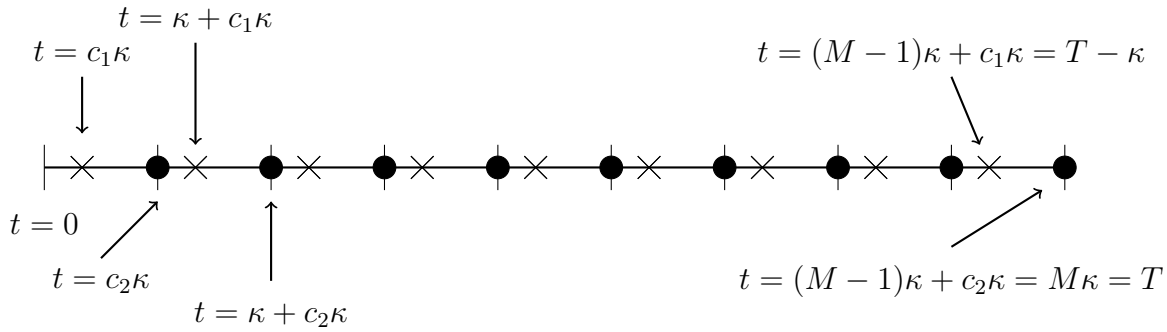

Figure 2.4: Structure of RKCQ approximation for a two stage stiffly accurate RK method. Circles represent the second stage (and also time step), while crosses are the points for the first stage.

(3) For every $\ell = 0, \ldots, N$, compute the eigendecomposition $\frac{1}{\kappa}\Delta(R\zeta_{N+1}^{-\ell}) = \mathbf{P}_\ell \mathbf{\Lambda}_\ell \mathbf{P}_\ell^{-1}$ *and compute*

$$\widehat{\mathbf{v}}_\ell := \widehat{\mathrm{F}}_\ell \widehat{\mathbf{h}}_\ell = (\mathbf{P}_\ell \otimes \mathbf{I}_Y)\mathrm{diag}(\mathrm{F}(\lambda_1), \ldots, \mathrm{F}(\lambda_p))(\mathbf{P}_\ell^{-1} \otimes \mathbf{I}_X)\widehat{\mathbf{h}}_\ell.$$

(4) Compute the IDFT

$$\mathbf{v}_n := \frac{1}{N+1}\sum_{\ell=0}^{N} \widehat{\mathbf{v}}_\ell \zeta_{N+1}^{\ell n}, \quad n = 0, \ldots, N.$$

(5) Scale back

$$\mathbf{u}_n := R^{-n}\mathbf{v}_n \in Y^p, \quad n = 0, \ldots, N.$$

If this is the last step of a sequence of convolutions, we can discard the internal stages and keep only the last step of $\mathbf{u}_n$ as an approximation to $u(t_{n+1})$. Because the RKCQ method counts stages, which are groups of steps, and not the steps themselves, we do not compute an approximation at t_0, and the final time step takes us to t_{N+1} and not t_N.

The algorithm for forward convolutions can be easily modified to handle convolution equations. The only change is replacing the multiplication in step 3 with a solution to

$$\widehat{\mathrm{F}}_\ell^{-1}\widehat{\boldsymbol{v}}_m = \widehat{\mathrm{F}}_\ell \widehat{\boldsymbol{h}}_\ell = (\boldsymbol{P}_\ell \otimes I_Y)\mathrm{diag}(\mathrm{F}(\lambda_1)^{-1}, \ldots, \mathrm{F}(\lambda_p)^{-1})(\boldsymbol{P}_\ell^{-1} \otimes I_X)\widehat{\boldsymbol{v}}_\ell,$$

that is, we need to solve p equations associated to the operators $\mathrm{F}(\lambda_j)$.

Algorithm 2.10.3 (Computation of a piece of a convolution)**.** *The algorithm to compute*

$$\boldsymbol{g}_n := \sum_{m=0}^{Q} W_n^{\mathrm{F}}(\kappa)\boldsymbol{u}_m, \qquad n = Q+1, \ldots, M,$$

renumbered in the form

$$\widetilde{\boldsymbol{g}}_k := \sum_{m=0}^{Q} W_{k+Q+1-m}^{\mathrm{F}}(\kappa)\boldsymbol{u}_m, \qquad k = 0, \ldots, M-Q-1,$$

starting from vectors $\boldsymbol{u}_m \in X^p$ and outputting values in Y^p, and using approximations

$$W_n^{\mathrm{F}}(\kappa) \approx \frac{R^{-n}}{N+1} \sum_{\ell=0}^{N} \widehat{\mathrm{F}}_\ell \zeta_{N+1}^{n\ell}, \qquad \widehat{\mathrm{F}}_\ell := \mathrm{F}(\tfrac{1}{\kappa}\Delta(R\zeta_{N+1}^{-\ell})) \tag{2.35}$$

(for positive and negative n) is derived in an entirely similar way to what we did for scalar CQ. The parameter $N \geq M$ is a design parameter that influences the size of the computation, but also the precision to which the approximations are carried out.

(1) Scale and augment data

$$\boldsymbol{w}_m := \begin{cases} R^m \boldsymbol{u}_m, & 0 \leq m \leq Q, \\ \boldsymbol{0}, & Q+1 \leq m \leq N. \end{cases}$$

(2) Compute the DFT $\widehat{\boldsymbol{w}}_\ell$ ($\ell = 0, \ldots, N$) of the vectors in (1).

(3) For every $\ell = 0, \ldots, N$, find the spectral decomposition $\frac{1}{\kappa}\Delta(R\zeta_{N+1}^{-\ell}) = \boldsymbol{P}_\ell \boldsymbol{\Lambda}_\ell \boldsymbol{P}_\ell^{-1}$ and compute

$$\widehat{\boldsymbol{h}}_\ell := \zeta_{N+1}^{\ell(Q+1)} \widehat{\mathrm{F}}_\ell \widehat{\boldsymbol{w}}_\ell = \zeta_{N+1}^{\ell(Q+1)} (\boldsymbol{P}_\ell \otimes I_Y) \mathrm{diag}(\mathrm{F}(\lambda_1), \ldots, \mathrm{F}(\lambda_p)) (\boldsymbol{P}_\ell^{-1} \otimes I_X) \widehat{\boldsymbol{w}}_\ell.$$

(4) Compute the IDFT of the sequence in (3), $\boldsymbol{h}_\ell$ ($\ell = 0, \ldots, N$).

(5) Scale and chop the resulting sequence

$$\widetilde{\boldsymbol{g}}_k := R^{-k-Q-1} \boldsymbol{h}_\ell, \qquad k = 0, \ldots, M-Q-1.$$

2.11 Convergence Results for RKCQ

We state here the main theorem of [12] on the convergence of Runge-Kutta Convolution Quadrature. We require first a few assumptions on the convolution kernel and Runge-Kutta method. We suppose that the convolution kernel F is analytic in the half-plane $\operatorname{Re} s \geq \sigma$ and satisfies for some real exponent μ and bounding factor M

$$|\mathrm{F}(s)| \leq M|s|^{-\mu} \quad \text{for } \operatorname{Re} s \geq \sigma.$$

In particular, the convolution kernels described in Definition A.3.1 satisfy these hypotheses. We assume that the Runge-Kutta method satisfies the following:

(1) The RK method is A stable with classical order p and stage order $q \leq p$,

(2) the stability function satisfies $|R(iy)| < 1$ for all real $y \neq 0$,

(3) $R(\infty) = 0$, and

(4) the RK coefficient matrix A is invertible.

For such convolution kernels and RK methods, the authors prove the following

Theorem 2.11.1. *For data $g \in \mathcal{C}^p[0,T]$ there is an $h_0 > 0$ such that for $0 < h \leq h_0$ and $nh \leq T$ the error of the Convolution Quadrature approximation is bounded as*

$$\begin{aligned} |u_n - u(t_n)| \leq & C \sum_{\ell=0}^{q} h^{\min(p,\ell+\mu)} |g^{(\ell)}(0)| \\ & + Ch^{\min(p,q+1+\mu)} \left(\sum_{\ell=q+1}^{p-1} |g^{(\ell)}(0)| + \max_{0\leq\tau\leq t_n} |g^{(p)}(\tau)| \right). \end{aligned}$$

The constant C depends on T.

Chapter 3

INTEGRAL METHODS FOR TRANSIENT STOKES FLOW

This chapter presents analysis and simulation of the single layer potential and operator for transient Stokes flow in the exterior of a bounded domain in two or three dimensions. We present a Laplace domain analysis of the Brinkman equations with the goal of deriving of CQ-type estimates for the Stokes problem in the time domain. For spatial discretization, we use a Galerkin-BEM approach that can be cast as an exotic transmission problem in the space variables. We are able to show stability and convergence for the Dirichlet Stokes problem using an indirect single layer representation. Technical challenges arise when considering the pressure potential in the two-dimensional case. We are able to show through a novel asymptotic argument in the pressure that we only miss being in $L^2(\mathbb{R}^2)$ in the first order term, and so a simple correction results in an appropriately bounded pressure potential. The results of this chapter appear in *Boundary integral solvers for an evolutionary exterior Stokes problem* (with C. Bacuta, G. Hsiao, and F.–J. Sayas) [6].

The literature on numerical methods for integral representations of parabolic problems has focused extensively on the heat equation. Most theoretical results are based on the single layer representation, leading to a Volterrà-Fredholm integral equation that can be formally considered to be of the first kind. (We note that the mapping properties of the integral operators make the integral equations of the second kind for parabolic problems not to be a smooth perturbation of the identity, due to the mapping properties in the time variable. Additional complications arise when the boundary is not smooth.) This analysis was sparked by the work of Arnold and Noon [4] and Costabel [23], with some sequels as [43]. The work of Lubich and Schneider [62] offered

a numerical treatment of the heat equation single layer operator equation. Other formulations, including fast multiplication techniques, appear in recent work of Tausch [79, 80, 66]. The mathematical literature for the unsteady exterior Stokes problem using integral equations seems to be quite limited: see, for instance, [39], [40]. A general overview of the state of the art of time domain integral equations one decade ago can be found in [24].

For our analysis we will rely on properties of the Brinkman single layer potential. We will however take a different approach than the one given in [47, 46, 48], since we need to study the behavior of all the bounds as functions of the parameter in the Brinkman model. We will adopt a Laplace domain approach similar to the one used in [7] for the wave equation. For some technical issues, we will rely on recent results on the Stokes potentials on general Lipschitz domains [75]. The passage to the time-domain will be done with a modification of a result in [62]. Following [52] we will analyze the semidiscretization in space in a systematic way, showing that a postprocessed solution (the velocity field) can have better properties than the preprocessed solution (the boundary density and, therefore, the pressure field, which is postprocessed with a steady-state operator). Finally, we will apply a general multistep-based Convolution Quadrature strategy and analyze it using the results in [58]. We note that this final step will be the only one where we will not be able to analyze how the constants that appear in the error estimates depend on time (as the latter grows to infinity).

The Stokes system will be written in the following form

$$\begin{aligned} \dot{\mathbf{u}} - \nu \Delta \mathbf{u} + \nabla p &= \mathbf{0} \\ \nabla \cdot \mathbf{u} &= 0, \end{aligned}$$

where ν is the hydrodynamic viscosity, $\mathbf{u}$ is a velocity field and p denotes the pressure. The Laplace transformed Stokes system (resolvent Stokes system)

$$s\mathbf{u} - \nu \Delta \mathbf{u} + \nabla p = 0, \qquad \nabla \cdot \mathbf{u} = 0$$

can be identified (when $s > 0$) with the equations of Brinkman flow.

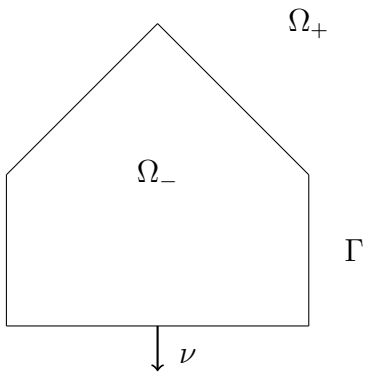

Figure 3.1: A sketch of the geometry for the exterior Stokes problem.

3.1 Notation and Sobolev Spaces

For our analysis, we will make use of a complex number not on the negative real axis:

$$s \in \mathbb{C}_\star := \mathbb{C} \setminus (-\infty, 0]. \tag{3.1}$$

We also need the space of Solenoidal vector fields

$$\widehat{\mathbf{V}}(\mathbb{R}^d) := \{\mathbf{u} \in \mathbf{H}^1(\mathbb{R}^d) \ : \ \operatorname{div} \mathbf{u} = 0\}.$$

We will make use of the triplet of inner products defined for open sets $\Omega \subset \mathbb{R}^d$ and scalar-valued, vector-valued, and tensor-valued functions:

$$(u, v)_\Omega = \int_\Omega uv, \quad (\mathbf{u}, \mathbf{v})_\Omega = \int_\Omega \mathbf{u} \cdot \mathbf{v}, \quad (\mathrm{U}, \mathrm{V})_\Omega = \int_\Omega \mathrm{U} : \mathrm{V},$$

where in the last we have used the Frobenius inner product, $\mathrm{U} : \mathrm{V} = \sum_{i,j} \mathrm{U}_{ij}\mathrm{V}_{ij}$. Our geometry will consist of a bounded Lipschitz domain Ω_- with a connected boundary Γ. We will denote its unbounded exterior $\Omega_+ := \mathbb{R}^d \setminus \overline{\Omega_-}$. For operators defined on both sides of Γ, we will indicate on which side we take a limit or restriction with $\pm$. For example, the exterior trace will be γ^+ and the interior trace will be γ^-. The angled brackets $\langle \cdot, \cdot, \rangle_\Gamma$ will refer to the $L^2(\Gamma)$ or $\mathbf{L}^2(\Gamma)$ inner products on the boundary Γ, as well as their extensions to the duality products of $H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)$ and their

vector counterparts. For a locally $\mathbf{H}^1$ function, we can define the jump of its trace by $[\![\gamma \mathbf{v}]\!] := \gamma^- \mathbf{v} - \gamma^+ \mathbf{v}$. The negative hydrodynamic stress is defined as

$$\boldsymbol{\sigma} := -2\nu\, \varepsilon(\mathbf{u}) + p\mathbf{I}, \quad \varepsilon(\mathbf{u}) := \tfrac{1}{2}(D\mathbf{u} + (D\mathbf{u})^T)$$

where $\mathbf{I}$ is the identity matrix and $(D\mathbf{u})_{ij} = u_{i,j}$. If $\mathbf{u}$ and p are such that $\operatorname{div} \boldsymbol{\sigma} \in \mathbf{L}^2(\mathbb{R}^d \setminus \Gamma)$ (where the divergence is applied to the rows of $\boldsymbol{\sigma}$) and we set

$$\mathbf{f} := -2\nu \operatorname{div} \varepsilon(\mathbf{u}) + \nabla p \in L^2(\mathbb{R}^d \setminus \Gamma),$$

then we can define the linear functionals $\mathbf{t}^{\pm}(\mathbf{u}, p) \in \mathbf{H}^{-1/2}(\Gamma)$ by

$$\begin{aligned} \langle \mathbf{t}^-(\mathbf{u}, p), \gamma \mathbf{v} \rangle_\Gamma &:= 2\nu(\varepsilon(\mathbf{u}), \varepsilon(\mathbf{v}))_{\Omega_-} - (p, \operatorname{div} \mathbf{v})_{\Omega_-} - (\mathbf{f}, \mathbf{v})_{\Omega_-} \quad \forall \mathbf{v} \in \mathbf{H}^1(\Omega_-), \\ \langle \mathbf{t}^+(\mathbf{u}, p), \gamma \mathbf{v} \rangle_\Gamma &:= -2\nu(\varepsilon(\mathbf{u}), \varepsilon(\mathbf{v}))_{\Omega_+} + (p, \operatorname{div} \mathbf{v})_{\Omega_+} + (\mathbf{f}, \mathbf{v})_{\Omega_+} \quad \forall \mathbf{v} \in \mathbf{H}^1(\Omega_+). \end{aligned}$$

This allows us to define the jump in the normal stress $[\![\mathbf{t}(\mathbf{u}, p)]\!] := \mathbf{t}^-(\mathbf{u}, p) - \mathbf{t}^+(\mathbf{u}, p)$. As a consequence, we have

$$\begin{aligned} \langle [\![\mathbf{t}(\mathbf{u}, p)]\!], \gamma \mathbf{v} \rangle_\Gamma = a(\mathbf{u}, \mathbf{v}) - (p, \operatorname{div} \mathbf{v})_{\mathbb{R}^d} + (-2\nu \operatorname{div} \varepsilon(\mathbf{u}) + \nabla p, \mathbf{v})_{\mathbb{R}^d \setminus \Gamma} \\ \forall \mathbf{v} \in \mathcal{D}(\mathbb{R}^d)^d, \end{aligned} \tag{3.2}$$

where $a(\mathbf{u}, \mathbf{v}) = 2\nu(\varepsilon(\mathbf{u}), \varepsilon(\mathbf{v}))_{\mathbb{R}^d}$ and $\mathcal{D}(\mathbb{R}^d)$ is the set of $\mathcal{C}^\infty$ compactly supported functions (see Appendix B).

3.2 Integral Forms of the Stokes Problem

We now present the single layer pressure and velocity potentials for the Stokes problems in 2 and 3 dimensions. The following definitions can be found in [46], [48], [47, p.81]. For a given density $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma)$, we define the **Stokes pressure potential**

$$(\mathrm{S}_p \boldsymbol{\lambda})(\mathbf{z}) := \langle \mathbf{e}_p(\mathbf{z} - \cdot), \boldsymbol{\lambda} \rangle_\Gamma, \quad \mathbf{z} \in \mathbb{R}^d \setminus \Gamma,$$

where

$$\mathbf{e}_p(\mathbf{r}) := \frac{1}{2(d-1)\pi} \frac{1}{|\mathbf{r}|^d} \mathbf{r}$$

is the negative gradient of the fundamental solution to the Laplacian and $\mathbf{r}_{ij} = x_i - x_j$. This is the fundamental solution to the pressure component of the Stokes equation. In two dimensions, taking $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma)$ is not sufficient to give a rapidly enough decaying pressure at infinity, so we require $\boldsymbol{\lambda}$ to be in the space

$$\mathbf{H}_0^{-1/2}(\Gamma) := \{\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma) \ : \ \langle \boldsymbol{\lambda}, \mathbf{a} \rangle_\Gamma = 0 \quad \forall \mathbf{a} \in \mathbf{P}_0(\Gamma)\}.$$

Because the pressure part of the Brinkman and Stokes problem are the same, we have the following result [75, Propositions 5.2 and 7.2]:

Proposition 3.2.1. *(a) When $d = 3$, $\mathrm{S}_p : \mathbf{H}^{-1/2}(\Gamma) \to L^2(\mathbb{R}^3)$ is bounded.*

(b) When $d = 2$, $\mathrm{S}_p : \mathbf{H}_0^{-1/2}(\Gamma) \to L^2(\mathbb{R}^2)$ is bounded.

Asymptotics of the pressure in the two dimensional case

The condition that the density $\boldsymbol{\lambda} \in \mathbf{H}_0^{-1/2}(\Gamma)$ in the two-dimensional case only impacts the behavior of the pressure at infinity. To understand how the pressure behaves without the zero integral condition, we can show the first-order asymptotics of the pressure to be

$$\frac{1}{2\pi} \langle \mathbf{e}_p(\mathbf{z}), \boldsymbol{\lambda} \rangle_\Gamma = \frac{1}{2\pi} \frac{1}{1 + |\mathbf{z}|^2} \langle \mathbf{z}, \boldsymbol{\lambda} \rangle_\Gamma + \mathcal{O}(|\mathbf{z}|^{-2})$$

as $|\mathbf{z}| \to \infty$. Therefore, we are able to capture the leading order term which is not in $L^2(\mathbb{R}^2)$ and a remainder that is in $L^2(\mathbb{R}^2)$. We can then correct for the leading term as in the following proposition.

Proposition 3.2.2. *Define*

$$\mathbf{p}_\infty(\mathbf{x}) := \frac{1}{2\pi} \frac{1}{1 + |\mathbf{x}|^2} \mathbf{x},$$
$$j_\ell(\boldsymbol{\lambda}) := \langle \boldsymbol{\lambda}, \mathbf{e}_\ell \rangle_\Gamma, \quad \ell = 1, 2,$$

where $\{\mathbf{e}_1, \mathbf{e}_2\}$ is the canonical basis of $\mathbb{R}^2$. Then

$$\mathrm{S}_p - \sum_{\ell=1}^{2} (\mathbf{p}_\infty \cdot \mathbf{e}_\ell) j_\ell : \mathbf{H}^{-1/2}(\Gamma) \to \mathbf{L}^2(\mathbb{R}^2)$$

is bounded.

For $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma)$, we define the **Brinkman velocity potential**

$$\left(\mathrm{S}_u(s)\boldsymbol{\lambda}\right)(\mathbf{z}) := \langle \mathrm{E}_u(\mathbf{z}-\cdot\,;s), \boldsymbol{\lambda}\rangle_\Gamma, \quad \mathbf{z} \in \mathbb{R}^d \setminus \Gamma$$

where

$$\mathrm{E}_u(\mathbf{r};s) := \frac{1}{4(d-1)\pi\nu}\left(\frac{A_d(\sqrt{s}|\mathbf{r}|)}{|\mathbf{r}|^{d-2}}\mathrm{I} + \frac{B_d(\sqrt{s}|\mathbf{r}|)}{|\mathbf{r}|^d}\mathbf{r}\otimes\mathbf{r}\right).$$

The functions A_d and B_d vary in $d = 2$ and $d = 3$ dimensions, and are given by the expressions

$$\begin{aligned}
A_3(z) &:= e^{-z}(1+z^{-1}+z^{-2}) - 2z^{-2} = 2z^{-2}(e^{-z}(z^2+z+1)-1),\\
B_3(z) &:= -2e^{-z}(1+3z^{-1}+3z^{-2}) + 6z^{-2} = -2z^{-2}(e^{-z}(z^2+3z+3)-3),\\
A_2(z) &:= 2(K_0(z) + z^{-1}K_0(z) - z^{-2}),\\
B_2(z) &:= 2(-K_0(z) - 2z^{-1}K_1(z) + 2z^{-2}) = 2(2z^{-2} - K_2(z)).
\end{aligned}$$

Here K_ℓ is the modified Bessel function of order ℓ. In three dimensions, A_3 and B_3 are entire and satisfy $A_3(0) = B_3(0) = 1$. In two dimensions, A_2 and B_2 are analytic in $\mathbb{C}_\star$ with a branch cut along the negative real axis $(-\infty, 0]$. We now proceed with a careful study of the velocity potential.

3.3 Variational Study of the 3D Single Layer Potential

Proposition 3.3.1. *Let* $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma)$ *and consider* $\mathbf{u}_\lambda := \mathrm{S}_u(s)\boldsymbol{\lambda} \in \mathbf{H}^1(\mathbb{R}^3)$ *and* $p_\lambda := \mathrm{S}_p\boldsymbol{\lambda} \in L^2(\mathbb{R}^3)$. *Then*

$$-2\nu\,\mathrm{div}\,\varepsilon(\mathbf{u}_\lambda) + s\mathbf{u}_\lambda + \nabla p_\lambda = \mathbf{0} \quad \textit{in } \mathbb{R}^3\setminus\Gamma, \tag{3.3a}$$

$$\mathrm{div}\,\mathbf{u}_\lambda = 0 \quad \textit{in } \mathbb{R}^3\setminus\Gamma, \tag{3.3b}$$

$$[\![\gamma\mathbf{u}_\lambda]\!] = 0, \tag{3.3c}$$

$$[\![\mathbf{t}(\mathbf{u}_\lambda, p_\lambda)]\!] = \boldsymbol{\lambda}. \tag{3.3d}$$

Moreover, a pair $(\mathbf{u}_\lambda, p_\lambda) \in \mathbf{H}^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ *is a solution of equation* (3.3) *if and only if*

$$\mathbf{u}_\lambda \in \mathbf{H}^1(\mathbb{R}^3),\ p_\lambda \in L^2(\mathbb{R}^3), \tag{3.4a}$$

$$a(\mathbf{u}_\lambda, \mathbf{v}) + s(\mathbf{u}_\lambda, \mathbf{v})_{\mathbb{R}^3} - (p_\lambda, \operatorname{div} \mathbf{v})_{\mathbb{R}^3} = \langle \boldsymbol{\lambda}, \gamma \mathbf{v} \rangle_\Gamma \quad \forall \mathbf{v} \in \mathbf{H}^1(\mathbb{R}^3), \tag{3.4b}$$

$$(\operatorname{div} \mathbf{u}_\lambda, q)_{\mathbb{R}^3} = 0 \quad \forall q \in L^2(\mathbb{R}^3). \tag{3.4c}$$

Proof. Our use of the integral representation of the solution gives the required regularity for $\mathbf{u}_\lambda$ and p_λ. The fundamental solutions satisfy the differential equations strongly, and therefore distributionally. Continuity of the trace of the velocity field follows because we have that $\mathbf{u}_\lambda \in \mathbf{H}^1(\mathbb{R}^3)$. The last equation in (3.3) follows from the PDE and (3.2). The equivalence of (3.3) and (3.4) is straightforward. □

We can also formulate the velocity part of the Brinkman equation in solenoidal Sobolev spaces as follows.

Proposition 3.3.2. *If* $(\mathbf{u}_\lambda, p_\lambda) \in \mathbf{H}^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ *is a solution to* (3.3)*, then* $\mathbf{u}_\lambda$ *satisfies*

$$\begin{aligned} &\mathbf{u}_\lambda \in \widehat{\mathbf{V}}(\mathbb{R}^3), \\ &a(\mathbf{u}_\lambda, \mathbf{v}) + s(\mathbf{u}_\lambda, \mathbf{v})_{\mathbb{R}^3} = \langle \boldsymbol{\lambda}, \gamma \mathbf{v} \rangle_\Gamma \quad \forall \mathbf{v} \in \widehat{\mathbf{V}}(\mathbb{R}^3). \end{aligned} \tag{3.5}$$

In addition, (3.5) *is well-posed.*

Proof. If we consider equation (3.4) with a test function $\mathbf{v} \in \widehat{\mathbf{V}}(\mathbb{R}^3)$, then $\mathbf{u}_\lambda$ satisfies (3.5). Applying Korn's first inequality

$$\|\mathbf{u}\|^2_{1,\mathbb{R}^3} \leq 2\|\varepsilon(\mathbf{u})\|^2_{\mathbb{R}^3} + \|\mathbf{u}\|^2_{\mathbb{R}^3} \leq 2\|\mathbf{u}\|^2_{1,\mathbb{R}^3} \quad \forall \mathbf{u} \in \mathcal{D}(\mathbb{R}^3).$$

and filling by density, the bilinear form in (3.5) is coercive, and therefore the problem is well-posed. □

We also have the following.

Corollary 3.3.3. *Problem* (3.4) *has a unique solution.*

Proof. If $(\mathbf{u}, p)$ satisfies (3.4) with $\boldsymbol{\lambda} = \mathbf{0}$, then by Proposition (3.3.2), $\mathbf{u} = \mathbf{0}$. Therefore $p \in L^2(\mathbb{R}^3)$ and $\nabla p = \mathbf{0}$, so $p = 0$. □

Corollary 3.3.4. $\mathrm{S}_u(s)\mathbf{n} \equiv \mathbf{0}$.

Proof. It is clear that $(\mathbf{0}, -\chi_{\Omega_-})$ is a solution of (3.4) with $\boldsymbol{\lambda} = \mathbf{n}$. By uniqueness, this is the layer potential. □

3.4 The Two Dimensional Case

The analysis for the Brinkman equations differs in two dimensions because of the zero integral condition required on the boundary density. This is triggered because the relevant weighted Sobolev spaces admit constant functions in $\mathbb{R}^2$, but not in $\mathbb{R}^3$. Details regarding these spaces can be found in [75]. We make use of the previous asymptotic expansion of the pressure to show well-posedness of the two dimensional problem.

Proposition 3.4.1. *If* $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma)$ *and we consider* $\mathbf{u}_\lambda := \mathrm{S}_u(s)\boldsymbol{\lambda} \in \mathbf{H}^1(\mathbb{R}^2)$ *and* $p_\lambda := \mathrm{S}_p\boldsymbol{\lambda} \in L^2_{loc}(\mathbb{R}^2)$. *Then*

$$-2\nu \operatorname{div} \varepsilon(\mathbf{u}_\lambda) + s\mathbf{u}_\lambda + \nabla p_\lambda = \mathbf{0} \quad \text{in } \mathbb{R}^2 \setminus \Gamma, \tag{3.6a}$$

$$\operatorname{div} \mathbf{u}_\lambda = 0 \quad \text{in } \mathbb{R}^2 \setminus \Gamma, \tag{3.6b}$$

$$[\![\gamma \mathbf{u}_\lambda]\!] = 0, \tag{3.6c}$$

$$[\![\mathbf{t}(\mathbf{u}_\lambda, p_\lambda)]\!] = \boldsymbol{\lambda}. \tag{3.6d}$$

Proof. This follows from the potential representation. □

Proposition 3.4.2. *Let* $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma)$, *and define* $\mathbf{u}_\lambda := \mathrm{S}_u(s)\boldsymbol{\lambda}$. *Then* $\mathbf{u}_\lambda$ *is the unique solution to the problem*

$$\mathbf{u}_\lambda \in \widehat{\mathbf{V}}(\mathbb{R}^2),$$
$$a(\mathbf{u}_\lambda, \mathbf{v}) + s(\mathbf{u}_\lambda, \mathbf{v})_{\mathbb{R}^2} = \langle \boldsymbol{\lambda}, \gamma \mathbf{v} \rangle_\Gamma \quad \forall \mathbf{v} \in \widehat{\mathbf{V}}(\mathbb{R}^2).$$

Proof. We define

$$(D\mathbf{p}_\infty)(\mathbf{x}) = \frac{1}{2\pi}\frac{1}{1+|\mathbf{x}|^2}\left(\mathrm{I} - \frac{2}{1+|\mathbf{x}|^2}\mathbf{x}\otimes\mathbf{x}\right),$$
$$\mathbf{g}_\ell := (D\mathbf{p}_\infty)\mathbf{e}_\ell = \nabla(\mathbf{p}_\infty\cdot\mathbf{e}_\ell).$$

From Proposition (3.3.2) we can write the pressure as

$$p_\lambda = \sum_{\ell=1}^{2} j_\ell(\boldsymbol{\lambda})\mathbf{p}_\infty\cdot\mathbf{e}_\ell + p_{reg,\lambda}, \quad p_{reg,\lambda}\in L^2(\mathbb{R}^2),$$

and so

$$\nabla p_\lambda = \sum_{\ell=1}^{2} j_\ell(\boldsymbol{\lambda})\mathbf{g}_\ell + \nabla p_{reg,\lambda}, \quad \mathbf{g}_\ell\in\mathbf{L}^2(\mathbb{R}^2).$$

By linearity, we have

$$[\![\mathbf{t}(\mathbf{u}_\lambda,p_\lambda)]\!] = [\![\mathbf{t}(\mathbf{u}_\lambda,p_{reg,\lambda})]\!] + \sum_{\ell=1}^{2}[\![\mathbf{t}(\mathbf{0},\mathbf{p}_\infty\cdot\mathbf{e}_\ell)]\!] = [\![\mathbf{t}(\mathbf{u}_\lambda,p_{reg,\lambda})]\!].$$

Therefore the pair $(\mathbf{u}_\lambda,p_\lambda)\in\mathbf{H}^1(\mathbb{R}^2)\times L^2(\mathbb{R}^2)$ is a solution to the problem

$$-2\nu\,\varepsilon(\mathbf{u}_\lambda) + s\mathbf{u}_\lambda + \nabla p_{reg,\lambda} = -\sum_{\ell=1}^{2} j_\ell(\boldsymbol{\lambda})\mathbf{g}_\ell \quad \text{in } \mathbb{R}^2\setminus\Gamma, \tag{3.7a}$$
$$\operatorname{div}\mathbf{u}_\lambda = 0 \quad \text{in } \mathbb{R}^2\setminus\Gamma, \tag{3.7b}$$
$$[\![\gamma\mathbf{u}_\lambda]\!] = 0, \tag{3.7c}$$
$$[\![\mathbf{t}(\mathbf{u}_\lambda,p_{reg,\lambda})]\!] = \boldsymbol{\lambda}. \tag{3.7d}$$

This problem is equivalent to the variational problem

$$(\mathbf{u}_\lambda,p_{reg,\lambda})\in\mathbf{H}^1(\mathbb{R}^2)\times L^2(\mathbb{R}^2), \tag{3.8a}$$
$$a(\mathbf{u}_\lambda,\mathbf{v}) + s(\mathbf{u}_\lambda,\mathbf{v})_{\mathbb{R}^2} - (p_{reg,\lambda},\operatorname{div}\mathbf{v})_{\mathbb{R}^2}$$
$$= \langle\boldsymbol{\lambda},\gamma\mathbf{v}\rangle_\Gamma - \sum_{\ell=1}^{2} j_\ell(\boldsymbol{\lambda})(\mathbf{g}_\ell,\mathbf{v})_{\mathbb{R}^2} \quad \forall\mathbf{v}\in\mathbf{H}^1(\mathbb{R}^2), \tag{3.8b}$$
$$(\operatorname{div}\mathbf{u}_\lambda,q)_{\mathbb{R}^2} = 0 \quad \forall q\in L^2(\mathbb{R}^2). \tag{3.8c}$$

If we take as a test and trial spaces $\widehat{\mathbf{V}}(\mathbb{R}^2)$, then the pressure terms drop out and leave the variational problem

$$\mathbf{u}_\lambda \in \widehat{\mathbf{V}}(\mathbb{R}^2), \tag{3.9a}$$

$$a(\mathbf{u}_\lambda, \mathbf{v}) + s(\mathbf{u}_\lambda, \mathbf{v})_{\mathbb{R}^2} = \langle \boldsymbol{\lambda}, \gamma \mathbf{v} \rangle_\Gamma - \sum_{\ell=1}^{2} j_\ell(\boldsymbol{\lambda})(\mathbf{g}_\ell, \mathbf{v})_{\mathbb{R}^2} \quad \forall \mathbf{v} \in \widehat{\mathbf{V}}(\mathbb{R}^2). \tag{3.9b}$$

Now we claim $\mathbf{p}_\infty \cdot \mathbf{e}_\ell \in W^2(\mathbb{R}^2) := \{u : \mathbb{R}^2 \to \mathbb{R} \ : \ \rho u \in L^2(\mathbb{R}^2), \quad \nabla u \in \mathbf{L}^2(\mathbb{R}^2)\}$ where the weight ρ is given by [75, 3]

$$\rho(\mathbf{x}) := \frac{1}{1 + \frac{1}{2}\log(1 + |\mathbf{x}|^2)} \frac{1}{\sqrt{1 + |\mathbf{x}|^2}}.$$

Because $\mathcal{D}(\mathbb{R}^2)$ is a dense subset of $W^2(\mathbb{R}^2)$ [75, 3], we can consider a sequence $\{\varphi_n\} \subset \mathcal{D}(\mathbb{R}^2)$ such that $\nabla \varphi_n \to \mathbf{g}_\ell = \nabla(\mathbf{p}_\infty \cdot \mathbf{e}_\ell)$. Considering the terms in the sum in the right-hand-side of (3.9), we have

$$(\mathbf{g}_\ell, \mathbf{v})_{\mathbb{R}^2} = \lim_{n\to\infty} (\nabla \varphi_n, \mathbf{v})_{\mathbb{R}^2} = - \lim_{n\to\infty} (\varphi_n, \operatorname{div} \mathbf{v})_{\mathbb{R}^2} = 0.$$

This shows that problem (3.8) is the same as problem (3.9). □

3.5 Laplace Domain Bounds

Thus far, we have shown the well-posedness of the Brinkman equations in $\mathbb{R}^d$ for $d = 2, 3$. To be able to derive estimates in the time domain for the transient Stokes problem, we require a careful analysis in the Laplace domain of the potential $\mathrm{S}_u(s)$, the operator $\mathrm{V}(s) := \gamma \mathrm{S}_u(s)$, and their composition $\mathrm{S}_u(s)\mathrm{V}^{-1}(s)$. Our goal is to construct bounds in terms of $|s|$ that can then be used to derive estimates in the time domain. We will make significant use of the following space:

$$\mathbf{H}_n^{1/2}(\Gamma) := \left\{ \boldsymbol{\xi} \in \mathbf{H}^{1/2}(\Gamma) \ : \ \int_\Gamma \boldsymbol{\xi} \cdot \mathbf{n} = 0 \right\}.$$

With this we have the following lemma.

Lemma 3.5.1. *The trace operator*

$$\gamma : \widehat{\mathbf{V}}(\mathbb{R}^d) \to \mathbf{H}_n^{1/2}(\Gamma)$$

is surjective.

Proof. In [75, Proposition 4.4] there is a right inverse for the trace operator whose range contains only compactly supported functions. The same right inverse is valid here. □

Suppose X, Y, and Z are Banach spaces such that $Y, Z \subset X$. We say the decomposition $X = Y \oplus Z$ is **stable** when

- for all $x \in X$ there is a unique $y \in Y$ and $z \in Z$ such that $x = y + z$, and
- $\|y\| + \|z\| \leq C\|x\|$ for some $C > 0$.

We remark that if Z is finite dimensional, it is enough to show that $\|y\| \leq C\|x\|$ to prove the decomposition is stable. We now consider decompositions of the boundary spaces.

Proposition 3.5.2 ([75] Propositions 4.1 and 4.2)**.** *Let*

$$\mathbf{H}_m^{-1/2}(\Gamma) := \{\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma) \ : \ \langle \boldsymbol{\lambda}, \mathbf{m} \rangle_\Gamma = 0\}, \quad \mathbf{m}(\mathbf{x}) := \mathbf{x} - \frac{1}{|\Gamma|} \int_\Gamma \mathbf{x}.$$

Then the decompositions

$$\mathbf{H}^{1/2}(\Gamma) = \mathbf{H}_n^{1/2}(\Gamma) \oplus \operatorname{span}\{\mathbf{m}\} \quad \textit{and} \quad \mathbf{H}^{-1/2}(\Gamma) = \mathbf{H}_m^{-1/2}(\Gamma) \oplus \operatorname{span}\{\mathbf{n}\}$$

are stable, and there is a constant $C > 0$ such that

$$\|\boldsymbol{\lambda}\|_{-1/2,\Gamma} \leq C \sup_{\mathbf{0} \neq \xi \in \mathbf{H}_n^{1/2}(\Gamma)} \frac{|\langle \boldsymbol{\lambda}, \boldsymbol{\xi} \rangle_\Gamma|}{\|\boldsymbol{\xi}\|_{1/2,\Gamma}} \qquad \forall \boldsymbol{\lambda} \in \mathbf{H}_m^{-1/2}(\Gamma).$$

In addition to these lemmas, we need to establish some details regarding the norms we will be using. For a complex number $s \in \mathbb{C}_\star$, we take its square root to be $s^{1/2} = |s|^{1/2} \exp(\frac{i}{2} \operatorname{Arg} s) \in \mathbb{C}_+$ where $\operatorname{Arg} s \in (-\pi, \pi)$ is the principal determination of the argument, and denote

$$\omega := \operatorname{Re} s^{1/2} = \operatorname{Re} \overline{s}^{1/2}, \quad \underline{\omega} := \min\{1, \omega\} = \min\{1, \operatorname{Re}|s|^{1/2}\}.$$

Our analysis will make use of the norms

$$|\!|\!| \mathbf{u} |\!|\!|_{(s)}^2 := 2\nu \|\varepsilon(\mathbf{u})\|_{\mathbb{R}^d}^2 + |s| \|\mathbf{u}\|_{\mathbb{R}^d}^2$$

which satisfy

$$\alpha_1(s)\,|||\mathbf{u}|||_{(1)} \le |||\mathbf{u}|||_{(s)} \le \alpha_2(s)\,|||\mathbf{u}|||_{(1)} \quad \forall \mathbf{u} \in \mathbf{H}^1(\mathbb{R}^d), \quad \forall s \in \mathbb{C}_\star$$

where

$$\alpha_1(s) := \min\{1, |s|^{1/2}\} \ge \underline{\omega}, \quad \alpha_2(s) := \max\{1, |s|^{1/2}\} \le \frac{|s|^{1/2}}{\underline{\omega}} \quad \forall s \in \mathbb{C}_\star. \tag{3.10}$$

With this, we will use the norm $|||\mathbf{u}|||_{(1)}$ as the standard norm in $\mathbf{H}^1(\mathbb{R}^d)$. Finally, we have the inequality

$$|a(\mathbf{u},\mathbf{v}) + s(\mathbf{u},\mathbf{v})_{\mathbb{R}^d}| \le |||\mathbf{u}|||_{(s)}\,|||\mathbf{v}|||_{(s)}\,.$$

Proposition 3.5.3. *For the single layer operator* $\mathrm{V}(s)$*, we have the following:*

(1) (Symmetry)

$$\langle \boldsymbol{\lambda}, \mathrm{V}(s)\boldsymbol{\mu}\rangle_\Gamma = \langle \boldsymbol{\mu}, \mathrm{V}(s)\boldsymbol{\lambda}\rangle_\Gamma \quad \forall \boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\Gamma).$$

(2) (Positivity)

$$\mathrm{Re}\,\langle \overline{s}^{1/2}\overline{\boldsymbol{\lambda}}, \mathrm{V}(s)\boldsymbol{\lambda}\rangle_\Gamma = \omega\,|||\mathrm{S}_u(s)\boldsymbol{\lambda}|||^2_{(s)} \quad \forall \boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma).$$

(3) $\mathrm{Ker}\,\mathrm{V}(s) = \mathrm{span}\{\mathbf{n}\}$.

(4) (Coercivity) There is a constant $C > 0$ *such that for all* $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}_m(\Gamma)$

$$|\langle \overline{\boldsymbol{\lambda}}, \mathrm{V}(s)\boldsymbol{\lambda}\rangle_\Gamma| \ge C\frac{\omega}{|s|^{1/2}\max\{1,|s|\}}\|\boldsymbol{\lambda}\|^2_{-1/2,\Gamma} \ge C\frac{\omega\underline{\omega}^2}{|s|^{3/2}}\|\boldsymbol{\lambda}\|^2_{-1/2,\Gamma},$$

therefore $\mathrm{V}(s) : \mathbf{H}^{-1/2}_m(\Gamma) \to \mathbf{H}^{1/2}_n(\Gamma)$ *is invertible.*

Proof. Define $u_\lambda := \mathrm{S}_u(s)\boldsymbol{\lambda}$ and $u_\mu := \mathrm{S}_u(s)\boldsymbol{\mu}$. Then

$$\langle \boldsymbol{\lambda}, \mathrm{V}(s)\boldsymbol{\mu}\rangle_\Gamma = \langle \boldsymbol{\lambda}, \gamma\mathbf{u}_\mu\rangle_\Gamma = a(\mathbf{u}_\lambda, \mathbf{u}_\mu) + s(\mathbf{u}_\lambda, \mathbf{u}_\mu)_{\mathbb{R}^d},$$

which establishes (1). Now consider

$$\overline{s}^{1/2}\langle \overline{\boldsymbol{\lambda}}, \mathrm{V}(s)\boldsymbol{\lambda}\rangle_\Gamma = \overline{s}^{1/2}\langle \boldsymbol{\lambda}, \mathrm{V}(s)\overline{\boldsymbol{\lambda}}\rangle_\Gamma = \overline{s}^{1/2}a(\mathbf{u}_\lambda, \overline{\mathbf{u}_\lambda}) + s^{1/2}|s|(\mathbf{u}_\lambda, \overline{\mathbf{u}_\lambda})_{\mathbb{R}^d}. \tag{3.11}$$

This establishes (2). Suppose $\mathbf{v} \in \widehat{\mathbf{V}}(\mathbb{R}^d)$. Then

$$\langle \mathbf{n}, \gamma \mathbf{v} \rangle_\Gamma = \int_\Gamma \gamma \mathbf{v} \cdot \mathbf{n} = \int_{\Omega_-} \operatorname{div} \mathbf{v} = 0,$$

and so $\mathrm{S}(s)\mathbf{n} = \mathbf{0}$. If $\mathrm{V}(s)\boldsymbol{\lambda} = 0$, then (2) shows that $\mathbf{u}_\lambda = \mathbf{0}$. Therefore the pressure p_λ satisfies $\nabla p_\lambda = \mathbf{0}$ in $\mathbb{R}^d$ and decays at infinity. Thus $p_\lambda \in \operatorname{span}\{\chi_{\Omega_-}\}$, and so $\boldsymbol{\lambda} = [\![\mathbf{t}(\mathbf{u}_\lambda, p_\lambda)]\!] = [\![\mathbf{t}(\mathbf{0}, p_\lambda)]\!] \in \operatorname{span}\{\mathbf{n}\}$. This proves (3). Lemma 3.5.1 shows that there is a bounded operator

$$\gamma^\dagger : \mathbf{H}_n^{1/2}(\Gamma) \to \widehat{\mathbf{V}}(\mathbb{R}^d) \quad \gamma\gamma^\dagger \boldsymbol{\phi} = \boldsymbol{\phi} \quad \forall \boldsymbol{\phi} \in \mathbf{H}_n^{1/2}(\Gamma).$$

For $\boldsymbol{\lambda} \in \mathbf{H}_m^{-1/2}(\Gamma)$, define $\mathbf{u}_\lambda = \mathrm{S}_u(s)\boldsymbol{\lambda}$. Then

$$\begin{aligned} |\langle \boldsymbol{\lambda}, \boldsymbol{\phi} \rangle_\Gamma| &= |\langle \boldsymbol{\lambda}, \gamma\gamma^\dagger \boldsymbol{\phi} \rangle_\Gamma| \\ &= |a(\mathbf{u}_\lambda, \gamma^\dagger \boldsymbol{\phi}) + s(\mathbf{u}_\lambda, \gamma^\dagger \boldsymbol{\phi})_{\mathbb{R}^d}| \\ &\leq |\!|\!| \mathbf{u}_\lambda |\!|\!|_{(s)} \, |\!|\!| \gamma^\dagger \boldsymbol{\phi} |\!|\!|_{(s)} \\ &\leq C_\Gamma \alpha_2(s) \, |\!|\!| \mathbf{u}_\lambda |\!|\!|_{(s)} \, \|\boldsymbol{\phi}\|_{1/2,\Gamma}. \end{aligned}$$

Taking the supremum over all $\boldsymbol{\phi}$ shows

$$\|\boldsymbol{\lambda}\|_{-1/2,\Gamma} \leq C\alpha_2(s) \, |\!|\!| \mathbf{u}_\lambda |\!|\!|_{(s)} \,. \tag{3.12}$$

By (2) we have

$$\operatorname{Re} \langle \overline{s}^{1/2} \overline{\boldsymbol{\lambda}}, \mathrm{V}(s)\boldsymbol{\lambda} \rangle_\Gamma = \omega \, |\!|\!| \mathbf{u}_\lambda |\!|\!|_{(s)}^2 \geq C \frac{\omega}{\alpha_2(s)^2} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma}^2 \quad \forall \boldsymbol{\lambda} \in \mathbf{H}_m^{-1/2}(\Gamma).$$

Taking absolute values gives the estimate

$$|\langle \boldsymbol{\lambda}, \mathrm{V}(s)\boldsymbol{\lambda} \rangle_\Gamma| \geq C \frac{\omega}{|s|^{1/2} \max\{1, |s|\}} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma}^2,$$

which establishes the result. □

Proposition 3.5.4. *There exists a $C > 0$ such that*

$$\alpha_1(s) \, |\!|\!| \mathrm{S}_u(s)\boldsymbol{\lambda} |\!|\!|_{(1)} \leq |\!|\!| \mathrm{S}_u(s)\boldsymbol{\lambda} |\!|\!|_{(s)} \leq C \frac{\alpha_2(s)}{\omega} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma} \quad \forall \boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\Gamma).$$

Proof. Let $\mathbf{u}_\lambda := \mathrm{S}(s)\boldsymbol{\lambda}$. Then

$$\begin{aligned}
\omega \left\|\!\left| \mathbf{u}_\lambda \right|\!\right|_{(s)}^2 &= \mathrm{Re}\, \langle \overline{s}^{1/2}\overline{\boldsymbol{\lambda}}, \mathrm{V}(s)\boldsymbol{\lambda}\rangle_\Gamma \\
&\leq |s|^{1/2} |\langle \overline{\boldsymbol{\lambda}}, \gamma \mathbf{u}_\lambda \rangle_\Gamma| \\
&\leq C_\Gamma |s|^{1/2} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma} \left\|\!\left| \mathbf{u}_\lambda \right|\!\right|_{(1)} \\
&\leq C_\Gamma \frac{|s|^{1/2}}{\alpha_1(s)} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma} \left\|\!\left| \mathbf{u}_\lambda \right|\!\right|_{(s)} \\
&= C_\Gamma \alpha_2(s) \|\boldsymbol{\lambda}\|_{-1/2,\Gamma} \left\|\!\left| \mathbf{u}_\lambda \right|\!\right|_{(s)},
\end{aligned}$$

from which the result follows. □

Proposition 3.5.5. *Let* $\boldsymbol{\phi} \in \mathbf{H}_n^{1/2}(\Gamma)$ *and* $\mathbf{u} = \mathrm{S}_u(s)\mathrm{V}^{-1}(s)\boldsymbol{\phi}$. *Then*

$$\left\|\!\left| \mathbf{u} \right|\!\right|_{(1)} \leq C \frac{\alpha_1(s)}{\alpha_2(s)} \frac{|s|^{1/2}}{\omega} \|\boldsymbol{\phi}\|_{1/2,\Gamma} = C \frac{\max\{1,|s|\}}{\omega} \|\boldsymbol{\phi}\|_{1/2,\Gamma} \leq C \frac{|s|}{\underline{\omega}^2 \omega} \|\boldsymbol{\phi}\|_{1/2,\Gamma}.$$

Proof. Define $\mathbf{u}_0 := \mathbf{u} - \gamma^\dagger \boldsymbol{\phi}$, where $\gamma^\dagger$ is the lifting operator defined in Lemma 3.5.1. Then $\mathbf{u}_0$ satisfies

$$a(\mathbf{u}_0, \overline{\mathbf{u}_0}) + s(\mathbf{u}_0, \overline{\mathbf{u}_0})_{\mathbb{R}^d} = -a(\gamma^\dagger \boldsymbol{\phi}, \overline{\mathbf{u}_0}) - s(\gamma^\dagger \boldsymbol{\phi}, \overline{\mathbf{u}_0})_{\mathbb{R}^d}$$

and so

$$\omega \left\|\!\left| \mathbf{u}_0 \right|\!\right|_{(s)}^2 = \mathrm{Re}\left(\overline{s}^{1/2} a(\mathbf{u}_0, \overline{\mathbf{u}_0}) + s^{1/2} |s| (\mathbf{u}_0, \overline{\mathbf{u}_0})_{\mathbb{R}^d} \right) \leq |s|^{1/2} \left\|\!\left| \mathbf{u}_0 \right|\!\right|_{(s)} \left\|\!\left| \gamma^\dagger \boldsymbol{\phi} \right|\!\right|_{(s)}.$$

This shows that

$$\left\|\!\left| \mathbf{u} \right|\!\right|_{(s)} \leq \left(1 + \frac{|s|^{1/2}}{\omega} \right) \left\|\!\left| \gamma^\dagger \boldsymbol{\phi} \right|\!\right|_{(s)} \leq C \alpha_2(s) \frac{|s|^{1/2}}{\omega} \|\boldsymbol{\phi}\|_{1/2,\Gamma}$$

Applying the estimate $\alpha_1(s) \left\|\!\left| \mathbf{u} \right|\!\right|_{(1)} \leq \left\|\!\left| \mathbf{u} \right|\!\right|_{(s)}$, the result follows. □

We now summarize the Laplace domain estimates for the operators $\mathrm{V}(s)$, $\mathrm{V}(s)^{-1}$, the potential $\mathrm{S}_u(s)$ and their composition $\mathrm{S}_u(s)\mathrm{V}(s)^{-1}$ we have derived in the last

propositions. All norms are the natural operator norms in the spaces $\mathbf{H}^1(\mathbb{R}^d)$, $\mathbf{H}^{1/2}(\Gamma)$, and $\mathbf{H}^{-1/2}(\Gamma)$:

$$\begin{aligned}
\|\mathrm{S}_u(s)\| + \|\mathrm{V}(s)\| &\leq C\frac{\alpha_2(s)}{\omega\alpha_1(s)} = C\frac{1}{\omega}\max\{|s|^{1/2}, |s|^{-1/2}\},\\
\|\mathrm{V}(s)^{-1}\| &\leq C\frac{|s|^{1/2}\max\{1,|s|\}}{\omega},\\
\|\mathrm{S}_u(s)\mathrm{V}(s)^{-1}\| &\leq C\frac{\alpha_2(s)}{\alpha_1(s)}\frac{|s|^{1/2}}{\omega} = C\frac{\max\{1,|s|\}}{\omega}.
\end{aligned}$$

We can transform these estimates into slightly simpler ones with the following inequalities:

$$\frac{\alpha_2(s)}{\alpha_1(s)} \leq \frac{|s|^{1/2}}{\underline{\omega}^2} \quad \text{and} \quad \max\{1,|s|\} \leq \frac{|s|}{\underline{\omega}^2}.$$

We thus have

$$\|\mathrm{S}_u(s)\| + \|\mathrm{V}(s)\| \leq C\frac{|s|^{1/2}}{\omega\underline{\omega}^2}, \tag{3.13a}$$

$$\|\mathrm{V}(s)^{-1}\| \leq C\frac{|s|^{3/2}}{\omega\underline{\omega}^2}, \tag{3.13b}$$

$$\|\mathrm{S}_u(s)\mathrm{V}(s)^{-1}\| \leq C\frac{|s|}{\omega\underline{\omega}^2}, \tag{3.13c}$$

which we will use to derive estimates in the time domain.

3.6 Time Domain Estimates for the Single Layer Potential and Operator

Given a Banach space X, we denote the set of causal $\mathcal{C}^k$ functions taking values on X by

$$\mathcal{C}^k_+(\mathbb{R};X) := \{\phi : \mathbb{R} \to X \ : \ \phi \in \mathcal{C}^k(\mathbb{R};X),\ \phi(t) = 0\ \forall t \leq 0\}.$$

If we consider the estimates from (3.13) and apply the Payley-Weiner Theorem, there is a causal distribution $\mathcal{S}$ with values in $\mathcal{B}(\mathbf{H}^{-1/2}(\Gamma), \mathbf{H}^1(\mathbb{R}^d))$ whose Laplace transform is S. The convolution operator $\mathcal{S} * \boldsymbol{\lambda}$, for any causal distribution $\boldsymbol{\lambda}$ taking values in $\mathbf{H}^{-1/2}(\Gamma)$, is the single layer potential for the Stokes problem in the time domain. The distribution $\mathcal{V} * \boldsymbol{\lambda} = \gamma(\mathcal{S} * \boldsymbol{\lambda})$ with Laplace transform V is the single layer operator for the Stokes problem in the time domain.

Proposition 3.6.1. *Let $\boldsymbol{\lambda} \in \mathcal{C}^1_+(\mathbb{R}; \mathbf{H}^{-1/2}(\Gamma))$. Then $\mathcal{S} * \boldsymbol{\lambda}$ and $\mathcal{V} * \boldsymbol{\lambda}$ are continuous functions of t and*

$$\|(\mathcal{S} * \boldsymbol{\lambda})(t)\|_{1,\mathbb{R}^d} \leq C \max\{1, t^2\} \max_{0 \leq \tau \leq t} \|\dot{\boldsymbol{\lambda}}(\tau)\|_{-1/2,\Gamma} \quad \forall t \geq 0,$$

$$\|(\mathcal{V} * \boldsymbol{\lambda})(t)\|_{1/2,\Gamma} \leq C \max\{1, t^2\} \max_{0 \leq \tau \leq t} \|\dot{\boldsymbol{\lambda}}(\tau)\|_{-1/2,\Gamma} \quad \forall t \geq 0.$$

Proof. The distributions $\mathcal{S}$ and $\mathcal{V}$ satisfy (A.1) and (A.2) with $\mu = 1/2$ and $\ell = 3$, and so by Proposition A.4.1 the result follows. □

Proposition 3.6.2. *Let $\boldsymbol{\phi} \in \mathcal{C}^2_+(\mathbb{R}; \mathbf{H}^{1/2}_n(\Gamma))$. Then there is a unique causal distribution $\boldsymbol{\lambda}$ with values in $\mathbf{H}^{-1/2}_m(\Gamma)$ such that $\mathcal{V} * \boldsymbol{\lambda} = \boldsymbol{\phi}$. Moreover $\boldsymbol{\lambda} \in \mathcal{C}_+(\mathbb{R}; \mathbf{H}^{-1/2}(\Gamma))$ and the associated potential $\mathbf{u} = \mathcal{S} * \boldsymbol{\lambda}$ is a continuous function of t. We also have*

$$\|\boldsymbol{\lambda}(t)\|_{-1/2,\Gamma} \leq C \max\{1, t^2\} \max_{0 \leq \tau \leq t} \|\ddot{\boldsymbol{\phi}}(\tau)\|_{1/2,\Gamma} \quad \forall t \geq 0$$

$$\|\mathbf{u}(t)\|_{1,\mathbb{R}^d} \leq C \max\{1, t^{5/2}\} \max_{0 \leq \tau \leq t} \|\ddot{\boldsymbol{\phi}}(\tau)\|_{1/2,\Gamma} \quad \forall t \geq 0.$$

Proof. Because $\boldsymbol{\phi}$ is causal, we can assume it is compactly supported in time. Then $\boldsymbol{\phi}$ has a Laplace transform $\boldsymbol{\Phi}$. By the Payley-Weiner Theorem and the estimates (3.13) there is a unique $\boldsymbol{\lambda}$ whose Laplace transform is $\mathrm{V}(s)^{-1}\boldsymbol{\Phi}$. With existence and uniqueness established, the energy estimates follow from Corollary A.4.2 with $\mu = 1/2$, $\ell = 3$. For $\mathbf{u} = \mathcal{S} * \mathcal{V}^{-1} * \boldsymbol{\phi}$ we apply Corollary A.4.2 with $\mu = 0$ and $\ell = 3$. □

3.7 The Exterior Dirichlet Problem

We begin with a velocity field $\boldsymbol{\phi}$ such that $\boldsymbol{\phi} \in \mathcal{C}^2(\mathbf{H}^{1/2}_n(\Gamma))$. We then produce

$$\boldsymbol{\lambda} \in \mathcal{C}_+(\mathbb{R}; \mathbf{H}^{-1/2}_m(\Gamma)) \quad \text{and} \quad \mathbf{u} \in \mathcal{C}_+(\mathbb{R}; \widehat{\mathbf{V}}(\mathbb{R}^d)) \tag{3.14}$$

from the equations

$$\mathcal{V} * \boldsymbol{\lambda} = \boldsymbol{\phi} \quad \text{and} \quad \mathbf{u} = \mathcal{S} * \boldsymbol{\lambda}. \tag{3.15}$$

The pressure field is time-independent, and is constructed with the single layer potential for the pressure:

$$p(t) := \mathrm{S}_p \boldsymbol{\lambda}(t). \tag{3.16}$$

We have shown previously that the pressure has the regularity

$$p \in \mathcal{C}_+(\mathbb{R}; L^2(\mathbb{R}^3)) \quad \text{or} \quad p \in \mathcal{C}_+(\mathbb{R}; L^2(B)) \quad \text{for any bounded set } B \subset \mathbb{R}^2.$$

We remark that if ∂_{x_i} is differentiation in the i^{th} space variable, then $\partial_{x_i} : L^2(\mathbb{R}^d \setminus \Gamma) \to H^{-1}(\mathbb{R}^d \setminus \Gamma)$ is bounded.

Proposition 3.7.1. *Let* $\mathbf{u}$ *and* p *be given by the integral representations in* (3.14)-(3.16)*. Then*

$$\dot{\mathbf{u}}(t) - \nu\Delta\mathbf{u}(t) + \nabla p(t) = 0 \qquad \forall t \geq 0, \tag{3.17a}$$

$$\operatorname{div} \mathbf{u}(t) = 0 \qquad \forall t \geq 0, \tag{3.17b}$$

$$\gamma\mathbf{u}(t) = \boldsymbol{\phi}(t) \quad \forall t \geq 0, \tag{3.17c}$$

$$\mathbf{u}(0) = \mathbf{0}. \tag{3.17d}$$

For any $t \geq 0$ *equations* (3.17a)-(3.17d) *are to be understood in the sense of distributions in* $\mathbb{R}^d \setminus \Gamma$*. We also have*

$$\mathbf{u} \in \mathcal{C}^1_+(\mathbb{R}; \mathbf{H}^{-1}(\mathbb{R}^d \setminus \Gamma)).$$

Proof. First, $\operatorname{div} \mathbf{u}(t) = 0$ for all t because we impose that $\mathbf{u}(t)$ takes values in the space $\widehat{\mathbf{V}}(\mathbb{R}^d)$. The initial condition is satisfied because $\mathbf{u}$ is continuous and causal. By causality, we can assume that $\boldsymbol{\phi}^{(k)}(t)$ is bounded for $k \leq 2$ (this does not affect the generality of the result), and therefore the Laplace transforms of $\mathbf{u}$, $\boldsymbol{\phi}$, and p exist for $s \in \mathbb{C}_\star$. In addition, we have

$$\mathbf{U}(s) = \mathrm{S}(s)\mathbf{V}(s)^{-1}\boldsymbol{\Phi}(s), \qquad P(s) = \mathrm{S}_p(s)\mathbf{V}(s)^{-1}\boldsymbol{\Phi}(s),$$

and therefore

$$s\mathbf{U}(s) - \nu\Delta\mathbf{U}(s) + \nabla P(s) = \mathbf{0} \qquad \forall s \in \mathbb{C}_\star,$$

and

$$\gamma\mathbf{U}(s) = \boldsymbol{\Phi}(s) \quad \forall s \in \mathbb{C}_\star.$$

The last equality proves that the boundary condition is satisfied in the time domain. Now notice that $\Delta\mathbf{u} \in \mathcal{C}_+(\mathbb{R}; \mathbf{H}^{-1}(\mathbb{R}^d \setminus \Gamma))$. In three dimensions, the pressure satisfies $\nabla p \in \mathcal{C}_+(\mathbb{R}; \mathbf{H}^{-1}(\mathbb{R}^3 \setminus \Gamma))$. In two dimensions, we make use of the decomposition in Proposition 3.3.2 and the fact $\nabla(\mathbf{p}_\infty \cdot \mathbf{e}_\ell) \in \mathbf{L}^2(\mathbb{R}^2)$ to prove that $\nabla p \in \mathcal{C}_+(\mathbb{R}; \mathbf{H}^{-1}(\mathbb{R}^2 \setminus \Gamma))$. Finally, $\mathbf{u} \in \mathcal{C}_+(\mathbb{R}; \mathbf{H}^{-1}(\mathbb{R}^d \setminus \Gamma))$ and therefore $\dot{\mathbf{u}}$ is a causal distribution with values in $\mathbf{H}^{-1}(\mathbb{R}^d \setminus \Gamma)$. By taking Laplace transforms of the time dependent problem and using $s\mathbf{U}(s) - \nu\Delta\mathbf{U}(s) + \nabla P(s) = 0 \ \forall s \in \mathbb{C}_\star$, we have that $\dot{\mathbf{u}} - \nu\Delta\mathbf{u} + \nabla p = 0$ pointwise in time. This is therefore a distributional equation in $\mathbb{R}^d \setminus \Gamma$ for all t. □

3.8 Galerkin Spatial Semidiscretization

Suppose that $\mathbf{X}_h \subset \mathbf{H}_m^{-1/2}(\Gamma)$ is a finite dimensional space. The spatially semi-discrete boundary integral equation for the exterior Dirichlet problem begins with causal data $\boldsymbol{\phi} : \mathbb{R} \to \mathbf{H}_n^{1/2}(\Gamma)$ and seeks a causal density $\boldsymbol{\lambda}^h : \mathbb{R} \to \mathbf{H}_m^{-1/2}(\Gamma)$ satisfying

$$\langle \boldsymbol{\mu}^h, (\mathcal{V} * \boldsymbol{\lambda}^h)(t) \rangle_\Gamma = \langle \boldsymbol{\mu}^h, \boldsymbol{\phi}(t) \rangle_\Gamma \quad \forall \boldsymbol{\mu}_h \in \mathbf{X}_h, \quad \forall t \tag{3.18}$$

and then constructs the potentials

$$\mathbf{u}^h := \mathcal{S} * \boldsymbol{\lambda}^h, \quad p^h := \mathrm{S}_p \boldsymbol{\lambda}^h. \tag{3.19}$$

We first study the operator $\mathrm{G}_h(s) : \mathbf{H}_n^{1/2}(\Gamma) \to \mathbf{X}_h$ defined by $\boldsymbol{\lambda}^h := \mathrm{G}_h(s)\boldsymbol{\phi}$, where

$$\boldsymbol{\lambda}^h \in \mathbf{X}_h \quad \text{s.t.} \quad \langle \boldsymbol{\mu}^h, \mathrm{V}(s)\boldsymbol{\lambda}^h \rangle_\Gamma = \langle \boldsymbol{\mu}^h, \boldsymbol{\phi} \rangle_\Gamma \quad \forall \boldsymbol{\mu}^h \in \mathbf{X}_h. \tag{3.20}$$

We will call the operator $\mathrm{G}_h(s)$ the **Galerkin solver**. We will also make extensive use of the space

$$\mathbf{X}_h^\circ := \{\mathbf{v} \in \mathbf{H}^{1/2}(\Gamma) \ : \ \langle \mathbf{v}, \mathbf{w} \rangle_\Gamma = 0 \ \ \forall \mathbf{w} \in \mathbf{X}_h\}.$$

We then have the following result.

Proposition 3.8.1. *There exists a constant C independent of the mesh size h such that*

$$\|\mathrm{G}_h(s)\| \leq C \frac{|s|^{3/2}}{\omega \underline{\omega}^2} \quad \textit{and} \quad \|\mathrm{S}(s)\mathrm{G}_h(s)\| \leq C \frac{|s|}{\omega \underline{\omega}^2}.$$

Proof. To prove the first inequality, we make use of the coercivity estimate from Proposition 3.5.3. Since Galerkin semidiscretizations inherit coercivity, we have

$$\begin{aligned}\|\boldsymbol{\lambda}^h\|^2_{-1/2,\Gamma} &\leq C\frac{|s|^{3/2}}{\omega\underline{\omega}^2}\left|\langle\overline{\boldsymbol{\lambda}^h},\mathrm{V}(s)\boldsymbol{\lambda}^h\rangle_\Gamma\right| \\ &\leq C\frac{|s|^{3/2}}{\omega\underline{\omega}^2}\|\boldsymbol{\lambda}^h\|_{-1/2,\Gamma}\|\boldsymbol{\phi}\|_{1/2,\Gamma},\end{aligned}$$

and so

$$\|\boldsymbol{\lambda}^h\|_{-1/2,\Gamma} = \|\mathrm{G}_h(s)\boldsymbol{\phi}\|_{1/2,\Gamma} \leq C\frac{|s|^{3/2}}{\omega\underline{\omega}^2}\|\boldsymbol{\phi}\|_{1/2,\Gamma},$$

which, upon taking the supremum over all $\boldsymbol{\phi}$ gives the desired result. For the second inequality, consider $\boldsymbol{\lambda}^h = \mathrm{G}_h(s)\boldsymbol{\phi}$. We then have that $\mathbf{u}^h$ is the unique solution to the problem

$$\begin{aligned}&\mathbf{u}^h \in \widehat{\mathbf{V}}(\mathbb{R}^d), \quad \gamma\mathbf{u}^h - \boldsymbol{\phi} \in \mathbf{X}_h^\circ, \\ &a(\mathbf{u}^h,\mathbf{v}) + s(\mathbf{u}^h,\mathbf{v})_{\mathbb{R}^d} = \langle\boldsymbol{\lambda},\gamma\mathbf{v}\rangle_\Gamma \quad \forall\mathbf{v}\in\widehat{\mathbf{V}}(\mathbb{R}^d).\end{aligned}$$

We consider the closed subspace

$$\begin{aligned}\widehat{\mathbf{V}}_h(\mathbb{R}^d) :&= \{\mathbf{v}\in\widehat{\mathbf{V}}(\mathbb{R}^d) \ : \ \gamma\mathbf{v}\in\mathbf{X}_h^\circ\} \\ &= \{\mathbf{v}\in\widehat{\mathbf{V}}(\mathbb{R}^d) \ : \ \langle\boldsymbol{\mu}^h,\gamma\mathbf{v}\rangle_\Gamma = 0 \ \forall\,\boldsymbol{\mu}^h\in\mathbf{X}_h\}.\end{aligned}$$

We now decompose $\mathbf{u}^h = \mathbf{w}^h + \gamma^\dagger\boldsymbol{\phi}$ where $\mathbf{w}^h \in \widehat{\mathbf{V}}_h(\mathbb{R}^d)$. We now proceed as in the proof of Proposition 3.5.5. We have that

$$a(\mathbf{w}^h,\overline{\mathbf{w}^h}) + s(\mathbf{w}^h,\overline{\mathbf{w}^h})_{\mathbb{R}^d} = -a(\gamma^\dagger\boldsymbol{\phi},\overline{\mathbf{w}^h}) + s(\gamma^\dagger\boldsymbol{\phi},\overline{\mathbf{w}^h})_{\mathbb{R}^d}$$

and so

$$\begin{aligned}\omega\left|\!\left|\!\left|\mathbf{w}^h\right|\!\right|\!\right|^2_{(s)} &= \mathrm{Re}\left(\overline{s}^{1/2}a(\mathbf{w}^h,\overline{\mathbf{w}^h}) + s^{1/2}|s|(\mathbf{w}^h,\overline{\mathbf{w}^h})_{\mathbb{R}^d}\right) \\ &\leq |s|^{1/2}\left|\!\left|\!\left|\gamma^\dagger\boldsymbol{\phi}\right|\!\right|\!\right|_{(s)}\left|\!\left|\!\left|\mathbf{w}^h\right|\!\right|\!\right|_{(s)},\end{aligned}$$

which shows

$$\left|\!\left|\!\left|\mathbf{w}^h\right|\!\right|\!\right|_{(s)} \leq \frac{|s|^{1/2}}{\omega}\left|\!\left|\!\left|\gamma^\dagger\boldsymbol{\phi}\right|\!\right|\!\right|_{(s)}.$$

It then follows that

$$\left|\!\left|\!\left|\mathbf{u}^h\right|\!\right|\!\right|_{(s)} \leq C\alpha_2(s)\frac{|s|^{1/2}}{\omega}\|\boldsymbol{\phi}\|_{1/2,\Gamma},$$

from which the final bound is derived. □

We will now study the error operator, from which we can derive convergence estimates. We begin with the operator $\mathrm{G}_h(s)\mathrm{V}(s) : \mathbf{H}_m^{-1/2}(\Gamma) \to \mathbf{X}_h$, or, equivalently, by taking $\boldsymbol{\lambda}^h$ as the solution to

$$\boldsymbol{\lambda}^h \in \mathbf{X}_h \quad \text{s.t.} \quad \langle \boldsymbol{\mu}^h, \mathrm{V}(s)\boldsymbol{\lambda}^h \rangle_\Gamma = \langle \boldsymbol{\mu}^h, \mathrm{V}(s)\boldsymbol{\lambda} \rangle_\Gamma \quad \forall \boldsymbol{\mu}^h \in \mathbf{X}_h. \tag{3.21}$$

We will be interested in the complementary projection, which corresponds to the error of the Galerkin semidiscretization. Thus, we define the **Galerkin error operator** as $\mathrm{E}_h(s) := \mathrm{G}_h(s)\mathrm{V}(s) - \mathrm{I}$ and the error operator for the postprocessing by $\mathrm{S}(s)\mathrm{E}_h(s)$. Notice that while $\mathrm{G}_h(s)\mathrm{V}(s)$ is a projection onto $\mathbf{X}_h$ for every s, the range of the operator $\mathrm{E}_h(s)$ varies with s. We then have the following proposition for the error operator.

Proposition 3.8.2. *There is a constant C independent of h such that*

$$\|\mathrm{E}_h(s)\| \leq C\frac{|s|}{\omega\underline{\omega}^2} \quad \textit{and} \quad \|\mathrm{S}(s)\mathrm{E}_h(s)\| \leq C\frac{|s|^{1/2}}{\omega\underline{\omega}^2}.$$

Proof. Let $\boldsymbol{\lambda} \in \mathbf{H}_m^{-1/2}(\Gamma)$ and $\mathbf{w}^h := \mathrm{S}(s)\mathrm{E}_h(s)\boldsymbol{\lambda} = \mathrm{S}(s)(\boldsymbol{\lambda}^h - \boldsymbol{\lambda})$, where $\boldsymbol{\lambda}^h$ is the solution to (3.21). We then have

$$\begin{aligned}
\omega \left|\!\left|\!\left| \mathbf{w}^h \right|\!\right|\!\right|_{(s)}^2 &= \mathrm{Re}\, \langle \overline{s}^{1/2}(\overline{\boldsymbol{\lambda}^h} - \boldsymbol{\lambda}), \mathrm{V}(s)(\boldsymbol{\lambda}^h - \boldsymbol{\lambda}) \rangle_\Gamma \\
&= -\mathrm{Re}\, \langle \overline{s}^{1/2}\overline{\boldsymbol{\lambda}^h}, \mathrm{V}(s)(\boldsymbol{\lambda}^h - \boldsymbol{\lambda}) \rangle_\Gamma \\
&\leq C_\Gamma |s|^{1/2} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma} \left|\!\left|\!\left| \mathbf{w}^h \right|\!\right|\!\right|_{(1)}.
\end{aligned}$$

Therefore we have the bounds

$$\left|\!\left|\!\left| \mathbf{w}^h \right|\!\right|\!\right|_{(s)} \leq C\frac{|s|^{1/2}}{\omega\underline{\omega}} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma} \quad \text{and} \quad \left|\!\left|\!\left| \mathbf{w}^h \right|\!\right|\!\right|_{(1)} \leq C\frac{|s|^{1/2}}{\omega\underline{\omega}^2} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma}.$$

The latter bound gives the estimate for $\|\mathrm{S}(s)\mathrm{E}_h(s)\|$. Finally, we have

$$\|\mathrm{E}_h(s)\boldsymbol{\lambda}\|_{-1/2,\Gamma} = \|\boldsymbol{\lambda}^h - \boldsymbol{\lambda}\|_{-1/2,\Gamma} \leq C\frac{|s|^{1/2}}{\underline{\omega}} \left|\!\left|\!\left| \mathbf{w}^h \right|\!\right|\!\right|_{(s)} \leq C\frac{|s|}{\omega\underline{\omega}^2} \|\boldsymbol{\lambda}\|_{-1/2,\Gamma},$$

which finishes the proof. □

We are now prepared to derive estimates for the transient Stokes problem using the previously constructed tools for the Brinkman problem.

Proposition 3.8.3 (Stability). *Let* $\boldsymbol{\phi} \in \mathcal{C}^2_+(\mathbb{R}; \mathbf{H}^{1/2}_n(\Gamma))$ *and let* $\boldsymbol{\lambda}^h$ *be the solution to* (3.18) *and* $\mathbf{u}^h$ *be given by* (3.19). *Then*

$$\boldsymbol{\lambda}^h \in \mathcal{C}_+(\mathbb{R}; \mathbf{X}_h), \quad \mathbf{u}^h \in \mathcal{C}_+(\mathbb{R}; \mathbf{H}^1(\mathbb{R}^d))$$

and

$$\|\boldsymbol{\lambda}^h(t)\|_{-1/2,\Gamma} \leq C \max\{1, t^2\} \max_{0\leq\tau\leq t} \|\ddot{\boldsymbol{\phi}}(\tau)\|_{1/2,\Gamma}$$
$$\|\mathbf{u}^h(t)\|_{1,\mathbb{R}^d} \leq C \max\{1, t^{5/2}\} \max_{0\leq\tau\leq t} \|\ddot{\boldsymbol{\phi}}(\tau)\|_{1/2,\Gamma}.$$

Proof. This is an immediate consequence of Corollary A.4.2 and Proposition 3.8.1. □

To prove error estimates, we introduce the orthogonal projection operator $\boldsymbol{\Pi}_h : \mathbf{H}^{-1/2}_m(\Gamma) \to \mathbf{X}_h$. Since $\mathrm{I} - \mathrm{E}_h(s) + \mathrm{I} = \mathrm{G}_h(s)\mathrm{V}(s)$ is a projection onto $\mathbf{X}_h$, we have

$$\mathrm{E}_h(s) = \mathrm{E}_h(s)(\mathrm{I} - \boldsymbol{\Pi}_h). \tag{3.22}$$

Proposition 3.8.4 (Error for Galerkin semidiscretization I). *If* $\boldsymbol{\lambda} \in \mathcal{C}^1_+(\mathbb{R}; \mathbf{H}^{-1/2}_m(\Gamma))$, *then*

$$\|\mathbf{u}^h(t) - \mathbf{u}(t)\|_{1,\mathbb{R}^d} \leq C \max\{1, t^2\} \max_{0\leq\tau\leq t} \|\dot{\boldsymbol{\lambda}}(\tau) - \boldsymbol{\Pi}_h\dot{\boldsymbol{\lambda}}(\tau)\|_{-1/2,\Gamma}.$$

Proof. This follows from Propositions 3.8.2 and A.4.1 with $\mu = 1/2$ and $\ell = 2$ and the identity (3.22) to introduce the orthogonal projection. □

Proposition 3.8.5 (Error for Galerkin semidiscretization II). *If* $\boldsymbol{\lambda} \in \mathcal{C}^2_+(\mathbb{R}; \mathbf{H}^{-1/2}_m(\Gamma))$, *then*

$$\|\boldsymbol{\lambda}^h(t) - \boldsymbol{\lambda}(t)\|_{-1/2,\Gamma} \leq C \max\{1, t^{5/2}\} \max_{0\leq\tau\leq t} \|\ddot{\boldsymbol{\lambda}}(\tau) - \boldsymbol{\Pi}_h\ddot{\boldsymbol{\lambda}}(\tau)\|_{-1/2,\Gamma},$$
$$\|p^h(t) - p(t)\|_B \leq C \max\{1, t^{5/2}\} \max_{0\leq\tau\leq t} \|\ddot{\boldsymbol{\lambda}}(\tau) - \boldsymbol{\Pi}_h\ddot{\boldsymbol{\lambda}}(\tau)\|_{-1/2,\Gamma},$$

where $B = \mathbb{R}^3$ *or is an open bounded set in* $\mathbb{R}^2$.

Proof. This is a consequence of Corollary A.4.2 and Proposition 3.8.1. □

3.9 Analysis of the Full Discretization

At this point, we are ready for a temporal discretization of equations (3.18) and (3.19) using Convolution Quadrature. Fix a basis for $\mathbf{X}_h$, denoted $\{\boldsymbol{\mu}_j \ : \ j = 1, \dots, N\}$ and a uniform time step $\kappa > 0$. We then consider a uniform time grid $t_n := n\kappa$ for $n \geq 0$. We sample the boundary data $\boldsymbol{\phi}(t)$ in time and test it against the basis of $\mathbf{X}_h$ to produce vectors

$$\boldsymbol{\phi}_j \in \mathbb{R}^N, \quad \phi_{n,j} := \langle \boldsymbol{\mu}_j, \boldsymbol{\phi}(t_n) \rangle_\Gamma.$$

The transfer operator corresponding to the convolution with $\mathcal{V}$ is defined as a matrix-valued function of $s \in \mathbb{C}_\star$:

$$\mathbf{V}(s) \in \mathbb{C}^{N \times N}, \quad \mathbf{V}_{ij}(s) = \langle \boldsymbol{\mu}_i, \mathrm{V}(s) \boldsymbol{\mu}_j \rangle_\Gamma.$$

As explained in Chapter 2, a CQ discretization of the convolution equation (3.21) begins with a Taylor expansion

$$\mathbf{V}\left(\frac{1}{\kappa}\delta(\zeta)\right) = \sum_{m=0}^{\infty} \mathbf{V}_m(\kappa)\zeta^m, \quad \text{where} \quad \delta(\zeta) := \sum_{\ell=1}^{p} \frac{1}{\ell}(1-\zeta)^\ell.$$

We then seek a sequence $\boldsymbol{\lambda}_n \in \mathbb{R}^N$ satisfying

$$\mathbf{V}_0(\kappa)\boldsymbol{\lambda}_n = \boldsymbol{\phi}_n - \sum_{m=1}^{n} \mathbf{V}_m(\kappa)\boldsymbol{\lambda}_{n-m}, \quad n \geq 0.$$

If the entries at time step n of the vector are $\boldsymbol{\lambda}_n = (\lambda_{n,1}, \dots, \lambda_{n,N})$, we construct the discrete density $\boldsymbol{\lambda}_n^h := \sum_{j=1}^N \lambda_{n,j}\boldsymbol{\mu}_j \in \mathbf{X}_h$. From the discrete density at each time step, we can compute

$$p_n^h := \mathrm{S}_p \boldsymbol{\lambda}_n^h.$$

Since the velocity field has convolution in time structure, we must postprocess with the discrete densities to produce

$$\mathbf{u}_n^h = \sum_{m=0}^{n} \mathrm{S}_m(\kappa)\boldsymbol{\lambda}_{n-m}, \qquad \mathrm{S}\left(\frac{1}{\kappa}\delta(\zeta)\right) := \sum_{m=0}^{\infty} \mathrm{S}_m(\kappa)\zeta^m.$$

Combining the Laplace domain estimates from Proposition 3.8.1 and Theorem 2.6.2, we have the following.

Proposition 3.9.1. *Let p be the order of the BDF method applied for the CQ discretization, and assume that $\boldsymbol{\phi} \in \mathcal{C}_+^{p+1}(\mathbb{R}; \mathbf{H}^{1/2}(\Gamma)) \cap \mathcal{C}^{p+2}([0,\infty); \mathbf{H}^{1/2}(\Gamma))$. Then*

$$\|\mathbf{u}^h(t_n) - \mathbf{u}_n^h\|_{1,\mathbb{R}^d} \leq C_1 \kappa^p \max_{0\leq\tau\leq t} \|\boldsymbol{\phi}^{(p+2)}(\tau)\|_{1/2,\Gamma},$$

$$\|p^h(t_n) - p_n^h\|_B \leq C_2 \kappa^p \max_{0\leq\tau\leq t} \|\boldsymbol{\phi}^{(p+2)}(\tau)\|_{1/2,\Gamma},$$

where $B = \mathbb{R}^3$ or any bounded open set in $\mathbb{R}^2$. The constants C_1 and C_2 depend on t, and C_2 depends on the bounded set B in the two dimensional case. For small t, $C_1 \leq Ct$ and $C_2 \leq Ct^{1/2}$.

3.10 Numerical Experiments

A first experiment

For the first numerical experiment, we choose our data so that we are able to compare the computed solution with a known exact solution. We simulate flow in the domain $\Omega = [-1,1]^2$, and choose the boundary data so that the exact solution is

$$\mathbf{u}(t)(x,y) = \sin^9(t) H(t) \begin{bmatrix} 2x \\ -2y \end{bmatrix}, \quad p(t)(x,y) = -9\sin^8(t)\cos(t) H(t)(x^2 - y^2),$$

where $H(t)$ is the Heaviside function. Because we are using an indirect method, the exact density $\boldsymbol{\lambda}(t)$ is not known. Note that even if the solution is smooth, there is no guarantee that $\boldsymbol{\lambda}(t)$ will be smooth in the space variable. We run the simulation from $t = 0$ to $t = 1$, using BDF(3) based CQ for the time discretization. For spatial discretization we divide $\Gamma = \partial\Omega_-$ into N equally sized elements $\{e_1, \ldots, e_N\}$ where N is a multiple of four. We then have the spaces

$$\mathbf{X}_h^+ := \{\boldsymbol{\lambda}^h : \Gamma \to \mathbb{R}^2 \ : \ \boldsymbol{\lambda}|_{e_j} \in \mathbb{P}_1(e_j)^2 \ \ \forall j\}, \quad \mathbf{X}_h := \mathbf{X}_h^+ \cap \mathbf{H}_m^{-1/2}(\Gamma).$$

The space $\mathbb{P}_1$ is the space of polynomials of degree less than or equal to one. We will use Lagrange multipliers to enforce the density to be in $\mathbf{X}_h$ rather than explicitly constructing a basis. We run the simulation using M time steps to reach $t = 1$, and report the errors

$$\max_j |\mathbf{u}(1)(x_j, y_j) - \mathbf{u}_M^h(x_j, y_j)|, \qquad \max_j |p(1)(x_j, y_j) - p_M^h(x_j, y_j)|,$$

where we have sampled the solution at the points

$$(x_1, y_1) := (-0.5, -0.5), \quad (x_2, y_2) := (0.3, 0.7), \quad (x_3, y_3) := (0.6, 0.2).$$

We do not know if $\boldsymbol{\lambda}$ is a smooth function of the space variables, but if it was, the convergence theory would predict an order of convergence of $\kappa^3 + h^{2.5}$ where $h = 1/N$ is the mesh size and $\kappa = 1/M$ is the time step size. The results are reported in Table 3.1.

N	M	errU	e.c.r.	errP	e.c.r
4	10	1.6448e-02	-	6.9116e-02	-
8	20	9.5414e-03	0.79	6.3904e-02	0.11
16	40	1.2200e-03	2.97	2.4554e-03	4.70
32	80	5.8683e-05	4.38	8.4062e-04	1.55
64	160	1.7639e-05	1.7	1.3247e-04	2.67
128	320	2.2716e-06	2.96	1.0263e-05	3.70
256	640	1.9787e-07	3.52	2.9564e-07	5.12

Table 3.1: Convergence history for the velocity and pressure fields, $\mathbb{P}_1$ elements in space and BDF(3) based CQ in time.

A second experiment

The second numerical experiment makes use of the same solution as the previous example, but instead our domain of interest is the unit circle. The same errors are measured, but the solution is now sampled at three points placed at $(0, 0)$, $(1/2, 1/2)$ and $(-0.6, 0.1)$. Our spatial discretization method is based on the Nyström method described in [26], which can be understood as a reduced integration process applied to a $\mathbb{P}_0$ Galerkin BEM discretization. The results are reported in Table 3.2.

A simulation

We now present a simulation of transient fluid flow around the exterior of a smooth bounded obstacle. Our boundary data is of the form $\boldsymbol{\phi}(t) = f(t)(1/\sqrt{2}, 1/\sqrt{2})$. The function f is the smooth causal function shown in Figure 3.2. We discretize in space again with the order three method of [26] and in time with BDF(3) based CQ.

N	M	errU	e.c.r.	errP	e.c.r
20	20	1.2285e-03	-	3.9793e-03	-
40	40	1.3750e-04	3.16	4.0498e-04	3.30
80	80	1.7287e-05	2.99	4.9458e-05	3.04
160	160	2.1636e-06	2.99	6.1078e-06	3.02
320	320	2.7053e-07	3.00	7.5887e-07	3.01
640	640	3.3819e-08	3.00	9.4578e-08	3.00

Table 3.2: Convergence history for the velocity and pressure fields, discretized with order three collocation in space and BDF(3) based CQ in time.

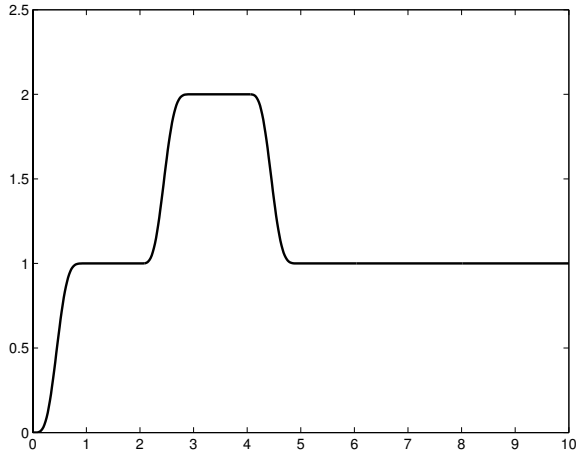

Figure 3.2: The function $f(t)$ used for the simulation.

3.11 An Equivalent Integral Formulation

Our final goal is to present an integral formulation that incorporates the restriction in the Brinkman bilinear form that the test and trial functions be elements of $\mathbf{H}_m^{-1/2}(\Gamma)$. To this end, we define the operator

$$\widetilde{\mathrm{V}}(s) := \mathrm{V}(s) + \langle \cdot\,, \mathbf{m}\rangle_\Gamma \mathbf{m} : \mathbf{H}^{-1/2}(\Gamma) \to \mathbf{H}^{1/2}(\Gamma).$$

This operator is associated to the bilinear form $\langle \boldsymbol{\mu}, \mathrm{V}(s)\boldsymbol{\lambda}\rangle_\Gamma + \langle \boldsymbol{\mu}, \mathbf{m}\rangle_\Gamma \langle \boldsymbol{\lambda}, \mathbf{m}\rangle_\Gamma$.

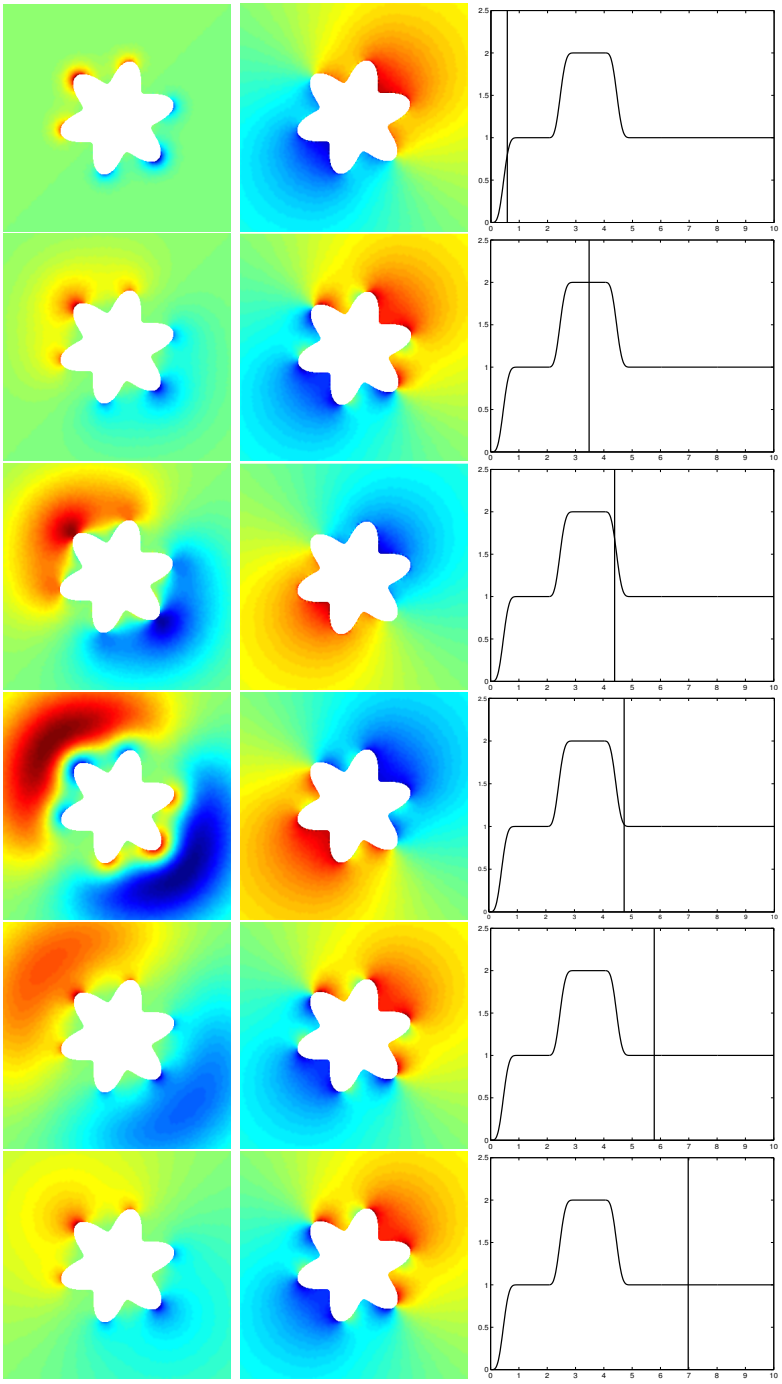

Figure 3.3: A simulation of transient flow around a Bouba-shaped obstacle. Discretized by order three collocation in space and BDF(3) CQ in time. From left to right, we plot the vorticity, the pressure, and the streamline of the incident field.

Proposition 3.11.1. *Let* $\boldsymbol{\phi} \in \mathbf{H}_n^{1/2}(\Gamma)$. *Then*

$$\mathrm{V}(s)\boldsymbol{\lambda} = \boldsymbol{\phi}, \quad \textit{and} \quad \langle \boldsymbol{\lambda}, \mathbf{m} \rangle_\Gamma = 0$$

if and only if

$$\widetilde{\mathrm{V}}(s)\boldsymbol{\lambda} = \boldsymbol{\phi}.$$

Moreover, $\widetilde{\mathrm{V}}(s) : \mathbf{H}^{-1/2}(\Gamma) \to \mathbf{H}^{1/2}(\Gamma)$ *is invertible for all* $s \in \mathbb{C}_\star$ *and*

$$\|\widetilde{\mathrm{V}}(s)^{-1}\| \leq C \frac{|s|^{3/2}}{\omega \underline{\omega}^2}.$$

Proof. The first equivalence is straightforward. To prove invertibility, we derive a coercivity estimate. We use the decomposition of Proposition 3.5.2 as follows:

$$\boldsymbol{\lambda} = \boldsymbol{\lambda}_0 + c(\boldsymbol{\lambda})\mathbf{n}, \quad c(\boldsymbol{\lambda}) := \frac{\langle \boldsymbol{\lambda}, \mathbf{m} \rangle_\Gamma}{\langle \mathbf{n}, \mathbf{m} \rangle_\Gamma}, \quad \boldsymbol{\lambda}_0 \in \mathbf{H}_m^{-1/2}(\Gamma).$$

It is then easy to show that

$$\langle \overline{\boldsymbol{\lambda}}, \widetilde{\mathrm{V}}(s)\boldsymbol{\lambda} \rangle_\Gamma = \langle \overline{\boldsymbol{\lambda}_0}, \mathrm{V}(s)\boldsymbol{\lambda}_0 \rangle_\Gamma + |c(\boldsymbol{\lambda})|^2 \langle \mathbf{n}, \mathbf{m} \rangle_\Gamma^2.$$

By (3.11)

$$|s|^{1/2} |\langle \overline{\boldsymbol{\lambda}}, \widetilde{\mathrm{V}}(s)\boldsymbol{\lambda} \rangle_\Gamma| \geq \mathrm{Re}\, \langle \overline{s}^{1/2} \overline{\boldsymbol{\lambda}}, \widetilde{\mathrm{V}}(s)\boldsymbol{\lambda} \rangle_\Gamma \geq C \frac{\omega}{\alpha_2(s)^2} \|\boldsymbol{\lambda}_0\|_{-1/2,\Gamma}^2 + C\omega |c(\boldsymbol{\lambda})|^2,$$

and therefore (using that $\underline{\omega} \leq |s|^{1/2}$ and the bounds (3.10)),

$$|\langle \overline{\boldsymbol{\lambda}}, \widetilde{\mathrm{V}}(s)\boldsymbol{\lambda} \rangle_\Gamma| \geq C \, \frac{\omega \underline{\omega}^2}{|s|^{3/2}} \Big(\|\boldsymbol{\lambda}_0\|_{-1/2,\Gamma}^2 + |c(\boldsymbol{\lambda})|^2 \Big),$$

which finishes the proof. □

For semidiscretization in space, we choose a finite dimensional space $\mathbf{X}_h^+ \subset \mathbf{H}^{-1/2}(\Gamma)$ such that $\mathbf{n} \in \mathbf{X}_h^+$. (In the case of polyhedral boundaries, this is easily verified if piecewise constant functions are elements of the space.) If we define the space $\mathbf{X}_h := \mathbf{X}_h^+ \cap \mathbf{H}_m^{-1/2}(\Gamma)$, we have a stable decomposition $\mathbf{X}_h^+ = \mathbf{X}_h \oplus \mathrm{span}\,\{\mathbf{n}\}$. The semidiscrete equations in the Laplace domain (3.20) are equivalent to

$$\boldsymbol{\lambda}_h \in \mathbf{X}_h^+ \qquad \text{s.t.} \qquad \langle \boldsymbol{\mu}_h, \widetilde{\mathrm{V}}(s)\boldsymbol{\lambda}_h \rangle_\Gamma = \langle \boldsymbol{\mu}_h, \boldsymbol{\phi} \rangle_\Gamma \quad \forall \boldsymbol{\mu}_h \in \mathbf{X}_h^+.$$

In the time domain, they correspond to looking for a causal function $\boldsymbol{\lambda}_h : \mathbb{R} \to \mathbf{X}_h^+$ such that

$$\langle \boldsymbol{\mu}_h, (\mathcal{V} * \boldsymbol{\lambda}_h)(t) \rangle_\Gamma + \langle \boldsymbol{\mu}_h, \mathbf{m} \rangle_\Gamma \langle \boldsymbol{\lambda}_h(t), \mathbf{m} \rangle_\Gamma = \langle \boldsymbol{\mu}_h, \boldsymbol{\phi}(t) \rangle_\Gamma \quad \forall \boldsymbol{\mu}_h \in \mathbf{X}_h^+, \quad \forall t.$$

Because of Proposition 3.11.1, all the preceding bounds for the semidiscrete case can be easily translated to this new formulation.

Chapter 4

SYMMETRIC COUPLING OF BOUNDARY AND FINITE ELEMENTS FOR TRANSIENT ACOUSTICS

In this chapter we study the transmission and scattering of acoustic waves by inclusions in free space. We focus on the case of a finite number of disjoint, bounded, inhomogeneous, and anisotropic inclusions. An incident acoustic wave interacts with the inclusions, producing transmitted and scattered fields. The wave transmitted through the inclusions is discretized in space with finite elements, while the scattered wave is reduced to two unknowns defined only on the boundary of the inclusions and is discretized in space with boundary elements. For time discretization, we make use of trapezoidal rule based Convolution Quadrature and trapezoidal rule time stepping. The scattered field can then be reconstructed from the boundary fields in a postprocessing step using Kirchhoff's formula. By imposing two continuity conditions across the boundary of the inclusions, we arrive at a symmetric BEM-FEM coupling scheme. The results of this chapter appear in *A fully discrete BEM-FEM scheme for transient acoustic waves* (with F.–J. Sayas) [38].

There has been extensive work on the study of coupling of boundary and finite elements for steady-state and time-harmonic problems, but the literature on coupling schemes for transient problems is relatively sparse. There are generally two types of coupling formulations, using one or two integral equations. The first ones (first analyzed by Johnson and Nédélec [44] for diffusion problems) lead to non-self adjoint formulations, while symmetric couplings (due to Costabel [22] and Han [35]) arrive at a symmetric system. Two-equation formulations are based on variational principles, and can be shown to always be stable, but at the cost of requiring all four of the operators of the Calderón projector associated to the underlying PDE. Single equation

coupling methods are simpler, but do not have an underlying energy principle, and may therefore become unstable when there are large jumps in the material parameters. The traditional two-equation coupling involves applying integral operators to the traces of finite element functions. There is an alternative formulation, using two fields on the boundary, that can keep the FEM and BEM modules better separated. For this work, we will study a two-equation, three-field coupling method. Because we are using a two-equation formulation, we require all four retarded boundary integral operators associated to the wave equation.

We next comment on some of the not very extensive existing literature on coupling of BEM and FEM for transient waves. The seminal paper [5] provides several variational formulations of BEM-FEM coupling for time-dependent electromagnetic waves, with proofs of stability and convergence for their formulations, using a full-Galerkin treatment of the integral equations. The papers [1, 14] deal with four-field formulations (two fields in the interior domain and two on the boundary) and aim at coupling an explicit interior time-stepping method with the retarded boundary integral equations on the boundary, differing in the use of Galerkin-in-time or CQ for the equations on the boundary. The papers [29, 27, 28] contain successful computational studies of one-equation couplings, although a theoretical understanding of their stability and convergence is still missing. A preliminary semidiscrete stability analysis in the Laplace domain of the coupling method we will study here appears in [52]. In a similar vein, there is also recent work [41] on the coupling of BEM and FEM for acoustic waves interacting with elastic media.

Traditional analysis of CQ discretizations of retarded integral equations has relied heavily on the use of the Laplace transform. Precise bounds in terms of the Laplace parameter can be translated into estimates for the time-dependent problem. The time domain estimates, however, are generally not sharp, because some regularity is lost by translating the problem to and from the Laplace domain. In [60] it is observed that the Laplace domain analysis can be avoided entirely, so that stability and convergence can be studied by directly considering the properties of the fully discrete (in space and

time) solution to the underlying PDE. This allows us to apply the theory of C_0 groups of isometries in Hilbert spaces to find sharper estimates than those provided by Laplace domain analysis. Our analysis follows the first-order-in-space-and-time methodology proposed in [36]. By transforming the second-order-in-space-and-time wave equation into a first order system, we are able to circumvent a number of technical challenges that arise in the second-order-in-space-and-time analysis of [74, 73]. Note that we make use of the same Sobolev space notation as in Chapter 3, although Ω_- may now be disconnected. Some of the potentials and spaces share the same names as in Chapter 3, but in this chapter they are defined differently.

4.1 Background and Problem Setting

We begin with the geometric setting and coefficients. Let $\Omega_j \subset \mathbb{R}^d$ $(j = 1, \ldots, N)$ be connected open sets lying on one side of their Lipschitz connected boundaries $\partial\Omega_j$ and such that their closures do not intersect. Let then $\Omega_- := \cup_{j=1}^N \Omega_j$, $\Gamma := \partial\Omega_-$, and $\Omega_+ := \mathbb{R}^d \setminus \overline{\Omega_-}$. In Ω_- we have two coefficients:

$$\kappa : \Omega_- \to \mathbb{R}^{d\times d}_{\mathrm{sym}}, \qquad c : \Omega_- \to \mathbb{R},$$

where $\mathbb{R}^{d\times d}_{\mathrm{sym}}$ is the space of symmetric $d \times d$ real matrices. We assume that $c \in L^\infty(\Omega_-)$ and $c \geq c_0 > 0$ almost everywhere, so that $c^{-1} \in L^\infty(\Omega_-)$. We also assume that $\kappa \in L^\infty(\Omega_-)^{d\times d}$ is uniformly positive definite, i.e., there exists $\kappa_0 > 0$ such that

$$\mathbf{d} \cdot (\kappa\mathbf{d}) \geq \kappa_0 |\mathbf{d}|^2, \qquad \forall \mathbf{d} \in \mathbb{R}^d, \qquad \text{almost everywhere in } \Omega_-.$$

Before we state the transmission problem in a rigorous form we need to introduce some spaces and operators related to the space variables. The solution will take values in the spaces

$$H^1_\kappa(\Omega_-) := \{u \in H^1(\Omega_-) : \operatorname{div}(\kappa\nabla u) \in L^2(\Omega_-)\}, \tag{4.1a}$$

$$H^1_\Delta(\Omega_+) := \{u \in H^1(\Omega_+) : \Delta u \in L^2(\Omega_+)\}. \tag{4.1b}$$

We will also need two trace operators $\gamma^\pm : H^1(\Omega_\pm) \to H^{1/2}(\Gamma)$ and the associated interior-exterior normal derivative operators $\partial^\pm_\nu : H^1_\Delta(\Omega_\pm) \to H^{-1/2}(\Gamma)$, defined in the

usual weak form through Green's identities. For functions defined only in the interior domain Ω_- we will not use a superscript for the trace. We will also use the interior conormal derivative operator $\partial_{\kappa,\nu} : H^1_\kappa(\Omega_-) \to H^{-1/2}(\Gamma)$. We refer to Appendix B for more details related to these Sobolev spaces.

To begin our exposition, we assume that the incident wave is defined in a way such that

$$\beta_0 := \gamma u^{\text{inc}} \in \text{TD}(H^{1/2}(\Gamma)), \qquad \beta_1 := \partial_\nu u^{\text{inc}} \in \text{TD}(H^{-1/2}(\Gamma)).$$

We refer the reader to Appendix A for the definition of the space $\text{TD}(\mathbb{X})$. This is a statement about 'smoothness' of the incident wave in the space variables close to the boundary, as well as about causality of the traces of the incident wave. We look for

$$(u, u_+) \in \text{TD}(H^1_\kappa(\Omega_-)) \times \text{TD}(H^1_\Delta(\Omega_+)) \tag{4.2a}$$

satisfying

$$c^{-2}\ddot{u} = \text{div}(\kappa \nabla u) \qquad (\text{in } L^2(\Omega_-)), \tag{4.2b}$$

$$\ddot{u}_+ = \Delta u_+ \qquad (\text{in } L^2(\Omega_+)), \tag{4.2c}$$

$$\gamma u = \gamma^+ u_+ + \beta_0 \qquad (\text{in } H^{1/2}(\Gamma)), \tag{4.2d}$$

$$\partial_{\kappa,\nu} u = \partial^+_\nu u_+ + \beta_1 \qquad (\text{in } H^{-1/2}(\Gamma)). \tag{4.2e}$$

Each of the equations in (4.2) is satisfied as an equality of distributions taking values in the space in parentheses on the right-hand-side of the equation. We note that the vanishing initial conditions for u are implicitly imposed by the condition (4.2a). Existence and uniqueness of solution to (4.2) follows by taking Laplace transforms [52, Section 6].

In the model equations (4.2), u and u_+ are a velocity potential for an acoustic fluid or solid. The parameters c and κ are chosen for mathematical convenience. We will deal with the very general case when κ is matrix-valued and c is scalar, both of the allowed to be variable in space. For the acoustic model, $\kappa = 1/\rho$, where ρ is the mass

density (so κ is a multiple of the identity) and the function multiplying the second time derivative should be $1/(c^2\rho)$, where c is the speed of sound.

The retarded layer potentials for the acoustic wave equation can be introduced using a uniquely solvable transmission problem. Let $\psi \in \mathrm{TD}(H^{1/2}(\Gamma))$ and $\eta \in \mathrm{TD}(H^{-1/2}(\Gamma))$. The problem that looks for $u \in \mathrm{TD}(H^1_\Delta(\mathbb{R}^d \setminus \Gamma))$ satisfying

$$\ddot{u} = \Delta u \qquad (\text{in } L^2(\mathbb{R}^d \setminus \Gamma)), \tag{4.3a}$$

$$[\![\gamma u]\!] = \psi, \qquad (\text{in } H^{1/2}(\Gamma)), \tag{4.3b}$$

$$[\![\partial_\nu u]\!] = \eta, \qquad (\text{in } H^{-1/2}(\Gamma)), \tag{4.3c}$$

admits a unique solution. Using Laplace transforms and the theory of layer potentials for the resolvent operator of the Laplacian, it can be shown that there exist

$$\mathcal{D} \in \mathrm{TD}(\mathcal{B}(H^{1/2}(\Gamma), H^1_\Delta(\mathbb{R}^d \setminus \Gamma))), \qquad \mathcal{S} \in \mathrm{TD}(\mathcal{B}(H^{-1/2}(\Gamma), H^1_\Delta(\mathbb{R}^d \setminus \Gamma))),$$

such that the solution of (4.3) can be written using the weak Kirchhoff formula (see [51] for a direct introduction to these operators in the three dimensional case)

$$u = \mathcal{S} * \eta - \mathcal{D} * \psi.$$

As in Chapters 2 and 3, the convolution symbol $*$ refers specifically to the convolution of a causal operator-valued distribution with a causal vector-valued distribution. The four retarded boundary integral operators are given by convolution with the averages of the Cauchy traces of the single and double layer retarded potentials:

$$\begin{aligned}
\mathcal{V} &:= \{\!\{\gamma \mathcal{S}\}\!\} = \gamma^{\pm} \mathcal{S} \in \mathrm{TD}(\mathcal{B}(H^{-1/2}(\Gamma), H^{1/2}(\Gamma))), \\
\mathcal{K} &:= \{\!\{\gamma \mathcal{D}\}\!\} \in \mathrm{TD}(\mathcal{B}(H^{1/2}(\Gamma), H^{1/2}(\Gamma))), \\
\mathcal{K}^t &:= \{\!\{\partial_\nu \mathcal{S}\}\!\} \in \mathrm{TD}(\mathcal{B}(H^{-1/2}(\Gamma), H^{-1/2}(\Gamma))), \\
\mathcal{W} &:= -\{\!\{\partial_\nu \mathcal{D}\}\!\} = -\partial_\nu^{\pm} \mathcal{D} \in \mathrm{TD}(\mathcal{B}(H^{1/2}(\Gamma), H^{-1/2}(\Gamma))).
\end{aligned} \tag{4.4}$$

A fully detailed introduction to the retarded layer potentials and operators is given in [74, Chapters 2 and 3], based on the Laplace domain analysis of Bamberger and HaDuong [7, 8].

Let u_+ be the exterior part of the solution of (4.2) and let

$$\phi := \gamma^+ u_+, \qquad \lambda := \partial_\nu^+ u_+.$$

Then, by definition of the layer potentials and operators,

$$u_+ = \mathcal{D} * \phi - \mathcal{S} * \lambda \qquad (\text{in } H^1_\Delta(\Omega_+)), \tag{4.5a}$$

$$\gamma^+ u_+ = \tfrac{1}{2}\phi + \mathcal{K} * \phi - \mathcal{V} * \lambda \qquad (\text{in } H^{1/2}(\Gamma)), \tag{4.5b}$$

$$0 = \mathcal{W} * \phi + \tfrac{1}{2}\lambda + \mathcal{K}^t * \lambda \qquad (\text{in } H^{-1/2}(\Gamma)). \tag{4.5c}$$

The coupled boundary-field system consists of: (a) a variational-in-space formulation of (4.2b) using (4.2e), (b) a non-local boundary condition obtained by substitution of (4.2d) in (4.5b), and (c) the identity (4.5c) to 'symmetrize' the coupled system. We look for

$$(u, \lambda, \phi) \in \mathrm{TD}(H^1(\Omega_-)) \times \mathrm{TD}(H^{-1/2}(\Gamma)) \times \mathrm{TD}(H^{1/2}(\Gamma)) \tag{4.6a}$$

satisfying

$$(c^{-2}\ddot{u}, w)_{\Omega_-} + (\kappa \nabla u, \nabla w)_{\Omega_-} - \langle \lambda, \gamma w \rangle = \langle \beta_1, \gamma w \rangle \quad \forall w \in H^1(\Omega_-) \quad (\text{in } \mathbb{R}), \tag{4.6b}$$

$$\gamma u + \mathcal{V} * \lambda - \tfrac{1}{2}\phi - \mathcal{K} * \phi = \beta_0 \qquad (\text{in } H^{1/2}(\Gamma)), \tag{4.6c}$$

$$\tfrac{1}{2}\lambda + \mathcal{K}^t * \lambda + \mathcal{W} * \phi = 0 \qquad (\text{in } H^{-1/2}(\Gamma)). \tag{4.6d}$$

The equivalence of the transmission problem with the boundary-field formulation (4.6) is given in the next proposition. Its proof follows from taking Laplace transforms and using well-known results on integral representations of the solutions of elliptic equations [64].

Proposition 4.1.1. *Problem (4.6) has a unique solution for arbitrary $\beta_0 \in \mathrm{TD}(H^{1/2}(\Gamma))$ and $\beta_1 \in \mathrm{TD}(H^{-1/2}(\Gamma))$. If (u, ϕ, λ) solves (4.6) and $u_+ = \mathcal{D} * \phi - \mathcal{S} * \lambda$, then (u, u_+) is the unique solution of (4.2). Reciprocally, if (u, u_+) is the solution of (4.2) and $\phi := \gamma^+ u_+$, $\lambda := \partial_\nu^+ u_+$, then (u, λ, ϕ) is the solution of (4.6).*

We now introduce three finite dimensional subspaces

$$U_h \subset H^1(\Omega_-), \qquad X_h \subset H^{-1/2}(\Gamma), \qquad Y_h \subset H^{1/2}(\Gamma).$$

While we will keep Galerkin notation for the discretization of the variational equation (4.6b), we will use the notation of Chapter 3 and shorten Galerkin semidiscrete-in-space equations on the boundary using polar spaces. If $\alpha \in \mathrm{TD}(H^{1/2}(\Gamma))$, we will write

$$\alpha \in X_h^\circ \quad (\text{in } H^{1/2}(\Gamma)) \quad \text{to denote} \quad \langle \mu^h, \alpha \rangle = 0 \quad \forall \mu^h \in X_h \quad (\text{in } \mathbb{R}).$$

Similary, if $\rho \in \mathrm{TD}(H^{-1/2}(\Gamma))$, we will write

$$\rho \in Y_h^\circ \quad (\text{in } H^{-1/2}(\Gamma)) \quad \text{to denote} \quad \langle \rho, \psi^h \rangle = 0 \quad \forall \psi^h \in Y_h \quad (\text{in } \mathbb{R}).$$

These conditions can also be described by taking Laplace transforms and imposing the respective tests with elements of X_h and Y_h to vanish for all values of the Laplace domain parameter s. We will also write conditions of the form

$$\eta \in X_h \quad (\text{in } H^{-1/2}(\Gamma)) \qquad \text{and} \qquad \psi \in Y_h \quad (\text{in } H^{1/2}(\Gamma)). \tag{4.7}$$

For instance, if $\Pi_h^X : H^{-1/2}(\Gamma) \to X_h$ is the orthogonal projection onto X_h, the first condition in (4.7) can be defined as $\Pi_h^X \eta = \eta$ as $H^{-1/2}(\Gamma)$-valued distributions. The semidiscrete version of (4.6) is the search for

$$(u^h, \lambda^h, \phi^h) \in \mathrm{TD}(U_h) \times \mathrm{TD}(H^{-1/2}(\Gamma)) \times \mathrm{TD}(H^{1/2}(\Gamma)) \tag{4.8a}$$

satisfying

$$\lambda^h \in X_h \quad (\text{in } H^{-1/2}(\Gamma)), \qquad \phi^h \in Y_h \quad (\text{in } H^{1/2}(\Gamma)). \tag{4.8b}$$

and

$$(c^{-2}\ddot{u}^h, w^h)_{\Omega_-} + (\kappa \nabla u^h, \nabla w^h)_{\Omega_-} = \langle \lambda^h + \beta_1, \gamma w^h \rangle \quad \forall w^h \in U_h \quad (\text{in } \mathbb{R}), \tag{4.8c}$$

$$\gamma u^h + \mathcal{V} * \lambda^h - \tfrac{1}{2}\phi^h - \mathcal{K} * \phi^h - \beta_0 \in X_h^\circ \quad (\text{in } H^{1/2}(\Gamma)), \tag{4.8d}$$

$$\tfrac{1}{2}\lambda^h + \mathcal{K}^t * \lambda^h + \mathcal{W} * \phi^h \in Y_h^\circ \quad (\text{in } H^{-1/2}(\Gamma)). \tag{4.8e}$$

A semidiscrete exterior solution is then defined with Kirchhoff's formula

$$u^\star = \mathcal{D} * \phi^h - \mathcal{S} * \lambda^h. \tag{4.9}$$

In (4.9) we have preferred not to name the output of the representation formula u_+^h because we will be interested in this output as a distribution with values in $H^1_\Delta(\mathbb{R}^d \setminus \Gamma)$ instead of $H^1_\Delta(\Omega_+)$. Existence and uniqueness of solution to (4.8) can be proved using the Laplace transform [52, Section 6]. The technique relates the semidiscrete problem to an exotic transmission problem with two fields in the interior domain and one field in the exterior domain.

Proposition 4.1.2. *Let (u^h, λ^h, ϕ^h) be the solution of (4.8) and let $u^\star$ be defined by (4.9). The pair*

$$(u^h, u^\star) \in \mathrm{TD}(U_h) \times \mathrm{TD}(H^1_\Delta(\mathbb{R}^d \setminus \Gamma)) \tag{4.10a}$$

satisfies

$$(c^{-2}\ddot{u}^h, w^h)_{\Omega_-} + (\kappa \nabla u^h, \nabla w^h)_{\Omega_-} + \langle [\![\partial_\nu u^\star]\!], \gamma w^h \rangle$$
$$= \langle \beta_1, \gamma w^h \rangle \quad \forall w^h \in U_h \qquad (\text{in } \mathbb{R}), \tag{4.10b}$$
$$\ddot{u}^\star = \Delta u^\star \qquad (\text{in } L^2(\mathbb{R}^d \setminus \Gamma)), \tag{4.10c}$$
$$([\![\gamma u^\star]\!], [\![\partial_\nu u^\star]\!]) \in Y_h \times X_h \qquad (\text{in } H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)), \tag{4.10d}$$
$$(\partial_\nu^- u^\star, \gamma u^h - \gamma^+ u^\star - \beta_0) \in Y_h^\circ \times X_h^\circ \qquad (\text{in } H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)). \tag{4.10e}$$

Reciprocally, if $(u^h, u^\star)$ is the unique solution of (4.10) and

$$\phi^h = -[\![\gamma u^\star]\!], \qquad \lambda^h = -[\![\partial_\nu u^\star]\!],$$

the triple (u^h, λ^h, ϕ^h) is the unique solution of (4.8).

To study the difference between the solutions of (4.6) and (4.8) we will use another exotic transmission problem. We first introduce the elliptic projection $\Pi_h^V : H^1(\Omega_-) \to U_h$ by solving the equations

$$(\kappa \nabla(\Pi_h^V u - u), \nabla w^h)_{\Omega_-} = 0 \quad \forall w^h \in U_h, \tag{4.11}$$

subject to the restrictions

$$\int_{\Omega_j} \Pi_h^V u = \int_{\Omega_j} u \qquad j = 1, \dots, N, \tag{4.12}$$

where Ω_j are the connected components of Ω_-.

Proposition 4.1.3. *Let (u, λ, ϕ) and (u^h, λ^h, ϕ^h) be the respective solutions of (4.6) and (4.8) and let*

$$\varepsilon^h := u^h - \Pi_h^V u, \qquad \theta^h := \Pi_h^V u - u,$$

$$\varepsilon^\lambda := \lambda^h - \lambda, \qquad \varepsilon^\phi := \phi^h - \phi, \qquad \varepsilon^\star := u^\star - \mathcal{D} * \phi + \mathcal{S} * \lambda = \mathcal{D} * \varepsilon^\phi - \mathcal{S} * \varepsilon^\lambda.$$

Then

$$(\varepsilon^h, \varepsilon^\star) \in \mathrm{TD}(U_h) \times \mathrm{TD}(H^1_\Delta(\mathbb{R}^d \setminus \Gamma)) \tag{4.13a}$$

satisfies

$$\begin{aligned}
&(c^{-2}\ddot{\varepsilon}^h, w^h)_{\Omega_-} + (\kappa \nabla \varepsilon^h, \nabla w^h)_{\Omega_-} + \langle [\![\partial_\nu \varepsilon^\star]\!], \gamma w^h \rangle \\
&\qquad = -(c^{-2}\ddot{\theta}^h, w^h)_{\Omega_-} \qquad \forall w^h \in U_h \qquad (\text{in } \mathbb{R}), && (4.13b)\\
&\qquad \ddot{\varepsilon}^\star = \Delta \varepsilon^\star \qquad (\text{in } L^2(\mathbb{R}^d \setminus \Gamma)), && (4.13c)\\
&\qquad \gamma \varepsilon^h - \gamma^+ \varepsilon^\star + \gamma \theta^h \in X_h^\circ \qquad (\text{in } H^{1/2}(\Gamma)), && (4.13d)\\
&\qquad [\![\gamma \varepsilon^\star]\!] - \phi \in Y_h \qquad (\text{in } H^{1/2}(\Gamma)), && (4.13e)\\
&\qquad [\![\partial_\nu \varepsilon^\star]\!] - \lambda \in X_h \qquad (\text{in } H^{-1/2}(\Gamma)), && (4.13f)\\
&\qquad \partial_\nu^- \varepsilon^\star \in Y_h^\circ \qquad (\text{in } H^{-1/2}(\Gamma)). && (4.13g)
\end{aligned}$$

Reciprocally, if (u, λ, ϕ) is the solution of (4.6), $\theta^h := \Pi_h^V u - u$, and $(\varepsilon^h, \varepsilon^\star)$ is the solution of (4.13), then $(u^h, \lambda^h, \phi^h) = (\varepsilon^h + \Pi_h^V u, \lambda - [\![\partial_\nu \varepsilon^\star]\!], \phi - [\![\gamma \varepsilon^\star]\!])$ is the unique solution of (4.8).

4.2 Analysis of an Equivalent First Order System

We will analyze problems (4.10) and (4.13) simultaneously. We thus look for

$$(u^h, u^\star) \in \mathrm{TD}(U_h) \times \mathrm{TD}(H^1_\Delta(\mathbb{R}^d \setminus \Gamma)) \tag{4.14a}$$

satisfying

$$(c^{-2}\ddot{u}^h, w^h)_{\Omega_-} + (\kappa\nabla u^h, \nabla w^h)_{\Omega_-} + \langle [\![\partial_\nu u^\star]\!], \gamma w^h\rangle$$

$$= \langle \beta, \gamma w^h\rangle + (c^{-2}r, w^h)_{\Omega_-} \quad \forall w^h \in U_h \qquad (\text{in } \mathbb{R}), \tag{4.14b}$$

$$\ddot{u}^\star = \Delta u^\star \qquad (\text{in } L^2(\mathbb{R}^d \setminus \Gamma)), \tag{4.14c}$$

$$\gamma u^h - \gamma^+ u^\star - \alpha \in X_h^\circ \qquad (\text{in } H^{1/2}(\Gamma)), \tag{4.14d}$$

$$[\![\gamma u^\star]\!] - \phi \in Y_h \qquad (\text{in } H^{1/2}(\Gamma)), \tag{4.14e}$$

$$[\![\partial_\nu u^\star]\!] - \lambda \in X_h \qquad (\text{in } H^{-1/2}(\Gamma)), \tag{4.14f}$$

$$\partial_\nu^- u^\star \in Y_h^\circ \qquad (\text{in } H^{-1/2}(\Gamma)), \tag{4.14g}$$

for given data $\alpha, \beta, \lambda, \phi$ and r taking values in the appropriate spaces. We will first transform (4.14) into a first order system. To do that we introduce the antidifferentiation operator: given $f \in \mathrm{TD}(X)$, $\partial^{-1} f$ is the only element of $\mathrm{TD}(X)$ whose distributional derivative is f. The operator ∂^{-1} is a weak version of

$$(\partial^{-1} f)(t) = \int_0^t f(\tau) d\tau.$$

We will need the Sobolev space [30]

$$\mathbf{H}(\mathrm{div}, \mathbb{R}^d \setminus \Gamma) := \{\mathbf{v} \in \mathbf{L}^2(\mathbb{R}^d) := L^2(\mathbb{R}^d)^d \,:\, \nabla \cdot \mathbf{v} \in L^2(\mathbb{R}^d \setminus \Gamma)\},$$

endowed with its natural norm, which we will denote $\|\cdot\|_{\mathrm{div}, \mathbb{R}^d \setminus \Gamma}$. For an element $\mathbf{v}$ of this space we can define the two sided normal components on Γ, $\gamma_\nu^\pm \mathbf{v}$ and the corresponding jump $[\![\gamma_\nu \mathbf{v}]\!] := \gamma_\nu^- \mathbf{v} - \gamma_\nu^+ \mathbf{v}$. We need finally the weighted orthogonal projection $P_h : L^2(\Omega_-) \to U_h$

$$P_h r \in U_h, \qquad (c^{-2}(P_h r - r), w^h)_{\Omega_-} = 0 \qquad \forall w^h \in U_h,$$

a second discrete space $\mathbf{V}_h := \nabla U_h = \{\nabla u^h \,:\, u^h \in U_h\}$, and the discrete operators $\mathrm{div}_h^\kappa : \mathbf{L}^2(\Omega_-) \to U_h$ and $\gamma_h^t : H^{-1/2}(\Gamma) \to U_h$, given by the relation

$$(c^{-2}(\mathrm{div}_h^\kappa \mathbf{v} + \gamma_h^t \eta), w^h)_{\Omega_-} = -(\kappa \mathbf{v}, \nabla w^h)_{\Omega_-} + \langle \eta, \gamma w^h\rangle \qquad \forall w^h \in U_h. \tag{4.15}$$

The first order formulation involves two new unknowns $\mathbf{v}^h := \partial^{-1}\nabla u^h$ and $\mathbf{v}^\star := \partial^{-1}\nabla u^\star$. It looks for

$$(u^h, u^\star, \mathbf{v}^h, \mathbf{v}^\star) \in \mathrm{TD}\left(U_h \times H^1(\mathbb{R}^d \setminus \Gamma) \times \mathbf{V}_h \times \mathbf{H}(\mathrm{div}, \mathbb{R}^d \setminus \Gamma)\right) \tag{4.16a}$$

satisfying

$$\dot{u}^h = \mathrm{div}_h^\kappa \mathbf{v}^h - \gamma_h^t[\![\gamma_\nu \mathbf{v}^\star]\!] + \gamma_h^t \partial^{-1}\beta + P_h r, \qquad (\text{in } U_h), \tag{4.16b}$$

$$\dot{u}^\star = \nabla \cdot \mathbf{v}^\star \qquad (\text{in } L^2(\mathbb{R}^d \setminus \Gamma)), \tag{4.16c}$$

$$\dot{\mathbf{v}}^h = \nabla u^h \qquad (\text{in } \mathbf{V}_h), \tag{4.16d}$$

$$\dot{\mathbf{v}}^\star = \nabla u^\star \qquad (\text{in } \mathbf{L}^2(\mathbb{R}^d \setminus \Gamma)), \tag{4.16e}$$

$$\gamma u^h - \gamma^+ u^\star - \alpha \in X_h^\circ \qquad (\text{in } H^{1/2}(\Gamma)), \tag{4.16f}$$

$$[\![\gamma u^\star]\!] - \phi \in Y_h \qquad (\text{in } H^{1/2}(\Gamma)), \tag{4.16g}$$

$$[\![\gamma_\nu \mathbf{v}^\star]\!] - \partial^{-1}\lambda \in X_h \qquad (\text{in } H^{-1/2}(\Gamma)), \tag{4.16h}$$

$$\gamma_\nu^- \mathbf{v}^\star \in Y_h^\circ \qquad (\text{in } H^{-1/2}(\Gamma)). \tag{4.16i}$$

Proposition 4.2.1. *Problems* (4.14) *and* (4.16) *are equivalent.*

Consider the space

$$\mathcal{H} := U_h \times L^2(\mathbb{R}^d \setminus \Gamma) \times \mathbf{V}_h \times \mathbf{L}^2(\mathbb{R}^d \setminus \Gamma),$$

endowed with the inner product whose associated norm is

$$\|U\|_{\mathcal{H}}^2 = \|(u^h, u^\star, \mathbf{v}^h, \mathbf{v}^\star)\|_{\mathcal{H}}^2 := \|c^{-1}u^h\|_{\Omega_-}^2 + \|u^\star\|_{\mathbb{R}^d\setminus\Gamma}^2 + \|\kappa^{1/2}\mathbf{v}^h\|_{\Omega_-}^2 + \|\mathbf{v}^\star\|_{\mathbb{R}^d\setminus\Gamma}^2.$$

We also introduce the unbounded operator

$$\mathcal{A}U = \mathcal{A}(u^h, u^\star, \mathbf{v}^h, \mathbf{v}^\star) := (\mathrm{div}_h^\kappa \mathbf{v}_h - \gamma_h^t[\![\gamma_\nu \mathbf{v}^\star]\!], \nabla \cdot \mathbf{v}^\star, \nabla u^h, \nabla u^\star) \tag{4.17}$$

defined in the domain $D(\mathcal{A}) := \mathcal{U} \times \boldsymbol{\mathcal{V}}$, where

$$\begin{aligned} \mathcal{U} &:= \{(u^h, u^\star) \in U_h \times H^1(\mathbb{R}^d \setminus \Gamma) \,:\, \gamma u^h - \gamma^+ u^\star \in X_h^\circ, \quad [\![\gamma u^\star]\!] \in Y_h\}, \\ \boldsymbol{\mathcal{V}} &:= \{(\mathbf{v}^h, \mathbf{v}^\star) \in \mathbf{V}_h \times \mathbf{H}(\mathrm{div}, \mathbb{R}^d \setminus \Gamma)) \,:\, [\![\gamma_\nu \mathbf{v}^\star]\!] \in X_h, \quad \gamma_\nu^- \mathbf{v}^\star \in Y_h^\circ\}. \end{aligned}$$

For basic concepts of contractive C_0-semigroups of operators on Hilbert spaces (and the associated groups of isometries), we refer to [45, Chapter 4] and the more comprehensive [67].

Proposition 4.2.2. *The operators $\pm\mathcal{A} : D(\mathcal{A}) \subset \mathcal{H} \to \mathcal{H}$ are maximal dissipative. Therefore $\mathcal{A}$ is the infinitesimal generator of a C_0-group of isometries in $\mathcal{H}$.*

Proof. We first need to prove that

$$(\mathcal{A}\,U, U)_{\mathcal{H}} = 0 \qquad \forall U \in D(\mathcal{A}), \tag{4.18}$$

which means, by definition, that $\pm\mathcal{A}$ are dissipative. To prove (4.18) we proceed as follows: given $U = (u^h, u^\star, \mathbf{v}^h, \mathbf{v}^\star) \in D(\mathcal{A})$,

$$\begin{aligned}
(\mathcal{A}\,U, U)_{\mathcal{H}} &= (c^{-2}(\mathrm{div}_h^\kappa \mathbf{v}_h - \gamma_h^t[\![\gamma_\nu \mathbf{v}^\star]\!]), u^h)_{\Omega_-} + (\kappa\nabla u^h, \mathbf{v}^h)_{\Omega_-} \\
&\quad + (\nabla\cdot\mathbf{v}^\star, u^\star)_{\mathbb{R}^d\setminus\Gamma} + (\nabla u^\star, \mathbf{v}^\star)_{\mathbb{R}^d\setminus\Gamma} \\
&= -\langle[\![\gamma_\nu \mathbf{v}^\star]\!], \gamma u^h\rangle + \langle\gamma_\nu^- \mathbf{v}^\star, \gamma^- u^\star\rangle - \langle\gamma_\nu^+ \mathbf{v}^\star, \gamma^+ u^\star\rangle \\
&= -\langle[\![\gamma_\nu \mathbf{v}^\star]\!], \gamma^+ u^\star\rangle + \langle\gamma_\nu^- \mathbf{v}^\star, \gamma^+ u^\star\rangle - \langle\gamma_\nu^+ \mathbf{v}^\star, \gamma^+ u^\star\rangle = 0.
\end{aligned}$$

We have applied: the definition of the discrete operators and the weak divergence theorem (definition of $\gamma_\nu^\pm$) in the second equality, and the transmission conditions included in the definitions $\mathcal{U}$ and $\boldsymbol{\mathcal{V}}$ for the third equality.

To prove maximal dissipativity, we need to show that $\mathcal{I} \pm \mathcal{A} : D(\mathcal{A}) \to \mathcal{H}$ are surjective. We will only show the details for $\mathcal{I} - \mathcal{A}$, since the other case is essentially identical. Given $F = (f^h, f^\star, \mathbf{g}^h, \mathbf{g}^\star) \in \mathcal{H}$, we solve the coercive variational problem

$$(u^h, u^\star) \in \mathcal{U}, \tag{4.19a}$$

$$\begin{aligned}
&(c^{-2}u^h, w^h)_{\Omega_-} + (\kappa\nabla u^h, \nabla w^h)_{\Omega_-} + (u^\star, w^\star)_{\mathbb{R}^d} + (\nabla u^\star, \nabla w^\star)_{\mathbb{R}^d\setminus\Gamma} \\
&\quad = (c^{-2}f^h, w^h)_{\Omega_-} - (\kappa\mathbf{g}^h, \nabla w^h)_{\Omega_-} + (f^\star, w^\star)_{\mathbb{R}^d} - (\mathbf{g}^\star, \nabla w^\star)_{\mathbb{R}^d\setminus\Gamma} \qquad \forall (w^h, w^\star) \in \mathcal{U},
\end{aligned} \tag{4.19b}$$

and define

$$\mathbf{v}^h = \nabla u^h + \mathbf{g}^h, \qquad \mathbf{v}^\star = \nabla u^\star + \mathbf{g}^\star. \tag{4.20}$$

If we test (4.19b) with $(0, w^\star) \in \{0\} \times \mathcal{D}(\mathbb{R}^d \backslash \Gamma) \subset \mathcal{U}$ and substitute the second equation in (4.20), it follows that

$$(u^\star, w^\star)_{\mathbb{R}^d \backslash \Gamma} + (\mathbf{v}^\star, \nabla w^\star)_{\mathbb{R}^d \backslash \Gamma} = (f^\star, w^\star)_{\mathbb{R}^d \backslash \Gamma} \qquad \forall w^\star \in \mathcal{D}(\mathbb{R}^d \setminus \Gamma).$$

Therefore

$$u^\star = \nabla \cdot \mathbf{v}^\star + f^\star, \tag{4.21}$$

which implies that $\mathbf{v}^\star \in \mathbf{H}(\mathrm{div}, \mathbb{R}^d \setminus \Gamma)$. Substituting now (4.20) and (4.21) in (4.19b), we obtain

$$(c^{-2} u^h, w^h)_{\Omega_-} + (\kappa \mathbf{v}^h, \nabla w^h)_{\Omega_-} + (\nabla \cdot \mathbf{v}^\star, w^\star)_{\mathbb{R}^d \backslash \Gamma} + (\mathbf{v}^\star, \nabla w^\star)_{\mathbb{R}^d \backslash \Gamma} = (c^{-2} f^h, w^h)_{\Omega_-} \tag{4.22}$$

for all $(w^h, w^\star) \in \mathcal{U}$. However, by the definition of the discrete operators (4.15) and the weak divergence theorem, we can equivalently (after some term rearrangement) write (4.22) as

$$\begin{aligned} &(c^{-2}(u^h - f^h - \mathrm{div}_h^\kappa \mathbf{v}^h + \gamma_h^t [\![\gamma \mathbf{v}^\star]\!]), w^h)_{\Omega_-} \\ &\qquad + \langle \gamma_\nu^- \mathbf{v}^\star, [\![\gamma w^\star]\!] \rangle + \langle [\![\gamma_\nu \mathbf{v}^\star]\!], \gamma^+ w^\star - \gamma w^h \rangle \;\; = \;\; 0 \quad \forall (w^h, w^\star) \in \mathcal{U}. \end{aligned} \tag{4.23}$$

Let then $(\psi^h, \xi^h) \in Y_h \times X_h^\circ \subset H^{1/2}(\Gamma)^2$ and $w^h \in U_h$. We can choose $w^\star \in H^1(\mathbb{R}^d \setminus \Gamma)$ satisfying the trace conditions $\gamma^+ w^\star = \gamma w^h + \xi^h$ and $\gamma^- w^\star = \gamma^+ w^\star + \psi^h$. This proves that the operator

$$\mathcal{U} \ni (w^h, w^\star) \longmapsto (w^h, [\![\gamma w^\star]\!], \gamma^+ w^\star - \gamma w^h) \in U_h \times Y_h \times X_h^\circ$$

is surjective. Therefore, (4.23) is equivalent to

$$u^h = \mathrm{div}_h^\kappa \mathbf{v}^h - \gamma_h^t [\![\gamma \mathbf{v}^\star]\!] + f^h \tag{4.24}$$

and the transmission conditions

$$\gamma_\nu^- \mathbf{v}^\star \in Y_h^\circ, \qquad [\![\gamma_\nu \mathbf{v}^\star]\!] \in X_h. \tag{4.25}$$

These conditions imply that $(\mathbf{v}^h, \mathbf{v}^\star) \in \boldsymbol{\mathcal{V}}$. Therefore $U = (u^h, u^\star, \mathbf{v}^h, \mathbf{v}^\star) \in D(\mathcal{A})$, and, finally, the collection of (4.20), (4.21), and (4.24) implies that $U = \mathcal{A}U + F$. This finishes the proof of surjectivity of $\mathcal{I} - \mathcal{A}$. □

The next step is the construction of a lifting operator to move all non-homogeneities in the transmission conditions of (4.16) (this includes the action of β in the right-hand-side of (4.16b)) to a right-hand-side of an operator equation $\dot{U} = \mathcal{A}U + F$. This operator is defined in Proposition 4.2.3. Note that we do not give a bound for the norm of $\mathbf{v}^h$ because it will not be used in the sequel. As in Chapter 3, the expression *C is independent of h* will be used to refer to a constant C that is allowed to depend on parameters of the equation and on the geometry, but not on the choice of the three discrete subspaces involved.

Proposition 4.2.3. *Given $(\varphi, \psi, \eta, \mu) \in H^{1/2}(\Gamma)^2 \times H^{-1/2}(\Gamma)^2$, there exists a unique*

$$(u^h, u^\star, \mathbf{v}^h, \mathbf{v}^\star) \in U_h \times H^1(\mathbb{R}^d \setminus \Gamma) \times \mathbf{V}_h \times \mathbf{H}(\mathrm{div}, \mathbb{R}^d \setminus \Gamma) \tag{4.26a}$$

such that

$$u^h = \mathrm{div}_h^\kappa \mathbf{v}^h - \gamma_h^t [\![\gamma_\nu \mathbf{v}^\star]\!] + \gamma_h^t \eta, \qquad u^\star = \nabla \cdot \mathbf{v}^\star, \tag{4.26b}$$

$$\mathbf{v}^h = \nabla u^h, \qquad \mathbf{v}^\star = \nabla u^\star, \tag{4.26c}$$

$$\gamma u^h - \gamma^+ u^\star - \varphi \in X_h^\circ, \qquad [\![\gamma u^\star]\!] - \psi \in Y_h, \tag{4.26d}$$

$$[\![\gamma_\nu \mathbf{v}^\star]\!] - \mu \in X_h, \qquad \gamma_\nu^- \mathbf{v}^\star \in Y_h^\circ. \tag{4.26e}$$

Furthermore, there exists $C > 0$, independent of h, such that

$$\|u^h\|_{1,\Omega_-} + \|u^\star\|_{1,\mathbb{R}^d\setminus\Gamma} + \|\mathbf{v}^\star\|_{\mathrm{div},\mathbb{R}^d\setminus\Gamma} \\ \leq C(\|\varphi\|_{1/2,\Gamma} + \|\psi\|_{1/2,\Gamma} + \|\eta\|_{-1/2,\Gamma} + \|\mu\|_{-1/2,\Gamma}).$$

Proof. Problem (4.26) is equivalent to the problem that looks for

$$(u^h, u^\star) \in U_h \times H^1_\Delta(\mathbb{R}^d \setminus \Gamma), \tag{4.27a}$$

satisfying

$$(c^{-2}u^h, w^h)_{\Omega_-} + (\kappa \nabla u^h, \nabla w^h)_{\Omega_-} + \langle [\![\partial_\nu u^\star]\!], \gamma w^h \rangle = \langle \eta, \gamma w^h \rangle \qquad \forall w^h \in U_h, \tag{4.27b}$$

$$u^\star = \Delta u^\star, \tag{4.27c}$$

$$\gamma u^h - \gamma^+ u^\star - \varphi \in X_h^\circ, \quad [\![\gamma u^\star]\!] - \psi \in Y_h, \tag{4.27d}$$

$$[\![\partial_\nu u^\star]\!] - \mu \in X_h, \qquad \partial_\nu^- u^\star \in Y_h^\circ, \tag{4.27e}$$

and then computes $\mathbf{v}^h = \nabla u^h$ and $\mathbf{v}^\star = \nabla u^\star$. The variational formulation of (4.27) is

$$(u^h, u^\star) \in U_h \times H^1(\mathbb{R}^d \setminus \Gamma), \tag{4.28a}$$

$$[\![\gamma u^\star]\!] - \psi \in Y_h, \qquad \gamma^+ u^\star - \gamma u^h - \varphi \in X_h^\circ, \tag{4.28b}$$

$$\begin{aligned}(c^{-2}u^h, w^h)_{\Omega_-} + (\kappa \nabla u^h, \nabla w^h)_{\Omega_-} \\ + (u^\star, w^\star)_{\mathbb{R}^d} + (\nabla u^\star, \nabla w^\star)_{\mathbb{R}^d \setminus \Gamma} = \langle \eta - \mu, \gamma w^h \rangle + \langle \mu, \gamma^+ w^\star \rangle \quad \forall (w^h, w^\star) \in \mathcal{U}.\end{aligned} \tag{4.28c}$$

The solution of (4.28) can be written as the sum $(0, u^\star_{nh}) + (u^h, u^\star_0)$, where $[\![\gamma u^\star_{nh}]\!] = \psi$, $\gamma^+ u^\star_{nh} = \varphi$ and the pair $(u^h, u^\star_0) \in \mathcal{U}$ is the solution of a coercive variational problem in $\mathcal{U}$ with coercivity and boundedness constants independent of h. □

Before we state our main theorem, we prepare some notation. For the proof, we refer the reader to [36, Section 3]. Suppose that $\mathbb{H}, \mathbb{V}$, $\mathbb{M}_1$, and $\mathbb{M}_2$ are Hilbert spaces, and that $\mathbb{V} \subset \mathbb{H}$ with continuous and dense embedding. Let $\mathsf{A}_\star : \mathbb{V} \to \mathbb{H}$ be a bounded linear operator such that the graph norm of $\mathsf{A}_\star$ is equivalent to the norm in the space $\mathbb{V}$. Suppose $\mathsf{G} : \mathbb{M}_1 \to \mathbb{H}$ and $\mathsf{B} : \mathbb{V} \to \mathbb{M}_2$ are bounded linear operators. Define the unbounded operator $\mathsf{A} := \mathsf{A}_\star|_{D(\mathsf{A})} \subset \mathbb{H} \to \mathbb{H}$, where $D(\mathsf{A}) = \mathsf{Ker}(\mathsf{B})$. We also assume $\pm\mathsf{A}$ are maximal dissipative operators. We are then interested in the abstract differential equation

$$U \in \mathrm{TD}(\mathbb{H}), \qquad \dot{U} = \mathsf{A}_\star U + \mathsf{G}\xi + F, \qquad \mathsf{B}U = \chi, \tag{4.29}$$

for data $(\xi, \chi) \in \mathrm{TD}(\mathbb{M}_1 \times \mathbb{M}_2)$. The final hypothesis is related to the lifting of boundary conditions: we assume that the steady-state problem

$$U \in \mathbb{V}, \qquad U - \mathsf{A}_\star U = \mathsf{G}\xi, \qquad \mathsf{B}U = \chi,$$

has a unique solution for all $(\xi, \chi) \in \mathbb{M}_1 \times \mathbb{M}_2$ and that there exists $C_{\mathrm{lift}} > 0$ such that

$$\|U\|_{\mathbb{H}} + \|U\|_{\mathbb{V}} \le C_{\mathrm{lift}} \|(\xi, \chi)\|_{\mathbb{M}_1 \times \mathbb{M}_2}.$$

We will also make use of the Sobolev spaces

$$\begin{aligned}\mathcal{C}^k_+(X) &:= \{f \in \mathcal{C}^k(\mathbb{R}; X) \ : \ f(t) = 0 \quad t \le 0\}, \\ W^k_+(X) &:= \{f \in \mathcal{C}^{k-1}_+(\mathbb{R}; X) \ : \ f^{(k)} \in L^1(\mathbb{R}; X), \ f^{(\ell)}(0) = 0 \quad \ell \le k-1\}.\end{aligned}$$

Note that we have the inclusion $W^k_+(X) \subset \mathrm{TD}(X)$. We then have the following theorem:

Theorem 4.2.4. [36, Theorem 3.3] *If $F \in W^1_+(\mathbb{H})$ and $\Xi := (\xi, \chi) \in W^2_+(\mathbb{M}_1 \times \mathbb{M}_2)$, then equation (4.29) has a unique solution $U \in \mathcal{C}^1_+(\mathbb{H}) \cap \mathcal{C}_+(\mathbb{V})$ and for all $t \geq 0$:*

$$\|U(t)\|_{\mathbb{H}} \leq C_{\text{lift}} \left(\int_0^t \|\Xi(\tau)\|_{\mathbb{M}_1 \times \mathbb{M}_2} d\tau + 2 \int_0^t \|\dot{\Xi}(\tau)\|_{\mathbb{M}_1 \times \mathbb{M}_2} d\tau \right) + \int_0^t \|F(\tau)\|_{\mathbb{H}} d\tau, \tag{4.30a}$$

$$\|\dot{U}(t)\|_{\mathbb{H}} \leq C_{\text{lift}} \left(\int_0^t \|\dot{\Xi}(\tau)\|_{\mathbb{M}_1 \times \mathbb{M}_2} d\tau + 2 \int_0^t \|\ddot{\Xi}(\tau)\|_{\mathbb{M}_1 \times \mathbb{M}_2} d\tau \right) + \int_0^t \|\dot{F}(\tau)\|_{\mathbb{H}} d\tau. \tag{4.30b}$$

We will now explain how problem (4.16b) fits in this general abstract framework. The spaces are

$$\begin{aligned} \mathbb{H} &:= \mathcal{H} = \mathcal{U}_h \times L^2(\mathbb{R}^d \setminus \Gamma) \times \mathbf{V}_h \times \mathbf{L}^2(\mathbb{R}^d \setminus \Gamma), \\ \mathbb{V} &:= \mathcal{U}_h \times H^1(\mathbb{R}^d \setminus \Gamma) \times \mathbf{V}_h \times \mathbf{H}(\mathrm{div}; \mathbb{R}^d \setminus \Gamma), \\ \mathbb{M}_1 &:= H^{-1/2}(\Gamma), \qquad \mathbb{M}_2 := X_h^* \times (Y_h^\circ)^* \times (X_h^\circ)^* \times Y_h^*, \end{aligned}$$

where the asterisk is used to denote the dual space. The operator $\mathsf{A}_\star$ is given by the same expression as the operator $\mathcal{A}$ defined in (4.17), but its domain is $\mathbb{V}$. The boundary conditions are taken care of by the operators

$$\mathsf{G}\eta := (-\gamma_h^t \eta, 0, 0, 0), \qquad \mathsf{B}U := ((\gamma u^h - \gamma^+ u^\star)|_{X_h}, [\![\gamma u^\star]\!]|_{Y_h^\circ}, [\![\gamma_\nu \mathbf{v}^\star]\!]|_{X_h^\circ}, \gamma_\nu^- \mathbf{v}^\star|_{Y_h}),$$

where γ_h^t is defined in (4.15). We can understand what we mean by the various restrictions in B as follows. Note that the difference in the traces $(\gamma u^h - \gamma^+ u^\star) \in H^{1/2}(\Gamma) = H^{-1/2}(\Gamma)^*$, and so we can recognize $(\gamma u^h - \gamma^+ u^\star)|_{X_h} : X_h \to \mathbb{R}$ as an element of X_h^*, defined by $X_h \ni \mu_h \mapsto \langle \mu_h, (\gamma u^h - \gamma^+ u^\star) \rangle_\Gamma$. The same explanation holds for the remaining components of $\mathsf{B}U$. The vector $\chi = (\alpha|_{X_h}, \phi|_{Y_h^\circ}, \partial^{-1}\lambda|_{X_h^\circ}, 0)$ contains the transmission data. Note that $D(\mathcal{A}) = \mathsf{Ker}(\mathsf{B})$ and $\mathsf{A} = \mathcal{A}$. Finally $F = (P_h r, 0, 0, 0)$. We can now

apply Theorem 4.2.4 (the hypotheses have been verified in Propositions 4.2.2 and 4.2.3) to problem (4.16). For convenience, we denote

$$H_k(f,t|X) := \sum_{j=0}^{k} \int_0^t \|f^{(j)}(\tau)\|_X d\tau$$

and $\mathbf{H}^{\pm 1/2}(\Gamma) := (H^{\pm 1/2}(\Gamma))^2$.

Proposition 4.2.5. *Let $\alpha, \phi \in W^2_+(H^{1/2}(\Gamma))$, $\beta, \lambda \in W^1_+(H^{-1/2}(\Gamma))$, and $r \in W^1_+(L^2(\Omega_-))$. Then (4.16) has a unique solution satisfying for all $t \geq 0$*

$$\begin{aligned}\|c^{-1}u^h(t)\|_{\Omega_-} + \|\kappa\nabla u^h(t)\|_{\Omega_-} + \|u^\star(t)\|_{1,\mathbb{R}^d\setminus\Gamma} + \|[\![\gamma u^\star(t)]\!]\|_{1/2,\Gamma} \\ \leq C\Big(H_2((\alpha,\phi),t|\mathbf{H}^{1/2}(\Gamma)) + H_2(\partial^{-1}(\beta,\lambda),t|\mathbf{H}^{-1/2}(\Gamma)) \\ + H_1(P_h r,t|L^2(\Omega_-))\Big),\end{aligned} \tag{4.31}$$

where the constant C does not depend on the time t or h. For $\alpha, \phi \in W^3_+(H^{1/2}(\Gamma))$, $\beta, \lambda \in W^2_+(H^{-1/2}(\Gamma))$, and $r \in W^2_+(L^2(\Omega_-))$ we have for all $t \geq 0$

$$\begin{aligned}\|[\![\partial_\nu u^\star(t)]\!]\|_{-1/2,\Gamma} \leq C\Big(H_2((\dot\alpha,\dot\phi),t|\mathbf{H}^{1/2}(\Gamma)) + H_2((\beta,\lambda),t|\mathbf{H}^{-1/2}(\Gamma)) \\ + H_1(P_h\dot r,t|L^2(\Omega_-))\Big).\end{aligned} \tag{4.32}$$

With this main result in hand, stability and semidiscretization error estimates follow as simple corollaries.

Corollary 4.2.6 (Stability)**.** *For data $\beta_0 \in W^2_+(H^{1/2}(\Gamma))$ and $\beta_1 \in W^1_+(H^{-1/2}(\Gamma))$ the semidiscrete scattering problem (4.10) has a unique solution $(u^h, u^\star)$ such that*

$$\begin{aligned}\|c^{-1}u^h(t)\|_{\Omega_-} + \|\kappa\nabla u^h(t)\|_{\Omega_-} + \|u^\star(t)\|_{1,\mathbb{R}^d\setminus\Gamma} + \|\phi^h(t)\|_{1/2,\Gamma} \\ \leq C\Big(H_2(\beta_0,t|H^{1/2}(\Gamma)) + H_2(\partial^{-1}\beta_1,t|H^{-1/2}(\Gamma))\Big).\end{aligned}$$

For $\beta_0 \in W^3_+(H^{1/2}(\Gamma))$ and $\beta_1 \in W^2_+(H^{-1/2}(\Gamma))$ we have the estimate

$$\|\lambda^h(t)\|_{-1/2,\Gamma} \leq C\Big(H_2(\dot\beta_0,t|H^{1/2}(\Gamma)) + H_2(\beta_1,t|H^{-1/2}(\Gamma))\Big).$$

The constant C is independent of h and t.

Proof. We apply Proposition 4.2.5 with $\alpha = \beta_0 \in W_+^2(H^{1/2}(\Gamma))$, $\beta = \beta_1 \in W_+^1(H^{-1/2}(\Gamma))$, $\phi = 0$, $\lambda = 0$, and $r = 0$. □

Corollary 4.2.7 (Semidiscretization error)**.** *Let*

$$\Pi_h^X : H^{1/2}(\Gamma) \to X_h \quad \textit{and} \quad \Pi_h^Y : H^{-1/2}(\Gamma) \to Y_h$$

be the orthogonal projections into the spaces X_h and Y_h, respectively, and let Π_h^V be the elliptic projection operator defined by (4.11) and (4.12). Suppose

$$\phi \in W_+^m(H^{1/2}(\Gamma)), \quad \lambda \in W_+^{m-1}(H^{-1/2}(\Gamma)), \tag{4.33a}$$

$$u \in W_+^m(H^1(\Omega_-)) \cap W_+^{m+1}(L^2(\Omega_-)). \tag{4.33b}$$

If (4.33a)–(4.33b) holds with $m = 2$, then the Galerkin semidiscretization error $(\varepsilon^h, \varepsilon^\star) := (u^h - u, u^\star - \mathcal{D} * \phi + \mathcal{S} * \lambda)$ that solves equations (4.13) satisfies for all $t \geq 0$

$$\begin{aligned}
&\|c^{-1}\varepsilon^h(t)\|_{\Omega_-} + \|\kappa\nabla\varepsilon^h(t)\|_{\Omega_-} + \|\varepsilon^\star(t)\|_{1,\mathbb{R}^d\setminus\Gamma} + \|\phi^h(t) - \phi(t)\|_{1/2,\Gamma} \\
&\qquad \leq C\Big(H_2(u - \Pi_h^V u, t|H^1(\Omega_-)) + H_1(\ddot{u} - \Pi_h^V \ddot{u}, t|L^2(\Omega_-)) \\
&\qquad\qquad + H_2(\partial^{-1}(\lambda - \Pi_h^Y \lambda), t|H^{-1/2}(\Gamma)) + H_2(\phi - \Pi_h^Y \phi, t|H^{1/2}(\Gamma))\Big).
\end{aligned}$$

If the exact solution (λ, ϕ, u) satisfies (4.33a)–(4.33b) with $m = 3$, then we have the estimate

$$\begin{aligned}
\|\lambda^h(t) - \lambda(t)\|_{-1/2,\Gamma} \leq C\Big(&H_2(\dot{u} - \Pi_h^V \dot{u}, t|H^1(\Omega_-)) + H_1(\dddot{u} - \Pi_h^V \dddot{u}, t|L^2(\Omega_-)) \\
&+ H_2(\lambda - \Pi_h^Y \lambda, t|H^{-1/2}(\Gamma)) + H_2(\dot{\phi} - \Pi_h^Y \dot{\phi}, t|H^{1/2}(\Gamma))\Big).
\end{aligned}$$

Proof. Note that the solution (4.16) with $\alpha = 0$, $\beta = 0$, $r = 0$, $\phi = \Pi_h^Y \phi$, and $\lambda = \Pi_h^X \lambda$ (i.e., the data ϕ and λ take values in the discrete spaces) is the trivial solution. If we now apply Proposition 4.2.5 with $\alpha = \gamma(u - \Pi_h^V u)$, $\beta = 0$, $r = \Pi_h^V \ddot{u} - \ddot{u}$, and (ϕ, λ) as in the hypotheses of the corollary, the result follows. □

4.3 Fully Discrete Analysis

The fully discrete method consists of applying the trapezoidal rule based CQ to the semidiscrete equations (4.8). Even if CQ, in practice, only produces solutions at

discrete times, the method gives a theoretical extension of this solution to continuous time [58, 37, 74]. The fully discrete solution will be denoted as $(u_k^h, \lambda_k^h, \phi_k^h)$. The boundary solutions are then input to a CQ discretized Kirchhoff formula, outputting a field $u_k^\star$. From the point of view of implementation (see also Section 4.4) the monolithic application of CQ to the semidiscrete equations (4.8) and to the representation formula (4.9) is equivalent to the use of CQ for the retarded integral equations (4.8d, 4.8e) and for the representation formula, coupled with a trapezoidal rule approximation of the linearly implicit second order differential equation (4.8c) (see [52, Proposition 12]). An interesting feature of CQ applied to time domain boundary integral equations is the fact that the method is equivalent to applying the underlying ODE solver (in this case, the trapezoidal rule) to the evolutionary PDE satisfied by the potential post-processing. This was already observed in [60] and has been exploited for analysis in [11] and [74, Chapter 9]. In our case this will amount to carrying out the analysis directly on the variables $(u_k^h, u_k^\star)$.

For the remaining analysis, we need to define the averaging and differencing operators

$$\alpha_k g(t) := \frac{1}{2}\left(g(t) + g(t-k)\right), \quad \partial_k g(t) := \frac{1}{k}\left(g(t) - g(t-k)\right),$$

and their squares

$$\begin{aligned}\alpha_k^2 g(t) &= \frac{1}{4}\left(g(t) + 2g(t-k) + g(t-2k)\right),\\ \partial_k^2 g(t) &= \frac{1}{k^2}\left(g(t) - 2g(t-k) + g(t-2k)\right).\end{aligned}$$

The fully discrete method looks for

$$(u_k^h, u_k^\star) \in \mathrm{TD}(U_h) \times \mathrm{TD}(H^1_\Delta(\mathbb{R}^d \setminus \Gamma)) \tag{4.34}$$

satisfying

$$(c^{-2}\partial_k^2 u_k^h, w^h)_{\Omega_-} + (\alpha_k^2 \kappa \nabla u_k^h, \nabla w^h)_{\Omega_-} + \langle [\![\alpha_k^2 \partial_\nu u_k^\star]\!], \gamma w^h \rangle$$
$$= \langle \alpha_k^2 \beta_1, \gamma w^h \rangle \quad \forall w^h \in U_h, \tag{4.35a}$$
$$\partial_k^2 u_k^\star = \alpha_k^2 \Delta u_k^\star, \tag{4.35b}$$
$$([\![\gamma u_k^\star]\!], [\![\partial_\nu u_k^\star]\!]) \in Y_h \times X_h, \tag{4.35c}$$
$$(\partial_\nu^- u^\star, \gamma u_k^h - \gamma^+ u_k^\star - \beta_0) \in Y_h^\circ \times X_h^\circ, \tag{4.35d}$$

i.e., we have applied the trapezoidal rule to the second order differential equation (4.10).

We define the consistency error for the trapezoidal rule time discretization for the interior and exterior fields by

$$\chi_k^h := \partial_k^2 u^h - \alpha_k^2 \ddot{u}^h \qquad \text{and} \qquad \chi_k^\star := \partial_k^2 u^\star - \alpha_k^2 \ddot{u}^\star.$$

Subtracting equations (4.35) from (4.10) we find the error quantities $e_k^h := u^h - u_k^h$ and $e_k^\star := u^\star - u_k^\star$

$$(e_k^h, e_k^\star) \in \mathrm{TD}(U_h) \times \mathrm{TD}(H^1_\Delta(\mathbb{R}^d \setminus \Gamma))$$

satisfy the equations

$$(c^{-2}\partial_k^2 e_k^h, w^h)_{\Omega_-} + (\alpha_k^2 \kappa \nabla e_k^h, \nabla w^h)_{\Omega_-} + \langle [\![\partial_\nu \alpha_k^2 e_k^\star]\!], \gamma w^h \rangle_\Gamma$$
$$= (c^{-2}\chi_k^h, w^h)_{\Omega_-} \quad \forall w^h \in U_h, \tag{4.36a}$$
$$\partial_k^2 e_k^\star = \alpha_k^2 \Delta e_k^\star + \chi_k^\star, \tag{4.36b}$$
$$([\![\gamma e_k^\star]\!], [\![\partial_\nu e_k^\star]\!]) \in Y_h \times X_h, \tag{4.36c}$$
$$(\partial_\nu^- e_k^\star, \gamma e_k^h - \gamma^+ e_k^\star) \in Y_h^\circ \times X_h^\circ. \tag{4.36d}$$

The following lemma is the key integration by parts formula for our analysis.

Lemma 4.3.1. *If $e_k^\star$ is a continuous function of t then the following Green's Identity holds for all $t \geq 0$:*

$$(\Delta e_k^\star(t), w^\star)_{\mathbb{R}^d \setminus \Gamma} + (\nabla e_k^\star(t), \nabla w^\star)_{\mathbb{R}^d \setminus \Gamma} = \langle [\![\partial_\nu e_k^\star(t)]\!], \gamma w^h \rangle_\Gamma \quad \forall (w^h, w^\star) \in \mathcal{U}.$$

Proof. The following chain of equalities

$$\begin{aligned}(\Delta e_k^\star, w^\star)_{\mathbb{R}^d\setminus\Gamma}+(\nabla e_k^\star(t), \nabla w^\star)_{\mathbb{R}^d\setminus\Gamma} - \langle[\![\partial_\nu e_k^\star(t)]\!], \gamma w^h\rangle_\Gamma \\ = \langle \partial_\nu^- e_k^\star(t), \gamma^- w^\star\rangle_\Gamma - \langle \partial_\nu^+ e_k^\star(t), \gamma^+ w^\star\rangle_\Gamma - \langle[\![\partial_\nu e_k^\star(t)]\!], \gamma w^h\rangle_\Gamma \\ = \langle[\![\partial_\nu e_k^\star(t)]\!], \gamma^+ w^\star - \gamma w^h\rangle_\Gamma + \langle \partial_\nu^- e_k^\star(t), [\![\gamma w]\!]\rangle_\Gamma = 0\end{aligned}$$

holds for all $(w^h, w^\star) \in \mathcal{U}$. This proves the result. □

Theorem 4.3.2. *Suppose that $\beta_0 \in W_+^6(H^{1/2}(\Gamma))$ and $\beta_1 \in W_+^5(H^{-1/2}(\Gamma))$. Then the natural error quantities*

$$\widehat{e}_k^h := \alpha_k e_k^h, \quad \widehat{f}_k^h := \partial_k e_k^h, \quad \widehat{e}_k^\star := \alpha_k e_k^\star, \quad \widehat{f}_k^\star := \partial_k e_k^\star$$

for a trapezoidal rule in time discretization of (4.10) satisfy for all $t \geq 0$

$$\|\widehat{f}_k^h(t)\|_{\Omega_-} + \|\kappa\nabla\widehat{e}_k^h(t)\|_{\Omega_-} + \|\widehat{f}_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} + \|\nabla\widehat{e}_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} \leq Ck^2 tH(\beta_0^{(3)}, \beta_1^{(3)}, t), \quad (4.37)$$

where $H(\eta_0, \eta_1, t) := H_3(\eta_0, t|H^{1/2}(\Gamma)) + H_2(\eta_1, t|H^{-1/2}(\Gamma))$. We also have the L^2 error estimate

$$\|e_k^h(t)\|_{\Omega_-} + \|e_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} \leq Ck^2t^2H(\beta_0^{(3)}, \beta_1^{(3)}, t). \quad (4.38)$$

The error for $[\![\gamma e_k^\star]\!] = \phi_k^h - \phi^h$ is bounded as

$$\|\alpha_k^2[\![\gamma e_k^\star(t)]\!]\|_{1/2,\Gamma} \leq Ck^2 \max\{t, t^2\}H(\beta_0^{(3)}, \beta_1^{(3)}, t). \quad (4.39)$$

For $\beta_0 \in W_+^7(H^{1/2}(\Gamma))$ and $\beta_1 \in W_+^6(H^{-1/2}(\Gamma))$, the error for $[\![\partial_\nu e_k^\star]\!] = \lambda_k^h - \lambda^h$ is bounded as

$$\|\alpha_k^2[\![\partial_\nu e_k^\star(t)]\!]\|_{-1/2,\Gamma} \leq Ck^2 \max\{1, t\}H(\beta_0^{(4)}, \beta_1^{(4)}, t). \quad (4.40)$$

Proof. Using the definition of the hatted variables, (4.36a), (4.36b), and Lemma 4.3.1 it follows that

$$\begin{aligned}\partial_k\left(\widehat{f}_k^h(t), w^h\right)_{\Omega_-} + \partial_k\left(\widehat{f}_k^\star(t), w^\star\right)_{\mathbb{R}^d\setminus\Gamma} + \alpha_k\left(\kappa\nabla\widehat{e}_k^h(t), \nabla w^h\right)_{\Omega_-} + \alpha_k\left(\nabla\widehat{e}_\kappa^\star(t), \nabla w^\star\right)_{\mathbb{R}^d\setminus\Gamma} \\ = (\chi_k^h(t), w^h)_{\Omega_-} + (\chi_k^\star(t), w^\star)_{\mathbb{R}^d\setminus\Gamma} \quad \forall (w^h, w^\star) \in \mathcal{U}.\end{aligned}$$

We know by (4.36c) and (4.36d) that $(\widehat{e}_k^h(t), \widehat{e}_k^\star(t)) \in \mathcal{U}$ for all t. We can then test the latter identity with $2\partial_k(\widehat{e}_k^h(t), \widehat{e}_k^\star(t)) = 2\alpha_k(\widehat{f}_k^h(t), \widehat{f}_k^\star(t))$ and re-order terms to obtain

$$\left|\!\left|\!\left| \left(\widehat{e}_k^h(t), \widehat{e}_k^\star(t), \widehat{f}_k^h(t), \widehat{f}_k^\star(t)\right) \right|\!\right|\!\right|^2 = \left|\!\left|\!\left| \left(\widehat{e}_k^h(t-k), \widehat{e}_k^\star(t-k), \widehat{f}_k^h(t-k), \widehat{f}_k^\star(t-k)\right) \right|\!\right|\!\right|^2 + k\left(\chi_k^h(t), 2\alpha_k \widehat{f}_k^h(t)\right)_{\Omega_-} + k\left(\chi_k^\star(t), 2\alpha_k \widehat{f}_k^\star(t)\right)_{\mathbb{R}^d\setminus\Gamma},$$

where

$$|\!|\!|(u, u^\star, v, v^\star)|\!|\!|^2 := \|c^{-1}v\|_{\Omega_-}^2 + \|\kappa^{1/2}\nabla u\|_{\Omega_-}^2 + \|v^\star\|_{\mathbb{R}^d\setminus\Gamma}^2 + \|\nabla u^\star\|_{\mathbb{R}^d\setminus\Gamma}^2.$$

By induction,

$$\left|\!\left|\!\left| \left(\widehat{e}_k^h(t), \widehat{e}_k^\star(t), \widehat{f}_k^h(t), \widehat{f}_k^\star(t)\right) \right|\!\right|\!\right|^2 = k\sum_{j\geq 0}\left(\left(\chi_k^h(t-t_j), 2\alpha_k \widehat{f}_k^h(t-t_j)\right)_{\Omega_-} + \left(\chi_k^\star(t-t_j), 2\alpha_k \widehat{f}_k^\star(t-t_j)\right)\right)_{\mathbb{R}^d\setminus\Gamma},$$

where for each t the sum is finite because all of the functions are causal. We now take $t^\star \leq t$ such that

$$\left|\!\left|\!\left| \left(\widehat{e}_k^h(t^\star), \widehat{e}_k^\star(t^\star), \widehat{f}_k^h(t^\star), \widehat{f}_k^\star(t^\star)\right) \right|\!\right|\!\right| = \max_{0\leq\tau\leq t} \left|\!\left|\!\left| \left(\widehat{e}_k^h(\tau), \widehat{e}_k^\star(\tau), \widehat{f}_k^h(\tau), \widehat{f}_k^\star(\tau)\right) \right|\!\right|\!\right|$$

and therefore we can bound

$$\left|\!\left|\!\left| \left(\widehat{e}_k^h(t^\star), \widehat{e}_k^\star(t^\star), \widehat{f}_k^h(t^\star), \widehat{f}_k^\star(t^\star)\right) \right|\!\right|\!\right|^2 \leq 2t^\star \left|\!\left|\!\left| \left(\widehat{e}_k^h(t^\star), \widehat{e}_k^\star(t^\star), \widehat{f}_k^h(t^\star), \widehat{f}_k^\star(t^\star)\right) \right|\!\right|\!\right| \max_{0\leq\tau\leq t^\star} \left(\|\chi_k^h(\tau)\|_{\Omega_-} + \|\chi_k^\star(\tau)\|_{\mathbb{R}^d\setminus\Gamma}\right). \quad (4.41)$$

A simple Taylor expansion shows the following estimate of the consistency error for the trapezoidal rule

$$\|\chi_k^h(\tau)\|_{\Omega_-} + \|\chi_k^\star(\tau)\|_{\mathbb{R}^d\setminus\Gamma} \leq Ck^2\left(\max_{\tau-2k\leq\rho\leq\tau} \|(u^h(\rho))^{(4)}\|_{\Omega_-} + \max_{\tau-2k\leq\rho\leq\tau} \|(u^\star(\rho))^{(4)}\|_{\mathbb{R}^d\setminus\Gamma}\right),$$

which, combined with (4.41), yields the error estimate

$$\left|\!\left|\!\left| \left(\widehat{e}_k^h(t), \widehat{e}_k^\star(t), \widehat{f}_k^h(t), \widehat{f}_k^\star(t)\right) \right|\!\right|\!\right| \leq Ck^2 t\left(\max_{0\leq\tau\leq t} \|(u^h(\tau))^{(4)}\|_{\Omega_-} + \max_{0\leq\tau\leq t} \|(u^\star(\tau))^{(4)}\|_{\mathbb{R}^d\setminus\Gamma}\right).$$

Applying the estimates from Corollary 4.2.6, we have the final bound in the natural energy norm

$$\left|\!\left|\!\left| \left(\widehat{e}_k^h(t), \widehat{e}_k^\star(t), \widehat{f}_k^h(t), \widehat{f}_k^\star(t) \right) \right|\!\right|\!\right| \leq Ck^2 t H(\beta_0^{(3)}, \beta_1^{(3)}, t),$$

where the constant C is independent of h and t. This proves (4.37). If we expand the differencing operator acting on the quantities $e_k^h(t)$ and $e_k^\star(t)$, we find

$$\|e_k^h(t)\|_{\Omega_-} + \|e_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} \leq \|e_k^h(t-k)\|_{\Omega_-} + \|e_k^\star(t-k)\|_{\mathbb{R}^d\setminus\Gamma} + k\|f_k^h(t)\|_{\Omega_-} + k\|f_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma}.$$

We may then proceed as before and show the $L^2(\Omega_-) \times L^2(\mathbb{R}^d)$ error bound

$$\|e_k^h(t)\|_{\Omega_-} + \|e_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} \leq Ck^2 t^2 H(\beta_0^{(3)}, \beta_1^{(3)}, t),$$

which establishes (4.38). To prove (4.39) we apply the trace theorem and the previous $L^2(\mathbb{R}^d \setminus \Gamma)$ and $H^1(\mathbb{R}^d \setminus \Gamma)$ estimates:

$$\begin{aligned}
\|\alpha_k^2 [\![\gamma e_k^\star(t)]\!]\|_{1/2,\Gamma} &\leq C \left(\|\alpha_k \nabla \widehat{e}_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} + \|\alpha_k^2 e_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} \right) \\
&\leq C \left(\max_{0\leq\tau\leq t} \|\nabla \widehat{e}_k^\star(\tau)\|_{\mathbb{R}^d\setminus\Gamma} + \max_{0\leq\tau\leq t} \|e_k^\star(\tau)\|_{\mathbb{R}^d\setminus\Gamma} \right) \\
&\leq Ck^2 \max\{t, t^2\} H(\beta_0^{(3)}, \beta_1^{(3)}, t).
\end{aligned}$$

Note that

$$\begin{aligned}
\|\alpha_k^2 [\![\partial_\nu e_h^\star(t)]\!]\|_{-1/2,\Gamma} \leq& C \left(\|\alpha_k^2 \nabla e_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} + \|\alpha_k^2 \Delta e_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} \right) \\
\leq& C \left(\max_{0\leq\tau\leq t} \|\nabla \widehat{e}_k^\star(\tau)\|_{\mathbb{R}^d\setminus\Gamma} + \|\partial_k \widehat{f}_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} + \|\chi_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} \right) \\
\leq& C \left(\max_{0\leq\tau\leq t} \|\nabla \widehat{e}^\star(\tau)\|_{\mathbb{R}^d\setminus\Gamma} + \max_{0\leq\tau\leq t} \left\| \frac{d}{dt} \widehat{f}_k^\star(\tau) \right\|_{\mathbb{R}^d\setminus\Gamma} + \|\chi_k^\star(t)\|_{\mathbb{R}^d\setminus\Gamma} \right),
\end{aligned}$$

where we have applied (4.36b) and the Mean Value Theorem. The final bound (4.40) follows from the previous estimates and the fact that the error corresponding to data $(\dot{\beta}_0, \dot{\beta}_1)$ is the time derivative of the error. This is due to the fact that all operators involved are convolution operators. This finishes the proof. □

4.4 Algorithm

We fix a basis for the finite dimensional space U_h (the FEM space) and for the spaces X_h and Y_h (the BEM spaces). Let $\mathrm{V}_h(s)$, $\mathrm{K}_h(s)$, $\mathrm{W}_h(s)$, and I_h be the matrix representations of the bilinear forms

$$\langle \cdot, V(s)\cdot \rangle : X_h \times X_h \to \mathbb{C}, \quad \langle \cdot, K(s)\cdot \rangle : X_h \times Y_h \to \mathbb{C},$$
$$\langle W(s)\cdot, \cdot \rangle : Y_h \times Y_h \to \mathbb{C}, \quad \langle \cdot, \cdot \rangle : X_h \times Y_h \to \mathbb{R}.$$

These matrix-valued functions of s involve only the boundary element spaces. Let M_h and S_h be the finite element mass and stiffness matrices, that is, the matrix representation of the symmetric bilinear forms

$$(c^{-2}\cdot, \cdot)_{\Omega_-} : U_h \times U_h \to \mathbb{R}, \qquad (\kappa \nabla \cdot, \nabla \cdot)_{\Omega_-} : U_h \times U_h \to \mathbb{R}.$$

Finally, let Γ_h be the matrix representation of $\langle \cdot, \gamma \cdot \rangle : X_h \times U_h \to \mathbb{R}$. This is the only matrix that connects the finite and boundary element spaces, a connection simply established through inner products.

For simplicity of exposition, let us assume that the functions $\beta_0(t_n)$ and $\beta_1(t_n)$ have been projected or interpolated onto the spaces Y_h and X_h, respectively. The corresponding vectors of coefficients will be denoted $\boldsymbol{\beta}_{1,n}$ and $\boldsymbol{\beta}_{0,n}$. The marching-on-in-time scheme for discretization inverts the same large coupled operator at each time step, and then updates the right hand side with past values of the solution. It can be interpreted in the following form: in the interior domain we have a trapezoidal rule discretization of the FEM-semidiscrete wave equation with Neumann (unknown) boundary conditions

$$\begin{aligned} \frac{4}{k^2}\mathrm{M}_h \mathbf{u}_n + \mathrm{S}_h \mathbf{u}_n - \Gamma_h^t \boldsymbol{\lambda}_n =& \Gamma_h^t \left(\boldsymbol{\beta}_{1,n} + 2\boldsymbol{\beta}_{1,n-1} + \boldsymbol{\beta}_{1,n-2} - 2\boldsymbol{\lambda}_{n-1} + \boldsymbol{\lambda}_{n-2} \right) \\ & - \frac{1}{k^2}\mathrm{M}_h \left(2\mathbf{u}_{n-1} - \mathbf{u}_{n-2} \right) + \mathrm{S}_h \left(2\mathbf{u}_{n-1} - \mathbf{u}_{n-2} \right), \end{aligned} \tag{4.42}$$

while in the exterior domain a trapezoidal rule CQ scheme discretizes a symmetric Galerkin-BEM system with given (yet unknown) Dirichlet data

$$\begin{bmatrix} \Gamma_h \mathbf{u}_n \\ 0 \end{bmatrix} + \begin{bmatrix} \mathrm{V}_h(2/k) & -\frac{1}{2}\mathrm{I}_h + \mathrm{K}_h(2/k) \\ \frac{1}{2}\mathrm{I}_h^t + \mathrm{K}_h^t(2/k) & \mathrm{W}_h(2/k) \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}_n \\ \boldsymbol{\phi}_n \end{bmatrix} = \begin{bmatrix} \mathrm{I}_h \boldsymbol{\beta}_{0,n} \\ 0 \end{bmatrix} - \sum_{m=1}^{n} \begin{bmatrix} \omega_m^{\mathrm{V}_h}(k) & \omega_m^{\mathrm{K}_h}(k) \\ \omega_m^{\mathrm{K}_h^t}(k) & \omega_m^{\mathrm{W}_h}(k) \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}_{n-m} \\ \boldsymbol{\phi}_{n-m} \end{bmatrix}. \tag{4.43}$$

As we progressively compute the vectors $\mathbf{u}_n$, $\boldsymbol{\lambda}_n$, and $\boldsymbol{\phi}_n$, we can input the latter two in the CQ-discretized potential expression (using the basis representation for elements of Y_h and X_h):

$$u_k^\star(t_n) = \sum_{m=0}^{n} \omega_m^{\mathrm{D}_h}(k) \boldsymbol{\phi}_{n-m} - \sum_{m=0}^{n} \omega_m^{\mathrm{S}_h}(k) \boldsymbol{\lambda}_{n-m}.$$

The convolution weights $\omega_m^J(k)$ for $J \in \{\mathrm{V}_h, \mathrm{K}_h, \mathrm{K}_h^t, \mathrm{W}_h, \mathrm{S}_h, \mathrm{D}_h\}$ are computable based on the Taylor expansion of the appropriate transfer function. Alternatively, the memory term in the right-hand side of (4.43) and the potential representations can be evaluated using FFT-based techniques [17, 37].

Let us now focus on the case when Ω_- is a polygon or polyhedron that has been partitioned into triangles or tetrahedra. We choose U_h to be the space of continuous piecewise polynomial functions of degree at most $p \geq 1$, Y_h to be the space of continuous piecewise polynomial functions of degree at most p on the inherited partition of the boundary, and X_h to be the space of discontinuous piecewise polynomial functions of degree at most $p-1$ on the same partition of the boundary. Note that the use of the inherited partition on the boundary is done for the sake of simplicity but is not a necessary theoretical assumption. For this choice of spaces, Y_h can be identified with the trace space of U_h, and therefore, the matrix Γ_h can be computed from I_h identifying degrees of freedom of Y_h with the boundary degrees of freedom of U_h. In the two dimensional case, X_h and Y_h have the same dimension, and therefore all boundary matrices are square.

We can now give a simple error estimate for the case of smooth solutions of our problem. Suppose, for instance, that c and the components of the matrix-valued

function κ are $\mathcal{C}^\infty$, that $c \equiv 1$ in a neighborhood of Γ, and $\kappa \equiv \mathrm{I}$ (the identity matrix) in a neighborhood of Γ as well. Let the incident wave be a plane wave $u^{\mathrm{inc}}(t)(\mathbf{x}) = \psi(\mathbf{x}\cdot\mathbf{d} - t - t_0)$, where ψ is a smooth causal function, $|\mathbf{d}| = 1$, and t_0 is taken so that the support of u^{inc} does not intersect Ω_- at time $t = 0$. In this case the solutions of (4.2) are smooth functions of space and time and the restriction of the boundary unknowns λ and ϕ to the faces of Γ are smooth. Using Corollary 4.2.7 and standard estimates for approximations by piecewise polynomials, we can prove that the semidiscrete error satisfies

$$\|u(t) - u^h(t)\|_{1,\Omega_-} + \|\phi(t) - \phi^h(t)\|_{1/2,\Gamma} + \|\lambda(t) - \lambda^h(t)\|_{-1/2,\Gamma} = \mathcal{O}(h^p).$$

Consider now the quantities

$$e_n^u := u^h(t_n) - u_k^h(t_n), \quad e_n^\lambda := \lambda^h(t_n) - \lambda_k^h(t_n), \quad \text{and} \quad e_n^\phi := \phi^h(t_n) - \phi_k^h(t_n).$$

Then, by Theorem 4.3.2, we can prove

$$\left\|\tfrac{1}{2}(e_n^u + e_{n-1}^u)\right\|_{1,\Omega_-} + \left\|\tfrac{1}{4}(e_n^\phi + 2e_{n-1}^\phi + e_{n-2}^\phi)\right\|_{1/2,\Gamma} + \left\|\tfrac{1}{4}(e_n^\lambda + 2e_{n-1}^\lambda + e_{n-2}^\lambda)\right\|_{-1/2,\Gamma} = \mathcal{O}(k^2).$$

In equations (4.42) and (4.43), we can see that the finite element time stepping component of the solution has a short tail, i.e. it has a memory of only two time steps, while the boundary integral right hand sides have contributions from every previously computed time step. Computing the convolutional tails for the boundary integral equations can become expensive. To overcome this bottleneck, we use a reduction to the boundary method that decouples the solution process into three steps: solving first for an intermediate variable $\mathbf{w}$ (the result of solving an interior Neumann problem corresponding to the action of the incident wave), solving next for the boundary densities, and finally solving for the interior unknown. While this seems to require more solves than the time stepping method, this strategy does not require the computation of the convolutional tail at each time and can therefore be implemented in parallel. The all-steps-at once CQ method of [16] (see also Chapter 2, Section 7) is used for the parallel

time stepping. Consider the Finite Element matrix $\mathrm{F}_h(s) := \mathrm{S}_h + s^2\mathrm{M}_h$, which is the Laplace transform of the FEM-semidiscrete wave equation in the interior domain. The method consists of the following sequential steps:

1. Compute the intermediate variable $\mathbf{w}_n$ by solving the convolution

$$\sum_{m=0}^{n} \omega_m^{\mathrm{F}_h}(k)\mathbf{w}_{n-m} = \Gamma_h^t \boldsymbol{\beta}_{1,n} \qquad n = 0, \ldots, N$$

in parallel across the time steps. Equivalently, use the trapezoidal rule (with zero initial values) for the differential equation $\mathrm{M}_h\ddot{\mathbf{w}}(t) + \mathrm{S}_h\mathbf{w}(t) = \Gamma_h^t\boldsymbol{\beta}_1(t)$, where $\boldsymbol{\beta}_1(t)$ is the projection onto X_h of the actual transmission data.

2. Instead of time-stepping to compute the boundary unknowns $\boldsymbol{\lambda}_n$ and $\boldsymbol{\phi}_n$ by

$$\sum_{m=0}^{n} \begin{bmatrix} \omega_m^{\mathrm{V}_h}(k) + \Gamma_h \omega_m^{\mathrm{F}_h^{-1}}(k)\Gamma_h^t & \omega_m^{\mathrm{K}_h}(k) \\ \omega_m^{\mathrm{K}_h^t}(k) & \omega_m^{\mathrm{W}_h}(k) \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}_{n-m} \\ \boldsymbol{\phi}_{n-m} \end{bmatrix} + \frac{1}{2}\begin{bmatrix} -\mathrm{I}_h^t\boldsymbol{\phi}_n \\ \mathrm{I}_h\boldsymbol{\lambda}_n \end{bmatrix} = \begin{bmatrix} \boldsymbol{\beta}_{0,n} - \Gamma_h\mathbf{w}_n \\ 0 \end{bmatrix}, \quad n = 0, \ldots, N,$$

we apply the all-steps-at-once strategy to approximate CQ solutions [16]. This requires solving in parallel systems with matrix

$$\mathrm{B}_h(s) := \begin{bmatrix} \mathrm{V}_h(s) + \Gamma_h\mathrm{F}_h^{-1}(s)\Gamma_h^t & -\frac{1}{2}\mathrm{I}_h + \mathrm{K}_h(s) \\ \frac{1}{2}\mathrm{I}_h^t + \mathrm{K}_h^t(s) & \mathrm{W}_h(s) \end{bmatrix}$$

for a large number of complex frequencies s (with non-zero real part). Note that the construction of the above matrix (if a direct method is to be used) requires the solution of one linear system related to $\mathrm{F}_h(s)$ for each column of Γ_h^t.

3. Compute the interior unknown by

$$\sum_{m=0}^{n} \omega_m^{\mathrm{F}_h}(k)\mathbf{u}_{n-m} = \Gamma_h^t\left(\boldsymbol{\beta}_{1,n} + \boldsymbol{\lambda}_n\right), \qquad n = 0, \ldots, N$$

or use an equivalent trapezoidal method for an interior problem (with the correct boundary data now that we have computed $\boldsymbol{\lambda}_n$), or use an all-steps-at-once to compute $\mathbf{u}_n$ using a parallel algorithm.

The exterior solution can be postprocessed at the end of the second step. If we use an iterative method for the solution of a system associated to the matrix $\mathrm{B}_h(s)$, every matrix-vector multiplication requires the solution of a sparse linear system associated to the interior domain. Efficient methods to handle this discrete scheme are the goal of further investigation. In all the numerical experiments below, system solves are handled with Matlab's backslash operator.

4.5 Numerical Experiments and Simulations

We perform some numerical experiments to demonstrate the coupling scheme and corroborate our theoretical results. The first numerical experiment is created by studying an artificial scattering problem on the domain $[-0.5, 0.5]^2$. Instead of an incident wave, we generate transmission data on Γ so that the solution in the interior and exterior domains is known exactly. In the interior, we take the solution to be a plane wave moving in the direction $(1/\sqrt{2}, 1/\sqrt{2})$ and transmitting the signal $\sin(2t)\chi(t)$ where $\chi(t)$ is a smooth cutoff function so the signal has compact support in time. The exterior solution is a cylindrical wave due to a source point at the origin transmitting the signal $\sin^6(4t)H(t)$ where $H(t)$ is the Heaviside function. We take $c \equiv 1$ and

$$\kappa(x,y) = \begin{bmatrix} 1 + 0.5\,(x^2+y^2) & 0.25 + 0.5\,(x^2+y^2) \\ 0.25 + 0.5\,(x^2+y^2) & 3 + 0.5\,(x^2+y^2) \end{bmatrix}.$$

A body force term $f(x,y,t)$ is added in the interior domain (the equation is thus $c^{-2}\ddot{u} = \mathrm{div}(\kappa\nabla u) + f$) so that the chosen function (a plane wave) satisfies the wave equation in Ω_-. We discretize in space with standard $\mathbb{P}_1$ FEM for the interior variable and $\mathbb{P}_1 \times \mathbb{P}_0$ BEM (i.e., Y_h and X_h are respectively spaces of continuous $\mathbb{P}_1$ and discontinuous $\mathbb{P}_0$ functions) for the boundary unknowns. The simulation is run from $t = 0$ to $t = 3$ so that by the final time the exact solution is non-zero in both sides of the transmission boundary. Time discretization is carried out with trapezoidal rule based CQ.

For our error quantities, we use the following measures:

$$\mathrm{E}^u_{L^2}(t) := \|u(t) - u^h_k(t)\|_{\Omega_-}, \qquad \mathrm{E}^u_{H^1}(t) := \|u(t) - u^h_k(t)\|_{1,\Omega_-},$$
$$\mathrm{E}^\lambda(t) := \|\lambda(t) - \lambda^h_k(t)\|_\Gamma, \qquad \mathrm{E}^\phi(t) := \|\phi(t) - \phi^h_k(t)\|_\Gamma,$$
$$\mathrm{E}^{\mathrm{obs}}(t) := \max_j |u_+(t)(\mathbf{x}_j) - u^*_k(t)(\mathbf{x}_j)|.$$

In $\mathrm{E}^{\mathrm{obs}}(t)$, $\{\mathbf{x}_j\}$ is a finite collection of points in Ω_+. Note that we do not have any result asserting superconvergence in the $L^2(\Omega_-)$ norm for u, superconvergence in the $L^2(\Gamma)$ norm for ϕ, or convergence in the $L^2(\Gamma)$ norm for λ.

Tables 4.1 and 4.2 summarize the results from the convergence study. We use uniform triangulations with N_{FEM} elements in Ω_- and N_{BEM} elements on the boundary and perform M time steps to reach the final time $t = 3$.

N_{FEM}	M	$\mathrm{E}^u_{L^2}(3)$	e.c.r.	$\mathrm{E}^u_{H^1}(3)$	e.c.r.
32	20	2.4029e-02	-	2.6050e-01	-
128	40	5.6609e-03	2.0857	1.2017e-01	1.1162
512	80	1.4013e-03	2.0143	6.0233e-02	0.99642
2048	160	3.4927e-04	2.0043	3.0235e-02	0.99432
8192	320	8.7041e-05	2.0046	1.5147e-02	0.99721
32678	640	2.2092e-05	1.9782	7.5796e-03	0.99884

Table 4.1: Convergence of the interior variable with $\mathbb{P}_1$ FEM (coupled with $\mathbb{P}_1 \times \mathbb{P}_0$ BEM) and trapezoidal rule time stepping.

N_{BEM}	M	$\mathrm{E}^{\lambda}(3)$	e.c.r.	$\mathrm{E}^{\phi}(3)$	e.c.r	$\mathrm{E}^{\mathrm{obs}}(3)$	e.c.r
16	20	4.7204e-01	-	9.1250e-02	-	2.7533e-02	-
32	40	1.3196e-01	1.8388	2.4295e-02	1.9092	2.0929e-02	0.39563
64	80	4.9760e-02	1.4071	6.0872e-03	1.9968	2.8444e-03	2.8793
128	160	1.8880e-02	1.3981	1.5196e-03	2.0021	6.2183e-04	2.1935
256	320	7.2700e-03	1.3768	3.8422e-04	1.9837	1.5322e-04	2.0210
512	640	3.0133e-03	1.2706	1.0697e-04	1.8448	3.8211e-05	2.0035

Table 4.2: Convergence of boundary and exterior variables with $\mathbb{P}_1 \times \mathbb{P}_0$ BEM (coupled with $\mathbb{P}_1$ FEM) and trapezoidal rule based CQ. Note that we are measuring errors for λ in a stronger norm than the one used in the theory.

We repeat the previous experiment with the same, replacing the spatial discretization by $\mathbb{P}_2$ FEM coupled with $\mathbb{P}_2 \times \mathbb{P}_1$ BEM. Our theory predicts order two convergence in all variables for this experiment, which was not seen in the previous example because of the use of lower order FEM and BEM. We see comparable errors to the first experiment with reduced discretization parameters.

Tables 4.3 and 4.4 summarize the results from this convergence study. We again use uniform triangulations with N_{FEM} elements in Ω_- and N_{BEM} elements on the boundary and perform M time steps to reach the final time $t = 3$.

N_{FEM}	M	$\mathrm{E}^u_{L^2}(3)$	e.c.r.	$\mathrm{E}^u_{H^1}(3)$	e.c.r.
8	10	7.9596e-02	-	3.9938e-01	-
32	20	1.6335e-02	2.2847	1.6148e-01	1.3064
128	40	3.7889e-03	2.1081	2.4973e-02	2.6929
512	80	8.5690e-04	2.1446	5.1730e-03	2.2713
2048	160	2.0934e-04	2.0333	1.2740e-03	2.0217
8192	320	5.2069e-05	2.0074	3.3478e-04	1.9281

Table 4.3: Convergence of the interior variable with $\mathbb{P}_2$ FEM and trapezoidal rule time stepping.

N_{BEM}	M	$\mathrm{E}^\lambda(3)$	e.c.r.	$\mathrm{E}^\phi(3)$	e.c.r	$\mathrm{E}^{\mathrm{obs}}(3)$	e.c.r
8	10	4.0011e+00	-	2.7841e-01	-	2.1634e-02	-
16	20	6.6196e-01	2.5956	4.9454e-02	2.4931	2.3736e-02	-0.1338
32	40	5.8355e-02	3.5038	1.0361e-02	2.2549	8.1811e-03	1.5367
64	80	1.3106e-02	2.1546	2.5240e-03	2.0374	4.7098e-04	4.1186
128	160	3.4291e-03	1.9343	6.1230e-04	2.0434	9.1814e-05	2.3589
256	320	1.4502e-03	1.2416	1.5236e-04	2.0068	2.3948e-05	1.9388

Table 4.4: Convergence of boundary and exterior variables with $\mathbb{P}_2 \times \mathbb{P}_1$ BEM and trapezoidal rule based CQ.

A second numerical experiment makes use of the Runge-Kutta CQ method of [13, 15, 61] (see Chapter 2). The analysis of RKCQ methods was carried out in [12, 13] using abstract arguments in the Laplace domain: in principle, we expect the convergence order to be limited to the stage order, although potential postprocessings enjoy the full classical order of the RK method. (We also note that RKCQ methods

have been reported to enjoy better dispersion properties than multistep-CQ schemes [17].) The experiment below is set on the same example and triangulations as the first experiment, but is discretized in space with $\mathbb{P}_2$ FEM and $\mathbb{P}_2 \times \mathbb{P}_1$ BEM and in time with CQ based on the two-stage Radau IIa scheme, a method of classical order 3 and stage order 2. Tables 4.5 and 4.6 below demonstrates convergence order more than three, which was otherwise impossible using CQ based on a linear multistep method.

N_{FEM}	M	$\mathrm{E}^u_{L^2}(3)$	e.c.r.	$\mathrm{E}^u_{H^1}(3)$	e.c.r.
8	20	7.2998e-02	-	5.8872e-01	-
32	40	2.8039e-02	1.3804	2.8675e-01	1.0378
128	80	5.5717e-03	2.3313	1.1027e-01	1.3787
512	160	6.8020e-04	3.0341	3.1564e-02	1.8047
1024	320	7.9143e-05	3.1034	8.3212e-03	1.9234
2048	640	9.6606e-06	3.0343	2.1209e-03	1.9721

Table 4.5: Convergence of the interior variable when using $\mathbb{P}_2$ FEM and two-stage Radau IIa time stepping.

N_{BEM}	M	$\mathrm{E}^\lambda(3)$	e.c.r.	$\mathrm{E}^\phi(3)$	e.c.r	$\mathrm{E}^{\mathrm{obs}}(3)$	e.c.r
4	20	9.2094e-01	-	2.4561e-01	-	6.0797e-02	-
8	40	4.0652e-01	1.1798	6.5693e-02	1.9026	2.8148e-02	1.1109
16	80	1.3784e-01	1.5603	9.8444e-03	2.7384	2.7418e-03	3.3598
32	160	3.4386e-02	2.0031	9.3028e-04	3.4036	2.1949e-04	3.6429
64	320	7.3343e-03	2.2291	6.2996e-05	3.8843	1.4604e-05	3.9097
128	640	1.1850e-03	2.6297	3.8242e-06	4.0420	9.9590e-07	3.8743

Table 4.6: Convergence of boundary and exterior variables when using $\mathbb{P}_2 \times \mathbb{P}_1$ BEM and two-stage Radau IIa based RKCQ.

Next, we perform a simulation of a scattering problem with a known incident plane wave and unknown exact solution. An incident plane wave traveling in the direction $(1/\sqrt{2}, 1/\sqrt{2})$ interacts with the obstacle $\Omega_- = [-0.5, 0.5]^2$. The material properties in Ω_- have a Gaussian lensing effect described by a non-homogeneous multiple of the identity tensor

$$\kappa(x, y) = (1 - 1.65e^{-1/(1-r^2)})\mathrm{I},$$

where $r = \sqrt{x^2 + y^2}$, and we take $c \equiv 1$. The spatial discretization makes use of $\mathbb{P}_3$ finite elements in the interior with 8192 interior elements and $\mathbb{P}_3 \times \mathbb{P}_2$ boundary elements with 256 boundary elements on Γ. The CQ time step is $k = 4.375 \times 10^{-3}$ and we integrate from $t = 0$ to $t = 3.5$. Some snapshots of the scattering process are shown in Figure 4.1.

The next experiment demonstrates the coupling scheme applied to multiple obstacles with different material properties. An incident plane wave interacts with the four small boxes. The top left and bottom right boxes have material properties described by the matrix $\kappa = \mathrm{diag}(4, 1/4)$ while the top right and bottom left boxes have material matrix $\kappa = \mathrm{diag}(2, 1/2)$. In all four obstacles $c \equiv 1$. Again we use $\mathbb{P}_3$ FEM and $\mathbb{P}_3 \times \mathbb{P}_2$ BEM. There are a total of 1792 finite elements and 192 boundary elements for the spatial discretization. The time step is $k = 2 \times 10^{-2}$ and the simulation is run from $t = 0$ to $t = 4$. Figure 4.2 displays some different times of the experiment.

The last simulation takes place on a non-convex and trapping obstacle. Again we use $\mathbb{P}_3$ FEM for the interior and $\mathbb{P}_3 \times \mathbb{P}_2$ BEM for the boundary densities. The interior of the obstacle is partitioned into 11,968 finite elements, and the boundary is partitioned into 472 elements. The time step size is $k \approx 6.7 \times 10^{-3}$, and we integrate from $t = 0$ to $t = 2.5$. Wave propagation within the obstacle is determined by the parameters $c \equiv 1$ and the diagonal matrix $\kappa = \mathrm{diag}(0.25, 0.125)$. The large difference in wave speeds between the interior and exterior produces a strong scattered wave and a highly focused and long-lived wave within the obstacle. Some of the scattered wave is trapped within the void outside of the domain Ω_-. The results are shown in Figure 4.3.

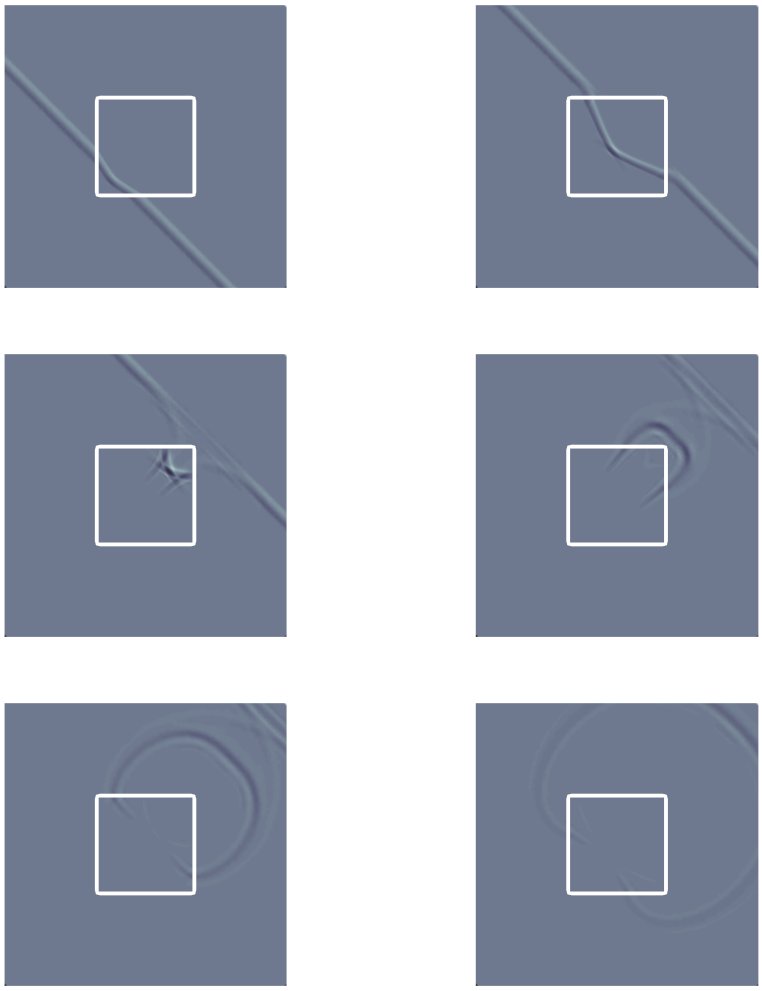

Figure 4.1: Scattering of a plane wave by an obstacle with Gaussian lensing properties.

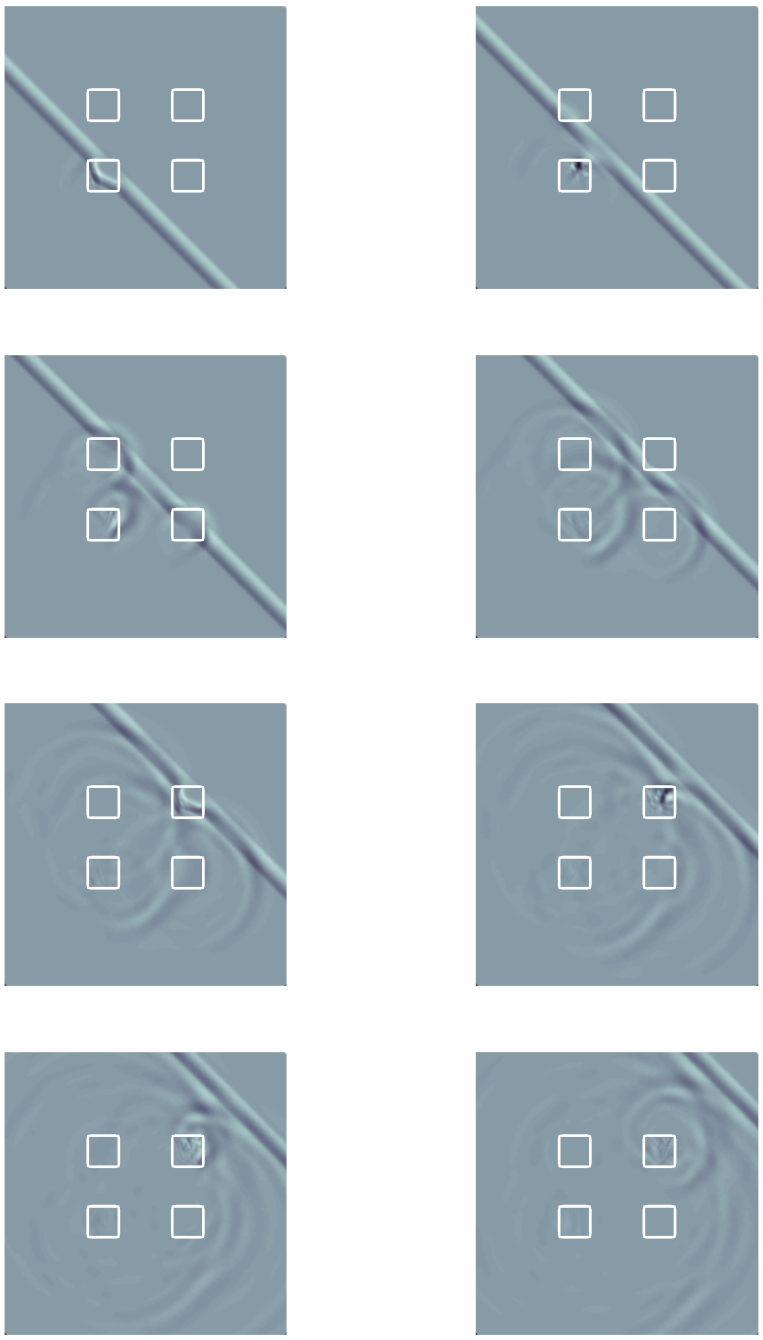

Figure 4.2: Scattering of a plane wave by four homogeneous anisotropic obstacles with different material parameters.

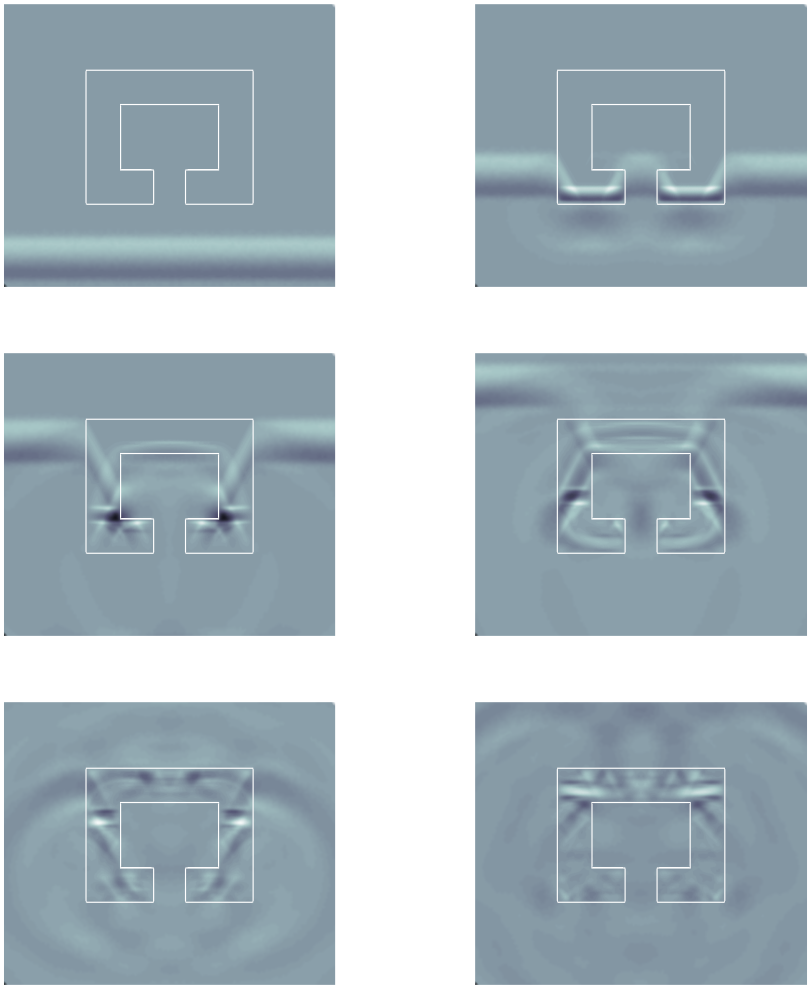

Figure 4.3: Scattering and transmission of a wave by a non-convex domain.

Chapter 5

DISCUSSION OF REDUCED BEM-FEM COUPLING SCHEMES FOR TRANSIENT ACOUSTICS

In this chapter we will present some results and numerical experiments related to two different reduced coupling schemes for transient acoustic waves. In Chapter 4 we saw a three-field symmetric coupling scheme that kept the BEM and FEM unknowns well separated: they only communicated through a discrete trace operator that required only the computation of inner products between the bases of the finite and boundary element spaces. The following two schemes eliminate one of the unknowns (the trace of the exterior field) by recognizing from the equation $\gamma u = \gamma^+ u_+ + \beta_0$ that the interior and exterior traces are approximating the same quantity, up to the incident wave [73]. For both formulations, we make use of a reduction-to-the-boundary strategy to parallelize the solves across the time steps as we did in Chapter 4.

5.1 Reduced Symmetric Coupling of Boundary and Finite Elements

We consider now our first reduced coupling formulation based on the BEM-FEM scheme of Costabel [22] and Han [35] for steady-state problems. We are interested in the same transmission problem as the previous chapter, given by equations (4.2).

Our unknown quantities will be the interior field u and the exterior normal derivative of the exterior field, $\lambda := \partial_\nu^+ u_+$. We can derive the coupling scheme as follows. Our potential ansatz with Kirchhoff's formula makes use of the continuity of the total wave across Γ:

$$u_+ := \mathcal{D} * (\gamma u - \beta_0) - \mathcal{S} * \lambda.$$

In this way we have eliminated the redundant approximation of the Dirichlet data on Γ. We weakly enforce the interior wave equation and apply the continuity of the normal derivative of the total wave across Γ:

$$\begin{aligned}(c^{-2}\ddot{u}, v)_{\Omega_-} + (\kappa\nabla u, \nabla v)_{\Omega_-} &= \langle \partial_{\nu,\kappa} u, \gamma v\rangle_\Gamma \\ &= \langle -\mathcal{W} * (\gamma u - \beta_0) + (\tfrac{1}{2} - \mathcal{K}^t) * \lambda + \beta_1, \gamma v\rangle_\Gamma \\ &\qquad\qquad \forall v \in H^1(\Omega_-).\end{aligned}$$

If we rearrange some terms, we arrive at the first equation in the coupling scheme:

$$(u, \lambda) \in \mathrm{TD}(H^1_\kappa(\Omega_-) \times H^{-1/2}(\Gamma)), \tag{5.1a}$$

$$\begin{aligned}(c^{-2}\ddot{u}, v)_{\Omega_-} + (\kappa\nabla u, \nabla v)_{\Omega_-} + \langle \mathcal{W} * \gamma u, \gamma v\rangle_\Gamma - \langle (\tfrac{1}{2} - \mathcal{K}^t) * \lambda, \gamma v\rangle_\Gamma \\ = \langle \beta_1 + \mathcal{W} * \beta_0, \gamma v\rangle_\Gamma \quad \forall v \in H^1(\Omega_-).\end{aligned} \tag{5.1b}$$

The second equation simply enforces that the trace of the exterior field is zero within the scatterer

$$\langle \mu, \tfrac{1}{2}\gamma u - \mathcal{K} * \gamma u\rangle_\Gamma + \langle \mu, \mathcal{V} * \lambda\rangle_\Gamma = \langle \mu, \tfrac{1}{2}\beta_0 - \mathcal{K} * \beta_0\rangle_\Gamma \quad \forall \mu \in H^{-1/2}(\Gamma). \tag{5.1c}$$

We translate this coupled system to a first-order-in-space-and-time system and cast it as an exotic transmission problem in the time domain. In the semidiscrete setting the coupling scheme then becomes the search for

$$(u^h, u^\star, \mathbf{v}^h, \mathbf{v}^\star) \in \mathrm{TD}\left(U_h \times H^1(\mathbb{R}^d \setminus \Gamma) \times \mathbf{V}_h \times \mathbf{H}(\mathrm{div}; \mathbb{R}^d \setminus \Gamma)\right) \tag{5.2a}$$

satisfying

$$\dot{u}^h = \mathrm{div}_h^\kappa \mathbf{v}^h + \gamma_h^t(\partial_\nu^+ \mathbf{v}^\star + \partial^{-1}\beta_1), \tag{5.2b}$$

$$\dot{u}^\star = \nabla \cdot \mathbf{v}^\star, \tag{5.2c}$$

$$\dot{\mathbf{v}}^h = \nabla u^h, \tag{5.2d}$$

$$\dot{\mathbf{v}}^\star = \nabla u^\star, \tag{5.2e}$$

$$[\![\gamma u^\star]\!] + \gamma u^h = \beta_0, \tag{5.2f}$$

$$\gamma^- u^\star \in X_h^\circ, \tag{5.2g}$$

$$[\![\gamma_\nu \mathbf{v}^\star]\!] \in X_h. \tag{5.2h}$$

For the sake of analysis we require the two spaces

$$\mathcal{U} := \left\{(u^h, u^*) \in U_h \times H^1(\mathbb{R}^d \setminus \Gamma) \ : \ [\![\gamma u^\star]\!] + \gamma u^h = 0, \ \gamma^- u^\star \in X_h^\circ\right\},$$
$$\mathbf{V} := \left\{(\mathbf{v}^h, \mathbf{v}^\star) \in \mathbf{V}_h \times \mathbf{H}(\mathrm{div}; \mathbb{R}^d \setminus \Gamma) \ : \ [\![\gamma_\nu \mathbf{v}^\star]\!] \in X_h\right\},$$

so we can define an unbounded operator

$$\mathcal{A}U := (\mathrm{div}_h^\kappa \mathbf{v}^h + \gamma_h^t \gamma_\nu^+ \mathbf{v}^\star, \nabla \cdot \mathbf{v}^*, \nabla u^h, \nabla u^\star),$$

in its domain

$$D(\mathcal{A}) := \mathcal{U} \times \mathbf{V}.$$

As we continue to verify that this system fits the general formulation presented in Chapter 4, we have the Hilbert spaces

$$\mathbb{H} := \mathcal{U}_h \times L^2(\mathbb{R}^d \setminus \Gamma) \times \mathbf{V}_h \times \mathbf{L}^2(\mathbb{R}^d \setminus \Gamma)$$
$$\mathbb{V} := \mathcal{U}_h \times H^1(\mathbb{R}^d \setminus \Gamma) \times \mathbf{V}_h \times \mathbf{H}(\mathrm{div}; \mathbb{R}^d \setminus \Gamma),$$

two operators related to boundary conditions

$$\mathsf{G} := (\gamma_h^t, 0, 0, 0), \qquad \mathsf{B} := ([\![\gamma u^\star]\!] + \gamma u^h, \gamma^- u^\star\big|_{X_h^\circ}, [\![\gamma_\nu \mathbf{v}^\star]\!]|_{X_h^*}),$$

and the related Sobolev spaces

$$\mathbb{M}_1 := H^{-1/2}(\Gamma), \qquad \mathbb{M}_2 := H^{1/2}(\Gamma) \times (X_h^\circ)^* \times X_h^*.$$

With the abstract result of Section 4.4 and these new ingredients, we can state the following stability and semidiscrete error theorems. Their proofs follow exactly the same lines as the ones seen in Chapter 4.

Theorem 5.1.1 (Stability)**.** *For $\beta_0 \in W_+^2(H^{1/2}(\Gamma))$ and $\beta_1 \in W_+^1(H^{-1/2}(\Gamma))$, problem (5.2) has a unique solution satisfying*

$$\|u^h(t)\|_{1,\Omega_-} + \|u^\star(t)\|_{1,\mathbb{R}^d\setminus\Gamma} \leq C\left(H_2(\beta_0, t|H^{1/2}(\Gamma)) + H_2(\partial^{-1}\beta_1, t|H^{-1/2}(\Gamma))\right),$$

where the constant C is independent of time t and h. For data with regularity $\beta_0 \in W_+^3(H^{1/2}(\Gamma))$ and $\beta_1 \in W_+^2(H^{-1/2}(\Gamma))$ we have the bound

$$\|[\![\partial_\nu u^\star(t)]\!]\|_{-1/2,\Gamma} \leq C\left(H_2(\dot{\beta}_0, t|H^{1/2}(\Gamma)) + H_2(\beta_1, t|H^{-1/2}(\Gamma))\right)$$

where again C is independent of h and t.

Theorem 5.1.2 (Semidiscrete error)**.** *Suppose the exact solution to the scattering problem (5.1a)-(5.1c) satisfies*

$$\lambda \in W_+^{m-1}(H^{-1/2}(\Gamma)) \quad \text{and} \quad u \in W_+^m(H^1(\Omega_-)) \cap W_+^{m-1}(L^2(\Omega_-)) \tag{5.3}$$

with $m = 2$. Then

$$\begin{aligned}\|\varepsilon^h(t)\|_{1,\Omega_-} + \|\varepsilon^\star(t)\|_{1,\mathbb{R}^d\setminus\Gamma} \leq C\big(&H_2(u - \Pi_h^V u, t|H^1(\Omega_-)) + H_1(\ddot{u} - \Pi_h^V \ddot{u}, t|L^2(\Omega_-)) \\ &+ H_2(\partial^{-1}(\lambda - \Pi_h^X \lambda), t|H^{-1/2}(\Gamma))\big).\end{aligned}$$

If the solution to (5.1a)-(5.1c) satisfies (5.3) with $m = 3$, then

$$\begin{aligned}\|\lambda(t) - \lambda^h(t)\|_{-1/2,\Gamma} \leq C\big(&H_2(\dot{u} - \Pi_h^V \dot{u}, t|H^1(\Omega_-)) + H_1(\dddot{u} - \Pi_h^V \dddot{u}, t|L^2(\Omega_-)) \\ &+ H_2(\lambda - \Pi_h^X \lambda, t|H^{-1/2}(\Gamma))\big).\end{aligned}$$

In both estimates, the constant is independent of h and t.

Before we present numerical experiments, we show the reduction-to-the-boundary strategy for this coupling scheme. This is analogous to the reduction-to-the-boundary strategy we used in Section 4.4. The scheme for the Costabel-Han system is somewhat more involved, however, because of the more condensed nature of the system. As we did for the three-field coupling scheme, we must introduce some compositions of operators. Using the notation of Chapter 4, we define the discrete operators (matrix-valued functions of the complex number $s \in \mathbb{C}_+$)

$$\begin{aligned}\mathrm{A}_h(s) &:= \mathrm{S}_h + s^2\mathrm{M}_h + \Gamma_h^t \mathrm{W}_h(s)\Gamma_h, \\ \mathrm{B}_h(s) &:= \mathrm{V}_h(s) + \left(\tfrac{1}{2}\mathrm{I}_h - \mathrm{K}_h(s)\right)\Gamma_h \mathrm{A}_h^{-1}(s)\Gamma_h^t(\tfrac{1}{2}\mathrm{I}_h^t - \mathrm{K}^t(s)),\end{aligned}$$

and the right hand sides

$$\mathbf{b}_n := \Gamma_h^t \boldsymbol{\beta}_{1,n} + \Gamma_h^t \sum_{m=0}^{n} \omega_m^{\mathrm{W}_h}(\kappa) \boldsymbol{\beta}_{0,n}, \qquad n = 0, \ldots, M.$$

The reduction-to-the-boundary algorithm then proceeds as follows.

1. Compute the first intermediate variable

$$\mathbf{w}_n = \sum_{m=0}^{n} \omega_m^{\mathrm{A}_h}(k) \mathbf{b}_{n-m}, \qquad n = 0, \ldots, M,$$

   in parallel across the time steps.

2. Solve the discrete convolutional equation

$$\sum_{m=0}^{n} \omega_m^{\mathrm{B}_h}(k) \boldsymbol{\lambda}_{n-m} = \tfrac{1}{2}(\mathrm{I}_h \boldsymbol{\beta}_{0,n} - \Gamma_h \mathbf{w}_n) - \sum_{m=0}^{n} \omega_m^{\mathrm{K}_h}(k)(\boldsymbol{\beta}_{0,n-m} + \Gamma_h \mathbf{w}_{n-m}),$$

   for $n = 0, \ldots, M$ in parallel across the time steps for the boundary unknown $\boldsymbol{\lambda}_n$.

3. Compute the second intermediate variable

$$\mathbf{v}_n = \tfrac{1}{2}\mathrm{I}_h^t \boldsymbol{\lambda}_n - \sum_{m=0}^{n} \omega_m^{\mathrm{K}_h^t}(k) \boldsymbol{\lambda}_{n-m}, \qquad n = 0, \ldots, M,$$

   in parallel across time steps.

4. Solve the discrete convolutional equation

$$\sum_{m=0}^{n} \omega_m^{\mathrm{A}_h}(k) \mathbf{u}_{n-m} = \mathbf{b}_n + \Gamma_h^t \mathbf{v}_n, \qquad n = 0, \ldots, M,$$

   for the interior unknown $\mathbf{u}_n$ at all times. This can also be done in parallel across the time steps.

5. Compute the exterior solution $\mathbf{u}_n^\star$ with the discrete Kirchhoff's formula

$$\mathbf{u}_n^\star = \sum_{m=0}^{n} \omega_m^{\mathrm{D}_h}(k) \left(\Gamma_h \mathbf{u}_{n-m} - \boldsymbol{\beta}_{0,n-m}\right) - \sum_{m=0}^{n} \omega_m^{\mathrm{S}_h}(k) \boldsymbol{\lambda}_{n-m}, \qquad n = 0, \ldots, M.$$

   This forward convolution can be computed in parallel across all time steps.

For numerical experiments, we use the same methodology as the three-field coupling scheme studied previously. We test convergence of our numerical discretization with a transmission problem on the square $\Omega_- = [0.5, 0.5]^2$. We generate synthetic transmission data so that the exact interior and exterior solutions are known. In Ω_- we choose a plane wave propagating in the direction $(1/\sqrt{2}, 1/\sqrt{2})$ and carrying the signal $\sin(2t)\chi(t)$ where $\chi(t)$ is a smooth cutoff function. The exterior solution is a cylindrical wave due to a point source at the origin transmitting the signal $\sin^6(4t)H(t)$ where $H(t)$ is the Heaviside function. We take $c \equiv 1$ and

$$\kappa(x, y) := \begin{bmatrix} 1 + 0.5\,(x^2 + y^2) & 0.25 + 0.5\,(x^2 + y^2) \\ 0.25 + 0.5\,(x^2 + y^2) & 3 + 0.5\,(x^2 + y^2) \end{bmatrix}.$$

A body force term $f(x, y, t)$ is added in the interior domain so that the chosen plane wave satisfies the wave equation in Ω_-. We discretize in space with standard $\mathbb{P}_1$ FEM for the interior variable and $\mathbb{P}_0$ BEM for the boundary unknown. We run the simulation from $t = 0$ to $t = 2$ with M time steps. Temporal discretization is carried out with trapezoidal rule based CQ. Our error quantities are defined as follows:

$$\mathrm{E}^u_{L^2}(t) := \|u(t) - u^h_k(t)\|_{\Omega_-}, \quad \mathrm{E}^u_{H^1}(t) := \|u(t) - u^h_k(t)\|_{1,\Omega_-},$$
$$\mathrm{E}^\lambda(t) := \|\lambda(t) - \lambda^h_k(t)\|_\Gamma, \qquad \mathrm{E}^{\mathrm{obs}}(t) := \max_j |u_+(t)(\mathbf{x}_j) - u^*_k(t)(\mathbf{x}_j)|,$$

where the four observation points are

$$\mathbf{x}_1 = [-0.75, -0.75], \quad \mathbf{x}_2 = [0.75, -0.75], \quad \mathbf{x}_3 = [0.75, 0.75], \quad \mathbf{x}_4 = [-0.75, 0.75].$$

We refine simultaneously in space (using a red refinement of the finite element mesh) and time (doubling the number of time steps for each experiment). Figures 5.1 and 5.2 present the convergence history for this experiment.

Previous stability analysis in the Laplace domain [52] and in the time domain [73] indicate that this method can be expected to attain the optimal order of convergence upon a Galerkin spatial discretization and a CQ discretization in time. Our numerical results are consistent with the theory. We conclude with some snapshots

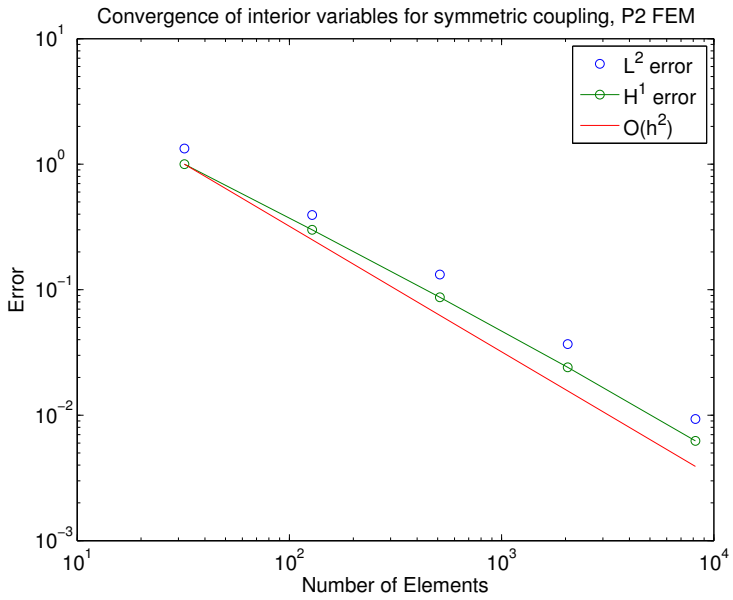

Figure 5.1: Convergence of the interior variable for two field symmetric coupling.

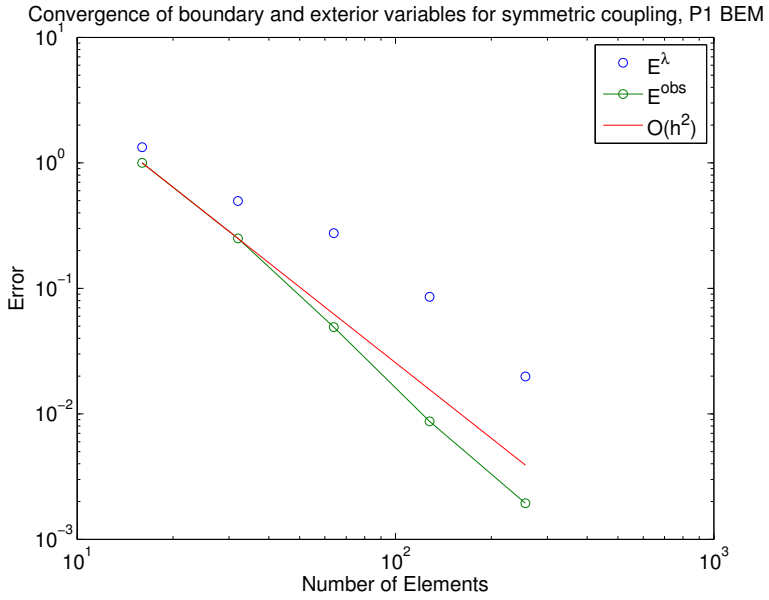

Figure 5.2: Convergence of the boundary and exterior variables for two field symmetric coupling.

given in Figure 5.3 of a simulation that is discretized using the Costabel-Han coupling method. The material matrix is given by

$$\kappa := \operatorname{diag}(1/r^2, 1/r^2)$$

where $r(x, y) := \sqrt{x^2 + y^2}$. A plane incident wave interacts with a Π-shaped scatterer such that $(0, 0) \notin \Omega_-$. We discretize with $\mathbb{P}_3$ FEM and $\mathbb{P}_2$ BEM, and integrate from $t = 0$ to $t = 3$ with trapezoidal rule based Convolution Quadrature.

5.2 Single Equation Coupling

Thus far, our coupling schemes have demanded that the representation formula satisfies two equations, at the cost of requiring all four of the operators of the Calderón Projector for wave equation. This final coupling scheme in the style of Johnson and Nédélec [44, 72] imposes only one condition on the potential representation, which avoids the use of all four of the boundary integral operators for the wave equation. However, we lose symmetry of the system, and direct in time analysis suggests that this coupling scheme does not generate a C_0-group of isometries like the other two we have studied [73]. Our experiments do show convergence of the method, however. While this fact does not deliver a fatal blow to its use in the time domain, we should be wary of potential instabilities that can occur when the material coefficients of the obstacle Ω_- are discontinuous. In [29], the authors perform a number of computational studies to search for instabilities with one-equation coupling, but they did not find any evidence for instabilities.

The Johnson-Nédélec coupled system seeks two unknowns

$$(u, \lambda) \in \mathrm{TD}\left(H^1(\Omega_-) \times H^{-1/2}(\Gamma)\right)$$

such that

$$\begin{aligned}
(c^{-2}\ddot{u}, v)_{\Omega_-} + (\kappa \nabla u, \nabla v)_{\Omega_-} - \langle \lambda, \gamma v \rangle_\Gamma &= \langle \beta_1, \gamma v \rangle_\Gamma && \forall v \in H^1(\Omega_-), \\
\langle \mu, \tfrac{1}{2}\gamma u - \mathcal{K} * \gamma u \rangle_\Gamma + \langle \mu, \mathcal{V} * \lambda \rangle_\Gamma &= \langle \mu, \tfrac{1}{2}\beta_0 - \mathcal{K} * \beta_0 \rangle_\Gamma && \forall \mu \in H^{-1/2}(\Gamma).
\end{aligned}$$

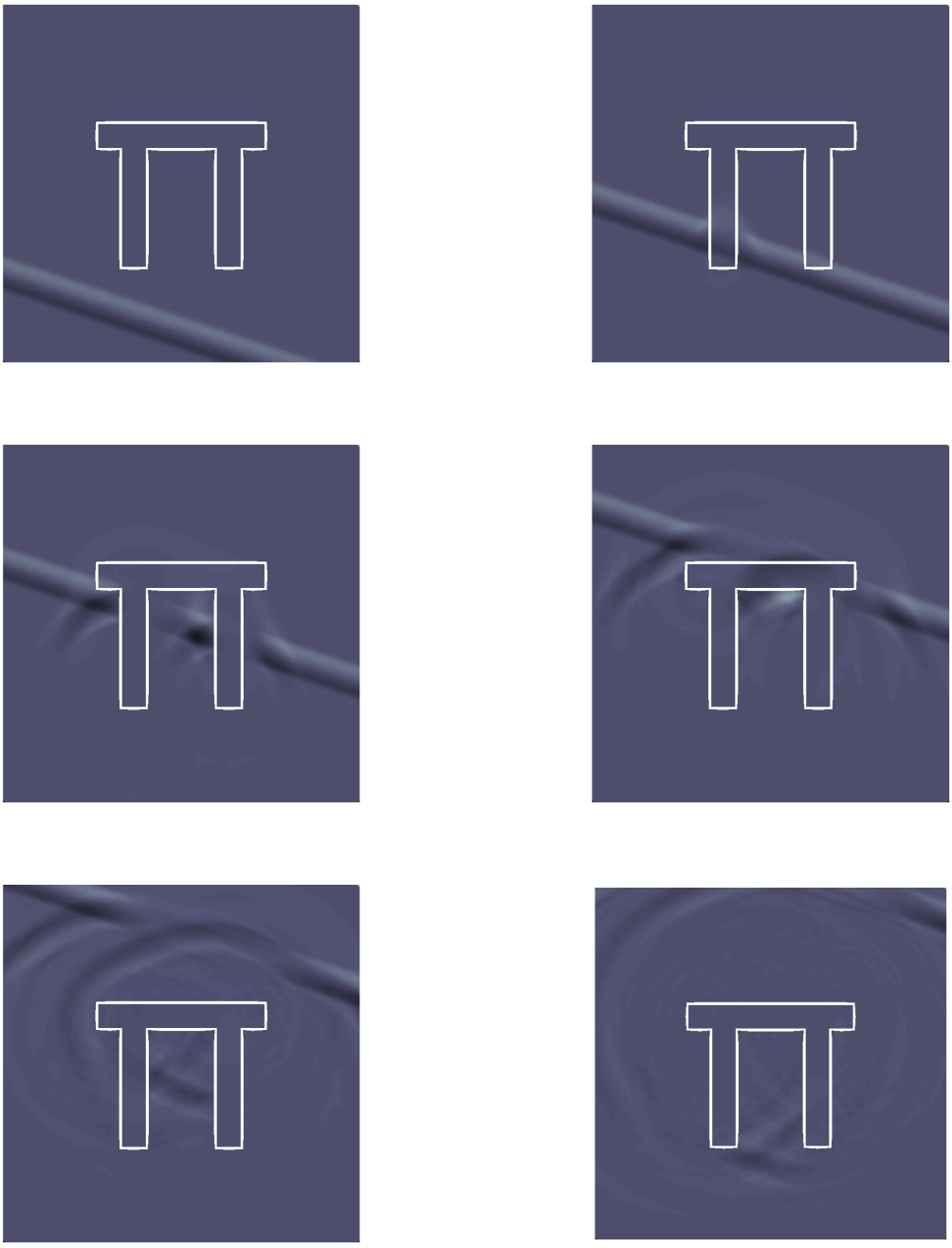

Figure 5.3: A simulation of scattering with Costabel-Han coupling.

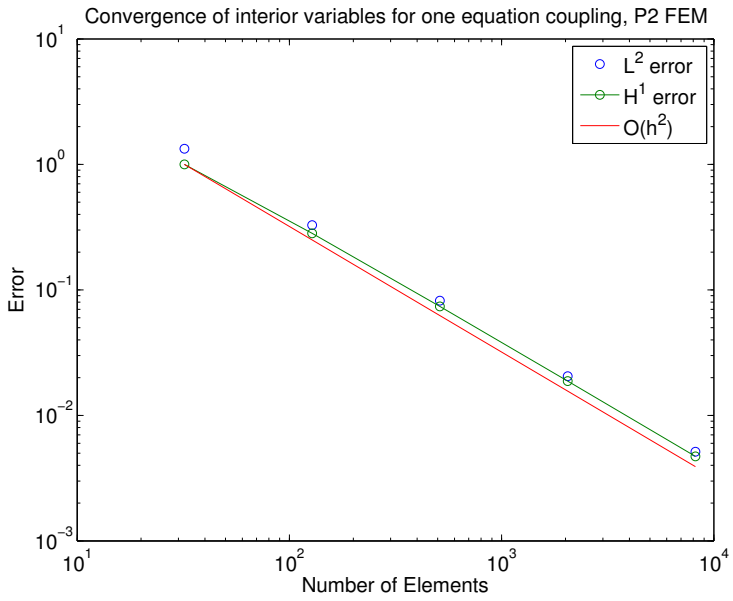

Figure 5.4: Convergence of the interior variable for one equation coupling.

Notice that this shares the same boundary integral equation as the Costabel-Han system, but does not include the coupling of the interior and exterior fields through the normal derivative.

We repeat the same experiments as for the two field symmetric coupling scheme and report our results for $\mathbb{P}_2$ FEM and $\mathbb{P}_1$ BEM in Figure 5.4 and Figure 5.5. We see order two convergence in all variables (we are prevented from seeing higher order because of our restriction to A-stable linear multistep CQ).

As a test of the stability of the Johnson-Nédélec coupling, we perform two tests where the interior material parameters have a significant jump across the boundary Γ compared to the exterior wave speed. To further test the method, we use a non-convex scatterer $\Omega_- = [-0.6, 0.4]^2 \setminus [-0.6, -0.1]^2$. The matrix for the interior wave equation is

$$\kappa(x, y) = \begin{bmatrix} 10 & 0 \\ 0 & 20 \end{bmatrix}.$$

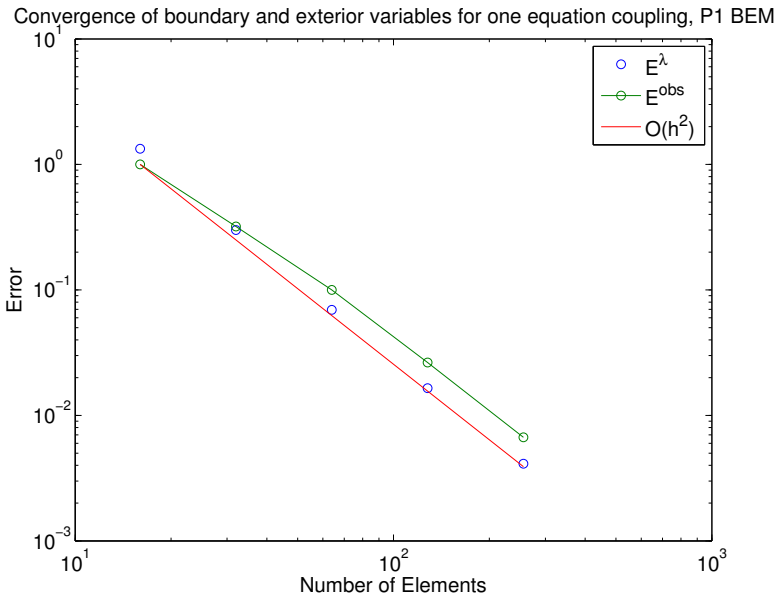

Figure 5.5: Convergence of the boundary and exterior variables for one equation coupling.

As before, we generate synthetic transmission data with known interior and exterior solutions. We take the exact solution in Ω_- to be a plane wave, but this time propagating the signal $\sin(16t)\chi(t)$, and the exterior solution is a wave due to a point source at the origin transmitting the signal $\sin^6(4t)$. We report in Figure 5.6 and Figure 5.7 the convergence history for this problem discretized with $\mathbb{P}_2$ FEM and $\mathbb{P}_1$ BEM. We do not see any signs of instability.

We perform one last test to search for possible instabilities. We use the same approach and known solution as the previous example, but now with the material matrix

$$\kappa(x, y) = \begin{bmatrix} 100 & 0 \\ 0 & 500 \end{bmatrix}.$$

We report our findings in Figures 5.8 and 5.9 and see no evidence of instabilities.

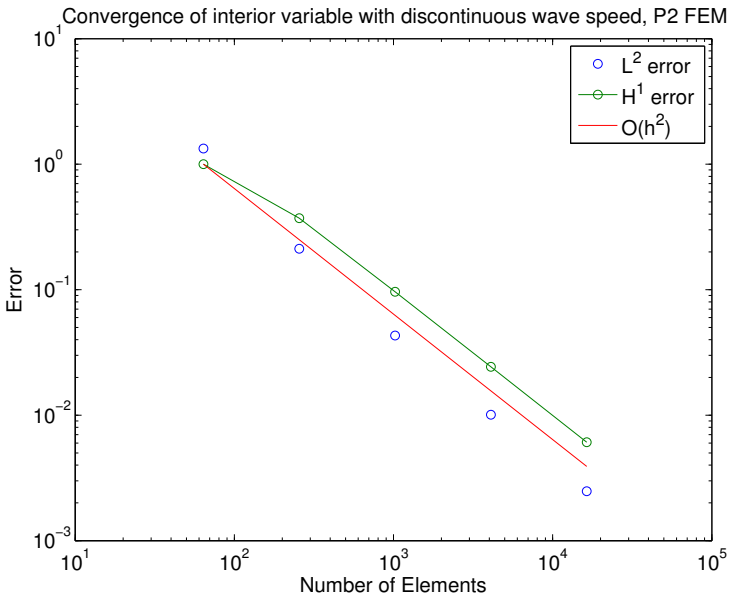

Figure 5.6: Convergence of the interior variable for one equation coupling with discontinuous wave speed.

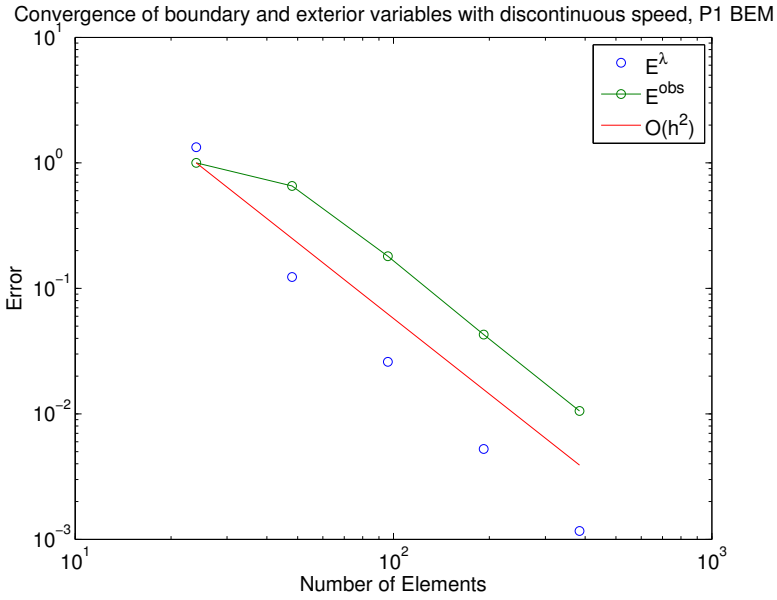

Figure 5.7: Convergence of the boundary and exterior variables for one equation coupling with discontinuous wave speed.

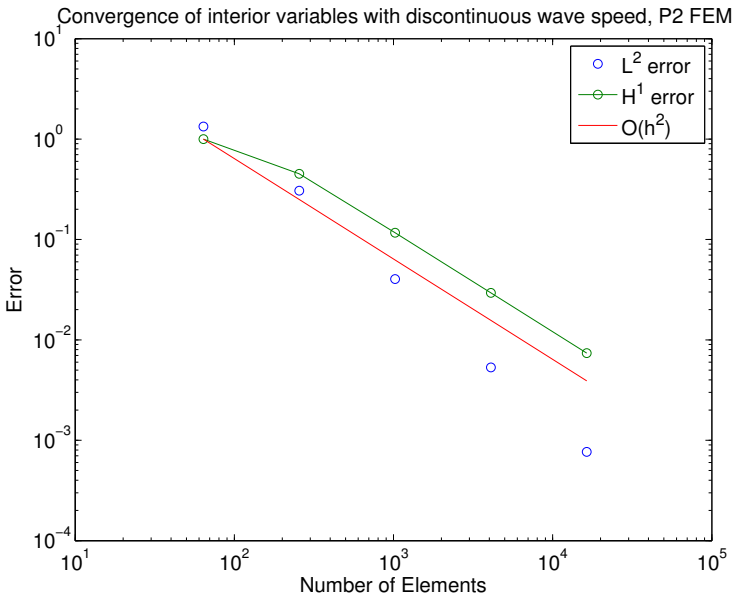

Figure 5.8: Convergence of the interior variable for one equation coupling with large jumps in wave speed.

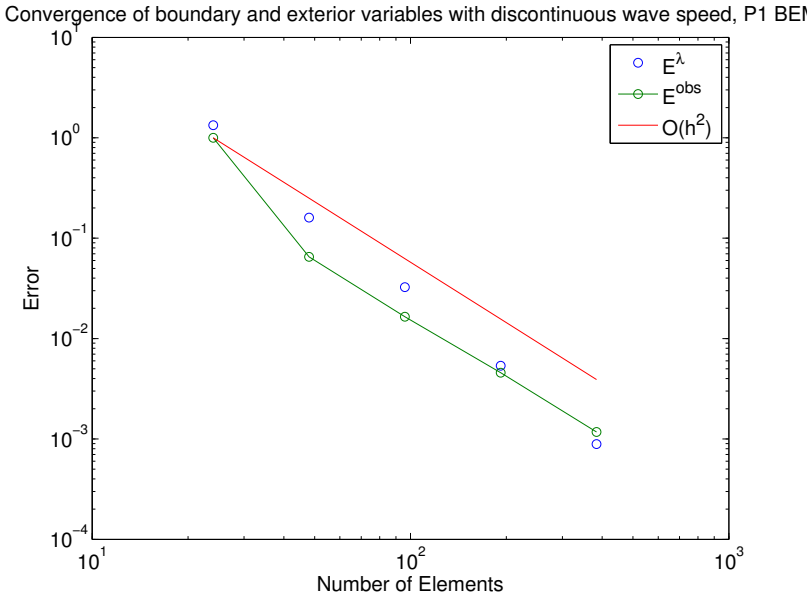

Figure 5.9: Convergence of the boundary and exterior variables for one equation coupling with large jumps in wave speed.

Chapter 6

CONCLUSIONS AND OUTLOOK

We have studied various applications of time domain boundary integral equations to the solution of transient PDEs. For discretization of the retarded potentials and integral operators associated to the underlying PDEs we have used Galerkin methods in space (including deltaBEM under that general heading) and Convolution Quadrature in time. The two general flavors of analysis for the fully discrete methods have been seen here as well. In the case of the Stokes problem, we take a route through the Laplace domain to derive stability and convergence estimates for the fully discrete problem in the time domain, using the original methods of Christian Lubich [58]. The BEM-FEM coupling analysis uses a different route that works with the problem directly in the time domain: we show that the evolution of the semidiscrete PDE is led by a C_0-group of isometries in an appropriate Hilbert space, and then apply simple finite-difference style analysis to show the convergence of the fully discrete method. The advantage of the direct-in-time analysis is seen in the growth of the stability constants with respect to time.

In itself, the first order methodology for the direct-in-time analysis is quite new. Previously, analysis was carried out directly on the second-order system [73, 74]. That analysis was complicated by spaces of rigid motions and the need for analysis only on compact subsets of free space. The first-order-in-space-and-time method was launched in [36] and circumvents these challenges entirely. There are still many open questions and problems of interest in the application CQ for the temporal disctretization of TDIEs. The direct-in-time analysis presented in Chapter 4 has thus far only been successfully carried out for Backward Euler and trapezoidal rule based CQ discretizations [74]. Extensions of this method to higher-order BDF methods as well as

to Runge-Kutta based CQ methods are still absent and are the subject of ongoing research.

In the BEM-FEM coupling direction, we have explored two other coupling schemes computationally. Previous analysis in both the Laplace [52] and time domain [73], as well as our own time domain analysis shows that the two field symmetric coupling scheme is stable and will converge at the correct order upon an appropriate discretization. On the other hand, the one-equation coupling formulation of Johnson and Nédélec can be shown in the time domain not to generate a strongly continuous group. We have made some computational studies of the one-equation coupling scheme and did not find instabilities in the face of large jumps in the material coefficients. There has been other work [29] that have also studied one-equation coupling in the time domain, and they have not found experimental evidence for instabilities, either. Recent work has studied coupling of BEM and FEM for linear elastic waves interacting with elastic and piezoelastic media [70, 71], and there is ongoing research into elastic waves interacting with thermoelastic media [42].

These are only a small part of the many possibilities to come out of coupling of BEM and FEM. From the inverse problems point of view, coupling schemes allow for the simulation of waves interacting with inhomogeneities, which would be of interest to researchers in sonar, oil prospecting, non-destructive testing, and defect detection [19]. When fully inhomogeneous and anisotropic media are not required for the physical model, we can instead couple boundary element computations for both the interior and exterior fields. As long as the wave speeds are constant in each obstacle, BEM-BEM coupling offers an alternate route. Time domain analysis for one particular BEM-BEM coupling formulation was analyzed in [68]. For analysis of acoustic scattering by layered media with constant coefficients in each layer, there is ongoing work in [69].

The work presented here on the simulation of transient Stokes flow with integral methods is quite cursory and leaves much to be completed. CQ-BEM discretizations of parabolic PDEs has focused almost exclusively on the Heat Equation. Our analysis of the transient Stokes Single Layer potential and operator is only one part of the complete

Calderón Projector for the Stokes problem, and a full analysis and implementation would open up many interesting possibilities. Besides the Stokes equations, there is an alternative linearization of Navier-Stokes known as Oseen flow. While transient Stokes can be seen as a flow around a moving obstacle, Oseen flow allows for both the obstacle and background fluid to be moving (albeit at a constant velocity and in a constant direction). Much effort has not led the author to the fundamental solution to the resolvent Oseen equations for a CQ-BEM discretization of that PDE. While only a small generalization of the Stokes problem, it would be an interesting step in understanding not only the Oseen problem, but the computation of particularly difficult Laplace transforms.

One drawback of a generic implementation of boundary elements is that the method suffers from a large overhead in memory and computational time. BEM discretizations result in full matrices, so storage grows quadratically with the number of degrees of freedom, and direct solves of the linear systems grow cubically. There is an entire field of work on developing fast and memory-efficient solvers for integral equations, which we have not touched upon at all in this thesis. These include tools like the Fast Multipole Method [31], H-Matrices [32] and H^2-Matrices [33]. These have the ability to reduce the complexity of the BEM solves to linear complexity, and can also reduce the storage costs to linear or near linear (up to log terms) complexity. Convolution Quadrature also has also been the target of research with the goal of reducing the computation time of the CQ weights. The work [76] started with reduced weight computations for parabolic problems and 3D wave equations. This involves deforming the elliptical integration region to a parabola that extends into the left half of the complex plane. The exponential decay of the convolution kernel for parabolic-type problems is then exploited in this regime, so many of the CQ weights can be safely replaced by zero. Only recently [54] has there been work on reducing the cost of computing weights associated to 2D hyperbolic symbols and dissipative wave equations. There is also the ability to include adaptive time stepping with CQ, which has been studied in [55]. This has the potential to further reduce computation time if coupled with fast

and data sparse methods in space.

While we have not studied them here, there are two other schools of thought in the numerical analysis of BIEs. The "full Galerkin" community uses a Galerkin method in space and time for full discretization. This was the original approach taken in [7] and continues to be a popular option. However, full Galerkin requires the fundamental solution to the dynamic problem, which is accessible for certain PDEs, but is unknown, for instance, for some problems in elastodynamics. This is an advantage the CQ-BEM route has: fundamental solutions are often known in the Laplace domain even when they are unknown in the time domain, and are also usually analytic functions of the Laplace parameter, even when the fundamental solution in the time domain is distributional. Recently, Weile has developed a method [82] to connect CQ and Galerkin-in-time to accelerate the computation of convolutional tails when solving TDIEs in a marching-on-in-time framework. This has the added bonus of reducing the artificial diffusion introduced when making a CQ discretization, though, as he points out, the differences in the errors themselves are negligible. On the other end of the spectrum, there are proponents of Nyström methods for spatial discretization. This limits the possibility of extending the problem to the time domain, since Nyström methods work almost exclusively with second-kind integral equations, while theory for TDIEs works well only for first kind integral equations.

Overall, there are still many interesting questions in the application of TDIEs to the solution of transient PDEs. This thesis has touched upon some of the key issues and problems in the field, both in theoretical and algorithmic aspects.

BIBLIOGRAPHY

[1] T. Abboud, P. Joly, J. Rodríguez, and I. Terrasse. Coupling discontinuous Galerkin methods and retarded potentials for transient wave propagation on unbounded domains. *J. Comput. Phys.*, 230(15):5877–5907, 2011.

[2] R. Adams and J. Fournier. *Sobolev spaces*, volume 140 of *Pure and Applied Mathematics (Amsterdam)*. Elsevier/Academic Press, Amsterdam, second edition, 2003.

[3] C. Amrouche, V. Girault, and J. Giroire. Espaces de Sobolev avec poids et équation de Laplace dans $\mathbf{R}^n$. I. *C. R. Acad. Sci. Paris Sér. I Math.*, 315(3):269–274, 1992.

[4] D. N. Arnold and P. J. Noon. Coercivity of the Single Layer heat potential. *J. Comput. Math.*, 7(2):100–104, 1989. China-US Seminar on Boundary Integral and Boundary Element Methods in Physics and Engineering (Xi'an, 1987–88).

[5] A. Bachelot, L. Bounhoure, and A. Pujols. Couplage éléments finis–potentiels retardés pour la diffraction électromagnétique par un obstacle hétérogène. *Numer. Math.*, 89(2):257–306, 2001.

[6] C. Bacuta, M. E. Hassell, G. C. Hsiao, and F.-J. Sayas. Boundary integral solvers for an evolutionary exterior Stokes problem. *SIAM J. Numer. Anal.*, 53(3):1370–1392, 2015.

[7] A. Bamberger and T. H. Duong. Formulation variationnelle espace-temps pour le calcul par potentiel retardé de la diffraction d'une onde acoustique. I. *Math. Methods Appl. Sci.*, 8(3):405–435, 1986.

[8] A. Bamberger and T. H. Duong. Formulation variationnelle pour le calcul de la diffraction d'une onde acoustique par une surface rigide. *Math. Methods Appl. Sci.*, 8(4):598–608, 1986.

[9] L. Banjai. Multistep and multistage Convolution Quadrature for the wave equation: algorithms and experiments. *SIAM J. Sci. Comput.*, 32(5):2964–2994, 2010.

[10] L. Banjai. Time-domain boundary integral treatment of the wave equation with a non-linear impedance boundary condition. Talk at Computational and Numerical Analysis of Transient Problems in Acoustics, Elasticity, and Electromagnetism, Banff International Research Station, 2016.

[11] L. Banjai, A. R. Laliena, and F.-J. Sayas. Fully discrete Kirchhoff formulas with CQ-BEM. *IMA J. Numer. Anal.*, 35(2):859–884, 2015.

[12] L. Banjai and C. Lubich. An error analysis of Runge-Kutta Convolution Quadrature. *BIT*, 51(3):483–496, 2011.

[13] L. Banjai, C. Lubich, and J. M. Melenk. Runge-Kutta Convolution Quadrature for operators arising in wave propagation. *Numer. Math.*, 119(1):1–20, 2011.

[14] L. Banjai, C. Lubich, and F.-J. Sayas. Stable numerical coupling of exterior and interior problems for the wave equation. *Numer. Math.*, 129(4):611–646, 2015.

[15] L. Banjai, M. Messner, and M. Schanz. Runge-Kutta Convolution Quadrature for the boundary element method. *Comput. Methods Appl. Mech. Engrg.*, 245/246:90–101, 2012.

[16] L. Banjai and S. Sauter. Rapid solution of the wave equation in unbounded domains. *SIAM J. Numer. Anal.*, 47(1):227–249, 2008/09.

[17] L. Banjai and M. Schanz. Wave propagation problems treated with Convolution Quadrature and BEM. In *Fast boundary element methods in engineering and industrial applications*, volume 63 of *Lect. Notes Appl. Comput. Mech.*, pages 145–184. Springer, Heidelberg, 2012.

[18] T. Betcke, N. Salles, and W. Smigaj. Overresolving in the Laplace domain for Convolution Quadrature methods. 2014. arXiv:1603.01761.

[19] A. Carpio and M. L. Rapún. Topological derivatives for shape reconstruction. In *Inverse problems and imaging*, volume 1943 of *Lecture Notes in Math.*, pages 85–133. Springer, Berlin, 2008.

[20] J. F.-C. Chan and P. Monk. Time dependent electromagnetic scattering by a penetrable obstacle. *BIT*, 55(1):5–31, 2015.

[21] Q. Chen, P. Monk, X. Wang, and D. Weile. Analysis of Convolution Quadrature applied to the time-domain electric field integral equation. *Commun. Comput. Phys.*, 11(2):383–399, 2012.

[22] M. Costabel. Symmetric methods for the coupling of finite elements and boundary elements. In *Boundary elements IX, Vol. 1 (Stuttgart, 1987)*, pages 411–420. Comput. Mech., Southampton, 1987.

[23] M. Costabel. Boundary integral operators for the heat equation. *Integral Equations Operator Theory*, 13(4):498–552, 1990.

[24] M. Costabel. Time-dependent problems with boundary integral equation method. In E. Stein, R. de Borst, and T. J. R. Hughes, editors, *Encyclopedia of computational mechanics. Vol. 1.* John Wiley & Sons, Ltd., Chichester, 2004.

[25] R. Dautray and J.-L. Lions. *Mathematical analysis and numerical methods for science and technology. Vol. 5*. Springer-Verlag, Berlin, 1992. Evolution problems. I, With the collaboration of Michel Artola, Michel Cessenat and Hélène Lanchon, Translated from the French by Alan Craig.

[26] V. Domínguez, S. L. Lu, and F.-J. Sayas. A Nyström flavored Calderón calculus of order three for two dimensional waves, time-harmonic and transient. *Comput. Math. Appl.*, 67(1):217–236, 2014.

[27] S. Falletta and G. Monegato. An exact non reflecting boundary condition for 2D time-dependent wave equation problems. *Wave Motion*, 51(1):168–192, 2014.

[28] S. Falletta and G. Monegato. Exact non-reflecting boundary condition for 3D time-dependent multiple scattering–multiple source problems. *Wave Motion*, 58:281–302, 2015.

[29] S. Falletta, G. Monegato, and L. Scuderi. A space-time BIE method for nonhomogeneous exterior wave equation problems. The Dirichlet case. *IMA J. Numer. Anal.*, 32(1):202–226, 2012.

[30] V. Girault and P.-A. Raviart. *Finite element methods for Navier-Stokes equations*, volume 5 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 1986. Theory and algorithms.

[31] L. Greengard and V. Rokhlin. A fast algorithm for particle simulations. *J. Comput. Phys.*, 73(2):325–348, 1987.

[32] W. Hackbush. A sparse matrix arithmetic based on H-matrices. Part I: Introduction to H-matrices. *Computing*, 62:89–108, 1999.

[33] W. Hackbush and S. Sauter. On H^2-matrices. *Lectures on Applied Mathematics*, 62:9–29, 2002.

[34] E. Hairer, C. Lubich, and M. Schlichte. Fast numerical solution of nonlinear Volterra convolution equations. *SIAM J. Sci. Statist. Comput.*, 6(3):532–541, 1985.

[35] H. Han. A new class of variational formulations for the coupling of finite and boundary element methods. *J. Comput. Math.*, 8(3):223–232, 1990.

[36] M. Hassell, T. Qiu, T. Sánchez-Vizuet, and F.-J. Sayas. A new and improved analysis of the time domain boundary integral operators for acoustics (submitted).

[37] M. Hassell and F.-J. Sayas. Convolution Quadrature for Wave Simulations. arXiv:1407.0345. To appear in SEMA-SIMAI Springer Series, 2014.

[38] M. Hassell and F.-J. Sayas. A fully discrete BEM-FEM scheme for transient acoustic waves. *Comput. Methods Appl. Mech. Engrg.*, May 2016. In revision.

[39] F.-K. Hebeker and G. C. Hsiao. On Volterra boundary integral equations of the first kind for nonstationary Stokes equations. In *Advances in boundary element techniques*, Springer Ser. Comput. Mech., pages 173–186. Springer, Berlin, 1993.

[40] F.-K. Hebeker and G. C. Hsiao. An initial-boundary value problem for a viscous compressible flow. *Georgian Math. J.*, 14(1):123–134, 2007.

[41] G. Hsiao, T. Sánchez-Vizuet, and F.-J. Sayas. Boundary and coupled boundary-finite element methods for transient wave-structure interaction. *IMA J. Numer. Anal.* In revision.

[42] G. Hsiao, T. Sánchez-Vizuet, and F.-J. Sayas. Scattering of waves by media with thermoelastic properties. In preparation, 2016.

[43] G. C. Hsiao and J. Saranen. Integral equation solution of some heat conduction problems. In *Integral equations and inverse problems (Varna, 1989)*, volume 235 of *Pitman Res. Notes Math. Ser.*, pages 107–114. Longman Sci. Tech., Harlow, 1991.

[44] C. Johnson and J.-C. Nédélec. On the coupling of boundary integral and finite element methods. *Math. Comp.*, 35(152):1063–1079, 1980.

[45] S. Kesavan. *Topics in functional analysis and applications*. John Wiley & Sons Inc., New York, 1989.

[46] M. Kohr. The Dirichlet problems for the Stokes resolvent equations in bounded and exterior domains in $\mathbf{R^n}$. *Math. Nachr.*, 280(5-6):534–559, 2007.

[47] M. Kohr and I. Pop. *Viscous incompressible flow for low Reynolds numbers*, volume 16 of *Advances in Boundary Elements*. WIT Press, Southampton, 2004.

[48] M. Kohr and W. L. Wendland. Boundary integral equations for a three-dimensional Brinkman flow problem. *Math. Nachr.*, 282(9):1305–1333, 2009.

[49] R. Kress. *Linear integral equations*, volume 82 of *Applied Mathematical Sciences*. Springer, New York, third edition, 2014.

[50] A. R. Laliena. *Theoretical And Algorithmic Aspects of the Convolution Quadrature Method Applied To Scattering of Acoustic Waves*. PhD thesis, Universidad de Zaragoza, 2011.

[51] A. R. Laliena and F.-J. Sayas. A distributional version of Kirchhoff's formula. *J. Math. Anal. Appl.*, 359(1):197–208, 2009.

[52] A. R. Laliena and F.-J. Sayas. Theoretical aspects of the application of convolution quadrature to scattering of acoustic waves. *Numer. Math.*, 112(4):637–678, 2009.

[53] J. Li, P. Monk, and D. Weile. Time domain integral equation methods in computational electromagnetism. In *Computational electromagnetism*, volume 2148 of *Lecture Notes in Math.*, pages 111–189. Springer, Cham, 2015.

[54] M. López-Fernández. Fast and oblivious algorithms for dissipative and 2D wave equations. Talk, Jan 2016. Computational and Numerical Analysis of Transient Problems in Acoustics, Elasticity, and Electromagnetism, Banff International Research Station.

[55] M. López-Fernández, C. Lubich, and A. Schädle. Adaptive, fast, and oblivious convolution in evolution equations with memory. *SIAM J. Sci. Comput.*, 30(2):1015–1037, 2008.

[56] M. López-Fernández and S. Sauter. Generalized Convolution Quadrature with variable time stepping. *IMA J. Numer. Anal.*, 33(4):1156–1175, 2013.

[57] M. López-Fernández and S. Sauter. Generalized Convolution Quadrature with variable time stepping. Part II: Algorithm and numerical results. *Appl. Numer. Math.*, 94:88–105, 2015.

[58] C. Lubich. Convolution Quadrature and discretized operational calculus. I. *Numer. Math.*, 52(2):129–145, 1988.

[59] C. Lubich. Convolution Quadrature and discretized operational calculus. II. *Numer. Math.*, 52(4):413–425, 1988.

[60] C. Lubich. On the multistep time discretization of linear initial-boundary value problems and their boundary integral equations. *Numer. Math.*, 67(3):365–389, 1994.

[61] C. Lubich and A. Ostermann. Runge-Kutta methods for parabolic equations and convolution quadrature. *Math. Comp.*, 60(201):105–131, 1993.

[62] C. Lubich and R. Schneider. Time discretization of parabolic boundary integral equations. *Numer. Math.*, 63(4):455–481, 1992.

[63] P. G. Martinsson. A direct solver for variable coefficient elliptic PDEs discretized via a composite spectral collocation method. *J. Comput. Phys.*, 242:460–479, 2013.

[64] W. McLean. *Strongly elliptic systems and boundary integral equations*. Cambridge University Press, Cambridge, 2000.

[65] M. Messner and M. Schanz. A symmetric Galerkin boundary element method for 3d linear poroelasticity. *Acta Mech.*, 223(8):1751–1768, 2012.

[66] M. Messner, M. Schanz, and J. Tausch. A fast Galerkin method for parabolic space-time boundary integral equations. *J. Comput. Phys.*, 258:15–30, 2014.

[67] A. Pazy. *Semigroups of linear operators and applications to partial differential equations*, volume 44 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1983.

[68] T. Qiu and F.-J. Sayas. The Costabel-Stephan system of boundary integral equations in the time domain. *Math. Comp.*, 2015. To appear.

[69] T. Qiu and F.-J. Sayas. Boundary integral simulation of transient acoustic waves across layered media. In preparation, 2016.

[70] T. Sánchez-Vizuet and F.-J. Sayas. Boundary and coupled boundary-finite element methods for transient wave-structure interaction. *IMA J. of Num. Anal.*, 2016. To appear.

[71] T. Sánchez-Vizuet and F.-J. Sayas. Boundary-finite element discretization of time dependent acoustic scattering by elastic obstacles with piezoelectric behavior. Submitted, 2016.

[72] F.-J. Sayas. The validity of Johnson-Nédélec's BEM-FEM coupling on polygonal interfaces. *SIAM J. Numer. Anal.*, 47(5):3451–3463, 2009.

[73] F.-J. Sayas. Energy estimates for Galerkin semidiscretizations of time domain boundary integral equations. *Numer. Math.*, 124(1):121–149, 2013.

[74] F.-J. Sayas. *Retarded potentials and time domain integral equations: a roadmap*. Springer Series in Computational Mathematics. Springer International Publishing, Berlin, 2016.

[75] F.-J. Sayas and V. Selgas. Variational views of Stokeslets and stresslets. *S$\widetilde{\text{e}}$MA J.*, 63:65–90, 2014.

[76] A. Schädle, M. López-Fernández, and C. Lubich. Fast and oblivious Convolution Quadrature. *SIAM J. Sci. Comput.*, 28(2):421–438 (electronic), 2006.

[77] M. Schanz. *Wave Propagation in Viscoelastic and Poroelastic Continua: A Boundary Element Approach*. Springer, 2001.

[78] L. Schwartz. *Méthodes mathématiques pour les sciences physiques*. Enseignement des Sciences. Hermann, Paris, 1961.

[79] J. Tausch. A fast method for solving the heat equation by layer potentials. *J. Comput. Phys.*, 224(2):956–969, 2007.

[80] J. Tausch. Nyström discretization of parabolic boundary integral equations. *Appl. Numer. Math.*, 59(11):2843–2856, 2009.

[81] F. Trèves. *Topological vector spaces, distributions and kernels*. Academic Press, New York-London, 1967.

[82] D. S. Weile. Numerical dispersion mitigation for Convolution Quadrature approaches to electromagnetic scattering simulation. Talk at Computational and Numerical Analysis of Transient Problems in Acoustics, Elasticity, and Electromagnetism, Banff International Research Station, 2016.

Appendix A

DISTRIBUTIONS OF ONE REAL VARIABLE TAKING VALUES ON A BANACH SPACE

Here we will present the basics of vector-valued distribution theory of a single variable that is needed for the development of Convolution Quadrature and time domain boundary integral equations. The standard reference for scalar distributions is [78], while for vector-valued distributions we refer to the works [81] and [25].

A.1 Causal distributions

Definition A.1.1. *The space $\mathcal{D}(\mathbb{R})$ is the set of C^∞ compactly supported functions on $\mathbb{R}$. We say a sequence $\{\varphi_n\} \subset \mathcal{D}(\mathbb{R})$ converges to an element $\varphi \in \mathcal{D}(\mathbb{R})$ if*

1. *there exists a compact set K such that $\operatorname{supp}\varphi_n \subset K$ for all n, and*
2. *$\max_{x\in K} \left|\partial^{(k)}\varphi_n(x) - \partial^{(k)}\varphi(x)\right| \to 0$ as $n \to \infty$ for all $k \in \mathbb{N}$.*

Definition A.1.2. *A distribution is a sequentially continuous linear map from $\mathcal{D}(\mathbb{R})$ to $\mathbb{R}$. The space of distributions is denoted $\mathcal{D}'(\mathbb{R})$.*

Definition A.1.3. *A distribution $f : \mathcal{D}(\mathbb{R}) \to \mathbb{X}$ is said to be causal when*

$$\langle f, \varphi\rangle = 0 \quad \textit{if} \quad \operatorname{supp}\varphi \subset (-\infty, 0).$$

Causal functions provide simple examples of causal distributions: if $f : \mathbb{R} \to \mathbb{R}$ is continuous, then we can define

$$\langle f, \varphi\rangle := \int_0^\infty f(t)\varphi(t)dt,$$

where the integral can be understood simply as a Riemann integral. We can also define the tensor product of a causal distribution with an element $x \in \mathbb{X}$ by:

$$\langle x \otimes \delta_{t_0}, \varphi \rangle := \varphi(t_0)x.$$

For $t_0 \geq 0$, $x \otimes \delta_{t_0}$ defines a causal distribution, whereas for $t_0 < 0$ the tensor product defines a non-causal distribution. Distributional differentiation is carried out in the standard way:

$$\langle \dot{f}, \varphi \rangle := -\langle f, \dot{\varphi} \rangle,$$

and so the distributional derivative of a causal distribution is again a causal distribution.

A.2 The Laplace Transform

This section will develop the distributional version of the Laplace transform for a restrictive class of causal distributions. We will begin with the Schwartz class. For a general introduction to the Laplace transforms of scalar distributions, we refer to [78].

Definition A.2.1. *The Schwartz class is the set*

$$\mathcal{S}(\mathbb{R}) := \{\varphi \in C^\infty(\mathbb{R}) \ : \ p_m \tfrac{d^m}{dt^m}\varphi \in L^\infty(\mathbb{R}) \ \forall m \geq 0\}$$

where $p_m(t) := 1 + t^{2m}$. *We say a sequence* $\{\varphi_n\} \subset \mathcal{S}(\mathbb{R})$ *converges to* $\varphi \in \mathcal{S}(\mathbb{R})$ *when* $p_m\varphi_n^{(m)} \to p_m\varphi^{(m)}$ *uniformly in* $\mathbb{R}$ *for all* $m \geq 0$.

It can be shown that $\mathcal{D}(\mathbb{R})$ is a dense subset of $\mathcal{S}(\mathbb{R})$. We will use this fact in the construction of a distributional Laplace transform. We now define a smooth cutoff function $h : \mathbb{R} \to \mathbb{R}$ such that

$$h \in \mathcal{C}^\infty(\mathbb{R}), \quad 0 \leq h \leq 1, \quad h \equiv 1 \text{ in } [-\tfrac{1}{2}, \infty), \quad h \equiv 0 \text{ in } (-\infty, -1].$$

If we let $s \in \mathbb{C}_+ := \{s \in \mathbb{C} \ : \ \operatorname{Re} s > 0\}$, then the function $\varphi_s(t) := h(t)e^{-st} \in \mathcal{S}(\mathbb{R})$. Therefore there is a sequence $\{\varphi_{n,s}\} \subset \mathcal{D}(\mathbb{R})$ converging to φ_s as elements of $\mathcal{D}(\mathbb{R})$.

If we let f be a causal $\mathbb{X}$-valued distribution, then we say that f has a distributional Laplace transform when the limit

$$\lim_{n\to\infty} \langle f, \varphi_{n,s} \rangle$$

exists for all $s \in \mathbb{C}_+$. We define the function $\mathrm{F}(s) := \lim_{n\to\infty} \langle f, \varphi_{n,s} \rangle$, sometimes also denoted by $\mathrm{F}(s) = \mathcal{L}\{f\}(s)$. The distributional Laplace transform does not depend on the choice of h, so long as it is smooth, vanishes on $(-\infty, a]$ and is identically 1 on some interval $[b, \infty)$ for $a < b < 0$.

The following formal manipulation shows how the Laplace Transform maps causal convolutions in the time domain to multiplication in the Laplace domain:

$$\begin{aligned}
\int_0^\infty (f * g) e^{-st} dt &= \int_0^\infty e^{-st} \int_0^t f(t-\tau) g(\tau) d\tau dt \\
&= \int_0^\infty e^{-s\tau} \int_\tau^\infty e^{-s(t-\tau)} f(t-\tau) dt g(\tau) d\tau \\
&= \int_0^\infty e^{-st} f(t) dt \int_0^\infty e^{-s\tau} g(\tau) d\tau \\
&= \mathcal{L}\{f(t)\}\mathcal{L}\{g(t)\}.
\end{aligned}$$

Examples of distributional Laplace Transforms

The Laplace transform of $x \otimes \delta_{t_0}$ is

$$\langle x \otimes \delta_{t_0}, e^{-st} \rangle = \langle \delta_{t_0}, e^{-st} \rangle x = e^{-st_0} x.$$

The Laplace transform of $x \otimes H$ is

$$\langle x \otimes H, e^{-st} \rangle = \langle H, e^{-st} \rangle x = \left(\int_0^\infty e^{-st} dt \right) x = \frac{1}{s} x.$$

If the Laplace transform of an X-valued distribution f exists and $A : X \to Y$ is a bounded linear steady-state operator, then the Laplace transform of Af is

$$\langle Af(t), e^{-st} \rangle = A \langle f(t), e^{-st} \rangle = A\mathrm{F}(s).$$

Differentiation

Suppose that f has a distributional Laplace transform. It is then easy to show that $\dot{\psi}_s(t) = -s\psi_s(t) + \varphi_s(t)$, where $\operatorname{supp}\varphi_s \subset (-\infty, 0)$. Then $\dot{f}$ has a Laplace transform given by

$$\begin{aligned}\mathcal{L}\{\dot{f}(t)\} = \langle \dot{f}(t), \psi_s(t)\rangle = -\langle f(t), s\psi_s(t) - \varphi_s(t)\rangle = -\langle f(t), s\psi_s(t)\rangle \\ = \langle sf(t), \psi_s(t)\rangle = s\mathrm{F}(s).\end{aligned}$$

Notice how this differentiation result differs from the classical Laplace transform, where $\mathcal{L}\{\dot{f}(t)\} = s\mathrm{F}(s) - f(0)$. The value of $f(0)$ is missing from our distributional definition because of the assumed causality of f. We can relate the classical and distributional transforms as follows. Suppose $f : [0, \infty) \to \mathbb{X}$ is a rapidly decaying smooth function, which we can extend by zero to the negative axis, and assume that its classical derivative $f' : [0, \infty) \to \mathbb{X}$ is also rapidly decaying. Then

$$\dot{f} = f(0) \otimes \delta_0 + f'.$$

Then we have

$$\mathcal{L}\{f'\}(s) = \mathcal{L}\{f'\}(s) - \mathcal{L}\{f(0) \otimes \delta_0\} = s\mathrm{F}(s) - f(0).$$

Some technical details

We note that the theory of functions of a single complex variable can be extended almost exactly to functions of a complex variables taking values in a general Banach space $\mathbb{X}$. It is quite easy to show that if f is causal and has a Laplace transform, then the map $\mathbb{C} \ni s \mapsto \mathrm{F}(s)$ is differentiable in the s variable, and is therefore an holomorphic function taking values on $\mathbb{X}$. We have also glossed over the fact the spaces $\mathcal{D}(\mathbb{R})$ and $\mathcal{S}(\mathbb{R})$ are real-valued, while $\psi_s = h(t)e^{-st}$ takes complex values. Our Laplace transform then needs to be understood as

$$\mathrm{F}(s) = \langle f, \psi_s\rangle := \langle f, \operatorname{Re}\psi_s\rangle + \langle f, \operatorname{Im}\psi_s\rangle.$$

Our applications will always focus on a real Banach space $\mathbb{X}$, and so $\mathrm{F}(s)$ will take values in its complexification $\mathbb{X} + i\mathbb{X}$. When $\mathbb{X}$ is already complex, this does not change

the space. An important result for complexified Banach spaces is that they admit a conjugation operator and Laplace transforms taking values on such a space satifying

$$\mathrm{F}(\overline{s}) = \overline{\mathrm{F}(s)}.$$

A.3 Laplace inversion theory for hyperbolic symbols

Before we can carefully study convolution operators and their Laplace transforms, we need to develop some functional analysis tools. We follow the method introduced in [50] and simplified in [74].

Definition A.3.1. *Let $\mathbb{X}$ be a Banach space and $\mu \in \mathbb{R}$. We say $\mathrm{F}(s) \in \mathcal{A}(\mu, \mathbb{X})$ when $\mathrm{F} : \mathbb{C}_+ \to \mathbb{X}$ is an analytic function such that*

$$\|\mathrm{F}(s)\| \leq C_F(\operatorname{Re} s)|s|^\mu \quad \forall s \in \mathbb{C}_+$$

where $C_F : (0, \infty) \to (0, \infty)$ is a non-increasing function such that $C_F(\sigma) \leq \frac{C}{\sigma^m} \quad \forall \sigma \in (0, 1]$.

We also have the following proposition from [74, Prop. 3.1.1-3.1.3] to complete our theory.

Proposition A.3.2. *(a) If $\mathrm{F} \in \mathcal{A}(\mu, \mathbb{X})$ with $\mu < 1$, then F is the Laplace transform of a continuous causal function $f : \mathbb{R} \to \mathbb{X}$ with polynomial growth.*

(b) Let $\mathrm{F} \in \mathcal{A}(\mu, \mathbb{X})$ with $\mu \in \mathbb{R}$ and let $k := \max\{0, \lfloor \mu + 2 \rfloor\}$. Then there exists a continuous causal function $\phi : \mathbb{R} \to \mathbb{X}$ with polynomial growth such that $\mathrm{F} = \mathcal{L}\{\phi^{(k)}\}$.

(c) If $f : \mathbb{R} \to \mathbb{X}$ is a continuous function with polynomial growth, then $\mathrm{F} \in \mathcal{A}(\mu, \mathbb{X})$ for some $\mu \in \mathbb{R}$. Therefore the set of symbols

$$\bigcup_{\mu \in \mathbb{R}} \mathcal{A}(\mu, \mathbb{X}).$$

is the set of the Laplace transforms of continuous causal functions $\mathbb{R} \to \mathbb{X}$ with polynomial growth and their distributional derivatives. For brevity, we will denote this space by $\mathrm{TD}(\mathbb{X})$.

From these results, it is clear that if we have two operator-valued distributions $\mathrm{A} \in \mathcal{A}(\mu, \mathbb{X})$ and $\mathrm{B} \in \mathcal{A}(\nu, \mathbb{X})$, then their composition $\mathrm{AB} \in \mathcal{A}(\mu+\nu, \mathbb{X})$. This allows us to give the distributional definition of convolution. The following proposition [74, Prop. 3.2.2.] gives an idea for the type of bounds that we can find for hyperbolic symbols using the Laplace inversion theory.

Proposition A.3.3. *Let* $\mathrm{A} = \mathcal{L}\{a\} \in \mathcal{A}(\mu, \mathcal{B}(X,Y))$ *with* $\mu \geq 0$ *and let*

$$k := \lfloor \mu + 2 \rfloor, \quad \varepsilon := k - (\mu + 1) \in (0, 1].$$

If $g \in \mathcal{C}^{k-1}(\mathbb{R}, X)$ *is causal and* $g^{(k)}$ *is integrable, then* $a * g \in \mathcal{C}(\mathbb{R}, Y)$ *is causal and*

$$\|(a * g)(t)\| \leq 2^{\mu} C_{\varepsilon}(t) C_A(t^{-1}) \int_0^t \|\mathcal{P}_k g(\tau)\| d\tau,$$

where

$$C_{\varepsilon}(t) := \frac{1+\varepsilon}{\pi\varepsilon} \frac{t^{\varepsilon}}{(1+t)^{\varepsilon}}$$

and

$$(\mathcal{P}_k g)(t) := e^{-t}(e^{\cdot} g)^{(k)}(t) = \sum_{\ell=0}^{k} \binom{k}{\ell} g^{(\ell)}(t).$$

A.4 Convolution operators for some parabolic symbols

To apply the Laplace inversion theory and derive estimates for the Stokes problem, we start with an operator valued holomorphic function $\mathrm{F} : \mathbb{C}_{\star} \to \mathcal{B}(X,Y)$ such that

$$\|\mathrm{F}(s)\| \leq C_{\mathrm{F}}(\operatorname{Re} s^{1/2}) |s|^{\mu} \quad \forall s \in \mathbb{C}_{\star}, \quad 0 \leq \mu < 1, \tag{A.1}$$

where

$$C_{\mathrm{F}} : (0,\infty) \to (0,\infty) \text{ is non-increasing and } C_{\mathrm{F}}(\omega) \leq C\omega^{-\ell} \quad \omega \to 0,\ \ell > 0. \tag{A.2}$$

For such an F there is a $\mathcal{B}(X,Y)$-valued causal distribution f whose Laplace transform is $\mathrm{F}(s)$. Following [62, Lemma 2.2] we prove the following proposition. We note that we require more regularity in the data, but also gain precise control over the growth of the convolution $(f * g)(t)$ with respect to t.

Proposition A.4.1. *Let f be such that its Laplace transform satisfies (A.1) and (A.2) and suppose $g \in \mathcal{C}^1_+(\mathbb{R}; X)$. Then $f * g \in \mathcal{C}_+(\mathbb{R}; Y)$ and*

$$\|(f * g)(t)\|_Y \leq C_\mu \max\{1, t^{\ell/2+1-\mu}\} \max_{0\leq\tau\leq t} \|\dot{g}(\tau)\|_X \quad \forall t \geq 0.$$

Proof. Since the result gives estimates of the convolution $f*g$, when $g \in \mathcal{C}^1_+(\mathbb{R}; X)$, and the convolution with f is a causal operator, we can assume (without loss of generality) that g and $\dot{g}$ are uniformly bounded. The following function

$$a(s,t) := \frac{d}{dt}\int_0^t e^{s(t-\tau)} g(\tau) d\tau = \int_0^t e^{s(t-\tau)} \dot{g}(\tau) d\tau$$

is well defined for all $t \in [0, \infty)$ and $s \in \mathbb{C}$. It is then possible to show (see [62, Lemma 2.2]) that

$$(f * g)(t) = \frac{1}{2\pi\imath} \int_\Gamma s^{-1} \mathrm{F}(s) a(s,t) ds \tag{A.3}$$

for a variety of integration contours. (This is shown by proving that the Laplace transform of the function in the right-hand side of (A.3) is F G.) Here we choose a two-parameter family of contours (see Figure A.1), formed by three pieces:

$$\begin{aligned} (-\infty, -c] \ni \rho &\longmapsto z_-(\rho) := -\rho\, e^{-\imath(\pi-\phi)}, \\ [-(\pi-\phi), \pi-\phi] \ni \rho &\longmapsto z_0(\rho) := c e^{\imath\rho}, \\ [c, \infty) \ni \rho &\longmapsto z_+(\rho) := \rho\, e^{\imath(\pi-\phi)}. \end{aligned}$$

The parameter $c > 0$ will play a decisive role in the estimates below, while $\phi \in (0, \pi/2)$ does not seem to be relevant for the following bounds. We first note that for all $t \geq 0$ and $s \in \mathbb{C}$,

$$\|a(s,t)\| \leq \|\dot{g}\|_t \begin{cases} t\, e^{t \operatorname{Re} s} & \operatorname{Re} s \geq 0, \\ t, & \operatorname{Re} s \leq 0, \\ \frac{1}{|\operatorname{Re} s|}, & \operatorname{Re} s < 0, \end{cases} \qquad \text{where} \qquad \|\dot{g}\|_t := \max_{0\leq\tau\leq t} \|\dot{g}(\tau)\|. \tag{A.4}$$

We start by bounding the part of the contour integral (A.3) that arises from the central path $\Gamma_0 = \{z_0(\rho) : |\rho| \leq \pi - \phi\}$. Using

$$|z_0(\rho)| = |z_0'(\rho)| = c, \;\; \operatorname{Re} z_0(\rho)^{1/2} = \sqrt{c} \cos\tfrac{\theta}{2} \geq \sqrt{c} \cos\tfrac{\pi-\phi}{2} = \sqrt{c} \sin\tfrac{\phi}{2}, \;\; \operatorname{Re} z_0(\rho) \leq c,$$

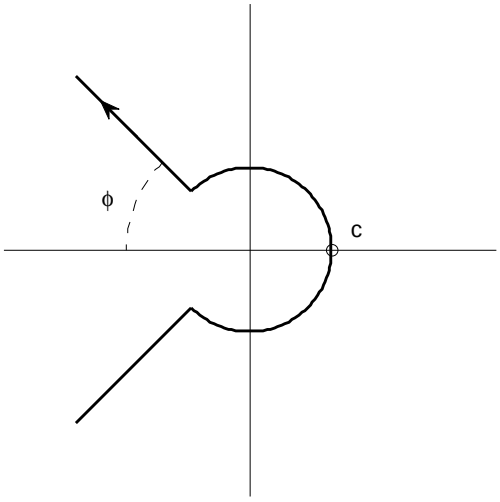

Figure A.1: The contours in the proof of Proposition A.4.1

and (A.4), we can bound

$$\|s^{-1}\mathrm{F}(s)\| \le C_{\mathrm{F}}(\sqrt{c}\,\sin\tfrac{\phi}{2})\,c^{\mu-1} \qquad \|a(s,t)\| \le te^{ct}\|\dot{g}\|_t, \qquad s\in\Gamma_0$$

and therefore

$$\Big\|\int_{\Gamma_0} s^{-1}\mathrm{F}(s)a(s,t)ds\Big\| \le 2(\pi-\phi)C_{\mathrm{F}}(\sqrt{c}\sin\tfrac{\phi}{2})\,c^{\mu}\,e^{ct}\,t\,\|\dot{g}\|_t. \tag{A.5}$$

In $\Gamma_+ := \{z_+(\rho) : \rho \ge c\}$, we have

$$|z_+(\rho)| = \rho,\ \ |z'_+(\rho)| = 1,\ \ \mathrm{Re}\, z_+(\rho)^{1/2} = \sqrt{\rho}\sin\tfrac{\phi}{2} \ge \sqrt{c}\sin\tfrac{\phi}{2},\ \ |\mathrm{Re}\, z_+(\rho)| = \rho\cos\phi,$$

and therefore (the bound in Γ_- can be done simultaneously)

$$\begin{aligned}\Big\|\int_{\Gamma_\pm} s^{-1}\mathrm{F}(s)a(s,t)ds\Big\| &\le C_{\mathrm{F}}(\sqrt{c}\sin\tfrac{\phi}{2})\|\dot{g}\|_t\frac{1}{\cos\phi}\int_c^\infty \theta^{\mu-2}d\theta \\ &= C_{\mathrm{F}}(\sqrt{c}\sin\tfrac{\phi}{2})\|\dot{g}\|_t\frac{1}{\cos\phi}\,\frac{c^{\mu-1}}{1-\mu}.\end{aligned} \tag{A.6}$$

When $t \le 1$, we can take $c = 1$ in (A.5) and (A.6) to bound

$$\|(f*g)(t)\| \le 2\Big((\pi-\phi)t + \frac{1}{(1-\mu)\cos\phi}\Big)\,C_{\mathrm{F}}(\sin\tfrac{\phi}{2})\,\|\dot{g}\|_t \qquad t\le 1.$$

When $t \geq 1$, we take $c = 1/t$ and obtain

$$\|(f * g)\| \leq 2\Big((\pi - \phi)t + \frac{1}{(1-\mu)\cos\phi}\Big) t^{1-\mu}\, C_{\mathrm{F}}(t^{-1/2}\sin\tfrac{\phi}{2})\, \|\dot{g}\|_t \qquad t \geq 1.$$

Using (A.2) bound of the statement is established. Continuity of $f * g$ follows from the representation (A.3) and the Dominated Convergence Theorem.

□

Corollary A.4.2. *Let f be such that its Laplace transform $\mathrm{F} : \mathbb{C}_\star \to \mathcal{B}(X, Y)$ satisfies*

$$\|\mathrm{F}(s)\|_{X\to Y} \leq C_{\mathrm{F}}(\operatorname{Re} s^{1/2})|s|^{1+\mu} \quad s \in \mathbb{C}_\star, \quad 0 \leq \mu < 1,$$

where C_{F} satisfies (A.2). Then for all $g \in \mathcal{C}^2_+(\mathbb{R}; X)$ we have that $f * g \in \mathcal{C}_+(\mathbb{R}; Y)$ and

$$\|(f * g)(t)\|_Y \leq C_\mu \max\{1, t^{\ell/2+1-\mu}\} \max_{0\leq\tau\leq t} \|\ddot{g}(\tau)\|_X, \quad \forall t \geq 0.$$

Proof. Let $\partial_t^{-1} f$ be the distribution whose transform is $s^{-1}\mathrm{F}(s)$. Then $f * g = \partial_t^{-1} f * \dot{g}$, and we can apply Proposition (A.4.1) to $\partial_t^{-1} f$ and $\dot{g}$. □

Appendix B

A SOBOLEV SPACE DIGEST

Here we will gather for ease of reference some definitions and notation that are used throughout this thesis. We begin with Sobolev spaces for domains laying on one side of their Lipschitz boundary, followed by the same spaces defined for domains that lay on both sides of their Lipschitz boundary.

B.1 On one side of the boundary

Let $\mathcal{O}$ be an open subset of $\mathbb{R}^d$ lying on one side of its boundary. We denote the test space as $\mathcal{D}(\mathcal{O})$, i.e. the space of $\mathcal{C}^\infty$ compactly supported functions. Recall from Appendix A that there there is a specific notion of convergence in this space. For more details, we refer the reader to [2]. The space $\mathcal{D}'(\mathcal{O})$ is the space of sequentially continuous linear functionals from $\mathcal{D}(\mathcal{O})$ to $\mathbb{R}$, also known as distributions. There is distributional differentiation defined with these two spaces, by

$$\langle \partial_{x_i} T, \varphi \rangle_{\mathcal{D}' \times \mathcal{D}} := -\langle T, \partial_{x_i} \varphi \rangle_{\mathcal{D}' \times \mathcal{D}} \qquad \forall \varphi \in \mathcal{D}(\mathcal{O}).$$

We will make significant use of the following three Sobolev spaces (listed with their associated norms)

(a) $L^2(\mathcal{O})$, with the norm $\|\cdot\|_{\mathcal{O}}$,

(b) $H^1(\mathcal{O}) := \{u \in L^2(\mathcal{O}) \ : \ \nabla u \in \mathbf{L}^2(\mathcal{O}) := L^2(\mathcal{O})^d\}$ with norm $\|u\|^2_{1,\mathcal{O}} := \|\nabla u\|^2_{\mathcal{O}} + \|u\|^2_{\mathcal{O}}$, and

(c) $\mathbf{H}(\mathrm{div}; \mathcal{O}) := \{\mathbf{u} \in \mathbf{L}^2(\mathcal{O}) \ : \ \nabla \cdot \mathbf{u} \in L^2(\mathcal{O})\}$, with the norm $\|\mathbf{u}\|^2_{\mathrm{div},\mathcal{O}} := \|\nabla \cdot \mathbf{u}\|^2_{\mathcal{O}} + \|\mathbf{u}\|^2_{\mathcal{O}}$.

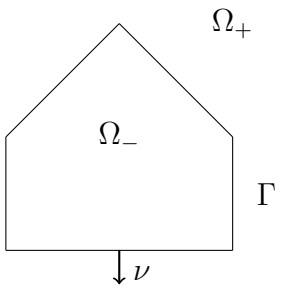

Figure B.1: A Lipschitz domain Ω_-, its boundary Γ, and exterior $\Omega_+ := \mathbb{R}^d \setminus \overline{\Omega_-}$.

Elements of the space $H^1(\mathcal{O})$ have well-defined restrictions to $\partial\mathcal{O}$ by way of the trace operator $\gamma : H^1(\mathcal{O}) \to H^{1/2}(\partial\mathcal{O})$. The trace operator is surjective from $H^1(\mathcal{O})$ to $H^{1/2}(\partial\mathcal{O})$. Moreover, $H^{1/2}(\partial\mathcal{O})$ is a Sobolev space equipped with an intrinsic norm $\|u\|_{1/2,\mathcal{O}}$ which is equivalent to

$$H^{1/2}(\mathcal{O}) \ni \xi \mapsto \inf\{\|u\|_{1,\mathcal{O}} \ : \ \gamma u = \xi\}.$$

The dual space of $H^{1/2}(\partial\mathcal{O})$ is denoted $H^{-1/2}(\partial\mathcal{O})$, and is also a Sobolev space with the dual norm $\|\cdot\|_{-1/2,\partial\mathcal{O}}$.

For a function $\mathbf{v} \in \mathbf{H}(\mathrm{div};\mathcal{O})$, we can define its normal trace $\gamma_\nu \mathbf{v} \in H^{-1/2}(\partial\mathcal{O})$ through Green's formula

$$\langle \gamma_\nu \mathbf{v}, \gamma w\rangle_\Gamma := (\nabla\cdot\mathbf{v}, w)_\mathcal{O} + (\mathbf{v}, \nabla w)_\mathcal{O} \qquad \forall w \in H^1(\mathcal{O}).$$

B.2 On both sides of the boundary

For sets that lay on both sides of their Lipschitz boundary Γ, we can define the necessary Sobolev spaces on each side of Γ. A sketch of this scenario is given in Figure B.1. We have the same Sobolev spaces as before, but this time on each side of Γ.

(a) $L^2(\Omega_\pm)$, with the norm $\|\cdot\|_{\Omega_\pm}$,

(b) $H^1(\Omega_\pm)$, with the norm $\|\cdot\|_{1,\Omega_\pm}$, and

(c) $\mathbf{H}(\mathrm{div};\Omega_\pm)$, with the norm $\|\cdot\|_{\mathrm{div},\Omega_\pm}$.

Traces can be defined from both sides of the boundary now, and will be denoted as $\gamma^{\pm}$. With this, we can define the jump and average value of the trace of a function defined on both sides of Γ

$$\begin{aligned}\llbracket \gamma v \rrbracket &:= \gamma^{-} v - \gamma^{+} v, \\ \{\!\{ \gamma v \}\!\} &:= \tfrac{1}{2} \left(\gamma^{+} v + \gamma^{-} v \right).\end{aligned}$$

If $\boldsymbol{\nu}$ is the unit outward-pointing vector field on Γ, we denote the interior and exterior normal traces by $\gamma_{\nu}^{\pm}$, and can therefore define the interior and exterior normal derivatives by $\partial_{\nu}^{\pm} := \gamma_{\nu}^{\pm} \nabla$. We finally have the space

$$H^1_{\Delta}(\Omega_{\pm}) := \left\{ u \in H^1(\Omega_{\pm}) : \Delta_{\pm} u \in L^2(\Omega_{\pm}) \right\},$$

for which normal derivatives $\gamma_{\nu}^{\pm}$ are defined on both sides of Γ.

As a final ingredient, let us recall that every bounded surjective linear operator between Hilbert spaces admits a bounded linear right-inverse. This fact will often be used to create "liftings" of different trace operators.

Appendix C

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