TRANSPARENT BOUNDARY CONDITIONS – THE POLE CONDITION APPROACH

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Abstract

A new approach to derive transparent boundary conditions (TBCs) for wave, Schrödinger and drift-diffusion equations is presented. It relies on the pole condition approach and distinguishes physical reasonable and unreasonable solutions by the location of the singularities of the spatial Laplace transform U of the exterior solution. By the condition that U is analytic in some region TBCs are established. To realize the pole condition numerically, a Möbius transform is used to map the region of analyticity to the unit disc. There the Laplace transform is expanded in a power series. The equations coupling the coefficients of the power series with the interior provide the TBC. Numerical result for the damped wave equation show that the error introduced by truncating the power series decays exponentially in the number of coefficients.

Introduction

Transparent boundary conditions are a key ingredient for the simulation of wave propagation on unbounded domains. In this talk work in progress is presented.

Prototypes of the governing equations under consideration are the wave, drift-diffusion and Schrödinger equations on the real line for $t > 0$ given by

$$\begin{aligned} \partial_{tt} u &= \partial_{xx} u - k^2 u, && (1)\\ \partial_t u &= \partial_{xx} u + 2d\partial_x u, && (2)\\ i\partial_t u &= \partial_{xx} u - k^2 u. && (3) \end{aligned}$$

All of these have to complemented by appropriate initial values. To treat (1) - (3) simultaneously the symbol $p(\partial_t)$ is introduced. Hence the generic equation is

$$p(\partial_t)u = \partial_{xx} u + 2d\partial_x u - k^2 u. \qquad (4)$$

For the procedure to derive exact non-local transparent boundary conditions we refer to the recent review articles [1]. The pole condition approach is an alternative and as we hope to show a more flexible way of deriving transparent boundary conditions. Almost immediately the pole condition approach yields an algorithm to implement approximate local transparent boundary conditions. The pole condition for time-harmonic problems is studied in [2], where it is shown that it coincides with the Sommerfeld radiation condition.

Alternative derivation of TBCs

Suppose we are only interested in the solution u restricted to the interval $[-a, a]$. Furthermore suppose that the initial value(s) are compactly supported in $[-a, a]$. To truncate the computational domain TBCs are needed. The exact TBCs are in general convolution in time, i.e. they are non-local.

Variational formulation

Multiplying (4) by a test function and integrating over the real line yields

$$\int p(\partial_t)uv\,dx = \int -\partial_x u\partial_x v + 2d\partial_x uv - k^2 uv\,dx. \qquad (5)$$

As test functions we chose $v(x) = \mathrm{e}^{-s(x-a)}$ for $x > a$ and $v(x) = \mathrm{e}^{s(x+a)}$ for $x < -a$ with a complex parameter s with $\Re s > 0$. The integral over the real line is split into three parts: an integral from $-\infty$ to $-a$, from $-a$ to a and from a to ∞. Defining

$$U^{(r)}(t, s) := \int_0^\infty u(t, x + a)\mathrm{e}^{-sx},$$

which is the Laplace transform of the solution u in the right exterior, and similar $U^{(l)}$ one obtains after some simple manipulations

$$\begin{aligned} &\int_{-a}^{a} p(\partial_t)uv\,dx + p(\partial_t)U^{(r)} + p(\partial_t)U^{(l)} = \\ &\quad\int_{-a}^{a} -\partial_x u\partial_x v + 2d\partial_x uv - k^2 uv\,dx \\ &\quad+s(sU^{(l)} - u_{-a}) - 2d(s(U^{(l)} - u_{-a})) - k^2 U^{(l)} \\ &\quad+s(sU^{(r)} - u_a) + 2d(s(U^{(r)} - u_a)) - k^2 U^{(r)}, \end{aligned}$$

where $u_{\pm a}$ are the boundary values of u at the left and right boundary.

Pole Condition

Consider the equation for the right exterior only, suppose for the moment that u is given on $[-a, a]$ and set

$$u' := \int_{-a}^{a} p(\partial_t)uv\,dx + \partial_x u\partial_x v - 2d\partial_x uv + k^2 uv\,dx$$

then the equation for $U^{(r)}$ is given by

$$s(sU^{(r)} - u_a) + 2d(sU^{(r)} - u_a) - k^2 U^{(r)} - p(\partial_t)U^{(r)} = u'\,.$$

Taking a Laplace transform in time with dual variable ω, $p(\partial_t)$ corresponds to a multiplication with $p(\omega) = \omega$, $p(\omega) = i\omega$ or $p(\omega) = \omega^2$ depending on the type of equation. Solving for $U^{(r)}(s)$ one obtains

$$U^{(r)}(s) = (s^2 + 2ds - k^2 - p(\omega))^{-1}(u' + su_a + 2du_a).$$

Clearly $U^{(r)}(s)$ is analytic in s except for two poles (or more generally for several singularities). If s_- and s_+ are the roots of $(s^2 + 2ds - k^2 - p(\omega))$ one can write by Cauchy's integral formula

$$\begin{aligned} U^{(r)}(s) &= \frac{1}{2\pi}\oint_{\gamma_-}\frac{(\sigma^2+2d\sigma-k^2-p(\omega))^{-1}}{\sigma-s}d\sigma \\ &\quad +\frac{1}{2\pi}\oint_{\gamma_+}\frac{(\sigma^2+2d\sigma-k^2-p(\omega))^{-1}}{\sigma-s}d\sigma \end{aligned}$$

where $\gamma_\pm$ are paths enclosing $s_\pm$. In this simple setting this is equivalent to a partial-fraction decomposition.

$$U^{(r)}(s) = \frac{r_+(s,u',u_a)}{s_+ - s} + \frac{r_-(s,u',u_a)}{s_- - s},$$

with $r_\pm = 1/2(u_a \pm (u' + 2du_a)/\sqrt{p(\omega)+k^2+d^2})$. Transforming back to space domain we have the correspondence

$$\frac{1}{s_- - s} \leftrightarrow \mathrm{e}^{s_- x} \quad \text{and} \quad \frac{1}{s_+ - s} \leftrightarrow \mathrm{e}^{s_+ x}.$$

Suppose that we can identify $\mathrm{e}^{s_+ x}$ as an incoming wave or a exponentially increasing solution. Thus depending on the location of the poles $s_\pm$ we can now distinguish incoming/exponentially increasing waves from outgoing/exponentially decreasing waves. So we are in the position to formulate TBCs as a *condition on* $U^{(r)}(s)$. The pole condition says: A wave is outgoing if $U^{(r)}(s)$ is an analytic function in the half plane E of possible locations of s_+. This is equivalent to the condition that $r_+ = 0$, which yields the classical transparent boundary condition. But we are not required to form the expression for r_+.

Pole Condition in Hardy space

How to handle the pole condition numerically? Analytic functions can be expanded into power serieses, which convergence in some ball, yet the pole condition is a condition set on a complex half plane. The Möbius transform is a conformal transformation that transforms a half plane to the unit ball. The Möbius transform is thus the key ingredient to make our algorithm fly. Let $s \mapsto \tilde{s} = M(s)$ be the Möbius transform that maps the half plane E to the unit ball. We can now reformulate the pole condition: A wave is outgoing if $U^{(r)}(\tilde{s})$ is analytic in the unit ball. Expanding

$$U^{(r)}(\tilde{s}) = \sum_{\ell=0}^{\infty} a_\ell \tilde{s}^\ell \tag{6}$$

one has to deduce equations for the a_ℓ. Then simply truncating the series expansion by setting $a_\ell = 0$ for $\ell > L$ an algorithm is obtained, to realize TBCs.

The details are as follows. The Möbius transform

$$s \mapsto \tilde{s} = M(s) := \frac{s+s_0}{s-s_0}$$

maps the half plane $\{z : \Re(-z/s_0) < 0\}$ onto the unit disk. (e.g. for positive real s_0 the left half plane is mapped onto the unit ball; the imaginary axis is mapped to the unit circle; $-s_0$ is mapped to 0; and 0 is mapped to -1.) The inverse is again a Möbius transform

$$\tilde{s} \mapsto s = M^{-1}(\tilde{s}) := s_0\frac{\tilde{s}+1}{\tilde{s}-1}.$$

Space discretization

For the sake of clearness we consider the case $d = 0$ only. Space discretization is done using third order finite elements resulting in the standard local mass and stiffness matrices, that are assemble to a global system. At the right boundary (and similar for the left boundary) we use the special *exp*-element as test function

$$v_s(x) = \begin{cases} \mathrm{e}^{-s(x-a)} & x \geq a \\ \frac{x-(a-h)}{h} & a-h \leq x \leq a \end{cases}$$

and obtain

$$\begin{aligned} &p(\omega)U^{(r)} + p(\omega)u_a^{(0)} = u_a^{(2)} - k^2 u_a^{(0)} + \\ &s_0\frac{\tilde{s}+1}{\tilde{s}-1}\left(s_0\frac{\tilde{s}+1}{\tilde{s}-1}U^{(r)} - u_a\right) - k^2 U^{(r)}, \end{aligned} \tag{7}$$

where $u_a^{(0)}$ and $u_a^{(2)}$ are the boundary contributions

$$u_a^{(0)} = \sum_j \int_{a-h}^{a} u_j\phi_j v_s\,dx\,;\; u_a^{(2)} = \sum_j \int_{a-h}^{a} u_j\phi_j' v_s\,dx$$

Setting $u_a' = (p(\omega)+k^2)u_a^{(0)} - u^{(2)}$, multiplying (7) by $(\tilde{s}-1)^2$ and rearranging terms yields

$$\begin{aligned} &\left(s_0^2(\tilde{s}+1)^2 - (\tilde{s}-1)^2(p(\omega)+k^2)\right)U^{(r)} \\ &\qquad = (\tilde{s}-1)^2 u_a' + s_0(\tilde{s}^2-1)u_a. \end{aligned}$$

Inserting the power series (6), sorting for powers of $\tilde{s}$ and comparing coefficients yields equations for the a_j:

$$\left(s_0^2 - p - k^2\right) a_0 = u_a' - s_0 u_a, \tag{8}$$

$$2\left(s_0^2 + p + k^2\right) a_0 + \left(s_0^2 - p - k^2\right) a_1 = -2u_a', \tag{9}$$

$$\begin{aligned} &\left(s_0^2 - p - k^2\right) a_0 + 2\left(s_0^2 + p + k^2\right) a_1 \\ &\quad + \left(s_0^2 - p - k^2\right) a_2 = u_a' + s_0 u_a, \end{aligned} \tag{10}$$

$$\begin{aligned} &\left(s_0^2 - p - k^2\right) a_{\ell-1} + 2\left(s_0^2 + p + k^2\right) a_\ell \\ &\quad + \left(s_0^2 - p - k^2\right) a_{\ell+1} = 0, \quad \ell = 1, \ldots, L \end{aligned} \tag{11}$$

with $a_{L+1} = 0$. Similar equations hold for the left boundary. Transforming back to time-domain equations (8) to (11) yield a system of ordinary differential equations for the coefficients a_j for $j = 1, \ldots, L$.

Take a closer look at (8). If one would choose s_0 to be time or ω dependent, $s_0 = \sqrt{p(\omega) + k^2}$ then (8) is the well-known exact non-local TBC; equations (8) to (11) decouple and all a_ℓ vanish for $\ell \geq 2$. Choosing s_0 to be constant gives local approximate TBCs.

In case of the wave equation (i.e. $p(\omega) = \omega^2$) choosing $s_0 = \omega$ gives local TBCs. In case $k = 0$ this choice gives the exact TBCs.

Numerical results

The numerical results for the wave equation (1) integrated from $t = 0, \ldots, 20$ with an extremely small stepsize of $\Delta t = 10^{-4}$ using the trapezoidal rule are shown below. The computational domain is $[-5, 5]$, $k = 5$, the initial value is a Gaußian $u(x, 0) = \exp(-x^2)$ and the initial velocity is set to zero. Space discretization is done by third order finite elements on an equidistant grid with $\Delta x = 0.002$. The reference solution is calculated on a domain $[-15, 15]$; this way the dominating error component should be the truncation error in the power series representation. Figure 1 shows the evolution of the error in energy norm for different L. Figure 2 shows the error in energy-norm vs. the number of coefficients L in the power series.

Extensions and future work

The concepct is easily extended to systems

$$Mp(\partial_t)u = A\partial_{xx}u + 2D\partial_x u - Ku.$$

with matrices M, A, D and K. These type of systems arise for example for two dimensional problems on a strip $\{(x, y), |y| < b, \infty < x < \infty\}$ after a discretisation of the y component. The extension to general two or three dimensional problems is currently under investigation.

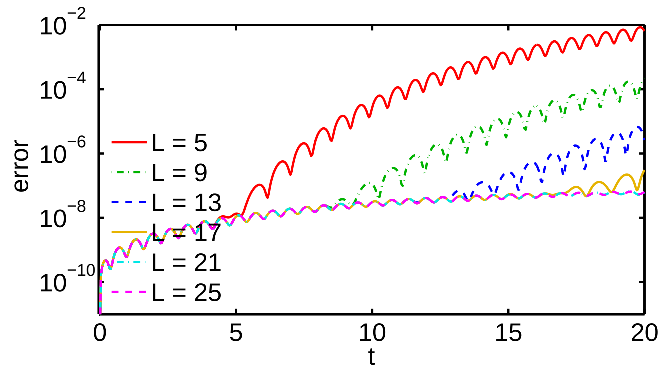

Figure 1: Evolution of the error for different L.

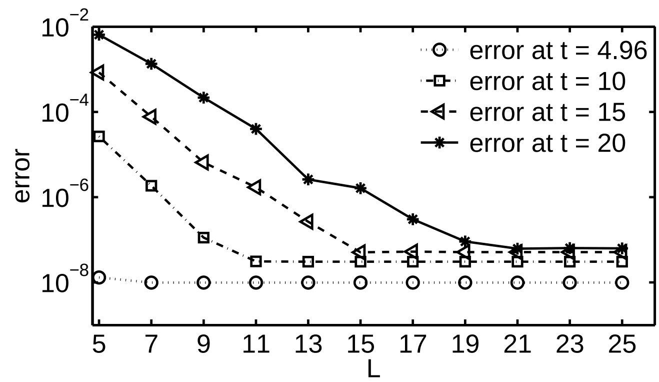

Figure 2: Error vs. L at different t.

References

[1] T. Hagstrom, "Radiation boundary conditions for numerical simulation of waves", Acta Numerica, vol. 8, pp. 47–106, 1999.

[2] T. Hohage, F. Schmidt, and L. Zschiedrich, "Solving Time-Harmonic Scattering Problems Based on the Pole Condition I: Theory", SIAM J. Math. Anal., vol. 35, pp. 183–210, 2003.