The Pole Condition: A Padé Approximation of the Dirichlet to Neumann Operator

Martin J. Gander[1] and Achim Schädle[2]

[1] Mathematics Section, University of Geneva, CH-1211, Geneva, Switzerland, Martin.gander@unige.ch

[2] Mathematisches Institut, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany

1 Introduction

When a problem is posed on an unbounded domain, the domain needs to be truncated in order to perform computations, and the pole condition is a new technique developed over the last few years for this purpose. The subject of domain truncation is already an established research field. It was started in 1977 in a seminal paper by Enquist and Majda [6], where a systematic method to obtain absorbing boundary conditions (ABCs) is introduced for wave propagation phenomena. Absorbing boundary conditions are approximations of transparent boundary conditions (TBCs), which, when used to truncate the unbounded domain, lead by definition precisely to the restriction of the original solution on the unbounded domain. Unfortunately transparent boundary conditions often involve expensive non-local operators and are thus inconvenient. Absorbing boundary conditions became immediately a field of interest of mathematicians in approximation theory, see for example [3, 9]. Recent reviews on non-reflecting or absorbing boundary conditions concerning the wave equation are [8] by Hagstrom and more recently Givoli [7]. Non-reflecting boundary conditions for the transient Schrödinger equation are reviewed by Antoine et al. [1].

For the description of resonances for Schrödinger operators, the exterior complex scaling (ECS) method was introduced by Simon [14] in 1979. In the early nineties, a technique called perfectly matched layers (PMLs) was developed by Bérenger [4]. Here the idea is to add a layer just outside where the domain is truncated. In this layer, a modified equation is solved, which can be interpreted as an area with different artificial material, which absorbs outgoing waves, without creating reflections. The PML can be interpreted as a complex coordinate stretching in the layer, by which the original equation is transformed into a new one with appropriate properties, see [5, 15]. Hence it is equivalent to ECS.

Absorbing boundary conditions and perfectly matched layers are two competing techniques with the same purpose, namely to truncate an unbounded domain for computational purposes. In 2003, a new technique for the derivation and approximation of transparent boundary conditions was proposed by Schmidt, Hohage and Zschiedrich [11], based on the so called pole condition:

> "The pole condition is a general concept for the theoretical analysis and the numerical solution of a variety of wave propagation problems. It says that the Laplace transform of the physical solution in the radial direction has no poles in the lower complex half-plane."

The pole condition leads to a numerical method for domain truncation which is easy to implement and has shown great promise in numerical experiments for a variety of problems, see [10, 12, 13]. We show in this paper for a model problem of diffusive nature an error estimate for the numerical method based on the pole condition: the domain truncation achieved is a Padé approximation of the transparent boundary condition.

2 Model Problem

We consider on the domain $\Omega_g := \mathbb{R} \times (0, \pi)$ the elliptic model problem

$$\begin{aligned} (\eta - \Delta)u = f \ \text{ in } \Omega_g, \\ u(x, 0) = u(x, \pi) = 0, \end{aligned} \tag{1}$$

where $\eta > 0$, and we seek bounded solutions. For an illustration, see Fig. 1. In order

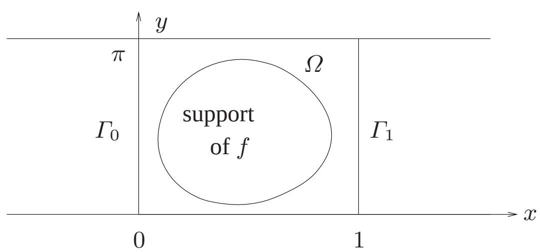

Fig. 1. Domain and support of f.

to perform computations on this problem, we truncate the domain in the unbounded x-direction. We assume that f is compactly supported in $\Omega := (0, 1) \times (0, \pi)$, which suggests to truncate the domain along $\Gamma_j = j \times (0, \pi)$, $j = 0, 1$, see Fig. 1, using an artificial boundary conditions of the form

$$\mathcal{B}_0(u)(0) = 0, \quad \mathcal{B}_1(u)(1) = 0. \tag{2}$$

Expanding the solution u in eigenmodes in the y direction, which in our case is a sine-expansion for constant η and the homogeneous Dirichlet conditions at the top and bottom, yields

$$\begin{aligned} (\eta - \partial_{xx} + k^2)\hat{u} = \hat{f}, \\ \beta_0 \hat{u}(0) = 0, \quad \beta_1 \hat{u}(1) = 0, \end{aligned} \tag{3}$$

where β_j, $j = 0, 1$ are the symbols of the artificial boundary conditions, and $\hat{f} = \mathcal{F}(f)$ denotes the sine transform of f. A direct calculation shows that if $\beta_j = \partial_n + \sqrt{\eta + k^2}$, the truncated solution and the global solution restricted to Ω coincide, and therefore the exact or transparent boundary conditions (TBCs) are

$$\partial_n \hat{u}(0,k) + \sqrt{\eta + k^2}\hat{u}(0,k) = 0, \quad \partial_n \hat{u}(1,k) + \sqrt{\eta + k^2}\hat{u}(1,k) = 0, \tag{4}$$

and we see the well known Dirichlet to Neumann operator $\mathcal{F}^{-1}(\sqrt{\eta + k^2})$ appear. In order to obtain an absorbing boundary condition, one could therefore approximate the square root either by a polynomial or a rational function.

3 The Pole Condition

In order to explain the pole condition, we follow the quote above and perform now a Laplace transform in the radial direction, which in our case is the x direction, with dual variable $\tilde{s}$, and obtain on the right boundary

$$(\eta + k^2 - \tilde{s}^2)U(\tilde{s},k) + \partial_n \hat{u}(1,k) + \tilde{s}\hat{u}(1,k) = 0, \tag{5}$$

and a similar result on the left of the interface Γ_0. Solving for U, we obtain

$$U(\tilde{s},k) = -\frac{\partial_n \hat{u} + \tilde{s}\hat{u}}{\eta + k^2 - \tilde{s}^2}, \tag{6}$$

and thus $U(\tilde{s},k)$ has two singularities (poles), at $\tilde{s} = \pm\sqrt{\eta + k^2}$. When looking outward from the computational domain, we are interested in bounded solutions, and hence the singularities in the right half plane $\mathbb{R}(\tilde{s}) > 0$ are undesirable, as they correspond to exponentially increasing solutions. Using a partial fraction decomposition, we find

$$U(\tilde{s},k) = \frac{\hat{u}(1,k) - \frac{\partial_n \hat{u}(1,k)}{\sqrt{\eta+k^2}}}{2(\tilde{s} + \sqrt{\eta + k^2})} + \frac{\hat{u}(1,k) + \frac{\partial_n \hat{u}(1,k)}{\sqrt{\eta+k^2}}}{2(\tilde{s} - \sqrt{\eta + k^2})}, \tag{7}$$

and we see again that if $\hat{u}$ satisfies the TBC (4), the undesirable pole represented by the second term of (7) is not present, since the numerator vanishes identically. The key idea of the pole condition is to enforce that the second term can not be present, by imposing analyticity of $U(\tilde{s},k)$ in the right half of the complex plane $\mathbb{R}(\tilde{s}) > 0$. In order to do so, it is convenient to first use the Möbius transform M_{s_0} for $s_0 \in \mathbb{C}$ with positive real part, see Fig. 2, and map the right half plane into the unit circle,

$$M_{s_0} : \tilde{s} \mapsto s = \frac{\tilde{s} - s_0}{\tilde{s} + s_0}, \qquad M_{s_0}^{-1} : s \mapsto \tilde{s} = -s_0\frac{s+1}{s-1}.$$

We now exclude singularities of the solution $U(\tilde{s},k)$ in the right half of the complex plane by enforcing the representation of U in the new variable s by the power-series

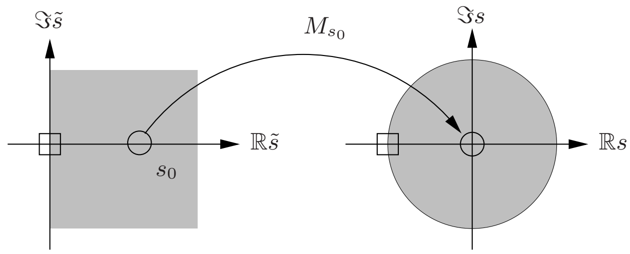

Fig. 2. Möbius transform.

$$U(s,k) = \frac{s-1}{2s_0}\Big((s-1)\sum_{n=0}^{\infty} a_n s^n - \hat{u}\Big). \tag{8}$$

We chose this particular ansatz, because it satisfies automatically the condition from Laplace transform theory that if $\hat{u}$ exists, we must have

$$\lim_{\tilde{s}\to\infty} \tilde{s}U(\tilde{s},k) = \lim_{s\to 1} -s_0\frac{s+1}{s-1}U(s,k) = \hat{u}(1,k).$$

To simplify the notation, we set $\tilde{\eta} := \eta + k^2$ in what follows. Inserting the power-series expansion (8) into Eq. (5), and collecting terms, we obtain

$$\left(\frac{\tilde{\eta}(s-1)^2}{2s_0} - \frac{s_0(s+1)^2}{2}\right)\sum_{n=0}^{\infty} a_n s^n = \left(\frac{\tilde{\eta}(s-1)}{2s_0} - s_0\frac{s+1}{2} - \partial_\nu\right)\hat{u}(1,k). \tag{9}$$

Matching powers of s, we obtain the equations for the power series coefficients a_n,

$$\left(\tilde{\eta} - s_0^2\right) a_0 + \left(s_0^2 + \tilde{\eta}\right)\hat{u}(1,k) = -2s_0\partial_\nu\hat{u}(1,k), \tag{10}$$

$$\left(\tilde{\eta} - s_0^2\right) a_1 - 2\left(\tilde{\eta} + s_0^2\right) a_0 - \left(\tilde{\eta} - s_0^2\right)\hat{u}(1,k) = 0, \tag{11}$$

$$\left(\tilde{\eta} - s_0^2\right) a_{n+1} - 2\left(\tilde{\eta} + s_0^2\right) a_n + \left(\tilde{\eta} - s_0^2\right) a_{n-1} = 0, \quad n = 1,\dots L-2, \tag{12}$$

$$-2\left(\tilde{\eta} + s_0^2\right) a_{L-1} + \left(\tilde{\eta} - s_0^2\right) a_{L-2} = 0, \tag{13}$$

where we truncated the power series expansion at the L-th term. We observe that the expansion coefficients satisfy a three term recurrence relation similar to the relation satisfied by the original solution in the x direction, when a five point finite difference stencil is used for the discretization, and since the expansion coefficients depend on k, and $\tilde{\eta} = \eta + k^2$, the recurrence relation shows that the expansion coefficients also satisfy a second order differential equation in the y direction. This permits an easy implementation of the expansion coefficients on the same grid as the solution, as illustrated in Fig. 3, and is the reason why it is so easy to use the pole condition truncation. Note that this is the same system of equations for the a_n as obtained using a Galerkin ansatz in the Hardyspace of the unit disc by Hohage and Nannen [10].

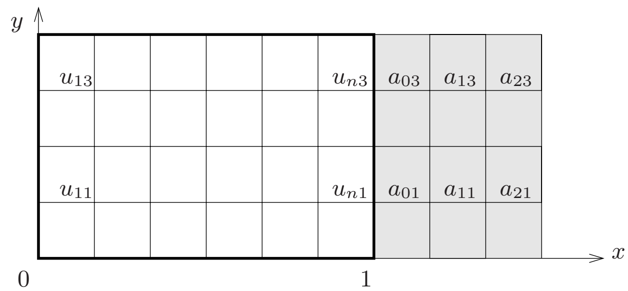

Fig. 3. Implementation of the expansion coefficients on the same grid as the interior unknowns.

4 Error Estimate

In order to gain insight into the approximation we obtain from the truncation at the L-th term, we define

$$b := \frac{\tilde{\eta} + s_0^2}{\tilde{\eta} - s_0^2} = \frac{\eta + k^2 + s_0^2}{\eta + k^2 - s_0^2}, \tag{14}$$

and we start resolving the recurrence relation from the last term (13), which implies

$$a_{L-1} = \frac{1}{2b} a_{L-2}.$$

Using this result and (12) for $n = L - 2$ then gives

$$a_{L-2} = \frac{1}{2b - \frac{1}{2b}} a_{L-3} = \frac{1}{2b-} \frac{1}{2b} a_{L-3},$$

and continuing like this, we arrive when using (12) for $n = 1$ at

$$a_1 = a_0 \frac{1}{2b - \frac{1}{2b - \dots \frac{1}{2b}}} = a_0 \frac{1}{2b-} \frac{1}{2b-} \frac{1}{2b-} \dots \frac{1}{2b} = \sum_{n=1}^{L-1} \frac{1}{2b-},$$

a truncated continued fraction expansion. Using now (11) and (10), and rearranging terms, we obtain the representation of the approximate operator which is defined by the pole condition, namely

$$\partial_\nu \hat{u}(1,k) + \frac{\eta + k^2 - s_0^2}{2s_0} \left(b - \sum_{n=1}^{L} \frac{1}{2b-} \right) \hat{u}(1,k) = 0. \tag{15}$$

Comparing this relation with the TBC from (4), we see that the term containing the continued fraction expansion must represent an approximation of the DtN operator $\sqrt{\eta + k^2}$.

Theorem 1. *If the truncation level L of the continued fraction expansion (15) is going to infinity, it represents the exact Dirichlet to Neumann operator,*

$$\frac{\eta + k^2 - s_0^2}{2s_0}\left(b - \sum_{n=1}^{\infty}\frac{1}{2b-}\right)\hat{u}(1,k) = \sqrt{\eta + k^2}\hat{u}(1,k) = -\partial_\nu \hat{u}(1,k), \tag{16}$$

independently of the expansion point s_0, and therefore the truncation condition obtained from the pole condition converges to the TBC.

Proof. The continued fraction in (16) maybe rewritten as

$$b - \sum_{n=1}^{\infty}\frac{1}{2b-} = b - \frac{1}{2b - \frac{1}{x}} \quad \text{with} \quad x = 2b - \frac{1}{x}. \tag{17}$$

The roots of $x^2 - 2bx + 1$ are $x_{1,2} = \pm\sqrt{b^2 - 1} + b$. Inserting $x = \sqrt{b^2 - 1} + b$ into (17), and using the identity

$$b - \frac{1}{b + \sqrt{b^2 - 1}} = \sqrt{b^2 - 1},$$

we find from (15) and using the definition for b in (14) that

$$\frac{\eta + k^2 - s_0^2}{2s_0}\left(\left(\frac{\eta + k^2 + s_0^2}{\eta + k^2 - s_0^2}\right)^2 - 1\right)^{\frac{1}{2}}\hat{u} = -\partial_\nu \hat{u},$$

which can be simplified to give the result. □

We are now interested in obtaining an error estimate if the power series is truncated at the L-th term. To this end, we use the following well known result for truncated continued fraction expansions.

Theorem 2 (Sect. 4 [2]). *The L-th truncated continued fraction expansion can be represented by*

$$a_0 + \sum_{n=1}^{L}\frac{b_n}{a_n +} = \frac{A_L}{B_L},$$

where A_n and B_n are defined by the recurrence relations

$$\begin{aligned} A_{-1} = 1,\ A_0 = a_0, \quad & A_{n+1} = a_{n+1}A_n + b_{n+1}A_{n-1}, \\ B_{-1} = 0,\ B_0 = 1, \quad & B_{n+1} = a_{n+1}B_n + b_{n+1}B_{n-1}. \end{aligned} \tag{18}$$

In what follows we will call $(a_n)_n$ the denominator sequence and $(b_n)_n$ the numerator sequence.

Theorem 3. *The truncated recurrence relation (10), (11), (12) and (13) from the pole condition represents an (L+1,L)-Padé approximation of the symbol of the DtN operator $s_0\sqrt{1+z}$ about $z = 0$, where $z = \frac{\eta + k^2 - s_0^2}{s_0^2}$.*

Proof. The Padé approximation of $(1+z)^{\frac{1}{2}}$ expanded at $z=0$ is given by the continued fraction

$$(1+z)^{\frac{1}{2}} = 1 + \frac{\frac{1}{2}z}{1+}\frac{\frac{1}{2}z}{2+}\frac{\frac{1}{2}z}{1+}\frac{\frac{1}{2}z}{2+}\dots .$$

Hence the denominator sequence is $a_0 = 1$ and $a_n = \frac{3+(-1)^n}{2}$, $n \geq 1$, whereas the numerator sequence is given by $b_n = \frac{1}{2}z$, see [2], equation (6.4) on page 139. Using Theorem 2, the L-th approximation is given by the fraction of A_L and B_L. Using the recurrence relations (18) with leading terms $2n+1$, $2n$, and $2n-1$, the even terms can be eliminated to give

$$\begin{aligned} &A_{-1} = 1,\ A_1 = \tfrac{z+2}{2},\ A_{2n+1} = (2+z)A_{2n-1} - \tfrac{z^2}{4}A_{2n-3}, \\ &B_{-1} = 0,\ B_1 = 1, \quad\ \ B_{2n+1} = (2+z)B_{2n-1} - \tfrac{z^2}{4}B_{2n-3}. \end{aligned} \tag{19}$$

Using the variable $z = \frac{\eta+k^2-s_0^2}{s_0^2}$ in the continued fraction representation for the square root stemming from the pole condition (15), we find that the denominator sequence is

$$c_0 = \frac{\eta + k^2 + s_0^2}{2s_0} = s_0\frac{z+2}{2},\ c_n = 2\frac{\eta+k^2+s_0^2}{\eta+k^2-s_0^2} = \frac{2(2+z)}{z}, \quad \text{for } n \geq 1,$$

and the numerator sequence is

$$d_1 = -\frac{\eta+k^2-s_0^2}{2s_0} = -s_0\frac{z}{2},\ d_n = -1, \quad \text{for } n \geq 2.$$

Using again Theorem 2, the L-th approximation is given by the fraction of C_L and D_L, which are given by

$$\begin{aligned} &C_{-1} = 1,\ C_0 = s_0\tfrac{z+2}{2},\ C_1 = s_0(\tfrac{z}{2}+4+\tfrac{4}{z}),\ C_{n+1} = \tfrac{2(2+z)}{z}C_n - C_{n-1}, \\ &D_{-1} = 0,\ D_0 = 1, \qquad D_1 = \tfrac{2}{z}(2+z), \qquad D_{n+1} = \tfrac{2(2+z)}{z}D_n - D_{n-1}. \end{aligned}$$

If we define $\tilde{C}_n := (z/2)^n C_n$, $\tilde{D}_n := (z/2)^n D_n$, we obtain for $n \geq 0$

$$\begin{aligned} &\tilde{C}_0 = s_0\tfrac{z+2}{2},\ \tilde{C}_1 = s_0\tfrac{z}{2}(\tfrac{z}{2}+4+\tfrac{4}{z}),\ \tilde{C}_{n+1} = (2+z)\tilde{C}_n - \tfrac{z^2}{4}\tilde{C}_{n-1}, \\ &\tilde{D}_0 = 1, \qquad \tilde{D}_1 = 2+z, \qquad \tilde{D}_{n+1} = (2+z)\tilde{D}_n - \tfrac{z^2}{4}\tilde{D}_{n-1}, \end{aligned} \tag{20}$$

which is the same recurrence as (19). Since $\tilde{C}_0 = s_0 A_1$, $\tilde{C}_1 = s_0 A_3$, $\tilde{D}_0 = B_1$ and $\tilde{D}_1 = B_3$, the proof is complete. □

References

1. X. Antoine, A. Arnold, C. Besse, M. Ehrhardt, and A. Schädle. A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations. *Commun. Comput. Phys.*, 4(4):729–796, 2008.

2. G.A. Baker. *Padé Approximants Part I: Basic Theory*. Encyclopedia of Mathematics and Its Applications. Addison-Wesley, Reading, MA, 1981.
3. A. Bayliss and E. Turkel. Radiation boundary conditions for wave-like equations. *Commun. Pure Appl. Math.*, 33(6):707–725, 1988.
4. J.P. Bérenger. A perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Phys.*, 114(2):185–200, 1994.
5. W.C. Chew and W.H. Weedon. A 3d perfectly matched medium from modified Maxwell's equations with stretched coordinates. *Microwave Opt. Technol. Lett.*, 7(13):599–604, 1994.
6. B. Engquist and A. Majda. Absorbing boundary conditions for the numerical simulation of waves. *Math. Comput.*, 31(139):629–651, 1977.
7. D. Givoli. High-order local non-reflecting boundary conditions: a review. *Wave Motion*, 39(4):319–326, 2004.
8. T. Hagstrom. Radiation boundary conditions for the numerical simulation of waves. *Acta Numer.*, 8:47–106, 1999.
9. L. Halpern. Absorbing boundary conditions for the discretization schemes of the one-dimensional wave equation. *Math. Comput.*, 38(158):415–429, 1982.
10. T. Hohage and L. Nannen. Hardy space infinite elements for scattering and resonance problems. *SIAM J. Numer. Anal.*, 47:972–996, 2009.
11. T. Hohage, F. Schmidt, and L. Zschiedrich. Solving time-harmonic scattering problems based on the pole condition. I: Theory. *SIAM J. Math. Anal.*, 35:183–210, 2003.
12. D. Ruprecht, A. Schädle, F. Schmidt, and L. Zschiedrich. Transparent boundary conditions for time-dependent problems. *SIAM J. Sci. Comput.*, 30:2358–2385, 2008.
13. F. Schmidt, T. Hohage, R. Klose, A. Schädle, and L. Zschiedrich. Pole condition: A numerical method for Helmholtz-type scattering problems with inhomogeneous exterior domain. *J. Comput. Appl. Math.*, 218(1):61–69, 2008.
14. B. Simon. The definition of molecular resonance curves by the method of exterior complex scaling. *Phys. Lett.*, 71A(2,3):211–214, 1979.
15. F.L. Teixeira and W.C. Chew. General closed-form PML constitutive tensors to match arbitrary bianisotropic and dispersive linear media. *IEEE Microwave Guided Wave Lett.*, 8(6):223–225, 1998.