Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Linear Algebra and its Applications 415 (2006) 455–468
LINEAR ALGEBRA AND ITS APPLICATIONS
www.elsevier.com/locate/laa

Low order approximation of the spherical nonreflecting boundary kernel for the wave equation☆

Jing-Rebecca Li *

Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, NY 10012-1110, USA

Received 2 May 2003; accepted 1 October 2003
Available online 9 December 2003
Submitted by P. Benner

Abstract

We find low order approximations to the spherical nonreflecting boundary kernel for the wave equation in three dimensions. First we express the Laplace transform of the kernel as a rational function by solving for the zeros of a modified Bessel function. Then we formulate a linear time-invariant dynamical system whose transfer function is this rational function. Finally we use the Balanced Truncation method to generate low order approximations. We compare our approach with a direct L^2 minimization approach where a rational approximation is expressed as the ratio of two polynomials.

Keywords: Nonreflecting boundary condition; Rational approximation

☆ The work of this author was supported by the US Department of Energy under grant DE-FGO2-00ER25053 and by the National Science Foundation under grant DMS-9983190.

* Present address: Projet Ondes INRIA, Domaine de Voluceau—Rocquencourt, B.P. 105, Le Chesnay Cedex 78153, France. Tel.: +33 1 39 63 53 55; fax: +33 1 39 63 58 84.
E-mail addresses: jingrebecca.li@inria.fr, jingli@cims.nyu.edu

0024-3795/$ - see front matter
doi:10.1016/j.laa.2003.10.020

1. Introduction

When solving the wave equation in an unbounded domain, one can impose a nonreflecting boundary condition on an artificial boundary to produce a finite computational domain. Simple examples of an artificial boundary are a circle in two dimensions and a sphere in three dimensions. There are many approaches for these two boundaries which begin with an *exact* nonreflecting boundary condition, including [7,8,13]. This condition can be couched in terms of what has been referred to in [2] as a nonreflecting boundary kernel, which is simply the inverse Laplace transform of an expression that includes the logarithmic derivative of a modified Bessel function, of whole order for the circular boundary, and of half order for the spherical boundary. Approximating this expression by a low order rational function, expressed as a sum of poles, means that the kernel can be approximated by a sum of exponentials. This representation allows the convolution integral in the nonreflecting boundary condition to be evaluated recursively (in history) at great savings in computation and storage.

In [2] low order rational approximations were found by L^2 minimization on the polynomials in the numerator and the denominator of a rational approximation. However, in three dimensions, another approach is possible because the Laplace transform of the spherical nonreflecting boundary kernel is exactly a rational function (of possibly high order). The problem of approximating a high order rational function by a low order one can be approached from the point of view of linear time-invariant model reduction, which is a mature field with a large body of literature [3,6,11]. A rational function can be formulated as the transfer function of a linear time-invariant dynamical system and model reduction is the approximation of the original system by a smaller one whose transfer function approximates that of the original. In particular, Balanced Truncation [11] is a method which produces a low order system whose transfer function has several good properties. One is that there is a L^∞ bound on the approximation error, which in turn can be used to bound the L^2 error in the convolution integral with the approximate kernel. Another is that if all the poles of the original system are stable, then so are all the poles of the reduced system. Stability preservation is highly desirable for the application of nonreflecting boundary conditions.

Our approach consists of finding all the zeros of a half order modified Bessel function to set up a linear time-invariant dynamical system whose transfer function is the Laplace transform of the spherical nonreflecting boundary kernel, performing Balanced Truncation to produce a reduced system, and finding a sum of poles representation for the transfer function of the reduced system, which is our low order approximation.

We will compare our approach to the direct L^2 minimization approach used in [2]. We show that for a given order of reduction our approach in general produces a better approximation (with smaller L^∞ error) than the L^2 minimization approach. Moreover, our approach is able to produce higher order (more accurate) approximations (represented as a sum of poles) when the L^2 minimization approach failed to produce a sum of poles representation from a ratio of polynomials. However, we

note that our approach cannot be directly applied to the circular boundary in two dimensions because the Laplace transform of the circular kernel (involving a whole order modified Bessel function) is not a rational function. In this case the approach of [2] can be used with good results.

This paper is organized as follows. Section 2 motivates the low order approximation of the nonreflecting boundary kernels for the wave equation. Section 3 describes how to obtain a representation of the Laplace transform of the spherical kernel as a sum of poles. Section 4 transforms the sum of poles representation into the transfer function of a linear dynamical system and uses Balance Truncation to obtain low order approximations. Section 5 gives numerical results and makes comparison with the direct L^2 minimization approach used in [2]. Section 6 contains the conclusions.

2. Low order approximation of nonreflecting boundary kernels

Consider the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u$$

in two and three dimensions. The general solution can be expressed as

$$\begin{aligned} u(\rho, \phi, t) &= \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}n\phi} u_n(\rho, t) \\ &= \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}n\phi} \mathscr{L}^{-1}\left[a_n(s) K_n\left(\frac{\rho s}{c}\right) + b_n(s) I_n\left(\frac{\rho s}{c}\right)\right](t) \end{aligned} \tag{1}$$

in polar coordinates in two dimensions and

$$\begin{aligned} u(\rho, \phi, \theta, t) &= \sum_{n=-\infty}^{\infty} \sum_{m=-n}^{n} Y_{nm}(\phi, \theta) u_{nm}(\rho, t) \\ &= \sum_{n=-\infty}^{\infty} \sum_{m=-n}^{n} Y_{nm}(\phi, \theta) \\ &\quad \times \mathscr{L}^{-1}\left[a_{nm}(s) \frac{K_{n+\frac{1}{2}}(\rho s/c)}{\sqrt{\rho s/c}} + b_{nm}(s) \frac{I_{n+\frac{1}{2}}(\rho s/c)}{\sqrt{\rho s/c}}\right](t) \end{aligned} \tag{2}$$

in spherical coordinates in three dimensions, where K_ν and I_ν are modified Bessel functions. If $\rho = \rho_1$ is to be used as a nonreflecting boundary, we can assume that there are no sources outside of $\rho = \rho_1$ and so the coefficients $b_n(s)$ (or $b_{nm}(s)$) are zero. In two dimensions, the nonreflecting boundary condition on each coefficient function $u_n(\rho, t)$ at $\rho = \rho_1$ is

$$\frac{\partial}{\partial\rho}u_n(\rho,t)+\frac{1}{c}\frac{\partial}{\partial t}u_n(\rho,t)+\frac{1}{2\rho}u_n(\rho,t)=\int_0^t\sigma_n(t-\tau)u_n(\rho,\tau)\,\mathrm{d}\tau, \tag{3}$$

where

$$\sigma_n(t)=\mathscr{L}^{-1}\left[\frac{s}{c}+\frac{1}{2\rho}+\frac{s}{c}\frac{K_n'(\rho s/c)}{K_n(\rho s/c)}\right](t). \tag{4}$$

In three dimensions, the nonreflecting boundary condition on the coefficient function $u_{nm}(\rho,t)$ at $\rho=\rho_1$ is

$$\frac{\partial}{\partial\rho}u_{nm}(\rho,t)+\frac{1}{c}\frac{\partial}{\partial t}u_{nm}(\rho,t)+\frac{1}{\rho}u_{nm}(\rho,t)=\int_0^t\omega_n(t-\tau)u_{nm}(\rho,\tau)\,\mathrm{d}\tau, \tag{5}$$

where

$$\omega_n(t)=\mathscr{L}^{-1}\left[\frac{s}{c}+\frac{1}{2\rho}+\frac{s}{c}\frac{K'_{n+\frac{1}{2}}(\rho s/c)}{K_{n+\frac{1}{2}}(\rho s/c)}\right](t). \tag{6}$$

If the expressions inside the inverse Laplace transform in (4) and (6) can be approximated by a rational function then the nonreflecting boundary kernels $\sigma_n(t)$ and $\omega_n(t)$ can be approximated by a sum of exponentials. The advantage of evaluating the convolution integrals on the right-hand side of (3) and (5) when the kernel is a sum of exponentials is that the integral can be done recursively in history. For example, in two dimensions for the exponential $\mathrm{e}^{q_l t}$, the integral in (3) can be written as

$$\begin{aligned}\int_0^t \mathrm{e}^{q_l(t-\tau)}u_n(\rho,\tau)\,\mathrm{d}\tau &= \mathrm{e}^{q_l\Delta t}\int_0^{t-\Delta t}\mathrm{e}^{q_l(t-\Delta t-\tau)}u_n(\rho,\tau)\,\mathrm{d}\tau\\ &\quad+\int_{t-\Delta t}^t \mathrm{e}^{q_l(t-\tau)}u_n(\rho,\tau)\,\mathrm{d}\tau.\end{aligned} \tag{7}$$

Thus, at each time step, the first quantity on the right-hand side is already available from the previous time step and only the second integral, which is local in time, needs to be computed. The work required to compute the convolution integral in the nonreflecting boundary condition for K time steps is $\mathrm{O}(K)$ due to the splitting of the integral into a history and a local part (compared to $\mathrm{O}(K^2)$ if the integral from 0 to t must be recomputed at each time step).

In a wave propagation problem, one truncates the infinite expansion in (1) or (2) after a finite number of terms and we want to approximate the kernel $\sigma_n(t)$ or $\omega_n(t)$ by

$$\mathscr{L}^{-1}\left[\sum_{l=1}^r\frac{p_l}{s-q_l}\right](t)=\sum_{l=1}^r p_l\mathrm{e}^{q_l t} \tag{8}$$

for all needed terms n. Clearly, a rational approximation needs to be given in the sum of poles form in order to be useful. The size of the approximation in (8) to

achieve a given error tolerance of course may be different for different n. Typically, it is adequate for most applications to have O(1000) discretization points on the artificial boundary, so we are most interested in approximating $\sigma_n(t)$ and $\omega_n(t)$ for $n \leqslant 1000$.

We are primarily interested in the accuracy of the low order approximations rather than the complexity of the work required to generate them because we assume that these approximations are to be precomputed and stored. Once approximations to kernels of up to a certain order have been obtained, they may be used for any wave propagation problem which uses an expansion of no higher than that order. Since obtaining the low order approximations only needs to be done one time, the work required to generate them is not an important factor. It is entirely separate from the simulation part. Nevertheless, in Section 5 we give the work required to generate low order approximations.

The L^2 error in the convolution with an approximate kernel is bounded by the L^∞ error in the Laplace transform:

$$\|\sigma * v - \alpha * v\|_2 \leqslant \left(\sup_{s\in \mathrm{i}\mathbb{R}} |\hat{\sigma} - \hat{\alpha}|\right) \|v\|_2. \tag{9}$$

3. Spherical nonreflecting boundary kernel

Now we focus on the spherical nonreflecting boundary kernel in three dimensions. It was shown in [2] that the expression inside the inverse Laplace transform in (6) (taking $\rho = 1$ and $c = 1$) is a proper rational function of the form:

$$f(z) := z + \frac{1}{2} + z\frac{K'_{n+\frac{1}{2}}(z)}{K_{n+\frac{1}{2}}(z)} = \sum_{l=1}^{n} \frac{k_{n+\frac{1}{2},l}}{z - k_{n+\frac{1}{2},l}}, \tag{10}$$

where $k_{n+\frac{1}{2},1}, \ldots, k_{n+\frac{1}{2},n}$ are the zeros of $K_{n+\frac{1}{2}}(z)$, which number exactly n and lie on an arc in the open left half plane (see Fig. 1). The zeros have strictly negative real parts and are distributed symmetrically about the real axis. The intersections of the arc with the axes are $(0, -n)$, $(-na, 0)$, and $(0, n)$, where $a \approx 0.66274$ (see [1]). The zeros closest to the imaginary axis are

$$k_{n+\frac{1}{2},1} \sim z_0 := \mathrm{i}\left(n + \frac{1}{2}\right) + \left(\cos\frac{5\pi}{6} + \mathrm{i}\sin\frac{5\pi}{6}\right)\left(\frac{n+\frac{1}{2}}{2}\right)^{\frac{1}{3}}(-a_1),$$
$$-a_1 \approx 2.338, \tag{11}$$

and its complex conjugate.

Clearly (10) gives an exact (in infinite precision arithmetic) sum of poles representation for the Laplace transform of the spherical nonreflecting kernel. We only

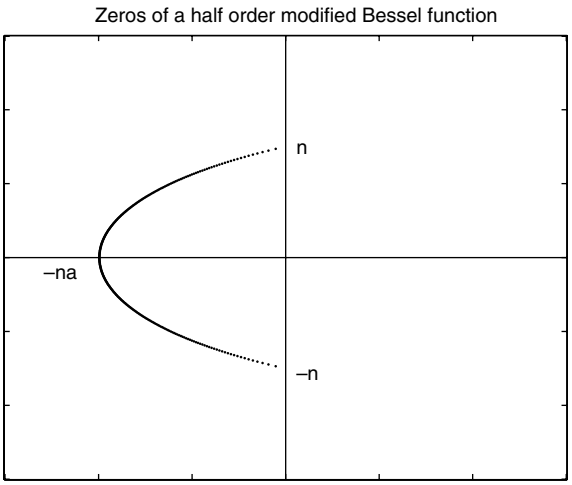


Fig. 1. Zeros of a half order modified Bessel function.

need to find all n zeros of $K_{n+\frac{1}{2}}(z)$. We do this by using the routine nag_nlin_sys provided by the NAG Fortran 90 Library which solves for a root of a system of nonlinear equations given an initial guess. The initial guesses need to be carefully chosen to find all n zeros. We describe this procedure in Algorithm 1. The idea is that if not all the zeros are found in one sweep of the curve in Fig. 1 then the curve is fitted more accurately using the zeros which have already been found. This algorithm successfully found all n zeros of $K_{n+\frac{1}{2}}(z)$ for any $n \leqslant 1000$ in negligible time.

We seek to approximate $f(z)$ by a low order rational function to within a given error tolerance. The number of terms needed in the approximation depends on n and on the error tolerance.

4. Model reduction

Transforming the sum of poles representation in (10) into the transfer function of a linear dynamical system is simple. We assume the poles are ordered as

$$k_{n+\frac{1}{2},1}, \ldots, k_{n+\frac{1}{2},n2}, k_{n+\frac{1}{2},n2+1}, \overline{k_{n+\frac{1}{2},n-n2}}, \ldots, \overline{k_{n+\frac{1}{2},1}},$$

where $n2 := \text{floor}\,\frac{n}{2}$ and the real pole $k_{n+\frac{1}{2},n2+1}$ does not appear if n is even. We define a linear dynamical system ($A \in \mathbb{R}^{n\times n}, b \in \mathbb{R}^{n\times 1}, c \in \mathbb{R}^{1\times n}$) with transfer function

$$c(zI - A)^{-1}b = \sum_{l=1}^{n} \frac{k_{n+\frac{1}{2},l}}{z - k_{n+\frac{1}{2},l}},$$

where the matrices are

$$c = (1 \quad \cdots \quad 1 \quad 1),$$

$$A = \begin{bmatrix} A_{11} & 0 & \cdots & & 0 & 0 \\ 0 & \ddots & & & & \vdots \\ \vdots & \ddots & A_{ii} & \ddots & \vdots & \\ & & & \ddots & 0 & \vdots \\ 0 & & \cdots & 0 & A_{n2n2} & 0 \\ 0 & \cdots & & \cdots & 0 & A_{(n2+1)(n2+1)} \end{bmatrix}, \tag{12}$$

$$b = \begin{pmatrix} b_1 \\ \vdots \\ b_{n2} \\ b_{n2+1} \end{pmatrix},$$

and

$$A_{ii} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad a_{11} = \operatorname{Re} k_{n+\frac{1}{2},i}, \quad a_{22} = a_{11},$$

$$a_{21} = \sqrt{-a_{11}a_{22} + \left(k_{n+\frac{1}{2},i}\right)\left(\overline{k_{n+\frac{1}{2},i}}\right)}, \quad a_{12} = -a_{21},$$

$$b_i = \begin{pmatrix} 1 & 1 \\ -a_{22} + a_{21} & -a_{11} + a_{12} \end{pmatrix}^{-1} \begin{pmatrix} 2\operatorname{Re} k_{n+\frac{1}{2},i} \\ -2\operatorname{Re} k_{n+\frac{1}{2},i}\left(\overline{k_{n+\frac{1}{2},i}}\right) \end{pmatrix}.$$

The quantities

$$A_{(n2+1)(n2+1)} = k_{n+\frac{1}{2},n2+1}, \quad b_{n2+1} = k_{n+\frac{1}{2},n2+1}$$

do not appear if n is even. The linear dynamical system with the coefficient matrices in (12) can be reduced using Balanced Truncation [11] and we use the Square Root method [12,14] to implement it. We obtain ($A_r \in \mathbb{R}^{r\times r}$, $b_r \in \mathbb{R}^{r\times 1}$, $c_r \in \mathbb{R}^{1\times r}$) so that the transfer function of the reduced system approximates that of the original. There is a L^∞ error bound on the transfer function approximation:

$$\sup_{s=\mathrm{i}\mathbb{R}} \left|c_r(sI - A_r)^{-1}b_r - c(sI - A)^{-1}b\right| \leqslant 2\sum_{l=r+1}^{n} \sigma_l,$$

where $\sigma_1, \ldots, \sigma_n$ are the Hankel singular values of the original system in (12) which can be obtained by solving two matrix equations involving A, b, and c (see [3,11]). This quantity can be used to bound the L^2 error in the convolution integral according to (9).

A sum of poles representation of $c_r(zI - A_r)^{-1}b_r$ can be obtained by diagonalizing A_r. Let $A_r = TDT^{-1}$ be the eigendecomposition of A_r and we define $\tilde{c} := c_r T$, $\tilde{b} := T^{-1}b_r$, then

$$q_l = D(l,l), \quad p_l = \tilde{c}_l\tilde{b}_l, \quad l = 1,\ldots,r, \tag{13}$$

are the poles and the residues of the rational approximation, respectively.

5. Numerical results

In this section we give numerical results and make comparison with the approach used in [2] where the following L^2 minimization problem was posed:

$$\min_{P,Q}\int_{-\infty}^{\infty}\left|\frac{P(\mathrm{i}w)}{Q(\mathrm{i}w)} - \left(\mathrm{i}w - \frac{1}{2} + \mathrm{i}w\frac{K'_{n+\frac{1}{2}}(\mathrm{i}w)}{K_{n+\frac{1}{2}}(\mathrm{i}w)}\right)\right|^2 \mathrm{d}w. \tag{14}$$

The algorithm used in [2] to solve (14) to within a given error tolerance is rather involved and we do not give details here. The authors of that paper made their code available to us and we used it to generate the approximations with which we compare ours in this section. In that approach, after the solution of (14), a sum of poles representation was obtained by finding the zeros of $Q(x)$ using Newton iteration and then computing the residues using recurrence relations. We note that finding all the zeros of $Q(x)$ from the monomial coefficients (given recursively in the approach of [2]) failed when the polynomial degree was relatively large ($r \geqslant 30$). On the other hand, finding the eigendecomposition of A_r to compute poles and residues via (13) did not fail in any of the numerical experiments.

Another difference in the two approaches involves the numerical computation of the Laplace transform of the spherical kernel. We denote by $f^{\mathrm{poles}}(z)$ the numerical computation of $f(z)$ using the sum of poles expression in (10) (our approach), and in contrast, we denote by $f^{\mathrm{recur}}(z)$ the computation via the following recurrence relations (use in [2]):

$$g_{\frac{1}{2}} = -z - \tfrac{1}{2}, \tag{15}$$

$$g_{n+\frac{1}{2}} = \frac{-z^2}{n - 1 + \frac{1}{2} - g_{n-1+\frac{1}{2}}} - \left(n + \tfrac{1}{2}\right), \tag{16}$$

$$f^{\mathrm{recur}}(z) = g_{n+\frac{1}{2}} + z + \tfrac{1}{2}. \tag{17}$$

Unfortunately, due to finite precision arithmetic, these two ways of evaluation differ irreconcilably when n is large. Even if all the zeros of the modified Bessel function are computed accurately (to 16 digits in double precision) $f^{\mathrm{poles}}(z)$ differs from $f^{\mathrm{recur}}(z)$ with the loss of all significant digits when $n > 300$ (see Fig. 2). Thus, numerical comparison of these two approaches can be made only for kernels of a moderate

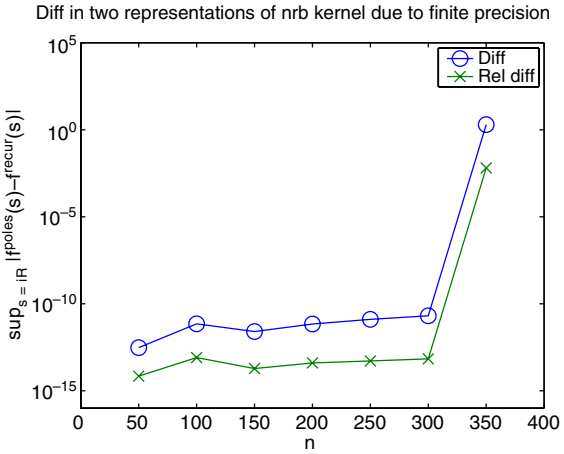


Fig. 2. Two ways of computing the Laplace transform of the spherical kernel differ in all significant digits when $n > 300$.

Table 1
Approximation of $f(z)$, $n = 50, 100, \ldots, 300$ by a rational function of order $r = 5, 10, \ldots, 50$ using Balanced Truncation

Approximation error in L^∞ norm: $\mathrm{err}^\infty_{\mathrm{balred}} := \sup_{s=i\mathbb{R}} \lvert f_r^{\mathrm{balred}}(s) - f(s)\rvert$						
	$n = 50$	$n = 100$	$n = 150$	$n = 200$	$n = 250$	$n = 300$
$r = 5$	1.2664e−01	5.5500e−01	1.1871e+00	1.9926e+00	2.9159e+00	3.8983e+00
$r = 10$	5.0717e−05	7.7091e−04	2.8508e−03	6.5626e−03	1.2134e−02	1.9352e−02
$r = 15$	5.8152e−09	4.7834e−07	3.5233e−06	1.2221e−05	2.9753e−05	5.8485e−05
$r = 20$	7.0232e−13	1.5227e−10	2.5484e−09	1.4321e−08	4.8159e−08	1.2111e−07
$r = 25$	6.6594e−13	8.0733e−12	2.5770e−12	1.6096e−11	6.2642e−11	1.8270e−10
$r = 30$	6.9461e−13	8.0810e−12	1.3511e−12	5.2822e−12	1.3464e−11	2.0379e−11
$r = 35$	6.6831e−13	8.0491e−12	1.3672e−12	5.3111e−12	1.3543e−11	2.0280e−11
$r = 40$	6.9661e−13	8.0988e−12	1.4023e−12	5.1822e−12	1.3656e−11	1.9725e−11
$r = 45$	6.9517e−13	8.0635e−12	1.4449e−12	5.2080e−12	1.3618e−11	1.9725e−11
$r = 50$	6.8732e−13	8.0886e−12	1.4955e−12	5.3267e−12	1.3728e−11	1.9930e−11

The exact value $f(z)$ is computed via the recurrence relations in (15)–(17).

order. For $n > 300$, it is not possible to compare them as they use drastically different values for the exact Laplace transform. To be consistent, we made the arbitrary choice of using $f^{\mathrm{recur}}(z)$ as the exact value throughout when measuring approximation error.

We denote a rational approximation of order r obtained from Balanced Truncation by $f_r^{\mathrm{balred}}(z)$ and a rational approximation obtained from direct L^2 minimization by $f_r^{l2\,\min}(z)$. In Table 1 we show the L^∞ errors of various Balance Truncation approximations. The error is measured against $f^{\mathrm{recur}}(z)$.

Table 2
Approximation of $f(z)$, $n = 50, 100, \ldots, 300$ by a rational function of order $r = 5, 10, \ldots, 50$

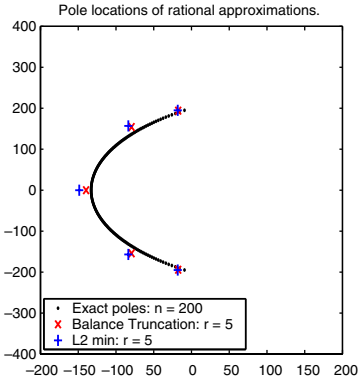
$\mathrm{err}^{\infty}_{l2\,\min} - \mathrm{err}^{\infty}_{\mathrm{balred}} := \sup_{s=i\mathbb{R}} \lvert f_r^{l2\,\min}(s) - f(s)\rvert - \sup_{s=i\mathbb{R}} \lvert f_r^{\mathrm{balred}}(s) - f(s)\rvert$						
	$n = 50$	$n = 100$	$n = 150$	$n = 200$	$n = 250$	$n = 300$
$r = 5$	−2.1309e−03	**6.4237e−03**	**5.0753e−02**	**8.5569e−02**	**9.1025e−02**	**8.2737e−02**
$r = 10$	−1.8405e−06	−1.0516e−05	**2.2774e−05**	**2.8651e−04**	**7.2658e−04**	**1.6700e−03**
$r = 15$	−2.7014e−10	−1.1462e−08	**3.3364e−08**	**1.6205e−06**	**5.9656e−06**	**1.3132e−05**
$r = 20$	**4.4554e−12**	**1.7029e−11**	**2.6346e−10**	**3.3427e−09**	**1.0396e−08**	**6.0160e−09**
$r = 25$	*no sp*	*no sp*	**1.2602e−11**	**3.5959e−11**	**1.2005e−10**	**7.3424e−11**
$r = 30$	**3.5714e−12**	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*
$r = 35$	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*
$r = 40$	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*
$r = 45$	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*
$r = 50$	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*	*no sp*

The entries where f_r^{balred} has a smaller L^{∞} error than $f_r^{l2\,\min}$ are shown in boldface. In the other entries $f_r^{l2\,\min}$ has a smaller L^{∞} error. The entry '*no sp*' indicates that a sum of poles representation was not obtainable from $f_r^{l2\,\min}(z)$. Such a representation was always obtainable from $f_r^{\mathrm{balred}}(z)$. The exact value $f(z)$ is computed via the recurrence relations in (15)–(17).

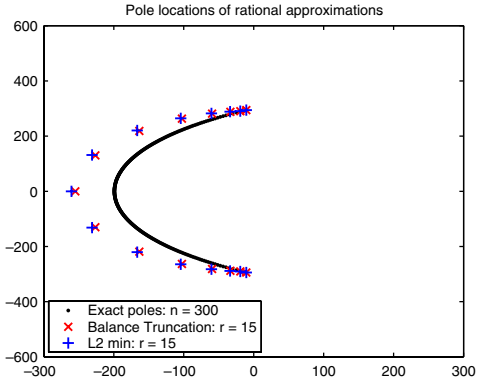
In Table 2 we show the difference in the L^{∞} errors of the approximations $f_r^{\mathrm{balred}}(z)$ and $f_r^{l2\,\min}(z)$. Again, the value $f(z)$ is computed via the recurrence relations in (15)–(17). The approximation error of $f_r^{l2\,\min}(z)$ is smaller in five entries (preceded by a minus sign). In the rest of the entries $f_r^{\mathrm{balred}}(z)$ has a smaller error (shown in boldface). It can also be seen that a sum of poles representation was not obtainable from $f_r^{l2\,\min}(z)$ for many entries when r is high. This comes from the fact that solving for the roots of $Q(z)$ given the monomial coefficients (determined recursively in [2]) is not a stable procedure. Admittedly in those cases fairly accurate approximations (error at most $\mathrm{O}(10^{-10})$) have already been found at lower r. On the other hand, we were always able to obtain a sum of poles representation from $f_r^{\mathrm{balred}}(z)$.

In Fig. 3 we show the difference between $f_r^{l2\,\min}(z)$ and $f_r^{\mathrm{balred}}(z)$ for $n = 200$, $r = 5$ and $n = 300$, $r = 15$ over a range of frequencies, with $f_r^{\mathrm{balred}}(z)$ achieving a lower L_{∞} error in both cases.

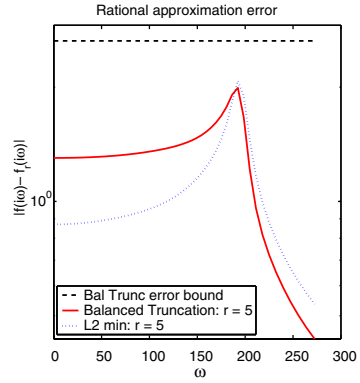
In terms of computational efficiency, our approach requires finding all the zeros of a modified Bessel functions whereas the L^2 minimization approach does not, and once they have been found, Balanced Truncation requires matrix operations of $\mathrm{O}(n^3)$ complexity after which one can easily obtain approximations of any size. On the other hand the L^2 minimization approach requires only repeated evaluations of the Laplace transform of the kernel (via recurrence relations) and a number of linear system solves of the size of the intended reduction (for a given error tolerance, this size was proved to be $\mathrm{O}(\log(n))$ in [2]). It is not known a priori how many linear system solves will be required because the algorithm used is iterative. But in practice, the number is small in both our experience and that of the authors in [2]. Again, we emphasize that we are



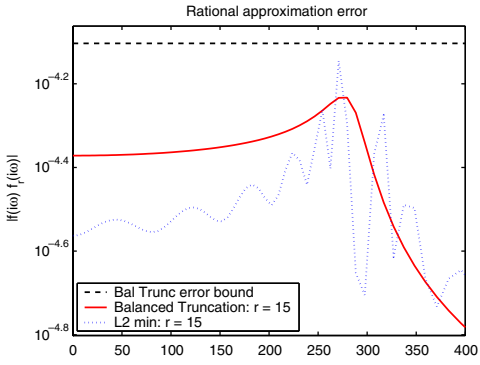
(a) n = 200, r = 5



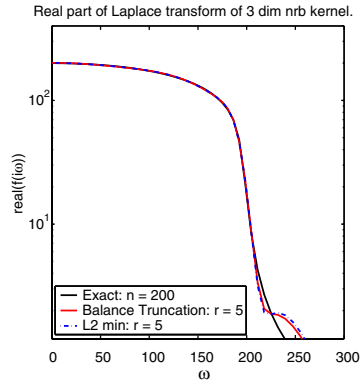
(d) n = 300, r = 15



(b) n = 200, r = 5



(e) n = 300, r = 15



(c) n = 200, r = 5

Fig. 3. Rational approximation of the Laplace transform of the spherical nonreflecting boundary kernel. Comparison of Balanced Truncation and L^2 minimization.

primarily interested in the accuracy of the low order approximations. We assume that these approximations are to be precomputed and stored, and then used for any wave propagation problem which uses an expansion of no higher than that order. Thus, in this paper we do not investigate the use of other model reduction methods which have lower orders of complexity but which are not as accurate as Balance Truncation [4,5,9,10].

6. Conclusions

We presented a method of finding low order approximations to the three dimensional spherical nonreflecting boundary kernel and showed that the approximations can achieve good accuracy. We compared it with a direct L^2 minimization approach where a rational approximation was represented as a ratio of polynomials and showed that our approach in general produced more accurate approximations and is better at generating a sum of poles representation. However, our approach is limited to the case of the spherical boundary in three dimensions. The direct L^2 minimization approach should be used for the two dimensional circular nonreflecting boundary kernel which involves a whole order modified Bessel function.

Algorithm 1. Finding all n zeros of $K_{n+\frac{1}{2}}(z)$.

1. Find $k_{n+\frac{1}{2},1}$ by calling nag_nlin_sys and give the initial guess $\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \begin{pmatrix} \operatorname{Re} z_0 \\ \operatorname{Im} z_0 \end{pmatrix}$ where z_0 is given in (11). Supply the Jacobian

$$J(x, y) = \begin{bmatrix} \operatorname{Re} K'_{n+\frac{1}{2}}(z) & -\operatorname{Im} K'_{n+\frac{1}{2}}(z) \\ \operatorname{Im} K'_{n+\frac{1}{2}}(z) & \operatorname{Re} K'_{n+\frac{1}{2}}(z) \end{bmatrix}$$

where $K'_{n+\frac{1}{2}}(z)$ is determined recursively by

$$K'_{n+\frac{1}{2}}(z) = -\frac{K_{n+1+\frac{1}{2}}(z) + K_{n-1+\frac{1}{2}}(z)}{2}.$$

2. Let $n2 :=$ floor $\frac{n}{2}$ and set $n\text{zero} = 1$.
   While ($n\text{zero} < n2$)
   (a) Interpolate a piecewise cubic Hermite function $x = h(y)$ through

$$\left\{ \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} := \begin{pmatrix} 0 \\ n \end{pmatrix}, \begin{pmatrix} \operatorname{Re} k_{n+\frac{1}{2},1} \\ \operatorname{Im} k_{n+\frac{1}{2},1} \end{pmatrix}, \ldots, \begin{pmatrix} \operatorname{Re} k_{n+\frac{1}{2},n\text{zero}} \\ \operatorname{Im} k_{n+\frac{1}{2},n\text{zero}} \end{pmatrix}, \begin{pmatrix} x_f \\ y_f \end{pmatrix} := \begin{pmatrix} -na \\ 0 \end{pmatrix} \right\}.$$

   (b) Do $n\text{step} = 0$ to $100 \times$ iter

      i. $\Delta y := \frac{n\text{step}}{100\text{iter}}$.

ii. Call nag_nlin_sys with initial guess $\begin{pmatrix} x = h(y) \\ y = y_0 + (y_f - y_0)\Delta y \end{pmatrix}$. Obtain a root $\begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix}$.

iii. If $\tilde{y} <$ machine ϵ, iter := iter + 1, GOTO 2a

iv. Elseif $\begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix} \notin \left\{ \begin{pmatrix} \mathrm{Re}\, k_{n+\frac{1}{2},1} \\ \mathrm{Im}\, k_{n+\frac{1}{2},1} \end{pmatrix}, \ldots, \begin{pmatrix} \mathrm{Re}\, k_{n+\frac{1}{2},n\mathrm{zero}} \\ \mathrm{Im}\, k_{n+\frac{1}{2},n\mathrm{zero}} \end{pmatrix} \right\}$, set $k_{n+\frac{1}{2},n\mathrm{zero}+1} := \begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix}$ and $n\mathrm{zero} := n\mathrm{zero} + 1$.

3. If n is odd, find $k_{n+\frac{1}{2},n2+1}$ by calling nag_nlin_sys and give the initial guess $\begin{pmatrix} -na \\ 0 \end{pmatrix}$.

4. Set $k_{n+\frac{1}{2},n-i} := \overline{k_{n+\frac{1}{2},i}}$, $i = 1, \ldots, n2$.

References

[1] M. Abramowitz, I.A. Stegun (Eds.), Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, Dover Publications, New York, 1992. Reprint of the 1972 edition.

[2] B. Alpert, L. Greengard, T. Hagstrom, Rapid evaluation of nonreflecting boundary kernels for time-domain wave propagation, SIAM J. Numer. Anal. 37 (4) (2000) 1138–1164. (electronic).

[3] D.F. Enns, Model reduction with balanced realizations: an error bound and frequency weighted generalizations, in: Proceedings of the 23rd Conference on Decision and Control, Las Vegas, NV, December 1984, pp. 127–132.

[4] P. Feldmann, R.W. Freund, Efficient linear circuit analysis by Padé approximation via the Lanczos process, IEEE Trans. Comput. Aided Design Integrated Circuits Syst. 14 (5) (1995) 639–649.

[5] K. Gallivan, E. Grimme, P. Van Dooren, A rational Lanczos algorithm for model reduction, Numer. Algorithms 12 (l–2) (1996) 33–63.

[6] K. Glover, All optimal Hankel-norm approximations of linear multivariable systems and their L^∞-error bounds, Internat. J. Control 39 (6) (1984) 1115–1193.

[7] M.J. Grote, J.B. Keller, Exact nonreflecting boundary conditions for the time dependent wave equation, SIAM J. Appl. Math. 55 (2) (1995) 280–297. Perturbation Methods in Physical Mathematics (Troy, NY, 1993).

[8] T. Hagstrom, S.I. Hariharan, R.C. MacCamy, On the accurate long-time solution of the wave equation in exterior domains: asymptotic expansions and corrected boundary conditions, Math. Comput. 63 (208) (1994) 507–539, S7–S10.

[9] I.M. Jaimoukha, E.M. Kasenally, Oblique projection methods for large scale model reduction, SIAM J. Matrix Anal. Appl. 16 (2) (1995) 602–627.

[10] J.-R. Li, J. White, Reduction of large circuit models via low rank approximate Gramians, Internat. J. Appl. Math. Comput. Sci. 11 (5) (2001) 1151–1171. Numerical analysis and systems theory (Perpignan, 2000).

[11] B.C. Moore, Principal component analysis in linear systems: controllability, observability, and model reduction, IEEE Trans. Automat. Control 26 (l) (1981) 17–32.

[12] M.G. Safonov, R.Y. Chiang, A Schur method for balanced-truncation model reduction, IEEE Trans. Automat. Control 34 (7) (1989) 729–733.

[13] I.L. Sofronov, Artificial boundary conditions of absolute transparency for two- and three-dimensional external time-dependent scattering problems, European J. Appl. Math. 9 (6) (1998) 561–588.
[14] M.S. Tombs, I. Postlethwaite, Truncated balanced realization of a stable nonminimal state-space system, Internat. J. Control 46 (4) (1987) 1319–1330.