Characteristics methods for transient analysis of wave propagation in unbounded media

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Abstract

A method based on characteristics was developed recently for the analysis of wave propagation in unbounded layered media \cite{Guddati2000}. In this paper, the method is extended to problems involving spherical and cylindrical computational boundaries. The procedure resulting from straightforward extension of the method meets with several difficulties in stability and accuracy. Modifications based on radial scaling and upwinding are applied to circumvent these difficulties. The resulting boundary conditions have all the properties desired in an artificial boundary condition. Numerical experiments are presented to illustrate the effectiveness of the procedure. © 1998 Elsevier Science S.A. All rights reserved.

1. Introduction

Accurate analysis of wave propagation in unbounded domains is of great importance in several fields of engineering and science. There has been a continuing effort to develop efficient and accurate methods of analysis for these problems. Analysis under time-harmonic excitation received considerable attention and there have been several successful methods for that purpose \cite{BemFelsen1964, Gegel1976, Guddati1998}. Transient analysis of unbounded media still provides a great challenge to researchers in several fields. This paper presents an efficient alternative to existing methods of analyzing transient analysis of unbounded media.

Typical problems involving unbounded domains contain an interior domain which is of main interest. The standard way of analyzing this type of problems is to truncate the unbounded domain around the main domain of interest and apply appropriate boundary conditions on the computational boundary surrounding the truncated domain (Fig. 1). These boundary conditions are expected to simulate the effect of the exterior unbounded domain on the truncated interior. The most natural boundary condition would be a relation between the Neumann data and the Dirichlet data on the computational boundary. This approach fits well especially when a variational formulation is employed for the interior problem. The map is generally referred to as the exterior stiffness matrix, or, more generally, the Dirichlet-to-Neumann (DtN) map. It is well known that the exact DtN map is global in both space and time and takes the form of a convolution operator, i.e.

\[
\frac{\partial u}{\partial n} = B * u ,
\]

where \( \partial u / \partial n \) is the Neumann data and \( u \) is the Dirichlet data. We emphasize here that \( B \) is global in space and belongs to the general space of distributions in time. We would like to split this operator into singular and regular parts (in time). Thus, our aim is to obtain a DtN map of the following form:

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where $K$ is a linear local (differential) operator in time and $h$ is the effect of past history. For various reasons, we would like the above boundary condition to have the following properties:

- **Accuracy**: The method should have the capability of obtaining any desired accuracy.
- **Well-posedness**: The resulting boundary condition should not create spurious stability problems when combined with the interior problem.
- **Compatibility**: The method for the exterior domain should be compatible with the numerical procedure used for analyzing the interior.
- **Computational time**: The time of computation should be reasonable so as to justify the practicality of the method.
- **Storage**: It is preferable for the method to require minimal storage.
- **Time stepping**: Ideally, the boundary condition should be such that it does not impose restrictions on time discretization of the interior problem coupled with the boundary condition.
- **Sparsity**: It is desirable to have a boundary condition with a sparse coefficient matrix $K$, if the coefficient matrix for the interior happens to be sparse. This will control the possible increase in computational cost for solving the linear system.

Most of the methods developed so far can be classified into two categories: local and global. Local boundary conditions take a form containing differential operators in space and time, whereas global boundary conditions preserve the nonlocality of the exact operator in time, space or both. Typically, local boundary conditions are relatively crude approximations of the global convolution operator, and are generally valid for a rather narrow range of wavelengths. These methods, however, are very efficient due to their local nature. The conditions developed by Engquist and Majda [4,5], Higdon [9] for straight boundaries, and the curved boundaries developed by Bayliss and Turkel [2] fall into this category. A survey of local methods can be found in [6].

The class of global methods include boundary element methods [3] and methods based on convolution with Green’s function of the exterior domain [6,13]. These methods are often prohibitively expensive for direct time-domain analyses because of their fully coupled nature: they tend to demand extremely high computational time and storage. Several methods of this category can be found in [6,13,14].

Recently, we presented an efficient method based on characteristics for the analysis of scalar wave propagation in unbounded homogeneous layers [7]. It was shown that the approach results in a global method with a computational cost less than that of existing global methods. The characteristics method is based on a new two-step procedure involving semidiscretization and space–time analysis. The unbounded domain is first discretized in the direction along the boundary and the resulting semidiscrete equations are solved in the space–time domain in an efficient manner. This paper is devoted to the generalizations of the characteristics method. The method is extended to other geometries of practical interest: cylindrical and spherical geometries. This extension is not straightforward, and we give the necessary steps to obtain a desirable boundary condition.

The outline of the rest of the paper is as follows: Section 2 states the basic problems of interest. In Section 3, the semidiscretization procedure is explained and the resulting semidiscrete problems are stated. Section 4 contains a brief review of the characteristics method for a layer and some critical observations. Section 5 deals
with the development of the characteristics method for circular and spherical geometries. Computational cost is discussed in Section 6. In Section 7, we illustrate the effectiveness of the procedures developed in this paper with the use of numerical experiments. Section 8 summarizes the paper with some concluding remarks.

2. Problem statement

The scalar wave equation governs several physical phenomena such as the motion of acoustic fluids and out-of-plane deformation of elastic solids [1,15]. The governing equations for these problems can be written in the following general form:

\[ \rho \frac{\partial^2 u}{\partial t^2} - \nabla \cdot (G \nabla u) = f \]  \hspace{1cm} (3)

Three types of geometries of practical interest are considered: two-dimensional layers, two- and three-dimensional half/full spaces. The exterior domain is assumed to be homogeneous. In the case of a layer, we assume the computational boundary \( \Gamma \) to be a straight edge transverse to the layer. Dirichlet conditions are applied at the bottom and Neumann conditions are applied on the top. The layer is assumed to start from rest. The problem setting is clearly shown in Fig. 2. For reasons that will be apparent later, we write the statement of the initial-boundary value problem in terms of the specific coordinate system of the layer. The source term \( f \) is taken to be zero and the boundary conditions are chosen to be homogeneous. The cases of non-zero source term and non-homogeneous boundary conditions can be dealt with in a straightforward manner [7] and thus are omitted for the sake of simplicity. The scalar wave problem takes the following form.

Problem CLayer: Find the map \( \mathbf{D}tN: \mathbf{u}_r \rightarrow s \) in which \( \mathbf{u}_r \) is the field variable at the boundary \( (x = 0) \) and \( s = -Gu_\nu \) is the traction on the boundary. The field variable satisfies the following differential equation, boundary conditions and initial conditions:

\[ \rho u_{rt} - Gu_{\nu x} - (Gu_\nu)_z = 0 \hspace{1cm} \text{for} \hspace{1cm} x > 0, \ z \in (-H,0), \ t > 0 \]  \hspace{1cm} (4)

\[ u(x, z, t) = 0 \hspace{1cm} \text{at} \hspace{1cm} z = -H \]  \hspace{1cm} (5)

\[ Gu_\nu (x, z, t) = 0 \hspace{1cm} \text{at} \hspace{1cm} z = 0 \]  \hspace{1cm} (6)

\[ u(x, z, 0) = u_x(x, z, 0) = 0 \]  \hspace{1cm} (7)

For the case of a three-dimensional half space, the computational boundary is taken as a spherical surface of radius \( R \) and the boundary conditions on the surface are assumed to be invariant in the radial direction (Fig. 3). Once again, we assume homogeneity of the exterior domain. The scalar wave propagation problem is stated as follows:

Problem CSpherical: Find the map \( \mathbf{D}tN: \mathbf{u}_r \rightarrow s \) in which \( \mathbf{u}_r \) is the field variable at the boundary \( (r = R) \) and \( s = -Gu_\nu \) is the traction on the boundary. The field variable satisfies the following differential equation, boundary conditions and initial conditions:

\[ \rho u_{tt} - G \left( u_{rr} + \frac{2}{r} u_r \right) - \frac{1}{r^2} \nabla_\theta \cdot (G \nabla_\theta u) = 0 \hspace{1cm} \text{for} \hspace{1cm} r > R, \ \theta \in \Theta, \ t > 0 \]  \hspace{1cm} (8)

Fig. 2. Wave propagation in a semi-infinite layer.
Fig. 3. Wave propagation in three-dimensional half space.

Fig. 4. Wave propagation in two-dimensional half space.

\[ u(r, \theta, t) = 0 \quad \text{for} \quad r > R, \theta \in I^D_{\theta} \]

\[ \frac{G}{r} \mu_{\phi}(r, \theta, t) = 0 \quad \text{for} \quad r > R, \theta \in I^N_{\theta} \]

\[ u(r, \theta, 0) = u_{\phi}(r, \theta, 0) = 0 \]

Here, \( \theta \) is the (spherical) angle and \( \Theta \) is the domain of \( \theta \) (i.e. exterior domain, \( R_e = (R, \infty) \times \Theta \)), and \( I_{\theta} \) is the boundary of \( \Theta \). \( I^D_{\theta} \) and \( I^N_{\theta} \) are the Dirichlet and Neumann partitions \( I_{\theta} \). \( \bar{V}_{\theta} \) is the gradient on the spherical surface.

In the case of two-dimensional half/full space (Fig. 4), we merely replace the spherical Laplacian by the cylindrical one and arrive at the following problem.

**Problem CPolar**: Find the map \( D_{rN} : u_{r} \rightarrow s \) in which \( u_{r} \) is the field variable at the boundary \( (r = R) \) and \( s = -Gu_{r} \) is the traction on the boundary. The field variable satisfies the following conditions.

\[ \rho u_{tt} - G \left( u_{rr} + \frac{1}{r} u_{r} \right) + \frac{1}{r^2} (Gu_{\theta})_{\theta} = 0 \quad \text{for} \quad r > R, \theta \in (\theta_1, \theta_2), t > 0 \]

\[ u(r, \theta, t) = 0 \quad \text{at} \quad \theta = \theta_1 \]

\[ \frac{G}{r} u(r, \theta, t) = 0 \quad \text{at} \quad \theta = \theta_2 \]

\[ u(r, \theta, 0) = u_{\phi}(r, \theta, 0) = 0 \]

### 3. Semidiscretization

In this section, the first level of approximation is performed: The boundary is discretized to reduce the spatial dimension of the problem to one. This is facilitated by the special geometries of the computational boundary. The method is explained in detail for the cases of two- and three-dimensional half spaces. The semidiscrete problem for the layer is also stated.

#### 3.1. Two- and three dimensional half spaces

The following approximation is used for the displacement field:

\[ u^h = \sum_{i=1}^{N} \phi_i(\Theta) u_i(r, t) = \Phi^T(\Theta) U(r, t) \]
In the above, $\Phi(\theta)$ can be viewed as the basis function vector on the boundary and $U(r, t)$ is the vector of nodal degrees of freedom. To enable easy coupling of the interior and exterior, the basis function vector $\Phi(\theta)$ is chosen such that the discretization of the interior coincides with that of the exterior. A schematic illustration of the semidiscretization procedure is given in Fig. 5.

We apply the standard Galerkin method using the above approximation. The test function is of the same form as the solution:

$$\delta u^h = \sum_{i=1}^{N} \phi_i(\theta) \delta u_i(r, t) = \Phi^T(\theta) \delta U(r, t).$$  \hspace{1cm} (17)

We get the Galerkin approximation of the variational form of the original equation as

$$\int_\theta \delta u^h \left(-Gu^h_{,,r} - \frac{G}{r} u^h_r - \frac{1}{r^2} \nabla_u \cdot (G\nabla_u u^h) + \rho u^h_n \right) d\theta = 0. \hspace{1cm} (18)$$

Integrating by parts in $\theta$, we get

$$\frac{G}{r^2} \int_\theta \nabla_u \delta u^h \cdot \nabla u^h d\theta - G \int_\theta \delta u^h u^h_{,,r} d\theta - \frac{G}{r} \int_\theta \delta u^h u^h_r d\theta + \rho \int_\theta \delta u^h u^h_n d\theta = 0 \hspace{1cm} (19)$$

Substituting the approximation for $u^h$ and $\delta u^h$, we get

$$\delta U^T G \int_\theta \Phi \Phi^T d\theta \ U_{,,r} + \delta U^T \frac{G}{r} \int_\theta \Phi \Phi^T d\theta \ U_r - \delta U^T G \int_\theta \nabla_u \Phi \nabla_u \Phi^T d\theta \ U - \delta U^T \rho \int_\theta \Phi \Phi^T d\theta \ U_n = 0 \ \ \forall \ \delta U \in \mathbb{R}^N \hspace{1cm} (20)$$

which reduces to the following form:

$$A \left( U_{,,r} + \frac{U_r}{r} - \frac{1}{r^2} U_n \right) - GU = 0, \hspace{1cm} (21)$$

in which $A$ and $G$ are constant $N \times N$ matrices:

$$A = \int_\theta \Phi G \Phi^T d\theta, \hspace{1cm} (22)$$

$$G = \int_\theta \nabla_u \Phi G \nabla_u \Phi^T d\theta. \hspace{1cm} (23)$$

Note that the matrix $A$ is of Grammian type, and thus positive definite. Matrix $G$ is positive semidefinite.

Our modified problem is to find a map between the displacement vector $U_r$ and the traction vector consistent with the approximation made in displacement, i.e. if $S$ is the traction vector, we need to satisfy the variational equivalence:

![Fig. 5. Semidiscretization of a two-dimensional half space](image-url)
\[ 8U^T S = \int_{\Gamma} 8u^h s^h d\Gamma = R^{(n^d-1)} \int_\theta 8u^h s^h d\theta , \]  
(24)

where \( s^h \) is the approximation of the traction \( s \). As \( s = -Gu, \) from Eq. (16), we have \( s^h = -\Phi^T GU, \) This results in the following relation:

\[ 8U^T S = -8U^T R^{(n^d-1)} \int_\theta \Phi G \Phi^T dz U, \quad \forall \delta U \in \mathbb{R}^N. \]  
(25)

From Eq. (22), we conclude that the traction vector is nothing but

\[ S = -R^{(n^d-1)} AU, \]  
(26)

We now present the discrete version of our original problem.

**Problem DSpace:** Find the map \( D_{\Omega} : U_{\Omega}(t) \rightarrow S(t) \) where \( U_{\Omega} \) is the displacement vector at \( r = R \) and \( S = -R^{(n^d-1)} AU, \) is the corresponding traction vector. The field variable \( U \) satisfies the following differential equation and initial conditions.

\[ AU_{xx} - \frac{n^d}{r^2} AU_{r} - GU = 0 \quad \text{for } r > R, t > 0 \]  
(27)

\[ U = U_0 = 0 \quad \text{at } t = 0. \]  
(28)

In the above, \( A \) is symmetric and positive definite, whereas \( G \) is symmetric and positive semidefinite.

### 3.2. Semi-infinite layer

For problem \( D_{\Omega} \), we choose the approximation similar to the one chosen for previous cases:

\[ u^h = \sum_{i=1}^{N} \phi_i(z) u_i(x, t) = \Phi^T(z) U(x, t). \]  
(29)

Following the procedure described above, we arrive at the following discrete problem for the layer.

**Problem DLayer:** Find the map \( D_{\Omega} : U_{\Omega}(t) \rightarrow S(t) \) where \( U_{\Omega} \) is the displacement vector at \( x = 0 \) and \( S = -AU, \) is the corresponding traction vector. We satisfy the following differential equations and initial conditions:

\[ AU_{xx} - \frac{1}{c^2} AU_{tt} - GU = 0 \quad \text{for } x > 0, t > 0 \]  
(30)

\[ U = U_0 = 0 \quad \text{at } t = 0. \]  
(31)

Again, \( A \) is symmetric and positive definite and \( G \) is symmetric and positive semidefinite.

### 4. Characteristics method for a layer

Before proceeding with the cases of circular and spherical computational boundaries, for the sake of completeness, we review the characteristics method for problem \( D_{\Omega} \) and explain some of the important issues involved. Details, results and discussion of performance can be found elsewhere [7].

The first step in the characteristics method is to decouple the system of equations by spectral decomposition of \( G \) with respect to \( A \). The system can be written as

\[ QQ^T U_{xx} - \frac{1}{c^2} QQ^T U_{tt} - QAQ^TU = 0 \]  
(32)

where, \( Q \) is the modal matrix and \( A \) is the diagonal matrix containing the eigenvalues of \( G \) with respect to \( A \). Premultiplying both sides of this equation by \( Q^{-1} \) gives:
in which $\hat{U} = Q^T U$.

Each of the above equations can be solved independently. All these variables are zero in the $x > ct$ section of the domain. This follows from the fact that the layer starts from rest and the disturbances at $x = 0$ travel at speed $c$. The problem thus reduces to solving for the field variable between the line $x = 0$ and $x = ct$ in the space–time domain. The Cauchy data on the characteristic $x = ct$ is specified ($u = 0$). We assume the field variable to be specified at $x = 0$ and would like to find the spatial derivative $u_x$ at the boundary $x = 0$.

All the decoupled equations (Eq. (33)) are transformed into the characteristic coordinate system:

$$\xi = \frac{x + ct}{2} \quad \text{and} \quad \eta = \frac{x - ct}{2}. \tag{34}$$

Then, the equations look like

$$\hat{U}_{\xi} - \mathbf{A}\hat{U} = 0. \tag{35}$$

We assume that the field variable is known on the characteristic $\xi = cT_{n-1}/2$ and try to obtain the field variable on the $\xi = cT_n/2$ characteristic. The space–time domain is divided into cells with edges parallel to the characteristics (Fig. 6). $\hat{U}$ is assumed to be bilinear in each cell. We would then require the values of $\hat{U}$ at the grid points only. The following notation is used for the purposes of presentation: $\hat{U}_\xi^n$ is the value of $\hat{U}$ when $\xi = cT_n/2$ and $\eta = -cT_n/2$. The interval between $T_{n-1}$ and $T_n$ is considered as the $n$th interval. We now describe the procedure for obtaining the values of $\hat{U}$ on the $\eta$ characteristic corresponding to the current time $T_n$, i.e., $\xi = cT_n/2$. The set of cells that are active in this step are shown in Fig. 6. The ordering of the analysis is also shown in the same figure: we start from cell $(n, 1)$ and proceed till $(n, n - 1)$. For each cell $(n, k)$, we need to obtain $\hat{U}_\eta^k$, given $\hat{U}_{\eta-1}^{k-1}$, $\hat{U}_{\eta-1}^k$ and $\hat{U}_{\eta-1}^{k-1}$. Cell-centered finite difference technique is used for this purpose. The differential equation is satisfied at the center of the cell:

$$\frac{\hat{U}_n^k - \hat{U}_{n-1}^{k-1} + \hat{U}_{n-1}^k + \hat{U}_{n-1}^{k-1}}{\Delta\xi_n \Delta\eta_k} - \mathbf{A} \frac{\hat{U}_n^k + \hat{U}_{n-1}^{k-1} + \hat{U}_{n-1}^k + \hat{U}_{n-1}^{k-1}}{4} = 0. \tag{36}$$

As we have $\Delta\xi_n = c \Delta T_n/2$ and $\Delta\eta_k = -c \Delta T_k/2$ (we are sweeping in negative $\eta$ direction), we arrive at the following form:
where
\[\alpha_i = \frac{4}{c^2 \Delta T_n \Delta T_k} - \frac{A(i)}{4} - \frac{4}{c^2 \Delta T_n \Delta T_k} + \frac{A(i)}{4}.\] (38)

In the above equations, \( \hat{U}(i) \) stands for the \( i \)th element of \( \hat{U} \). \( A(i) \) is the \( i \)th diagonal element of the matrix \( A \).

Note here that the coefficient \( \alpha_i \) is always less than unity for any mode. It is expected that this fact is crucial for the stability of the method. A proof of stability is not available at this time. Numerical experiments indicate that the method is stable, as long as \( \alpha_i < 1 \). A general proof of stability and accuracy of the characteristics method is currently under investigation.

Once the field variable is obtained on the \( \xi = c T_n / 2 \) characteristic, we can obtain \( \hat{U}_\eta \) by simple interpolation. The spatial derivative \( \hat{U}_x \) can be obtained using the chain rule.

\[\hat{U}_\eta = \hat{U}_x - \frac{1}{c} \hat{U}_t,\] (39)

It can be shown that the boundary condition resulting from this procedure leads to negative definite contribution to the coefficient matrix. This spoils the most important property of positive definiteness and can result in an unstable analysis procedure.

As an alternative, we obtain \( \hat{U}_x \) from \( \hat{U}_\eta \) instead of \( \hat{U}_\xi \). \( \hat{U}_\xi \) can be obtained by integrating Eq. (35) with respect to \( \eta \) on the \( \xi = c T_n / 2 \) characteristic.

\[\hat{U}_\xi|_{x=0, t=T_n} = \int_{\eta=-c T_n / 2}^{\eta=0} A \hat{U}(\xi, \eta) \, d\eta.\] (40)

By the chain rule, we obtain the following expression for \( \hat{U}_x \) at \( x = 0, t = T_n \).

\[\hat{U}_x|_{x=0, t=T_n} = \int_{\eta=-c T_n / 2}^{\eta=0} A \hat{U}(\xi, \eta) \, d\eta - \frac{1}{c} \hat{U}_t.\] (41)

As \( \hat{U} \) is known on the characteristic \( \xi = c T_n / 2 \), we can use standard numerical integration. The most appealing integration procedure would be the one which is consistent with the approximation of \( \hat{U} \) over the mesh. This suggests piecewise linear interpolation on the characteristic and trapezoidal rule is used for numerical integration. It should be noted that higher-order difference schemes or finite element schemes could also be used for the updating, and consistent integration schemes be used for the integration. This procedure leads to the following expression for \( \hat{U}_x \):

\[\frac{\partial \hat{U}_x}{\partial x} = \frac{\Delta \eta_n}{2} A \hat{U}_x^n - \frac{1}{c} \frac{\partial \hat{U}_x}{\partial t} + \sum_{k=1}^{n-1} \left[ \frac{\Delta \eta_k + \Delta \eta_{k+1}}{2} A \hat{U}_x^k \right].\] (42)

Premultiplying both sides of the above equation by \(-Q\) and by rearranging, we obtain the following relation between traction \( S \) and displacement \( U \) at the boundary.

\[S = KU + C \frac{\partial U}{\partial t} + H,\] (43)

where
\[K = \frac{c \Delta T_n}{4} G,\] (44)
\[C = \frac{1}{c} A,\] (45)

and
We notice that both the coefficient matrices $K$ and $C$ are symmetric and positive definite. Thus, for conventional time-stepping schemes, we get a symmetric positive definite coefficient matrix from the boundary which has definite advantage for linear solution purposes. Also, this approach of obtaining the traction through integration over the characteristic is expected to be more accurate than the local extraction of traction through interpolation. To summarize, we have derived in this section a boundary condition which relates the displacement vector on the boundary with the corresponding traction vector. The relationship is global in space, but local whenever the interpolation functions are local. It is pseudo-local in time as it uses only the displacement vector and the time derivative in a direct sense. However, the past history is accounted for in a different form with the displacement vector stored along the characteristics.

5. Extension to other geometries

Extension of the characteristics method to problems $DSpace2$ and $DSpace3$ is not straightforward. In this section, we outline the basic problem involved and suggest a way of applying the characteristics method in an effective manner.

5.1. Fundamental problem

We start by looking at the semidiscretized equation for half-spaces:

$$
A \left( U_{rr} + \frac{n^{sd} - 1}{r} U_r - \frac{1}{c^2} U_n \right) - \frac{1}{r^2} GU = 0
$$

(47)

When the above equation is transformed into the characteristic coordinates, it takes the form:

$$
A \left( U_{\xi\eta} + \frac{n^{sd} - 1}{r} \left( U_{\xi} + U_{\eta} \right) \right) - \frac{1}{r^2} GU = 0,
$$

(48)

where the characteristic variables are defined in a slightly different manner:

$$
\xi = \frac{r - R + ct}{2} \quad \text{and} \quad \eta = \frac{r - R - ct}{2}.
$$

(49)

For constant time step size, the cell-centered finite difference equation takes the form (compare with Eq. (36)):

$$
- \frac{4}{c^2 \Delta T^2} (\hat{U}_n^k - \hat{U}_n^{k-1} - \hat{U}_n^{k-1} + \hat{U}_n^{k-1}) + \frac{n^{sd} - 1}{r} \frac{\hat{U}_n^{k-1} - \hat{U}_n^{k-1}}{c \Delta T} - \frac{1}{r^2} A \frac{\hat{U}_n^k + \hat{U}_n^{k-1} + \hat{U}_n^{k-1} + \hat{U}_n^{k-1}}{4} = 0.
$$

(50)

where $r$ is the radial coordinate computed at the center of the cell. The above equation gives rise to the following updating procedure:

$$
\hat{U}_n^k(i) = \alpha \hat{U}_n^{k-1}(i) + \beta \hat{U}_n^{k-1}(i) - \gamma \hat{U}_n^{k-1}(i),
$$

(51)

where

$$
\alpha = \frac{4}{c^2 \Delta T^2} \frac{A(i)}{4r^2} + \frac{n^{sd} - 1}{r c \Delta T},
$$

$$
\beta = \frac{4}{c^2 \Delta T^2} \frac{A(i)}{4r^2}
$$

(52)

The coefficients $\beta$ and $\gamma$ are not of any significance to our discussion. Note that for small time steps, the contribution from $A(i)$ is diminished and $\alpha$ tends to be larger than unity. This implies that the updating
procedure is expected to be unstable, and is verified to be so by numerical experiments. Furthermore, the integral form of the spatial derivative takes the form:

\[
\hat{U}_r = \int_0^{-cT_n/2} \left( \frac{1}{r^2} \hat{A} \hat{U} + \frac{(n^{sd} - 1)}{r} \frac{\hat{U}_r + \hat{U}_q}{2} \right) \, d\eta - \frac{1}{c} \hat{U}_r.
\]  

(53)

For accurate computation of the integral, it is necessary to compute \( \hat{U}_r \) in an accurate manner. However, \( \hat{U}_r \) cannot be computed as accurately as \( \hat{U} \) and we would like to have only \( \hat{U} \) in the integrand.

It is clear that the presence of the term \( U \) creates several difficulties and we would like to eliminate it. To this end, we propose to use a modified field variable \( V \) as the variable of analysis. \( V \) is taken as a simple scaled version of \( U \):

\[
V = r^{n^{sd}-1/2} U
\]  

(54)

This radial scaling of the field variable is consistent with the asymptotic behavior of the field variable under time-harmonic excitation: the field variable has the asymptotic form of \( A e^{ikr/r^{(n^{sd}-1)/2}} \). Thus, the variable \( V \) has a harmonic variation as \( r \to \infty \). This is similar to the variation of the field variable in the case of the layer and thus, it is expected that this scaling makes the performance of the characteristics method better. Using Eq. (54), the governing semidiscrete equation takes the form:

\[
A \left( V_{rr} - \frac{1}{c^2} V_{tt} \right) - \left( G - \frac{1}{A} \right) \frac{1}{r^2} V = 0 \quad \text{for} \quad n^{sd} = 2
\]

\[
A \left( V_{rr} - \frac{1}{c^2} V_{tt} \right) - G \frac{1}{r^2} V = 0 \quad \text{for} \quad n^{sd} = 3
\]

(55)

(56)

This equation closely resembles the semidiscrete equation for a semi-infinite layer (Eq. (30)), but with decaying dispersion term (coefficient of \( U \)). Note that, in the two-dimensional problem, the dispersion matrix is not necessarily positive definite. This poses some difficulties and will be dealt with later in this section.

### 5.2. Three-dimensional case

For problem \( DSpace3 \), the dispersion term is always positive, and the characteristics method is immediately applicable. Standard cell-centered finite difference technique results in the following updating procedure similar to Eq. (37):

\[
\hat{V}_k(i) = \alpha_i (\hat{V}_{n-1}^k(i) + \hat{V}_{n-1}^{k-1}(i)) - \hat{V}_{n-1}^{k-1}(i),
\]

where

\[
\alpha_i = \frac{4}{c^2 \Delta T_n \Delta T_k} - \frac{1}{r^2} \frac{A(i)}{4}
\]

\[
= \frac{4}{c^2 \Delta T_n \Delta T_k} + \frac{1}{r^2} \frac{A(i)}{4}.
\]

(57)

(58)

The integral form for the spatial derivative is

\[
\hat{V}_r = \int_0^{-cT_n/2} \frac{1}{r^2} \hat{V} \, d\eta - \frac{1}{c} \hat{V}_r.
\]

(59)

The presence of the term \( 1/r^2 \) renders the trapezoidal integration procedure erroneous, especially when the radius of the boundary \( R \) is small compared to \( c \Delta T \). To improve the accuracy of integration, we suggest that the integration be performed exactly, assuming piecewise linear variation of the modified field variable \( V \) on the characteristic. The integration is performed using the following identity:

\[
\int_{r_1}^{r_2} f(r) \frac{dr}{r^2} = \left( \frac{f(r_1)}{r_1} - \frac{f(r_2)}{r_2} \right) + \left( f(r_2) - f(r_1) \right) \frac{\ln(r_2) - \ln(r_1)}{r_2 - r_1}.
\]

(60)

In the above, \( f(r) \) is a function of \( r \) varying linearly between \( r_1 \) and \( r_2 \).
Application of the characteristics method with the above updating and integration procedures results in the following relation between the modified field variable $V$ and the modified traction $-AV$:

$$-AV_{r} - KV + C \frac{\partial V}{\partial t} + H,$$

where

$$K = \frac{1}{R} \left( 1 - \ln \left( 1 + c \frac{\Delta t_{n} / 2R}{c \Delta T_{n} / 2} \right) \right) G,$$

$$C = \frac{1}{c} A,$$

and

$$H = -Q \sum_{k=1}^{n-1} \left[ \left( \frac{\ln \left( 1 + c \frac{\Delta T_{k} / 2R}{c \Delta T_{k} / 2} \right)}{c \Delta T_{k} / 2} + \frac{\ln \left( 1 - c \frac{\Delta T_{k+1} / 2R}{c \Delta T_{k+1} / 2} \right)}{c \Delta T_{k+1} / 2} \right) AV_{n}^{k} \right].$$

where, $\xi = cT_{n} / 2$; $\eta = -cT_{n} / 2$.

Substitution of $V = rU$ and further manipulations give rise to the following boundary condition relating the traction $S = -R^2 AU_{r}$ with the displacement $U$:

$$S = KU + C \frac{\partial U}{\partial t} + H,$$

where

$$K = R \left( 1 - \frac{\ln \left( 1 + c \frac{\Delta T_{n} / 2R}{c \Delta T_{n} / 2} \right)}{c \Delta T_{n} / 2R} \right) G + RA,$$

$$C = \frac{R^2}{c} A,$$

and

$$H = -Q \sum_{k=1}^{n-1} \left[ \left( \frac{\ln \left( 1 + c \frac{\Delta T_{k} / 2R}{c \Delta T_{k} / 2} \right)}{c \Delta T_{k} / 2} + \frac{\ln \left( 1 - c \frac{\Delta T_{k+1} / 2R}{c \Delta T_{k+1} / 2} \right)}{c \Delta T_{k+1} / 2} \right) AV_{n}^{k} \right].$$

As in the case of the layer, the coefficient matrices are symmetric and positive definite. They are also sparse depending on the local nature of the shape functions for the semidiscretization. We note from Eq. (65) that the singular part of the map, $RA + (R^2A / c) \partial U / \partial t$, is exactly the first order local boundary condition for the spherical case. It can also be observed that, for a spherically symmetric harmonic ($G = A = 0$), this approximation is exact.

5.3. Two-dimensional case

The case of two-dimensional wave propagation is made more complicated by the possibility of having negative dispersion. The standard cell-centered finite difference technique gives rise to an updating procedure similar to the one for three-dimensional wave propagation (Eq. 57):

$$\dot{V}_{\xi}(i) = \alpha_{t}(\dot{V}_{\xi+1}^{1}(i) + \dot{V}_{\xi-1}^{1}(i)) - \dot{V}_{\xi-1}^{1}(i).$$

However, in the case of two-dimensional wave propagation, $\alpha_{t}$ is given by
\[
\alpha_i = \frac{4}{c^2 \Delta T_n \Delta T_k} - \frac{1}{4r^2} \left( A(i) - \frac{1}{4} \right)
\]

(70)

It can be seen that \( \alpha_i \) can be more than unity and the updating procedure is unstable. To stabilize this, we borrow the concept of upwinding from the computational fluid dynamics literature: instead of the center of the cell, we satisfy the governing PDE at the bottom node of the cell, i.e. at \( \xi = cT_{n-1}/2; \eta = -cT_{k-1}/2 \). This gives rise to the following modified updating procedure:

\[
\hat{V}_n^k(i) - \hat{V}_{n-1}^k(i) + \beta_i \hat{V}_{n-1}^{k-1}(i) ,
\]

(71)

where

\[
\beta_i = 1 - \frac{c^2 \Delta T_n \Delta T_k}{4r^2} \left( \frac{1}{4} - A(i) \right)
\]

(72)

It can be seen that \( \beta_i \ll 1 \) for \( A(i) \ll 1/4 \) and \( \alpha_i \ll 1 \) for \( A(i) \gg 1/4 \). Thus, to ensure stability of the updating, one should use Eq. (69) when \( A(i) \ll 1/4 \) and Eq. (71) otherwise. Note that the updating in Eq. (71) is only first-order accurate as opposed to the second-order accuracy obtained from cell-centered finite differences. We thus sacrifice accuracy for unconditional stability of the scheme.

Following the procedure identical to that described for three-dimensional wave propagation, we obtain the following relation between the traction and displacement.

\[
S = KU + C \frac{\partial U}{\partial t} + H ,
\]

(73)

where

\[
K = \left( 1 - \frac{\ln(1 + c \Delta T_n / 2R)}{c \Delta T_n / 2R} \right) G + \left[ \frac{1}{2} - \frac{1}{4} \left( 1 - \frac{\ln(1 + c \Delta T_n / 2R)}{c \Delta T_n / 2R} \right) \right] A ,
\]

(74)

\[
C = \frac{R}{c} A ,
\]

(75)

and

\[
H = -\sqrt{RQ} \sum_{k=1}^{n-1} \left[ \left( \frac{\ln(1 + c \Delta T_k / 2R_k)}{c \Delta T_k / 2} + \frac{\ln(1 - c \Delta T_{k+1} / 2R_k)}{c \Delta T_{k+1} / 2} \right) \left( A - \frac{1}{4} I \right) V_n^k \right] ,
\]

(76)

where \( I \) is the identity matrix. It can be verified that the coefficient of \( A \) in Eq. (74) is positive for all values of \( \Delta T_n \). This implies that \( K \) is positive definite and so is the matrix \( C \). Again, these matrices are sparse, provided that the semidiscrete shape functions are local in space. Similar to the spherical case, the singular part of the map, \( A / 2 + (RA/c) \beta / \partial t \), coincides with the first-order local boundary condition for the cylindrical geometry and is exact as \( \omega \to \infty \). However, differently from the case of the spherically symmetric harmonic, the singular part is not exact for the cylindrically symmetric harmonic.

6. Computational cost

The computational expense involved in using the Characteristics method for cylindrical and spherical geometries is comparable to that for a layer problem. In this section, the computational cost is analyzed and compared with the cost involved in using other global methods, i.e. methods based on convolution.

Storage: similar to the case of a layer, we store the matrices \( G, A \) and \( Q \), and the values of \( \hat{U} \) on the current characteristic. Assuming most general discretization on the boundary, i.e. if \( G \) and \( A \) are dense, we require \( 3N^2 \) initial storage, where \( N \) is the number of degrees of freedom on the boundary. For practical discretizations, \( G \) and \( A \) are sparse, and the required initial storage is much smaller. Storage of \( \hat{U} \) on the characteristic
corresponding to \( k \)th time step requires space for \( k \times N \) numbers. This storage is reduced to \( k \times \bar{N} \), when only \( \bar{N} \) of the \( N \) modes are used for the analysis. The number of active modes \( (\bar{N}) \) can be chosen depending on the type of loading and can be much smaller than \( N \) resulting in considerable savings. Thus, the maximum storage required during the whole analysis process involving \( n \) time steps is \( 3N^2 + nN \).

**Computational time:** the initial spectral decomposition of \( G \) with respect to \( A \) requires \( O(N^3) \) time. For the \( k \)th time step, we need to perform \( k \) cell-updates and integration over the characteristic for \( N \) modes. This process requires \( O(N) \) operations. After the integration, premultiplication by \( Q \) requires \( N \bar{N} \) operations. Thus, the \( k \)th time step involves \( O(k \bar{N}^2) \) operations, making the total computational time to be \( O(N^3 + n^2 \bar{N} + nN) \) for \( n \) time steps. Although of the same order, the computational time required for cylindrical and spherical boundaries is slightly more than that for layer cases, due to the need for evaluating logarithmic functions while computing the integral (Eqs. (68) and (76)).

For methods based on convolution, the computational cost involved is two-fold: the cost of computing the Green’s function, and the cost of convolution. The cost involved in Green’s function computation is method-dependent, and in general very high. We do not include this cost in the comparison, but use only the convolution cost. The Green’s function is global in both space and time, i.e., it consists of \( n \) dense matrices of size \( N \times N \). Thus, the storage required for convolution based methods is \( nN^2 \). For the \( k \)th time step, convolution involves \( k \) matrix-vector multiplications, and for total analysis for \( n \) time steps, it involves \( n^2N/2 \) matrix-vector multiplications. Thus the total time involved convolution is \( O(n^2N^2) \).

It is clear from the above discussion that the required storage for the characteristics method is minimal: only the field variable is stored on the current characteristic. Essentially, this is equivalent to storing just the history on the boundary as it requires only storage of \( \bar{N} \) in addition to the initial storage of less than \( 3N^2 \) required for matrices \( G, A \) and \( Q \). The convolution based methods, on the other hand, require storage of \( nN^2 \), which is of higher order than the characteristics method. Neglecting the initial cost, the \( O(n^2\bar{N} + nN) \) time required for characteristics method is an order of magnitude less than that of convolution \( O(n^2N^2) \). Furthermore the initial cost involved in characteristics method is only that of spectral decomposition. On the other hand, the cost of obtaining the Green’s function for transient analysis is in general extremely high. Another advantage of the characteristics method arises when the method is coupled with the conventional finite element/finite difference analysis procedure for the interior. The augmented matrices (Eqs. (65) and (73)) are sparse, preserving the sparsity of the interior coefficient matrix. The methods based on convolution, on the other hand, render the interior coefficient matrix dense, and thus increase the cost of solving the interior linear system. In summary, the characteristics method is more efficient than convolution based methods in all respects.

We conclude this section with a note on local boundary conditions. It is clear that the characteristics boundary is more expensive than local boundary conditions such as the ones proposed by Bayliss and Turkel [2]. However, these local boundaries tend to perform poorly when placed close to the source of excitation. The characteristics boundary does not have this restriction and can be placed right next to the load. The only error involved in the characteristics method is the discretization error and it is thus appropriate to compare it with the methods based on convolution. A comparison of the characteristics method with local boundaries taking into account the cost of analyzing the larger interior is possible, but rather strongly problem-dependent and is out of the scope of this paper. A comprehensive cost comparison will be attempted at a later time, especially after exploring the possible improvements of the characteristics method such as the space-time mesh truncation suggested in the final section.

### 7. Numerical examples

The effectiveness of the proposed procedures is verified by the use of illustrative examples representing the problems involved in modeling wave propagation in unbounded media. The same problems are also solved using the first-order Bayliss–Turkel boundary condition in place of the characteristics method. The main purpose for this comparison is to illustrate the accurate performance of the method in cases where local boundaries tend to fail.

We start our verification process by first investigating the performance for modeling individual spherical and cylindrical harmonics. This would serve as a simple illustration of the accuracy of the proposed methods. To
verify the applicability and accuracy of the method when coupled with interior finite element method, a more representative problem of the response of a half-space under a strip load is also analyzed.

7.1. Three-dimensional wave propagation

We focus our analysis on a spherical cavity of unit radius \( R = 1 \) in an infinite acoustic medium. The material properties \( \rho \) and \( G \) are chosen to be unity. The Dirichlet data is specified on the wall of the cavity and the characteristics method is used to obtain the resulting traction. The applied displacement has the form of a spherical harmonic:

\[
    u|_{r=R} = Y_{lm}(\theta)f(t),
\]

It is clear that the resulting field variable has similar variation in \( \theta \).

\[
    u = Y_{lm}(\theta)U(r, t).
\]

The governing equation can be written in the following form:

\[
    G\left(U_{rr} + \frac{2}{r} U_r - l(l + 1)U\right) - \rho U_{tt} = 0
\]

The characteristics method is now applied to this equation. The variation of the excitation in time is chosen to be a squared-sine pulse:

\[
    f(t) = \sin^2(\Omega t) \quad \text{for } 0 \leq \Omega t < \pi
\]

\[
    0 \quad \text{otherwise}
\]

The system is analyzed to obtain the Neumann data for two cases: \( \Omega = 1 \) and \( \Omega = 2 \). The time step is chosen to be 1/8th of the duration of the loading, i.e. \( \Delta T = \pi/(8\Omega) \).

The first-order Bayliss–Turkel boundary condition [2] (which is the spherical damper in three-dimensional case), is also used to obtain the traction:

\[
    G \frac{\partial u}{\partial r} = \sqrt{\rho G} \frac{\partial u}{\partial t} + \frac{G}{R} u.
\]

For comparison purposes, frequency-domain computations in conjunction with Fourier transformation are used to obtain the exact Neumann data. \( f \) is first transformed into the frequency-domain. The exact frequency-domain stiffness is given by:

\[
    K(\omega) = \frac{\omega}{c} \frac{H_{1+3/2}(\omega R/c)}{H_{1+1/2}(\omega R/c)} - \frac{l}{R},
\]

where \( H_n \) is the Hankel function of second kind and order \( \alpha \). The exact stiffness is applied to the transformed Dirichlet data to obtain the Neumann data in frequency domain, which is then transformed back to the time domain. Note that the singular part of the exact frequency-domain stiffness is treated analytically and only the regular part is transformed. All the computations are carried out with sufficient precision such that the result can be considered exact for all practical purposes.

The above procedure is applied to a harmonic with \( l = 1 \). Figs. 7 and 8 show the comparison of the tractions resulting from the characteristics method and spherical damper with the exact one. It is clear from the figures that the characteristics method performs very well even for very coarse time discretization. The comparison for a harmonic with \( l = 2 \) is also excellent (Figs. 9 and 10). On the other hand, as expected, the spherical damper performs very poorly and the results are erroneous.

7.2. Two-dimensional wave propagation

Similar to the three-dimensional case, we analyze a circular cavity in a two-dimensional space. The applied Dirichlet data is a circular harmonic:

\[
    u|_{r=R} = \sin(n\theta)f(t).
\]
Then, the governing equation takes the form:

$$G \left( U_{rr} + \frac{1}{r} U_r - n^2 U \right) - \rho U_{tt} = 0, \quad (84)$$

and the characteristics method is now applied to this equation. The first-order Bayliss–Turkel boundary condition for two dimensions [2] is the same as the cylindrical damper:

$$G \frac{\partial u}{\partial r} = \sqrt{\rho G} \frac{\partial u}{\partial t} + \frac{G}{2R} u. \quad (85)$$

The exact frequency-domain stiffness for this harmonic is given by

$$K(\omega) = \frac{\omega}{c} \frac{H_{n+1}(\omega R/c)}{H_n(\omega R/c)} - \frac{n}{R}, \quad (86)$$

where, $H_n$ is the Hankel function of second kind and order $\alpha$.

Following a procedure similar the one for the three-dimensional case, we compare the results for the first
harmonic \((n = 1)\) in Figs. 11 and 12. The characteristics method again performs very well, whereas the cylindrical damper results in erroneous tractions.

To assess the performance of the upwinding procedure described in Section 5.3, we apply the characteristics method to axisymmetric excitation \((n = 0)\). From Figs. 13 and 14, it can be seen that the results are very accurate. It appears that the cylindrical damper also produces fairly accurate results. But it is expected that, once the representative frequency \((\Omega)\) of the applied displacement is made small, the cylindrical damper is expected to perform poorly. This is clearly illustrated in Fig. 15, which contains the results for \(\Omega = 0.25\). The characteristics method, on the other hand, retains its accuracy even at this low frequency.

7.3. Coupling with FEM

To illustrate the applicability and performance of the exterior characteristics method when coupled with the interior finite element method, a 2-D half-space is analyzed under strip loading. The details of the problem are clearly illustrated in Fig. 16(a). The variation of the traction with time is taken as a triangular pulse of width 3, so that a wide range of frequencies are excited. The objective of the analysis is to obtain the displacement response at different points on the surface of the half space, more specifically, at the left, center and right points.
under the load. Exact solution can be computed with the use of the available Green’s function for a half space [1]: An impulse of intensity \( P \) at \( x = 0, t = 0 \) produces a displacement response of the following form for \( t > 0 \):

\[
    u(t, R) = \frac{P}{\pi G} \frac{1}{\sqrt{t^2 - (R/c)^2}} H(ct - R).
\]

(87)

where \( H \) is the Heaviside function. This impulse response function is convoluted with the loading function in both space and time to obtain the displacement at desired locations.

The analysis procedure is as follows: a half-disk of unit diameter is chosen as the interior domain of analysis and the artificial boundary condition is applied on the semi-circular boundary (see Fig. 16(b)). To make the test of performance as stringent as possible, the load is applied immediately next to the computational boundary (Fig. 16(b) Loading Case – A). Finite element discretization of the interior is shown in Fig. 17: 600 bilinear finite elements with 641 nodes are used to discretize the interior. Constant average acceleration with constant time step size of 0.1 is used for time integration.

Two analyses were performed with different methods used for the exterior: one with characteristics method, and the other with first order Bayliss–Turkel boundary condition (cylindrical damper). The displacements at left, center and right points under the load are compared with the exact solution in Figs. 18, 19 and 20, respectively.
Fig. 17. Finite element mesh for the interior (600 bilinear elements).

Fig. 18. Comparison of the responses at the left of the load from different methods.

Fig. 19. Comparison of the responses at the center of the load from different methods.

Fig. 20. Comparison of the responses at the right of the load from different methods.

Fig. 21. The effect of placement of computational boundary for different methods.
The results from the characteristics method are almost indistinguishable from the exact displacements. The cylindrical damper, however, performs very poorly and the results have up to 35\% error.

To further verify the validity of placing the boundaries next to the load, the load is moved to the center, and the analyses are performed again (Loading Case - B in Fig. 16). The displacement response at the center of the load is compared for different analyses (see Fig. 21). The response does not vary with the placement of the load for the characteristics method, whereas, there is significant difference for the case of cylindrical damper. It is clear that placing the load at the center makes the cylindrical damper’s performance considerably better, but still does not compare with the results from the characteristics method. Notice that the long-term response from the cylindrical damper remains erroneous regardless of the location of the load with respect to the boundary. Thus, the characteristics boundary kept right next to the load outperforms the cylindrical damper even when it is placed far away from the load.

8. Concluding remarks

In this paper, the characteristics method developed for transient wave propagation analysis of semi-infinite layer [7] is generalized to cylindrical and spherical geometries. The characteristics method consists of a two-step procedure. First the exterior domain is discretized in the direction of the boundary such that the discretizations of the exterior and the interior coincide at the computational boundary. The resulting system of hyperbolic partial differential equations is solved efficiently using a characteristics method. This results in an efficient boundary condition that can be used with the interior problem. The simplest form of the characteristics method is applicable to the case of a homogeneous layer. For cylindrical and spherical geometries, the method is not applicable in a straightforward manner due to some stability and accuracy problems. Two main modifications are made to circumvent these problems: radial scaling of the field variable and modified integration rule for near-singular functions. The case of two-dimensional wave propagation poses further difficulties of stability because of apparent negative dispersion. The concept of upwinding from the computational fluid dynamics literature is used to stabilize this method. Numerical examples suggest that these modifications still preserve the method’s accuracy (but not the convergence properties) for practical analyses.

The boundary condition obtained from the characteristics method possesses all the desirable properties listed in the introductory section. Preliminary numerical experiments indicate that the method is convergent. They also indicate unconditional stability of the method when combined with the interior finite element formulations, suggesting that the method does not impose any restrictions on the time step size. Proofs for convergence or unconditional stability are not available at this time and are subjects of ongoing research. The characteristics boundary augments a positive definite coefficient matrix to the interior matrix and thus preserves the well-posedness of the interior problem. Compatibility of the method is always ensured as the semidiscretization of the exterior coincides with the discretization of the interior domain at the computational boundary. The computational cost for both time and storage is shown to be an order of magnitude smaller that that required for other global methods. This cost could be further reduced by truncating the growing space–time mesh. Local boundaries and their implementations for characteristic methods will be investigated at a later time. Finally, the coefficient matrices from the boundary condition are sparse and preserve the exact same sparse structure of the interior matrix.

An efficient extension of the characteristics method to azimuthally inhomogeneous media (i.e., the material properties vary only in the direction of the boundary) does not seem feasible. This is mainly due to the complicated mode coupling and presence of multiple wave speeds. For analyzing transversely inhomogeneous elastic and acoustic layers, an element-by-element procedure based on a space–time Galerkin technique has been developed [8]. Possible extensions of the characteristics method to more complicated geometries are topics of further research.

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