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Fast convolution quadrature for the wave equation in three dimensions [☆]L. Banjai ^{a,1}, M. Kachanovska ^{b,*}^a School of Mathematical & Computer Sciences, Heriot-Watt University, EH14 4AS Edinburgh, UK^b Max Planck Institute for Mathematics in the Sciences, Inselstr. 22, 04103 Leipzig, Germany

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ABSTRACT

This work addresses the numerical solution of time-domain boundary integral equations arising from acoustic and electromagnetic scattering in three dimensions. The semidiscretization of the time-domain boundary integral equations by Runge–Kutta convolution quadrature leads to a lower triangular Toeplitz system of size N . This system can be solved recursively in an almost linear time ($O(N \log^2 N)$), but requires the construction of $O(N)$ dense spatial discretizations of the single layer boundary operator for the Helmholtz equation. This work introduces an improvement of this algorithm that allows to solve the scattering problem in an almost linear time.

The new approach is based on two main ingredients: the near-field reuse and the application of data-sparse techniques. Exponential decay of Runge–Kutta convolution weights $w_n^h(d)$ outside of a neighborhood of $d \approx nh$ (where h is a time step) allows to avoid constructing the near-field (i.e. singular and near-singular integrals) for most of the discretizations of the single layer boundary operators (near-field reuse). The far-field of these matrices is compressed with the help of data-sparse techniques, namely, \mathcal{H} -matrices and the high-frequency fast multipole method. Numerical experiments indicate the efficiency of the proposed approach compared to the conventional Runge–Kutta convolution quadrature algorithm.

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1. Introduction

Many physical applications, e.g. transient acoustic or electromagnetic scattering, require the solution of the three-dimensional scalar or vector wave equation outside of a bounded obstacle. An elegant approach to treating problems that are posed in unbounded domains is offered by the use of boundary integral equations. However, compared to the field of elliptic problems, efficient solvers for time domain boundary integral equations (TDBIE) are not that extensively developed. A comprehensive review of the available methods at the time of publishing is given in [1].

[☆] A brief review of the main results of this paper has been published in the Proceedings of the 6th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2012).

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A rigorous theory of retarded potentials for the acoustic wave equation dates back to 1986 [2,3]. The numerical solution of corresponding integral equations is traditionally performed using time-domain Galerkin methods [4–8], collocation methods [9,10] or Laplace-domain approaches (see [1], as well as [11,12] for the application of the method to problems of elasticity).

Galerkin methods [4] often require the underlying spatial quadrature to be evaluated with high accuracy and become extremely complicated in the case of curved boundary elements. This kind of issue was recently overcome with the help of specially designed time basis functions, see [8,13,14].

To achieve higher accuracies, marching-on-in-time (MOT) solvers (collocation in time) require that time steps are chosen very small, which can lead to instabilities on long time intervals. To solve this problem, in [15] a new procedure for the accurate MOT matrix element evaluation was suggested. The field of fast solvers that are based on MOT is relatively well-developed. Recent advances in this field include the seminal works [16,17] on the plane-wave time-domain algorithm, [18,19] on time-domain adaptive integral equation methods and [20,21] on the nonuniform (Cartesian) grid time-domain algorithms.

An alternative approach to treating time-domain boundary integral equations was suggested by C. Lubich [22–24]. The convolution quadrature (CQ) method combines Laplace transform techniques and the usual time-stepping approach and results in a stable and efficient algorithm.

The history of the application of convolution quadrature to problems of wave propagation starts with the work [24] where multistep CQ was employed to discretize the indirect time-domain boundary integral formulation for the wave equation. In [25–27] convolution quadrature was applied to discretize the TDBIE arising from visco- and poroelasticity. For such applications convolution quadrature is of particular importance, since it requires only the Laplace transform of the fundamental solution to be explicitly known. In [28] convolution quadrature was applied to the time-domain boundary integral formulation of the wave equation with non-zero initial conditions.

In [29–31] a range of numerical experiments demonstrating properties of the convolution quadrature was conducted. The use of Runge–Kutta CQ allows to achieve arbitrary high convergence rates, see [32,33]. The use of the method does not require the application of sophisticated spatial quadratures, and hence it can be straightforwardly applied when boundary elements are curvilinear. Compared to multistep convolution quadrature, Runge–Kutta convolution quadrature has low dissipation and dispersion, see [34,35] for a quantifiable definition and analysis of these properties, as well as numerical experiments in [29]. Recent works [36,37] provide the analysis of multistep convolution quadrature combined with the Galerkin discretization for the scattering by a sound-hard obstacle, as well as suggest the procedure of the reduced convolution weight computation. In [38] the convolution quadrature formulation for the Maxwell equations was studied analytically and numerically.

To our knowledge, despite many attractive features of CQ, there exist very few fast convolution quadrature methods. Particularly, the method of [39–41], namely sparse convolution quadrature, though offering a great improvement both in the asymptotic complexity and in constants in complexity estimates, does not allow to compute the solution in linear time. Another fast algorithm, directional FMM accelerated convolution quadrature of [42], requires the solution of many Helmholtz integral formulations with wavenumbers that have large real and small imaginary part, see also [29]. Currently there are, to our knowledge, no efficient preconditioners for this kind of problems. In [43] the authors developed a multistep CQ method based on the fast multipole accelerated BEM of [44,45]. However, the complexity of this algorithm is not linear.

In this paper we propose an improved algorithm for the solution of the time-domain boundary integral equations with retarded potentials based on the Runge–Kutta convolution quadrature discretization [46]. As a model problem we consider acoustic wave scattering in three dimensions. The use of the method results in the sparsity of convolution weights [47], a property that our approach heavily relies on. We show how the application of this property combined with data-sparse techniques allows to reduce storage and computational costs required by the conventional recursive algorithm of [23]. The sparsification of convolution weights has already been employed in [39–41], but our approach is different. We construct the algorithm based on the method of originally linear complexity rather than quadratic used in [41]. Due to the recursive nature of the algorithm we are able to employ fast techniques based on analytic expansions (namely, the high-frequency fast multipole method). We also use Runge–Kutta methods instead of linear multistep ones.

This work is organized as follows. In Section 2 we state the boundary integral formulation for the wave equation, apply Runge–Kutta convolution quadrature to it and discuss some properties of Runge–Kutta convolution weights. Next, we briefly describe the conventional recursive algorithm our approach is based on. This algorithm relies on the construction of many Galerkin discretizations of single layer boundary operators for the Helmholtz equation with decay. Hence, the use of data-sparse techniques (\mathcal{H} -matrices and high-frequency fast multipole method of [48,49]) is required.

However, a simple application of these methods does not allow to avoid the evaluation of singular and near-singular Galerkin integrals (so called near-field), which in practice takes a significant part of the total computation time. For the high-frequency fast multipole method this was demonstrated in [50, Tables 3.2–3.3], and for the \mathcal{H} -matrix approximation of the Laplace boundary operators in [51] (though in the latter case the assembly of the near-field is shown to take a smaller part of the total matrix construction time). In Section 4 we review the main ideas of data-sparse techniques. In the end of the section we present a heuristic that allows to determine whether \mathcal{H} -matrices or the high-frequency fast multipole method should be applied to approximate a matrix in the course of the convolution quadrature algorithm. In Section 5 we describe an approach that allows to evaluate only a small part of singular and near-singular integrals. In the final sections

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