A superconvergent convolution quadrature method for time-dependent dynamical energy analysis

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Abstract
Dynamical Energy Analysis (DEA) was introduced in 2009 as a novel method for predicting high-frequency acoustic and vibrational energy distributions [1]. In this work we detail how DEA can be reformulated in the time-domain by means of a convolution integral operator and apply a modified multistep-based Convolution Quadrature (CQ) method to discretise in time. Stable time-stepping based on multistep CQ schemes has typically been limited to second-order convergence as a consequence of the second Dahlquist barrier. In this work we apply a simple modification to the traditional second-order backward-difference multistep scheme, which leads to third-order convergence of the time discretisation in time-dependent DEA. The final result is a fully time-dependent DEA method that can accurately track the propagation of high-frequency transient signals through phase-space.

1 Introduction

Boundary integral methods for modelling time-dependent wave propagation were originally proposed in the 1960s [2, 3]. The considerable increase in available computer power during the latter part of the twentieth century made numerical solutions over longer time intervals feasible, and with this advance long-time instabilities in the numerical solutions also became evident [4, 5, 6]. The cause of these instabilities has been linked to internal resonances of the wave scatterer for exterior problems [5], or the region being modelled for interior problems. For this reason, combined field integral equations, such as the time-dependent Burton and Miller formulation, have been proposed to tackle these stability issues [7, 8]. However, these formulations introduce additional computational overheads and the need to evaluate hypersingular boundary integral operators. An alternative is to apply the CQ method, see for example Refs. [9, 10, 11], which is able to provide stable results based on standard integral equation formulations. The reason for the preferable stability properties of CQ essentially relate to the reconstruction of the time domain solution, or alternatively the time domain boundary integral operator, through a numerical inverse Laplace transform where the contour is taken over Laplace domain frequencies with strictly positive real part. Since the resonances lie on the imaginary axis in the Laplace domain, then they do not affect the result in the time domain.

For high-frequency time-dependent wave problems, such as those arising in seismology or room acoustics, ray-tracing methods are often preferred to full wave models, see for example [12, 13, 14]. Traditional ray based methods work well for applications where only a few reflections need to be considered, but not so well for problems including multiple scattering and chaotic dynamics. In this case, multiple reflections of the rays can give an exponentially growing number of trajectories to track. Dynamical Energy Analysis (DEA) is a phase-space boundary integral method that models wave energy densities [1]. DEA is a frequency domain method formed by seeking solutions of the stationary Liouville equation, circumventing issues regarding the exponentially growing number of rays to track as time increases [15].

Time-domain simulations are important for various applications such as modelling electromagnetic scattering from conductors [16], shock-responses in structural mechanics [17] and auralisation of room acoustics [13]. In this proceedings paper we outline a methodology for extending DEA to the time-domain based on the CQ method. The computational cost of time-domain DEA should scale only linearly with the modelled time period regardless of the ray dynamics, comparing favourably with conventional ray-tracers. Furthermore, we outline a simple modification to the basic CQ method that leads to third-order convergence of our time-discretisation, even though it is based on a second-order backward-difference formula, that is, super-convergence. This methodology was recently proposed by Lehel Banjai and co-workers, with application to the wave equation, see [18, 19]. Notably, the third-order convergence of the approach is proved in [18] for a class of boundary integral operators that includes the operator arising in (time-domain) DEA.

2 Methodology

2.1 Multistep CQ for DEA in the time domain

In order to develop a time-dependent DEA method for a domain $\Omega \subset \mathbb{R}^2$ with associated wave or ray propagation speed c, the first step is to reformulate the DEA phase-space boundary integral operator to have explicit time dependence. The result is a one-sided convolution (in time t) operator $\mathcal{B}$ given by

$$(\mathcal{B}\rho_0)(t,s,p) = \int_{c|p'|\leq 1}\int_{\Gamma}(k*\rho_0)(t,s',p')\,\mathrm{d}\Gamma(s')\mathrm{d}p', \tag{1}$$

which is applied to a specified initial density distribution of rays ρ_0 on the boundary Γ. Here k is the time-dependent kernel of our boundary integral operator, which is given by a multidimensional Dirac delta generalised function specifying the propagation of a ray through time, position and momentum. The variables (s',p') relate respectively to the position (parameterised by arclength around Γ) and momentum of the starting position of a ray emanating from Γ and (s,p) corresponds to the arrival position and momentum on Γ, respectively, following a specular reflection. Note that a damping factor must be applied to obtain convergence in frequency domain DEA, but this is not necessary in the time-dependent formulation owing to the fact that we only model a finite time duration $0 \leqslant t \leqslant T$.

The CQ method can be applied for the time discretisation of one-sided convolution operators such as $\mathcal{B}$ (1), see for example [9, 10, 11]. In doing so, the convolution $(k*\rho_0)$ appearing in (1) is approximated by a discrete convolution of the form

$$(k *_{\Delta t} \rho_0)(t_n) = \sum_{j=0}^{n} w_{n-j}\,\rho_0(t_j),$$

where $t_j = j\Delta t$ and $\Delta t = T/N$ is the time-step assuming N steps in total. The convolution weights w_j are defined implicitly through the $\mathcal{Z}$-transform as

$$\sum_{j=0}^{\infty} w_j\,\zeta^j = K\left(\frac{\gamma(\zeta)}{\Delta t}\right),$$

where K denotes the Laplace transform of k and γ is the quotient of generating polynomials for the linear multistep method underlying the CQ discretisation. In this work we will use the second-order backward-difference formula (BDF2), for which

$$\gamma(\zeta) = \frac{1}{2}\zeta^2 - 2\zeta + \frac{3}{2}.$$

After applying the time-discretisation, we then need to discretise in the position and momentum variables in order to obtain a fully discrete problem. Here we may use any of the discretisation methods previously applied for frequency domain DEA amongst others, see for example [1, 15, 20] for more details. However, for the modified scheme outlined in the next section, it will be important that the spatial discretisation is performed using a boundary element method where the basis functions have only local support.

2.2 Modified CQ method

The modified CQ introduced in [18, 19] was proposed to reduce the dispersion and artificial dissipation errors arising in standard multistep CQ schemes. This modified scheme can be applied to one-sided convolutions of the form (1) provided that the kernel k is zero for early times. The approach is therefore well suited for wave or ray propagation operators where these early time zero values are associated with the time taken for a signal to reach a receiver point. In time-dependent DEA, k takes the form

$$k(t) = \delta(t - c^{-1}\|\boldsymbol{r} - \boldsymbol{r}'\|)g(s', p'), \tag{2}$$

where we have suppressed the dependence of k on the spatial and momentum variables (s', p') to simplify the presentation. Here, we have introduced g to represent the time-independent part of k, which is equivalent to the kernel of the integral operator from standard frequency-domain DEA without damping - see [20] for details. The positions $\boldsymbol{r}'$, $\boldsymbol{r}$ are the Cartesian coordinates associated with the boundary sending and receiving positions described by the arclength parameters s', s, respectively. The properties of the Dirac delta in (2) mean that $k(t) = 0$ for $t < c^{-1}\|\boldsymbol{r} - \boldsymbol{r}'\|$. The modified CQ makes use of this property by starting the convolution quadrature at a later time $t_{m+1} = (m+1)\Delta t$ corresponding to the first integer multiple of Δt for which $(k *_{\Delta t} \rho_0)(t_{m+1}) \neq 0$. Note therefore that t_m is taken to be as large as possible given that it must satisfy $t_m \leqslant c^{-1}|\boldsymbol{r} - \boldsymbol{r}'\|$ and will be defined locally relative to a boundary element discretisation in space. That is, t_m is related to the minimal travel time along all rays connecting a specified pair of boundary elements. In terms of practical implementation, we pre-compute a square matrix of t_m values whose dimension is the number of boundary elements.

Once t_m has been defined, the modified CQ method is implemented by defining a modified kernel

$$\hat{k}(t) = \delta(t - c^{-1}\|\boldsymbol{r} - \boldsymbol{r}'\| + t_m)g(s', p'),$$

with Laplace transform

$$\hat{K}(z) = e^{zt_m}K(z) = e^{-z(c^{-1}|\boldsymbol{r}-\boldsymbol{r}'\|-t_m)}g(s', p'). \tag{3}$$

We then use the Laplace (Bromwich) inversion formula to rewrite the convolution from (1) in the form

$$(k * \rho_0)(t, s', p') = \int_0^t k(t - t')\rho_0(t', s', p')\mathrm{d}t' = \frac{1}{2\pi \mathrm{i}}\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty} K(z)P_0(z, s', p')e^{zt}\mathrm{d}z, \tag{4}$$

where P_0 is the Laplace transform of ρ_0. We now introduce a modified form of the convolution (4), which is discretised using CQ to provide a modified CQ method that exploits the early time (zero) behaviour of k. Consider therefore the modified convolution

$$(k *^m \rho_0)(t) := \begin{cases} \dfrac{1}{2\pi \mathrm{i}}\displaystyle\int_{\sigma-\mathrm{i}\infty}^{\sigma+\mathrm{i}\infty} \hat{K}(z)\, P_0(z, s', p')e^{z(t-t_m)}\mathrm{d}z & \text{if } t > t_m, \\ 0 & \text{otherwise,} \end{cases} \tag{5}$$

which after discretisation will have the desired property of starting the quadrature only after the initial time delay. Note that the $\exp(-zt_m)$ factor cancels out the factor introduced when replacing K with $\hat{K}$ (see (3)), meaning that (4) and (5) are equivalent. However, we will see in the next section that the implementation of a scheme based on the modified form of the convolution (5) leads to an increase in the order of convergence from second to third-order.

3 Numerical results

In this section we present numerical results for the propagation of time-dependent ray densities inside a unit square acoustic domain Ω with vertices $[x, y] = [0, 0]$, $[1, 0]$, $[1, 1]$ and $[0, 1]$ and having sound-hard specular reflections at the boundaries. A wider range of numerical results will be presented at the conference. The source term will correspond to a plane wave emanating from the left boundary in the direction of the internal normal vector. The temporal profile is chosen to correspond to a wave described by a high-frequency sinusoidal tone burst with a Gaussian envelope. The time-dependent DEA method is applied to track the square amplitude of this wave as it propagates through the domain.

For this example there is a simple exact solution that can be used to verify the method and study its convergence. The problem set-up described above corresponds to an initial ray density of the form

$$\rho_0(t,s,p) = \chi(s)\delta(p)\left|\exp\left(-\alpha c^2(t-t_0)^2\right)\right|^2,$$

where $s = 0$ corresponds to the origin and $\chi(s) = 0$ unless $3 < s < 4$, corresponding to a position along the left edge where $x = 0$. The parameters α and t_0 are used to prescribe the position and width of the Gaussian envelope function. The exact solution for the interior density ρ_Ω can then be determined using the method of images as follows

$$\rho_\Omega(t,\boldsymbol{x}) = \sum_{j=0}^{\infty}\left[\exp\left(-2\alpha(x+2j-c(t-t_0))^2\right) + \exp\left(-2\alpha(x-2(j+1)+c(t-t_0))^2\right)\right]. \quad (6)$$

Since in practice we only model a finite time duration $0 \leqslant t \leqslant T$, the exact solution will be given by a finite number of terms from the sum (6). In this study we take $\alpha = 32$, $t_0 = 1$, $c = 1$ and $T = 4$ and as a consequence we only need the $j = 0, 1$ terms from (6) to define our exact solution.

We apply both the standard and modified BDF2 based CQ discretisations in time and compare their accuracy. The spatial discretisation uses only four piecewise constant boundary elements (one per edge of the square) and we apply the momentum discretisation from [20] with only four (global) directions $\Phi_l = (l-1)\pi/2$, $l = 1, 2, 3, 4$. The exact solution (6) is constant along each boundary edge of the square and propagates only in the directions Φ_1 and Φ_3, and so this seemingly coarse approximation is able to model both the spatial and directional dependence of the solution exactly. This example is therefore useful for studying the error introduced by the time discretisation in isolation from other sources of error.

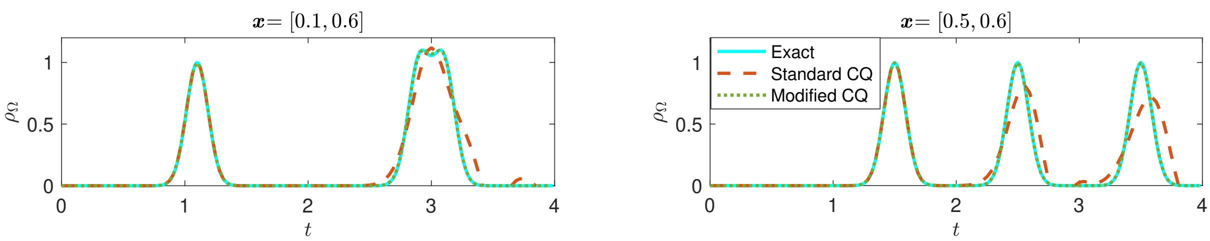

Figure 1: Comparison of the standard and modified CQ schemes for simple one-dimensional plane wave propagation at two points inside a unit square. Parameters: $N = 128$, $\alpha = 32$, $t_0 = 1$, $c = 1$ and $T = 4$.

Figure 1 clearly shows that the modified CQ scheme provides better accuracy than the standard scheme at the two interior points $\boldsymbol{x}$ considered when using $N = 128$ time-steps in each case. In order to study the enhanced accuracy of the modified CQ scheme in more detail we calculate the relative errors at both interior points via

$$\text{Error}(\boldsymbol{x}) = \sqrt{\frac{\sum_{n=1}^{N}\left(\hat{\rho}_\Omega(t_n,\boldsymbol{x}) - \rho_\Omega(t_n,\boldsymbol{x})\right)^2}{\sum_{n=1}^{N}\rho_\Omega(t_n,\boldsymbol{x})^2}}, \quad (7)$$

where $\hat{\rho}_\Omega$ is used to denote the numerical approximation to ρ_Ω given by either the standard or modified CQ scheme. For the standard CQ scheme we obtain $\text{Error}([0.1, 0.6]) = 0.1898$ and $\text{Error}([0.5, 0.6]) = 0.3519$, whereas with the modified CQ we achieve $\text{Error}([0.1, 0.6]) = 7.845 \times 10^{-3}$ and $\text{Error}([0.5, 0.6]) = 1.155 \times 10^{-8}$, showing the dramatic improvement achieved by using the modified CQ. We now study this improved performance in more detail at the interior solution point $\boldsymbol{x} = [0.1, 0.6]$.

Table 1 shows the convergence of both the standard and modified CQ schemes at the interior point $\boldsymbol{x} =$

Table 1: Relative error and estimated order of convergence (EOC) at the interior point $\boldsymbol{x} = [0.1, 0.6]$ as the time-step $\Delta t = 4/N$ is varied. Parameters: $\alpha = 32$, $t_0 = 1$, $c = 1$ and $T = 4$.

	Standard CQ		Modified CQ	
N	Error	EOC	Error	EOC
64	2.920E-1	-	5.267E-2	-
128	1.898E-1	0.62	7.845E-3	2.7
256	1.211E-1	0.65	9.477E-4	3.0
512	3.958E-2	1.6	1.834E-4	2.4
1024	1.019E-2	2.0	1.764E-5	3.4
2048	2.546E-3	2.0	2.038E-6	3.1
4096	6.360E-4	2.0	2.342E-7	3.1

$[0.1, 0.6]$ as the number of time-steps N is increased. The estimated order of convergence (EOC) was calculated using the logarithm to the base 2 of the ratio of each error value to the error value from the previous row in the table. The results show that the standard CQ eventually (for $N \geq 1024$) achieves the expected second order convergence rate inherited from the underlying BDF2 multistep scheme. However, the modified CQ method based on the same BDF2 formula achieves third-order convergence for the same range of N values. In addition, the baseline errors for the modified CQ are significantly smaller than those for standard CQ for small N values, achieving under 1% error for $N = 128$. The standard CQ scheme does not achieve errors of around 1% or lower until at least $N = 1024$. The modified CQ scheme can therefore provide significant computational cost savings when working to a fixed error tolerance.

4 Conclusions

In this short paper we have motivated and outlined a methodology to extend the DEA method for time-dependent problems, where the time-discretisation exhibits third-order convergence despite being based on a second-order multistep method. We have also presented numerical results for a simple test case providing evidence of this superconvergence. We will present an extended set of numerical results based on this work at the conference. Through these examples we will investigate whether the superconvergence phenomena observed for the simple test here is also observed for more complex geometries and different types of wave source.

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