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New high-order integral methods in computational electromagnetism

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Abstract: We present a new set of high-order algorithms and methodologies for the numerical solution of problems of scattering by complex bodies in three-dimensional space. These methods, which are based on integral equations, high-order integration and Fast Fourier Transforms, can be used in the solution of problems of electromagnetic and acoustic scattering by surfaces and penetrable scatterers—even in cases in which the scatterers contain geometric singularities such as corners and edges. The solvers presented here exhibit high-order convergence, they run on low memories and reduced operation counts, and they result in solutions with a high degree of accuracy.

1 Introduction

We present a new set of accurate Fourier methods for the numerical solution of problems of scattering by complex bodies in three-dimensional space. These methods, which are based on integral equations, high-order integration and Fast Fourier Transforms, can be used in the solution of problems of electromagnetic and acoustic scattering by surfaces and penetrable scatterers—even in cases in which the scatterers contain geometric singularities such as corners and edges. The solvers presented in this text exhibit high-order convergence, they run on low memories and reduced operation counts, and they result in solutions with a high degree of accuracy.

With regards to engineering relevance of the accuracy exhibited by high order numerical methods, it has been correctly argued that often an accuracy better than 1%-0.1% is not significant in engineering practice. (An important class of problems in which significantly higher accuracies are needed relate to low-observable applications, where the quantities of interest are small residuals of large incident fields.) In any case, it is our contention that high-order accuracy is extremely valuable in all applications, since, at the very least, it allows one to produce accurate estimates of the errors incurred in a given calculation. Indeed, estimation of the accuracy of a certain approximation requires, say, the possibility of evaluation of the solution to at least one additional digit of accuracy. With first order convergence (which necessarily results from a direct integration method or without use of high-order surface representations) this requires a refinement of a one dimensional mesh by a factor of ten. For the two-dimensional integrals we consider this translates into a factor of $10^2 = 100$ in the number of discretization points—and thus, in the number of unknowns in the problem! Clearly, refinement of a first order algorithm is generally not a viable approach for evaluation of the accuracy of a numerical solution. A high-order algorithm such as that used to produce Table 1 right, in turn, can give us an additional digit of accuracy (and, therefore, a good measure of the accuracy of a numerical solution) by a small increase in the overall size of the numerical problem. This is an extremely valuable feature in a numerical method; as indicated throughout the following text, our approaches produce such high-order accuracy by exploiting the high-order convergence of both, the integration through the trapezoidal rule and approximation via Fourier series for smooth periodic functions. Fast numerics in our algorithms results from use of $O(N\log(N)$ Fast Fourier Transforms.

This paper is organized as follows: after a brief general discussion in Section 2 on integration, interpolation and surface representation we present, in Sections 3 and 4, our direct integral solvers for surface and volumetric scattering, respectively.

2 High-order integration and interpolation of smooth functions

Many aspects of our methods resulted from consideration of the remarkable properties exhibited by the trapezoidal rule for integration of smooth periodic functions over d-dimensional cubes ($d = 1, 2, \ldots$). Of course the integrals arising in integral equation formulations involve

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surfaces which are much more complex that a square in 2-dimensions or a cube in 3-dimensions, and they require consideration of highly non-smooth integrands—which arise from both singularities in the Green functions and geometric singularities of the scatterer: edges, corners, etc. As we have shown, in spite of these singularities, appropriate transformations permit one to obtain high-order integrators for scattering problems from trapezoidal rules and Fourier series. Further, use of Fast Fourier Transforms for evaluation of Fourier series and convolutions allows for fast numerics in addition to high order accuracy. To demonstrate these facts in simple settings we preface our discussion with some considerations on the properties of the trapezoidal rule and Fourier series for one-dimensional functions under various periodicity and smoothness assumptions.

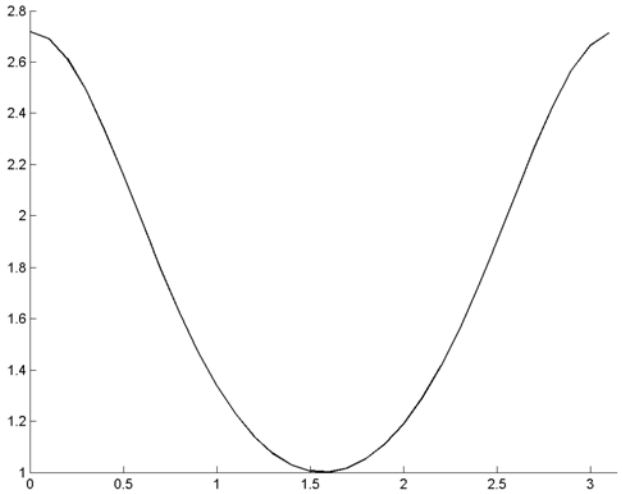


Figure 1 : $f(x) = e^{\cos^2(x)}$.

2.1 Trapezoidal-rule integration

Let us thus consider the problem of integration of a function $y = f(x)$ over a one-dimensional interval $[a,b]$. Table 1 displays relative errors and convergence ratios exhibited by the trapezoidal rule as applied to three problems—which encapsulate some relevant issues under consideration: $\int_0^{1/2} \sqrt{x}\,dx$; $\int_0^{\pi/4} e^{\cos^2(x)}\,dx$ and $\int_0^{\pi} e^{\cos^2(x)}\,dx$. From Table 1 we see that integration of the *non-smooth* function $\sqrt{x}$ results in errors larger than $O(h^2)$ for an N interval grid of mesh-size $h = (b-a)/N$: refinement of the mesh by a factor of 2 leads to error reductions by a factor smaller than 4. When applied to integration of the smooth function $f(x) = e^{\cos^2(x)}$ over the interval $[0,\pi/4]$, in turn, the trapezoidal rule results in quadratic errors: refinement of the mesh by a factor of 2 leads to error reductions by a factor of 4. In the last case in which the *smooth and periodic* function $f(x) = e^{\cos^2(x)}$ shown in Fig. 1 is integrated over its period, we see a much higher, exponential convergence rate.

The behavior exhibited by the trapezoidal rule is easy to explain. As is well known, for a general smooth function, the trapezoidal rule gives rise to quadratic errors $O(h^2)$ (see Table 1 center) since the error in the approximation of a function by its trapezoidal approximation is of the order of h^3 within each one of the $O(1/h)$ individual integration elements. As it can be checked, for the *non-smooth* function $f(x) = \sqrt{x}$, the overall errors is of the order of $h^{3/2}$ only, in accordance with the results of Table 1 left. A remarkable phenomenon takes place as the trapezoidal rule is applied to functions such as $e^{\cos^2(x)}$ which are periodic on the integration domain, and smooth for $-\infty < x < \infty$: in this case the integration errors decrease exponentially fast: see Table 1 right. Two basic facts make this extraordinary behavior possible, namely

1. The extremely fast convergence of Fourier series of smooth periodic functions [Courant and Hilbert (1953)], and,

2. The remarkable fact that, as it can be verified easily, the trapezoidal rule with $N+1$ points (N intervals) integrates exactly the Fourier harmonics $e^{i\ell x}$ for $\ell = -N \ldots N$.

From Table 1 we thus see that use of 8 integration intervals for integration of the smooth periodic function $f(x) = e^{\cos^2(x)}$ in its periodicity interval results in errors of the order of 10^{-10}. For the non-periodic integration problem in Table 1 center, an equivalent accuracy requires 8192 intervals. And, use of this highly refined mesh gives an accuracy of only 10^{-5} when the integration problem for the non-smooth function $\sqrt{x}$ is considered.

As discussed above, the integrands of the type occurring in integral equations of the type (2) below generally are neither one dimensional, nor smooth or periodic. The methods presented in the rest of this text, however, do reduce these general integration problems to problems of

N	Rel. Error	Ratio
1	4.69(-1)	
2	2.04(-1)	2.30
4	8.99(-2)	2.27
8	4.02(-2)	2.24
8192	2.72(-5)	

N	Rel. Error	Ratio
1	4.77(-2)	
2	1.19(-2)	4.03
4	2.95(-3)	4.02
8	7.36(-4)	4.01
8192	7.01(-10)	

N	Rel. Error	Ratio
1	5.50(-1)	
2	6.03(-2)	9.12
4	3.10(-4)	1.95e(+2)
8	7.17(-10)	4.32e(+5)
16	2.10(-23)	3.42e(+13)

Table 1 : Relative errors in trapezoidal-rule approximations for $\int_a^b f(x)dx$ using N intervals ($N+1$ discretization points). Left: $f(x) = \sqrt{x}$, $a = 0$, $b = 1/2$. Center: $f(x) = e^{\cos^2(x)}$, $a = 0$, $b = \pi/4$. Right: $f(x) = e^{\cos^2(x)}$, $a = 0$, $b = \pi$.

evaluation of sequences of one-dimensional integrals of smooth periodic functions.

2.2 High-order representation of functions and surfaces

Clearly, a high-order surface integrator must use high-order representations of the integration surfaces; as discussed repeatedly in the rest of this paper, further, high-order interpolation of known data is needed in the integration algorithms we use. Such high-order representations are generally not directly available, however: usually only triangulations of surfaces are provided, so that first order derivatives are discontinuous, or, at most, spline representation with continuous first order derivatives and discontinuous curvatures are provided. Since the curvature of the surface occurs as part of the double-layer integrands, a high order integration method requires several derivatives *of the curvature* to exist. Finally, high-order representation of surfaces near corners, edges and other geometric singularities, which also need to be provided, present certain special difficulties.

Previous approaches to this problem utilize piece-wise polynomial approximations, and, under certain assumptions concerning regularity of a given triangulation, have provided representations with continuous derivatives of first order. Higher order differentiability has not been produced by these means as yet, and the prospects for the feasibility of such extensions do not seem favorable: it appears that piecewise polynomial approximations may not be helpful in our context.

In the interest of brevity we only present a summary description of our approach to high-order representation (see [Bruno and Pohlman] for details). These methods arose from consideration of the properties of the trapezoidal rule and Fourier series, as described in the previous section, which suggest that representations of with high order accuracy can be produced by means of Fourier series. Further, as discussed below, a continuation method can be used for efficient high-order treatment of the surface representation problem. Clearly, the most significant obstacle for use of Fourier series in this context is presented by the Gibbs phenomenon: Fourier series of discontinuous functions converge very slowly and contain unacceptable oscillations.

A number of methods have been proposed over the years which eliminate to various extents the inaccuracies associated with the Gibbs phenomenon—and which can thus improve the convergence properties of Fourier series of discontinuous functions—, including methods that utilize frequency domain filters, Gegenbauer polynomials, basis functions with "built-in" discontinuities, and Padé approximations. Our new method, whose implementation is very simple indeed, yields super-algebraic convergence for Fourier series of discontinuous functions, it applies in an arbitrary number of dimensions, and it can be used even when only unevenly spaced data is available and in presence of irregular domains of definition. And, most importantly, it has significantly better properties of convergence and stability than other methods available at present. Our approach is based on a very simple but previously untested idea: continuation of each smooth branch of a piecewise-smooth function into a new function which, defined on a larger domain, is both smooth and periodic. These "continuation functions" have Fourier coefficients that decay super-algebraically, and thus result in high-order approximations of a given function throughout its domain of definition—even at points of discontinuity. A proof of the super-algebraic convergence of the continuation method is given in [Bruno and Pohlman], together with a variety of numerical examples demonstrating the capabilities of the continuation approach.

Results of a number of applications of our algorithm are

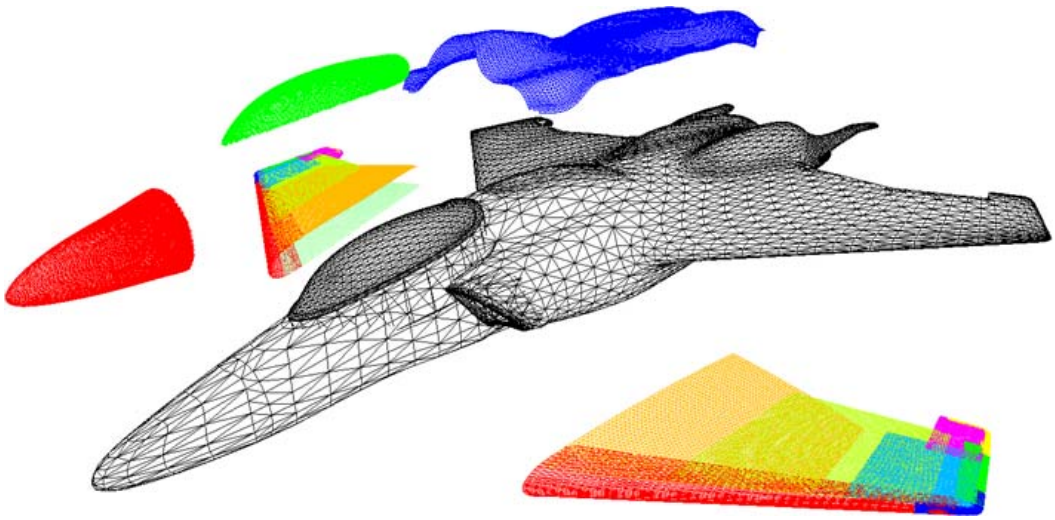


Figure 2 : Triangulation of an airplane and color-coded patches, each one of which is given by an explicit Fourier series.

presented in Figure 2: each one of the shaded surfaces is given by an *explicit* finite Fourier series.

3 Fast, high-order surface scattering solvers

(*Joint work with L. Kunyansky* [Bruno and Kunyansky (2001a), Bruno and Kunyansky (2001b), Kunyansky and Bruno]**)**

In this section we describe our Fourier-based high-order algorithms for the numerical solution of problems of scattering by surfaces in three-dimensional space. This algorithm evaluates scattered fields through fast, high-order solution of the corresponding boundary integral equations. The high-order accuracy of our solver is achieved through use of *partitions of unity* (that is, a set of windowing functions which add up to one throughout the surface), together with *analytical* resolution of kernel singularities. The acceleration, in turn, results from use of a novel approach which, based on high-order *"two-face" equivalent source* approximations, reduces the evaluation of far interactions to evaluation of 3-D FFTs. This approach is faster, substantially more accurate, and it runs on dramatically lower memories than other FFT and k-space methods. The present overall algorithm computes one matrix-vector multiply in $O\left(N^{6/5}\log N\right)$ to $O(N^{4/3}\log N)$ operations, where N is the number of surface discretization points. The latter estimate applies to smooth surfaces, for which our high order algorithm provides accurate solutions with small values of N; the former, more favorable count is valid for highly complex surfaces requiring significant amounts of subwavelength sampling. Further, our approach exhibits super-algebraic convergence, it can be applied to smooth and non-smooth scatterers, and, unlike other accelerated schemes it does not suffer from accuracy breakdowns of any kind (compare [Dembart and Yip (1998), Rokhlin (1990)] and [Labreuche (1998), p. 576]). In what follows we introduce the main algorithmic components in our approach, and we demonstrate its performance with a variety of numerical results. In particular, we show that the present algorithm can evaluate accurately in a personal computer scattering from bodies of acoustical sizes of several hundreds.

3.1 Fast high-order surface integration algorithm

For simplicity we restrict our presentation to the problem of acoustic scattering by a sound-soft obstacle. (In Section 3.2, however, numerical results for both electromagnetic and acoustic applications of our methods are given.) The relevant "combined field" integral equation is given by the appropriate combination of a single- and a double-layer potential (see e.g. [Colton and Kress (1998)])

$$(S\varphi)(\mathbf{r}') = \int_{\partial D} \Phi(\mathbf{r}',\mathbf{r})\varphi(\mathbf{r})ds(\mathbf{r}) \quad \text{and}$$

$$(K\varphi)(\mathbf{r}') = \int_{\partial D} \frac{\partial \Phi(\mathbf{r}',\mathbf{r})}{\partial \nu(\mathbf{r})}\varphi(\mathbf{r})ds(\mathbf{r}), \qquad (1)$$

Here $\Phi(\mathbf{r}',\mathbf{r}) = e^{ik|\mathbf{r}'-\mathbf{r}|}/4\pi|\mathbf{r}'-\mathbf{r}|$ is the Green function for the Helmholtz equation, and $\nu(\mathbf{r})$ is the external normal to the surface ∂D at point $\mathbf{r}$. Explicitly, given the values of the incoming wave $\psi^i(\mathbf{r})$ on ∂D, the scattered field can be obtained easily once the integral equation for the unknown density $\varphi(\mathbf{r})$

$$\frac{1}{2}\varphi(\mathbf{r}) + (K\varphi)(\mathbf{r}) - i\eta(S\varphi)(\mathbf{r}) = \psi^i(\mathbf{r}), \qquad \mathbf{r} \in \partial D \quad (2)$$

has been solved. Naturally, the possibility of producing fast and accurate solutions for our problems hinges on our ability to evaluate the integrals (1) accurately and efficiently. In attempting to develop such accurate and efficient integrators one faces two main problems, namely, accurate evaluation of the singular *adjacent interactions*—without undue compromise of speed—and fast evaluation of the voluminous number of *nonadjacent interactions* —without compromise in accuracy. In what follows we present a solution to these problems.

Partitions of unity. In order to deal with topological characteristics of closed surfaces, which are given in terms of the local parametrizations discussed in Section 2, we utilize partitions of unity. In detail, we use a covering of the surface ∂D by a number K of overlapping two-dimensional patches P^j, $j = 1, \cdots, K$, (called local charts in differential geometry) together with smooth mappings to coordinate sets H^j in two-dimensional space, where actual integrations are performed. Further, we utilize a partition of unity subordinated to this covering of ∂D, i.e. we introduce a set of non-negative smooth functions $\{w^j, j = 1, \ldots, K\}$, such that (i) w^j is defined, smooth and non-negative in ∂D, and it vanishes outside P^j, and (ii) $\sum_{j=1}^{K} w^j = 1$ throughout ∂D. This allows us to reduce the problem of integration of the density $\varphi(\mathbf{r})$ over the surface to a calculation of integrals of smooth functions φ^j compactly supported in the planar sets H^j.

Adjacent integration. Substantial difficulties in the high-order evaluation of *adjacent interactions* are caused by the singular nature of the integral kernels. While, certainly, the well-known strategy of "singularity subtraction" gives rise to bounded integrands, integration of such bounded functions by means of classical high-order methods does not exhibit high-order accuracy—since the subsequent derivatives of the integrand are themselves unbounded. The new basic high-order integrator we present is based on analytical resolution of singularities. The resolution is achieved by integration in polar coordinates centered around each singular point. The Jacobian of the corresponding change of variables has the effect of canceling the singularity, so that high order integration in the both radial and angular directions can be performed using the trapezoidal rule. Since the corresponding radial quadrature points do not lie on the Cartesian grid, a high-order, fast interpolation technique has been developed for evaluation of the necessary function values at the radial integrations points. Efficiency is of utmost importance here, since we use one such polar coordinate transformation *at each target point*. Our high order integrator exhibits super-algebraic convergence for smooth and non-smooth scattering surfaces [Bruno and Kunyansky (2001a), Kunyansky and Bruno].

Non-adjacent integration and acceleration. Our accelerator is closely related to two of the most advanced FFT methods developed recently [Bleszynski, Bleszynski, and Jaroszewicz (1996), Phillips and White (1997)]. An important common element between these two methods and our technique is a concept of equivalent (or auxiliary) sources, located on a subset of a 3-D Cartesian grid. In all three cases, the intensities of these sources are chosen to approximate the field radiated by the scatterer, which allows for fast computation of the "non-adjacent interactions" through the use of 3-D FFTs. Surface problems like the ones we consider are treated in [Bleszynski, Bleszynski, and Jaroszewicz (1996), Phillips and White (1997)] by means of equivalent sources located in a *volumetric* grid—in such a way that equivalent sources with non-zero intensities occupy *all Cartesian nodes adjacent to the scatterer*. Since the spacing of this Cartesian grid cannot be coarsened beyond some threshold for surface problems such a scheme requires a $O(N^{3/2})$ FFT. Therefore, previous FFT surface scattering solvers require $O(N^{3/2})$ units of RAM and they run in $O\left(N^{3/2}\log N\right)$ operations. Our algorithm, in contrast, subdivides the volume occupied by the scatterer into a number of (relatively large) cubic cells, and it places equivalent sources *on the faces* of those cells. As we have shown, such a design reduces significantly the sizes of the required FFTs—to as little as $O\left(N^{6/5}\right)$ to $O\left(N^{4/3}\right)$ points—with proportional improvement in storage requirements and operation count. Further, it results in super-algebraic convergence of the equivalent source approximations *as the size of the scatterer is increased*.

Resolution of singularities. To obtain resolution of the singular integrands around the ogive's conical singularities, for example, a combination of two changes of vari-

Type	Size	Unknowns	Iterations	Time/It.	ε_∞	ε_2
Non Accelerated	1λ	1568	20	69s	2.5×10^{-3}	$1.4\cdot10^{-3}$
Non Accelerated	1λ	6336	17	12m 45s	3.8×10^{-5}	$2.2\cdot10^{-5}$
Non Accelerated	1λ	25472	17	3h 27m	9.8×10^{-7}	$4.8\cdot10^{-7}$
Accelerated	10λ	34112	13	26m	3.8×10^{-4}	$2.1\cdot10^{-4}$
Accelerated	20λ	34112	14	14m	6.0×10^{-3}	$2.4\cdot10^{-3}$
Accelerated	20λ	72320	19	67m	5.4×10^{-5}	$2.1\cdot10^{-5}$

Table 2 : Scattering by an ogive. Results produced on a single processor 400MHz PC with 1Gb of RAM.

ables were used: a polar change of variables similar to that described in the section "Adjacent integration" above, followed by a polynomial change of variables which regularizes the Hölder-type singularity of the underlying density.

3.2 Surface Scattering: Numerical Results

We present results for well known and widely used test geometries: large spheres, ellipsoids, cubes and ogives; solutions with analogous accuracies and computing times for non-exact geometries have been presented elsewhere. In particular, we present comparisons with the FMM solver FISC [Song, Lu, Chew, and Lee (1998)]. The following caveat should be taken into account when considering these comparisons: our results for large spheres correspond to solutions of three-dimensional acoustic scattering problems—solutions of the Helmholtz equation— whereas the FISC data corresponds to solutions of the Maxwell equations. There are of course some differences between the Helmholtz and Maxwell problems; in particular the unknowns in the Maxwell integral equations are two-dimensional vectors, as opposed to the single scalar unknown arising in the Helmholtz integral equation. However, our methods apply to the full Maxwell problem—although our implementations do not yet include Maxwell solvers with equivalent source acceleration. Results provided by our non-accelerated Maxwell solver have already been obtained: for example, results for an electromagnetic cube of about one wavelength in diagonal were obtained with errors of the order of 10^{-4}. Implementations of our fully accelerated EM solvers for general, possibly singular surfaces are currently being produced.

Results for problems of scattering by large spheres are presented in Table 3. We see that the performance of the present methods compares very well with that of leading solvers.

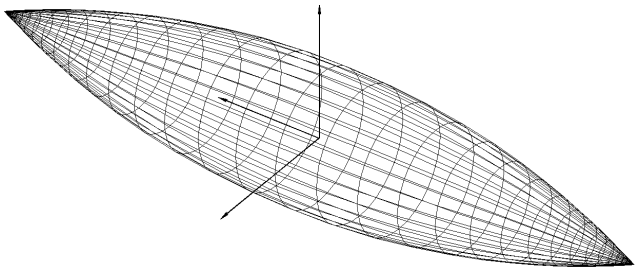


Figure 3 : Ogive geometry presented in reference [Woo, Wang, Schuh, and Sanders (1993)].

Table 3 presents results for problems of scattering by very large spheres; note the excellent accuracies provided by the algorithm in competitive running times. Table 2 displays a set of results obtained for scattering from a singular surface: the ogive depicted in Figure 3, for acoustical sizes (distances between tips) equal to 1λ, 10λ and 20λ. For the larger sizes we used the accelerator described above; note the substantial improvements in computing times resulting from the acceleration algorithm.

4 Fast, high-order volumetric scattering solvers

(*Joint work with McKay Hyde* [Bruno and Hyde (a), Bruno and Hyde (b), Hyde and Bruno] *and A. Sei* [Bruno and Sei (1997), Bruno and Sei (2000), Bruno and Sei (2003)])

Our approach to the problem of scattering by large volumetric scatterers is based, in part, on a concept of cancellation of errors: certain large errors in integrands arising by approximation of discontinuous functions by

Algorithm	Diameter	Time	RAM	Unknowns	RMS Error	Computer
FISC	120λ	$32\times 14.5h$	$26.7Gb$	9,633,792	4.6%	SGI Origin 2000 (32 proc.)
Present	80λ	$55h$	$2.5Gb$	1,500,000	0.005%	AMD 1.4GHz (1 proc.)
Present	100λ	$68h$	$2.5Gb$	1,500,000	0.03%	AMD 1.4GHz (1 proc.)

Table 3 : Scattering from large spheres.

their Fourier series can result in small errors in values of integrals—provided integrands and integrals are setup appropriately; see Section 4 below and references therein for details. Since the ideas of error cancellation have proven somewhat controversial we preface our discussion on volumetric scattering by a one dimensional example (given in the following paragraph), which illustrates this phenomenon in a simple setting. Then in Section 4 we present our volumetric scattering solver.

The proposed concept of error cancellation may be readily illustrated by means of an elementary numerical example: use of Fourier expansions to produce high-order numerical evaluations of an integral of the form $\int_0^1 f(\theta)g(\theta)d\theta$, where (i) f is a discontinuous periodic function, and where (ii) g is a function which is continuous together with its derivative, but whose second derivative is discontinuous. For this example we use the functions

$$f(\theta)=\begin{cases} 1 & 0\le\theta<1/4 \\ -1 & 1/4\le\theta<3/4 \\ 1 & 3/4\le\theta\le 1 \end{cases}$$

and

$$g(\theta)=\begin{cases} \theta^2/2 & 0\le\theta<1/4 \\ -\theta^2/2+\theta/2-0.0625 & 1/4\le\theta<3/4 \\ (\theta-1)^2/2 & 3/4\le\theta\le 1 \end{cases}$$

see Figure 4; we have $\int_0^1 f(\theta)g(\theta)d\theta=-1/48$. The discontinuities of f and the degree of smoothness of g correspond, respectively, to those of the refractive index n and the scattered field u *for a soft acoustic scatterer with a discontinuous refractive index*.

In analogy with some aspects of our method, here we proceed to evaluate the integral of fg by replacing f and g by their respective Fourier series truncated to order F—including modes between $-F$ and F only—, evaluating their *pointwise* product, and integrating the result by means of the trapezoidal rule—with N_θ points and mesh-size $h=1/(N_\theta-1)$. [We emphasize here that the Fourier coefficients of the discontinuous function f should be accurate, and could not therefore be produced by a simple integration rule. Fortunately, it is not hard to produce accurate Fourier coefficients for f, as it is generally the case for the Fourier coefficients of a given distribution n of refractive indexes: either closed expressions or simple one-dimensional high-order integration rules "by-pieces" can be used.] The accuracies resulting from these operations are displayed in Table 4. We see that the error in the approximate integral is of the order h^3, in spite of the Gibbs phenomenon and the low order convergence of the series for the discontinuous function f. This cancellation of errors can be explained through consideration of the error arising in the zero-th order coefficient of the function fg as a result of the truncations used, [Bruno and Hyde (a)]. Naturally, even higher order convergence results for smoother functions f and g (or n and u). We point out, however, that, even in the most singular case considered here, it suffices to use 64 points to produce results with an accuracy better than full single precision. Tight error estimates for the numerical method presented in this paper are given in [Bruno and Hyde (a)].

F	N_θ	Absolute Error	Ratio
2	4	3.0 (-4)	
4	8	4.8 (-5)	6.3
8	16	6.5 (-6)	7.4
16	32	8.3 (-7)	7.8
32	64	1.0 (-7)	8.3

Table 4 : Convergence test for the evaluation of $\int_0^1 f(\theta)g(\theta)d\theta$ as a function the number of modes N used for f and g.

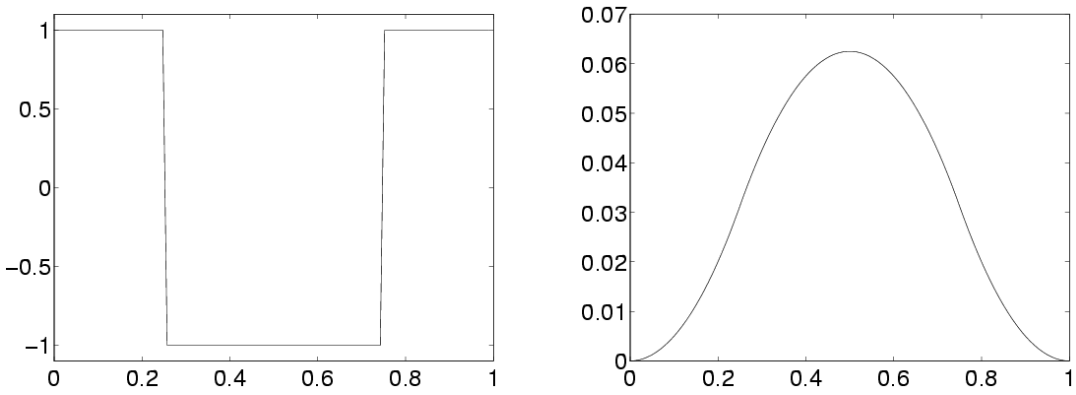


Figure 4 : The functions f and g.

In what follows we consider scattering of an incident field by an inhomogeneous medium, according to the Helmholtz equation: The total field $u = u^i + u^s$ solves both the Helmholtz equation [Colton and Kress (1998), p. 2],

$$\Delta u + \kappa^2 n^2(x) u = 0, \;\; x \in \mathbb{R}^3,$$

and the Lippmann-Schwinger integral equation [Colton and Kress (1998), p. 214]

$$u(x) \;\; = \;\; u^i(x) - \kappa^2 \int_\Omega g(x-y) m(y) u(y) dy, \qquad (3)$$

where $g(x) = \frac{1}{4\pi} \frac{e^{i\kappa|x|}}{|x|}$ is the Green's function for the Helmholtz equation in three dimensions and $m = 1 - n^2$.

As is well known, the complexity of the integration associated with this integral equation can be reduced to $O(N \log N)$ operations through use of the fast Fourier transform (FFT). Perhaps the most familiar such method is the *k*-space or conjugate-gradient FFT method (CG-FFT) [Bojarski (1982), Xu and Liu (2001), Zwamborn and Van den Berg (1992)], in which the convolution with the Green's function is computed via a Fourier transform (computed with an FFT) and multiplication in Fourier space. Although this method provides a reduced complexity, it is only first-order accurate. This low-order accuracy arises because the FFT provides a poor approximation to the Fourier transform when, as in this case, the function is not smooth and periodic.

Although our methods also use FFTs to achieve a reduced complexity, they yield, in addition, *high-order accuracy*. To our knowledge, only limited attempts have been made at devising high-order methods for this problem. Liu and Gedney [Liu and Gedney (2000)] proposed a $O(N^2)$ locally corrected Nyström scheme for scattering in two dimensions. This method provides high-order convergence rates that are not limited by the regularity of the scatterer, but it does not possess the desirable low operation counts of Fourier based methods. Vainikko [Vainikko], on the other hand, proposed a method for smooth scatterers that is related to our approach. In this method, the integral equation is modified to produce a periodic solution by cutting off the Green's function (either smoothly or discontinuously) outside a cube that is at least twice as large as the scatterer. The solution to the modified integral equation is smooth and periodic on this larger cube and, furthermore, agrees with the true solution on the support of the scatterer. Thus, for smooth scatterers, the solution is smooth and periodic and can, therefore, be approximated to high-order with a truncated Fourier series. However, the convergence rates of this approach lag significantly behind those of our approach—producing only first-order convergence in the case of discontinuous scatterers. Vainikko introduces a completely different approach for piecewise-smooth scatterers that produces $O(h^2(1+\log h))$ convergence in both the near and far fields, where h is the discretization spacing in each direction. This approach requires that for each level of discretization, one must approximate the volume fraction of each cell that lies on each side of a discontinuity in the refractive index. This seems rather difficult to obtain, especially for complicated scatterers in three dimensions. This contrasts with the limited geometrical requirements of our method, in which various portions of a scatterer can be treated separately to finally assemble the Fourier

series of the overall refractive index distribution as a sum of the Fourier series for the refractive indexes of the components.

Our goal is to obtain an FFT-based method (thereby yielding $O(N\log N)$ complexity) that is also high-order accurate. As is well known, the trapezoidal rule can be used to evaluate convolution integrals and Fourier coefficients and, in these cases, is algorithmically equivalent to the FFT. Also, FFTs can efficiently evaluate a truncated Fourier series on a set of equally-spaced grid points. However, the trapezoidal rule yields high-order convergence only for *smooth and periodic* integrands and similarly, truncated Fourier series exhibit high-order convergence only when approximating *smooth and periodic* functions.

For these reasons, a primary obstacle to the development of a high-order, FFT-based method is the lack of regularity in the scatterer. Hence, perhaps the most important aspect of our approach is the substitution of the scatterer by an appropriate Fourier-smoothed approximation. This approach counters conventional wisdom: a Fourier approximation of a discontinuous function necessarily yields low-order convergence. However, as shown in the example of Section 4 above, through our computational examples and as we have proven rigorously [Bruno and Hyde (a)], an *appropriate* numerical integration of such a Fourier approximated function does indeed yield high-order accuracy.

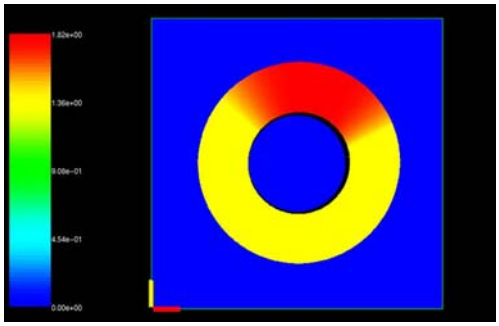
Another obstacle to the development of a high-order method concerns the Green's function. There are two ways to evaluate the convolution by means of FFT-based method. First, one could evaluate the convolution by means of the trapezoidal rule. However, even with the Fourier-smoothed scatterer, the polar singularity in the Green's function produces first-order convergence. Alternatively, one could approximate the convolution operator $K[u](x)$ (see (3)) itself by means of a truncated Fourier series. However, although $K[u](x)$ is smooth, because of the slowly decaying tail of the Green's function, it is not periodic. Hence, the Fourier series converges to first-order only.

To overcome these difficulties, we decompose the Green's function by means of a smooth partition of unity into 1) a smooth part with infinite support and 2) a singular part with compact support. The convolution with the smooth part of the Green's function is computed to high-order by means of the trapezoidal rule. Finally, the convolution with the singular part is computed to high-order by approximating the (now smooth and periodic) operator by a truncated Fourier series. Each one of these convolutions is computed using FFTs yielding high-order accuracy and a total complexity of $O(N\log N)$. We thereby obtain a method that is as simple and efficient as the CG-FFT method, but, which, unlike the CG-FFT, yields high-order accuracy.

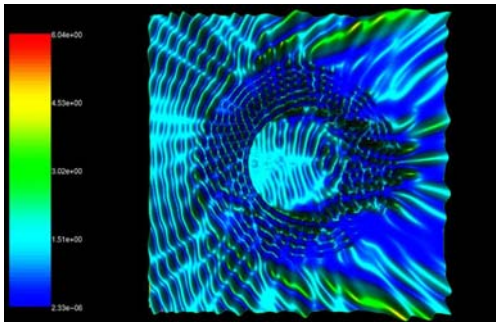
4.1 Large penetrable bodies: Numerical Results

The numerical results of this section demonstrate both, the $O(N\log N)$ complexity as well as the high-order convergence rate of our method. We first consider the two-dimensinonal scatterer containing the refractive index distribution indicated in Figure 5. Next, we present a problem of scattering for a piecewise-constant (discontinuous) layered sphere in three dimensions, for which the analytical solution is known. Finally, we consider in Figure 7 a $5\times 5\times 5$ array of scattering potentials. Except in the case in which the exact solution is known, errors are evaluated through comparison of the computed solution with the solution obtained for a significantly finer discretization.

These examples demonstrate both the $O(N\log N)$ complexity as well as the high-order convergence rate of the method. In particular, the method seems to yield significantly more than second-order convergence in the near field and third-order convergence in the far field for the discontinuous scatterers. Furthermore, the method allows one to construct quite complicated scatterers with limited effort.



(a) Scatterer ($q = -m = n^2 - 1$)

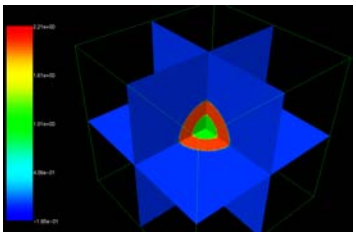


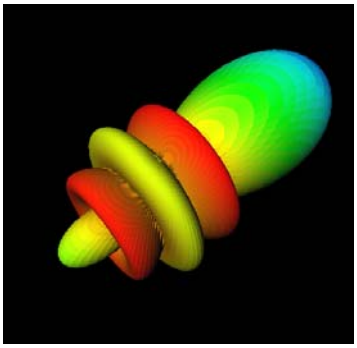
(b) Near Field Intensity ($|u|^2$)

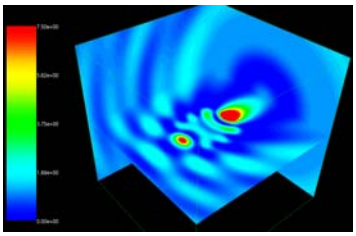
M	N_r	N	Memory	Iter.	Time	Near Error	Ratio	Far Error	Ratio
60	102	12K	19M	54	36s	2.16e-5		7.33e-9	
120	102	25K	39M	54	72s	4.81e-7	44.91	1.06e-11	691.51
240	102	50K	75M	54	160s	1.05e-8	45.81	4.50e-12	Conv.
480	102	99K	150M	54	331s	4.76e-10	22.06	4.52e-12	Conv.
960	102	198K	305M	54	561s	1.36e-11	35.0	4.61e-12	Conv.
1920	102	396K	609M	54	1172s	1.94e-12	Conv.	4.72e-12	Conv.

(c) Convergence Results

Figure 5 : Two-dimensional scatterer. Diameter $= 10\lambda$







(a) Scatterer ($q = n^2 - 1$) (b) Far Field Intensity ($|u_\infty|^2$) (c) Near Field Intensity ($|u|^2$)

Discretization	Time (s) $\times$ #CPUs	Max. Far Field Error
$10 \times 10 \times 10$	2.15×1	0.146
$20 \times 20 \times 20$	15.6×1	4.56(-3)
$40 \times 40 \times 40$	125×1	9.55(-4)
$80 \times 80 \times 80$	1119×1	5.43(-5)
$160 \times 160 \times 160$	475×32	7.11(-6)

(d) Convergence Results

Figure 6 : Layered Sphere – $\kappa a = 4$

(a) Scatterer ($q = n^2 - 1$) (b) Far Field Intensity ($|u_\infty|^2$) (c) Near Field Intensity ($|u|^2$)

N	Time (s) $\times$ #CPUs	ϵ_u^{nf}	Ratio	ϵ_u^{ff}	Ratio
$10 \times 10 \times 10$	2.15×32	3.70		43.0	
$20 \times 20 \times 20$	15.6×32	1.35	2.73	10.6	4.05
$40 \times 40 \times 40$	125×32	4.80(-2)	28.2	8.66(-2)	122
$80 \times 80 \times 80$	1119×32	8.28(-3)	5.79	4.47(-2)	1.94
$160 \times 160 \times 160$	475×32	6.48(-5)	128	7.76(-5)	576

(d) Convergence Results

Figure 7 : Array of Smooth Scatterers (Potentials)– $6\lambda \times 6\lambda \times 6\lambda$

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