Analysis of boundary element methods for high-frequency scattering simulations

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In the context of acoustic or electromagnetic waves, the classical issues that arise in connection with numerical simulations for other applications are additionally augmented with the intrinsic complexities (i.e. oscillations) of the quantities themselves. Still, very efficient methodologies (based on, for instance, finite elements, finite differences or boundary integral equations) have been devised to simulate the propagation of acoustic and electromagnetic waves in rather complicated settings. The very nature of these classical approaches, however, limits their applicability at high frequencies since the numerical resolution of field oscillations translates in a commensurately higher number of degrees of freedom and this, in turn, can easily lead to impractical computational times. For higher frequencies, accordingly, the only practical recourse is to resort to asymptotic methods (e.g. ray tracing) as these by-pass the need for frequency-dependent discretizations. These methods, on the other hand, are not error-controllable since they solve an approximate model instead of the original equations (e.g. the eikonal equation instead of the Helmholtz equation or the Maxwell system).

In this report, we survey a class of recently developed numerical schemes that *combine* the advantages of rigorous solvers (*error controllability*) with those of asymptotic methods (*frequency-independent discretizations*), and that therefore result in efficient and accurate simulators applicable throughout the frequency spectrum.

These algorithms pioneered by Bruno et. al. [4] in the context of singlescattering configurations (later extended by Bruno et. al. [5] to allow for the treatment of multiple scattering effects) are based on the solution of suitably chosen integral-equation formulations of the scattering problem, and they rely on three main elements, namely: 1) the use of an "ansatz" for the unknown surface currents which reduces the integral equation to one for a slowly varying modulation; 2) specialized quadrature rules for the new integral equation that take advantage of the highly-oscillatory nature of the kernel, and 3) full resolution of shadowing transitions with discretizations that are adapted to their boundary-layer structure. The results in [4] clearly demonstrate the attainability of solutions within a prescribed error-tolerance in times that do not depend on the wavenumber k. An actual proof that provides a rigorous upper bound for the operation count of $\mathcal{O}(k^{1/9})$ in the case of circular/spherical boundaries was recently established by Dominguez et. al. [7] for a p-version boundary element implementation of a similar approach where, using the exponential decay (with increasing wavenumber k) of the surface current in the deep shadow region, they approximate this quantity by zero there as in [4]. Our contribution in this direction has been the design of two new Galerkin schemes [6] where we have shown that the error in best approximation of the surface current grows at most at $\mathcal{O}(k^{\epsilon})$ (for any $\epsilon > 0$) for the first algorithm, and at $\mathcal{O}(\log k)$ for the second one (based on a novel change of variables around the transition regions) over the entire boundary.

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Returning to the treatment of multiple scattering effects, as we have found out, a fundamental step in understanding the high-frequency features of multiple scattering iterations is the derivation of accurate asymptotic expansions for the densities that are sequentially induced on the surface of the scatterers. Indeed, when a multiple scattering orbit is considered, the field diffracted from the surface of the m-th obstacle acts as an incidence impinging on the (m+1)-st surface and, thus, it generates a current therein. As we have shown in [1, 10], this allows one to recover the *symbolic classes* (in the sense of Hörmander) of the multiple scattering iterates; and this, in turn, enables one to derive their high-frequency asymptotic expansions that turn out to be *uniform* perturbations of order $\mathcal{O}(k^{-1})$ of a discrete dynamical system determined by the open billiard flow in the region exterior to the obstacles.

In two-dimensions [10, 11, 9], these expansions show that if an optical ray arrives at a point on the boundary of a scatterer after m transverse bounces, then (asymptotically) the current at that point equals the current at the (m-1)-st reflection-point times a continued fraction determined by geometric properties of the corresponding ray path; consequently, the current at that point is a perturbation of order $\mathcal{O}(k^{-1})$ of the product of m (recursively defined) continued fractions determined by the entire ray path. In three-dimensional settings, on the other hand, and for the scalar acoustic case [1], these continued fractions are replaced by expressions in the form of two-dimensional continued fractions; a distinctive property of these expressions, when compared to their two-dimensional counterparts, is that they depend smoothly on the relative angle of rotation between the principal axes of the successive reflection points of the optical rays. The fully three-dimensional vector electromagnetic expansions in [8], in turn, show that at each reflection the asymptotic currents are, as they ought to be, tangential to the surfaces and, most importantly, that they undergo a rotation and a projection onto the surface perpendicular to the reflection vector, followed by a second rotation and a projection onto the tangent space at the point of arrival.

To analyze these asymptotic expansions for a collection of convex structures, a fundamental observation relates to the convexity of wavefront sets corresponding to successive wave reflections. This has resulted in a rather technical analysis yielding a proof that the ratios of high-frequency asymptotic expansions of multiple scattering iterates on a periodic orbit converge to an *explicitly computable* complex number (vector) \mathcal{R}_k in the form of a wavenumber dependent phase term modulated by a (real) amplitude. Moreover, we have shown that this latter convergence is *exponential* in the number of reflections, *uniform* over the *entire* boundaries, and that the analysis is *optimal* with regards to the length of the periodic orbits.

Even though, as our work has shown, the multiple-scattering series converges spectrally, it is clearly desirable to design mechanisms to accelerate its convergence. In this connection, an essential consequence of our analysis is that the ratio of iterated currents differing by one period stabilizes after a *frequency dependent* number of reflections which grows only *logarithmically* with increasing frequency.

Accordingly, once stabilized, the behavior of the series resembles an $\mathcal{O}(k^{-1})$ perturbation of a geometric series which, in turn, can be well approximated by rational functions. This, as we have shown, completely *clarifies* the enhanced convergence properties of the Padé approximation procedure when applied to the multiple-scattering series [5].

Moreover, based on the stabilization properties of the series, we have further devised two alternative acceleration algorithms that, as opposed to Padé approximants, do not require the solution of a linear system. The first algorithm makes explicit use of the derived rate of convergence formulas and provides an $\mathcal{O}(k^{-1})$ improvement once the series stabilizes. The second, in contrast, is based on the fact that the series itself is a perturbation of a geometric series and it provides a further significant reduction in the number of single-scattering problems necessary to solve the overall problem within a desired accuracy. Finally, for cases wherein the aforementioned convergence is slow, we have shown that utilization of a new post-processing algorithm based on a novel use of Krylov-subspaces provides a further significant reduction in the number of iterations while still retaining the frequency-independent computational cost [2, 3].

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