Chapter 6

Conclusions

In this thesis, we have introduced a new, fast, high-order method for scattering by inhomogeneous media in three dimensions. This approach was motivated in part by the fast, high-order method in two dimensions introduced in [13]. In an attempt to allay the controversy generated by the claim of high-order accuracy, we proved, in Chapter 2, that this method indeed achieves high-order accuracy even in the case of discontinuous scatterers—yielding, in this case, second-order convergence in the near field and third-order convergence in the far field. We emphasized the interesting dependence of the convergence rate on the regularity of the scatterer, i.e., the convergence rates in the far field jump from third-order for discontinuous scatterers to fifth-order for $C^{0,\alpha}$ scatterers and to seventh-order for $C^{1,\alpha}$ scatterers (assuming they are also piecewise smooth).

In Chapter 3, we presented several improvements to the numerical implementation of this two-dimensional method. In particular, we achieved increased efficiency and stability through a new Chebyshev-based radial integration scheme and a new preconditioner. Also, the new method for computing scaled Bessel functions (see Appendix B) proved to be of great practical importance.

The high-order accuracy in the two-dimensional method is based on high-order trapezoidal rule integration and Fourier approximation of smooth and periodic functions. These ideas motivated the development of the three-dimensional method, as introduced in Chapter 4. By decomposing the Green's function into a smooth part with infinite support and a singular part with compact support, we were able to make use of both high-order trapezdoial rule integration and high-order Fourier approximation in computing the required convolutions. The rather counterintuitive method of Fourier smoothing played a central role in achieving high-order accuracy for discontinuous scatterers.

In Chapter 5, we demonstrated the efficiency and high-order accuracy of these numerical methods through several computational examples. These examples served to verify the theoretical convergence rates of the two-dimensional method. We also demonstrated the high-order convergence of the radial integration scheme. We illustrated the effectiveness of the preconditioner. Finally, we presented results from parallel runs of the three-dimensional method. In particular, we sought to emphasize the power and versatility of the three-dimensional method in constructing complicated scatterers for which high-order accurate solutions can then be computed.

Many interesting problems still remain. Perhaps one of the most important research problems is the development of a preconditioner for the three-dimensional case. The dramatic growth of the number of required iterations with problem size remains one of the most fundamental obstacles to solving realistic problems of hundreds or even thousands of wavelengths in size.

A related issue concerns the scaling of the unknowns with the wavelength. In three dimensions, doubling the frequency requires a doubling of the grid points in each direction, yielding a factor of *eight* increase in unknowns. This doubling of discretization points is required to resolve the highly oscillatory fields. If, instead, one could factor out the dominant, highly oscillatory modes of the solution so that one would not need to explicitly resolve them, then the remaining smoothly varying function could be discretized with relatively few points. A similar approach, often called enveloping, is taken in paraxial approximations since the dominant propagation direction is known [7, 21, 23]. Also, previous work focusing on the application of multigrid to scattering problems [11, 40] made use of similar ideas.

Since FFT-based methods require, in general, equally spaced discretization points, it is not straightforward to implement adaptive discretization strategies. At the same time, there are certainly problems for which the availability of an adaptive method could save considerable time and memory. Hence, we want to consider adaptive approaches such as (smoothly) decomposing the scatterer into several pieces, each of which has a different discretization level. Interactions between these pieces could be computed through use of equivalent sources (see [12] for more details).

Finally, we are interested in extending these methods to other specific application fields such as materials science, particularly electron diffraction. In electron diffraction, the

Lippman-Schwinger integral equation (1.6) arises from the Schrödinger equation [27, p. 141]. In spite of similarities with the problems considered in this text, such materials science problems give rise to important differences. In particular, a crystal lattice, because of its size relative to the lattice spacings, is considered an infinite periodic structure. Extension of our methods to this problems is not straightforward, but the benefits of a fast, high-order accurate method would, we believe, prove quite useful in this field.

We believe research along these lines would lead to significantly improved capabilities in computational scattering. It is our hope that such methods in computational scattering will play an important role in advancing scientific understanding and engineering capabilities in a variety of fields.