Nanostructures and Computation

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Introduction

Photonic crystals and nanophotonics employ nanoscale optical structures, on the scale of the wavelength of light, in order to produce optical phenomena far different from those in more homogeneous media. Our work has centered on three general categories of problems in nanophotonics: what new effects and devices can one achieve in such structures, how does one design devices given so many degrees of freedom, and what higher-level understanding can one develop for such complex systems. Electromagnetism also permits large-scale brute-force simulations that are essentially exact, and this has led us to a second topic of research, that of efficient numerical methods for large-scale computation. Not only have we studied advances in methods specific to electromagnetism, but we also investigate the theory and implementation of algorithms, such as FFTs, that are important for many ares of scientific computing.

1. Fast Algorithms for Spectral Methods and Signal Processing

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Project staff:
Prof. S. G. Johnson, Dr. M. Frigo

Fast Fourier Transform (FFT) algorithms play a central role in many areas of scientific computing, from digital signal processing to spectral methods for solving partial differential equations, and are one of the fundamental building blocks of numerical analysis. Although considerable effort has gone into the development of efficient FFT implementations on modern computers, and we have even developed automatic techniques to optimize FFT programs (Frigo and Johnson, 2005), there has been very little progress in the underlying theory of FFT algorithms, and in particular there had been almost no progress for nearly 40 years in the underlying arithmetic counts of the algorithms. In 2007, we published a new FFT algorithm that improved these counts for the first time since 1968.

All known algorithms compute an FFT of length N in $O(N \log N)$ arithmetic operations, but the fundamental limits of the algorithms are poorly understood. It is not even known whether $O(N \log N)$ is a lower bound on the complexity. Furthermore, there are many different FFT algorithms with different constant factors in the $O(N \log N)$, and one wishes to know what is the "optimal" algorithm in some sense. Because additions can often be traded off for multiplications or vice versa, the question is typically phrased: *what is the minimum exact total count of real additions and multiplications for an FFT of size* N*, in particular for* N *a power of 2*? No rigorous minimum is known, but since 1968 the minimum count had been exactly $4N \log_2 N - 6N + 8$, achieved by the split-radix algorithm, and not a single further multiplication or addition was saved for almost 40 years. Because of this complete lack of improvement, despite thousands of papers on the subject, by the 1990s split-radix was widely conjectured to be optimal in this regard.

In 2004, in unpublished work, a correspondent of ours (J. Van Buskirk) first broke the split-radix operation count via hand optimization for N=64. Subsequently, we have shown how to generalize these savings to arbitary power-of-two N via a straightforward recursive modification of the

conventional split-radix algorithm. In doing so, we showed that not only are some operations saved, but the asymptotic constant factor is reduced from $4N \log_2 N$ to ${}^{34}/_{9}\, N \log_2 N$. The basic idea of the new algorithm is simply a recursive rescaling of the sub-transforms of the split-radix FFT, where the sub-transforms are scaled in such a way as to cancel certain constant factors and hence to reduce the number of required multiplications. It turns out that the best choice of rescaling factor has a self-similar fractal pattern that is interesting in its own right, as shown in figure 1 below.

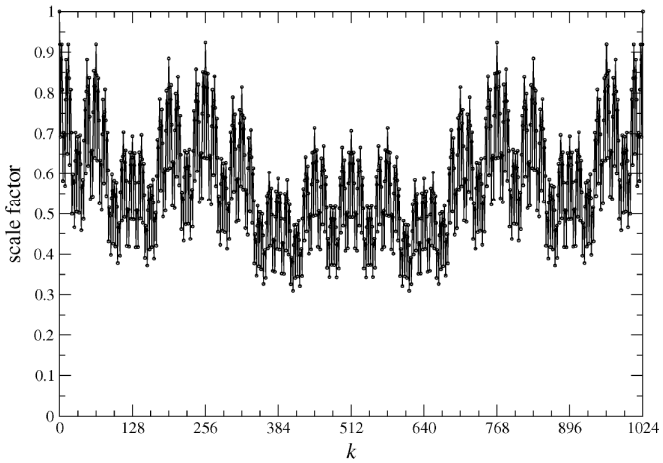

figure 1. The fractal rescaling factor for a sub-transform of size N=4096 in order to achieve the new minimum-operation FFT.

This 6% improvement in a count long thought to be optimal immediately re-opens the question of whether further improvements are possible. Furthermore, it leads to immediate improvements in related transforms, such as the discrete cosine transforms used for audio and image compression.

2. Numerical Methods for Design in Electromagnetism

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The most common and general computational methods for numerical electromagnetism typically involve discretizing Maxwell's equation over some form of grid or mesh. Most notably, the finite-difference time-domain (FDTD) method, one of the most widespread techniques, uses a uniform Cartesian grid. When faced with material interfaces where the refractive index changes discontinuously, however, such methods face degradation in their accuracy due to "staircasing" of the interface; more precisely, the accuracy degrades because of the discontinuities in the underlying electromagnetic fields. For example, standard FDTD schemes are reduced from second-order accuracy (error quadratic in the resolution) to linear accuracy (error linear in resolution). Besides the accuracy problems, the discretization of sharp interfaces causes problems for design of electromagnetic structures: because the geometry can only be changed one "pixel" at a time, powerful continuous optimization techniques are inapplicable. We address both of these techniques by showing that new developments in perturbative methods lead to an

accurate way to “smooth” the structure, removing discontinuous interfaces without degrading the structure.

Smoothing discontinuous interfaces in numerical methods is an old idea, and several such techniques have been proposed for FDTD. However, by smoothing the dielectric function, one is changing the geometry of the structure, and hence this smoothing can actually make the errors worse. A few years ago, however, we developed a correct perturbation theory for boundary perturbations in electromagnetism (Johnson et al., 2002), and we have now shown that such a perturbation theory directly leads to an accurate smoothing method (Farjadpour et al., 2006). In particular, one simply designs a smoothing of the dielectric function so that the resulting first-order perturbation in the solution is zero. This preserves the underlying second-order accuracy of the FDTD method, results in errors far lower than other smoothing methods, and is furthermore constructed to give the correct derivative when changing the geometry—the last property being critical for continuous optimization methods.

An example of the resulting improvement is shown in figure 2, below, for a two-dimensional eigenfrequency calculation in FDTD. The new method (hollow blue squares) exhibits by far the lowest absolute errors (often by an order of magnitude) when compared to other previous smoothing algorithms and also to no smoothing. By doubling the smoothing radius (or by extending the plots to higher resolution), we can also see that the new method (solid blue squares) restores the underlying quadratic convergence of FDTD, compared to the clear linear convergence displayed by the other smoothing methods (many of which have larger errors than no smoothing at all).

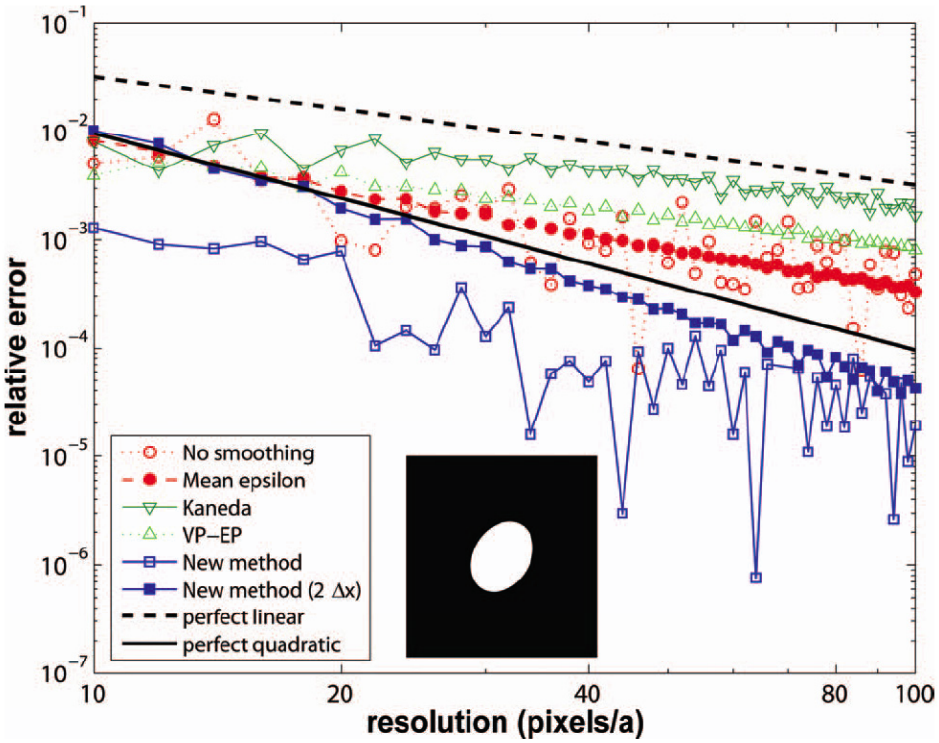

figure 2. Error in eigenfrequency, versus FDTD resolution, for a square lattice (period *a*) of elliptical air holes in dielectric (ε=12) (one unit cell is inset). Various smoothing methods are compared, along with no smoothing at all (hollow circles). No smoothing leads to erratic errors, while the new smoothing method leads to both the lowest absolute error, and also asymptotically restores quadratic convergence. Straight lines showing linear (dashed black) and quadratic (solid black) convergence are shown for comparison.

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