"The Nonuniform FFT, Image Reconstruction and Heat Flow"

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Summary

A major recent initiative in our group concerns nonstandard numerical applications of Fourier analysis. An essential algorithm in this context is the non-uniform fast Fourier transform (NUFFT). In a typical problem, one is given an irregular sampling of N points in the frequency domain and is interested in rapidly reconstructing the corresponding function at N points in the physical domain. The NUFFT carries out this computation in O(N log N) operations. Based in part on this algorithm, we have developed a fast and accurate reconstruction method for magnetic resonance imaging. We have also demonstrated that a new class of Fourier-space methods, making use of the NUFFT, is likely to have substantial impact on the design of robust methods for the solution of the heat equation in complex geometry. This approach has a natural extension to low speed, incompressible flows and we are planning to create a new class of design tools for microfluidics and other low Reynolds number applications in the next few years.

The non-uniform Fourier transform arises in a number of application areas, from medical imaging to the numerical solution of partial differential equations. In a typical problem, one is given an irregular sampling of N points in the frequency domain and is interested in reconstructing the corresponding function in the physical domain. When the sampling is uniform, the Fast Fourier Transform (FFT) allows this calculation to be computed in O(N log N) operations rather than O(N^2) operations. Unfortunately, when the sampling is non-uniform, the FFT does not apply.

Over the last decade, beginning with the work of Dutt and Rokhlin, a number of algorithms have been developed to overcome this limitation, which we will refer to generically as *non-uniform FFTs* (NUFFTs). These rely on a mixture of interpolation and the judicious use of the FFT on an oversampled grid. In a sequence of papers [*Greengard and Lee, SIAM Review (2004), Lee and Greengard, J. Comput. Phys. (2005)*], we observed that one of the standard interpolation or "gridding" schemes, based on Gaussians, can be accelerated by a significant factor without precomputation or storage of the interpolation weights. This is of particular value in two and three dimensional settings, accelerating the NUFFT schemes by an order of magnitude.

In magnetic resonance imaging, we have shown that the NUFFT together with a new approach to quadrature in the Fourier

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domain leads to fast and accurate image reconstruction using the kinds of experimental data acquired in "fast" imaging modalities [*Greengard, Lee and Inati, Comm. App. Math. and Comp. Sci (2006)*].

Heat Flow

We have developed a fast solver for the inhomogeneous heat equation in unbounded domains. While the most commonly used approaches are based on finite difference and finite element methods, these must be coupled to artificial (non-reflecting) boundary conditions imposed on a finite computational domain in order to simulate the effect of diffusion into an infinite medium. Our approach, which we refer to as the Fast Recursive Marching (FRM) method, is mathematically much more straightforward. The FRM method is based on evaluating the exact solution of the governing equation, using convolution in space and time with the free-space Green's function. This is carried out in the Fourier domain and relies on the spectral approximation of the free-space heat kernel [*Greengard and Lin, Appl. Comput. Harmonic Anal. (2000)*], coupled with the NUFFT. There are several advantages to this approach. The FRM method is explicit, unconditionally stable, and requires an amount of work of the order $O(NM \log N)$ where N is the number of discretization points in physical space and M is the number of time steps [*Li and Greengard, J. Comput. Phys., to appear*]. We have also developed NUFFT-based schemes for the rapid evaluation of heat potentials [*Li and Greengard, in progress*]. When coupled with the inhomogeneous solver described above, we will have completed the "core library" for the creation of a new generation of methods for the heat equation in complex geometry. This is of significant technical importance, because the computation of diffusion or heat flow arises as an important component in a wide variety of physical settings and the need for implicit time-stepping often emerges as a computational bottleneck. By adopting an integral-equation viewpoint, we have overcome that limitation. Robust, easy-to-use solvers are being constructed. The price to pay for this is a more complex set of core algorithms – all of which are now in place. We are planning to release our NUFFT library for one, two and three-dimensional problems in late summer, 2007.

Future Directions

As indicated above, one of the reasons we have concentrated on developing the core machinery for heat solvers in complex geometry is that these solvers play an important role in numerous applications, including the unsteady, incompressible Stokes and Navier-Stokes equations. We are planning to build fast solvers for these equations based on combining our heat flow tools to handle the diffusion of vorticity with the fast multipole method (developed previously) to handle the incompressibility constraint. These solvers will form the basis for a new class of microfluidic design tools and new modeling capabilities for biological and other low-speed flows.

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