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Geometrical Multiscale Analysis: Applications to Scientific Computing and Partial Differential Equations

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Summary of Past Research

In the last two decades or so, many multiscale algorithms have been proposed to enable large scale computations which were thought as nearly intractable. For example, the fast multipole algorithm and other similar ideas have allowed to considerably speed up fundamental computations in electromagnetism, and many other fields. The thesis underlying this proposal is that traditional multiscale methods have been well-developed and it is clear that we now need new ideas in areas where traditional spatial multiscaling is ill-suited. In this context, the proposal argues that clever phase-space computations is bound to play a crucial role in advancing algorithms and high-performance scientific computing.

Our research past accomplishments have shown the existence of ideas beyond the traditional scale-space viewpoint such as new multiscale geometric representations of phase-space. We have shown that these clever representations lead to enhanced sparsity. We have shown that enhanced sparsity has significant important implications both for analysis, and for numerical applications, where sparsity allows for faster algorithms. We have implemented these ideas and built computational tools to be used as new building blocks of a new generation of wave propagation solvers. Finally, we have deployed these ideas into novel algorithms. In this last year, we assembled all these techniques and made very significant progress in solving a variety of computational problems, which we then applied in selected areas of considerable scientific interest.

Report on the Technical Progress since August 15, 2005

The phase flow method

Many computational problems involve solving an ordinary differential equation (ODE) with many initial conditions. In the context of high-frequency propagation, we can think of propagating a wavefront which involves tracing out a very large number of rays. The standard approach, which consists in integrating the solution for each initial condition independently is, in general, extremely costly. Together with Lexing Ying, we have developed the phase flow method which is a completely novel method for computing the solution to ODEs. The phase flow method operates by constructing the *whole* phase map of the dynamical system under consideration. Given an arbitrary initial condition, one only needs to apply the phase map, an operation which only requires a small constant number of flops. The construction of the phase map is accurate, fast, and general so that it works for arbitrary systems of autonomous ordinary differential equations. The main idea is to exploit the smoothness and the group structure of the phase flow. The algorithm first constructs the phase map for a small time step using a standard ODE integration rule, and then builds up the phase map for progressively larger times with the help of a repeated squaring type algorithm which uses the group property of the phase flow. This method has provably high accuracy and low complexity. In fact, it is remarkably efficient since the computational cost of building the whole phase map by the phase flow method is usually that of tracing a few rays.

We have successfully applied the phase flow method in the field of high frequency wave propagation. Whenever the asymptotic behavior of the solution is of interest, the phase flow method has been used to rapidly propagate wave fronts, calculate wave amplitudes along these wave fronts, and evaluate multiple wave arrival times at arbitrary locations [7]. Figure 1 shows an example of wavefront calculation with this method. The phase flow method has also been applied to fast computation of geodesics on smooth manifolds [8].

Fast computation of Fourier integral operators

Together with Demanet and Ying, we have proposed a very efficient and novel algorithm for the numerical evaluation of Fourier integral operators (FIOs) [6]. This is significant because FIOs come up in a large number of applications. Examples in reflection seismology, radar imaging, ultrasound imaging, and electron microscopy all come to mind. Therefore, I suspect this will be used to speed up a lot of fundamental computations throughout science and engineering. Now this is connected to the main theme of these project which is the propagation of high-frequency waves in inhomogeneous media because one can express the hyperbolic Green's function for small times as an oscillatory integral, which is an FIO when acting on the Fourier transform of the initial data. Because an FIO is a dense matrix, a naive matrix vector product with an input given on a Cartesian grid of size N by N would require $O(N^4)$ operations. This paper develops a new numerical algorithm which requires $O(N^{2.5} \log N)$ operations, and as low as $O(\sqrt{N})$ in storage space (the constants in front of these estimates are small). In numerical tests, the speedup factor over the naive evaluation for grids of size 512 by 512 is close to 200. Overall, the algorithm can be thought of as an extension of the FFT for nontrivial phases and amplitudes.

The algorithm operates by localizing the integral over polar wedges with small angular aperture in the frequency plane. On each wedge, the algorithm factorizes the highly oscillatory kernel into two components: 1) a diffeomorphism which is handled by means of a nonuniform FFT and 2) a residual factor which is handled by numerical separation of the spatial and frequency variables. The key to the complexity and accuracy estimates is the fact that the separation rank of the residual kernel is provably independent of the problem size. We have demonstrated the numerical accuracy and low computational complexity of the

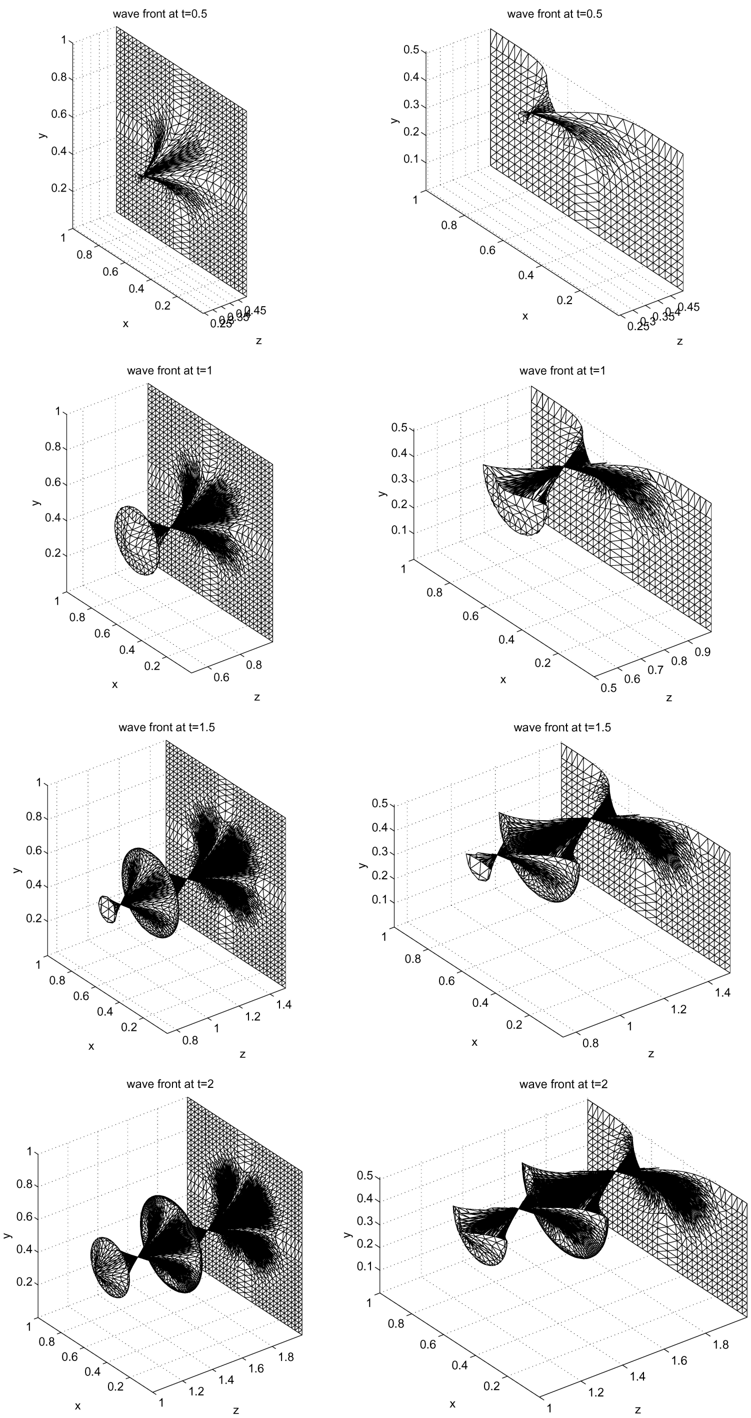

Figure 1: Wave front propagation in a 3D waveguide. The four rows show the wave front at times $t = 0.5, 1, 1.5$ and 2. In each row, the left frame plots the whole wave front, while the right frame only displays the lower half in order to show the interior. The mesh used to approximate the wave front is not uniform since our algorithm adaptively refines the grid as the wave front evolves. Many other figures of this type may be found in [7].

proposed methodology [6]. We also made clear how our ideas could be very effective in various applications such as reflection seismology.

Finally, we also know that under certain conditions on the smoothness of the separable representation, one might lower the complexity of evaluating the algorithm to $O(N^2 \log N)$. Such a reduction is nontrivial, and we hope to report on progress later.

Time upscaling of wave equations

Another research accomplishment of this past year is concerned with the time upscaling of wave equations, and is joint with Demanet and Ying. The idea, which motivated the proposal, is that sparser representations can speed up fundamental computations especially in the area of wave propagation. Our recent work had shown that new multiscale systems based on a notion of parabolic scaling such as curvelets offered optimally sparse decompositions of the wave propagator in smooth inhomogeneous media. We were recently able to transform this theoretical insight into effective algorithms and developed solvers for wave equations which are not constrained by the CFL condition on the time step. In effect, the method constructs the full wave propagator; that is, the time dependent Green's function of the wave equation in a basis where it is known to exhibit a sparse structure. We show that it is possible to build the propagator with optimal computational complexity up to a time which is far larger than the CFL time step. Once the full-propagator is available, one can then use it to perform gigantic upscaled time steps to solve the wave equation with arbitrary initial conditions.

Our strategy is an entirely novel approach for solving hyperbolic systems in the sense that it is not at all a refinement of existing ideas. On the one hand, there are theorems showing that the entire approach is mathematically sound. On the other hand, our early numerical experiments show that this novel algorithm accurately propagates highly oscillatory wavefields for far longer times than finite difference and finite element methods. The algorithm is also 5 to 10 times faster than standard spectral and pseudo-spectral methods with about the same accuracy. It is believed that this algorithm will help speed up computations in seismic imaging where one needs to propagate multiple wavefields in the same medium and we are currently exploring such opportunities.

Conclusions

We have achieved all the goals set forth in the proposal. First, we have developed the mathematical foundation of phase-space computing and developed ideas showing the promise of this viewpoint. Second, we have been able to operationalize these ideas and develop novel and effective algorithms for problems related to high-frequency wave propagation. Along the way, we have developed computational tools that may have a far reaching impact. The phase flow method is attracting some attention and there seems to be considerable interest in the Fast Discrete Curvelet Transform, both from academic groups and selected industries. Since we released software to the public, several companies—and especially oil companies—are exploring the potential of curvelets for seismic data processing, and we are aware of several research group worldwide, which are now routinely using our curvelet software for performing various tasks such as image enhancement, image restoration, seismic migration, velocity estimation in geophysics, and many others. Our work has resulted in 6 articles all published in top journals and I expect more to come. For example, one can extend our ideas to problems in reflection seismology such as wave migration. There, the generalized Radon transform, when cast as an FIO, has a nonsmooth phase but we believe that we can extend our algorithm to handle this important situation as well.

We have started something new and extremely promising (as emphasized earlier, this work is getting a lot of attention) and I would like to thank the DOE for making this possible. Under the auspices of this grant, I have been able to hire Dr. Ying who has expanded my research horizon and enriched my vision of the field; for instance, we started working on a variety of topics I would not have otherwise touched. I expect to collaborate with him for years to come.

Collaborators and Supported Personnel

The personnel who worked on this project were:

1. Professor Emmanuel Candès has of course worked on all the projects developed in connection with this proposal.

   Dr. Candès has received major awards since the beginning of this project in recognition of his work. Among others, he was awarded the James H. Wilkinson Prize in Numerical Analysis and Scientific Computing by SIAM in 2005. He is the recipient of the 2006 Alan T. Waterman Medal awarded by the US National Science Foundation, which is the highest honor bestowed by the National Science Foundation. He has been invited to give addresses at major international conferences such as the International Congress of Mathematicians (ICM 2006) and the International Congress on Industrial and Applied Mathematics (ICIAM 2007). Finally, since 2002, he has been promoted from Assistant Professor of Applied and Computational Mathematics to the Ronald and Maxine Linde Professor of Applied and Computational Mathematics, effective December 1st 2006.

2. Laurent Demanet was a Caltech graduate student in Applied and Computational Mathematics. He is now an Assistant Professor at Stanford University. Dr. Demanet has worked on the mathematical underpinning of the proposed research [1, 2, 3]. Dr. Demanet has worked on building the key computational tools underlying this project such as the Fast Digital Curvelet Transform [5]. He has co-developed the time upscaling method for wave equations. He co-authored the algorithm for rapidly computing the action of Fourier integral operators [6]. Demanet was awarded the Carey prize which recognizes a PhD thesis of exceptional quality in the mathematical sciences at Caltech. He has also won the SIAM Student Paper Competition for the paper [2].

3. Lexing Ying was a post-doctoral scholar hired in 2004 (he was the recipient of the prestigious 2004 Janet Fabri Prize for the most outstanding dissertation in Computer Science at New York University). Dr. Ying stayed at Caltech until August 2006, and he is now an Assistant Professor at the University of Texas. Dr. Ying has co-invented the phase flow method and applied it to selected problems in high-frequency wave propagation, and in problems involving the computations of geodesics over smooth manifolds. Dr. Ying has co-developed the time upscaling method for wave equations. He also co-authored the algorithm for rapidly computing the action of Fourier integral operators [6].

4. Paige Alicia Randall is a Caltech graduate student in Physics has worked on the development of simplified numerical experiments to test some ideas for practical significance. Ms. Randall was only partially supported DOE and will write her PhD thesis under my supervision.

Other collaborators included David L. Donoho from Stanford University and Guillaume Bal from Columbia University.

References

[1] E. J. Candès and L. Demanet. Curvelets and Fourier integral operators. *C. R. Acad. Sci. Paris Sér. I Math.*, 336:395–398, 2003.

[2] E. J. Candès and L. Demanet. The curvelet representation of wave propagators is optimally sparse. *Comm. Pure and Appl. Math.* **58**, 1472-1528, 2005.

[3] E. J. Candès, L. Demanet, and L. Ying Time-upscaling of wave equations. Technical report, California Institute of Technology, 2006. In preparation.

[4] E. J. Candès and D. L. Donoho. New tight frames of curvelets and optimal representations of objects with piecewise-C^2 singularities. *Comm. Pure and Appl. Math.* **57** (2004), 219-266.

[5] E. J. Candès, L. Demanet, D. L. Donoho and L. Ying. Fast Discrete Curvelet Transforms. *Multiscale Model. Simul.* **5**, 861899 (2006).

[6] E. J. Candès, E. J., L. Demanet, and L. Ying. Fast computation of Fourier integral operators. Submitted to *SIAM J. Sci. Comput.* (2006).

[7] L. Ying, and E. J. Candès. The phase flow method. *J. Comput. Phys.*, in press, 2006.

[8] L. Ying, and E. J. Candès. Fast geodesics computation with the phase flow method. *J. Comput. Phys.*, in press, 2006.