

New Perspectives for Spectral and High-Order Methods

With the next in a series of conferences on spectral and high-order methods scheduled for June 2004 at Brown University, a group of organizers and other proponents of these methods, with the help of Gail Pieper of Argonne National Laboratory, put together the following snapshot of the field for readers of *SIAM News*.

Spectral methods are great fun,” observes Michel Deville, a professor at l’Ecole Polytechnique Fédérale de Lausanne, Switzerland. “It’s always a numerical nirvana when—for the first time—one observes that adding one or two polynomials to a basis makes the error for smooth problems drop by a factor of 50 or even 100.”

Spectral methods have not always come in for such high praise. Although originating in early-20th-century work of Galerkin and Lanczos, and put to limited use by meteorologists in the 1950s, spectral methods came into their own as a powerful tool for scientific computing only with the advent of the fast Fourier transform. In the early 1970s, in a series of landmark papers, Steven Orszag showed that spectral methods, and the closely related pseudospectral methods, could be used to simulate incompressible turbulence with N^3 Fourier modes at a cost of only $O(N^3 \log N)$ operations per timestep with zero numerical dispersion and dissipation. In a historic computation, Orszag and his colleague G.S. Patterson undertook the first calculation of homogeneous isotropic turbulence at laboratory Reynolds numbers with a 32^3 pseudospectral discretization. Today, computations using spectral methods as large as 1024^3 are routine.

A Cube or the Whole Spectrum?

Spectral methods are named for the fact that the unknowns in the computation are the coefficients of eigenfunctions of the differential operators in the governing equation. The problem, in other words, is cast in terms of the spectrum of the unknown solution field.

The unparalleled accuracy and efficiency of spectral methods clearly set them apart from low-order finite difference and finite element techniques. Nevertheless, Deville says, spectral methods were regarded with skepticism for a decade after Orszag’s initial work. One of the major arguments against their use was that “people see the world through a cube, or a sphere, or a cylinder, or the like.” That argument fell in the 1980s,

when A.T. Patera published the first paper on spectral elements. Spectral elements combine the

rapid convergence rates of spectral methods with the geometric flexibility of the classical finite element methods of applied mechanics. Today, multidomain spectral methods are used to simulate a variety of physical phenomena in complex domains, including photolithography, blood flow (Figure 1), and electromagnetic scattering from aircraft (Figure 2).

Unstructured multidomain problems do require extra work, says Paul Fischer, a computer scientist in the Mathematics and Computer Science Division at Argonne National Laboratory. Fortunately, efficient preconditioning techniques have been developed for spectral methods, strongly enhancing their numerical performance. Preconditioning techniques are pervasive in modern iterative methods for the solution of large linear systems. Initially advocated for use in spectral methods to treat complicated geometries, preconditioning techniques are particularly effective in overcoming the ill-conditioning of high-order methods, Fischer points out. Several preconditioning approaches have been proposed, with the most promising based on domain decomposition strategies developed by Olof Widlund and co-workers.

Singularities present another challenge for researchers wishing to use spectral methods. An important milestone in this area was reached

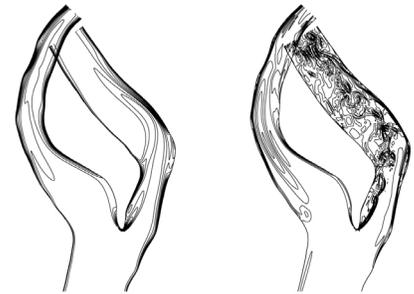


Figure 1. Vorticity contours in the cross-section of a stenosed (narrowed) carotid artery. The flow, laminar during the diastolic phase (left), transitions to a turbulent state during the systolic phase (right). The calculation employed 2544 hexa-hedral elements of order 7 and was carried out on 256 nodes of the TCS1 machine at the Pittsburgh Supercomputer Center by S. Lee, F. Loth, and P. Fischer.

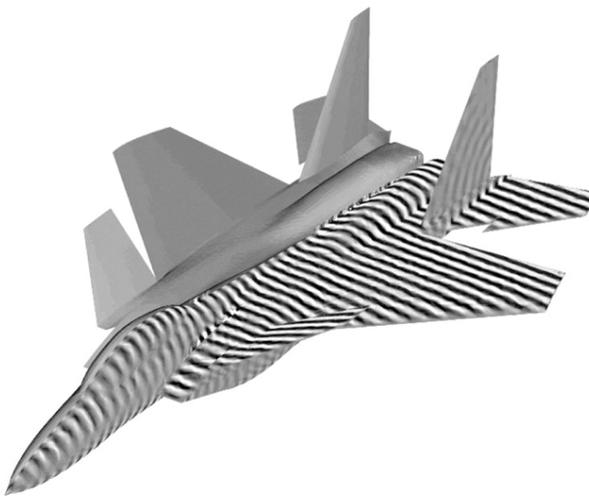


Figure 2. Scattered field solution of Maxwell’s equations, showing the E_x component of a horizontally polarized 600-MHz plane-wave illuminating an aircraft head on, computed in the time domain with the USEME (unstructured spectral element method) code developed by J. Hesthaven and T. Warburton. The computation uses a body-conforming unstructured grid with 250,000 fourth-order tetra-hedra.

in the mid-1990s, when David Gottlieb and Chi-Wang Shu showed that the Gibbs phenomenon associated with Fourier reconstruction of discontinuous functions could be overcome with filters, which allow extraction of the spectral information within the otherwise oscillatory solution.

Figure 3 shows the results of such an effort, a spectral calculation of two-dimensional density contours of the Richtmyer–Meshkov instability that occurs when a shock passes through an interface, separating materials—typically gases—of different densities. The instability deposits vortices on the perturbed interface, and the resulting rollup of the interface enhances the mixing of the gases. As shown in the figure, the detail in postprocessed spectral results can surpass that obtained with a fifth-order finite difference scheme, such as WENO.

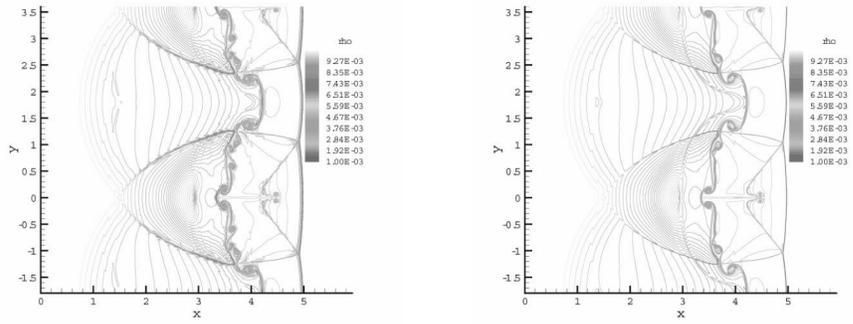


Figure 3. Density contour plots of Richtmyer–Meshkov instability as computed by spectral (left) and WENO-5 (right) schemes at time 50 microseconds. The resolution of the spectral scheme is 1024 Chebyshev polynomials and 512 trigonometric polynomials in the x and y directions, respectively. Calculation by W.S. Don and D. Gottlieb.

Moving to a Higher Order

Researchers now recognize that the desirable properties of spectral methods can be achieved with many high-order formulations. One such approach relies on *modal bases*. These hierarchical bases are made up of “bubbles,” approximations that vanish on the element edges or faces. Modal bases, which researchers have been applying to solid mechanics problems for three decades, yield excellent convergence rates for problems involving discontinuities, such as crack propagation. More recently, these methods have been extended to fluid dynamics.

In another approach, researchers have developed *nodal bases* for use with the triangles often employed to cover complicated geometries. M. Taylor and B. Wingate, for example, obtain stable nodal bases by minimizing the determinant of the van der Monde matrix; Jan Hesthaven and co-workers exploit the equivalence between Gaussian quadrature points and the distribution of freely moving electrostatic charges.

A popular alternative to spectral methods is the p -version finite element method pioneered in the 1970s by I. Babuška, J.T. Oden, B. Szabo, and others working in computational solid mechanics. Ernest Mund, a professor at l’Université Catholique de Louvain, describes the method: “As in the classical FEM, one begins with a decomposition of the domain into subdomains, or elements. Instead of using just linear basis functions within each element, however, p -FEM uses polynomials of degree p to effect rapid convergence to smooth solutions.”

The p -FEM approach achieves the exponential convergence properties of spectral methods, but the computational complexity is typically $O(Ep^6)$ for three-dimensional problems involving E elements. If the element types are restricted to tensor-product forms, as in the case of the spectral element method, the p -version complexity can be improved to $O(Ep^4)$. For small values of p , however, the constants in the complexity estimates can be quite important, and the $O(Ep^6)$ formulation is usually the most efficient.

A refinement added to many implementations of the p -version FEM also makes it possible to decrease the element size, h . This option is desirable when singularities are present, which slows the spectral convergence rate. Refinement strategies for these hp methods have been fully automated and optimized, guided by a rich theory developed by numerical analysts over the past three decades.

As simulation becomes increasingly commonplace in science and engineering, high-order methods will be needed for the solution of problems involving a broad range of spatial and temporal scales. High-order methods currently require considerable programming overhead, Mund says. He believes, however, that greater sophistication in simulation software will ease this difficulty.

A Glimpse at the Future of Spectral Methods

Climate modeling and weather forecasting have long been application areas for global spectral methods. With the development of multidomain spectral methods, oceanography has emerged as another geophysical application. New spectral schemes have been designed to cope with the complicated shapes of coastlines and river estuaries. In a recent paper, Mohamed Iskandarani and co-workers show the utility of spectral discretizations, with the mesh in this case built of hexahedra and prisms, for such problems. For reasons of data locality, spectral element methods are also gaining interest as an alternative to global spectral methods in climate modeling. For example, the HOMME (High-Order Multiscale Modeling Environment) code of Richard Loft and Stephen Thomas of NCAR is being developed as a dynamic core of future-generation community climate models.

The complex physics of non-Newtonian fluid flows presents many challenges to practitioners of spectral methods, including the so-called high-Weissenberg-number problem. The Weissenberg number is a measure of the elasticity in a flow. For values larger than 10–15, algorithms start to fail, and it is possible that convergence will never be achieved. Deville points out that the values of the Weissenberg number easily reach 100 in industrial applications. Despite several recent attempts to overcome the convergence problem, this remains an open area in which considerable research is still necessary. Clearly, advances are needed if simulations of real-world situations are to be carried out. Improved modeling will be as important as improved numerical methods.

Undaunted by such challenges, Deville points to the progress already made. “Panta rei,” he says, citing the famous axiom of the

Greek philosopher Heraclitus; “all things flow.” Today, spectral methods cover not only complex fluid flows but also Maxwell’s equations, image reconstruction, and quantum chemistry. “The range of applications of spectral methods,” Deville says, “has been considerably enlarged in recent years, demonstrating the versatility of these methods and the broad scope of problems they can tackle.”

Getting Started

In the 1977 SIAM monograph *Numerical Analysis of Spectral Methods: Theory and Applications*, Gottlieb and Orszag presented the first unified description of the field, with an emphasis on numerical analysis and algorithmic considerations. Published almost a decade later (1987, Springer-Verlag) was *Spectral Methods in Fluid Dynamics*, by C. Canuto, M.Y. Hussaini, A. Quarteroni, and T.A. Zang. Although more than a dozen texts on the topic are now available, these two volumes continue to serve as primary references for practitioners of spectral methods.

Those wishing to implement spectral methods will find libraries and routines for high-order differentiation and integration, including the *speclib* routines of Einar Rønquist, the *pseudopack* routines of Wai-Sun Don and Bruno Costa, and the *USEMe* code of Jan Hesthaven and Tim Warburton. Perhaps the easiest place to start is Nick Trefethen’s book, *Spectral Methods in Matlab* (SIAM, 2000), which provides a set of codes and examples for a variety of problems.

Another good source of information on spectral methods is the International Conference on Spectral and High-Order Methods, held every three years. The next meeting, organized by the scientific computing group at Brown University, will be held June 21–25, 2004. Researchers interested in delivering a paper or attending the lectures should visit the conference Web site: www.dam.brown.edu/icosahom2004.