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SPECTRAL METHODS IN FLUID DYNAMICS

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SPECTRAL METHODS IN FLUID DYNAMICS

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ABSTRACT

Fundamental aspects of spectral methods are introduced. Recent developments in spectral methods are reviewed with an emphasis on collocation techniques. Their applications to both compressible and incompressible flows, to viscous as well as inviscid flows, and also to chemically reacting flows are surveyed. The key role that these methods play in the simulation of stability, transition, and turbulence is brought out. A perspective is provided on some of the obstacles that prohibit a wider use of these methods, and how these obstacles are being overcome.

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INTRODUCTION

In certain areas of computational fluid dynamics spectral methods have become the prevailing numerical tool for large-scale calculations. This is certainly the case for such three-dimensional applications as direct simulation of homogeneous turbulence, computation of transition in shear flows, and global weather modeling. For many other applications, such as heat transfer, boundary layers, reacting flows, compressible flows, and magnetohydrodynamics, spectral methods have proven to be a viable alternative to the traditional finite difference and finite element techniques.

Spectral methods are characterized by the expansion of the solution in terms of global and, usually, orthogonal polynomials. Since the mid-nineteenth century this has been a standard analytical tool for linear, separable differential equations. Nonlinearities present considerable algebraic difficulties, even on a modern computer. These were surmounted effectively in the early 1970's, and only then did spectral methods become competitive with alternative algorithms. By the present time, however, spectral methods have been refined and extended to the point where many problems in fluid mechanics are only tractable by this technique.

Numerical spectral methods for partial differential equations were originally developed by meteorologists. Though this approach was proposed by Blinova in 1943 and Haurwitz and Craig in 1952, the first numerical computations were conducted by Silberman (1954). The expense of computing nonlinear terms remained a severe drawback until Orszag (1969) and Eliasen, et al (1970) developed the transform methods that still form the backbone of many large-scale spectral computations.

These methods and others used in fluid mechanics prior to 1970 are now termed spectral Galerkin methods: the fundamental unknowns are the expansion coefficients and the equations for these are derived by the techniques used in classical analysis. The advent of computers made feasible an alternative discretization, termed the spectral collocation technique, in which the fundamental unknowns are the solution values at selected, collocation points and the series expansion is used solely for the purpose of approximating derivatives. This approach was proposed by Kreiss and Oliger (1971) and Orszag (1972).

Many useful versions of spectral methods have been developed since 1971 and especially during the 1980's. This review will discuss many of the recent innovations and will focus on the collocation technique since it is the version most readily applicable to nonlinear problems. We will survey applications to both compressible and incompressible flows, to viscous as well as inviscid flows, and also to chemically reacting flows. In the interests of brevity we shall not cover the applications to meteorology, magnetohydrodynamics, astrophysics, and other related fields. Moreover, we will restrict ourselves to the three-dimensional applications of well-established algorithms while discussing some two- and even one-dimensional applications of more novel spectral methods.

Let us mention here some other articles for those interested in additional historical references, applications in other fields, and theoretical developments on the numerical analysis of spectral methods. The monograph by Gottlieb and Orszag (1977) describes the theory and applications developed prior to 1977. It will be referenced hereafter as GO. The following five years are covered in the proceedings edited by Voigt, et al (1984). Fluid dynamical applications, especially multigrid techniques, are discussed by Zang and Hussaini (1985c). Compressible flow applications are covered by Hussaini, Salas, and Zang (1985). The role of spectral methods in meteorology is explained by Jarraud and Baede (1985). The book by Canuto, et al (1987) contains a detailed description of many spectral algorithms and presents an exhaustive discussion of the theoretical aspects of these numerical methods. It will be referenced hereafter as CHQZ.

FUNDAMENTALS

The motivation for the use of spectral methods in numerical calculations stems from the attractive approximation properties of orthogonal polynomial expansions. Suppose, for example, that a function $u(x)$ is expanded in a truncated Chebyshev series on $[-1,1]$:

$$u_N(x) = \sum_{n=0}^{N} a_n T_n(x) \tag{1}$$

where $T_n(x) = \cos(n \text{ arc } \cos x)$. The classical form of the expansion coefficients (or spectra) is

$$a_n = (2/c_n) \int_{-1}^{1} u(x)\, T_n(x)(1 - x^2)^{-1/2}\, dx \tag{2}$$

where $c_0 = 2$, and $c_n = 1$ for $n > 1$. The substitution $x = \cos \theta$ converts this into a Fourier cosine series. A simple integration-by-parts argument (GO, Ch. 3) reveals that

$$n^p a_n \to 0, \qquad \text{as} \quad n \to \infty, \qquad \text{for all} \quad p > 0 \tag{3}$$

provided that u is infinitely differentiable. Consequently, the approximation error decreases faster than algebraically. This rapid convergence is referred to as infinite order accuracy, exponential convergence, or spectral accuracy. Our primary concern in this review is on numerical methods for partial differential equations that exhibit spectral accuracy for infinitely differentiable solutions.

The approximation just described is typical of spectral Galerkin methods. An alternative approximation, termed spectral collocation, is one of interpolation. It retains the expansion (1), but replaces the condition (2) for the expansion coefficients, with the condition

$$u_N(x_j) = u(x_j) \tag{4}$$

where x_j are special, so-called collocation, points in $[-1,1]$. For most problems, the optimal choice of these collocation points is

$$x_j = \cos(\pi j/N). \tag{5}$$

This choice of collocation points yields an extremely accurate approximation (CHQZ, Ch. 2) to the integral appearing in Eq. (2):

$$a_n = (2/N\bar{c}_n) \sum_{j=0}^{N} \bar{c}_j^{-1} u(x_j) T_n(x_j), \tag{6}$$

where, $\bar{c}_0 = \bar{c}_N = 2$ and $\bar{c}_n = 1$, otherwise. Whether (2) or (6) is used for the expansion coefficients, the expansion (1) is differentiated analytically to form the approximations to whatever derivatives are required for the problem at hand.

A graphical distinction between traditional approximations and spectral ones is provided in Figure 1 for the simple task of estimating the derivative of the function $1 + \sin(2\pi x + \pi/4)$ on $[-1,1]$ from the values of the function at a finite number of grid points. A finite difference or finite element method uses local information to estimate derivatives whereas a spectral method uses global information. In this figure a second-order (central) finite difference method is compared with a Chebyshev spectral collocation method. The finite difference approximation estimates the derivative at, say, $x = 0$, from the parabola which interpolates the function at $x = 0$ and the two adjacent grid points. A separate parabola is used at each grid point. The spectral approximation, on the other hand, uses all the available information about the function. If there are $N + 1$ grid points, then the interpolating polynomial from which the derivative is extracted has degree N and the same polynomial is used for all the grid points. Note that the local method produces a second-order accurate derivative, with the error decreasing as $1/N^2$, whereas the error from the global method decreases exponentially.

An essential aspect of any spectral method is the choice of expansion functions. Consider first the case of a bounded, cartesian domain. Fourier series are the most familiar expansion functions, but they are only appropriate for problems with periodic boundary conditions. The appropriate collocation points on $[0,2\pi]$ are

$$x_j = 2\pi j/N, \qquad j = 0,1,\cdots,N-1. \tag{7}$$

In the general, non-periodic case, normalized to $[-1,1]$, the appropriate class of functions is the Jacobi polynomials. The proper collocation points are generally -1, $+1$ and the extrema of the last polynomial retained (CHQZ, Ch. 2). The most commonly used Jacobi polynomials are the Chebyshev and Legendre ones.

On an unbounded domain, the obvious choices of Laguerre or Hermite polynomials are rarely advisable. Not only are fast transforms unavailable, but these expansion functions have relatively poor resolution properties (GO, Ch. 3). A better approach is to combine a mapping with a Fourier or Chebyshev series in the mapped variable. Boyd (1986) has shown that spectral accuracy can be achieved for $u(x)$ on $(-\infty, \infty)$ with the mapping $x = x_* \cot \xi$, and a full Fourier series in ξ, provided that $u(x)$ exhibits at least algebraic decay at ∞. Moreover, if $u(x)$ has exponential decay, then a Fourier cosine series will suffice. The latter case is equivalent to a Chebyshev series in η with $x = x_* \eta/\sqrt{(1 - \eta^2)}$. Spalart (1984) noted that the odd (or even) Chebyshev polynomials work well on $[0,\infty)$, when combined with an exponential mapping, provided that $u(x)$ decays faster than exponentially.

The process of numerical differentiation is particularly simple when the expansion functions are trigonometric polynomials. Starting from u_j, the values of u at x_j, one computes

$$a_k = (1/N) \sum_{j=0}^{N-1} u_j \exp(-ikx_j), \qquad k = -\frac{N}{2}, \frac{N}{2}+1, \cdots, \frac{N}{2}-1 \tag{8}$$

and then uses

$$\sum_{k=-N/2}^{N/2-1} ik\, a_k \exp(ikx_j) \tag{9}$$

to approximate du/dx at x_j. The Fast Fourier Transform (FFT) can be used to evaluate both the sums given above. The total cost of computing the derivative in this manner is $5N \log_2 N + N$ real operations. (All operation counts given in this review presume, for simplicity, that N is a power of 2 and that the complex FFT is used; however, FFTs which allow prime factors of 3 and 5 are just as efficient and are widely available and real to half-complex FFTs offer a 20% savings (Temperton (1983)).) The FFT can also be used to differentiate functions which are expanded in Chebyshev series, since expansions in these special Jacobi polynomials reduce to cosine series. Morever, in terms of the Chebyshev coefficients, derivatives are obtained by simple recursion relations (CHQZ, Ch. 2). For Chebyshev series the total operation count for differentiation is $5N \log_2 N + 16 N$.

For the classical expansion functions the matrix which represents differentiation, i.e., $d^q u/dx^q = D^q u$, is known in closed form (Gottlieb, et al (1984)). Unlike the differentiation matrices for alternative, local discretizations, these matrices are full. Hence, the matrix-vector multiplication which produces the derivative at the collocation points costs $2N^2$ operations. These operation counts suggest that for $N > 16$, transform methods are faster for differentiation than matrix multiplies. On modern scalar and vector computers the transform methods become faster than the matrix-vector multiply methods for N between 16 and 32 (CHQZ, Ch. 2).

An important issue in many applications of Chebyshev spectral methods is the manner in which the boundary conditions are enforced. Dirichlet boundary conditions are generally straightforward. Neumann boundary conditions may be enforced by altering the boundary values to ensure the desired normal derivative or by building the boundary condition into the differential operator (Streett, et al (1985)). For hyperbolic systems, characteristic boundary conditions are a virtual necessity (Gottlieb, et al (1981), Salas, et al (1985)). Canuto and Quarteroni (1986) discuss how to implement characteristic boundary conditions for implicit time discretizations. Chebyshev spectral methods have the advantages (over standard finite difference schemes) that they require the same number and type of boundary conditions as the analytical formulations of the problem, and that no special difference formulae are required at the boundary.

The spectra of the discrete differentiation operators D^q are an important characteristic of numerical methods. For Fourier approximations to periodic problems, these are obvious: purely imaginary and growing as $N/2$ for D^1, negative real and growing as $N^2/4$ for D^2. Indeed, for periodic problems such as $u_t + u_x = 0$, the Fourier eigenvalues are exactly equal to their analytic counterparts. This means that Fourier spectral methods propagate the numerical solution with zero phase error. This is illustrated in Figure 2 for the problem whose solution is $u(x,t) = \sin(\pi \cos(x-t))$. The lagging phase of the finite difference solution is apparent, whereas the Fourier solution is indistinguishable from the true one. Of course, in realistic problems, variable coefficients or nonlinear terms will introduce non-zero (but still relatively small) phase errors.

Figure 3 displays the eigenvalues of a Chebyshev approximation to d/dx on $[-1,1]$ with homogeneous Dirichlet boundary conditions at $x = +1$. The eigenvalues are predominantly imaginary but do have negative real parts. The absolute value of the largest eigenvalue grows as N^2. These eigenvalues may be surprising at first sight. After all, the periodic discrete problem has purely imaginary eigenvalues, whereas the non-periodic continuous problem has no discrete eignevalues. Nevertheless, Figure 3 does convey the nature of the eigenvalues of the discrete problem and these are crucial for both time differencing methods and iterative schemes. The eigenvalues of Chebyshev approximations to d^2/dx^2 with homogeneous Dirichlet boundary conditions at $x = -1$ and $x = +1$ are real and negative and the largest eigenvalue grows as N^4 (Gottlieb and Lustman (1983)).

In practice, when one is solving an evolution problem such as $u_t = Lu$, where the operator L contains all the spatial derivatives, one combines a spectral discretization of L with a standard finite difference technique for the time derivative. The Leap Frog, Adams-Bashforth, Crank-Nicolson, and Runge-Kutta schemes are the ones most commonly used (CHQZ, Ch. 4). The stability regions of these schemes depend upon the spatial operators. The stability properties of Fourier methods are qualitatively the same as those for second-order central difference spatial operators. However, the precise stability limit is typically a factor of $(1/\pi)^n$ smaller for Fourier approximations, where n is the order of the highest spatial derivative which appears in L.

The stability properties of Chebyshev methods are more subtle. For example, Leap Frog is unconditionally unstable for advection problems, such as $u_t + u_x = 0$, since the discrete eigenvalues of the spatial operator have negative real parts. On the other hand, second-order Adams-Bashforth and Runge-Kutta methods are strictly stable (and not weakly unstable like their Fourier counterparts) for the same reason.

The typical time-step limitations on Chebyshev methods are $1/N^2$ for first derivative operators and $1/N^4$ for second derivative ones. These are far more stringent than the analogous restrictions for uniform grid finite difference approximations. They arise from the crowding of the collocation points near the boundaries (see Figure 1). Although this crowding necessitates small time-steps, it is required for the high spatial resolution of the method and is quite advantageous for problems with boundary layers. This is, however, a substantial disadvantage for problems with very little structure near the boundaries. It can be alleviated to some degree by mapping, but a mapping to a uniform grid is counter-productive because it destroys the spatial accuracy.

This Chebyshev time-step limitation disappears when implicit time discretizations are employed. The principal difficulty is obtaining efficient solutions of the resulting implicit equations, since the matrices which represent the differentiation operators are full. In some special cases, fast direct solution methods are available. These typically require low-order polynomial coefficients and, in multidimensional problems, at most one non-periodic direction (GO, Chs. 9 and 10, Moser, et al (1983)).

The use of implicit techniques in more general situations requires iterative methods. This has been one of the major developments of the current decade (CHQZ, Ch. 5). Let us denote a typical linear, implicit system arising from a spectral discretization as $L_{sp}\ u = f$. The simplest iterative scheme -- Richardson's method -- is just

$$u \leftarrow u + \omega\left(f - L_{sp}\ u\right) \tag{10}$$

where ω is an acceleration parameter. The matrix L_{sp} will be full and will have eigenvalues which grow rapidly as the number of grid points increases. The fullness of the matrix does not preclude iterative methods since transform techniques for differentiation permit the matrix-vector product $L_{sp}\ u$ to be computed in $O(N \log_2 N)$ operations rather than $O(N^2)$. The slow convergence which results from the large eigenvalues of L_{sp} can be ameliorated by preconditioning. In this case the basic iterative scheme is

$$u \leftarrow u + \omega H^{-1}\left(f - L_{sp}\ u\right) \tag{11}$$

where H is a preconditioning matrix. This will accelerate convergence if H is a good approximation to L_{sp}, and it will be relatively inexpensive if H is readily inverted. The former condition is met by low-order finite difference (Orszag (1980)) and finite element (Deville and Mund (1985)) approximations to L_{sp}. Although the latter condition certainly holds for one dimensional problems, these particular preconditionings become increasingly expensive to invert as the dimensionality of the problem increases.

The most attractive approach to very large problems is to combine a less accurate but more readily inverted preconditioning with multigrid techniques. Spectral multigrid methods take advantage of the fact that most iterative methods are highly effective in reducing the error components corresponding to the upper half of the eigenvalue spectrum, but are very inefficient on the remaining, low frequency components. Thus, in a multigrid method one combines iterations on the desired grid with (much cheaper) iterations on successively coarser grids. The details of this method are admittedly subtle, but they have been carefully described in a series of papers (Zang, et al (1982, 1984), Streett, et al (1985), Phillips, et al (1986)). Brandt, et al (1985) have demonstrated that many periodic problems can be successfully solved in this manner without the need for any preconditioning.

Another recent innovation has been the development of spectral multidomain techniques. These allow spectral methods to be applied to geometries for which a single, global expansion is either impossible, or else inadvisable due to resolution requirements which vary widely over the domain. In a multidomain technique the full domain is partitioned into (not necessarily disjoint) subdomains. These may be patched together at interfaces or else they may overlap. The crucial part of the patched multidomain methods are the interface conditions. These may be expressed explicitly as continuity conditions (Orszag (1980), Kopriva (1986)), may arise from a variational principle (Patera (1984)), may consist of integral constraints (Macaraeg and Streett (1986)), or may be enforced by a penalty method (Delves and Hall (1979)). The spectral element method of Patera is to date the most highly developed of these. Many techniques, such as isoparametric elements (Korczak and Patera (1986)), have been borrowed from conventional finite element methodology. Indeed, there are many similarities in this approach to the p-version of the finite element method (Babuska and Dorr (1981)). Figure 4 illustrates a spectral element grid as well as the computed solution for flow past a cylinder (Karniadakis, et al (1986)). In all cases convergence is achieved with a fixed number of subdomains while the number of grid points on each subdomain increases. The spectral overlapping subdomain methods were devised by Morchoisne, et al (1983), and are currently being investigated extensively in Europe.

INVISCID FLOW

Perhaps the simplest fluid dynamical problems are those which are steady, inviscid, incompressible and irrotational. In terms of the velocity potential ϕ, these are described by the Laplace equation

$$\nabla^2 \phi = 0 \tag{12}$$

with Neumann conditions on the boundaries. Spectral methods can be quite effective on such elliptic problems and also on the slightly more general class of problems described by

$$\nabla^2 \phi - \lambda\phi = f \tag{13}$$

with Dirichlet, Neumann or mixed boundary conditions. These more general methods could easily be applied to the idealized flow problem described above.

Spectral methods have been developed for such Poisson/Helmholtz problems in a variety of geometries. Direct methods are straightforward when at most one of the directions requires non-periodic boundary conditions, and hence a Chebyshev polynomial representation. Constant coefficient equations become diagonal in the periodic directions. In a cartesian non-periodic direction the equation can be reduced to a quasi-tridiagonal form (GO, Ch. 10) if the domain is finite and a penta-diagonal form if it is infinite and the cotangent mapping is used (Cain, et al (1984)). Otherwise, a matrix diagonalization technique can be employed (Murdock (1977), Haidvogel and Zang (1979)). Direct methods for problems with 2 or more non-periodic directions have been discussed by Haidvogel and Zang (1979), Haldenwang, et al (1984), and LeQuere and Roquefort (1985). Some extensions to three non-periodic directions are described by Haldenwang, et al (1984) and Tan (1985). Iterative methods allow efficient treatment of more general geometries, especially for exterior problems. See Canuto, et al (1985) and Deville and Mund (1985) for some standard techniques. Especially for very large problems of this type, spectral multigrid methods appear to be the most efficient (Zang, et al (1982, 1984)).

Compressible potential flow is described by a similar, but nonlinear equation

$$\nabla \cdot (\rho \nabla \phi) = 0 \tag{14}$$

where the density ρ is a quadratic function of $\nabla\phi$. For subsonic flow this problem is elliptic. Streett, et al (1985) have demonstrated the great efficiency that spectral multigrid methods achieve for this case. They have applied these techniques to the two-dimensional flow past a circular cylinder. Using a mere 2000 grid points they have obtained an estimate for the free stream Mach number at which the flow first becomes sonic. It agrees to 6 digits with the results of van Dyke and Guttman (1983) based on a Rayleigh-Jensen expansion.

For transonic flow, the potential equation is of mixed type, with a supersonic pocket embedded in a subsonic flow. There will be a sonic line and usually a shock which terminates the supersonic region. The challenging numerical task is to obtain a converged solution to the discrete, nonlinear potential equation. Spectral multigrid methods have proven competitive with finite difference methods and achieve substantial economies in storage (Streett, et al (1985)).

Still within the confines of inviscid flow, one can obtain the effects of vorticity by resorting to the Euler equations

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \underline{q}) = 0 \\ &\frac{\partial \underline{q}}{\partial t} + \underline{q} \cdot \nabla \underline{q} = -\frac{1}{\rho} \nabla p. \\ &\frac{\partial S}{\partial t} + \underline{q} \cdot \nabla S = 0, \end{aligned} \tag{15}$$

where $\underline{q}$ is the velocity, p is the pressure, S is the entropy, and $p = \rho^{\gamma} e^{S/S_0}$. As is the case for all numerical methods, the real delicacy is the treatment of sonic lines and shock waves. The discontinuities arising from shocks are especially troublesome for spectral methods. The global nature of these approximations induces oscillations in the solution which are essentially of a Gibbs phenomenon type. The high frequency component of the solution decays very slowly. This part of the spectrum must be filtered to produce a presentable approximation. A detailed mathematical analysis of filtering techniques in Fourier spectral methods for linear, hyperbolic problems with discontinuous solutions has been presented by Majda, et al (1978). A post-processing procedure that involves matching the computed solution with simple discontinuities has been discussed by Abarbanel, et al (1985).

The first applications of spectral methods to compressible flows focused on the treatment of shock waves in one-dimensional problems (Gottlieb, et al (1981), Zang and Hussaini (1981), Taylor, et al (1981)). As is the case with finite difference methods, spectral methods for problems involving shocks require some type of explicit or implicit numerical dissipation. In solutions to partial differential equations the explicit dissipation may take the form of a linear, spectral filter, or it may consist of an artificial viscosity term which is added to the Euler equations. This artificial viscosity may be nonlinear. Approximations based on Chebyshev polynomials may be stable without any explicit dissipation since the Chebyshev derivative operator contains implicit dissipation (Gottlieb, et al (1981)).

Most investigations have confined themselves to problems whose solutions (even in two-dimensions, Sakell (1984)), were either piecewise constant or else piecewise linear. No one has yet exhibited a spectral solution to a problem with both shock waves and complex flow structure in which spectral accuracy was attained (Hussaini, et al (1985a)).

The difficulties that shock capturing spectral methods exhibit are not due to any intrinsic difficulty in resolving transonic and supersonic flows. Kopriva, et al (1984) solved the Ringleb flow problem, which is a smooth two-dimensional transonic flow with a closed form solution, by a Chebyshev spectral method. They were able to exhibit the usual spectral accuracy on this class of problems.

The shock-fitting approach popularized by Moretti (1968) for finite difference schemes was adapted to spectral discretizations by Salas, et al (1982). This technique avoids the Gibbs phenomenon by treating the shock as a boundary rather than as an interior region of the flow. It is applicable to flows which contain a few, geometrically simple shocks. Some problems for which high resolution results have been obtained by this method are the shock-vortex iteraction (Salas, et al (1982)), the shock-turbulence interaction (Zang, et al (1983), and the blunt body problem (Hussaini, et al (1985b)).

BOUNDARY LAYER

In many aerodynamic applications the boundary layer equations are an economical and useful model of viscous effects, especially when coupled interactively with an inviscid model for the outer flow (AGARD, 1981). In similarity variables the two-dimensional boundary layer is described by

$$\frac{\partial}{\partial \eta}\left(\nu \frac{\partial f}{\partial \eta}\right) - v \frac{\partial f}{\partial \eta} - \beta(f^2 - 1) - 2\xi f \frac{\partial f}{\partial \xi} = 0$$

$$\frac{\partial v}{\partial \eta} + f + 2\xi \frac{\partial f}{\partial \xi} = 0 \tag{16}$$

where f is the non-dimensional streamwise velocity, v is the normal velocity, η is the normal coordinate, and ξ is the streamwise coordinate. The boundary conditions are $f = v = 0$ at $\eta = 0$ and $f \to 1$ as $\eta \to \infty$. An inflow condition is required at some $\xi = \xi_0$.

Chebyshev spectral approximations to the similar version of this system $(\partial/\partial\xi = 0)$ are fairly straightforward to obtain by simple preconditioned iterative schemes (Streett, et al (1984)). This work demonstrated that a combination of domain truncation (typically at $\eta = 15$) and grid stretching (to pack grid points near the solid boundary) is quite effective. A mere 20 collocation points will usually yield values for the wall shear and displacement thickness that have 3-digit accuracy, while 30 points produce 5-digit accuracy.

The full non-similar equations are more challenging since there is a Chebyshev approximation in two directions. Streett, et al (1984) used an alternating direction type of preconditioning to obtain a solution. For non-similar flow roughly 20 polynomials in ξ (coupled with 25 in η) are required for 3-digit accuracy. They found that the Chebyshev approximation in ξ produced a substantial improvement over a simpler, mixed scheme which used finite differences in ξ together with Chebyshev collocation in η. The global nature of the streamwise approximation is especially useful for handling separated flow. In this case marching techniques in ξ are ineffective for finite difference approximations. Figure 5 displays the streamlines and skin friction from a fully spectral solution of separated boundary layer flow. The arrow marks the region of the flow which is most sensitive to the numerical resolution. To obtain 4-digit accuracy in the skin friction here requires 40 collocation points in the normal direction and 26 in the streamwise direction. The corresponding requirements for a standard second-order finite difference method are 240 and 200 points respectively. Moreover, the spectral solution requires only 10% of the CPU time taken by the finite difference method.

NAVIER-STOKES FLOW

Much of the current enthusiasm for spectral methods is attributable to their success on simple, yet computationally intensive problems in viscous, time-dependent, incompressible flow. The pioneering simulations of three-dimensional homogeneous, isotropic turbulence by Orszag and Patterson (1972) were particularly influential. Subsequent calculations of three-dimensional transition and turbulence in simple wall-bounded flows have also been persuasive. Algorithms for these problems are substantially more difficult and time-consuming than those for homogeneous flows. The presence of non-periodic boundary conditions makes purely Fourier methods inappropriate and detailed simulations of transition problems typically require an order of magnitude more time-steps than do turbulence problems. The simplest class of such problems consists of flows which are assumed to be periodic in two directions, e.g., Poiseuille flow and Taylor-Couette flow for cylinders of infinite length. In these cases, ones needs a Chebyshev discretization in only one direction. Several types of multidomain spectral techniques are currently being explored to extend further the class of viscous problems that are amenable to spectral methods.

In many applications the preferred version of the Navier-Stokes equations is

$$\frac{\partial \underline{q}}{\partial t} + \underline{\omega} \times \underline{q} = - \nabla P + \nu \nabla^2 \underline{q}$$

$$\nabla \cdot \underline{q} = 0. \tag{17}$$

The velocity is denoted by $\underline{q}$, the pressure by p, the vorticity by $\underline{\omega} = \nabla \times \underline{u}$, the pressure head by $P = p + (1/20|\underline{q}|^2$, and the kinematic viscosity by ν. This so-called "rotation" form is favored because, as noted by Orszag (1972), the use of the rotation form guarantees that Fourier collocation methods conserve kinetic energy. One can easily show that momentum is conserved as well. The conservation of kinetic energy is especially important for numerical reasons. In practice, it means that if the time differencing scheme is operated at time-steps below its stability limit, then nonlinear instabilities will not occur.

Homogeneous Turbulence

Homogeneous, isotropic turbulence is perhaps the one fluid dynamical problem for which strictly periodic boundary conditions in all spatial directions are justifiable. Hence, Fourier spectral methods are ideally suited for this class of problems. Moreover, since the nonlinearities of the Navier Stokes equations are at worst quadratic, Fourier Galerkin methods are the most natural and efficient spectral technique for this problem (Orszag and Patterson (1972). Rogallo (1981) developed a linear coordinate transformation that permits simulation of flows with constant strain, shear and rotation within the confines of periodic boundary conditions. Rogallo (1981) and Basdevant (1983) have discussed techniques for minimizing the storage, CPU time and I/O costs of such algorithms.

The original simulations of Orszag and Patterson were on 32^3 grids. By the early 1980's, 64^3 simulations were fairly routine. Rogallo (1981), Kerr (1985) and Lee and Reynolds (1985) have performed numerous 128^3 simulations. By fully exploiting the special symmetries of the Taylor-Green vortex, Brachet, et al (1983) achieved a simulation of this flow at a Reynolds number of 3000 with an effective resolution of 256^3.

Fourier collocation approximations to this problem are also possible. For these approximations use of the rotation form of the Navier-Stokes equations is crucial. (Galerkin approximations to the inviscid form of these equations will automatically conserve momentum and kinetic energy in the absence of time differencing errors).

The review by Rogallo and Moin (1984) discusses many applications of these techniques to problems in homogeneous turbulence. Here we need mention only the most recent applications. A primary goal of most of the simulations of isotropic turbulence has been to establish numerically the existence of an inertial range. The inertial range has, of course, been established experimentally, but only for Reynolds numbers exceeding 10,000. Even though the high resolution calculations of Brachet, et al (1983) were performed at a Reynolds number of 3000, which is uncomfortably low by experimental standards, they did achieve the first plausible inertial range in a numerical simulation of turbulence. Bardina, et al (1985) and Dang and Roy (1985) have simulated the evolution of turbulence intensity in rotating flow. Wu, et al (1985) have performed calculations of compressed turbulence. Lee and Reynolds (1985) have analyzed the structure of turbulence in axisymmetrically contracting and expanding flow. Moin, et al (1985) have used numerical simulations to extract the large-scale vortical structures of some turbulent shear flows. Kerr (1985) has examined high-order correlations and small-scale structure in isotropic turbulence involving passive scalars.

A few applications, all using the collocation technique, have been made to compressible, homogeneous turbulence. Feiereisen, et al (1981) simulated subsonic turbulent flows with uniform shear. They used a collocation method, in part because a Galerkin method is much more cumbersome and costly for problems with more than quadratic nonlinearities. Compressible, two-dimensional turbulence has been investigated by Leorat, et al (1985) and by Delorme (1984), the former with a fairly standard scheme and the latter with an implicit time-differencing method based on the ideas of Lerat, et al (1982).

Linear Stability

Most investigations of stability and transition in wall-bounded flows rely, at least in part, upon the results of linear stability theory. The Orr-Sommerfeld equation has been the basis for many investigations of the stability of incompressible parallel flows (Drazin and Reid (1981)). This eigenvalue problem is described by a fourth-order ordinary differential equation. The Chebyshev approximation developed by Orszag (1971) for the temporal stability problem has been adopted and extended by many investigators. (A separate development of Chebyshev methods for ordinary differential eigenvalue problems has been conducted by Ortiz. See Chaves and Ortiz (1968) and, more recently, Ortiz and Samara (1983).) Leonard and Wray (1982) developed a Galerkin method for pipe flow which uses special Jacobi polynomials. Spalart (1984) demonstrated that for exterior flows (such as the parallel boundary layer) the use of only half the usual Chebyshev basis was advisable. Boyd (1985) has developed methods in the complex plane which are useful for flows in which the critical layer is well-separated from the wall. Von Kerczek (1982) has used Chebyshev polynomials for assessing the stability of oscillatory plane Poiseuille flow. Mac Giolla Mhuiris (1986) has used the Galerkin technique to examine the linear stability of some axisymmetric flows which are relevant to the vortex breakdown problem.

The spatial stability versions of these problems are more difficult because the eigenvalue enters nonlinearly. Chebyshev methods for time-independent but spatially growing perturbations of Poiseuille flow are discussed by Bramley and Dennis (1982). Bridges and Morris (1984a, 1984b) solved by a spectral method the more difficult, general spatial stability problem of self-similar boundary layers.

These methods have been extended, in the manner of Floquet theory, to include weakly nonlinear effects. In addition to a Chebyshev discretization in the direction normal to the wall, one includes several Fourier harmonics in the streamwise direction. Orszag and Patera (1983) and Herbert (1983a) have used this approach to determine the neutral stability surface of finite amplitude two-dimensional Tollmien-Schlichting waves in channel flow. In turn, the linear stability of these neutral finite amplitude waves can be examined. Thus, the linear stability of some special, temporally and spatially varying flows can be examined. Orszag and Patera (1983) have used this technique to study the interaction of two-dimensional and three-dimensional Tollmien-Schlichting waves in channel flow. Herbert (1983a, 1983b, 1984) has performed a detailed study of channel and boundary layer flows. He has unravelled the details of fundamental and subharmonic instabilities in parallel flows.

Transition

Transition to turbulence is highly nonlinear and a full simulation of the Navier-Stokes equations is required for its investigation. The primary difficulty of algorithms for incompressible flows is the simultaneous enforcement of the incompressiblity constraint and the no-slip boundary condition. This constraint is most easily but least rigorously satisfied in splitting methods, of which the Orszag-Kells (1980) algorithm is the prototype. The splitting errors of this method are O(1) near the boundary for the normal pressure gradient and diffusion terms (Deville 1985). They appear to cause no serious errors in the channel flow problem. However, Marcus (1984a) decisively demonstrated that the boundary errors produce serious inaccuracies in Taylor-Couette flow -- as both the spatial and temporal discretizations are refined, the algorithm appears to converge to answers that disagree with experiments in the third digit. Marcus (1984a) and Kleiser and Schumann (1984) devised an influence matrix technique which completely eliminates the splitting errors at a modest extra cost. Marcus found that the results of this algorithm agreed with the experimental results to the full 4 digits that were available. He ascribed the sensitivity of the rotating cylinder problem to the fact that its dynamics are driven by the motion of the boundary rather than by a mean pressure gradient.

A procedure for reducing, although not entirely eliminating the splitting errors at the boundary, was devised by Fortin, et al (1971) for finite element methods (re-discovered later by Kim and Moin (1985)), and applied to spectral algorithms by Zang and Hussaini (1986). It consists of modifying the boundary conditions for the intermediate steps of the algorithm so that both the no-slip and divergence-free conditions are satisfied at the end of the full time-step to a higher order in the size of the time-step.

The big advantage of these splitting techniques is that they require the solution of only Poisson equations (for the pressure) or Helmholtz equations (from a Crank-Nicolson discretization of the viscous term). These positive definite, scalar equations are much easier to solve numerically that the indefinite, coupled equations that arise in unsplit methods. The Orszag-Kells, Marcus and Kleiser-Schumann algorithms resort to direct solution methods of the type discussed in section 3. The Zang-Hussaini algorithm employs iterative techniques so that it is applicable to a wider class of problems. The most sophisticated and powerful of the iterative techniques is the spectral multigrid method. It makes the cost of a single time-step of order $N^3 \log_2 N$, even for problems with variable geometric terms and transport coefficients. In contrast, a parallel flow problem, even with uniform transport coefficients, requires order N^4 operations per step by direct methods.

One way to avoid the splitting errors is to integrate the incompressible Navier-Stokes equations in a single step that couples the divergence-free constraint with the momentum equations. The numerical difficulty of this approach is that one must invert a larger set of equations (it involves the pressure as well as the three velocity components), which is indefinite. In a few special cases direct techniques are viable (Moin and Kim (1980)). The preconditioned iterative scheme of Malik, et al (1985) has been applied to channel flow (Zang and Hussaini (1985a)) and to the heated boundary layer (Zang and Hussaini (1985b)), a problem which involves variable transport coefficients, and also in a verification of weakly nonlinear stability theory for stagnation point flow (Hall and Malik (1986)).

Many of the numerical problems caused by the incompressibility constraint can be avoided by an expansion in functions which are divergence-free (Ladyzhenskaya 1969, Temam 1977). Leonard and Wray (1982) first applied this idea to spectral methods. They devised a set of basis functions for pipe flow which are both divergence-free and satisfy no-slip boundary conditions. Similar basis functions have been developed for straight and curved channels (Moser, et al (1983)) and for the parallel boundary layer (Spalart (1984)). This class of methods can be quite economical of storage since only two variables per grid point are required to specify the flow field. (However, in actual implementations it may be more efficient in terms of CPU time to store several additional quantities per grid point.) The efficiency of these methods is dependent upon the bandwidth of the matrices which arise from the implicit treatment of the viscous terms. In the examples cited above, the bandwidth is quite small, roughly of order 10. This requirement has dictated the use of special Jacobi polynomials rather than Chebyshev ones in pipe and boundary layer flow. As a consequence, transform methods are not applicable in the non-periodic direction. Hence, the cost of evaluating the nonlinear terms increases as N^4 rather than as $N^3 \log_2 N$. Moreover, in even slightly more general cases, the matrices can be completely full.

Orszag and Patera (1983) performed a parametric study of the secondary instability in channels and pipes, demonstrating that subcritical instabilities exist at Reynolds numbers as low as 1100. Kleiser and Schumann (1984) replicated many of the features of the Nishioka, et al (1980) experiments on channel flow transition. Both groups also obtained good quantitative agreement with the predictions of weakly nonlinear theory. The subharmonic instabilities that were predicted by Herbert's (1983b), (1984) weakly nonlinear analysis (and are also in evidence in boundary layer experiments, Saric, et al 1984), were reproduced by Spalart (1985) and Laurien (1986) for the boundary layer and by Zang and Hussaini (1985a), and by Singer, et al (1986) for channel flow. The existence of a similar nonlinear instability of center modes in channel flow was uncovered by Zang and Hussaini (1985a). A detailed comparision of nonlinear effects on the laminar flow control techniques of pressure gradient, suction and heating in boundary layer flow was made by Zang and Hussaini (1985b). Krist and Zang (1986) have performed a detailed study of the resolution requirements for simulation of the later stages of transition to turbulence in channel flow. The spanwise direction places the greatest demands on the resolution because of the very sharp spanwise gradients which occur near the tip of the characteristic hairpin vortex. Figure 6, which is extracted from that work, illustrates the structure.

Marcus (1984a, 1984b) has performed a careful numerical study of non-axisymmetric instabilities in classical Taylor-Couette flow. He has produced 4-digit agreement with the wave speeds measured by King, et al (1984) for both the one wavy-vortex and the two wavy vortex states. Marcus and Tuckerman (1986a, 1986b) have simulated axisymmetric spherical Couette flow. Unlike previous workers they did not assume equatorial symmetry. This was a crucial factor in their success in reproducing the transitions between 0, 1, and 2 vortex states observed by Wimmer (1976).

Inhomogeneous Turbulence

In several cases these algorithms have been used to simulate turbulence in wall-bounded flows. Orszag and Patera (1983) performed a 64^3 simulation of turbulent channel flow which reproduced the turbulent velocity profile, including the law of the wall behavior. Moser, et al

(1984) computed turbulent flow in a curved channel on a $128^2 \times 64$ grid. They reproduced some of the data on low-order turbulence statistics and exhibited some of the effects of curvature. Spalart and Leonard (1985) have done some analyses of pressure gradient effects in turbulent boundary layers.

More Realistic Geometries

As noted above, there is a substantial increase in cost when there is more than one inhomogeneous direction in the problem. The Kleiser-Schumann influence matrix technique has been extended to two non-periodic directions by LeQuere and Roquefort (1985), who used it to study thermal convection in a square cavity. Streett and Hussaini (1986) similarly extended the split algorithm of Zang and Hussaini (1986), and used it to study the effect of finite length cylinders in Taylor-Couette flow. Ku and Taylor (1985) have developed an algorithm for three non-periodic directions. This method presently treats only the pressure term implicitly. Thus, there can be a severe time-step limitation arising from the viscous terms. Morchoisne (1984) has developed a number of methods for problems with more than one non-periodic direction. In general iterative techniques are used for solving the resulting implicit equations. There has not yet been any systematic comparison of these methods. Leonard (1984) has derived a set of divergence-free basis functions for 2 nonperiodic directions, but an efficient solution technique for the implicit equations has not yet been devised.

Several of the multidomain spectral methods have been applied to viscous problems. Morchoisne (1984) has performed some sample calculations of channel flow. The spectral element has been used to calculate heat transfer in a two-dimensional, grooved channel (Ghaddar, et al (1984)) and to investigate stability and resonance phenomena in imbedded cavities in channel flows (Ghaddar, et al (1986a, 1986b)). Other applications include two-dimensional flow past a cylinder and flow past three-dimensional roughness elements (Karniadakis, et al (1986)).

Spectral/Finite Difference and Quasi-Spectral Methods

Heretofore, this review has been confined to numerical fluid dynamical work which employed spectral discretizations in all coordinate directions. There have, of course, been numerous computations which used mixed spectral/finite difference methods, i.e., algorithms with spectral discretizations in some directions and finite differences in the others. The parallel boundary layer transition calculations of Wray and Hussaini (1984) fall into this category. They used a Fourier spectral method in two periodic directions and second-order finite differences in the normal direction. They demonstrated that, despite the neglect of non-parallel effects, these simulations could reproduce features observed experimentally by Kovasznay, et al (1962), up to the so-called "two-spike stage" of transition. A slightly different spectral/finite difference method was used by Moin and Kim (1982) in their large-eddy simulations of turbulent channel flow and by Biringen (1985) in a study of active control in channel flows. More recently, Eidson, et al (1986) have used a similar algorithm in a high resolution direct simulation of a turbulent Rayleigh-Benard flow.

Another alternative to true spectral methods are what might be termed quasi-spectral methods. Such algorithms employ Fourier expansions in all directions but infinite-order accuracy is not attained due to non-periodic physical boundary conditions in at least one direction. The simulations by Riley and Metcalfe (1980) of a time-developing mixing layer fall into this category. In this idealized flow the mean velocity is solely a function of the transverse coordinate y. Although the flow extends to $y = \pm\infty$, Riley and Metcalfe computed on a finite domain in y and used sine or cosine expansion to enforce free-slip boundary conditions in y. Quasi-spectral methods have also been used by Curry, et al (1984) to study Benard convection.

True spectral methods have been developed for the time developing mixing layer. Cain, et al (1984) use a cotangent transformation in y combined with a Fourier method. Metcalfe, et al (1986) use hyperbolic tangent or algebraic transformations combined with a Chebyshev method.

Riley and Metcalfe (1980) find that large amplitude two-dimensional disturbances have a pronounced effect upon the evolution of a turbulent mixing layer. Metcalfe, et al (1986) find that the mixing layer exhibits three-dimensional secondary instabilities similar to those which occur in wall-bounded flows. They appear to account for the mushroom-shaped features which are observed experimentally. Cain, et al (1981) have performed large-eddy simulations of this problem.

REACTING FLOWS

An emerging application field for spectral methods is reacting flows. These flows are especially challenging because they contain sharp gradients in both space and time and because most real flows involve dozens or even hundreds of species. Flame fronts and shock waves are an additional complication. Some of the important features are mixing rates, ignition, and flame holding.

There are a number of simplifying assumptions which lead to more tractable, but less realistic, models of reacting flows. The most drastic of these is that the reactions proceed without heat release and that the Mach number is so low that the flow may be trated as incompressible. Riley, et al (1986) have performed some three-dimensional simulations of a 2 species, time-developing mixing layer. They used a quasi-spectral method and obtained good agreement with both similarity theory and experimental data.

McMurtry, et al (1986) employed a low Mach number approximation which includes some mild heat release effects but neglects the acoustic modes. They performed some two-dimensional calculations which indicate that the first-order effect of heat release is to reduce the rate of mixing.

Drummond, et al (1986) applied a Chebyshev spectral method to a supersonic quasi-one-dimensional diverging nozzle flow with a simple but quite stiff 2 species hydrogen-air reaction. The spectral method proved to be quite economical compared with a benchmark finite difference result. The Chebyshev grid point distribution was quite well-adapted to the sharp gradients at the nozzle inflow, but less well-suited to the fairly uniform outflow region.

PERSPECTIVE

A decade ago spectral methods appeared to be well-suited only to problems governed by ordinary differential equations or by partial differential equations with periodic boundary conditions. And, of course, the solution itself needed to be smooth. Some of the obstacles to wider application of spectral methods were: 1) sensitivity to boundary conditions; 2) treatment of discontinuous solutions; 3) resolution and time-step limitations imposed by the standard spectral grids; and 4) drastic geometric constraints.

Substantial progress has been made on the implementation of Neumann boundary conditions, on characteristic boundary conditions for hyperbolic systems, and on the use of pressure and intermediate boundary conditions in incompressible flow. There have been some theoretical advances on filtering techniques for discontinuous solutions to linear problems. Moreover, the development of shock-fitting techniques has opened a new field of applications to compressible flows with shock waves. Some efficient direct solution techniques have been devised which enable severe viscous time-step limitations to be overcome in certain special geometries. The development of preconditioned iterative methods and, in particular, spectral multigrid techniques have radically expanded the class of problems which can be handled efficiently by spectral methods. Moreover, they lend much greater flexibility (combined with mapping techniques) to the grid point distribution. Finally, various multidomain techniques have expanded the range of spectral methods to many problems of real, practical interest.

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CAPTIONS

1. Comparison of finite difference (left) and Chebyshev spectral (right) differentiation. The solid curves represent the exact function and the dashed curves their numerical approximations. The solid lines are the exact tangents at $x = 0$ and the dashed lines the approximate tangents. The error in slope is noted as is the number of intervals N.

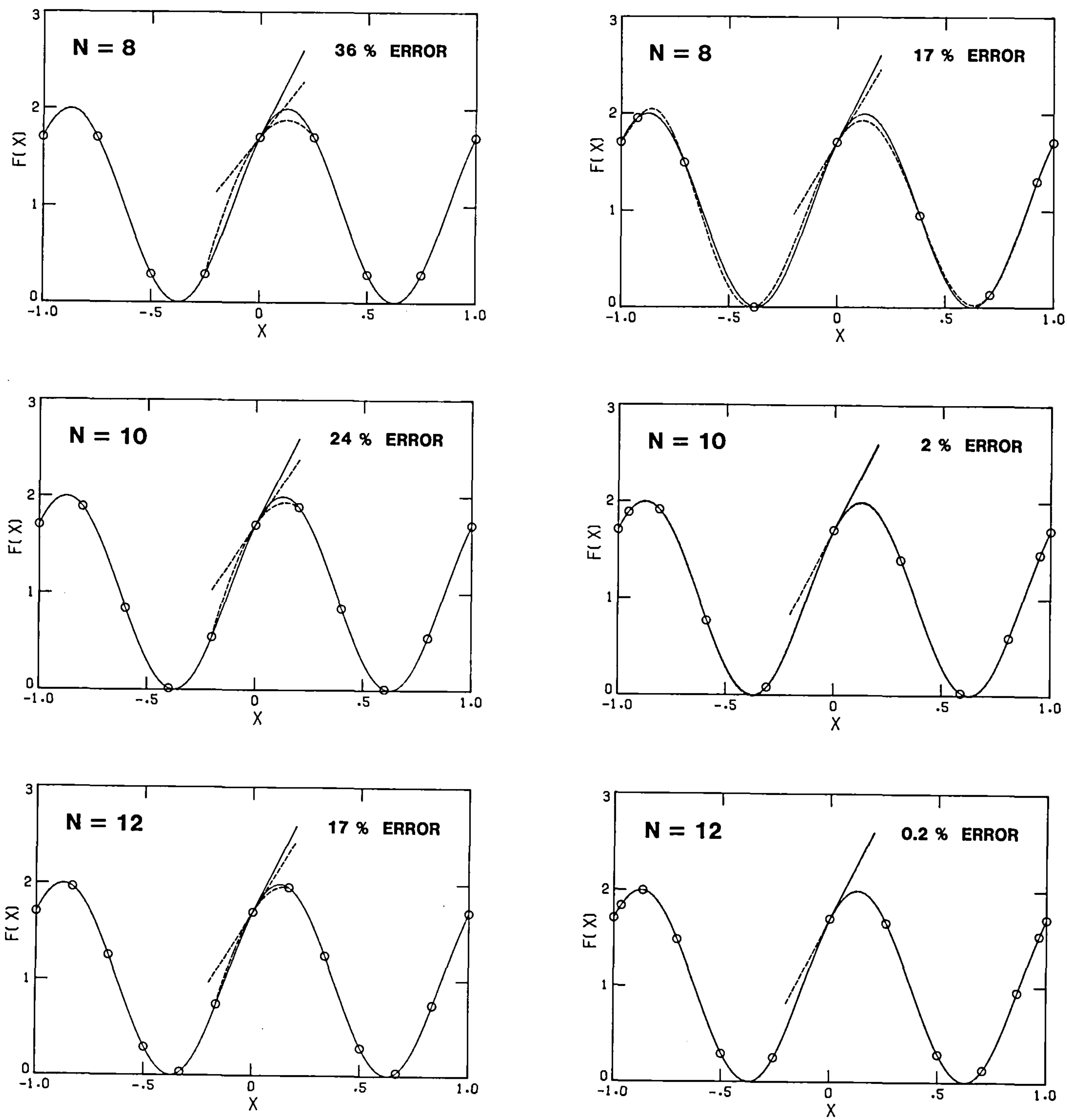
2. Finite difference (circles) and Fourier spectral (diamonds) approximations after one period to a simple wave equation whose exact solution is represented by the curve.

3. Eigenvalues of the Chebyshev first derivative operator for $N = 16$.

4. A spectral element grid (top) and the corresponding numerical solution for flow past a circular cylinder (courtesy of G. E. Karniadakis and A. T. Patera).

5. Streamlines (top) and skin friction (bottom) from a Chebyshev spectral solution of the boundary layer equations (courtesy of C. Streett).

6. Streamwise (left) and spanwise (right) vorticity at four streamwise locations for a hairpin vortex in low Reynolds number channel flow transition. Only the lower half of the channel is shown.



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36 % ERROR
N = 8
17 % ERROR
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24 % ERROR
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2 % ERROR
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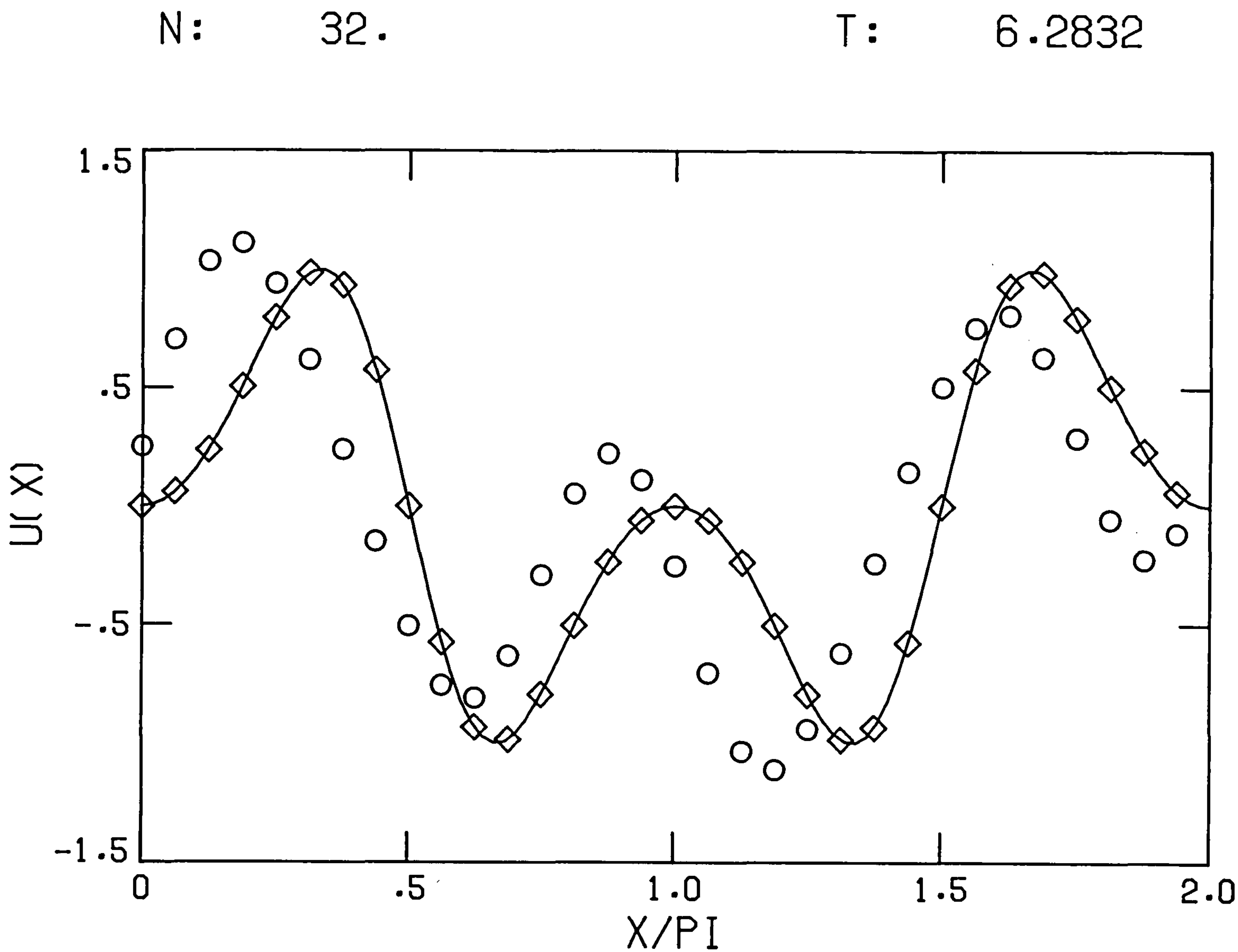
17 % ERROR
N = 12
0.2 % ERROR
F(X)
X

Figure 1



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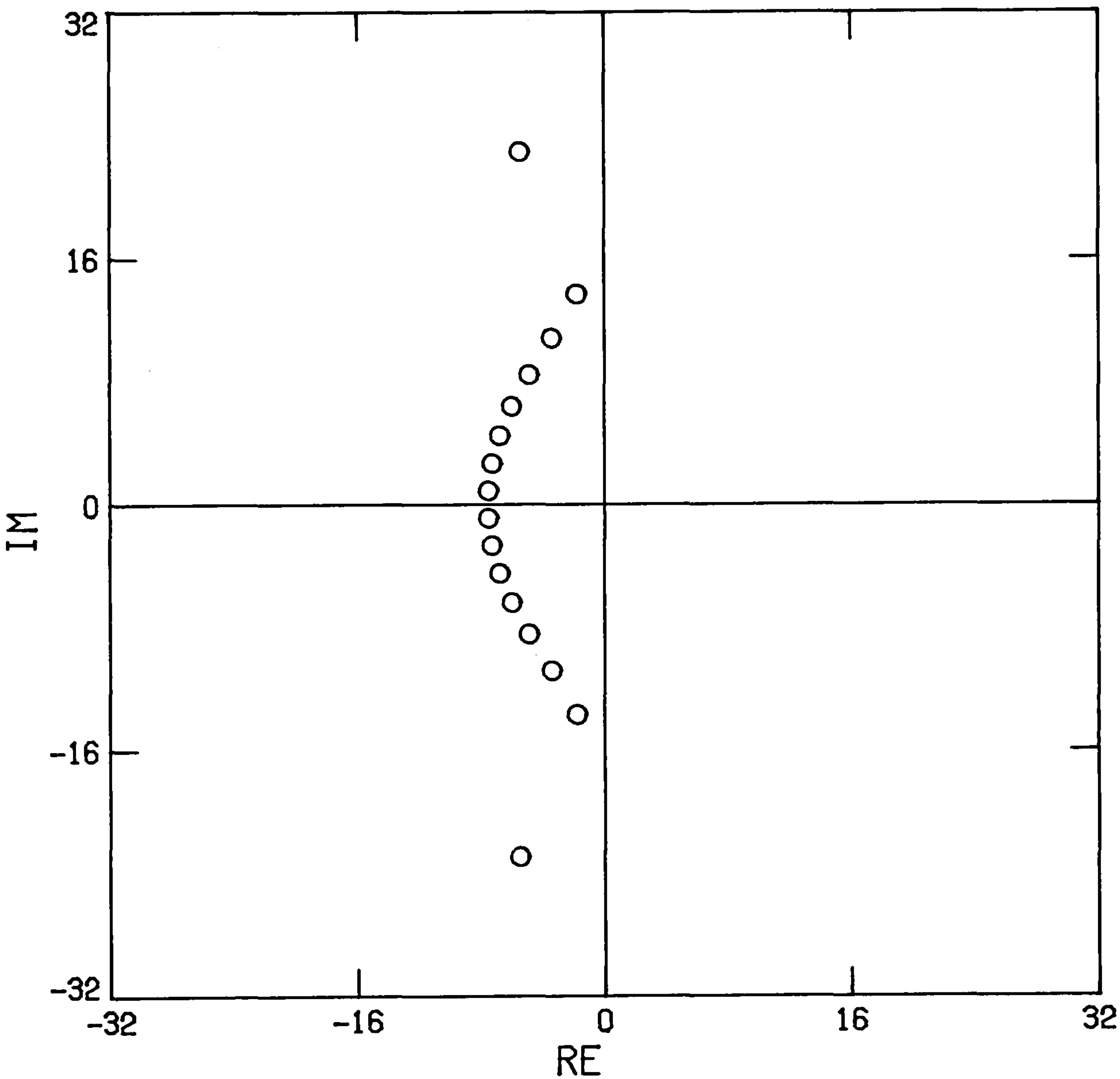

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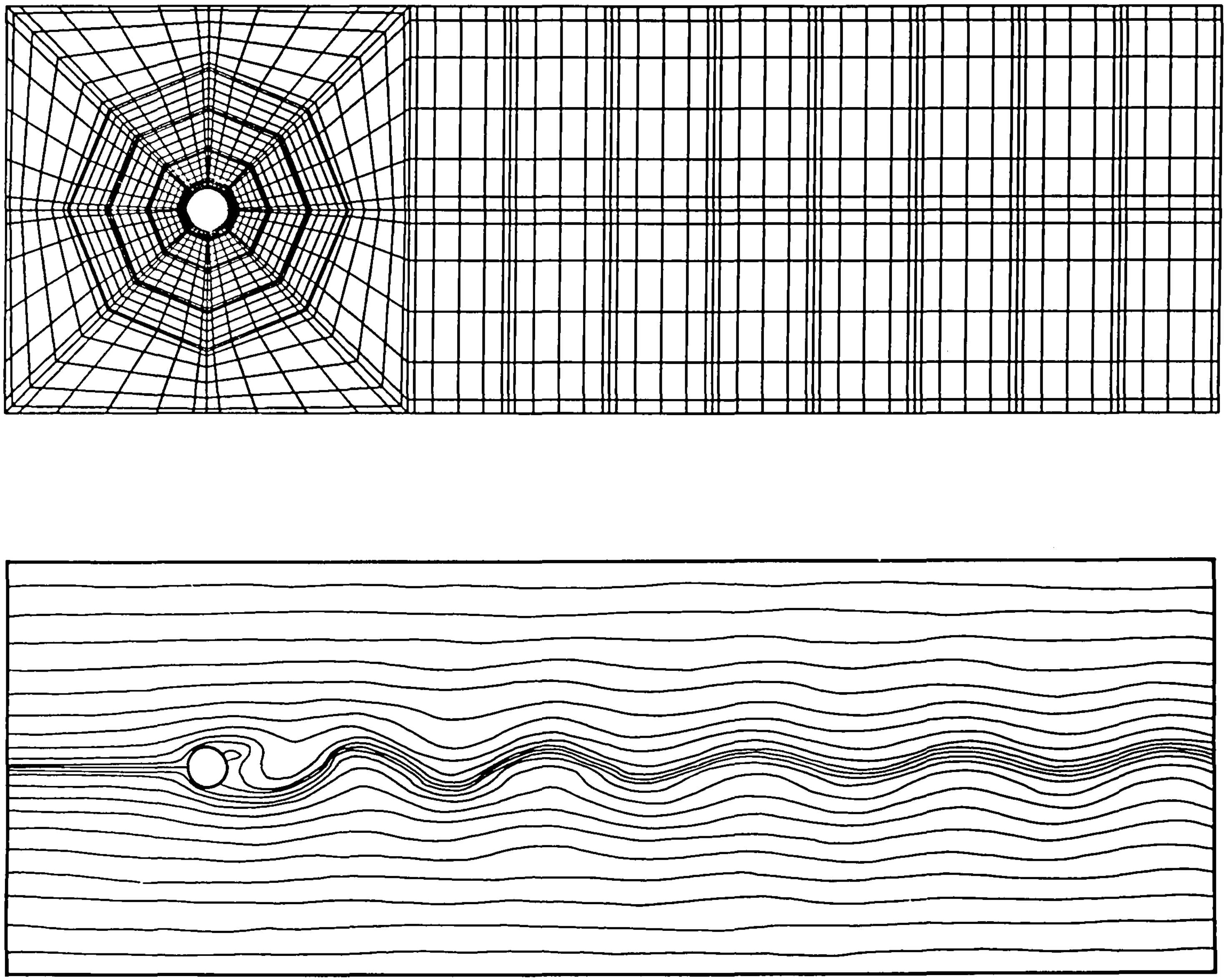

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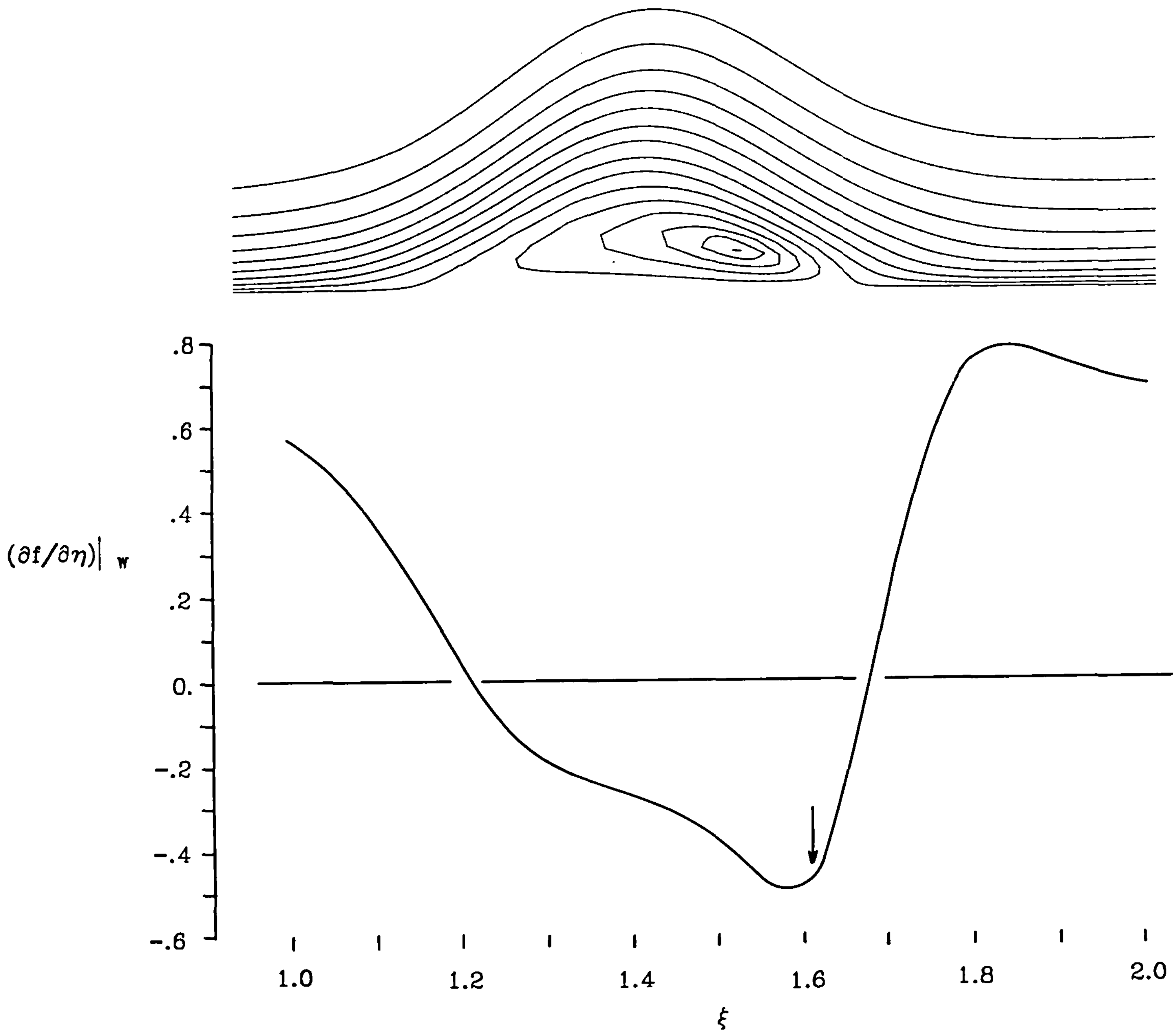

Figure 5

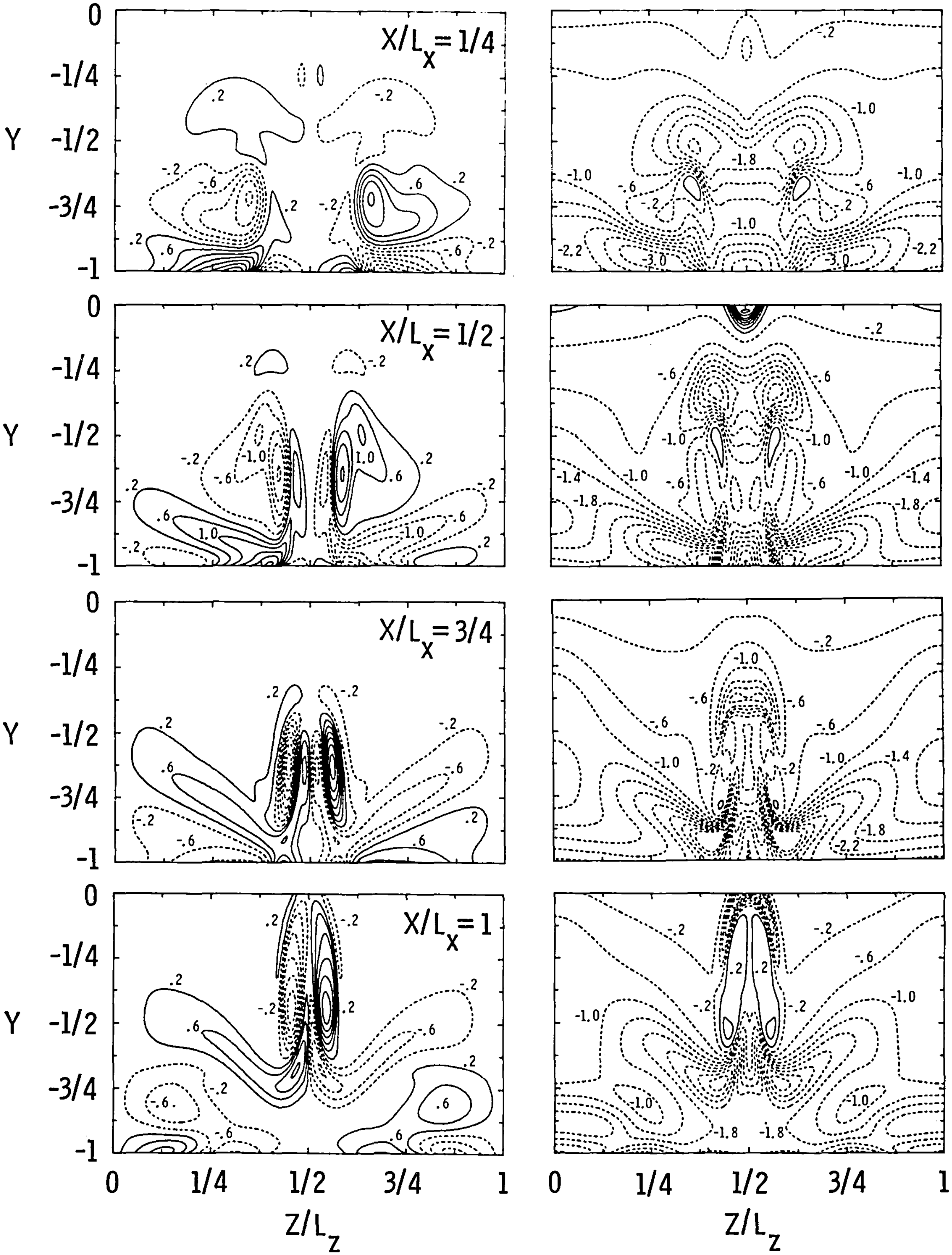

Figure 6

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16. Abstract

Fundamental aspects of spectral methods are introduced. Recent developments in spectral methods are reviewed with an emphasis on collocation techniques. Their applications to both compressible and incompressible flows, to viscous as well as inviscid flows, and also to chemically reacting flows are surveyed. The key role that these methods play in the simulation of stability, transition, and turbulence is brought out. A perspective is provided on some of the obstacles that prohibit a wider use of these methods, and how these obstacles are being overcome.

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