The investigator proved research on the use of spectral methods in computational fluid dynamics. In particular, he looked at their implementation for the solution of time dependent partial differential equations. Other topics pursued included the adaptation spectral methods for compressible flow problems involving shocks, and the exploration of information content in spectral calculations.
The following topics were researched:

1) Spectral methods for time dependent partial differential equations.

The theory of spectral methods for time dependent partial equations is reviewed. When the domain is periodic, Fourier methods are presented while for nonperiodic problems both Chebyshev and Legendre methods are discussed. The theory is presented for both hyperbolic and parabolic systems using both Galerkin and collocation procedures. While most of the review considers problems with constant coefficients, the extension to nonlinear problems is also discussed. Some results for problems with shocks are presented. (See Appendix 1)

2) Spectral methods for compressible flow problems.

In this article we review recent results concerning numerical simulation of shock waves using spectral methods. We discuss shock fitting techniques as well as shock capturing techniques with finite difference artificial viscosity. We also discuss the notion of the information contained in the numerical results obtained by spectral methods and show how this information can be recovered. (See Appendix 2)
3) Recovering pointwise values of discontinuous data within spectral accuracy.

We show how pointwise values of a function, \( f(x) \), can be accurately recovered either from its spectral or pseudospectral approximations, so that the accuracy solely depends on the local smoothness of \( f \) in the neighborhood of the point \( x \). Most notably, given the equidistant function grid values, its intermediate point values are recovered within spectral accuracy, despite the possible presence of discontinuities scattered in the domain. (Recall that the usual spectral convergence rate decelerates otherwise to first order, throughout.)

To this end we employ a highly oscillatory smoothing kernel in contrast to the more standard positive unit-mass mollifiers.

In particular, post-processing of a stable Fourier method applied to hyperbolic equations with discontinuous data recovers the exact solution modulo a spectrally small error. Numerical examples are presented. (See Appendix 3)

4) Information content in spectral calculations.

Spectral solutions of hyperbolic partial differential equations induce a Gibbs phenomenon near local discontinuities or strong gradients.

A procedure is presented for extracting the piecewise smooth behavior of the solution out of the oscillatory numerical solution data. The procedure is developed from the theory of linear partial differential equations. Its application to a non-linear system (the two-dimensional Euler equations of gas dynamics) is shown to be efficacious for the particular situation. (See Appendix 4)
5) Spectral methods for discontinuous problems.

We show that spectral methods yield high-order accuracy even when applied to problems with discontinuities, though not in the sense of pointwise accuracy. Two different procedures are presented which recover pointwise accurate approximations from the spectral calculations. (See Appendix 5)


A set of differential equations for the eigenvalues and eigenvectors of the stability matrix of a dynamical system, as well as for the Lyapunov exponents and the corresponding eigenvectors is derived. The rate of convergence of the Lyapunov eigenvectors is shown to be exponential. The eigenvectors of the stability matrix can be grouped into sets, each spanning a subspace which converges at an exponential rate. It is demonstrated that, generically, the real parts of the eigenvalues of the stability matrix equal the corresponding Lyapunov exponents. This statement has been tested numerically. The values of the Lyapunov exponents, \( \mu_i \), are shown to be related to the corresponding finite time values of the Lyapunov exponents (e.g. those deduced from a finite time numerical simulation), \( \mu_i(t) \), by:

\[
\mu_i(t) = \mu_i + \frac{b_i + \xi_i(t)}{t}
\]

The \( b_i \)'s are constants and \( \xi_i(t) \) are "noise" terms of zero mean. This observation leads to a method of extrapolation, which has been used to predict Lyapunov exponents from a finite amount of data. It is shown that the use of the standard (numerical) methods to compute Lyapunov exponents introduces an error \( \frac{a_i}{t} \) in the value of \( \mu_i(t) \), where the \( a_i \)'s are
constants. Thus the standard method has a rate of convergence which is the same as that of the exact \( u_i(t) \)'s. Finally, we have shown how one can compute the eigenvectors associated with each of the eigenvalues of the stability matrix as well as the Lyapunov eigenvectors. (See Appendix 6)

7) Boundary conditions for incompressible flows.

In this paper, we have analyzed the effect of boundary conditions on incompressible flows. We have explained and analyzed a numerical boundary layer of thickness \( \sqrt{\Delta t} \) that appears in many formulations of incompressible flow problems and we have explained techniques for the development of high-order methods.

For first- or second-order methods, we recommend the use of splitting methods in the form (4.1) - (4.5) or (7.1) - (7.5) with the tangential-derivative boundary conditions (7.16) or the modified velocity boundary conditions (7.28). To achieve higher-order accuracy, we may employ either the extrapolation methods outlined in Sec. 6 or, perhaps even better, we may use schemes of the form (1.11) with high-order pressure boundary conditions of the form (7.23) or iterative conditions of the form (7.25) [with only a few iterations per time step].

In this paper, we have shown that we can characterize methods for the solution of incompressible flow problems as belonging to either parabolic or elliptic type with regard to the determination of the pressure field. The elliptic schemes typically have smaller errors in the divergence field, with the errors decaying exponentially away from the boundaries of
the computational domain. On the other hand, the parabolic schemes have smooth solutions, without numerical boundary layers, but care should be exercised with respect to the boundary conditions in order the initial divergence errors be eliminated. This analysis explains why 'elliptic' schemes, like that introduced by Harlow & Welch (1965) have been found to be more accurate than parabolic schemes.

We have also shown, using Weyl's lemma for the decomposition of a flow into its solenoidal and irrotational components, that it is possible to derive accurate boundary conditions for the pressure that involve only the tangential derivative of the boundary vorticity. This form of the boundary condition tends to minimize the effects of numerical boundary layers induced by splitting methods. (See Appendix 7)

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