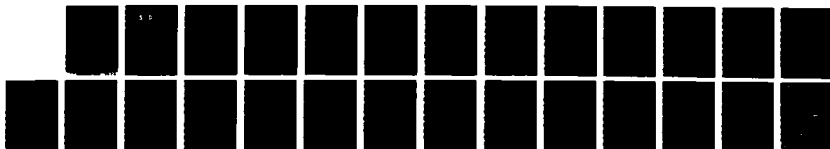
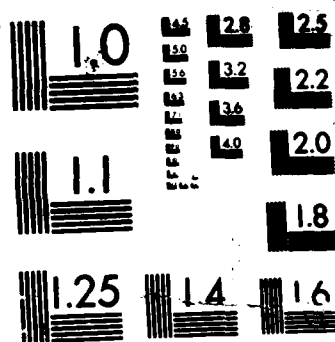


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Variable Reduction
Vectorization

Block 11

For Large-Eddy Simulation of Circular-Jet
Turbulence

UDR-TR-86-131

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**FAST ALGORITHM DEVELOPMENT FOR LARGE-EDDY
SIMULATION OF CIRCULAR-JET TURBULENCE**

L. Krishnamurthy, J. Burkardt, C. A. Hall,
J. S. Peterson, and T. A. Porsching

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SECTION I

INTRODUCTION

This first annual technical report documents the current status and accomplishments of the research performed by the University of Dayton for the Air Force Office of Scientific Research (AFOSR), Fast Algorithms Initiative. The research documented herein was carried out by the University of Dayton Research Institute (UDRI) as the prime contractor and by the University of Pittsburgh Institute for Computational Mathematics and Applications (ICMA) as the subcontractor.

1.1 BACKGROUND

The so-called turbulence problem in fluid mechanics remains unsolved, but not for a lack of theoretical interest or of practical importance. From the theoretical viewpoint, the understanding and prediction of turbulent shear flows from first principles have remained elusive and continue to provide challenging problems in fluid dynamics, computational physics and mathematics, and numerical algorithm development. From a practical viewpoint, many research and development problems of interest to the Air Force, ranging from combustion in jet engines and rocket motors to aerodynamics of wings and surfaces, give rise to the transport of mass, momentum, and energy that are predominantly governed by turbulent flows, thereby necessitating their understanding and prediction.

It is generally accepted that fluid mechanical turbulence begins in an erstwhile laminar flowfield as the onset and growth of hydrodynamic instabilities. According to this traditional viewpoint, as the energy driving the macroscopic instabilities cascades through higher and higher wavenumbers, culminating in what is commonly referred to as the fully developed turbulence,

the overall flowfield is characterized by the interaction of a very large number of disparate length and time scales. This viewpoint has led to the predictive approach which seeks the evolution of turbulence from the solution of the time-dependent Navier-Stokes equations. If these equations can be solved exactly for the entire range of the time and length scales prevailing in a realistic flowfield, then the resulting solutions explicitly describe and predict the turbulent flow. Unfortunately, this approach has been thwarted by the enormous computing requirements imposed by the time-dependent, multidimensional Navier-Stokes equations in simulating a realistic flow, which requirements are well beyond the capabilities of today's largest and fastest computers.

The only feasible approach for turbulent flow predictions at present comprises the direct computation of the complete equations on a coarsely resolved grid (dictated by the available computing resources) for describing the "large"-scale motions, the development of model(s) for the "small" subgrid-scale (SGS) turbulent mixing, and the proper coupling of the SGS modeling to the large-eddy simulation (LES). Indeed, the prospects for economical and accurate LES of turbulent shear flows have been greatly enhanced with the increasing availability of vector computers of greater and greater size and speed, the potential for major improvements in the development of efficient numerical algorithms, and the considerable scope for efficient matching of these algorithms to emerging computer architectures.

1.2 SCOPE AND OBJECTIVES

The overall goal of this UDRI-ICMA joint research is the computational investigation of the turbulent mixing layers of several prototype circular-jet configurations. Initial attention is directed at an examination of a single free jet expanding into a quiescent environment, with emphasis on the development of

suitable SGS turbulence models and the computation of large-scale motions. Specific areas addressed during the first year include the following:

- Investigation of the axisymmetric mixing layer of circular jets with LES and SGS modeling.
- Investigation and analysis of variable reduction algorithms, such as the dual variable method.
- Investigation and analysis of numerical algorithms based on weighted combinations of stable and unstable schemes.
- Investigation of vectorization of solution algorithms and its efficient implementation.

Our research to date has entailed a critical review and assessment of the LES and SGS modeling procedures prior to the selection of the specific avenues that have been explored. Furthermore, the research has involved several interdependent phases consisting of a number of tasks. Some of these tasks are independently conducted by UDRI (e.g., SGS turbulence modeling) and by ICMA (e.g., modification and adaptation of an existing two-dimensional procedure) and some have entailed joint efforts (e.g., boundary-condition modifications and algebraic-turbulence-model incorporation and testing). These are discussed in the next section.

1.3 OUTLINE OF REPORT

Section II discusses our accomplishments to date, and gives the current status of our research. Section III presents the documentation from research sponsored under this program. The research personnel at UDRI and ICMA supported by this program are shown in Section IV.

SECTION II

STATUS OF RESEARCH

There has been significant progress in achieving the research objectives outlined in the previous section. A brief summary of our accomplishments to date is presented below.

2.1 MATHEMATICAL DESCRIPTION

The prediction of jet turbulence in the present research has adopted the traditional viewpoint that it is based upon the solutions of the time-dependent Navier-Stokes equations. It must be emphasized, nevertheless, that these equations remain to be fully tested for completeness by computations. Be that as it may, the time-averaged information in a turbulent jet is obtained by solving the time-dependent equations and averaging the solutions. The prediction of the large-scale motion by LES requires the computation of the three-dimensional equations, since the large eddies are highly anisotropic. Thus, while the circular-jet geometry and its mean-flow characteristics preserve axisymmetry, such an assumption for LES is invalid. Within the constraints of the overall research program, however, the present predictive research is based upon the two-dimensional formulation. As regards the small-scale motion, even with our calculation methodology of LES the smallest scale explicitly resolved is very much larger than the Kolmogoroff [1940] scale for viscous dissipation. Thus, while the smallest scales are truly isotropic and possess universal characteristics, that is not the case at the (arbitrary) LES cutoff length scale. This necessitates a closure model for wavenumbers larger than that corresponding to the LES cutoff, with the consequent indeterminacy and the ad hoc introduction of turbulence modeling. The present SGS modeling approach is crude but provides a useful starting point for the incorporation of a variable viscosity in

our calculation procedure. These LES and SGS turbulence modeling approaches are discussed next.

2.1.1 Large-Scale Motion

The initial research effort has addressed the assessment and analysis of LES procedures with a view to arriving at suitable schemes for investigating circular-jet turbulence.

The basis for our predictive computation is the viewpoint that turbulence consists of chaotic motion (with persistent organized structures) at a range of length scales that increases rapidly with the Reynolds number. This range of scales stems from the convective terms of the Navier-Stokes equations. The entire range of scales can be numerically resolved with no modification of the convective terms only for sufficiently low Reynolds numbers (at which complete numerical simulation is possible with currently available computers, but turbulence can not be maintained). When the desired scale range exceeds the lower bound imposed by computer capacity (as in LES), the scales that are smaller than the LES cutoff are discarded, and the influence of these discarded scales upon the retained scales must be modeled. This necessitates the modification of the governing equations, since the computations involving the unmodified Navier-Stokes equations and the arbitrary cutoff in the resolution have no relation to the real fluid physics. This lack of realism can manifest itself in several ways:

- The numerical algorithm for the unmodified LES equations can become unstable as the smallest resolved scales accumulate energy.
- The use of energy-conserving numerical approximations can lead to a nonphysical equilibrium distribution of the energy among the finite degrees of freedom.

- When the viscosity is not zero but is too small to allow accurate resolutions of the dissipation scales, an energy-conserving algorithm collects energy at the smallest resolved scales until there is equilibrium between the dissipation and cascade rates. Indeed, it has been demonstrated that this excess energy, trapped at the mesh scale rather than cascading to the Kolmogoroff scale, produces too rapid an energy transfer from the large scales. Such an occurrence can well be expected if the small scales act on the large scales as an eddy viscosity with a value (proportional to the length and velocity scales of the trapped energy) that is enhanced by the entrapment.

Thus, one of the most important modifications of the Navier-Stokes equations prior to current LES computation is the incorporation of terms that provide the mechanism for removal of energy from the computed scales that mimics as closely as possible the physical cascade process. This aspect is currently under investigation.

Concurrently, LES investigations of an approximate nature have been initiated for addressing the single free jet issuing into an unbounded ambient domain. This research is based upon the ALgorithms for Gas Equations (ALGAE), which is a general-purpose computational procedure developed at ICMA. The version of ALGAE available at the start of this research program is capable of simulating transient, incompressible or compressible, laminar flows in two-dimensional planar and axisymmetric geometries. ALGAE makes use of the dual variable method for reducing the number of difference equations that need to be solved at each time interval. The availability of this particular feature and the potential for extension to address three-dimensional flows in future have led to our choice of ALGAE for investigating the large-scale motions, despite our

recognition of its current limitations in providing true LES of the circular-jet turbulence. Our present intent has been to treat ALGAE as a baseline procedure that can be refined and optimized for the problem at hand through successive implementation of a number of modifications. The modifications addressed during this research are discussed subsequently.

2.1.2 Small-Scale Motion

Several essential requirements must be met by the SGS turbulence model, if it is to provide the correct asymptotic decoupling from the LES computations. To start with, SGS model(s) must satisfy certain matching requirements at two distinguished limits of wavenumbers. These arise from the fact that the essential physics of turbulence is continuously distributed over the entire spectrum of wavenumbers, ranging from $k = 0$ to $k = k_d$ (k_d is the dissipation wavenumber corresponding to the Kolmogoroff microscale, and wavenumbers exceeding k_d belong to the realm of molecular motion and do not concern us), whereas the division of wavenumbers (or length scales) into "large eddies" and modeled "subgrid quantities" is simply arbitrary. Thus, the SGS model prediction must merge smoothly to the "laminar" limit at k_d on the one hand, and to the "grid-size" limit k_g (which is the largest resolvable wavenumber in LES) on the other. Unfortunately k_g can, and often does, change with available computing power (and also when, for example, the numerical resolution is doubled or halved). Therefore the SGS model predictions must also remain invariant of these macroscopic changes, when they are coupled to the LES computations.

SGS model(s) must go beyond the mere matching requirements. It is essential that they also provide for the phenomenological effects of the laminar viscosity, diffusivity, etc. (which represent the averages over the molecular dynamics).

Furthermore, additional coefficients of viscosity, diffusivity, etc. for the eddy motion are seen to arise from the averaging over the unresolved wavenumbers (that are bounded from below by k_g and from above by k_d). The effects of these coefficients on the large-scale motion must be incorporated as well by the SGS model. The model(s) must, of course, predict the onset of initial instability and its subsequent growth in an erstwhile laminar flow, with an increase in the parameter -- parameters of interest (e.g., Reynolds number). Finally, the model must be computationally efficient when it is coupled to the LES procedure.

The nature of small-scale motion could be further elucidated by examining an important field variable of turbulence. This is the local dissipation rate per unit mass defined as $\epsilon = (\nu/2) (\partial u_i / \partial x_j + \partial u_j / \partial x_i)^2$, where ϵ is averaged over volumes of $O(L)$, L being the energy scale of motion, with $L \gg 1/k_g$; x and u denote the coordinate and velocity, and $\nu = \mu/\rho$ is the kinematic viscosity, with ρ and μ respectively denoting the mass density and molecular viscosity coefficient. A characteristic property of turbulence is that ϵ increasingly varies with increasing Reynolds number. This random character of ϵ was suggested by Kolmogoroff [1962] and Obukhoff [1962] in a refinement of Kolmogoroff's original hypotheses [1940]. They argued that ϵ should not only be random but that its distribution be lognormal. Yaglom [1966] demonstrated that the assumption of a cascade process of energy transfer from the very large- to the very small-scale motions implies that $\ln(\epsilon)$ should be Gaussian if the transfer stages are statistically similar and independent. This lognormality prediction by Kolmogoroff, Obukhoff, and Yaglom has been subsequently verified by a number of experimental investigations. Thus, while the large-scale motions are properly treated deterministically through LES, the SGS turbulence model(s) must be treated statistically.

Moreover, if SGS turbulence is the key for a proper LES computation, the key for an acceptable SGS model is its ability to predict a return of energy from the subgrid scales to the large eddies. This return of energy would appear to necessitate new "de-averaging" models when the predictive calculations involve explicit computation for LES and modeling for SGS turbulence. This aspect could become crucial when a vortex which is subgrid somewhere (e.g., sufficiently far downstream from the jet origin) needs to be explicitly resolved elsewhere (e.g., where the grid is finer), since this implies the re-emergence of a structure from the SGS model into the resolved region of LES.

2.2 ACCOMPLISHMENTS

The different aspects of the large- and small-scale motions addressed by the present research are briefly discussed next.

2.2.1 SGS Modeling Procedure

Current effort is focused on one-point closure models. It is worth noting that most of the closure models attempted to date are either one-point or two-point models (depending on the number of spatial points appearing in the desired statistical results). Although the two-point closure models are much more complicated and have been limited so far to homogeneous (and usually isotropic) flows, their application to the circular-jet turbulence is clearly warranted. Our initial effort, however, has considered one-point closure models. The main motivation for considering the candidate model is to facilitate the incorporation of a variable-viscosity capability in ALGAE and to provide for a basis of benchmark comparison with a more sophisticated one-point model and possible two-point models that will be considered subsequently in our research.

As noted earlier, the averaging over the subgrid scales introduces a coefficient of viscosity for the eddy motion. Thus, the effective viscosity μ_e involved in the LES computations could be considered as the sum of the molecular viscosity of the fluid μ and a turbulent eddy viscosity μ_t . The candidate model for determining μ_t is the algebraic mixing-length model due to Launder et al. [1972]. The formulation discussed here applies to axisymmetric free-shear flows with monotonic velocity profiles. The velocity is the maximum at the centerline and decreases monotonically in the radially outward direction. Thus, no recirculating flow with an inflection point in the velocity profile can be considered. Clearly, this model is appropriate for addressing the single round free jet. This mixing-length model is one of the three turbulence models implemented by Cline [1981] in the VNAP2 procedure for solving the two-dimensional, time-dependent, compressible, turbulent flow.

The eddy viscosity, according to this model, is given by

$$\mu_t = \rho \ell^2 [(\partial w / \partial r)^2 + (\partial u / \partial z)^2]^{1/2}$$

where u and w are the radial and axial velocity components, r and z are the radial and axial coordinates, and ℓ is the mixing length. For monotonic velocity profiles, mixing length is expressed as

$$\ell = C |r_2 - r_1|,$$

where C is a constant ($= 0.11$ for axisymmetric flows), and r_2 and r_1 are radii that correspond to certain arbitrary values of normalized axial velocity. Thus,

$$r_1 = r \quad \text{for } (w - w_{\min}) / (w_{\max} - w_{\min}) = 0.1,$$

and

$$r_2 = r \quad \text{for } (w - w_{\min}) / (w_{\max} - w_{\min}) = 0.9.$$

Here w_{\min} and w_{\max} denote the minimum and maximum axial velocity components of the monotonically decreasing velocity profile. For the round jet of our interest, w_{\max} is the centerline velocity at a particular axial (z) location. For the jet issuing into quiescent ambient, w_{\min} is zero. For computational expediency, however, a nonzero value of $0.01 w_{\max}$ (i.e., 1.0% of the centerline velocity) is appropriate.

With the typical boundary conditions on the centerline (viz., $u=0$ and $\partial w/\partial r=0$, invoking symmetry), the equation for μ_t must be modified on the centerline. This is done by replacing the previous equation with

$$\mu_t = \rho l^3 |\partial^2 \omega / \partial r^2|$$

on the centerline.

2.2.2 ALGAE Modifications

The initial effort involving LES computations with ALGAE has focused on certain modifications aimed at improvement in physical modeling and code enhancements. The former aspect includes the incorporation of a variable eddy viscosity and the refinement of spatial resolution. The latter aspect includes vectorization and graphic display enhancements.

The variable eddy viscosity in ALGAE is determined from the algebraic mixing-length turbulence model discussed in the previous paragraph. Test computations have been in progress at ICMA to discern the influence of the variable eddy viscosity on the flowfield predictions.

The earlier version of ALGAE had a maximum number of 4800 finite-difference grid points for the two-dimensional computational domain. This has been increased to 6400 and is expected to result in more refined simulations of the large-scale motions.

The ongoing vectorization involves the conversion of ALGAE (originally written for DEC 1099) for operation on the FPS-164 at ICMA and the CRAY-XMP at the NSF Pittsburgh Supercomputer Center. Further optimizations for the CRAY are in progress.

Predictive calculations of the circular-jet turbulence with LES computations and SGS turbulence modeling can be greatly facilitated by the availability of enhanced graphic display capability. An appealing option is the computer-generated movie of the evolving flowfield. The software necessary to generate such 16mm movies using the ICMA Datagraphic Communications Unit has been developed and is currently being tested.

2.2.3 Far-Field Boundary Conditions

The specification of boundary conditions for the numerical computation of the free-jet development presents many difficulties. Ideally, our interest is the solution to the problem of the jet discharging into an unbounded domain. However, the present ALGAE-based approach requires that the problem be transformed into a pseudo boundary-value problem within the domain of the computational grid. For instance, since ALGAE is limited to treating confined flowfields, it is necessary to impose far-field conditions on certain artificially introduced boundaries.

Initial numerical simulations have centered on a model jet problem whose geometry is shown in Figure 1. The dashed lines R and T represent the pseudo boundaries in the quarter plane. Of

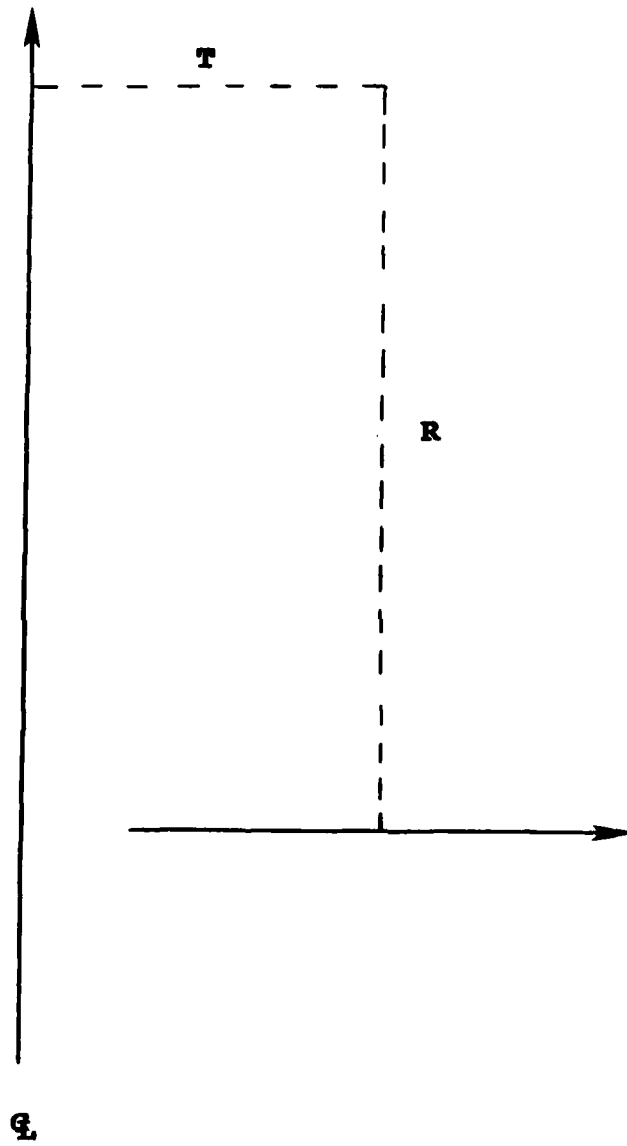


Figure 1. Model Jet Problem Geometry.

the variety of conditions tested so far, specification of the pressure on these boundaries appears to yield the most realistic behavior of the numerical solution. Appropriate pressure distributions may be obtained by assuming that the far-field conditions are approximately those of related model problems for which analytical solutions are known. For example, a linear distribution results from a Poiseuille flow-type assumption. Another possibility currently under consideration (Porsching [1986a]) is to use the pressure field corresponding to irrotational flow of a jet with free stream lines. This is a classic problem of a type first considered by Helmholtz [1868] for the flow out of a slot (plane jet). Its solution has been reproduced in many hydrodynamics texts (see, for example, Milne-Thompson [1955]). The solution technique uses a sequence of Schwarz-Christoffel transformations to obtain an implicit representation of the complex potential of the motion. Bernoulli's theorem may then be employed to relate the far field pressure on streamlines within the jet to the known pressure at infinity. Plots of the streamline and velocity fields resulting from an application of this technique to the plane-jet case may be seen in Porsching [1986a]. Analogous treatment of the circular jet remains to be carried out.

Another approach to obtain the far-field pressure distribution is through an asymptotic analysis of the fully developed region of the axisymmetric turbulent jet. A useful start is provided by the results of ongoing research of Bush and Krishnamurthy [1986] which have been shown to be consistent with the experimental results of Reichardt [1942] and theoretical results of Görtler [1942].

2.2.4 Weakly Dissipative Difference Methods.

Sustained numerical simulation of the vortex structures in the flowfield of a circular jet requires the use of difference

methods with small numerical dissipation. Unfortunately, in the absence (or near absence) of naturally occurring dissipative mechanisms, it is precisely the numerical viscosity that stabilizes the method. Thus, it is important to examine the prospect of constructing methods that are robust (with respect to their stability characteristics), but not uniformly overly dissipative.

A conceptually simple way to attenuate the dissipative effects of a difference method is to create a hybrid method by blending the given method with a less robust but more accurate one. The idea is to design the weights used in the blending process so that in regions where little numerical dissipation is needed, the accurate method is dominant, whereas in regions requiring significant numerical dissipation to preserve stability (or certain qualitative features of the solution such as monotonicity), the original scheme prevails. Such self-adjusting methods in computational fluid dynamics were apparently first considered by Harten and Zwas [1972], and a comprehensive account of the steps involved in the design of these methods is contained in the thesis of Wilders [1983].

Hybridization is also the notion behind the Flux Corrected Transport (FCT) schemes of Boris and Book [1973, 1976] and Book, Boris, and Hain [1975]. The FCT schemes, originally developed for one space dimension, were given a nontrivial multidimensional generalization by Zalesak [1979]. He also showed that they could be interpreted in terms of convex combination of flux terms related to low-order (strongly dissipative) and high-order (marginally dissipative) difference methods. The FCT weight selection process uses a "monotonicity constraint" on the numerical solution and has a particularly simple formulation in one dimension. Specifically, the weights are determined so as to maximize the effect of the high-order method's flux terms, subject to the condition that over any timestep no extrema are introduced that would not also be present in the low-order

solution at the new time. This implies that the total variation of the hybrid grid function does not exceed that of the low-order grid function. The same idea has been used to define total-variation-diminishing (TVD) schemes (Harten [1983], [1984]).

The monotonicity constraint is consistent with the behavior of a solution of the one-dimensional scalar convection equation (the total variation of such a solution does not increase in time), and in this case the FCT algorithms perform impressively. However, the situation is different for systems of nonlinear conservation laws. According to Woodward and Colella [1984]:

Then no such monotonicity constraint is implied by the differential equations, and the use of such a constraint can lead to difficulties. In particular, a smooth region with strong gradients can be turned into a sequence of discontinuous jumps, with the appearance of a staircase.

The unsuitability of a TVD condition in the design of difference methods for multidimensional quasilinear systems is also indicated by a recent result of Rauch [1986]. There it is shown that unless the commutators of all of the Jacobian matrices appearing in the system vanish, no multiple of the $W^{1,1}$ seminorm of the initial condition can bound this seminorm at a later time. Thus, it is unlikely that a numerical solution with a TVD property will converge to a solution of the original system.

In view of these difficulties with the TVD condition, it is appropriate to consider other weight selection criteria. One such alternative is based on the ability of the hybrid method to conserve (or nearly conserve) the discrete energy of the numerical solution that it produces. For the simple (constant coefficient) convection equation

$$f_t + uf_x = 0$$

in which the stable upwind-difference method is blended with the unstable centered-difference method, this leads to a hybrid method with the single weight θ given by the formula

$$\theta = [2\lambda - 1 + (1 - 4\lambda^2)^{1/2}] / 2\lambda,$$

where λ is the Courant number.

When applied to a standard square wave test problem, the resulting scheme produces a numerical solution that virtually coincides with that of the Lax-Wendroff and leapfrog scheme. This hybrid method is not TVD, but does reduce the numerical dissipation of the upwind method by about 21%. Furthermore, for this problem it appears possible to modify the analysis to permit weights that depend on the local character of the numerical solution (Porsching [1986b]). In this way TVD-like properties might also be incorporated into the method.

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SECTION III DOCUMENTATION

The following reports were supported in part by this research program:

Bush, W.B. and Krishnamurthy, L. "Asymptotic Analysis of the Fully Developed Region of an Incompressible, Free, Turbulent, Round Jet," in preparation.

Porsching, T.A., "A Note on the Analytic Solution of a Model Jet Problem," ICMA Tech. Memo. 1986.

Porsching, T.A., "On Weight Selection Procedure for Hybrid Difference Methods," in preparation.

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The following were supported in part by this research project:

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