JOURNAL OF COMPUTATIONAL PHYSICS 110, 190–195 (1994)

NOTE

The Effect of Interpolation Errors on the Lagrangian Analysis of Simulated Turbulent Channel Flow

1. INTRODUCTION

The proliferation of codes for the direct numerical simulation of turbulent flows has stimulated interest in performing analyses of Lagrangian turbulence statistics including the tracking of ensembles of fluid particle paths. Among the recent studies requiring Lagrangian data are those exploring the relationship between Eulerian and Lagrangian statistics [11, 16, 18], the physics of particle laden flows [4, 7, 13], and the studies of momentum and vorticity transport [2, 3, 8, 15].

A principal difficulty with Lagrangian calculations is the error associated with interpolation of the particle positions and velocities. Accurate interpolation is required in order to correctly follow particle paths as well as to secure useful predictions of the velocity derivatives, vorticity, and other higher order quantities along the trajectories. In fact, Yeung and Pope [17] found that for cases where the time step is small enough to satisfy the Courant condition, interpolation is the major source of error. The degree of accuracy required of interpolation methods when the particle vorticity and higher order Lagrangian statistics are desired is particularly critical due to the significant high wavenumber content of the velocity gradient fields.

The accuracy of an interpolation scheme is determined by its ability to resolve the smallest scales in the flow. A parameter which has been found useful in this regard is $k_{max}\eta$, where k_{max} is the largest resolved wavenumber, and η is the Kolmogorov length scale. Several studies of homogeneous and isotropic turbulence [1, 16, 17] have shown that if $k_{max}\eta > 1$ then the effect of interpolation errors on single point Lagrangian velocity correlations is relatively small, and that as $k_{max}\eta$ decreases the accuracy of the interpolation method becomes increasingly important. Yeung and Pope [17] also investigated higher order statistics such as the fourth-order structure function and found that values of $k_{max}\eta > 2$ were required for accuracy in this case. Prior studies of the interpolation errors associated with Lagrangian statistics have concentrated on isotropic flows where it was possible to maintain $k_{max}\eta > 1$. The effect of interpolation error on the statistics in wall-bounded and other engineering flows where $k_{max}\eta$ can become relatively small has not yet been directly addressed. In this paper the accuracy of specific interpolation schemes used in these flows and their effects on the turbulence statistics is examined.

Pseudo-spectral interpolation methods in which a direct summation of the finite Chebyshev–Fourier series is made at off-nodal points is known to offer optimal accuracy, limited only by the number of modes or collocation points used in a given calculation. However, the high cost of tracking significant numbers of particles for any reasonable length of time by this method usually eliminates this technique as a credible choice for production runs. Trilinear interpolation, on the other hand, executes much faster than pseudo-spectral methods, and has been used in some studies, e.g., [2, 16]. It is known, however, to be much less accurate than spectral interpolation and can be expected to generate unacceptable errors for some quantities of interest, particularly velocity derivatives and long time particle trajectories.

The need for interpolation schemes which provide a compromise between the speed of linear interpolation, and the accuracy of pseudo-spectral methods has led to the consideration of such approaches as 13-point cubic splines [17], partial Hermite interpolation [1, 10], and Lagrangian interpolation of various orders [10]. The present work analyzes the effect of interpolation error on particle paths and Lagrangian statistics in a turbulent channel flow for several different interpolation schemes including tricubic Hermite and B-splines. Additionally, frozen velocity fields of simulated channel flow are used to illustrate the relative magnitude of these errors and to examine interpolation of velocity derivatives. We conclude, in agreement with previous studies [1, 10], that Hermite interpolation offers significant advantages over other approaches. It is also shown that direct differentiation of the tricubic operator provides an efficient and reasonably accurate means of interpolating derivative fields.

2. INTERPOLATION METHODS

Four different interpolation methods, including pseudo-spectral, linear, cubic splines, and Hermite are compared. The pseudo-spectral interpolation method follows the development by Canuto *et al.* [5] and consists of a direct

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summation in spectral space of the contributions from each point in the flow. For channel flow, Fourier series in the spanwise and streamwise directions are used, with periodic boundary conditions applied to the sides of the computational box, while Chebyshev polynomials are used in the wall-normal direction, with no-slip and no-penetration boundary conditions applied at the walls. The linear interpolation method considered here is the standard eight-point scheme utilizing the grid points immediately surrounding the interpolation point.

The two other methods we examine represent schemes which are more accurate than linear interpolation and less expensive to compute with than pseudo-spectral interpolation. The first is the cubic B-spline routine obtained from the IMSL library, which is an extension of the 2D routine developed by De Boor [6]. The second scheme, tricubic interpolation, is an extension of the bicubic scheme of Press *et al.* [14] and is mathematically equivalent to the full 3D Hermite interpolation scheme proposed by Balachandar and Maxey [1]. Consequently, the terms tricubic and Hermite may be used interchangeably to describe this method. There are, however, some differences between the present approach and that of Balachandar and Maxey and Kontomaris *et al.* [10]. In particular, we allow for Hermite interpolation in all directions by estimating the velocity at a point (x, y, z), using the cubic polynomial

$$u(x, y, z) = \sum_{i=1}^{4} \sum_{j=1}^{4} \sum_{k=1}^{4} c_{ijk} t^{i-1} r^{j-1} s^{k-1},$$

where $x_i \leqslant x \leqslant x_{i+1}$, $y_j \leqslant y \leqslant y_{j+1}$, $z_k \leqslant z \leqslant z_{k+1}$, and $t = (x - x_i)/(x_{i+1} - x_i)$, $r = (y - y_j)/(y_{j+1} - y_j)$, $s = (z - z_k)/(z_{k+1} - z_k)$. The interpolation constants, c_{ijk}, are determined by requiring the velocity, first-order velocity derivatives, and higher order velocity derivatives such as $\partial^2 u/\partial x\, \partial y$ to agree with their exact values at the grid points surrounding (x, y, z). To duplicate the Hermite interpolation operator, the fields chosen are u, $\partial u/\partial x$, $\partial u/\partial y$, $\partial u/\partial z$, $\partial^2 u/\partial x\, \partial y$, $\partial^2 u/\partial x\, \partial z$, $\partial^2 u/\partial y\, \partial z$, and $\partial^3 u/\partial x\, \partial y\, \partial z$. Further details are given in [15].

The direct numerical simulation used in this study [9] is of a channel flow with a wall Reynolds number, R_τ, of 125, where $R_\tau = u_\tau h/\nu$, h is the channel half-width, $u_\tau = (\tau_w/\rho)^{1/2}$, τ_w is the wall shear stress, ν is the kinematic viscosity, and ρ is the density. A time splitting technique with a Green function correction was used to enforce continuity at the walls [12]. The streamwise and spanwise directions employed a uniform grid of $\Delta x^+ = 19.5$ and $\Delta z^+ = 9.8$, while a cosine mapping was used in the wall-normal direction so that the distance between grid points varied from $\Delta y^+ = 0.15$ near the wall to $\Delta y^+ = 6.1$ at the center of the channel, where $y^+ = u_\tau y/\nu$ and y is the coordinate normal to the boundary.

The Kolmogorov length scale was estimated using the relation $\eta = (\nu^3/\varepsilon)^{1/4}$, where ε is the isotropic dissipation rate. At $y^+ = 15$ where the peak turbulence production takes place, $k_{\max} \eta \approx 0.29$, based on the value of $\varepsilon^+ = 0.1113$, as determined from the direct numerical simulation, where $\varepsilon^+ = \nu\varepsilon/u_\tau^4$, and $k_{\max} \approx 20$ as a result of the chosen grid. It follows that interpolation inaccuracies can be expected to significantly affect the Lagrangian statistics.

3. FIXED TIME INTERPOLATION ERRORS

Single time velocity and velocity derivative fields were used to compare the accuracies of the interpolation schemes. Consistent with the results of Balachandar and Maxey [1], pseudo-spectral methods were found to require two orders of magnitude more CPU time per point than linear interpolation and an order of magnitude more time than Hermite or cubic spline interpolation. Both the tricubic and cubic spline interpolation methods, however, have some overhead or preprocessing associated with them. In the case of cubic splines, this takes the form of solving a $N_X \times N_Y \times N_Z$ system of equations in order to determine the spline functions, while the tricubic approach requires spectral computation of seven nodal velocity derivatives. Although the operation count suggests that the amount of overhead associated with the cubic splines would be smaller than that for the tricubic interpolation, in practice the widespread availability of optimized FFT routines often results in significantly less time being required. On a CRAY YMP-8, for example, the advantage between the tricubic approach over the optimized IMSL routine was found to be better than 50:1. In fact, over 5000 spectral interpolations could have been performed during the setup time for cubic splines. Because of the disparity in overhead, Hermite interpolation was found to be more economical than spline interpolation, except for exceptionally large numbers of particles. This is despite the additional fact that once the interpolation constants have been found, the execution time for cubic splines is slightly faster than that for Hermite interpolation.

The question of accuracy was studied here by comparing the results of the linear, cubic spline, and Hermite interpolation schemes to those for pseudo-spectral interpolation which is considered to be exact. Linear interpolation was found to be the least accurate, while Hermite interpolation conformed most closely with the spectral results, in agreement with Balachandar and Maxey [1] and Kontomaris *et al.* [10]. The interpolation error was quantified using the relative error estimate given by

$$E_u(y^+) = \left[\frac{1}{N_P} \sum_{n=1}^{N_P} \{u_{\text{spectral}}(y^+) - u_{\text{interp}}(y^+)\}^2\right]^{1/2} \Big/ u_{\text{rms}}(y^+), \qquad (1)$$

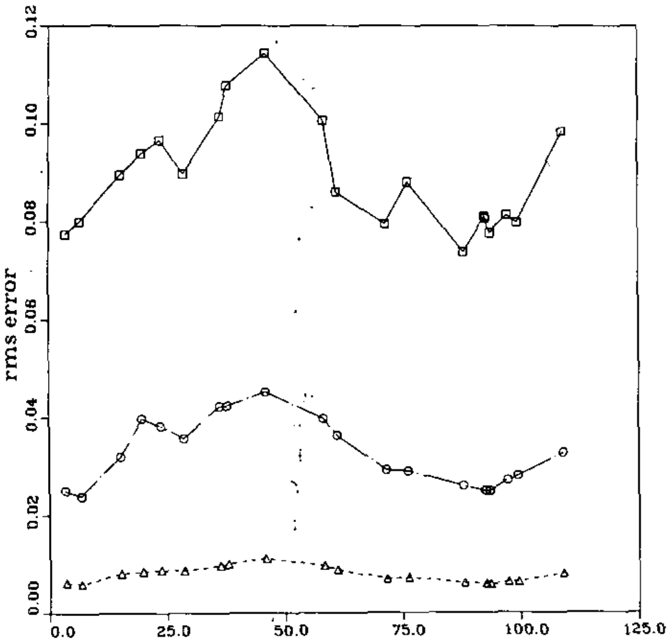

FIG. 1. Comparison of interpolation errors for a fixed time velocity field: □, trilinear; ○, spline; △, Hermite.

where N_P is the number of points tested on a given y^+ level, u_{spectral} represents the spectrally computed velocity, u_{interp} is the velocity determined using the interpolation method under consideration, and u_{rms} is the averaged rms velocity. The y^+ dependence of E_u is allowed here since we can expect the interpolation errors to be strongly effected by the varying mesh resolution across the channel and, as will become evident below, by the differences in the nature of the turbulence at different positions with respect to the wall.

Figure 1 shows the error for the interpolation of streamwise velocity, u, as a function of y^+ for 250 particles scattered randomly on each of 20 arbitrarily chosen y^+ levels. The results show that both cubic spline and tricubic interpolation offer much greater accuracy than does linear interpolation and that tricubic is superior to cubic spline interpolation. The rapid changes in E_u with y^+, particularly for linear interpolation may be attributed in part to the effect of intense underlying structures in the simulation, which can cause significant interpolation errors for individual fluid particles which happen to be under their influence. With increased sampling rates such variations in E_u should diminish, although the overall trend should remain. In particular, the largest errors seem to appear near $y^+ = 40$, where the vortical structures tend to be centered. The degree to which Hermite interpolation is insulated from such effects is a strong argument in its favor.

A similar comparison of interpolation error can be made for the velocity derivatives. The interpolation methods under consideration offer several ways to interpolate the velocity gradients at off nodal points. The most straightforward approach is to spectrally differentiate the velocity field, thereby creating a derivative field defined on the grid points, and then using the various interpolation methods as they have previously been developed. In the case of cubic spline and tricubic interpolation, however, this approach requires new values for the interpolation constants. An alternative approach, which avoids this extra overhead, is to compute velocity derivatives by evaluation of the differentiated forms of the previously derived velocity interpolation formulas.

Figure 2 compares the errors for the $\partial u/\partial y$ field for the following interpolation methods:

1. Linear interpolation of the spectrally differentiated velocity field.
2. Differentiation of the cubic spline operator.
3. Cubic spline interpolation of the differentiated velocity field.
4. Tricubic interpolation of the differentiated velocity field.
5. Differentiation of the tricubic operator.

Plotted in Fig. 2 is the rms error computed via an adaptation of (1) for the case of $\partial u/\partial y$. The enormously increased error associated with derivative interpolation is evident in the magnitude of the error here in comparison to E_u in Fig. 1.

Again the results indicate that Hermite interpolation of the differentiated velocity field gives the most accurate

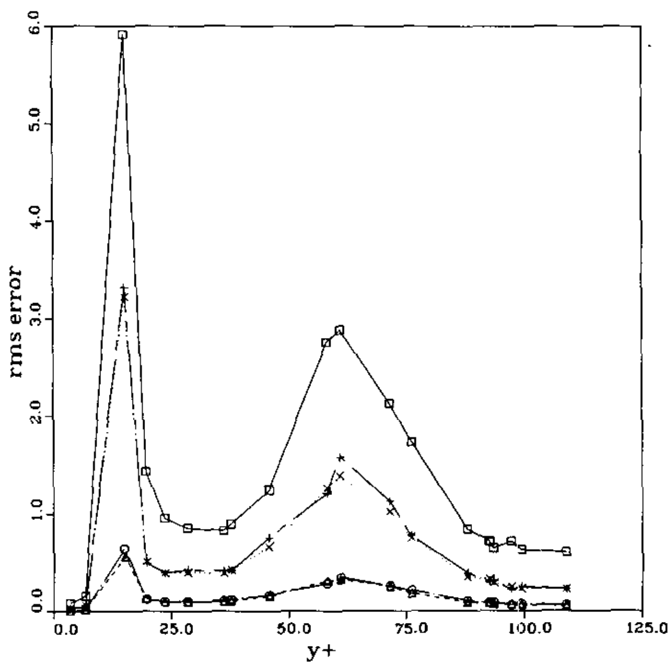

FIG. 2. Comparison of interpolation errors for a fixed time velocity derivative field $\partial u/\partial y$: □, trilinear interpolation of $\partial u/\partial y$; ○, derivative of Hermite u interpolation; △, Hermite interpolation of $\partial u/\partial y$; +, derivative of u spline interpolation; ×, spline interpolation of $\partial u/\partial y$.

results. However, the differentiated Hermite operator is nearly as accurate as the direct Hermite interpolation, yet has a significant advantage as far as the amount of computation time required in comparison to the direct method, since new interpolation constants are not computed. A similar result occurs when the cubic spline interpolation of the differentiated velocity field is compared to the differentiated spline operator. It is clear that both Hermite methods are significantly more accurate than cubic spline methods, which are in turn more accurate than linear interpolation. It also may be noted that the curves in Fig. 2 once again reflect the activity of coherent structures in the flow which generate locally intense regions of shear.

4. PARTICLE PATHS AND LAGRANGIAN STATISTICS

The interpolation errors associated with Lagrangian statistics, defined by actual fluid particles traveling through the time developing flow field, were explored using an ensemble of paths obtained using the various interpolation schemes. Sets of 250 particles with initial points randomly scattered on each of five y^+ levels on the top and bottom channel walls, so that statistics at each y^+ level are based on 500 particles, were generated. The particles were tracked forward in time for $t^+ = 9.4$ using a second-order Runge–Kutta predictor–corrector scheme, where $t^+ = tu_\tau^2/\nu$.

The ensemble averaged errors in the locations of the fluid particles starting at $y^+ = 17.8$ as a function of time are shown in Fig. 3, where the interpolation error is defined here as

$$E_x(\tau) = \frac{1}{N_p}\left(\sum_{n=1}^{N_p} |\mathbf{x}_{\text{interp}}(\tau) - \mathbf{x}_{\text{spectral}}(\tau)|^2\right)^{1/2}.$$

As before, the results of the pseudo-spectral interpolation are assumed to be exact. As seen in the figure, the position errors increase with time, indicating that the particles wander off from their correct paths for all of the non-spectral interpolation schemes. Hermite interpolation, however, can be seen to be approximately an order of magnitude more accurate than linear interpolation and about three times more accurate than cubic splines. This remained true at each of the y^+ locations tested.

As any particular particle moves through the flow, the rate at which its total positional interpolation error increases depends upon where the particle is in relation to the grid points, since all interpolation methods, by definition, agree at such points. This aspect of interpolation error is made evident by comparing the time histories of the Lagrangian velocity field associated with individual particles. Figure 4 shows this error in the interpolated velocity, namely, $|u_{\text{interp}} - u_{\text{spectral}}|$ for an arbitrarily selected particle as a function of time. The symbols plotted along each curve denote the times at which the particles have passed through a grid plane. Since the interpolation is likely to be temporarily more accurate when particles pass near grid planes, it is not surprising to see the quasi-periodic nature of the

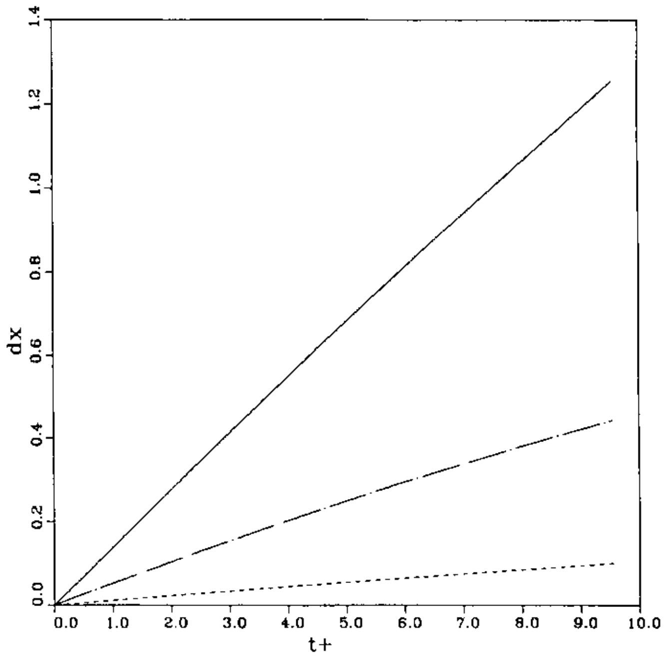

FIG. 3. RMS positional error for particles originating at $y^+ = 17.8$: ———, trilinear; —·—, spline; – – –, Hermite.

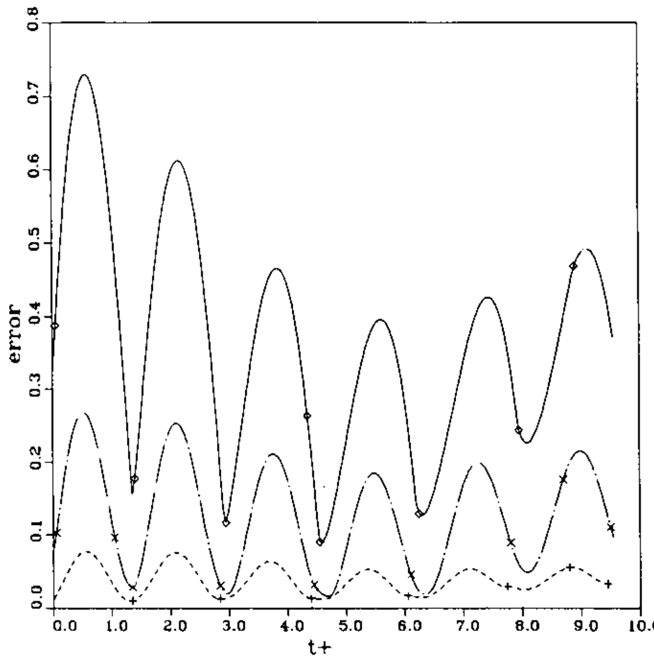

FIG. 4. Typical velocity error for convecting fluid particle originating at $y^+ = 24.6$: ———, trilinear; —·—, spline; – – –, Hermite.

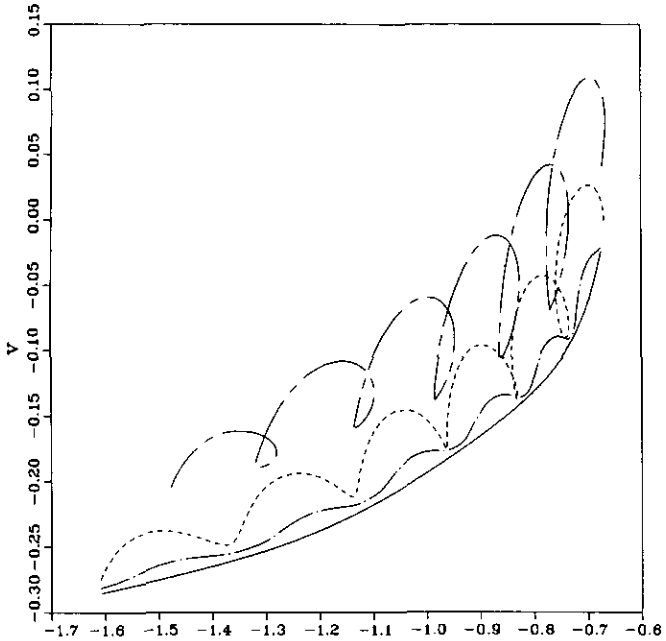

FIG. 5. $v-w$ hodograph for a typical convecting fluid particle originating at $y^+=24.6$: ———, spectral; —·—, Hermite; ---, spline; ———, trilinear.

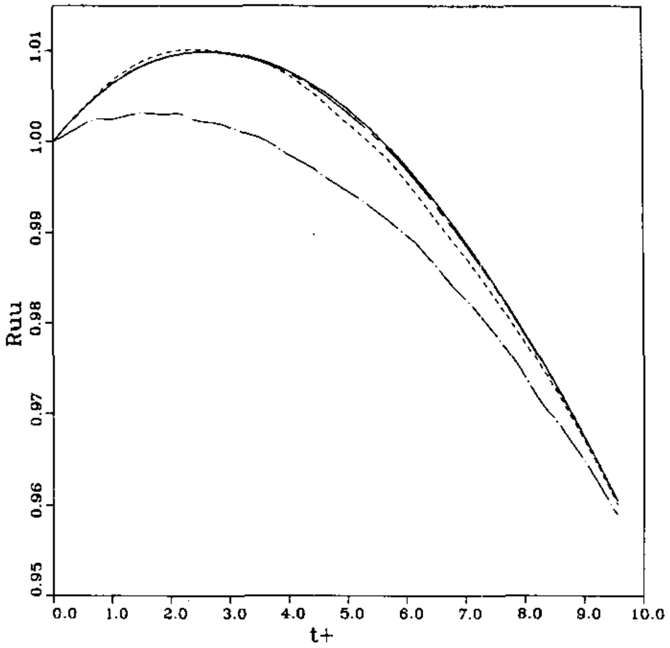

FIG. 6. Lagrangian autocorrelation coefficient R_{uu} for fluid particles originating at $y^+=12$: ———, spectral; ———, Hermite; ---, spline; —·—, trilinear.

error amplitude. The relative magnitude of the errors between the interpolation methods are consistent with the results of the previous section, so that both the amplitude and minimum value of the error are smallest for tricubic interpolation and largest for linear interpolation.

The peculiarities of interpolation error for convecting fluid particles are accented in the (v, w) hodograph plot for a typical particle given in Fig. 5, where v and w are the wall-normal and spanwise velocities, respectively. Here, interpolation-induced sinusoidal variations of particle velocity is reflected in the circular traces of the hodographs. The tricubic scheme is most closely able to follow the correct hodograph plot, while linear interpolation is entirely overwhelmed by errors.

The pronounced interpolation error for velocity can be expected to have some influence on statistics gleaned from the particle paths. A particularly interesting effect is illustrated in Fig. 6, showing a plot of the Lagrangian velocity autocorrelation coefficient, $R_{uu}(t)=\overline{u(0)\,u(t)}/\overline{u(0)\,u(0)}$ at $y^+=12.0$, computed using the various schemes. Hermite interpolation appears to do an excellent job of capturing this correlation while the splines also appear to be of acceptable accuracy. The trilinear scheme, on the other hand, tends to result in a lower peak value of R_{uu}, a much more rapid decay, and a very different shape near $t=0$. In fact, the interesting rise in R_{uu} to a value greater than one, which may be attributed to the presence of a Reynolds shear stress in the flow field [2], is not well captured by the linear scheme. As a result, the magnitude of such quantities as the turbulent microscale and integral scale will be substantially in error. These results contrast somewhat with those of Kontomaris *et al.* [10], who found that in the center of the channel the value of R_{uu} computed from linear interpolation tended to be greater than that obtained from a more accurate Lagrangian interpolation scheme.

5. CONCLUSIONS

Previous studies investigating the effect of interpolation error on turbulence statistics have shown that for cases where $k_{max}\eta > 1$, the flow is adequately resolved and the effects of interpolation error can be kept relatively small. In wall-bounded turbulence, such as considered here, however, it is often not feasible to maintain this condition for Reynolds numbers at which turbulence is self-sustained, since the Kolmogorov scale tends to become small and the number of Fourier modes included in the simulation is limited. The present study suggests that the accuracies of interpolation schemes do have a significant effect on Lagrangian statistics and that Hermite interpolation is substantially more accurate than either cubic splines or trilinear interpolation.

The level of accuracy of the interpolation of velocity derivatives is generally much less than that of velocities themselves, although Hermite interpolation appears to provide adequate performance. An important outcome of the present comparisons is that it is considerably more accurate to differentiate the cubic spline or tricubic operators directly in order to obtain derivatives, than to use linear interpolation from the spectrally differentiated velocity field. Additionally, differentiation of the Hermite operator represents a much less costly alternative to both pseudo-spectral interpolation and direct Hermite interpolation of the derivative field, with an acceptably small decrease in accuracy. The suitability of Hermite interpolation for computing derivatives is borne out in recent applications of Hermite interpolation to Lagrangian studies of vorticity transport [15] and the Reynolds stress [8] in which first- and second-order velocity derivatives are computed along particle paths.

Finally, the effect of interpolation error on Lagrangian velocities was shown to vary cyclically as fluid particles travel through the flow. The cumulative effect of such errors in position increases monotonically in time and can have a strong effect on Lagrangian correlations and the scales derived from them. Once again, Hermite interpolation appears to successfully predict these quantities at a reasonable computational expense in comparison to exact spectral interpolation.

ACKNOWLEDGMENTS

This work was supported by the fluid dynamics program at the Naval Research Laboratory, ONR Contract N00014-91-WX-24079 and NRL Grant 42-2010-91. The first author is a recipient of a NRC postdoctoral fellowship.

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Received August 3, 1992; revised March 5, 1993

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