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Project unit: AERO ENGR — Unit code: 22
Project director(s):
PDPI- YEUNG P AERO ENGR (404)894-9341

Sponsor : ENVIRON PROTECTION AGENCY/EPA - DC
Division Id: 129 / 3481
Award period: 01-OCT-1994 to 30-SEP-1998 (performance) 30-SEP-1998 (reports)

Sponsor amount	New this change	Total to date
Contract value:	0.00	174,028.00
Funded:	0.00	174,028.00
Cost sharing amount:	0.00	9,161.00

Does subcontracting plan apply?

Title: NUMERICAL SIMULATION OF TURBULENT DISPERSION AND RELATIVE DIFFUSION

PROJECT ADMINISTRATIVE DATA

OCA contact: Anita D. Rowland (404) 894-4820

Sponsor technical contact:
DERAN PASHAYAN
U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF EXPLORATORY RESEARCH, 8703
ROOM 3102, NEM

Phone: 2022602606
Fax: 401 M STREET, S.W.
Email: WASHINGTON, D.C. 20460

Sponsor issuing office:
ALICE THAVONGSA
U.S. ENVIRONMENTAL PROTECTION AGENCY
GRANTS OPERATIONS BRANCH (3903F)
GRANTS ADMINISTRATION DIVISION

Phone: 2022609281
Fax: 401 M STREET, S.W.
Email: WASHINGTON, D.C. 20460

Security class (U,C,S,TS): U
Defense priority rating :

ONR resident rep is ACO (Y/N): N
Supplemental sheet:

Equipment title vests with: S
NONE PROPOSED

Administrative comments -
AWARDS A NO-COST EXTENSION THRU 30 SEP 1998.(ORACLE update, processed in M204 on 3.31.97/Rev.5) *

PROJECT CLOSEOUT - NOTICE

Closeout Notice Date 10-NOV-1998

Project Number E-16-X52 Doch Id 45789

Center Number 10/24-6-R8339-0A0

Project Director YEUNG, PUI-KUEN

Project Unit AERO ENGR

Sponsor ENVIRON PROTECTION AGENCY/EPA - DC

Division Id 3481

Contract Number R 821340 Contract Entity GTRC

Prime Contract Number

Title NUMERICAL SIMULATION OF TURBULENT DISPERSION AND RELATIVE DIFFUSION

Effective Completion Date 30-SEP-1998 (Performance) 30-SEP-1998 (Reports)

Closeout Action:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	Y	
Final Report of Inventions and/or Subcontracts	Y	
Government Property Inventory and Related Certificate	Y	
Classified Material Certificate	N	
Release and Assignment	N	
Other	N	

Comments

Distribution Required:	
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Research Administrative Network	Y
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Georgia Tech Research Corporation	Y
Project File	Y

NOTE: Final Patent Questionnaire sent to PDPI

E-16-X52 #1 (New)

Georgia Tech

School of Aerospace Engineering

Georgia Institute of Technology
Atlanta, Georgia 30332-0150
USA
404•894•3000
Fax: 404•894•2760

Tel. (404)-894-9341
e-mail: yeung@peach.ae.gatech.edu

November 2, 1995

Dr. Deran Pashayan
Office of Exploratory Research (8703)
U.S. Environmental Protection Agency
401 M St. SW
Washington, DC 20460

Dear Dr. Pashayan:

I am pleased to enclose my first annual report for Grant No. R821340010. I apologize for being somewhat late with this report. Any comments you may have would be greatly appreciated.

Thank you for your support.

Yours sincerely,

P.K. Yeung, PhD
Assistant Professor

encl: Annual Progress Report

cc: Ms. Anita Rowland, Office of Contract Administration

EPA Grant No. R821340010
Annual Progress Report, 10/01/94-9/30/95

P.I.: Dr. P.K. Yeung
School of Aerospace Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0150

November 2, 1995

Introduction

This is the first annual report for research activities supported by EPA Grant No. R821340010, entitled "Numerical simulation of turbulent dispersion and relative diffusion". The objectives of the research are to study, using direct numerical simulations (DNS, reviewed by Reynolds 1990), the physics of the relative diffusion of material fluid elements which move apart from each other (on average) as a result of the dispersive nature of turbulence. The ultimate goal is to discover long-awaited physical insights that will facilitate the development of stochastic models of two particle motion, which can then be used to advantage in the context of air quality management (see Weil 1992).

In the sections below we report briefly on progress in different aspects of the research, and on plans for work to be performed during the succeeding period. The focus of our efforts in recent months has been on algorithmic development. Copies of a journal publication (Yeung 1994) based on research performed before the grant period (but corresponding to the first phase of the proposed research) and a conference manuscript on computational aspects (Yeung 1995; Yeung & Moseley 1995) have been forwarded to EPA previously.

Progress in the research has been greatly facilitated by significant upgrades of the local computer equipment (the core being IBM RS/6000 workstations) made possible by the equipment component of EPA project funds, as well as an NSF Engineering Research Equipment Grant (No. CTS-9411690) that the P.I. received in the period September 1994 to August 1995. In addition, the P.I. has been able to maintain a continuing allocation of supercomputing resources at the NSF-supported Cornell Theory Center, which allowed intensive high-resolution numerical simulations through massively parallel computing. In April and June 1995 the P.I. had given three invited seminars on the subject of "Parallel computations of turbulent mixing and dispersion" at the University of Maryland, the Institute for Computer Applications in Science and Engineering (ICASE, NASA Langley Research Center), and Rocketdyne Division, Rockwell International Corporation (Canoga Park, CA).

One-time statistics of relative diffusion

Substantial efforts were made in this area while the proposal (submitted January 1993) was being considered, in the simplest case of stationary isotropic turbulence. Although isotropic turbulence is idealized, it is the flow to which most current stochastic models apply, and its study greatly promotes fundamental understanding.

Direct numerical simulation (DNS) results for the relative diffusion of fluid particle pairs in statistically stationary isotropic turbulence at Taylor-scale Reynolds number 90 have been published in Yeung (1994). As predicted by early theories, the growth of two-particle separation is found to exhibit asymptotic stages at small and large diffusion times. It should be noted that, through the two-particle separation, Lagrangian particle-pair velocity correlations are closely related to the Eulerian spatial structure of the turbulence. At large times the square of the separation distance has a chi-square probability distribution. At the moderate Reynolds number of the simulations, for this asymptotic distribution to be reached before the particles begin to move independently of each other, the initial separation must be small compared to the Kolmogorov scale. In an inertial frame moving with the initial particle velocities, the velocity increments of two fluid particles become uncorrelated only if their initial velocities are uncorrelated, which in turn requires their initial separation be large compared to the integral length scale. For sufficiently large initial separations, the relative velocity increments and mean-square dispersion in this moving frame display a resemblance to inertial range scaling, but with a proportionality constant that is much smaller than classical estimates. At large times, the degree of preferential alignment between the separation and relative velocity vectors is weak, but the product of the separation distance and the velocity component projected along the separation vector is sustained on average.

The work of Yeung (1994) focussed on statistics of the relative displacement between fluid particle pairs, and their relative velocity. In the next phase of research, we will extract statistics of the relative acceleration (studied by Borgas & Sawford 1991) from our DNS database. It is also important to obtain results at higher Reynolds number, because most stochastic models are formulated using inertial-range type arguments for high Reynolds number turbulence. There are also interesting questions about Lagrangian similarity hypotheses (Monin & Yaglom 1975) which can be properly addressed only when the Reynolds number is high enough to give a wide range of scales (e.g., between the large-eddy integral length scale and the Kolmogorov scale for the small scale motions).

Single-particle statistics in homogeneous shear flow

Two-particle turbulent dispersion in homogeneous shear flow with a mean velocity field of the form $U = Sy$ (with uniform shear rate S) is the ultimate target of investigation in this project. Unlike the case of stationary isotropic turbulence, this flow is anisotropic (with directional dependences dictated by the mean flow) and non-stationary (because mean shear causes continued growth of the turbulence kinetic energy). Algorithmic extensions are required because of these considerations.

The DNS solution algorithm we use (Rogallo 1981) solves the equations for the turbulent velocity fluctuations in a set of coordinate axes moving with the mean flow. The solution domain is initially a cuboid (or orthogonal "box"), but, over time, deforms into a slanted parallelipiped. To prevent excessive distortion of flow scales due to the resulting anisotropy in the numerical mesh, a "remeshing" procedure is applied to the solution domain at regular time intervals. Because length scales in the flow are "stretched" in the streamwise direction, it is also advantageous to use a solution domain of unequal length or number of grid points in each direction. These numerical considerations require careful (although in principle straightforward) extensions of the code employed for cubic spline interpolation (Yeung & Pope 1988) of Lagrangian variables following fluid particles. These extensions are now complete, with tests showing the fourth-order accuracy expected of cubic splines. As discussed by Yeung & Pope (1988, 1989), the high-order accuracy and differentiability (twice) properties of cubic spline interpolation are very important, and are in fact superior attributes compared to some lower-order (e.g. linear) schemes used by other previous investigators.

A logical prerequisite for understanding two-particle relative diffusion in homogeneous shear flow is to study one-particle Lagrangian statistics in the same flow. A sample result is shown in Fig. 1, in which the growth of single-particle mean-square displacement over time is shown in non-dimensional form. The calculation used a solution domain lengthened in the streamwise direction with 128^3 grid points, and an ensemble of 8,192 fluid particles are released after sufficient time for the Eulerian (space-averaged) flow statistics to reach a developed state. The t^2 behavior at early times is just a consequence of fluid particles moving in straight lines over sufficiently small time intervals. At large times, however, the displacements in different directions exhibit different rates of asymptotic growth. The streamwise displacements grow approximately as t^3, consistent with early similarity theories. The measured exponents for the other two components are about 1.6, which is higher than theoretical values because the turbulence kinetic energy continues to grow in the simulations, instead of attaining a stationary state (Squires & Eaton 1991).

Massively parallel computing

This is an exciting new development of great potential in years to come. It is well known that the major limiting factor in the potential of DNS is the difficulty of achieving high Reynolds numbers. At present, massively parallel computing offers the best hope—by allowing faster calculations using more grid points which then can resolve a wider range of scales at higher Reynolds number. In the past year, the P.I. has successfully developed a production parallel version of his DNS code, including the particle-tracking capability needed to extract Lagrangian statistics. The new code is run on an 512-node IBM SP2 parallel supercomputer at the Cornell Theory Center, using the IBM-optimized Message Passing Library software for parallel communication constructs. Data structures have been optimized for Fast Fourier Transforms and cubic-spline interpolation, which are key tasks in the Eulerian and Lagrangian parts of the code respectively. Some interesting high-resolution results have already been achieved, at R_λ 160 using 256^3 grid points, with evidence of an inertial range in the energy spectrum. The wall time on a 256^3 grid using 64 nodes with 98,304 fluid particles (compared with 4,096 particles in Yeung & Pope 1989) is only 10 seconds per time step—the same order as for 64^3 on a relatively fast serial workstation.

A systematic timing study (Yeung & Moseley 1995) has been conducted to evaluate the performance of the parallel algorithm. For given hardware (number and type of processors), a primary factor is the data partitioning in the distributed-memory scheme. A special consideration for cubic-spline interpolation (and other interpolation schemes in general) is that, because each node stores only a slab of the Eulerian velocity field, the interpolation information needed for each particle location generally comes from different grid planes which reside across different slabs (on different nodes). Because the number of grid points in general will be much larger than the number of particles, the only practical approach for data partitioning within the memory capacity of each node is to distribute the cubic spline coefficients across the nodes, with each node carrying the full set of particles. Discrete communication calls are required to collect contributions from individual nodes, and as a result the performance of the Lagrangian part of the code does not scale with increasing number of nodes as well as the Eulerian part. Nevertheless, other investigators have also encountered similar difficulties, and it is believed that our timings compare favorably with those reported for other parallel architectures (e.g., Huang & Leonard 1995). Currently, a re-structuring of the data partition scheme for the Eulerian part is being considered with the objective of reducing memory requirements and possibly also the elapsed wall time on each node.

The P.I. was among a select group of test users for the Cornell SP2 before it went into full production in March 1995, and has received a substantial renewal allocation of 25,000 service units for additional high-resolution computations. We emphasize the potential of simulations at high Reynolds number in addressing fundamental questions and establishing the values of (presumed) universal constants that in turn play an important role in the latest stochastic models (e.g., Thomson 1990, Borgas & Sawford 1994) of relative diffusion. One such result, for which more robust answers are expected from planned parallel simulations, is illustrated in Fig. 2.

New developments and plans

We recall the four major research areas identified in the original proposal, namely:

1. Growth of mean separation
2. One-time statistics of relative diffusion
3. Two-time statistics
4. Effects of Reynolds number and mean shear

A flexible schedule allowing for responses to new opportunities (an example being our foray into massively parallel computing, as described above) is essential for good research. Overall, in the first project year we have achieved significant progress in areas 1, 2 and 4, whereas area 3 will be investigated in the next few months. Specifically, we intend to focus our efforts on the following aspects:

1. *Statistics of relative acceleration.* Because cubic splines are twice continuously differentiable, Lagrangian time series of acceleration can be obtained by simply differentiating the interpolated particle velocity in time. Borgas & Sawford (1991) presented arguments that suggest, contrary to early theories (e.g., Novikov 1963), two-particle acceleration correlations within the inertial range are *not* negligible. Our DNS data should be able to throw light on this issue, which is important for statistical theories of dispersion.

2. *Two-time statistics of relative diffusion.* As noted in the original proposal, very little is known about two-time statistics such as the correlation between the velocities of different particles at different times. In the statistical analysis we need to note the fact that relative diffusion in homogeneous turbulence is an accelerating, non-stationary process (with particles moving apart from each other), even if the velocity fluctuations are statistically stationary.

3. *Relative diffusion in homogeneous shear flow.* With our algorithms validated for single-particle statistics, extension to particle pairs in this case should be relatively straightforward. To facilitate the interpretation of results, we need to develop a suitable scheme for selecting the initial locations and separation between an ensemble of particle pairs. This scheme must take account of the anisotropic nature of the flow and of the solution domain.

4. *Towards high resolution simulations.* The largest simulations (of isotropic turbulence) we have conducted so far are at Taylor-scale Reynolds number 160 on a 256^3 grid. While this already is quite respectable and the computed energy spectrum does indicate approximate inertial range behavior, we propose the even more ambitious tasks of simulations using 384^3 and 512^3 grid points. A substantial allocation of computer time at the Cornell Theory Center has been granted for these purposes. We will first generate statistically stationary isotropic turbulence fields using the forcing scheme of Eswaran & Pope (1988). To spend our resources wisely, we will first explore strategies for further improvements of parallel performance.

5. *Effects of turbulence structure on dispersion.* Work by the P.I. (Yeung 1994) and other investigators (Fung, Hunt, Malik and Perkins 1992) have found that the

inertial-range constant in two-particle dispersion is *much* less than its classical estimate. Fung *et al.* (1992) has postulated that this is because the fluid particles undergo significant separation from each other only if they are in a region of instantaneously high strain rate, which occur intermittently. It would be interesting to probe this concept of "structural diffusion" further using our DNS database, using conditional sampling and other techniques. For this purpose, a capability of the DNS code in obtaining Lagrangian data for velocity gradients (Yeung, Pope & Girimaji 1990) will be updated.

6. *Insights for stochastic modeling.* A practical motivation for the present research is to provide guidance and testing information for stochastic models (for a review, see Pope 1994) of turbulent dispersion, many of which are formulated by researchers in the atmospheric or environmental science community. The P.I. is actively pursuing interactions with other researchers in this regard. A proposal for international collaboration is currently pending at the National Science Foundation (see below).

Publication efforts (including conference presentations) will be stepped up as the research progresses. To conclude this report we note two recent developments:

First, the P.I. has submitted a proposal (entitled "Numerical simulation and stochastic modeling of turbulent mixing and dispersion") to the Division of International Programs of NSF for the purpose of a two-year collaboration with a leading researcher in stochastic modeling of dispersion (Dr. Michael S. Borgas, of the CSIRO Division of Atmospheric Research, Australia). Funds from NSF (and an Australian counterpart agency) are requested to support (only) two approximately one-month exchange visits between the P.I. and Dr. Borgas in the years 1996 and 1997. The P.I. will also have the opportunity to observe first hand experiments conducted by the Australian atmospheric science researchers. We expect such a collaboration to be of high synergistic potential, combining our respective expertise in numerical simulations and stochastic modeling. Our complementary interests will also broaden the scope of this research, including the tracking of contaminant species molecules (in addition to material fluid particles). A funding decision may be known within the next couple of months.

Second, as part of continuing efforts by the P.I. to develop collaborations with others in the research community, he has spent two weeks this past summer as a visiting scientist at ICASE, NASA Langley Research Center to work with Dr. Y. Zhou, a Senior Staff Scientist. The current focus is on simulations of turbulence subject to uniform solid-body rotation, which is important in many applications such as turbomachinery and geophysical flows. Parallel simulations are being conducted at IBM SP2s at NASA Ames and Langley Research Centers. This work may conceivably lead to numerical simulations of dispersion in rotating turbulence, which would be of substantial interest in pollution control problems over large spatial distances.

Note on student support

Although the funding commenced in October 1994, there was a delay in selecting a suitably qualified graduate student to work on this project. Mr. P. Shen joined the P.I.'s group in February 1995, and recently passed his PhD oral qualifying exams in September. To compensate for the period Oct. 94 to Feb. 95, we may request a short extension beyond the end of the award period. Some indirect contributions have also been made by another student (Ms. C.A. Moseley) who is separately supported by NSF funds.

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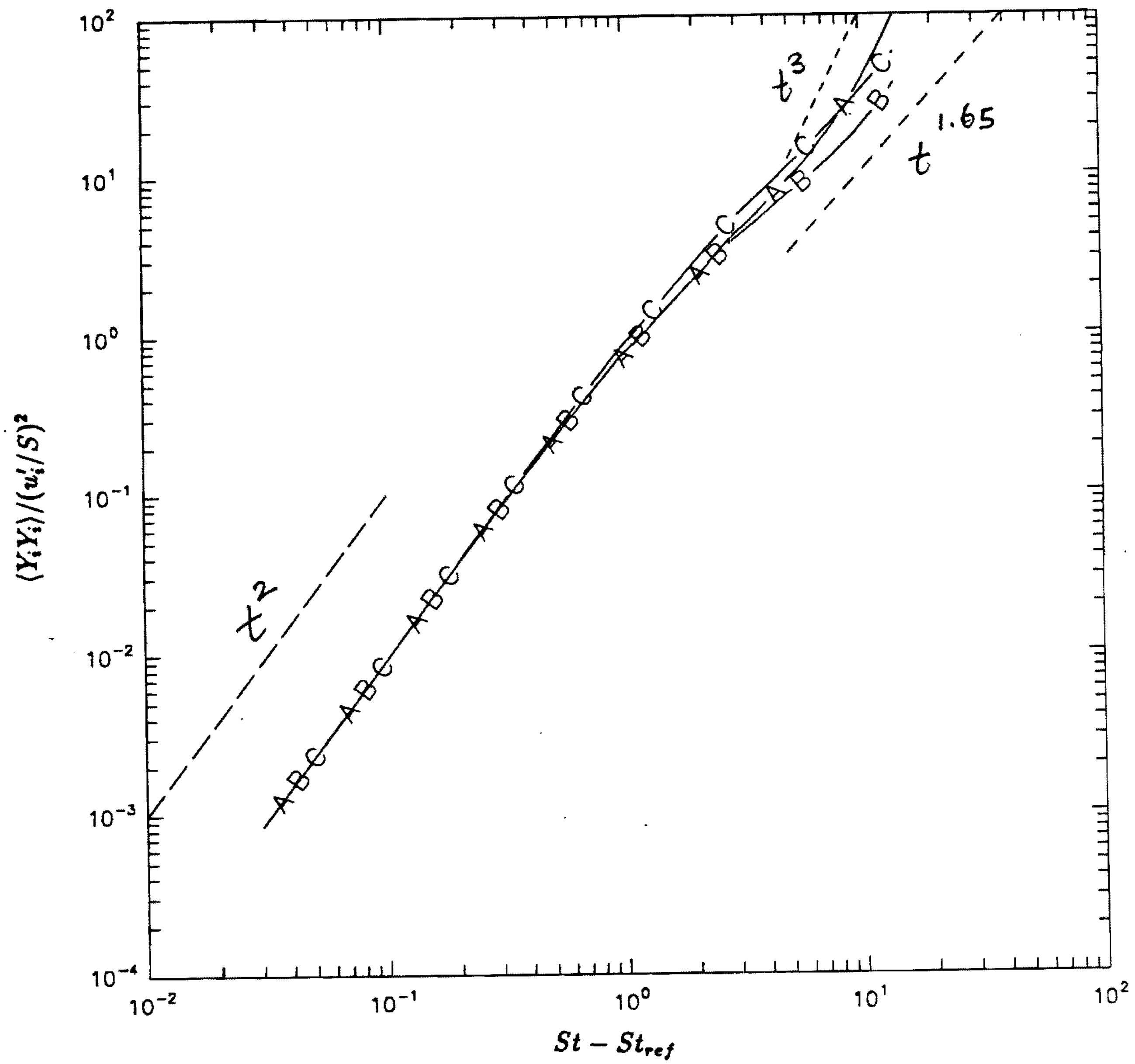

FIGURE 1. Growth of mean square displacements in different directions, $\langle Y_i Y_i \rangle$ ($i = 1, 2, 3$, as lines A, B, C respectively) for homogeneous turbulent shear flow. Time is non-dimensionalized by the shear rate S, whereas the displacements are normalized by the shear rate and component r.m.s. velocity fluctuations. Results at small and large times are compared with dashed lines of indicated slopes with log-log scales. Ensemble averaging has been taken over 8,192 particles released at time St_{ref}.

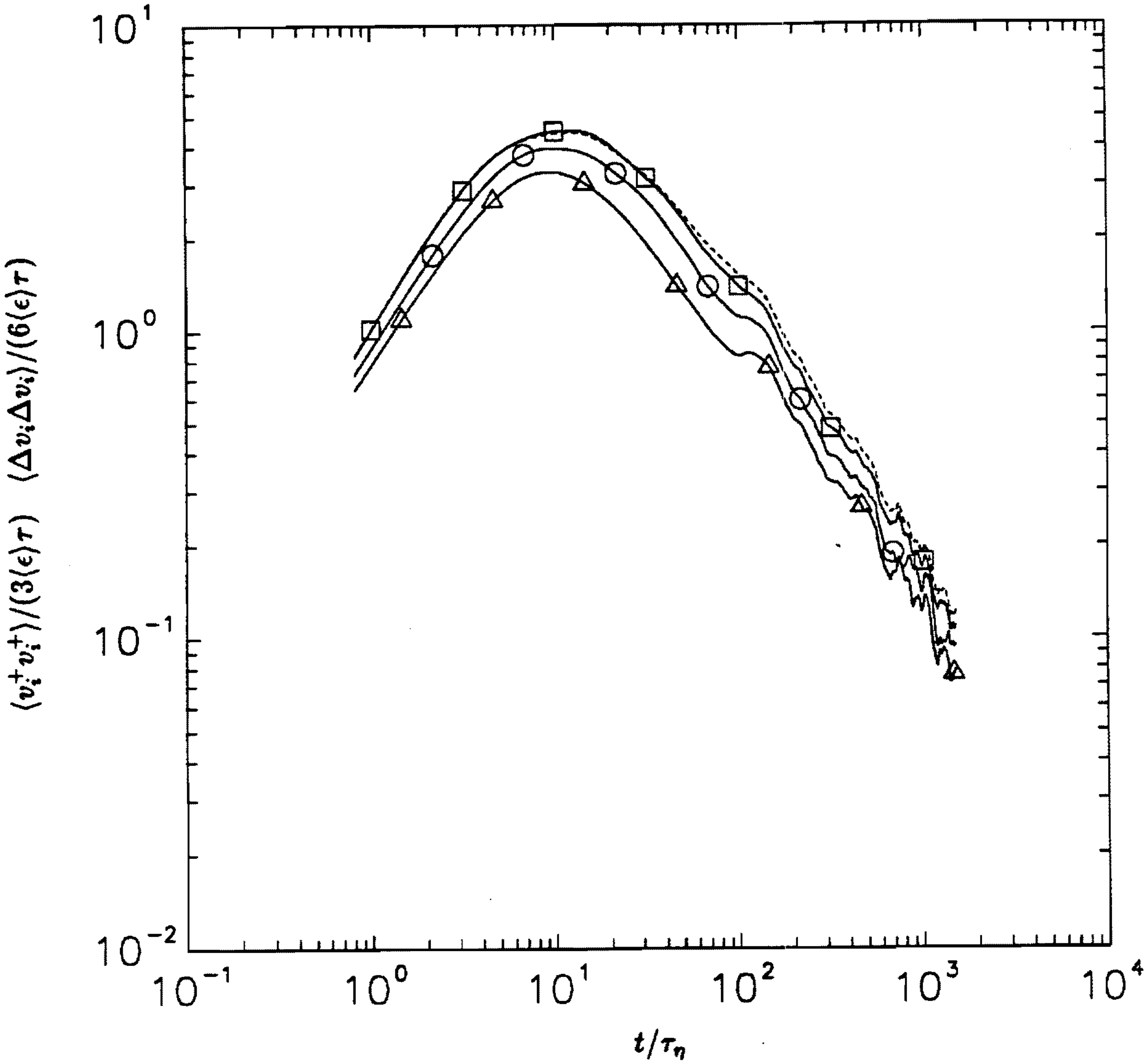

FIGURE 2. Variances of two-particle relative velocity increments over time intervals τ in normalized form ($\langle \Delta v_i \Delta v_i \rangle/(6\langle\epsilon\rangle\tau)$) compared with single-particle data ($\langle v_i^+ v_i^+ \rangle/(3\langle\epsilon\rangle\tau)$, dashed curve). (Here $\langle\epsilon\rangle$ is the energy dissipation rate, and η and τ_η the Kolmogorov length and time scales.) Two particle data are shown for initial separations l_0/η at 4 ($\triangle$), 16 ($\bigcirc$) and 64 ($\square$). Classical inertial scaling estimates imply a flat plateau at a universal constant value C_0 at intermediate times. However, at R_λ 90, the range of scales is too narrow for inertial scaling: $l_0/\eta = 64$ corresponds to 1.14 integral length scales. [Results from DNS, taken from Yeung 1994]

E-16-X52
#2

Georgia Institute of Technology

School of Aerospace Engineering
Atlanta, Georgia 30332-0150 U.S.A.
PHONE 404-894-3000
FAX 404-894-2760

Tel. (404)-894-9341
e-mail: yeung@peach.ae.gatech.edu

September 25, 1996

Dr. Deran Pashayan
Office of Exploratory Research (8703)
Rm 3102, NEM
Office of Research Development
U.S. Environmental Protection Agency
401 M St. SW
Washington, DC 20460

Dear Dr. Pashayan:

I am pleased to enclose the second annual report for research supported under Grant No. R821340010. Any comments you may have will be greatly appreciated.

I note that the EPA funds for the third project year (96-97) have arrived at Georgia Tech. I am most grateful for your continuing support.

Yours sincerely,

P.K. Yeung, PhD
Assistant Professor

encl: Annual Progress Report

cc: Ms. Anita Rowland, Office of Contract Administration

EPA Grant No. R821340010
Annual Progress Report, 10/01/95-9/30/96

P.I.: Dr. P.K. Yeung
School of Aerospace Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0150

September 25, 1996

Introduction

This is the second annual report for research activities supported by EPA Grant No. R821340010, entitled "Numerical simulation of turbulent dispersion and relative diffusion". The primary objective of the research is to study the fluid mechanics of contaminant dispersion caused by the spreading apart of material fluid elements in turbulent flow. Direct numerical simulations (DNS) of the basic equations of fluid motion are used to advance physical understanding, with a long-term view towards improving air-quality models which are at present relatively crude (see Weil *et al.* 1992). The DNS approach is essentially the only feasible method for obtaining the required information in a (Lagrangian) reference frame following the motion of material fluid elements, and hence offers special hope for model testing.

In the sections below we report briefly on progress in different aspects of the research, and outline our plans for work to be performed during the succeeding period. Recently, we have submitted a journal article (Yeung 1996a) for publication, and an abstract (Yeung 1996b) for presentation at a large national conference. Copies of these materials have previously been forwarded to the program manager (Dr. Deran Pashayan) at EPA.

Progress in the research has been greatly facilitated by an allocation of supercomputing resources (to be renewed) at the NSF-supported Cornell Theory Center, which has allowed the conduct of intensive high-resolution numerical simulations through massively parallel computing. In addition, with support from the Division of International Programs at NSF, the P.I. has recently spent a month (mid-August to mid-September) in Australia collaborating with a leading atmospheric dispersion modeling scientist to work on the use of our numerical simulation data for the development of advanced stochastic models of atmospheric dispersion. While in Australia the P.I. gave three invited seminars on the subject of "Studies of turbulent mixing and dispersion using high-resolution direct numerical simulations" at the University of Sydney, Monash University (in Melbourne) and the CSIRO Division of Atmospheric Research.

Further information on the research activities is given in the sections below.

High-resolution simulations by parallel computing

It is generally agreed that the method of direct numerical simulations (DNS, see Reynolds 1990 for a recent review) has contributed much to our fundamental understanding of turbulence, but that high Reynolds number simulations are still very computationally intensive. To increase the Reynolds number, high resolution simulations which can resolve a wide range of scales are required. To this end, the P.I. has expended considerable effort in developing a massively parallel DNS code with particle-tracking capabilities. The main ideas of the (distributed-memory) parallel algorithm have been described in the previous annual report, and in a conference manuscript (Yeung & Moseley 1995). The latter also contains the results of a systematic timing study which evaluated the impact of various factors on the performance of the parallel algorithm. In the last few months the data structure of the code has been further improved to reduce the per-processor memory requirements. The parallel code is run on an 512-node IBM SP2 parallel supercomputer at the Cornell Theory Center, using the IBM-optimized Message Passing Library (MPL) software for parallel communication constructs. We have begun the process of converting the MPL communication calls (which are supported only on IBM SP2's) into a more portable form, namely using the Message Passing Interface (MPI), which is being developed as an industry standard and is supported by multiple vendors.

Other than the MPL-to-MPI conversion effort described above, we are currently in a phase of actively making production runs with the parallel codes. The strategy is first to develop stationary isotropic Eulerian turbulent velocity fields at high resolution, and then to track Lagrangian fluid particles as well as obtain other important Eulerian statistics. At the time of writing, we have made a series of 384^3 grid simulations at Taylor-scale Reynolds number about 180. This is just marginally below the highest Reynolds numbers reported from similar numerical simulations in the literature (e.g., Wang, Chen, Brasseur & Wyngaard 1996). We have used the data to examine in a new light some important issues in high Reynolds number DNS, including the attainment of inertial range similarity, and the values of Kolmogorov and other universal constants. Other researchers (in particular, Prof. K.R. Sreenivasan of Yale University) have expressed considerable interest in the results.

Within the limits of the capacity of currently available parallel computer architectures, our ultimate goal is to perform 512^3 simulations (which involve as many as 134 million grid points) which should yield Taylor-scale Reynolds numbers greater than 200. With 64 parallel nodes used, each time step in a simulation without fluid particles is found to take just below one minute. Thus these ambitious computations are now feasible.

Two-particle acceleration statistics

In traditional theories (e.g., Novikov 1963, Monin & Yaglom 1975) of turbulent dispersion it is generally assumed that the acceleration of fluid particle pairs with an initial separation (l_0) much greater than the Kolmogorov length scale (η) is uncorrelated at all times. Similarly, in all Markovian models for fluid particle velocities the two-particle acceleration correlation is neglected. Application of this assumption for initial separations in the inertial range in which $\eta \ll l_0 \ll L_1$ (where L_1 is the integral length scale) would imply the two-particle covariance of temporal velocity increments is simply twice that of the single-particle result, without the need for a separate theory. However, recently Borgas & Sawford (1991) presented theoretical arguments that suggest the two-particle acceleration correlation remains important for significant periods of time, decaying as t^{-1} in the inertial range. An understanding of this issue is important for the development of dispersion models that can account for viscous effects properly at small times.

In Yeung (1996a) we have examined the nature of two-particle Lagrangian acceleration statistics in statistically stationary isotropic turbulence by direct numerical simulation, at Taylor-scale Reynolds number about 140. Because of the differentiability properties of cubic-spline interpolation (as opposed to piecewise polynomial schemes) for fluid particle velocities, accelerations are conveniently calculated by a simple finite difference of the velocity time series of each particle. Two-particle acceleration correlations are found to be non-negligible over significant periods of time, especially for particle pairs of small initial separation. Although the Reynolds number is perhaps not sufficiently high, results at intermediate times and for intermediate initial separations nevertheless offer qualitative support for t^{-1} scaling. A conditional sampling procedure is used to investigate the observation (Fig. 1) that the decay of the two-particle acceleration correlation with mean separation is much slower than that of the Eulerian two-point correlations in space. It is found that intermittency of the particle-pair separation plays a prominent role, especially at early times and for small initial separations. Under these conditions large values of separation are associated by fluid particles of large acceleration, whereas the majority of closer-together particle pairs tend to maintain the ensemble-averaged acceleration correlation.

Through the particle-pair separation, two-particle statistics are very sensitive to the spatial structure of turbulence. Consequently we are motivated to study the Eulerian statistics of the acceleration vector field. In Eulerian analyses it is useful to decompose the acceleration field into a dominant irrotational part (due to pressure gradients) and a much weaker solenoidal part (due to viscosity). We have found that longitudinal and transverse correlations display fundamental differences, and are not describable by classical inertial range arguments at intermediate spatial separations. At a conference to be held this November (Yeung 1996b) we plan to present numerical results obtained using a massively parallel algorithm at Taylor-scale Reynolds numbers up to 200 and beyond.

Stochastic modeling

As emphasized in the original proposal, a primary benefit anticipated from this research is the opportunity to use DNS data to develop improved stochastic models of dispersion that are needed to predict the variance of concentration fluctuations (Thomson 1990). This aspect is now actively pursued within an international collaboration (supported by the Division of International Programs at NSF) between the P.I and a leading researcher in stochastic modeling of turbulence, namely Dr. Michael S. Borgas of the Atmospheric Pollution Program at CSIRO Division of Atmospheric Research in Australia. Dr. Borgas and his colleague Dr. Brian L. Sawford have published extensively in the stochastic modeling literature (e.g., Borgas & Sawford 1991, 1994). NSF and Australian funds provide for a two-year program of one-month exchange visits between the lead researchers on each side. The P.I. has just recently returned from his first Australian trip, which also provided exposure to a world-class research program in atmospheric pollution.

A one-dimensional second-order stochastic model is currently being developed for particle-pair dispersion. Essentially, we model the rate of change (a) of the relative velocity magnitude (v) between the particles as a Markov process in a manner consistent with Eulerian two-point statistics, and then integrate twice in time to calculate the separation distance (r). Eulerian DNS data are parametrized in suitable forms as input for modeling. An example is given by Fig. 2, which shows the conditional expectation $< a|v >$ for several values of the separation. Considerable statistical jitter is apparent at values of the conditioning variable (v) far away from the mean because of sampling limitations, which will be addressed by performing ensemble averaging over time. Despite a certain amount of skewness, this result suggests that, within the limits of statistical uncertainty, the function $< a|v >$ may be described reasonably well by a parabolic fit of the form $\gamma_0 + \gamma_1 v^2$, where γ_0 and γ_1 are functions of r.

A Monte-Carlo computer code written to implement the stochastic model described above is currently being tested. An adaptive time-stepping procedure is used to ensure that the separation distance does not become unphysically negative as a result of random terms in the model. Input to the model includes parametrizations of Lagrangian DNS data (see Pope 1994).

In addition to working with Dr. Borgas, the P.I. has also provided detailed data to another researcher in stochastic modeling (Heppe 1996) who has made close comparisons with the P.I.'s DNS results of Yeung (1994). This further illustrates the unique value of DNS data for the testing of Lagrangian stochastic models.

Two-particle relative motion in homogeneous shear flow

Two-particle turbulent dispersion in homogeneous shear flow with a mean velocity field of the form $U = Sy$ (with uniform shear rate S) is a principal target of investigation in this project. Unlike the case of stationary isotropic turbulence, this flow is anisotropic (with directional dependences dictated by the mean flow) and non-stationary (because mean shear causes continued growth of the turbulence kinetic energy). Algorithmic extensions are required because of these considerations. In the DNS solution algorithm we use (Rogallo 1981), the transport equations for the turbulent velocity fluctuations are solved in a solution domain moving with the mean flow but which is periodically "remeshed" to prevent excessive distortion of the grid lines. Single-particle statistics of displacement and velocity are similar to those of Squires & Eaton (1991), whereas the two-particle statistics described below are believed to be new.

The Eulerian velocity field is first simulated for a sufficient length of time (using parameters similar to Rogers, Moin & Rogallo 1986), for the effects of shear to become dynamically established. Ensembles of fluid particle pairs are then released, using a generalized version of an initialization scheme described by Yeung (1996a) which allows both the orientation and magnitude of the initial separation vector in each ensemble to be readily specified. Asymptotic results at small and large times have been derived for all the nontrivial components of the dispersion tensor $\langle \Delta l_i \Delta l_j \rangle$ in a fixed (laboratory) frame, where $\Delta \underline{l}(t)$ is the change in the separation vector over time t. These results are well verified in the numerical simulations.

Because of the inherent anisotropy induced by mean shear in the flow, certain Lagrangian statistics which are sensitive to the large scales may be expected to deviate from traditional results based on isotropic turbulence. For example, at large times, although the Cartesian components of the separation vector $\underline{l}$ are Gaussian distributed, the component l_1 and l_2 (in the streamwise and cross-stream directions) are not statistically independent (but have a correlation coefficient theoretically equal to 0.866). Accordingly, the separation PDF (of the magnitude l) differs from the chi-square result of Yeung (1994).

Two-particle velocity statistics are currently actively studied. The two-particle correlation coefficient decreases (of course) in time as the particles move apart, but is found to be more persistent in the streamwise velocity component.

New developments and plans

We recall the four major research areas identified in the original proposal, namely:

1. Growth of mean separation

2. One-time statistics of relative diffusion
3. Two-time statistics
4. Effects of Reynolds number and mean shear

A flexible schedule allowing for responses to new opportunities (an example being our foray into massively parallel computing, as described above) is essential for good research. At this time (end of year 2) our work in areas 1 and 2 is nearly complete (and documented in Yeung 1994, 1996a). The focus in the final project year will be on areas 3 and 4, with increased publication efforts. Specifically, we intend to focus our efforts on the following aspects:

1. *Two-time statistics of relative diffusion.* As noted in the original proposal, very little is known about two-time statistics such as the correlation between the velocities of different particles at different times. In the statistical analysis we need to note the fact that relative diffusion in homogeneous turbulence is an accelerating, non-stationary process (with particles moving apart from each other), even if the velocity fluctuations are statistically stationary.

2. *Relative diffusion in homogeneous shear flow.* With the testing phase now complete, a production run using $256 \times 128 \times 128$ grid points is to be conducted shortly. The results will be carefully prepared for publication.

3. *Towards high resolution simulations.* Direct numerical simulations of isotropic turbulence at 384^3 and 512^3 resolution are currently in progress, with Taylor-scale Reynolds numbers that are higher than most published DNS studies. Subject to the continued availability of supercomputer resources, we will attempt to obtain both single- and two-particle statistics at higher Reynolds numbers using these high-resolution simulations. High Reynolds number results are expected to be instrumental in addressing similarity hypotheses (e.g. as given in Monin & Yaglom 1975).

4. *Stochastic modeling.* We will use ensemble-averaged DNS data to continue the development of the new second-order stochastic model of particle-pair dispersion. After adequate model performance is demonstrated at lower Reynolds numbers we will use the higher Reynolds number data from high-resolution simulations.

We expect to maintain and increase the momentum of our publication efforts (including conference presentations) within the next 12 months. Journal submissions are planned for the Eulerian properties of the acceleration field, two-particle statistics in homogeneous shear flow, and stochastic modeling. We are also considering submitting an abstract to the Conference on Boundary Layers and Turbulence sponsored by the American Meteorological Society in Vancouver, Canada in summer 1997.

In the third project year we will also submit a renewal proposal. Possible topics for further research are dispersion in turbulence subjected to uniform solid-body rotation and in turbulent boundary layers with thermal stratification. Both of these topics address physical phenomena important to practical problems of atmospheric pollutant dispersion.

Note on student support

The P.I. expects to request a no-cost extension for a few months beyond October 1997 in order to continue using project funds to support a PhD student (Mr. P. Shen) until February 1998.

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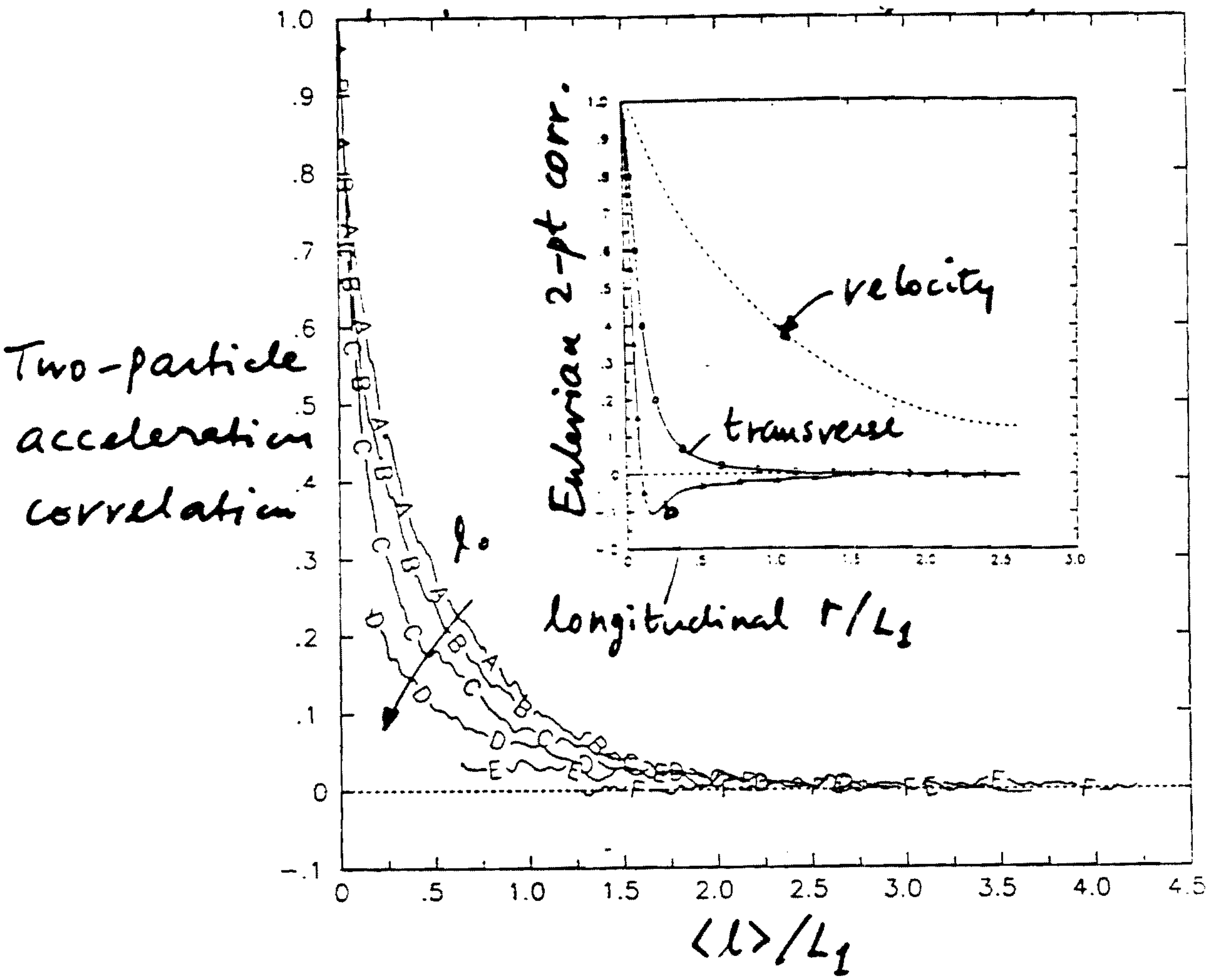

FIGURE 1. Comparison of two-particle acceleration correlations with Eulerian two-point correlations (inset), in isotropic turbulence at R_λ 140 simulated using 256^3 grid points. Lines A-F are for initial separations l_0 equal to 1/4, 1, 4, 16, 64 and 128 times of the Kolmogorov length scale (η). The mean particle-pair separation $\langle l \rangle$ and Eulerian spatial separation are both scaled by the longitudinal integral length scale (L_1).

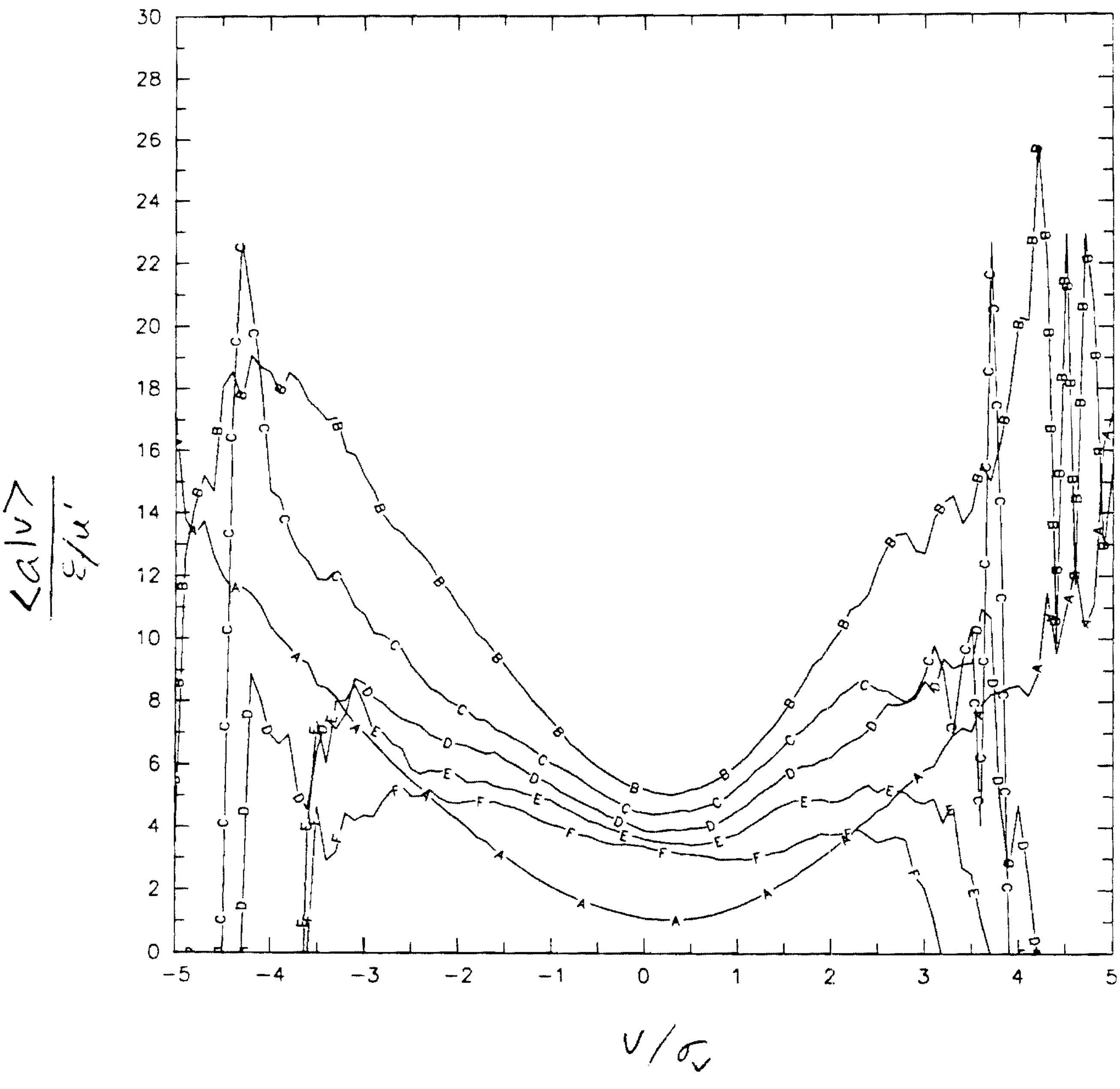

FIGURE 2. The conditional expectation $< a|v >$ for several values of the spatial separation (r), with v normalized by its standard deviation and a scaled by ϵ/u' (where ϵ is the energy dissipation rate and u' is the r.m.s. velocity). The values of r used correspond to 1.78 to 106.9 Kolmogorov scales (η) for lines A–F, in equal increments. This Eulerian result was extracted from one instantaneous velocity field at 128^3 resolution with the time-averaged Taylor-scale Reynolds number being 90.

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Georgia Institute of Technology

School of Aerospace Engineering
Atlanta, Georgia 30332-0150 U.S.A.
PHONE 404·894·3000
FAX 404·894·2760

Tel. (404)-894-9341
e-mail: yeung@peach.ae.gatech.edu

September 22, 1997

Dr. Deran Pashayan
Environmental Sciences Research Division (8723R)
National Center for Environmental Research and Quality Assurance
U.S. Environmental Protection Agency
401 M St. SW (8723R)
Workstation 51185
Washington, DC 20460

Dear Dr. Pashayan:

I am pleased to enclose the third annual report for research supported under Grant No. R821340010. Any comments you may have will be greatly appreciated.

Thank you for your support.

Yours sincerely,

P.K. Yeung, PhD
Assistant Professor

encl: Annual Progress Report

cc: Ms. Anita Rowland, Office of Contract Administration

EPA Grant No. R821340010
Annual Progress Report, 10/01/96-9/30/97

P.I.: Dr. P.K. Yeung
School of Aerospace Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0150

September 22, 1997

Introduction

This is the third annual report for research activities supported by EPA Grant No. R821340010, entitled "Numerical simulation of turbulent dispersion and relative diffusion". Whereas significant progress has been made, in order to further enhance the quality of the research results the P.I. has requested, and received approval for, a one-year extension beyond the original three-year project schedule.

The primary objective of the research is to study the fluid mechanics of contaminant dispersion caused by the spreading apart of material fluid elements in turbulent flow. Direct numerical simulations (DNS) of the basic equations of fluid motion are used to advance physical understanding, with a long-term view towards improving air-quality models in practice which are at present relatively crude (see Weil *et al.* 1992). The DNS approach is essentially the only feasible method for obtaining the required information in a (Lagrangian) reference frame following the motion of material fluid elements, and hence offers special hope for model testing. Progress in the research continues to be greatly facilitated by the availability of peer-reviewed parallel computer resources at national supercomputing centers, which is essential for the conduct of intensive high-resolution numerical simulations. Furthermore, the P.I's collaboration (supported by the Division of International Programs at NSF) with a leading atmospheric dispersion modeling scientist in Australia has been the source of much stimulus.

In the sections below we report briefly on progress in different aspects of the research, and outline our plans for work in the remaining project period (until September 1998). In the past 12 months our work has led to two journal articles (Yeung 1997a, Shen & Yeung 1997) accepted for publication, and two conference presentations (Yeung 1996, 1997b). Copies of these materials have previously been forwarded to the program manager (Dr. Deran Pashayan) at EPA. In addition, the P.I. has given invited seminars on the subject of turbulent dispersion at the National Center for Atmospheric Research (Boulder, CO, March 1997) and at the University of Queensland (Brisbane, Australia, August 1997).

Study of the fluid acceleration

In traditional theories (e.g., Novikov 1963, Monin & Yaglom 1975) of turbulent dispersion it is generally assumed that the acceleration of fluid particle pairs with an initial separation (l_0) much greater than the Kolmogorov length scale (η) is uncorrelated at all times. Similarly, in all Markovian models for fluid particle velocities the two-particle acceleration correlation is neglected. Application of this assumption for initial separations in the inertial range in which $\eta \ll l_0 \ll L_1$ (where L_1 is the integral length scale) would imply the two-particle covariance of temporal velocity increments is simply twice that of the single-particle result, without the need for a separate theory. However, recently Borgas & Sawford (1991) presented theoretical arguments that suggest the two-particle acceleration correlation remains important for significant periods of time, decaying as t^{-1} in the inertial range. An understanding of this issue is important for the development of dispersion models that can account for viscous effects properly at small times.

In Yeung (1997a) Lagrangian statistics of the fluid particle acceleration are studied by direct numerical simulation, in stationary isotropic turbulence (at three different Reynolds numbers) and homogeneous shear flow with uniform mean shear rate. The one-particle acceleration autocorrelation decays rapidly with time, with a zero-crossing at just over two Kolmogorov time scales. In contrast, two-particle correlations are relatively persistent, especially for particle pairs of small initial separation distance. Results for intermediate times at Taylor-scale Reynolds number 140 resemble a t^{-1} inertial-range scaling suggested in the literature, but even higher Reynolds numbers are needed for more definitive comparisons. Use of a theoretical argument and conditional sampling indicates that the two-particle correlation is determined by a coupling between a correlation localized in space and a particle-pair separation probability density of positive skewness. The scenario which emerges is that whereas some fluid particles accelerate rapidly away from each other, the majority of particle pairs can still be relatively close together and hence help maintain the two-particle correlation at significant levels. Acceleration correlations in homogeneous shear flow are found to display a tendency towards local isotropy.

Through the particle-pair separation, two-particle statistics are very sensitive to the spatial structure of turbulence. Consequently we are motivated to study the Eulerian statistics of the acceleration vector field. In Eulerian analyses it is useful to decompose the acceleration field into an irrotational part (due to pressure gradients) and a solenoidal part (due to viscosity). In general the irrotational part is found to be dominant. One consequence is that, in contrast to classical expectations, the mean-squared acceleration scaled by Kolmogorov variables appears to increase with Reynolds number (Yeung 1996), rather than approaching universal behavior.

Two-particle relative motion in homogeneous shear flow

Two-particle turbulent dispersion in homogeneous shear flow with a mean velocity field of the form $U = Sy$ (with uniform shear rate S) is a principal target of investigation in this project. Unlike the case of stationary isotropic turbulence, this flow is anisotropic (with directional dependences dictated by the mean flow) and non-stationary (because mean shear causes continued growth of the turbulence kinetic energy). Algorithmic extensions are required because of these considerations. In the DNS solution algorithm we use (Rogallo 1981), the transport equations for the turbulent velocity fluctuations are solved in a solution domain moving with the mean flow but which is periodically "remeshed" to prevent excessive distortion of the grid lines. Single-particle statistics of displacement and velocity are similar to those of Squires & Eaton (1991), whereas the two-particle statistics described below are believed to be new.

In Shen & Yeung (1997) the dispersion of Lagrangian fluid particle pairs in homogeneous turbulent shear flow is studied by direct numerical simulation using 256×128^2 grid points. It is emphasized that anisotropy requires the effects of both magnitude and orientation of the initial separation vector on two-particle statistics to be considered separately, especially at early times when these statistics are primarily determined by the Eulerian structure of the velocity gradient fluctuations. The effects of initial particle positions and pair-separation on displacement and dispersion statistics are examined in relation to classical theory. Particle-pair dispersion is found to be most effective in the streamwise direction, and especially so for particle pairs initially separated in the direction of the mean velocity gradient. Similarly, two-particle velocity correlations are anisotropic, being strongest in the streamwise component but weakest in the cross-stream component. The particle-pair separation distance probability density function differs significantly from a Gaussian form used in most dispersion models for air-quality applications. It is hoped that the new results will be helpful for extending two-particle stochastic models to anisotropic turbulent flows.

Two-particle, two-time statistics

The form of the governing equations suggests that the mean-squared particle-pair dispersion can be calculated if the correlation between the velocities of two particles (within each pair) at different times is known (or can be accurately modeled). In Yeung (1997b) we study the behavior of two-particle, two-time Lagrangian velocity correlations extracted from direct numerical simulations of isotropic turbulence with up to 256^3 grid points. It is found that these correlations are dominated by the single-particle autocorrelation, with a lesser effect due to the spatial separation between the particles. The numerical simulation data are used to evaluate two simple models based on the single-particle autocorrelation and a weighted average (according to the separation-distance probability distribution) of Eulerian two-point correlations. Effects of the Reynolds number and initial separation are also addressed. These results can be used to compute the two-particle eddy diffusivity, which is the integral of the two-time correlation of the relative velocity between the particles.

High-resolution simulations by parallel computing

It is generally agreed that whereas direct numerical simulations (DNS, see Reynolds 1990 for a recent review) have contributed much to our fundamental understanding of turbulence, simulations at high Reynolds numbers (typical of applications) are still very difficult for reasons of computational expense. To achieve higher Reynolds numbers, high-resolution simulations using a large number of grid points which can resolve a wide range of scales are required. To this end, the P.I. has expended considerable effort in developing a massively parallel DNS code (described in Yeung & Moseley 1995) with particle-tracking capabilities. The code currently runs on an IBM SP2 parallel supercomputer at the Cornell Theory Center, using the Message Passing Interface library (MPI, a portable standard) for inter-processor communication. Since MPI is portable we are in a good position to switch to other parallel architectures if circumstances so require; such a conversion has, in fact, been achieved for CRAY T3D and T3E's.

A prerequisite task for obtaining high-resolution Lagrangian data is to develop stationary isotropic Eulerian turbulent velocity fields at high resolution. Eulerian statistics from simulations using 512^3 grid points have been reported in Yeung & Zhou (1997), with a Taylor-scale Reynolds number above 200 and in the same range as the highest reported from similar numerical simulations in the literature (e.g., Wang, Chen, Brasseur & Wyngaard 1996). We have used the data to uncover some new insights on important issues in high Reynolds number DNS, including the attainment of inertial range similarity, and the values of Kolmogorov and other universal constants.

A new series of 512^3 simulations including particle tracking and passive scalar transport is currently in progress. The scope of these new calculations is pushing the limits of the capacity of currently available parallel computer architectures. Yet, with 64 IBM SP2 processors (of the latest "superchip" variety) each time step takes less than one minute, making these ambitious computations quite feasible.

Deta for stochastic modeling

As emphasized in the original proposal, a primary benefit anticipated from this research is the opportunity to use DNS data to develop improved stochastic models of dispersion that are needed to predict the variance of concentration fluctuations (Thomson 1990). This aspect is now actively pursued within an international collaboration (through one-month exchange visits supported by the Division of International Programs at NSF) between the P.I and a leading researcher in stochastic modeling of turbulence, namely

Dr. Michael S. Borgas of the Atmospheric Pollution Program at CSIRO Division of Atmospheric Research in Australia.

A new stochastic model for particle-pair dispersion has been developed which is based on representing the rate of change of the relative velocity between the particles (measured along the separation vector) as a Markovian process. The influence of the spatial structure of the turbulence on particle-pair separation is expressed in terms of Eulerian two-point statistics, for which suitable parameterizations have been proposed and tested (Borgas & Yeung 1997). Recently we have made actual comparisons between simulation and modeling results for two-particle dispersion using the DNS data of Yeung (1994) and Yeung (1997). A new journal article will be written upon completion of the 512^3 simulations and subsequent data analysis.

In addition to working with Dr. Borgas, the P.I. has also provided detailed data to another researcher in stochastic modeling (Heppe 1997) who has made close comparisons with the P.I.'s DNS results of Yeung (1994). This further illustrates the unique value of DNS data for the testing of Lagrangian stochastic models.

Planning for further research

We recall the four major research areas identified in the original proposal, namely:

1. Growth of mean separation
2. One-time statistics of relative diffusion
3. Two-time statistics
4. Effects of Reynolds number and mean shear

Significant progress has been made in four areas, as documented in journal articles (Yeung 1994, 1997a, Shen & Yeung 1997) and conference publications (Yeung 1997b). In addition, as described above we have made advances in the related subjects of massively parallel computing and stochastic modeling. In the next 12 months we will conclude the project by focusing our research and publication efforts on the following aspects:

1. *Further studies of relative diffusion in homogeneous shear flow.* The results in Shen & Yeung (1997) are based on only one simulation designed to show the characteristic effects of mean shear and anisotropy. In continuing work we are studying the quantitative effects of different shear rates via multiple simulations. We also plan to extend our work on two-time statistics and stochastic modeling comparisons in isotropic turbulence to the case of homogeneous shear flow. Some generalizations in concept are necessary: for example, the two-particle, two-time correlation is now a second-order tensor function of a vector (initial separation) argument.

2. *Conduct of high-resolution computations* As stated above a series of 512^3 simulations of isotropic turbulence simulations is currently in progress. This will provide a full range of both one- and two-particle Lagrangian statistics from DNS at the highest Reynolds number known for such data. Together with existing results at lower Reynolds numbers we will address questions of Reynolds number dependence and similarity hypotheses (e.g. in given in Monin & Yaglom 1975) which are important for the extrapolation of DNS results towards higher Reynolds numbers not yet attainable with current technologies.

3. *Use of data for stochastic modeling.* As stated above our unique Lagrangian DNS data are being used actively for the development of modeling. Already the degree of qualitative agreement is quite encouraging, and we expect that good quantitative agreement can be obtained in most of the important two-particle statistics with the new models being proposed. Successful completion of this task should help demonstrate the practical importance of this research project: namely that the simulation data can be (and has been) used to improve modeling procedures which in turn constitute the basis of current and future air-quality models.

The P.I also plans to submit a renewal proposal. Possible topics for further research include dispersion in turbulent boundary layers with thermal stratification and in turbulence subjected to uniform solid-body rotation. Both of these topics address physical phenomena important to practical problems of atmospheric pollutant dispersion.

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EPA Grant No. R821340010
Final Project Report

P.I.: Dr. P.K. Yeung
School of Aerospace Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0150

October 23, 1998

Introduction

This is the final report for research activities supported by EPA Grant No. R821340010, entitled "Numerical simulation of turbulent dispersion and relative diffusion".

The primary objective of the research was to study the fluid mechanics of contaminant dispersion caused by the spreading apart of material fluid elements in turbulent flow. A major motivation was that new physical understanding would be helpful in the long-term development of improved air-quality models in practice which are at present relatively crude (see Weil *et al.* 1992). To this end, Lagrangian data (in a reference frame following the motion of material fluid elements) obtained from the simulations has indeed provided physical insight, and the use of simulation data for modeling development is proceeding in earnest. The latter efforts have been enhanced by a two-year travel grant from the Division of International Programs at NSF which has enabled formal collaborations with a leading researcher in dispersion modeling (Dr Michael Borgas, CSIRO Atmospheric Research, Australia).

Work performed in this project has led to a substantial number of publications and presentations. In particular, these include four articles in archival journals published or in process (Yeung 1994, Yeung 1997a, Shen & Yeung 1997, Vedula & Yeung 1998), two conference manuscripts (Yeung & Moseley 1995, Yeung 1997b), and one doctoral thesis (Shen 1998). NSF support for the international collaboration referenced above has also led to related publications (Borgas & Yeung 1998, Yeung & Borgas 1998, Yeung, Borgas & Franzese 1998). In addition the research has an important part of invited seminars that the PI has given in the last four years at various institutions in the US and Australia (University of Maryland, NASA Langley Research Center, Rockwell International Corporation, University of Sydney, Monash University, CSIRO Atmospheric Research, National Center for Atmospheric Research, University of Brisbane, Kansas State University, City College of New York, and Yale University).

In the sections below we briefly summarize our technical accomplishments in several aspects of the research, including extensions beyond the original research areas which for reference are listed below.

1. Growth of mean separation
2. One-time statistics of relative diffusion
3. Two-time statistics
4. Effects of Reynolds number and mean shear

Dispersion in isotropic turbulence

The dispersion of fluid particle pairs diffusing relative to each other has been studied in the simplified case of stationary isotropic turbulence by direct numerical simulation. The main independent variable is the initial particle-pair separation distance, which is varied over a wide range covering both the smallest and largest dynamically relevant length scales present in the velocity fluctuations. The growth of two-particle separation exhibits asymptotic stages at small and large diffusion times. Through the two-particle separation, particle-pair velocity correlations are closely related to the Eulerian spatial structure of the turbulence. At large times the square of the separation distance has a chi-square probability distribution. The relative velocity between particle pairs is studied in both a fixed coordinate frame and an inertial frame which moves with the initial particle velocity. In the latter case the velocity increments of two fluid particles become uncorrelated only if their initial velocities are uncorrelated, which in turn requires their initial separation be large compared to the integral length scale. For sufficiently large initial separations, the relative velocity increments and mean-square dispersion in this moving frame display a resemblance to inertial range scaling, but with a proportionality constant that is much smaller than classical estimates. At large times, the degree of preferential alignment between the separation and relative velocity vectors is weak, but the product of the separation distance and the velocity component projected along the separation vector is sustained on average.

Basic dispersion results as described above were first given in Yeung (1994). Subsequently we have studied the slightly more complex case of homogeneous shear flow (below), extended our results to include statistics of fluid particle accelerations (Yeung 1997a), and towards higher Reynolds number (Yeung, Borgas & Franzese 1998). The importance of two-particle acceleration correlations is emphasized by Borgas & Sawford (1991). At higher Reynolds numbers we observe that both the separation distance and its rate of change (given by the projection of the relative velocity along the separation vector) are highly intermittent. This indicates dispersion regimes where most fluid particle pairs are close together but a small number are much farther apart. The practical implication is that this suggests finite probability of traces of pollutant reaching far from a localized source.

Dispersion in homogeneous turbulent shear flow

Two-particle turbulent dispersion in homogeneous shear flow with a mean velocity field of the form $U = Sy$ (with uniform shear rate S) is a principal target of investigation in this project. Unlike the case of stationary isotropic turbulence, this flow is anisotropic (with directional dependences dictated by the mean flow) and non-stationary (because mean shear causes continued growth of the turbulence kinetic energy). Algorithmic extensions are required because of these considerations. In the DNS solution algorithm we use (Rogallo 1981), the transport equations for the turbulent velocity fluctuations are solved in a solution domain moving with the mean flow but which is periodically "remeshed" to prevent excessive distortion of the grid lines. Single-particle statistics of displacement and velocity are similar to those of Squires & Eaton (1991), whereas the two-particle statistics described below are believed to be new.

In Shen & Yeung (1997) the dispersion of Lagrangian fluid particle pairs in homogeneous turbulent shear flow is studied by direct numerical simulation using 256×128^2 grid points. It is emphasized that anisotropy requires the effects of both magnitude and orientation of the initial separation vector on two-particle statistics to be considered separately, especially at early times when these statistics are primarily determined by the Eulerian structure of the velocity gradient fluctuations. The effects of initial particle positions and pair-separation on displacement and dispersion statistics are examined in relation to classical theory. Particle-pair dispersion is found to be most effective in the streamwise direction, and especially so for particle pairs initially separated in the direction of the mean velocity gradient. Similarly, two-particle velocity correlations are anisotropic, being strongest in the streamwise component but weakest in the cross-stream component. The particle-pair separation distance probability density function differs significantly from a Gaussian form used in most dispersion models for air-quality applications. Effects of the magnitude of shear are studied also in Shen (1998): higher shear rate is found to cause more rapid de-correlation of both one- and two-particle velocity correlations in time, which in turn implies more rapid growth (and mixing) in mean-squared displacement and particle-pair separation.

Two-time statistics

The form of the governing equations suggests that the mean-squared particle-pair dispersion can be calculated if the correlation between the velocities of two particles (within each pair) at different times is known (or can be accurately modeled). In Yeung (1997b) we study the behavior of two-particle, two-time Lagrangian velocity correlations extracted from direct numerical simulations of isotropic turbulence with up to 256^3 grid points. It is found that these correlations are dominated by the single-particle autocorrelation, with a lesser effect due to the spatial separation between the particles. The numerical simulation data are used to evaluate two simple models based on the single-particle autocorrelation and a weighted average (according to the separation-distance probability distribution) of Eulerian two-point correlations. Effects of the Reynolds number and initial separation are also addressed. These results can be used to compute the two-particle eddy diffusivity, which is the integral of the two-time correlation of the relative velocity between the particles.

The modeling of two-particle, two-time correlations in shear flow is also addressed briefly in Shen (1998). We compare the merits of two heuristic models cited by Sawford (1982) as well as extend these models to off-diagonal elements of the particle-pair velocity correlation tensor.

High-resolution computations

It is generally agreed that whereas direct numerical simulations are a very powerful research tool (Moin & Mahesh 1998), calculations at high Reynolds numbers (typical of applications) are still very difficult for reasons of computational expense. To achieve higher Reynolds numbers, high-resolution simulations using a large number of grid points which can resolve a wide range of scales are required. To this end, the P.I. has expended considerable effort in developing a massively parallel DNS code (described in Yeung & Moseley 1995) with particle-tracking capabilities. The code has run on IBM SP2 machines at NSF-supported national facilities at the Cornell Theory Center and San Diego Supercomputing Center. A high level of portability is achieved by using the Message Passing Interface library (MPI, a portable standard) for inter-processor communication. (In fact the code has been ported to CRAY T3E machines as well.)

The use of 64 IBM SP2 processors allows 512^3 computations (with 134 million grid points) to be performed at a speed of less than one minute per time step. These computations are at the highest resolution reported today, with the Reynolds number sufficiently high to achieve (limited) evidence of inertial-range scaling in the energy spectrum (Yeung & Zhou 1997), in a manner consistent with experimental data. Incidentally, this extensive DNS database has created many new opportunities in studying the structure of turbulence. For instance, we have used this data to study the Eulerian scaling properties of acceleration and (as its dominant component) the pressure gradient (Vedula & Yeung 1998). The availability of DNS data over a substantial Reynolds number range is seen to be important in discriminating between alternative scaling relations previously suggested in the literature. In addition several highly-respected researchers at other institutions have in fact expressed interest in using our data to study other important questions in turbulence structure, such as vorticity statistics and unsteady versus convective parts of the fluid acceleration.

Developments in stochastic modeling

As emphasized in the original proposal, a primary benefit anticipated from this research is the opportunity to use DNS data to develop improved stochastic models of dispersion that are needed to predict the variance of concentration fluctuations (Thomson 1990). This aspect is actively pursued in an international collaboration (in part through a series of one-month exchange visits) with a leading researcher in stochastic modeling of turbulence, namely Dr. Michael S. Borgas of the Atmospheric Pollution Program at CSIRO Atmospheric Research in Australia. (Note that CSIRO is Australia's premier research agency.)

A new stochastic model for particle-pair dispersion has been developed which is based on representing the rate of change of the relative velocity between the particles measured along the separation vector as a Markovian process. Essentially we focus on motions that tend to stretch the particle pairs apart, while motions in the plane orthogonal to the separation vector (which becomes important in anisotropic flows) are considered separately in Yeung & Borgas (1998). The influence of the spatial structure of the turbulence on particle-pair separation is expressed in terms of Eulerian two-point statistics, for which suitable parameterizations have been proposed and tested (Borgas & Yeung 1998). Recently we have made actual comparisons between simulation and modeling results for two-particle dispersion using the DNS data of Yeung (1994) and Yeung (1997). A new journal article is currently under preparation.

In addition to working with Dr. Borgas, the P.I. has also provided detailed data to another researcher in stochastic modeling (Heppe 1998) who has made close comparisons with the P.I.'s DNS results of Yeung (1994). Other researchers (Malik & Vassilicos 1998) have also referenced the results in Yeung (1994) in considerable detail. These developments further illustrate the unique value of DNS data for Lagrangian modeling purposes.

Closing remarks

In summary, we have largely fulfilled the technical objectives of this project, and in fact in some aspects (high-resolution computations and stochastic modeling) have achieved beyond the original plans. Our hope is that a future project focused on practical configurations like turbulent boundary layers with increased relevance to flow in the lower atmosphere will meet with a similar degree of success.

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