12:00:13 OCA PAD INITIATION - PROJECT HEADER INFORMATION 09/19/94

Active

Project #: E-16-X46 Cost share #: E-16-386 Rev #: 0
Center # : 10/24-6-R8283-0A0 Center shr #: 10/22-1-F8283-0A0 OCA file #:
Work type : RES
Contract#: CTS-9411690 Mod #: Document : GRANT
Prime #: Contract entity: GTRC

Subprojects ? : N CFDA: 47.041
Main project #: PE #: N/A

Project unit: AERO ENGR Unit code: 02.010.110
Project director(s):
YEUNG P K AERO ENGR (404)894-9341

Sponsor/division names: NATL SCIENCE FOUNDATION / GENERAL
Sponsor/division codes: 107 / 000

Award period: 940901 to 950831 (performance) 951130 (reports)

Sponsor amount	New this change	Total to date
Contract value	18,000.00	18,000.00
Funded	18,000.00	18,000.00
Cost sharing amount		18,442.00

Does subcontracting plan apply ?: N

Title: ENGINEERING RESEARCH EQUIPMENT: HIGH PERFORMANCE WORKSTATION UPGRADE TO ...

PROJECT ADMINISTRATION DATA

OCA contact: Jacquelyn L. Bendall 894-4820

Sponsor technical contact	Sponsor issuing office
MILTON J. LINEVSKY	PAULETTE L. GREEN
(703)306-1371	(703)306-1217
NATIONAL SCIENCE FOUNDATION	NATIONAL SCIENCE FOUNDATION
4201 WILSON BLVD.	4201 WILSON BLVD.
ARLINGTON, VA 22230	ARLINGTON, VA 22230

Security class (U,C,S,TS) : U ONR resident rep. is ACO (Y/N): N
Defense priority rating : N/A NSF supplemental sheet
Equipment title vests with: Sponsor GIT X

Administrative comments -
INITIATION OF PROJECT. THIS IS AN EQUIPMENT GRANT. GIT MUST MEET THE COST
SHARING REQUIREMENTS IN THE AMOUNT OF $18,442

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

4

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 12/05/95

Project No. E-16-X46 — Center No. 10/24-6-R8283-0A0

Project Director YEUNG P K — School/Lab AERO ENGR

Sponsor NATL SCIENCE FOUNDATION/GENERAL

Contract/Grant No. CTS-9411690 — Contract Entity GTRC

Prime Contract No. ____________

Title ENGINEERING RESEARCH EQUIPMENT: HIGH PERFORMANCE WORKSTATION UPGRADE TO .

Effective Completion Date 950831 (Performance) 951130 (Reports)

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

Comments
LETTER OF CREDIT APPLIES. 98A SATISFIES PATENT REQUIREMENT.

Subproject Under Main Project No. ____________

Continues Project No. ____________

Distribution Required:

Project Director	Y
Administrative Network Representative	Y
GTRI Accounting/Grants and Contracts	Y
Procurement/Supply Services	Y
Research Property Managment	Y
Research Security Services	N
Reports Coordinator (OCA)	Y
GTRC	Y
Project File	Y
Other	N
	N

E-16-X46 #1

Georgia Tech

School of Aerospace Engineering

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November 30, 1995

Dr. Roger Arndt
Division of Chemical and Transport Systems
National Science Foundation
4201 Wilson Boulevard
Arlington, VA 22230

Dear Dr. Arndt:

I am pleased to enclose the Final Report for my equipment grant CTS-9411690. Thank you for your support.

Yours sincerely,

P.K. Yeung, PhD
Assistant Professor

encl: Final project report

cc: Ms. Jacquelyn Bendall, Office of Contract Adminstration

E-16-X46 #1

OMB Number 345-0058

NATIONAL SCIENCE FOUNDATION
4201 Wilson Blvd.,
Arlington, VA 22230

PI/PD Name and Address

Pei-Kuen Yeung
School of Aerospace Engineering
[redacted]
Atlanta GA 30332-0150

NATIONAL SCIENCE FOUNDATION
FINAL PROJECT REPORT

PART I - PROJECT IDENTIFICATION INFORMATION

1. Program Official/Org. Robert L. Powell - CTS

2. Program Name FLUID,PARTICULATE & HYDRAULIC SYSTEMS PR

3. Award Dates (MM/YY) From: 05/94 To: 08/95

4. Institution and Address
[redacted]
Administration Building
Atlanta GA 30332

5. Award Number 9411690

6. Project Title
ENGINEERING RESEARCH EQUIPMENT: High-Performance Workstation Upgrade Beyond 100 Megaflops

This Packet Contains
NSF Form 98A
And 1 Return Envelope

PART IV — FINAL PROJECT REPORT — SUMMARY DATA ON PROJECT PERSONNEL

(To be submitted to cognizant Program Officer upon completion of project)

The data requested below are important for the development of a statistical profile on the personnel supported by Federal grants. The information on this part is solicited in resonse to Public Law 99-383 and 42 USC 1885C. All information provided will be treated as confidential and will be safeguarded in accordance with the provisions of the Privacy Act of 1974. You should submit a single copy of this part with each final project report. However, submission of the requested information is not mandatory and is not a precondition of future award(s). Check the "Decline to Provide Information" box below if you do not wish to provide the nformation.

Please enter the numbers of individuals supported under this grant.
Do not enter information for individuals working less than 40 hours in any calendar year.

	Senior Staff		Post-Doctorals		Graduate Students		Under-Graduates		Other Participants[1]	
	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.
A. Total, U.S. Citizens						1				
B. Total, Permanent Residents	1									
U.S. Citizens or Permanent Residents[2]:										
American Indian or Alaskan Native										
Asian.	1									
Black, Not of Hispanic Origin.										
Hispanic										
Pacific Islander.										
White, Not of Hispanic Origin						1				
C. Total, Other Non-U.S. Citizens										
Specify Country 1. China					1					
2.										
3.										
D. Total, All participants (A + B + C)	1				1	1				
Disabled[3]	1									

☐ Decline to Provide Information: Check box if you do not wish to provide this information (you are still required to return this page along with Parts I-III).

[1] Category includes, for example, college and precollege teachers, conference and workshop participants.

[2] Use the category that best describes the ethnic/racial status fo all U.S. Citizens and Non-citizens with Permanent Residency. *(If more than one category applies, use the one category that most closely reflects the person's recognition in the community.)*

[3] A person having a physical or mental impairment that substantially limits one or more major life activities; who has a record of such impairment; or who is regarded as having such impairment. *(Disabled individuals also should be counted under the appropriate ethnic/racial group unless they are classified as "Other Non-U.S. Citizens.")*

AMERICAN INDIAN OR ALASKAN NATIVE: A person having origins in any of the original peoples of North America and who maintains cultural identification through tribal affiliation or community recognition.

ASIAN: A person having origins in any of the original peoples of East Asia, Southeast Asia or the Indian subcontinent. This area includes, for example, China, India, Indonesia, Japan, Korea and Vietnam.

BLACK, NOT OF HISPANIC ORIGIN: A person having origins in any of the black racial groups of Africa.

HISPANIC: A person of Mexican, Puerto Rican, Cuban, Central or South American or ether Spanish culture or origin, regardless of race.

PACIFIC ISLANDER: A person having origins in any of the original peoples of Hawaii; the U.S. Pacific territories of Guam, American Samoa, and the Northern Marinas; the U.S. Trust Territory of Palau; the islands of Micronesia and Melanesia; or the Philippines.

WHITE, NOT OF HISPANIC ORIGIN: A person having origins in any of the original peoples of Europe, North Africa, or the Middle East.

NSF Grant Conditions (Article 17, GC-1, and Article 9, FDP-11) require submission of a Final Project Report (NSF Form 98A) to the NSF program officer no later than 90 days alter the expiration of the award. Final Project Reports for expired awards must be received before new awards can be made (NSF Grants Policy Manual Section 677).

Below, or on a separate page attached to this form, provide a summary of the completed projects and technical information. Be sure to include your name and award number on each separate page. See below for more instructions.

PART II - SUMMARY OF COMPLETED PROJECT (for public use)

The summary (about 200 words) must be self-contained and intelligible to a scientifically literate reader. Without restating the project title, it should begin with a topic sentence stating the project's major thesis. The summary should include, if pertinent to the project being described, the following items:

The primary objectives and scope of the project
The techniques or approaches used only to the degree necessary for comprehension
The findings and implications stated as concisely and informatively as possible

PART III - TECHNICAL INFORMATION (for program management use)

List references to publications resulting from this award and briefly describe primary data, samples, physical collections, inventions, software, etc. created or gathered in the course of the research and, if appropriate, how they are being made available to the research community. Provide the NSF Invention Disclosure number for any invention.

I certify to the best of my knowledge (1) the statements herein (excluding scientific hypotheses and scientific opinion) are true and complete, and (2) the text and graphics in this report as well as any accompanying publications or other documents, unless otherwise indicated, are the original work of the signatories or of individuals working under their supervision. I understand that willfully making a false statement or concealing a material fact in this report or any other communication submitted to NSF is a criminal offense (U.S. Code, Title 18, Section 1001).

	11/30/95
Principal Investigator/Project Director Signature	Date

IMPORTANT:
MAILING INSTRUCTIONS
Return this *entire* packet plus all attachments in the envelope attached to the back of this form. Please copy the information from Part I, Block I to the *Attention block* on the envelope.

NSF Grant No. CTS-9411690
Final Report

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

November 30, 1995

Introduction

This is the final report for research activities supported by NSF Grant No. CTS-9411690, entitled "Engineering Research Equipment: high-performance workstation upgrade beyond 100 Megaflops". The objectives of this project are to upgrade the local computer workstation equipment in order to enhance research supported by a separate NSF grant (CTS-9307973), as well as to pursue two new research initiatives. After a budgetary revision, the project funds provided for an upgrade of an IBM RS/6000 workstation to a Model 58H rated at a CPU speed of 101-Megaflops, a core memory of 256 Megabytes, an additional 2 Gigabytes of disk space, as well as a new X-terminal. All of the new hardware components were installed in March 1995, and have been functioning properly since then.

The subject area of the research is the process of greatly enhanced mixing in turbulent fluid flows. Direct numerical simulations solving fundamental conservation equations are carried out on the P.I.'s local facilities as well as on national supercomputers. In this report we first describe current progress, made possible by the enhanced equipment, in the study of differential diffusion of multiple scalars with different molecular diffusivities. Copies of relevant manuscripts or conference presentations (Moseley & Yeung 1995, Yeung 1995, Yeung & Luo 1995, Yeung & Moseley 1995) have all been sent previously to NSF (in the context of Grant CTS-9307973). We also discuss briefly progress on two new initiatives: namely (a) differential diffusion with reaction and heat release, and (b) Lagrangian studies of turbulence structure and scalar transport. Whereas progress in the two latter areas have not reached a publication stage, it should perhaps be noted that a long-term view is appropriate for an *equipment* grant. Indeed, the equipment upgrades made possible with the project funds are expected to have a beneficial impact on the P.I.'s research extending far beyond the nominal one-year project period. It is the P.I.'s intention to continue and expand efforts in the two new research directions.

Differential diffusion for multiple passive scalars

Direct numerical simulations are highly intensive in both CPU and memory requirements, which in our calculations are aggravated by the inclusion of multiple scalar fields (in addition to the velocity). The memory capacity of the P.I.'s workstation before the upgrade (at 160 Mb) was *not* sufficient to accommodate efficiently calculations with three scalars using 128^3 grid points (requiring 156 Mb of core memory), incurring substantial memory paging costs and causing a slowdown of other user processes on the system. The memory expansion to 256 Mb with project funds, together with a faster CPU and a new compiler has reduced the CPU time per time step from 225 seconds to 87 seconds. This level of performance is only about 10% slower than a so-called serial wide node on the IBM SP2 parallel supercomputer at the Cornell Theory Center. (This actually gives a faster turnaround time, since our local computer is dedicated for our own use.) Correspondingly, the feasibility of data analysis programs extracting statistics from 128^3 datasets is also much improved.

Together with supercomputer time allocated at Cornell (for calculations using more than 128^3 grid points), this upgrade of the local computing facility has allowed us to achieve the following. Direct numerical simulations of differential diffusion with three passive scalars have been carried out, and satisfactory phenomenological models have been devised to describe the simulation results, as reported in Yeung & Luo (1995). Both model and simulation suggest that, despite being a process of molecular origin, differential diffusion remains important in the small scales even at high Reynolds numbers. Multi-scalar spectral transfer characteristics have also been analyzed in detail, and the specific spectral mechanisms concerning the role of scale interactions in differential diffusion have been identified (Yeung 1995). More recently, conditional statistics that appear as unclosed terms in the probability density function (PDF) approach (Pope 1985) of turbulence modeling have been extracted from our DNS databases and presented by the P.I.'s student at a conference (Moseley & Yeung 1995). In addition, detailed timing studies have been performed with both serial and parallel (on the IBM SP2) codes to fully understand the effects of various numerical parameters on time and memory requirements (Yeung & Moseley 1995).

Differential diffusion with reaction and heat release

A new computer code is at present being developed for direct numerical simulations of reacting flow with the momentum, energy and species transport equations written in the low-Mach number approximation (McMurtry 1987). The low-Mach number approximation allows for variable density effects due to chemical heat release, as long as the Mach number is sufficiently low so that acoustic waves (which would require very small time steps for numerical stability) can be filtered out of the governing equations. The density equation is first advanced in time using a second-order Adams-

Bashforth scheme. The momentum equation is then advanced using a time-splitting scheme, with the pressure field obtained by solving a Poisson equation. Subsequently the time-advance cycle is completed by advancing the energy and species transport equations incorporating a suitable reaction scheme. Because we are interested in homogeneous turbulence, all spatial derivatives may be conveniently computed in a Fourier pseudo-spectral manner, with the aliasing errors arising in nonlinear terms controlled by a truncation of aliased high-wavenumber modes.

In our production calculations (to be performed) we will focus on the effects of heat release and consequent density fluctuations on the processes of momentum and scalar transport. Incompressible and isothermal initial conditions will be prescribed, with an initial flow field either taken from constant-density simulations or initialized according to a specified energy spectrum. Our attention will first be on the case of initially segregated species, corresponding to a diffusion flame if the chemistry is fast compared to the turbulence time scales. A typical segregated configuration can be ready constructed from a single variable (say θ) with an approximately bimodal distribution (see Fig. 1, characterized by broad regions in which θ is close to ± 1) as follows. If θ is interpreted as a mass fraction variable based on two species with concentrations ϕ_1 and ϕ_2, then two segregated species are given by

$$\phi_1 = \begin{cases} \theta & \text{if } \theta > 0 \\ 0 & \text{otherwise} \end{cases}$$

ϕ_2 similarly corresponding to the (absolute value of) negative part of θ.

Lagrangian studies of turbulence structure and scalar transport

Our objectives here are to use the backward tracking of fluid particle paths in time to investigate the dynamical origin of packets of high local concentration for scalar fields transported by turbulent flow. The major difficulty is in the need to store many sets of three-dimensional velocity and scalar fields at previous time steps in order to be able to retrieve information "from the past". This requires a huge amount of disk space, for which the 2 Gigabyte addition funded by this Grant will be of instrumental value.

A numerical issue that needs to be addressed is the accuracy of backward tracking. Usually, within the DNS codes, fluid particles are tracked in a forward-time manner: that is, given the current position $\underline{x}^+$ at time t_n, we we calculate (numerically) its position at a later time $t_{n+1} = t_n + \Delta t$. This is done by a second-order predictor-corrector method, through the formulas

$$\underline{x}^* = \underline{x}^+(t_n) + \Delta t \; \underline{u}^+(t_n) \tag{1}$$

(for the predictor position) and

$$\underline{x}^+(t_{n+1}) = \underline{x}^+(t_n) + \frac{1}{2}\Delta t[\underline{u}^+(t_n) + \underline{u}(\underline{x}^*, t_{n+1})] \ . \tag{2}$$

The velocities involved in this time advancement are the fluid particle velocity $\underline{u}^+$ at time t_n, and the value of the Eulerian velocity field at time level t_{n+1} taken at the predictor particle position. To track the particle backwards in time, however, we start with its velocity $\underline{u}^+$ at time t_{n+1}, and evaluate a time reversed "predictor" position by

$$\underline{x}' = \underline{x}^+(t_{n+1}) - \Delta t \ \underline{u}^+(t_{n+1}) \ . \tag{3}$$

This position $\underline{x}'$ is then used to evaluate a "corrector" velocity at time t_n. Because of the velocities involved in forward and backward tracking schemes are different, if we track a fluid particle forward and then backward again over a certain time interval, it would not (numerically) return exactly to its origin. This numerical error is expected to increase with the length of the tracking time period, but can be controlled by reducing the time step Δt. Our numerical tests suggest it is necessary to use velocity and scalar fields stored at intervals of approximately half a Kolmogorov time-scale (the time scale of the small eddies) apart. More comprehensive production calculations are expected in the near future.

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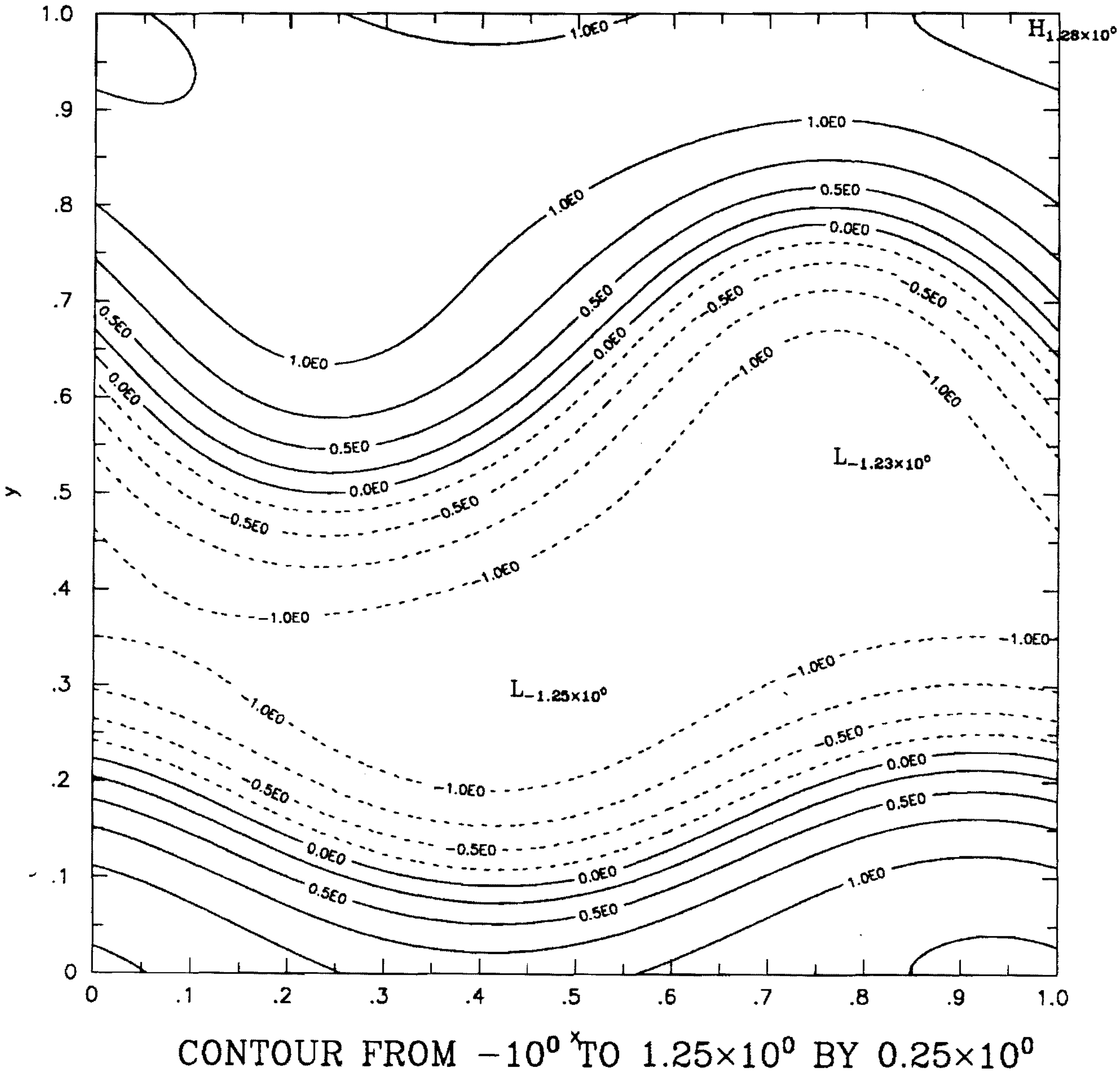

Figure 1. Two-dimensional contours (in an arbitrary cross-sectional plane) of a single variable having an approximately bimodal distribution. The initialization scheme is that of Eswaran & Pope (1988).