DOE F 241.1
(8-98) p. 1 of 2
(Formerly DOE F 1332.15)
(All other versions are obsolete)

OMB Control No
1910-1400

U. S. DEPARTMENT OF ENERGY
ANNOUNCEMENT OF U. S. DEPARTMENT OF ENERGY (DOE) SCIENTIFIC AND TECHNICAL INFORMATION (STI)

RECORD STATUS *(select one)*:
_X_ New ___Revised Data ___Revised STI Product

Part I: STI PRODUCT DESCRIPTION

A. STI PRODUCT TYPE *(select one)*:

___ 1. **Technical Report**
a.Type: ___Semiannual ___Annual _X_ Final ___Topical ___Other *(specify)* ______
b.Reporting Period *(mm/dd/yyyy)* 09 / 01 / 1998 thru 08 / 31 / 2001

___ 2. **Conference**
a.Product Type: ___Conference Proceedings _X_ Conference Paper or Other *(abstracts, excerpts, etc.)*
b.Conference Information *(title, location, dates)*
ASEE Annual Meeting and Exhibit, Albuquerque, New Mexico, June 24-27, 2001

___ 3. **Software Manual** *(The actual software package should be made available simultaneously. Follow instructions provided with ESTSC F 1 and ESTSC F 2.)*

___ 4. **Journal Article**
a.Type: ___Announcement citation only ___Preprint ___Postprint
b.Journal Name ______
c.Volume ______ d. Issue ______ e. Serial identifier *(e.g., ISSN or CODEN)* ______

___ 5. **S&TAccomplishment Report**

___ 6. **Book**

___ 7. **Patent Application**
a. Date Filed *(mm/dd/yyyy)* ___/___/______
b. Date Priority *(mm/dd/yyyy)* ___/___/______
c. Patent Assignee ______

___ 8. **Thesis/Dissertation**

B. STI PRODUCT TITLE "Alliance for Computational Science Collaboration, HBCU Partnership at AAMU"

C. AUTHOR(s) Dr. Z.T. Deng, Alabama A&M University
E-mail Address*(es)*: AAMZXD01@AAMU.EDU

D. STI PRODUCT IDENTIFIER
___ 1. Report Number*(s)* ______
___ 2. DOE Contract Number*(s)* DE-FG02-98ER25366
___ 3. R&D Project ID*(s)* ______
___ 4. Other Identifying Number*(s)* ______

E. ORIGINATING RESEARCH ORGANIZATION Alabama A&M University

F. DATE OF PUBLICATION *(mm/dd/yyyy)* 11 / 15 / 2001

G. LANGUAGE *(if non-English)* ______

(Grantees and Awardees: Skip to Description/Abstract section at the end of Part I)

H. SPONSORING ORGANIZATION Department of Energy

I. PUBLISHER NAME AND LOCATION *(if other than research organization)* ______

Availability *(refer requests to [if applicable])* ______

J. SUBJECT CATEGORIES *(list primary one first)* ______
Keywords High Performance Computing, Computational Fluid Dynamics

K. DESCRIPTION/ABSTRACT

The objective of this project was to conduct high performance computing research and teaching at AAMU, and to train African-American and other minority students and scientists in the computational science field for eventual employment with DOE. During the project period, eight tasks were accomplished. Student Research Assistant, Work Study, Summer Interns, Scholarship were proved to be one of the best way for us to attract top quality minority students. Under the support of DOE, through research, summer interns, collaborations, scholarships programs, AAMU has successfully provided research and educational opportunities to minority students in the field related to computational science.

Part II: STI PRODUCT MEDIA/FORMAT and LOCATION/TRANSMISSION

A. MEDIA/FORMAT INFORMATION

1. Medium of STI product is: X Paper ___Electronic document ___Computer medium ___Audiovisual material
2. Size of STI product ______
3. File format:
   a. If electronic document is posted at site, indicate: ___SGML ___HTML ___XML ___PDF Normal
   b. If electronic document is transmitted to OSTI, indicate: ___SGML ___HTML ___XML ___PDF Normal ___PDF Image
   ___ TIFFG4 ___WP–indicate Version *(5.0 or greater)* ______ platform/operating system ______
   ___ MS Word–indicate Version *(5.0 or greater)* ______ platform/operating system ______ ____ Postscript
4. If computer medium or audiovisual material:
   a.Quantity/type *(specify)* ______
   b.Machine compatibility *(specify)* ______ c. Sound: ___*(yes)* d. Color: ___*(yes)* e.Tables/Graphics ___*(yes)*
   f. Other information about product format a user needs to know: ______

B. LOCATION/TRANSMISSION INFORMATION

1. STI Product is available at site: Unique URL *(of specific STI Product)* ______
2. STI Product is being transmitted to OSTI:
   a. ___ Electronically via FTP
   b. X Via mail or shipment *(e.g., Federal Express) (Paper products, electronic documents on CD-ROM, diskettes, videocassettes, etc.)*
3. Information Product Filename *(of transmitted electronic format)* ______

C. ADDITIONAL INFORMATION *(concerning media/format or location/transmission; for OSTI internal use only)*: ______

(Grantees and Awardees: Skip to Contact section at the end of Part III)

Part III: STI PRODUCT REVIEW/RELEASE INFORMATION

A. ACCESS LIMITATION

___ 1. **Unlimited Announcement** *(available to U.S. and non-U.S. public)*
___ 2. **OpenNet** *(use OpenNet guidance for below)*:
   a.If additional source other than making it available through NTIS:
   (1) Accession Number ______
   (2) Document Location ______
   b.Field Office Acronym ______
   c.Declassification date *(mm/dd/yyyy)* ____ / ____ / ______
   d.Declassification Status:
   ___Declassified ___Sanitized ___Never classified
   e. OpenNet Document Categories ______
   f. OpenNet Addressee ______
___ 3. **U.S. Dissemination Only**
___ 4. **Copyrighted material;** Are there any restrictions based on copyright? ___ yes ___no. If yes, list the restrictions ______
___ 5. **Small Business Innovation Research** *(SBIR)* Release date *(mm/dd/yyyy)* ____ / ____ / ______
___ 6. **Small Business Technology Transfer** *(STTR)* Release date *(mm/dd/yyyy)* ____ / ____ / ______
___ 7. **Proprietary/Trade Secret**
___ 8. **Patent Pending**
___ 9. **Protected data** ___CRADA ___Other *(specify)* ______ Release date *(mm/dd/yyyy)* ____ / ____ /
___10. **Official Use Only** *(OUO)*
___11. **Program-Directed Special Handling** *(specify)* ______
___12. **Export Control/ITAR/EAR**
___13. **Unclassified Controlled Nuclear Information** *(UCNI)*
___14. **Classified** Classification Level/Category of:
   a.This form ______ b. The STI Product ______
___15. **Other information relevant to access** *(specify; for OSTI internal use only)* ______

B. OTHER *(information useful to include in published announcement record which is not suited for any other field on this form)*

C. CONTACT AND RELEASING OFFICIAL

1. Contact *(if appropriate, the organization or site contact to include in published citations who would receive any external questions about the content of the STI Product or the research information contained therein)*
   Name and/or Position Dr. Z.T. Deng, Department of ME, Alabama A&M University
   E-mail AAMZXD01@AAMU.EDU Phone 256-858-4142
   Organization Alabama A&M University
2. Releasing Official ___ I verify that all necessary reviews have been completed *(e.g. Patent, Copyright, ECI, UCNI, etc.)*
   Released by *(name)* ______ Date *(mm/dd/yyyy)* ____ / ____ / ______
   E-mail ______ Phone ______

(8-93)

U.S. DEPARTMENT OF ENERGY

NOTICE OF FINANCIAL ASSISTANCE AWARD

(See Instructions on Reverse)

der the authority of Public Law 95-91, U.S. Department of Energy Organization Act and

bject to legislation, regulations and policies applicable to *(cite legislative program title)*: Advanced Scientific Computing Research

ROJECT TITLE ance for Computational Science Collaboration HBCU tnership at Alabama A&M University	2. INSTRUMENT TYPE ☑ GRANT ☐ COOPERATIVE AGREEMENT
ECIPIENT *(Name, address, zip code, area code and telephone no.)* bama A&M University). Box 411, 4900 Meridian Street rmal, AL 35762 (256) 858-8184	4. INSTRUMENT NO. DE-FG02-98ER25366 5. AMENDMENT NO. A002 6. BUDGET PERIOD FROM: 09/01/2000 THRU: 08/31/2001 7. PROJECT PERIOD FROM: 09/01/1998 THRU: 08/31/2001
ECIPIENT PROJECT DIRECTOR *(Name and telephone No.)* engtao Deng [256/858-8183]	10. TYPE OF AWARD ☐ New ☐ Continuation ☐ Renewal ☑ Revision ☐ Supplement
ECIPIENT BUSINESS OFFICER *(Name and telephone No.)* rothy W. Huston [(256) 858-8184]	12. ADMINISTERED FOR DOE BY *(Name, address, zip code, telephone No.)* Tonja Stokes (630) 252-2136 U.S. Department of Energy/ACQ Chicago Operations Office 9800 South Cass Avenue Argonne, IL 60439
DOE PROJECT OFFICER *(Name, address, zip code, telephone No.)* aniel A. Hitchcock U. S. Department of Energy, SC-64 C-31 19901 Germantown Road 01) 903-5800 Germantown, MD 20874-1290	

RECIPIENT TYPE

☐ STATE GOV'T ☐ INDIAN TRIBAL GOV'T ☐ HOSPITAL ☐ FOR PROFIT ORGANIZATION ☐ INDIVIDUAL

☐ LOCAL GOV'T ☑ INSTITUTION OF HIGHER EDUCATION ☐ OTHER NONPROFIT ORGANIZATION ☐ C ☐ P ☐ SP ☐ OTHER *(Specify)*

. ACCOUNTING AND APPROPRIATIONS DATA

a. Appropriation Symbol	b. B & R Number	c. FT/AFP/OC	d. CFA Number
89X0222.91	KJ010101	WA/CH/410	N/A

15. EMPLOYER I.D. NUMBER 63-6001097

. BUDGET AND FUNDING INFORMATION

CURRENT BUDGET PERIOD INFORMATION		b. CUMULATIVE DOE OBLIGATIONS	
1) DOE Funds Obligated This Action	$90,000.00	(1) This Budget Period *[Total of lines a.(1) and a.(3)]*	$90,000.00
2) DOE Funds Authorized for Carry Over	$0.00		
3) DOE Funds Previously Obligated in this Budget Period	$0.00	(2) Prior Budget Periods	$120,000.00
(4) DOE Share of Total Approved Budget	$90,000.00		
(5) Recipient Share of Total Approved Budget	$0.00	(3) Project Period to Date *[Total of lines b.(1) and b.(2)]*	$210,000.00
(6) Total Approved Budget	$90,000.00		

7. TOTAL ESTIMATED COST OF PROJECT $ N/A

(This is the current estimated cost of the project. It is not a promise to award nor an authorization to expend funds in this amount.)

18. AWARD/AGREEMENT TERMS AND CONDITION

This award/agreement consists of this form plus the following:

a. Special terms and conditions.

b. Applicable program regulations *(specify)* 10 CFR Part 605 (Date) 01/01/2000

c. DOE Financial Assistance Rules, 10 CFR Part 600, as amended.

d. Application/proposal dated 5/27/98; 7/1/99; 5/15/00 ☑ as submitted ☐ with changes as negotiate

19. REMARKS

This amendment provides supplemental funding for the budget period specified in Block No. 6. The Budget Page, attached hereto, is substituted for the Budget Page No. 3, previously incorporated into this grant in Amendment No. A000. The Project Director has been changed to Zhengtao Deng, as indicated in Block No. 8. In addition, the Special Terms and Conditions for Financial Assistance Awards, coded SPRG-0700/APM, attached hereto, are substituted for the Special Terms and Conditions for Financial Assistance Awards, coded SPRG-0498/APM, previously incorporated into this grant. All oth terms and conditions remain unchanged.

20. EVIDENCE OF RECIPIENT ACCEPTANCE	21. AWARDED BY
(Signature of Authorized Recipient Official) *(Date)*	Christopher D. Swierczek 9/22 *(Signature)* (D
(Name)	Christopher D. Swierczek ~~Acquisition and Assistance Group~~ *(Name)*
(Title)	Contracting Officer *(Title)*

Form Approved
OMB No. 1902-0121

PATENT CERTIFICATION

Alabama A & M University
Awardee

☐ Interim Certification

DE-FG02-98ER25366
DOE Prime and/or Subcontract Nos.

☒ Final Certification

Awardee hereby certifies unless indicated to the contrary, that:

1. All procedures for identifying and disclosing subject inventions as required by the patent clause of the contract have been followed throughout the reporting period.

2. There were no subcontracts or purchase orders involving research, development, and demonstration except as follows: (a separate certification must be provided to DOE for each subcontract or purchase order awarded.)

   None

3. No inventions or discoveries were made or conceived in the course of or under this contract other than the following (Certification includes ☐, does not include ☐ all subcontracts):

TITLE	INVENTOR	DATE REPORTED	DOE "S" NO.*
None			

4. The completion date of this contract is as follows: August 31, 2001

5. The following period is covered by this certification:

September 1, 1998 to August 31, 2001
Month Day Year — Month Day Year

Alabama A & M University	
Contractor	Signature
P. O. Box 1163	Principal Investigator
	Title
Normal, AL 35762	November 15, 2001
Address	Date of Certification

* Also include Subcontract No. if available.

NOTE: A positive certification for this Item 3 does not negate the requirement for furnishing to DOE a fully executed Patent Certification from each subawardee identified in Item 2.

FINANCIAL ASSISTANCE
PROPERTY CERTIFICATION

AWARDEE Alabama A & M University AWARD NO. DE-FG02-98ER25366

The DOE Assistance Rules, 10 CFR 600, define property acquired under the terms of the grant as either exempt (purchased with DOE operating dollars) or non-exempt (acquired with DOE capital equipment dollars, Government-furnished or acquired from the Government excess property lists). Non-exempt property is normally identified in the award document as Government-owned and requires a Semi-Annual Summary Report of DOE-Owned Plant and Capital Equipment pursuant to DOE regulations.

In order to facilitate grant closeout, please review your property records and complete the applicable Item I, for exempt property, or Item II, for non-exempt property, of this certificate and return it to the Contracting Officer as soon as possible.

I. There was no reportable residual exempt property of any description at the completion of this award.

SIGNATURE Z. T. Deng

TITLE Assistant Professor / Principal Investigator DATE 11/15/01

II. A final inventory of residual non-exempt property is enclosed for the category (or categories) checked below:

( ) A. NONEXPENDABLE PERSONAL PROPERTY, Federally-Owned (acquired with Capital Equipment funds, Government-furnished equipment, or through excess)

( ) B. EXPENDABLE PERSONAL PROPERTY (SUPPLIES), if fair market value exceeds $1,000.

Except for the category (categories) checked above, no other reportable residual property of any description remained on this grant at its completion.

SIGNATURE __________

TITLE __________ DATE __________

AA-88
03/97

Alliance for Computational Science Collaboration
HBCU Partnership at Alabama A&M University

(DE-FG02-98ER25366)

Final Performance Technical Report

To

Department of Energy
Mathematical, Information, and
Computational Sciences Division

Submitted by

Dr. Z.T. Deng

Principal Investigator
Director for High Performance Computing Laboratory
Alabama A&M University
Huntsville, Alabama 35762
November 2001

Table of Content

ABSTRACT

This is the final report for the Department of Energy (DOE) project DE-FG02-98ER25366, entitled, "Alliance for Computational Science Collaboration, HBCU Partnership at Alabama A&M University". High performance computing project was initiated in 1999 at Alabama A&M University (AAMU) under the support of DOE Alliance for Computational Science Collaboration (ACSC) project. The project ended in August 31, 2001. In the past three years, many accomplishments have been made in the laboratory establishment, student research, summer interns and scholarship program.

The objective of this project was to conduct high performance computing research and teaching at AAMU, and to train African-American and other minority students and scientists in the computational science field for eventual employment with DOE. During the project period, eight tasks were accomplished.

(1). Supported graduate and undergraduate students research in computational science related area.
(2). Supported three undergraduate summer interns (10 weeks) at Oak Ridge National Lab computational science division.
(3). Provided 21 ACSC High Performance Computing Scholarships to AAMU undergraduate students in science and engineering majors within three years.
(4). Established high performance computing laboratory at AAMU.
(5). Conducted research on computational fluid dynamics (CFD), structural analysis, and data visualization. CFD codes such as WIND, FDNS, RPLUS were implemented on the HPC lab and benchmarked. Propulsion simulation and modeling were initiated for related research project.
(6). Supported AAMU faculties to obtain technical training related to high performance computing; Introduced high performance computing concepts to undergraduate student class.
(7). Supported campus wide parallel computing efforts.
(8). Supported collaborated research on computational science activities, publish research papers.

Student Research Assistant, Work Study, Summer Interns, Scholarship were proved to be one of the best way for us to attract top quality minority students. Under the support of DOE, through research, summer interns, collaborations, scholarships programs, AAMU has successfully provided research and educational opportunities to minority students in the field related to computational science.

1. Introduction

The Alliance for Computational Science Collaboration (ACSC) has operated since October 1997 with the overall goal of training African-American and other minority scientists in the computational science field for eventual employment with DOE. Historically Black Colleges and Universities (HBCUs) are the primary source of African-American scientists in the US, and HBCU participation is central to the Alliance.

Strategies designed to help produce future DOE minority scientists are

(1). To involve HBCU students and faculty members in computational science projects at national laboratories and research institutions;
(2). To assist HBCU faculty members in integrating interdisciplinary computational science courses into their undergraduate curricula, involving freshmen to senior students; and
(3). To provide support and expertise to HBCU researchers using state-of-the-art computational science technologies and methodologies.

Alabama A&M University (AAMU) is one of the HBCU members. AAMU is a land-grant historically black university. The University is located at the northeast outreach of Huntsville, Alabama, an important world center of expertise for advanced missile, space, electronic, research and development. The University provides scholarly environments for teaching and research. As a developing minority institution, the university seeks to address the special needs of capable students disadvantaged by systems and circumstances, which have thwarted their efforts and chances for normal educational opportunities. A continued responsibility for this element of our society is strongly embedded in the mission of the University.

The high performance computing ACSC program started first time at AAMU in 1999. The Department of Energy (DOE) funding support for AAMU ended in August 31, 2001. The key elements of this program at AAMU is to encourage faculty and students to involve in computational science activities through teaching high performance computing, student scholarship program, student internship program, student research work study program, collaborative research projects involving Oak Ridge National Lab (ORNL) scientists, and establishment of a high performance computing laboratory. The program promotes research and education relative to computational science and high performance computing. It broadens the research and educational capability at AAMU in a manner consistent with the overall growth in sponsored research and with the teaching mission of the University.

Many accomplishments have been made in the past three years. Continuation, enhancement and improvement of the established activities are essential for AAMU to provide high quality minority graduates for DOE.

2. Achievement

The objective of this project was to conduct high performance computing research and teaching at AAMU, and to train African-American and other minority students and scientists in the computational science field for eventual employment with DOE.

Dr. Scott von Laven, the previous project director, initially directed the establishment of the high performance-computing lab. Dr. Scott von Laven left Alabama A&M University in the spring of 2000 and Dr. Z.T. Deng resume the responsibility of the project director for the remaining one and half years. Dr. Andrew Scott, from Alabama Research and Education Network (AREN) and Computer Sciences Corporation, and Dr. Bruce Vu, Research Scientist at NASA Marshall Space Flight Center in Huntsville, Alabama have contributed their help to the establishment of the Laboratory.

During the overall three-year project period, eight tasks in research and education were accomplished.

2.1 Establishment of High Performance Parallel Computing Lab

Under the support of DOE computational science division, a High Performance Computing (HPC) Laboratory using 9 Pentium II PCs that run Linux (with the help of the School of Engineering and Technology) and MPI or PVM, or alternatively Windows NT, has been established. Two new Sun Ultra 10 workstations were purchased and were configured to run high performance computing applications. The Laboratory is located in Carver Complex North, room 220 where the School of Engineering and Technology is hosted. This Laboratory is available for use by project participants and by researchers, faculty and students. Students were from Mechanical Engineering, Electrical Engineering, Civil Engineering, Biology, and Computer Science Departments, who involved in high performance computing project or enrolled in appropriate classes during the Fall 1999, Spring 2000, Summer 2000, Fall 2000, Spring 2001, Summer 2001 and Fall 2001 semesters. All computers were equipped with Unix or LINUX/WINDOWS operating system with FORTRAN, C compilers and related scientific image processing and data visualization software.

Dr. Z.T. Deng, assistant professor at Mechanical Engineering Department and the project director at AAMU introduced high Performance Computing concept to one of the Mechanical Engineering class, ME 300, Mathematical Methods in Mechanical Engineering. The HPC laboratory and course elements help preparing students who are selected to participate in the summer internship program in computational science research at the Computational Science Division in Oak Ridge National Laboratory.

A similar effort to configure a cluster of PCs to perform low-cost parallel computing was conducted in the AAMU Civil Engineering Department for an ongoing NASA Research Grant. Dr. Z. T. Deng was a co-investigator on that research project. The goal of that research is to provide an unconventional parallel flow solver for hypersonic reusable lunch vehicle aerodynamics prediction at high altitude. Undergraduate student from Mechanical Engineering Department was involved in this research activity. Sharing of resources between these two PC labs enable us to accommodate a wider range of courses and to achieve higher processing performance.

Several scientific and engineering computing applications have been established in the HPC lab. For example, legacy computational fluid dynamics codes, GENIE++ (Grid Generation code for complex three-dimensional geometry), FDNS (Code contributed by NASA Marshall Space Flight Center Fluid Dynamics Group, Finite-Difference Navier-Stokes code), WIND (Developed by AEDC and Boeing company, a generic aerodynamics computation code), RPLUS (developed by NASA Glenn Research Center, used for computation of high speed chemically reacting flows) were installed on the Lab computers. The benchmark testing is in progress. Structural analysis code, ANSYS and HyperMesh were also installed and configured to perform high performance finite element analysis. Scientific visualization application TEPLOT was also installed on a LINUX based system. Except for ANSYS and TECPLOT, which are commercial codes that we purchased for this Lab, all the other codes were obtained through agreement with code distributors and AAMU is adopting those codes to conduct related research on campus.

The HPC Laboratory is currently connected to the campus network via 10Mbs ethernet and, in turn, to the Internet via a T1 digital circuit. Local Ethernet connections were established to conduct parallel computing. Two projects funded by the National Science Foundation plus another funded by the state of Alabama will supply critical components of a DS3 Internet feed to our campus during 2000 and 2001. AAMU will be able to complete the DS3 circuit with a relatively inexpensive fiber installation (underway as of this writing) and will qualify as an Internet 2 institution by virtue of its participation in the NSF projects. This will permit campus projects, such as the HPC laboratory, to be connected to their collaborators at other Internet 2 institutions at 45 Mbs provided the departments hosting those projects upgrade their local area networks (LANs) to fast ethernet or better.

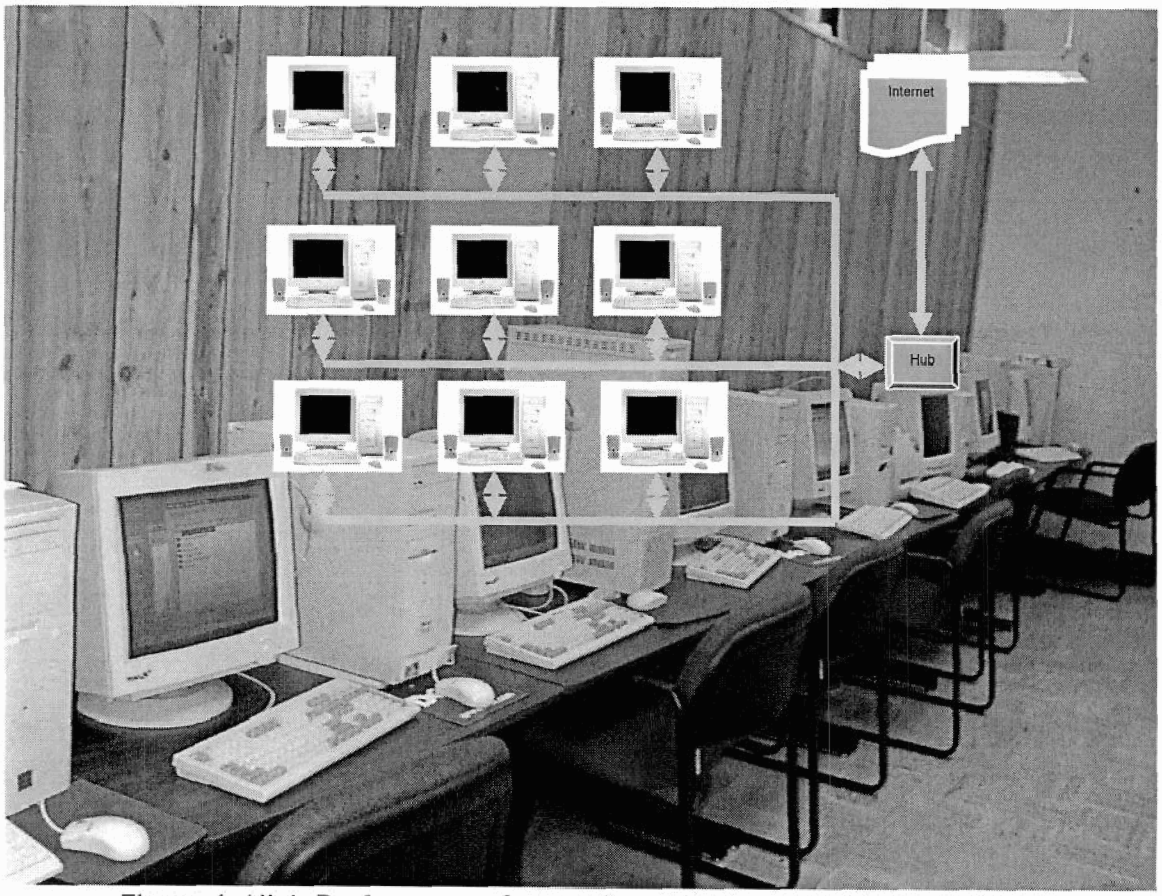


Figure 1. High Performance Computing Laboratory at AAMU, CCN 220.

Table 1 shows partially the WIND 4.0 simulation results on the LINUX Based PC in the High Performance Computing Lab for hypersonic flows over a 2D wedge. Figure 2 shows one of the hypersonic simulation results conducted by Dr. Z.T. Deng using NPARC (Previous version of WIND) code on one of the Sun Workstation.

Table 1. Sample Run of WIND 4.0 Code for Hypersonic Flow Over A Wedge

SYSTEM	WIND 4.0 RUN TIME INFORMATION Application time =User time (Seconds)	SYSTEM DISK INFORMATION	SYSTEM MEMORY (Megabytes)	CPU SPECS (MHz)
HPC1-LINUX	319.76user 0.62system 5:32.86elapsed 96%CPU, Tue Jun 12 10:17:01 CDT 2001	3.196 GB	30.652	334.095623
HPC2-LINUX	220.50user 0.18system 3:49.79elapsed 96% CPU, Mon Jun 11 12:33:45 CDT 2001	11.928 GB	63.032	498.855735
HPC3-LINUX	357.25user 0.13system 6:04.10elapsed 98% CPU, Mon Jun 11 11:36:51 CDT 2001	7.689 GB	63.092	299.752093
HPC4-LINUX	216.47user 0.10system 3:43.03elapsed 97% CPU, Tue Jun 12 10:09:55 CDT 2001	5.203 GB	63.032	498.857937
HPC8-LINUX	148.08user 0.08system 2:33.86elapsed 96% CPU, Tue Jun 12 10:22:33 CDT 2001	19.449 GB	257.492	730.968182
HPC9-LINUX	148.27user 0.08system 2:31.29elapsed 98% CPU, Tue Jun 12 09:38:31 CDT 2001	19.433 GB	257.492	730.974900

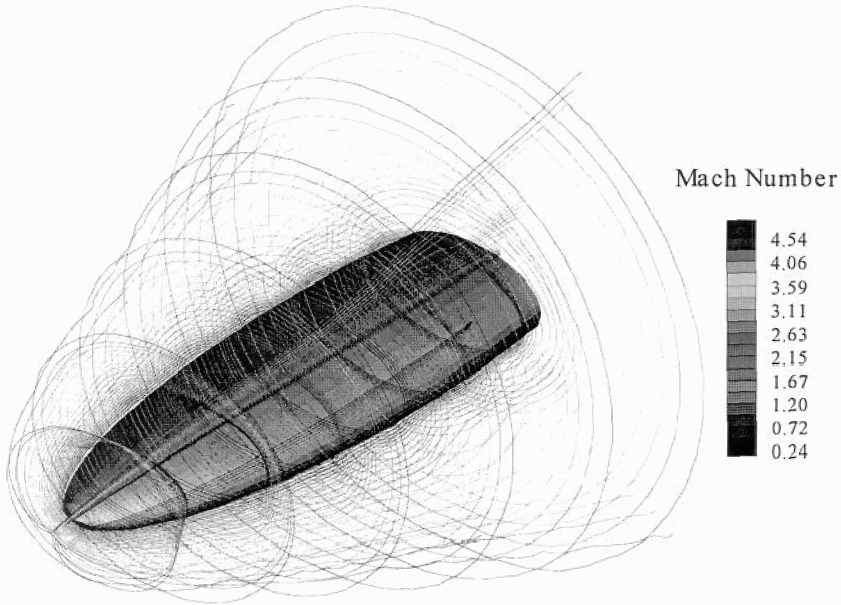


Figure 2. Hypersonic Flow Simulation for flow over an ellipsoid body.

2.2 Student Recruitment

As mentioned in the previous annual reports, many students have benefited from our efforts to promote computational science, first under NSF sponsorship and now under DOE sponsorship. One of our past students, a top graduate at AAMU, was named to USA Today's 1999 academic Second Team. Only 20 students nationwide are selected for each team. One student was one of the first graduates with Mechanical Engineering degree at AAMU.

Under DOE sponsorship, we hired two graduate students from computer sciences department at AAMU, and six undergraduate students (science and engineering majors), to assist with the configuration of PC laboratories and applications.

2.3 DOE Computational Science Scholarship Program

AAMU created a DOE Computational Science Scholarship program during FY 2000. Official application announcement was made through Admission office in November 1999. Appendix 1 shows the official announcement of the scholarship program. This announcement was then modified each year to recruit science, engineering and Mathematics major students working in the field of computational science. A scholarship award selection criterion was developed. To apply the scholarship, student needs to fill out the application form, as shown in Appendix 2, write an essay about their goal towards high performance computing, and a faculty recommendation letter is required. Upon receipt of the application package, careful selection was conducted based on the selection criteria. Once student was selected for award, student was informed about the selection, and student need to sign acceptance agreement, as shown in Appendix 3. In the agreement, student needs to agree to maintain GPA of 2.8 (undergraduates) and 3.0 for graduates. Student also need to successfully complete a minimum of 12 credit hours per semester, maintain a major in science, mathematics, engineering, or computer science. Student will have to pay for any course that fail or receive an incomplete grade. Student is responsible for any fees in excess of the minimum amounts provided by DOE, and student is required to accept student employment with the Department of energy each year if offered. In the past three years, totally 21 undergraduate scholarships were awarded to physics, computer sciences, biology, civil engineering, mechanical engineering and electrical engineering students. The scholarship recipient's names are listed in Table 2.

Table 2 DOE Computational Science Scholarship Recipients

Recipient	Major of Study
1999 ACADEMIC YEAR	
#1	Civil Engineering
#2	Computer Science
#3	Mechanical Engineering
2000 ACADEMIC YEAR	
#4	Biology/Chemistry
#5	Mechanical Engineering
#6	Mechanical Engineering
#7	Mechanical Engineering
#8	Mechanical Engineering
#9	Electrical Engineering
#10	Mechanical Engineering
#11	Mechanical Engineering
#12	Computer Science
2001 ACADEMIC YEAR	
#13	Civil Engineering
#14	Mechanical Engineering
#15	Mechanical Engineering
#16	Mechanical Engineering
#17	Mechanical Engineering
#18	Mechanical Engineering
#19	Civil Engineering
#20	Mechanical Engineering
#21	Mechanical Engineering

All scholarship recipients are trained in the multi-disciplinary area related to computational science. Table 3 listed the training area for scholarship recipients in academic year of 2000.

Table 3. DoE Computational Science Scholarship Student Assignment Sheet Academic Year 2000

Student	Major	Project
#1	ME	ANSYS on ME Lab
#2	ME	ANSYS on ME Lab
#3	ME	LabView on ME Lab
#4	CS	PVM&MPI HPC Lab
#5	ME	Missle Intelligence
#6	EE	PVM&MPI HPC Lab
#7	Biology & Chemistry	Missle Intelligence
#8	ME	LabView on ME Lab
#9	ME	Missle Intelligence

2.4 Faculty Training and Circulation of Faculty Profiles at ORNL

Several computer science and engineering faculties were supported to participate training and conference related to scientific computing. Collaboration with Oak Ridge National Lab Computational Science division was established and collaboration efforts on student summer interns are ongoing. Our primary point of contact at ORNL and UTK was Dr. Ruth Ann Manning previously. Ms. Debbie McCoy was the current RAMS contact. Dr. Manning has helped in our efforts to establish individual collaborative relationships between ORNL and AAMU scientists. Dr. Manning has forwarded AAMU faculty capabilities summaries to her contacts at ORNL. Several faculty members at AAMU were supported to participate American Institute of Aeronautics and Astronautics (AIAA), American Society of Mechanical Engineering (ASME) scientific computing conferences, and exchange information in the field related to computational fluid dynamics, structural finite element analysis, materials science, propulsion, combustion and control. Those Faculty members supported include Dr. Ruben Rojas-Oviedo (ME), Dr. Hung (Former Computer Science Faculty, also worked on the project), Dr. von Laven (Former AAMU Research Administrator), Dr. Qian (ME), Dr. Mobasher (ME), Dr. Jalloh (ME), and two faculty researchers from Plant and Soil Science research center at AAMU (Image processing). With the funding support of this project, Dr. Jalloh at Mechanical Engineering Department was able to attend ANSYS training in 2000, which enhance significantly the finite-element parallel computation capability at AAMU.

2.5 Student Summer Internship at ORNL

ORNL RAM summer internship program announcement were posted around the AAMU campus. With the collaborated work of RAMS directors at ORNL, previously Dr. Ruth Ann Manning, Previous RAM coordinator at ORNL, and currently Ms. Debbie McCoy (Current RAM director at ORNL) and Dr. Z.T. Deng, three undergraduate students were selected to participate ORNL RAM Summer Internship program. Students were paid in advance a total amount of $5000 for ten weeks stay at ORNL in the summer. Students participated in ORNL scientist' research projects and learn from them directly. In the end of the project, they were asked to make presentations and report their research progress. The student names are listed in Table 4. These students expressed their strong intension to work in the field of computational science after their graduation. Reports produced by students are listed in Appendix 4.

Table 4. Stiudent Summer Interns at Computational Science Division in ORNL

Student	Major of Study
#1	Civil Engineering
#2	Computer Science
#3	Mechanical Engineering

2.6 Graduate and Undergraduate Student Research Work Study

Two graduate students and six undergraduate students were hired to assist high performance computing in the high performance-computing Lab. All students participated in the on-going research with Dr. Deng and other faculty advisors. For example, three summer students were working with Dr. Deng on development of a new algorithm to numerically investigate hypersonic low-density flows around an ellipsoid body using WIND 4.0 code. Students also assist in the establishment of laboratory setting. Table 5 lists the names of the undergraduate research and work study students. They worked on installation of LINUX on WINDOWS-NT based PC platform. Students were supported to attend professional meetings related to scientific computing.

Table 5. Student Research Work Study

Student (Undergraduate)	Major of Study
#1	Mechanical Engineering
#2	Mechanical Engineering
#3	Mechanical Engineering
#4	Physics
#5	Mechanical Engineering
#6	Mechanical Engineering

2.7 Publications

Dr. Z.T. Deng has published a paper "high performance computing initiative at AAMU" to ASEE annual meeting in June 2001. Dr. C.C. Hung, former AAMU Computer Science Faculty of AAMU and Dr. Kwai Wong of UTK have produced parallel multispectral classification algorithms of interest to the remote sensing community. (Chih-Cheng Hung, S.A. von Laven, Kwai L. Wong, Kevin Chu, I. Chen, and Author J. Bond, "Establishment of the High-Performance Computing Laboratory at AAMU,"*ADMI Symposium on Computing at Minority Institutions*, Duluth, Minnesota, June 3-6, 1999.) Several presentations were made to encourage collaborations between AAMU and industry and government agencies. The paper, abstract and presentations are listed in Appendix 5. The selected presentation was made to Boeing Executives in May 2000. A web-page describing high performance computing activities at AAMU was created. The HTTP address is http://www.aamu.edu/MechanicalEngineering.

2.8 Supported Campus-Wide Research Activities on High Performance Computing

A very informative Research Collaboration Meeting with Mr. Michael Taylor from Computational Physics and Engineering Division at Oak Ridge National Laboratory was conducted in April 2000. The purpose of this collaboration meeting is to link the possible research collaborations at ORNL with AAMU. Mr. Taylor presented the research capabilities and interests of the Computational Physics and Engineering Division at ORNL especially in the areas of heat transfer and fluid flow, structural and engineering analysis, simulation and modeling, supercomputing, environmental science and materials science, and other scientific applications. He met with many AAMU faculties in the conference room of the Center for Irradiation of Materials and exchanged information with them.

Dr. Z.T. Deng submitted a research proposal in April, 2000, to NASA Marshal Space Flight Center, entitled "Numerical prediction of Drag Reduction for AJAX type Vehicle".

The research was funded in May 2001. This work adopted the parallel computing concepts and lab configuration, is partially supported by high performance computing lab at AAMU.

2.9 Conclusions

The ACSC program increases the quality and quantity of the Science, Engineering and Mathematics graduates in AAMU, especially increases minority student's interests in pursuing a career towards computational science fields. This program strongly supports faculty research in high performance computing. It also established a model laboratory for high performance computing using PC clusters.

Student Research Assistant, Work Study, Summer Interns, Scholarship were proved to be one of the best way for us to attract top quality minority students. Under the support of DOE, through research, summer interns, collaborations, scholarships programs, AAMU has successfully provided research and educational opportunities to minority students in the field related to computational science.

3. Challenges and Suggestions

The computational science research and education activities at AAMU, initiated by the DOE ACSC project, need to be continued, improved and enhanced in the following focused areas.

3.1 Focus Area one: Improvement of HPC Laboratory

The productivity of the HPC lab need to be maintained by upgrading the necessary hardware and software. Parallel applications need to be enhanced in the area of computational fluid dynamics, finite elements analysis, image processing, and scientific data visualization. Scientific computing and simulation codes such as WIND, FDNS, RPLUS need to be implemented and benchmarked using parallel computing and applied to related research projects. AAMU is ready to conduct a High Performance Computing Seminar and course unit on high performance computing application now to enhance education activities.

The HPC Laboratory is currently available for special workshops. Planned topics are parallel programming, computational science applications, and application tools.

3.2 Focus Area Two: Continue Efforts to Build Overall Ability of AAMU to Produce Best Minority Scientists through Work-Study, Summer Interns, and Scholarship Programs

Now that we have established the basic infrastructure for supporting student and faculty collaboration with ORNL, increasing our student and faculty participation is the immediate need. Student Research Assistant, Work Study, Summer Interns were proved to be one of the best way for us to attract top quality minority students. Students can be selected primarily from science, mathematics and engineering major in Mechanical Engineering, electrical engineering, civil engineering, computer science, mathematics and physics department. Scholarships constitute a new, more aggressive, component of our student. We anticipate that the large investment that these scholarship and interns represents will have a correspondingly high payoff in terms of minority scientists and engineers employed at DOE laboratories.

3.3 Focus Area Three: Continue Pursuit of Opportunities for Research and Education Collaborations with DOE and NASA Labs

The primary strategy for improving AAMU's ability to produce minority scientists and engineers in specialty areas of interest to DOE is to continue to seek funding in those areas from all available sources. AAMU will need to continue to establish contacts at ORNL, and NASA Labs. The research specialty areas at AAMU need to be enhanced in computational fluid dynamics, finite element analysis and image processing.

4. Acknowledgement

This project was supported by the Department of Energy Mathematical, Information, and Computational Sciences Division. Dr. Daniel A. Hitchcock is the program manager.

APPENDIX 1:

DOE COMPUTATIONAL SCIENCE SCHOLARSHIP PROGRAM ANNOUNCEMENTS

1. Announcement Flyer
2. Admission Office Announcement in Academic Year 1999
3. Updated Announcement in Academic Year 2000

ATTENTION: SCIENCE AND ENGINEERING MAJOR STUDENTS

The Department of Energy Computational Science Scholarships are immediately available for Science and Engineering major students at Alabama A&M University.

For Scholarship Application, Please see:

Dr. Z.T. Deng, Director, High Performance Computing Lab at AAMU, CCN 125A
Dr. Ruben Rojas-Oviedo, Chairman, Mechanical Engineering Department, CCN 221
Dr. T. Montgomery, Chairman, Electrical Engineering Department, CCN 222

Or please contact University Admission Office.

Alabama A&M University

Department of Energy Computational Science Scholarship

The Department of Energy (DOE) Computational Science Scholarship Program is designed to:

(1) **Attract a larger number of students with high academic potential to science and engineering.**
(2) **Provide a pool of graduates with the skills to work at Department of Energy laboratories, particularly Oak Ridge National Laboratory in Tennessee.**
(3) **Involve students in research collaborations between AAMU and DOE while they are participating in the scholarship program.**

All science, mathematics, and engineering students at AAMU are potentially eligible for the program.

Scholarships provide $3,000 toward college expenses, during each year of the program. <u>Each year that a scholarship is received obligates the student to a year of full-time employment at a DOE laboratory</u> (at the discretion of DOE).

Scholarship grants are payable in $1,500-per-semesters increments as long as the student maintains eligibility and contingent on continues DOE funding of the program. Eligibility for a scholarship from semester to semester is conditional upon maintenance of a minimum scholastic average of 3.25. When a student falls below the minimum grade point average, he/she will be informed that he/she is no longer eligible. Funds provided in the scholarship grant may be used for tuition, course fees, or room and board. Funds are not available for books or other items, or for expense incurred off campus.

All applicants for this program must be United States citizens or permanent residents.

Criteria for scholarships

(1) **Student must complete the Department of Energy (DOE) Computational Science Scholarship application.**
(2) **Student must have maintained a 3.25 or better grade point average and scored at least 27 on the ACT or 1220 on the SAT.**
(3) **Student must have a recommendation from a high-school counselor or faculty member.**

Applications must be submitted six weeks prior to the start of a semester to be eligible for consideration for that semester. However, early submission is recommended because: (1) Relatively few scholarships are available, and (2) scholarships are awarded on the basis of first-received first-awarded. The date that the admissions office receives all required items will be the official receipt date.

Office of Admissions
Alabama A&M University
Post Office Box 908
Normal, Alabama 35762

Telephone (256) 851-5245 or 1-800-553-0816
Fax No. (256) 851-5249
Web *http://www.aamu.edu*

<u>Scholarship Announcement:</u>

Alabama A&M University
Department of Energy
Computational Science Scholarship

The Department of Energy (DOE) Computational Science Scholarship Program is designed to:

(1) **Attract a larger number of students with high academic potential to science and engineering.**
(2) **Provide a pool of graduates with the skills to work at Department of Energy laboratories, particularly Oak Ridge National Laboratory in Tennessee.**
(3) **Involve students in research collaborations between AAMU and DOE while they are participating in the scholarship program.**

All science, mathematics, and engineering students at AAMU are potentially eligible for the program.

Scholarships provide $1500 toward college expenses, during each year of the program. <u>Each year that a scholarship is received obligates the student to a year of full-time employment at a DOE laboratory</u> (at the discretion of DOE).

Scholarship grants are payable in $1,500-per-semesters as long as the student maintains eligibility and contingent on continues DOE funding of the program. Eligibility for a scholarship from semester to semester is conditional upon maintenance of a minimum scholastic average of 3.25. When a student falls below the minimum grade point average, he/she will be informed that he/she is no longer eligible. Funds provided in the scholarship grant may be used for tuition, course fees, or room and board. Funds are not available for books or other items, or for expense incurred off campus.

All applicants for this program must be United States citizens or permanent residents.

Criteria for scholarships

(1) **Student must complete the Department of Energy (DOE) Computational Science Scholarship application.**
(2) **Student must have maintained a 3.25 or better grade point average and scored at least 27 on the ACT or 1220 on the SAT.**
(3) **Student must have a recommendation from a high-school counselor or faculty member.**

Applications must be submitted as soon as possible because: (1) Relatively few scholarships are available, and (2) scholarships are awarded on the basis of first-received first-awarded.

For Application, Contact to:

Dr. Z.T. Deng or Dr. Ruben Rojas-Oviedo
Department of Mechanical Engineering
Alabama A&M University
Post Office Box 1163
Normal, Alabama 35762

APPENDIX 2:

DOE COMPUTATIONAL SCIENCE SCHOLARSHIP PROGRAM APPLICATION FORM

ALABAMA AGRICULTURAL AND MECHANICAL UNIVERSITY
NORMAL, ALABAMA 35762

APPLICATION FOR DEPARTMENT OF ENERGY (DoE) COMPUTATIONAL SCIENCE SCHOLARSHIP

Name ____

Telephone No. ____________________ Social Security No. ____________________

Citizenship/Residency Status ______________ Gender _________ Race ______________

Home Address ____
Street and Number or Route and Box Number

____
City, State and Zip Code

If you have a tentative choice of occupation, please state it: ____________________

What subject have you enjoyed and why? ______________________________

____

What is your major or anticipated major? ______________________________

What other subject will you emphasize? ______________________________

How many students are/were in your high school graduating class? ______________

What is your Rank in that class? ______________________________

What is your grade point average? ______________________________

(You may need to consult your counselor or principal to answer the foregoing questions accurately).

Have you taken the Scholastic Aptitude Test (SAT) administered by the Educational Testing Service or the American College Test (ACT)? If so, which one? _________ When? _________

Please name at least two of your instructors of whom we may make inquiry concerning your eligibility for this scholarship: ____

In what extra-curricular and community affairs have you been especially active? ____________

____

____

Please state the name and occupations of your parents and guardian:

____

____

What amount of your own or family resources will be available to supplement any Scholarship funds granted? ____

Are you a current AAMU Student? ______________________________

If yes, what is your major? ______________________________

What is your current grade point average? ______________________________

When do you expect to enroll at the University? (Month/year) ______________

Submit a 250 word, handwritten essay citing reasons for applying for the academic scholarship award highlighting educational goals and computational/scientific research-related skills and abilities. Use separate sheets.

Signature ______________________________ Date ______________________

Application must be submitted six weeks prior to the start of a semester to be eligible for consideration for that semester. However, early submission is recommended because: (1) relatively few scholarships are available, and (2) scholarships are awarded on the basis of first-received first-awarded. The date that the admissions office receives all required items will be the official receipt date.

APPENDIX 3:

SCHOLARSHIP ACCEPTANCE AGREEMENT FORM

US DEPARTMENT
of
ENERGY

ALABAMA A&M UNIVERSITY
PO BOX 1387
NORMAL, AL 35762

DEPARTMENT of ENERGY
FINANCIAL ASSISTANCE ACCEPTANCE FORM

I, ______________________________________ _______________
Print First, Middle Initial, Last Name (SS Number)

Accept ____________________ Do Not Accept ______________________

the financial assistance offered by the US Department of Energy. I understand that I must maintain certain academic requirements and employment standards and if I fail to maintain those requirements, my financial assistance may be suspended or terminated.

I agree to:

- Maintain a cumulative grade point average of 2.8 (undergraduates) 3.0 (graduates)
- Successfully complete a minimum of 12 credit hours per semester
- Maintain a major in science, mathematics, engineering, or computer science
- **Perform interdisciplinary research work project and deliver a final project report**
- **Work four hours per week in a team supervised by engineering faculty**
- Pay for any course that I fail or receive an incomplete grade
- Be responsible for any fees in excess of the maximum amounts provided by DOE
- Accept student employment with the Department of Energy each year if offered.
- Demonstrate a continuing interest in a career with the Department of Energy.
- **Accept regular employment with the Department of Energy for a period equal to six months times the number of semester-scholarships accepted.**

______________________ SEMESTER

______________________ AMOUNT

______________________________________ ____________________
SIGNATURE DATE

APPENDIX 4:

STUDENT SUMMER INTER REPORTS

1. DeSantis Pride, Computer Science, Summer 2000.
2. Valarie Spencer, Mechanical Engineering, Summer 2001

The use of object oriented programming languages to make interactive Web pages

DeSantis Pride

Office of Science, Research Alliance for Minorities Program

Alabama A&M University

Oak Ridge National Laboratory

Oak Ridge, TN, 37831

August 1, 2000

Prepared in partial fulfillment of the requirements of the Office of Science, Department of Energy Research Alliance for Minorities Program under the direction of Dr. Mike Leuze in the Computer Science and Mathematics Division (CSMD) at Oak Ridge National Laboratory.

Participant: ______________________________

Signature

Research Advisor: ______________________________

Signature

Table of Contents

Abstract

The use of object oriented programming languages to make interactive Web pages. DeSantis T. Pride (Alabama A&M University, Huntsville, AL 35810) Dr. Mike Leuze & Dr. Ruthann Manning (Oak Ridge National Laboratory, Oak Ridge, TN 37831).

My research project or projects for the summer of 2000 consist of using two different object oriented languages. These languages I give mention to are Java and Perl. As you know Java was originally developed as a programming language that could be used to control access to information services, such as cable television. Although this was the original purpose for creating Java, researchers found that Java was also an ideal method for controlling the display of information over the Web. Similarly Perl is also an ideal programming language for certain Web applications. However, Perl is mainly used for applications, which are too complicated to code in C or some other Unix language. Therefore through the use of Perl, Web applications which require interaction between users of the Web and developers of Web pages can be done more easily and efficiently.

The first project, which I was assigned, requires me to use the programming language Java to make modifications to the ORNL/RAM Web site. The modification that I have to make require me to develop a Java applet that can be used to make animated images on the RAM Web site.

The next project I would like to talk about requires me to use the language Perl. Ultimately, I have been given the task of using Perl and HTML code to make up interactive registration forms for the RAM program. These forms which I am to create will ask for information about students such as school classification, GPA, and courses taken which will help Dr. Manning perform her task of paring each RAM intern up with an appropriate ORNL Mentor. The most intriguing aspect of this project is that it requires me to make forms, which will be filled out over the Web.

Introduction/Problem Description

The main problem to resolve is the use of the correct programming language or languages to complete the task of animating images and creating fill-out forms, which in turn could be used for various Web development applications. Currently, to do such task as these a programmer has a wide variety of languages to choose from. These languages I give mention to are languages such as Pascal, C++, Ada, Java, and Perl just to name a few. Despite, this wide variety of languages available to the programmer however, the main issue at hand is choosing a language when used by a programmer has plenty of leverage and flexibility.

Therefore, what is leverage and what is flexibility? The term leverage as it relates to programming means having the ability to write code and develop programs quickly, easily, and efficiently (Swartz and Christian 1997). The term flexibility as it relates to programming means having the ability to write code and develop programs that are portable and can be used on various platforms (Swartz and Christian 1997). Due to the fact that these ideas and concepts entail leverage and flexibility, a programmer seeking to develop animated images and fill-out forms for various Web development applications must keep these concepts and ideas in mind.

So, how do these ideas and concepts relate to Web development? Basically, they relate to the ultimate choice of choosing a language that interacts effectively with Web applications. Therefore, because of this great necessity for compatibility a programmer must find a language, which consist of the same basis as

Web applications. Therefore, this basis requires a language that is small yet; object oriented, provides for full graphical user interface and multimedia facilities, and provides threading features for multiple threading (Bishop 1998). Thus, the language or languages of choice are Java and Perl because they consist of this basis.

Materials and Methods

To use any programming languages to create animated images and fill-out forms for Web develop applications, a programmer must have an understanding of the language and it's specifications. For instance, every program designed for any language requires an environment in which each specific program can be written in it's program language, translated to machine language, and executed. Therefore, yet to get a better understanding of how these three elements relate to the task of creating animated imagines and fill-out forms for various web development applications, I will give a brief description of how to implement these principles for each task.

The first task is to create animated images using the programming language Java. Noting that you should have a Java environment in which to create Java programs. Therefore, download the Java development kit from www.java.soft.com. This kit from Sun Microsoft Systems contains the necessary facilities for writing, running, and executing Java programs. The main element in the Java Development kit is the Java Bin in which Java code is written and stored. This code is later, then compiled by using the MS DOS Prompt to test for errors in the written code. After which if no errors were found would generate a class file, which makes the program executable, giving a way for the programmer to test his or her code. Basically, the environment is fairly simple to use, the greatest task is writing code.

Similarly, creating fill-out forms in the programming language Perl there requires the same basic elements and steps. These same elements and steps consist of a Perl environment, instead of a Java environment, in which there is a Perl Bin, instead of the Java Bin, for writing, running, and executing code. Basically, using either of these environments is fairly simple the greatest task is writing the code for each.

Results

In order to develop animated images for Web development applications in Java requires the use of Java Applets. The reason this is so is because Java contains two different types of programs: one for Web integration (Applets) and the other for standalone applications (Perry 1997). Since, the purpose of my research requires the development of programs for Web development applications. There was no other alternative for myself but to develop a Java applet for this purpose.

Basically, the Java applet which I am to create will have to have the ability to read a number of images, the ability to see whether all images have been read, the ability to display those images, and the ability to display each image per time.

The form that I am to create in Perl requires me to know some HTML (Hypertext Markup language) for creating Web page forms. I will have to use the correct HTML form tags in order to create text fields and text areas in which individuals who view there Web pages can enter information and send this information via the Web. Even though, creating an HTML file containing these tags is very important. Writing Perl code is the most important process in this type of Web development application. The reason that the Perl interaction with the HTML form file is necessary is so that information being transmitted from the form can be stored into a file.

Discussion and Conclusion

There are a variety of languages used to create various types of programs. The issue at hand is to decide which programming language is suited to your particular purpose. In the case of Web development applications it's good to use languages such as Java and Perl because of their unique capabilities. Capabilities such as network control, interactive multimedia, platform independence, and multiple levels of security, which are intricate parts of today's Web development (Perry 1997).

Acknowledgements

I thank the United States Department of Energy – Office of Science for giving me the opportunity to participate in the Research Alliance for Minorities Program.

My thanks also goes to my mentors Dr. Mike Leuze (The Director of Collaborative Technologies Research Center) and Dr. Ruthann Manning (The Director of Research Alliance for Minorities) and the entire staff at the CSMD department at Oak Ridge National Laboratory in Oak Ridge, TN. Also, special thanks go out to Ron Lee, CSMD Lab Researcher and RAM Interns Randy Debasa and Andrew Obeng.

The research described in this paper was performed at the Computer Science and Mathematics Division, a national scientific user facility sponsored by the United States

Department of Energy's Office of High Speed Computing located at Oak Ridge National Laboratory.

References

Bishop, J. (1998). Java Gently:Programming Principles Explained, 2nd Edition. Addison Wesley Longman, Inc., Harlow, England. pp. 3-4.

Perry, P.J. (1997). Discover Visual J++. IDG Books Worldwide, Inc., Foster City, CA. pp. 1-20.

Schwartz, R. L., Christiansen, T. (1997). Learning Perl. O'Reilly & Associates, Inc., Sebastopol, CA. pp. 1-4.

Using Perl to Process your WEB Form: Writing CGI Programs in Perl, http://fpg.uwaterloo.ca/cgiperl/index.html

Sample Code

Example of Java applet developed by Morgan Johnson 99RAM Intern

```
//File myAnime.java

//create for RAM  06/22/00

//Author MLJ

import java.awt.*;

import java.awt.image.*;

public class myAnime extends java.applet.Applet implements Runnable

{           //tailor this to the number of images that you plane to have

            int NUM_IMAGES = 10;

            int frameNum  = 0;

            Thread        myThread;

            Graphics      bufferGraphic;

            Image         bufferImg;

            Image         images[];

            int           imgWdth,imgHght;

            //loop variable

            int i,j,k,l;

            //this justs tracks things while I load the images

            MediaTracker   tracker;

            public void init()

            {           images = new Image[NUM_IMAGES];

                        frameNum=0;

                        //should work with either ie or netscape

                        for(i=0;i<NUM_IMAGES;++i)

                        {//please make sure that the first name of all of you images is "frame"

                        //I am assuming that they are going to be .jpg files.  If not, you can change

                        //the ext below to .gif.  I have include some .jpg files for example

                        //purposes.

                        images[i]=getImage(getCodeBase(),"./frame" + i + ".jpg");
```

```
tracker=new MediaTracker(this);
tracker.addImage(images[i],0);
try
{           tracker.waitForID(0);
}catch (InterruptedException e) {return;};
}//emd of for loop
//grab the image dimensions off of the first image
//by the way, make sure the dimensions of all the images is the same
imgWdth=images[0].getWidth(this);
imgHght=images[0].getHeight(this);
bufferImg = createImage(imgWdth,imgHght);
bufferGraphic = bufferImg.getGraphics();
//I will just place the first image on the screen at init time
//bufferGraphic.drawImage(images[0],0,0,this);
resize(imgWdth,imgHght);
}//end of init!!!!!!!!
public void start()
{           if (myThread==null)
            {           myThread=new Thread(this);
                        myThread.start();
            }
}//start
public void stop()
{           myThread=null;
}//stop
//we should pause the thread so images dont go by to quickly
void pause(int sleepTime)
{           try{myThread.sleep(sleepTime);}
            catch(InterruptedException e) {}
}//pause
public void run()
{           //this is going to run for ever (at least until the thread dies a
            //natural death by you shutting down the applet
            while(true)
            {           //repaint the screen
```

```
                    repaint();
                    if(frameNum==NUM_IMAGES)
                    frameNum=0;
                    ++frameNum;
                    //try changing the pause time (it is in milliseconds)
                    //this will very the speed of animation
                     pause(120);
            }
        }//run
        public void update(Graphics g)
        {       paint(g);
        }//update
        public void paint(Graphics g)
        {       //for all images
                bufferGraphic.drawImage(images[frameNum], 0 , 0, this);
                g.drawImage(bufferImg,0,0,this);
        }//paint
} //end of myAnime Class
```

Sample Code

Example of HTML and Perl Form Code Provided by:

http://fpg.uwaterloo.ca/cgiperl/index.html

HTML Form Code

```
<FORM METHOD=POST ACTION="/cgi-bin/pride_form.pl">

What is your name?

<INPUT TYPE="text" NAME="name" VALUE="David Jonker"><BR>

What is your student id#?

<INPUT TYPE="text" NAME="id" VALUE="12345678" MAXSIZE=8><BR>

What was your evaluation of the course?

<SELECT NAME="evaluate">

<OPTION SELECTED>good

<OPTION>satisfactory

<OPTION>poor

</SELECT><BR>

<INPUT TYPE="submit" VALUE="Submit">

<INPUT TYPE="reset" VALUE="Reset">

</FORM>
```

Perl Code

```
#!/usr/bin/perl

read (STDIN,$in,$ENV{'CONTENT_LENGTH'});

$in =~ s/\+/ /g;

@pairs = split (/&/, $in);

foreach $pair (@pairs) {

  ($key[$num],$value[$num]) = split (/=/, $pair);

  ++$num;

}

print "Content-type: text/html\n\n";

print "<A HREF=\"/pride_form.html\">Return</A>\n";

$recipient = "dpide@aamu.edu";
```

```
$mailprog = '/usr/bin/mail';

open (MAIL, "|$mailprog $recipient");

print MAIL "Subject: Survey Using PERL to Process Your Web Form\n";

print MAIL "------------------------------------------------\n";

print MAIL "Name: $value[0]\n";

print MAIL "Id# : $value[1]\n";

print MAIL "Evaluation: $value[2]\n";

close MAIL;
```

An Introduction to Parallel Cluster Computing using PVM for Computer Modeling and Simulation of Engineering Problems

Presented by Valerie Spencer
Mentored by Jim Kohl

Oak Ridge National Laboratory RAM Internship
June 11 – August 17, 2001

Contents <u>**Page**</u>

List of Figures

Page

Acknowledgements

I appreciate Dr. Z. T. Deng's decision of selecting me to be a part of the Summer 2001 RAM Program. I appreciate Dr. Jim Kohl for guiding my research, dedicating time to discuss my findings, and facilitating resources from the Computer Science and Mathematics Division. This research was performed under the Research Alliance for Minorities Program administered through the Computer Science and Mathematics Division, Oak Ridge National Laboratory. This Program is sponsored by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research; U.S. Department of Energy. I would also like to acknowledge Mrs. Debbie McCoy for organizing the RAM Program that allowed me to spend the summer gaining significant information at ORNL. Other acknowledgements go out to Debbie Flanagan, Stephen Scott, and Cheryl Hamby. This work has been authored by a contractor of the U.S. Government at Oak Ridge National Laboratory managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

Abstract

An investigation has been conducted regarding the ability of clustered personal computers to improve the performance of executing software simulations for solving engineering problems. The power and utility of personal computers continues to grow exponentially through advances in computing capabilities such as newer microprocessors, advances in microchip technologies, electronic packaging, and cost effective gigabyte-size hard drive capacity. Many engineering problems require significant computing power. Therefore, the computation has to be done by high-performance computer systems that cost millions of dollars and need gigabytes of memory to complete the task. Alternately, it is feasible to provide adequate computing in the form of clustered personal computers. This method cuts the cost and size by linking (clustering) personal computers together across a network. Clusters also have the advantage that they can be used as stand-alone computers when they are not operating as a parallel computer. Parallel computing software to exploit clusters is available for computer operating systems like Unix, Windows NT, or Linux. This project concentrates on the use of Windows NT, and the Parallel Virtual Machine (PVM) system to solve an engineering dynamics problem in Fortran.

Introduction

There are two parts to the PVM system. The *daemon* is a special purpose process that runs on behalf of the system to handle all the incoming and outgoing message communication. It is represented by "pvmd3" or "pvmd" and any user with a valid login id can install and execute this on a machine. The other part of the system is a library of routines that enables parallel tasks on the computers to interact.

In order to use PVM in the computation of a problem, the problem must be able to be broken down into several tasks. This is known as parallelism, which is done in two ways. One way is "functional" and is accomplished by breaking the application into different tasks that perform different functions. The other way is "data" and this is done by having several similar tasks each solve one part of the data. PVM is a system that can be used for one of these methods or a combination of both.

C, C++, and Fortran are all languages that can be used to write PVM codes. This project is done using the Fortran language. Fortran language binders are carried out as subroutines instead of functions. This is because some compilers cannot combine Fortran functions with C functions. Therefore, Fortran applications (programs) have to be linked to the PVM Fortran library, the standard PVM library and the C socket library using these links libfpvm3.lib, libpvm3.lib, and wsock32.lib.

PVM codes are written following two main programming models. Using the master/worker model, the master task creates all other tasks that are designed to work on the problem, and then coordinates the sending of initial data to each task, and collects results from each task. However, in the hostless model the initial task spawns off copies of itself as tasks and then starts working on its portion of the problem while the created tasks immediately begin working on their portion. Input and output requirements are often handled by individual tasks, but it may be beneficial to have some results collected by a single task, especially if those results need to be broadcast back out to all the tasks.

In order to execute a program under PVM, the user adds calls to the PVM library routines that spawn off tasks to the other machines within the user's virtual machine and allow tasks to send and receive data.

Method

The problem to solve was a 3-D spring/mass system. Utilizing the ideas and concepts learned in my dynamics course, we applied the equations for spring force, velocity, and displacement such as:

$$\text{Force} = K_{spring}(DX)$$

$$X = X_0 + V_0\,DT + [a(DT)^2]/2 \quad \text{where } a = \text{Force/mass}$$

Therefore, we came up with the equations:

(1) Ftmp = (E0 - E) * Springs(I, J)

and

(2a) Fx(I) = Fx(I) + Ftmp * (X(I) - X(J)) / E
(2b) Fy(I) = Fy(I) + Ftmp * (Y(I) - Y(J)) / E
(2c) Fz(I) = Fz(I) + Ftmp * (Z(I) - Z(J)) / E

(2d) Fx(J) = Fx(J) + Ftmp * (X(J) - X(I)) / E
(2e) Fy(J) = Fy(J) + Ftmp * (Y(J) - Y(I)) / E
(2f) Fz(J) = Fz(J) + Ftmp * (Z(J) - Z(I)) / E

and

(3a) X(I) = X(I) + (Vx(I) * DT) + ((Fx(I) * DT**2)/(2 * Mass))
(3b) Y(I) = Y(I) + (Vy(I) * DT) + ((Fy(I) * DT**2)/(2 * Mass))
(3c) Z(I) = Z(I) + (Vz(I) * DT) + ((Fz(I) * DT**2)/(2 * Mass))

and

(4a) Vx(I) = Vx(I) + (Fx(I) * DT / Mass)
(4b) Vy(I) = Vy(I) + (Fy(I) * DT / Mass)
(4c) Vz(I) = Vz(I) + (Fz(I) * DT / Mass)

First, using equation (1) the spring force attached to any two masses is calculated and then is used to calculate the vector forces of mass 1 (2a-c) and mass 2 (2d-f). The forces accumulated in equations (2a-c) are then used to update all mass locations (3a-c) and velocities (4a-c) in vector form as the system vibrates back and forth in space. No boundary conditions are assumed. Before the velocities are updated (4a-c), they are also used in equations (3a-c). DT is the change in time, which is a constant value, as are mass and E0 (original extension of spring). Figure 1 shows a diagram of the program flow.

Results and Discussion

Figure 2 shows the performance of the average time in seconds that it took to run a sequential version of the program versus a parallel version of the program for the given number of masses. Only a single desktop PC was used and the number of computation iterations was set at five hundred. Each parallel run was set up to have one master task and two worker tasks. The results of the parallel program were poor because when a parallel program is run on a single computer, the overhead of running multiple processes parallel will always make the "parallel" code run slower than the sequential code.

Figure 3 shows the results after running the sequential program on a laptop and the desktop. The laptop, which is much slower than the desktop, has a huge effect on the performance.

In order to collect more efficient and correct data, we need to run the parallel code in a more balanced parallel environment. Figure 4 shows the results clustering the PC with the laptop to create our parallel environment. The PC, which obviously has more computing power, is slowed down by the laptop when running in parallel. A proper, balanced parallel cluster should give the desired results that when given a large and complex problem, clustering PCs together will compute much faster than a single computer. For the current configuration, the imbalance in computing power, plus the cost of parallel communication overhead, makes the sequential program faster.

Conclusion

This research has proved that clustering personal computers together can provide adequate computing power for large engineering problems. It has also proved that computers within the cluster can be used as stand alone computers because the desktop and laptop in this cluster served other purposes such as preparing a paper, this Power Point presentation, and a poster presentation. However, there are several optimizations that should be done to this project to improve the parallel performance. Avoiding unnecessary message packing and reducing the message sizes are two approaches that I plan to explore in the future upon my potential return to ORNL next summer.

References

Geist, Al, Beguelin, A., Dongarra, J., Jiang, W., Manchek, R., and Sunderam, V. (1994), *PVM: Parallel Virtual Machine*, London, Massachusetts: MIT Press.

Nyhoff, L., and Leestma, S. (1988), *Fortran 77 for Engineers and Scientists* (4th ed.), New York: Macmillan.

Resnick, R., and Halliday, David. (1977), *Physics: Part One* (3rd ed.), New York: John Wiley & Sons.

Appendix of Figures

Figure 1:
Program Flow

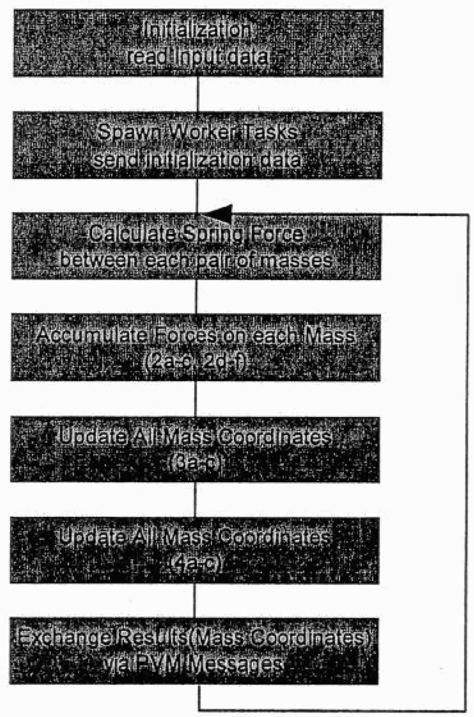
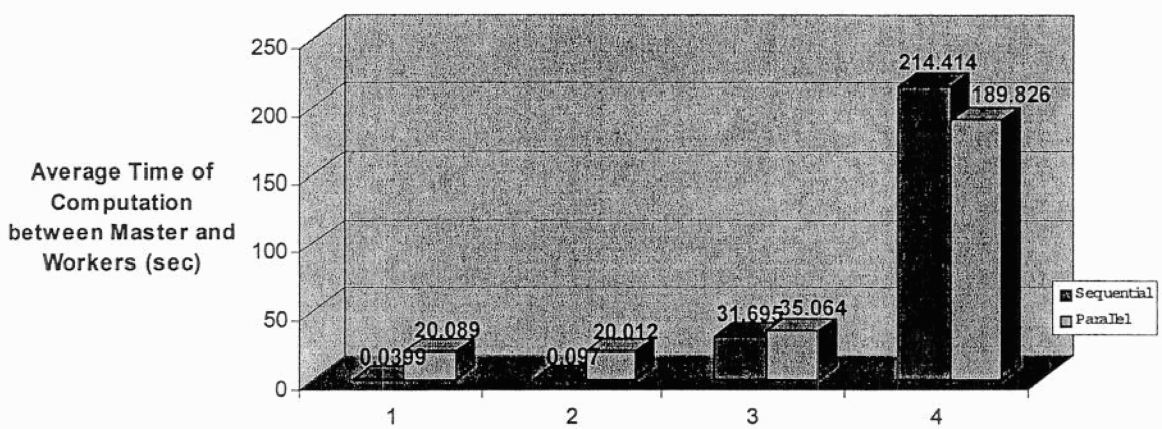
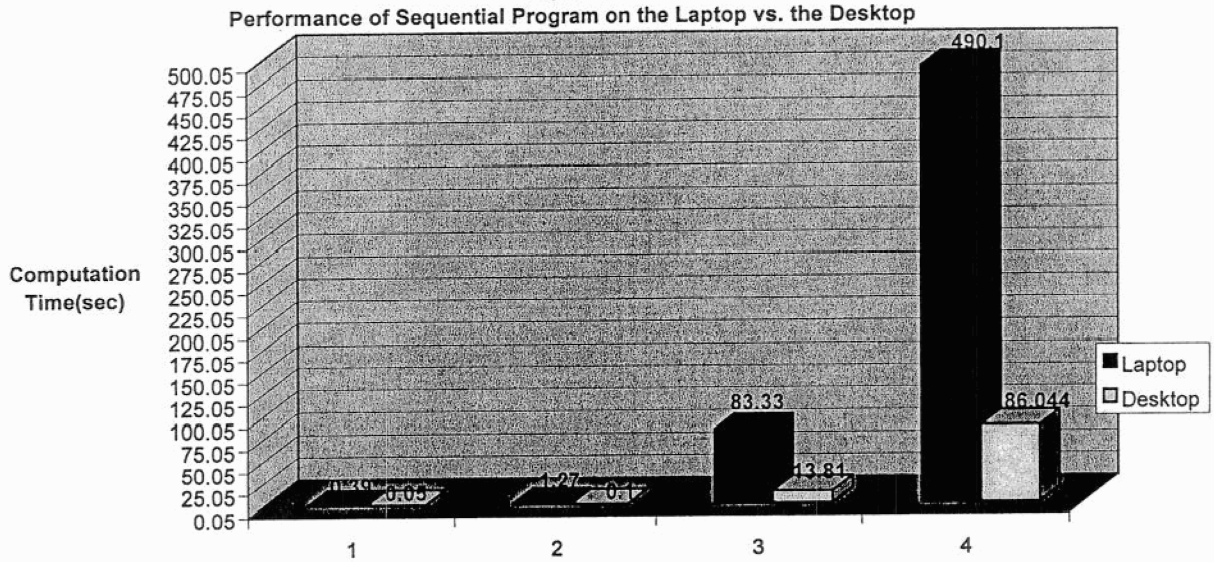


Figure 2:
Performance of Sequential Program vs.
Parallel Program on Desktop Only



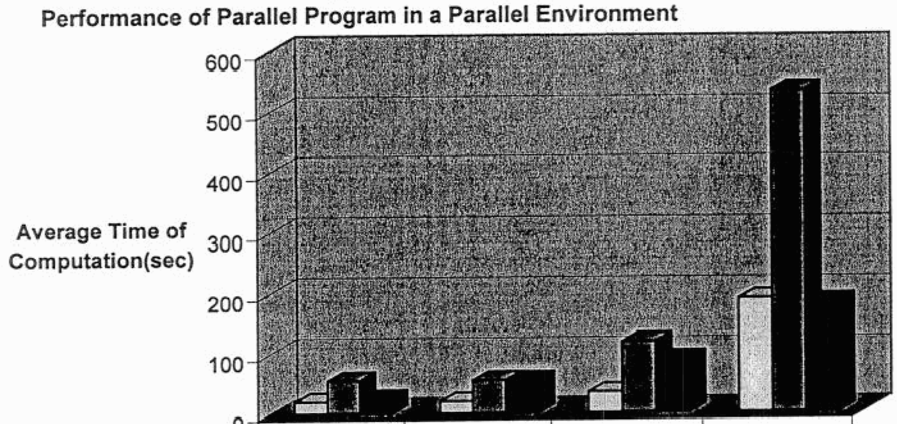
Number of Masses
1 = 27 masses
2 =64 maases
3 =729 masses
4 = 1728 masses

Figure 3:
Performance of Sequential Program on the Laptop vs. the Desktop



Number of Masses
1=27 masses
2=64 masses
3=729 masses
4=1728 masses

Figure 4:
Performance of Parallel Program in a Parallel Environment



	1	2	3	4
□Parallel(PC only)	20.089	20.012	35.064	189.826
▩Parallel(laptop and PC, PC:M/W Laptop:W)	55.079	54.976	118.454	534.83
■Parallel(laptop and PC, PC:2W Laptop:M)	24.994	54.996	89.579	183.836

Number of Masses
1=27 masses
2=64 masses
3=729 masses
4=1728 masses

APPENDIX 5:

PAPER, ABSTRACT AND PRESENTATION

1. ADMI Paper Abstract: Dr. C. Hung
2. ASEE Paper: Dr. Deng
3. High Performance Computing Lab Presentation to Boeing

Establishment of the High-Performance Computing Laboratory at AAMU

Chih-Cheng Hung, S.A. von Laven, Kwai Wong*, Kevin Chu, I. Chen and A. Bond#

Department of Mathematics and Computer Science,
#School of Engineering and Technology
Alabama A&M University, Normal, AL 35762 U.S.A.
*Joint Institute for Computational Science
University of Tennessee, Knoxville, TN U.S.A.

Abstract

Alabama A&M University (AAMU) is an active member of the Metacenter Regional Alliance (MRA) funded by the National Science Foundation (NSF). The University of Tennessee in Knoxville (UTK) has managed the MRA program. With the support from the MRA, a High-Performance Computing (HPC) Laboratory suitable for training and research in parallel processing is being established in the AAMU Mathematics and Computer Science Department at AAMU [1].

The fastest computers achieve their speed through highly parallel designs involving hundreds to thousands of processors, as well as substantial parallelism within the processor [2]. There are two main approaches to parallel processing [3]: algorithmic parallelism and data parallelism. In algorithmic parallelism, the task is split into a number of functions that are then implemented by different processors. In data parallelism, the data are split into several regions and different processors handle the different regions.

Many existing types of workstations/personal computers have been networked together to be utilized as parallel computers working in a distributed computing environment [3]. The Message Passing Interface (MPI) [4] environment is chosen for the testbed. MPI defines a reliable, efficient, portable commumication interface, with implementations available on a wide variety of platforms, ranging from networks of workstations to supercomputers. MPICH is Argonne National Laboratory's public-domain implementation of MPI; it supports a variety of platforms in homogeneous and heterogeneous configurations. MPICH is available at http://www.mcs.anl.gov/mpi.

The machines in our HPC Laboratory will initially have Windows NT, Linux, and MPI installed. They are configured with 300 MHz Pentium II processors and fast ethernet network cards. We have so far acquired eight clients and one server. More clients will be purchased to fit the needs of the parallel processing course and other courses. Testing of these clients has already begun. A student research assistant is conducting many of the tests. He attended the August 13-14, 1998 UTK workshop "Setting Up a PC Cluster for High-Performance Computing." The HPC lab will provide a platform for certain HPC course projects. The Mathematics and Computer Science Department will offer a parallel processing course (CMP490) during the Spring 1999 Semester. The course outline is shown in Appendix A [1]. This lab will also benefit our new Electrical Engineering program and other departments such as Chemistry, Physics, Civil Engineering, and Environmental Sciences for education and research. In addition to classroom training in high-performance computing and participation in faculty research, students will have the opportunity to visit Oak Ridge National Laboratory and speak

with computational scientists working directly on problems of interest to DOE [5]. Eventually we expect to implement Tango, a web-based distance learning and collaboration environment, and possibly other learning aids on these machines.

References

[1] von Laven, S. A., C. C. Hung, and Z. T. Deng, "Alabama A&M University's Participation in the Metacenter Regional Alliance," Final Report, August 1998.

[2] Messina, P., D. Culler, W. Pfeiffer, W. Martin, J. T. Oden, and G. Smith, "Architecture," COMMUNICATIONS of the ACM, Vol. 41, No. 11, November 1998, pp. 36-44.

[3] Kumar, V., A. Grama, A. Gupta, and G. Karypis, Introduction to Parallel Computing: Design and Analysis of Algorithms, The Benjamin/Cummings Publishing Company, Inc., 1994.

[4] Marc Snir, Steve Otto, Steven Huss-Lederman, David Walker, and Jack Dongarra, MPI: The Complete Reference, MIT Press, 1996. (also available from http://www.nwtlib.org/utk/papers/mpi-book/mpi-book.html)

[5] von Laven, S. A. and C. C. Hung, "Alliance for Computational Science Collaboration: HBCU Partnership at Alabama A&M University," Proposal to the Department of Energy, May 1998 **Appendix A**

Prerequisite:

MTH203, CMP305 & CMP380

Textbook:

Introduction to Parallel Computing: Design and Analysis of Algorithms by V. Kumar, A. Grama, A. Gupta, and G. Karypis, The Benjamin/Cummings Publishing Company, Inc., 1994

References:

1. Notes of UTK MRA Workshop on Parallel Computing in Undergraduate Education, JICS, University of Tennessee, Knoxville, TN, May 26-29, 1997.
2. Introduction to Parallel Algorithms and Architectures by F. T. Leighton, Morgan Kaufmann Publishers, 1992.
3. Parallel Programming with MPI by P. S. Pacheco, Morgan Kaufmann Publishers, Inc., 1997
4. Using MPI: Portable Parallel programming with the Message-Passing Interface by W. Gropp, E. Lusk, and A. Skjellum, The MIT Press, 1995
5. High Performance Computing and Its Applications in the Physical Sciences by D. A. Browne etc. (ed.), World Scientific publisher, 1994.

Course Objective:

The course is designed for undergraduate students majoring in computer science. The introduction of basic parallel processing concepts, design and performance analysis of parallel algorithms, parallel processing programming languages, hardware, and some popular commercial machines will be done in this entry level course.

Modes of Instruction:

Large group lectures, independent study, self-instructional techniques will be employed in the teaching of this course. You are encouraged to discuss any questions with your instructor.

Materials of Instruction:

Textbook, different reference books and supplementary materials will be used in this class. A survey of existing commercial machines will be done by each student enrolled in this course.

Course Description:

1. Introduction
2. An overview of parallel computing: Hardware and Software issues
3. Basic Communication Operations
4. Performance and Scalability of Parallel Systems
5. Basic Considerations concerning Data Structures
6. Parallel Algorithms: Sorting, Fast Fourier Transform, Linear Equations, and Dynamic Programming
7. Parallel Programming
8. Other suggested topics

High Performance Computing Initiative to Enhance Engineering Education

Z.T. Deng, Ruben Rojas-Oviedo, X, Qian, A. Jalloh and A. Mobasher

Department of Mechanical Engineering
Alabama A&M University
Huntsville, AL 35762
Phone: (256) 858-4142
E-Mail: aamzxd01@aamu.edu
rojaso@aamu.edu; cqian@aamu.edu; ajalloh@aamu.edu; amobasher@aamu.edu

Scott von Laven
Alabama Research and Education Network
Alabama Supercomputer Authority
Huntsville, Alabama
E-Mail: scott@asc.edu

Abstract

The power and utility of personal computers continues to grow exponentially through (1) advances in computing capabilities through newer microprocessors, (2) advances in microchip technologies, (3) electronic packaging, and (4) cost effective gigabyte-size hard-drive capacity. The engineering curriculum must not only incorporate aspects of these advances as subject matter, but must also leverage technological breakthroughs to keep programs competitive in terms of their infrastructure (i.e., delivery mechanisms, teaching tools, etc.).

An aspect of these computing advances is computer modeling and simulation of engineering problems. Many engineering problems require significant computing power, and some complex problems require massive computing power.

An example of a complex problem is a model that combines several aspects of a flight vehicle. Such a model might include fluid-solid interaction, heat transfer and dynamic loading of structures, all of which are coupled. Such models can easily consume massive computing resources, such as a supercomputer. To provide a conventional supercomputer on a dedicated basis to our faculty and upper level students is not feasible. It is feasible, however, to provide computing power adequate for teaching and student research in the form of clustered personal computers. Clusters can be acquired over time as individual computer purchases and configured by our own departmental personnel. Parallel computing software to exploit the clusters is available for computer operating systems like Unix, Windows NT or Linux. Clusters also have the advantage that they can be used as stand alone computers in a laboratory environment when they are not operating as a parallel computer.

This paper describes how the Mechanical Engineering program introduces engineering students to high performance computing, and parallel computing in particular, without adding courses to the curriculum. The Mechanical Engineering Department at Alabama A&M University has undertaken the High Performance Computing Initiative to Enhance Engineering Education. Under this initiative we not only introduce undergraduate students to high performance computing but also make it an integral part of the undergraduate curriculum.

Our high performance computing initiative was launched with funding from the Department of Energy (DOE) Alliance for Computational Science Collaboration (ACSC) project. A high-performance computing laboratory to support the initiative was established in the Mechanical Engineering Department.

This project provides faculty and students the opportunity to become involved in computational science projects of interest to national laboratories and research institutions. DOE support provides science, engineering and mathematics (SEM) undergraduate majors with scholarships to work under the mentorship of faculty members in projects involving high performance computing. There are currently twelve scholarship recipients. The recipients include students from Mechanical, Electrical, and Civil Engineering, Computer Science and Biology/Chemistry. Seven of them are from the Mechanical Engineering Department. Among these recipients, three multi-disciplinary teams were formed to conduct guided research. The projects include research and training in areas such as computational fluid dynamics, finite element analysis and advanced propellant characterization for propulsion. This paper describes the implementation process for introducing high performance computing to undergraduates and the assessment method to evaluate the effectiveness of this approach to enhance engineering education.

I. Introduction

For problems like global climate modeling, groundwater modeling, human genome mapping, weather forecasting, vehicle dynamics, molecular dynamics, and others., computer power is never sufficient. In the field of computational fluid dynamics (CFD), the problem size grows as the square (2D) or cube (3D) of the grid resolution. Large CFD problems, such as modeling the airflow around a complete aircraft, require hundreds of giga FLOPS (GFLOPS)) and tremendous memory allocations to complete in a reasonable time. Consider the following global climate modeling parameters.

> one grid point per square kilometer
> 15 vertical levels from sea level up to 14 kilometers,
> six primary time dependent variables (updated once per minute at each grid point

It is estimated that to cover the entire earth surface, it requires the computer to process three Gigabytes of data [1]. To run even higher resolution models than the one described may require an impractical amount of time and memory using a serial high performance computer. In the past few years, computer speeds have increased from Megaherz to GigaHerz, and faster chips are still to come. However, computer speeds may approach fundamental speed limits, in the next two or three decades. Also associated with the faster chips are problems of heat dissipation. It is generally agreed that continued performance gains beyond these limits can only be achieved by concurrent execution of programs on multiple processors. As indicated by [1], "the greatest gain in computing performance since 1989 has been through the move to large-scale parallelism."

High performance parallel processing can significantly reduce the wall clock time required to execute a program. It also facilitates a huge amount of total memory, which is necessary to solve the largest problems. It can be cost effective to use a cluster of workstations or PCs as a parallel computer. Parallel computing can be achieved through implementation of the Parallel Virtual Machine (PVM) or Message Passing Interface (MPI) libraries on such platforms. Great efforts have been made towards parallel computing applications for engineering in the past few years. Significant achievements have been accomplished in the field of computational fluid dynamics, in particular.

II. Need for Minority Scientists in Computational Science

> *"There is an urgent need to prepare an increasingly diverse population from a multi-cultural world for academic, government, and industry careers in Science, Mathematics, Engineering and Technology (SMET). According to the US 1990 census, the total US population was 248,709,873 in 1990. Of these, approximately 51% were women, 29,986,060 (or 12%) were African American, 22,354,059 (or 9%) Hispanic, and 1,878,285 (or 1 %) Native American. As of 1995, of the total US civilian labor force (132 million), only 627,000 had Ph.D. degrees in SMET and only 341,000 of these were employed in SMET fields. Of these 341,000, only 55,210 (or 16.2%) were women, 7270 (or 2.1%) Hispanic, 5500 (or 1.6%) African American, and 810 (or 0.2%) Native American."*

--- DOE Alliance for Computational Science Collaboration (ACSC) FY00 STRATEGIC PLAN [2].

The Department of Energy Alliance for Computational Science Collaboration has operated since October 1997 with the overall goal of training African-American and other minority scientists in computational science for eventual employment with DOE. Strategies designed to help produce future DOE minority scientists are

- to involve HBCU students and faculty members in computational science projects at national laboratories and research institutions;
- to assist HBCU faculty members in integrating interdisciplinary computational science courses into their undergraduate curricula, involving freshmen to senior students; and
- to provide support and expertise to HBCU researchers using state-of-the-art computational science technologies and methodologies.

Historically Black Colleges and Universities (HBCUs) are the primary source of African-American scientists in the US, and HBCU participation is central to the Alliance. Alabama A&M University is one of the HBCU members of the Alliance.

The question at hand is how to introduce engineering students to advanced computational resources without adding courses to the curriculum.

III. Mechanical Engineering Department at Alabama A&M University

Alabama A&M University (AAMU), is a land-grant historically black university. It is located in the northeast outreach of Huntsville, Alabama, an important world center of expertise for advanced missile, space transportation and electronics research and development. Among the leading industry and government organizations located in this area are NASA Marshall Space Flight Center, the Army Aviation and Missile Command (AMCOM), the Redstone Technical Test Center, Boeing, Northrup Grumman, Lockheed Martin and many others associated with high-tech. endeavors. These industries and government agencies require large numbers of highly trained engineers, in the areas of both manufacturing and also propulsion.

To better serve the state of Alabama and in particular the northern part of the state, the Mechanical Engineering program at AAMU was formulated with two options: Manufacturing and Propulsion Systems. To provide additional adaptability in the program, a third option was included and designated the General option. The Mechanical Engineering program strives to provide a strong foundation in engineering design, analysis, and the engineering sciences. Thermodynamics, Fluid Mechanics, and Heat and Mass Transfer are core courses common to all options. Students who pursue one of our more specialized options in Manufacturing or Propulsion Systems are exceptionally well prepared upon graduation. For example, high level propulsion courses include power system integration, power plant performances, analysis and synthesis of gas turbine components, gas dynamics, rocket propulsion, and two consecutive semesters of senior design in propulsion related project. In both options, scientific computing and the intelligent use of computers are given special attention. As part of the vertical and horizontal integration of design and project development, the ME program strongly encourages teamwork in class projects for courses in the major. This helps students to develop a design portfolio starting in their freshman year. Project training continues through their capstone design course. The projects assigned to students are often combined with on-going externally funded research. This aspect of program keeps the students in touch with leading-edge technology and current research activities in the real world.

IV. High Performance Computing Initiative at AAMU

The high performance computing initiative at AAMU was launched in 1999 under the support of the Department of Energy (DOE) Alliance for Computational Science Collaboration (ACSC) project. The key elements of this program at AAMU are to encourage faculty and students to become involved in computational science activities through student scholarships, student internships, student work study, collaborative research projects involving Oak Ridge National Lab (ORNL) scientists, and research proposal submission. The program promotes research and education relative to computational science and high performance computing. It broadens the research and educational capability at AAMU in a manner consistent with our overall growth in sponsored research and with the teaching mission of the University.

A High Performance Computing (HPC) Laboratory using Pentium II PCs that run Linux and PVM, or alternatively Windows NT, has been established. A new Sun Ultra 10 was configured to run high performance computing applications. Current applications include computational fluid dynamics, finite element analysis and grid generation. The Laboratory is located in Carver Complex North, where the school of Engineering and Technology is hosted. This Laboratory is available for use by project participants and by students from Mechanical Engineering, Electrical Engineering, Civil Engineering, and Computer Science Departments, who are either involved in high performance computing projects or enrolled in appropriate classes during the fall 1999 and spring 2000 semester.

The HPC Laboratory is currently connected to the campus network via 10Mbs ethernet and, in turn, to the Internet via a T1 digital circuit. Two projects funded by the National Science Foundation (NSF) plus another funded by the state of Alabama last year supplied critical components of an OC3 Internet feed to our campus.. The OC3 circuit became operational during the summer of 2000.AAMU can arrange to become an Internet 2 affiliate institution when the need arises. These steps will permit campus projects, such as the HPC laboratory, to be connected to their collaborators at other Internet 2 institutions at 155 Mbs provided the departments hosting those projects upgrade their local area networks (LANs) to gigabit ethernet.

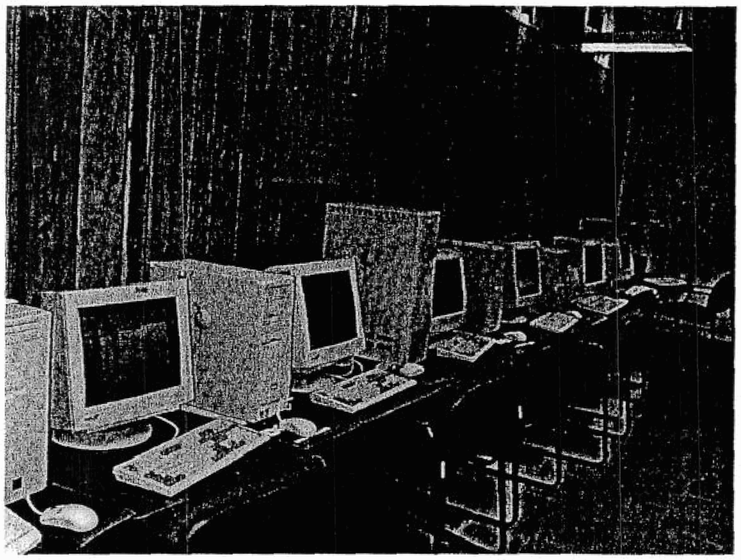


Figure 1. High-Performance Computing Laboratory at AAMU, CCN 220.

The initial effort to establish a high-performance computing laboratory was directed by Dr. Scott von Laven and Dr. Deng. Dr. Z.T. Deng was appointed as laboratory director in Fall 1999. The HPC Laboratory is a collaborate efforts among Alabama A&M University, the Alabama Research and Education Network (AREN), and Computer Sciences Corporation. Currently, the high performance computing applications are focused on parallel implementations of computational fluid dynamics codes and finite element structural dynamics codes.

High Performance Computing as a course topic was introduced in one of the Mechanical Engineering classes, ME 300, Mathematical Methods in Mechanical Engineering, taught by the current authors at Mechanical Engineering Department. The HPC laboratory and course elements help prepare students who are selected to participate in the summer internship program in computational science research at ORNL. The high performance computing lab provides access to the course materials and also serve as a teaching platform for other courses in the ME curriculum.

A number of students have benefited from our efforts to promote computational science under DOE sponsorship. Among our past students is a USA Today 1999 Academic Second Team member. Only 20 students nationwide are selected for each team. Another student was a member of the first graduating class (May 1999) to obtain B.S. degrees in ME at AAMU. Under DOE sponsorship so far, two graduate students from Computer Science and one undergraduate student from the Department of Mechanical Engineering have been hired to assist the faculty to conduct research on high performance computing.

AAMU created a DoE Computational Science Scholarship program during FY 2000. The official program announcement was made through the AAMU Admissions Office in November 1999. Scholarship award selection criteria were developed. To apply for the scholarship, a student needs to fill out the application form, write an essay about their goals as they relate to high performance computing, and obtain a faculty recommendation letter. Upon receipt of the application package, a careful selection process is conducted based on the selection criteria. The student needs to agree to maintain GPA of 3.0 or better. Students also need to successfully complete a minimum of 12 credit hours per semester, and maintain a major in science, mathematics, engineering, or computer science. Students will have to pay for any course they fail or in which they receive an incomplete grade. Students are responsible for any fees in excess of the minimum amounts provided by DoE. The student is required to accept employment with the Department of Energy (one-year of employment for each year of scholarship coverage) if offered. The most important part of this scholarship is that students work on interdisciplinary teams to assist faculty in high performance computing research and applications. Twelve students were awarded scholarships for the 2000-2001 academic year. Six are from Mechanical Engineering, two from Computer Science, two from Natural Sciences, one from Civil Engineering and one from Electrical Engineering. Three multi-disciplinary teams were formed to conduct guided research led by the Mechanical Engineering faculty. The student research projects include research and training in areas such as computational fluid dynamics, finite element analysis and advanced propellant characterization for propulsion (biology and chemistry students involved). Four undergraduate students (engineering and computer science majors) were selected to participate in the ORNL RAM Summer Internship program. These students expressed their strong intention to work in the field of computational science after their graduation.

VI. Assessment

The high-performance computing initiative was externally evaluated by a team from Oak Ridge National Laboratory. The project outcome was also evaluated by DOE, and funding was renewed by DoE based on program merit. Each scholarship recipient's performance is evaluated annually by faculty members. Their progress in research is evaluated primarily on project delivery.

VII. Conclusion

The High Performance Computing initiative was established at AAMU to introduce students in science, engineering and mathematics to the state-of-the-art computational science technology. Results indicate that interest in computational science in minority students has increased, particularly among engineering students. The initiative is geared to build stronger competence in modeling and simulation through parallel processing and to provide leading edge computational science resources to both faculty and students at AAMU. The success of the High Performance Computing initiative has been demonstrated, and as a result funding by DOE has been sustained through 2001.

Acknowledgement

This effort has been partially supported by DOE Grant DE-FG02-98-ER25366.

Bibliography/References:

1. Introduction to Parallel Processing, Christian Holloy, Kwai Wong and Asim yarkhan. JICS workshop Materials. March 2000.
2. DOE Alliance for Computational Science Collaboration (ACSC), FY00 STRATEGIC PLAN . Ruth Ann Manning, Computer Science and Mathematics Division, Oak Ridge National Laboratory (ORNL), November 1999.

ZENGTHAO DENG
Z.T. Deng is Assistant Professor of the Department of Mechanical Engineering at Alabama A&M University in Huntsville, AL. Dr. Deng has an extensive background and research experience in Computational Fluid Dynamics numerical simulation in particular high speed aerodynamics/flows with heat transfer phenomena. He earned his Ph.D. in Aerospace Engineering, from the University of Tennessee in 1991 and his Bachelor of Science, Aerospace and Mechanical Engineering, from Beijing University of Aeronautics and Astronautics in 1985.

RUBEN ROJAS-OVIEDO
Ruben Rojas-Oviedo is Chairperson and Associate Professor of the Department of Mechanical Engineering at Alabama A&M University in Huntsville AL. Dr. Rojas-Oviedo has international engineering experience working both in academe and industry. He has an engineering consulting company and conducts applied research. He earned a Ph. D. in Aerospace Engineering from Auburn University. He has two Masters degrees, one in Mechanical Engineering from N.C. State at Raleigh and the other in Applied Mathematics from Auburn. He earned a B.S. degree in Aeronautical Engineering from the National Polytechnic Institute – Escuela Superior de Ingenieria Mecanica y Electrica in Mexico City, Mexico.

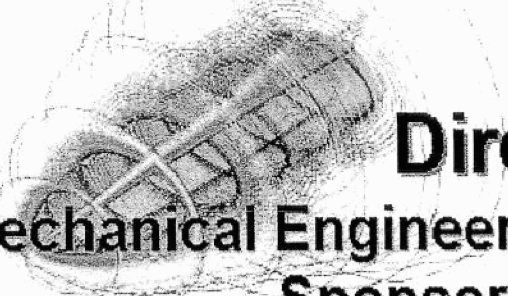
XIAOQING QIAN
X.Qian is Assistant Professor of the Department of Mechanical Engineering at Alabama A&M University in Huntsville, AL. Dr. Qian earned her Ph.D. and M.S. in Mechanical Engineering from the University of Tennessee. Dr. Qian has been working at industry for five years as a Senior System Engineer. She has an extensive experience in instrumentation, measurements, numerical simulation in particular heat transfer phenomena, and system engineering.

ABDUL JALLOH
A. Jalloh is Assistant Professor of the Department of Mechanical Engineering at Alabama A&M University in Huntsville, AL. Dr. Jalloh earned his Ph.D.in Mechanical Engineering, with a minor in Engineering Mechanics from the University of Arizona, he obtained his M.S. Mechanical Engineering also from the University of Arizona, and he holds a B.Eng. in Mechanical Engineering from University of Sierra Leone. His research interests are in the areas of mechanical vibrations, structural dynamics, structural mechanics, applied elasticity, probabilistic design, finite element analysis, manufacturing and reliability.

AMIR MOBASHER
Amir Mobasher is Assistant Professor of the Department of Mechanical Engineering at Alabama A&M University in Huntsville, AL. He holds a Ph.D. degree in Mechanical Engineering from the University of Alabama in Huntsville. He has research interest in the areas of Computational Fluid Dynamics, Biomechanics, and Control and Automation. After graduating from UAH, he worked at U.S. Army Aeromedical Research Laboratory at Fort Rucker, Alabama. During his employment there, his research focused on aircrew protection and head-supported mass and center of mass placement for the U.S. Army aviation.

SCOTT VON LAVEN
Dr. Scott von Laven is currently the Computational Specialties Director of the Alabama Supercomputer Center in Huntsville, Alabama and an employee of Computer Science Corporation. He holds a Ph.D. degree in Physics from Dartmouth College. His research interests include particle accelerators, electron-beam driven coherent radiation, novel RF devices, and signal processing.

High Performance Computing Laboratory



Director: Dr. Z.T. Deng

Mechanical Engineering Department, Alabama A&M University

Sponsor: Department of Energy (DOE)

Parallel Computing using PC Clusters

Presented to Boeing executive

Dr. Z.T. Deng
Dr. Bruce Vu
Dr. Ruben Rojas-Oviedo

May 2001

Alliance for Computational Science Collaboration:

Project Objective

- Promote High Performance Computing
- Create a Local High Performance Computing Laboratory,Cluster of PCs doing Parallel Computing
- Graduate and Undergraduate Research
- Undergraduate Scholarships (12 Scholarships)
- Support Summer Interns in ORNL (2)

Support

Supporting Agency:	Project Duration:
Department of Energy	9-1999 --- 9-2001

Contributing Agencies:

Alabama A&M University
NASA Marshall Space Flight Center (Dr. Bruce Vu)
Alabama Super Computer Authority
Oak Ridge National Laboratory

Hardware

- **High Performance PCs:**

  9 PC running RedHat Linux and Windows NT

  Connected by 100 Mb/s Ethernet networks

  2 Pentium III 750 MHz, 256M RAM, 16 GB disk

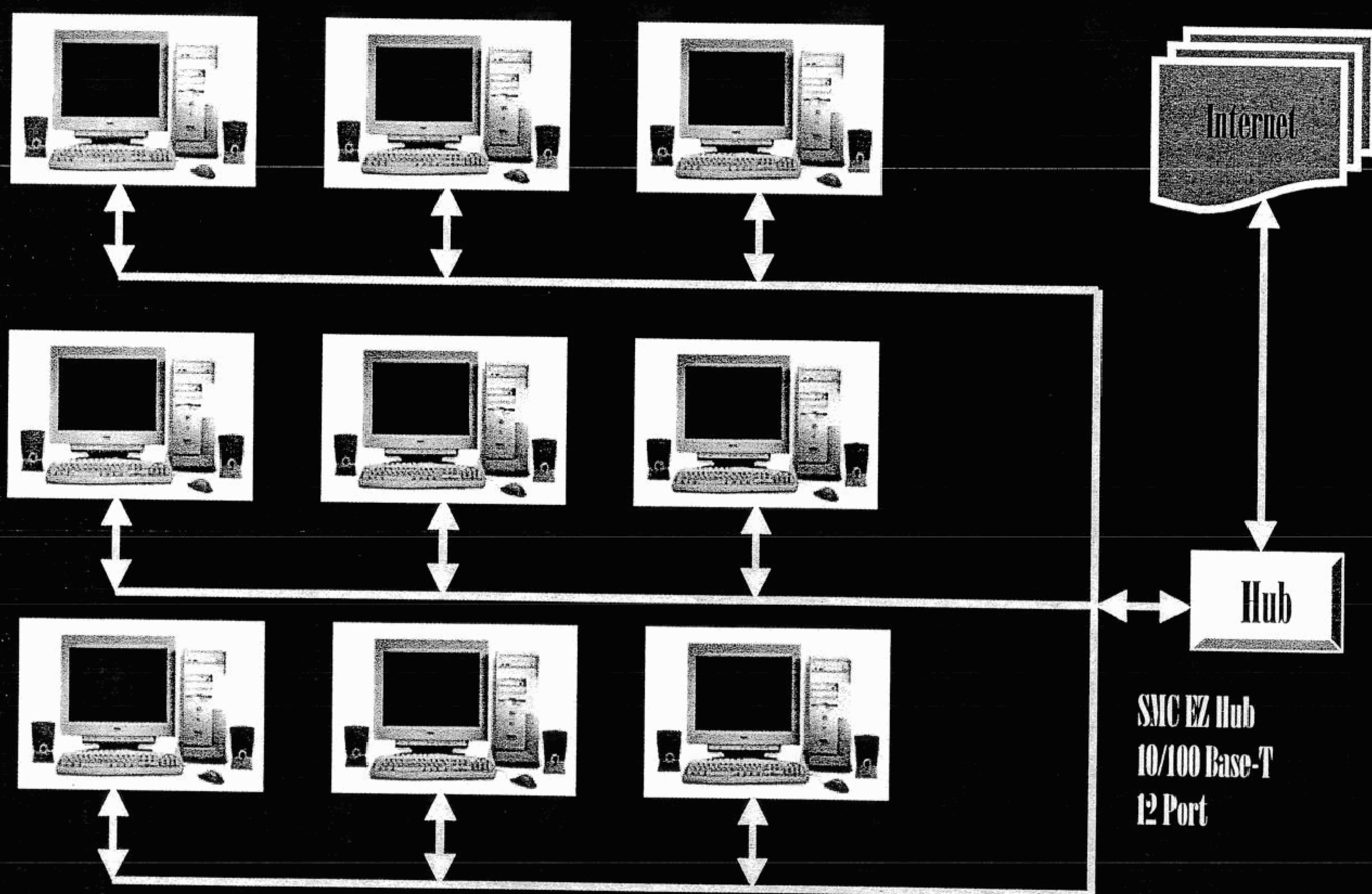
  2 Pentium III 500 MHz, 64M RAM, 13 GB disk

  2 Pentium II 333 MHz, 32M RAM, 5 GB disk

- **Workstations:**

  Sun Ultra 10 and SGI Onyx workstations connected via 10-Base-T Internet secure shell.

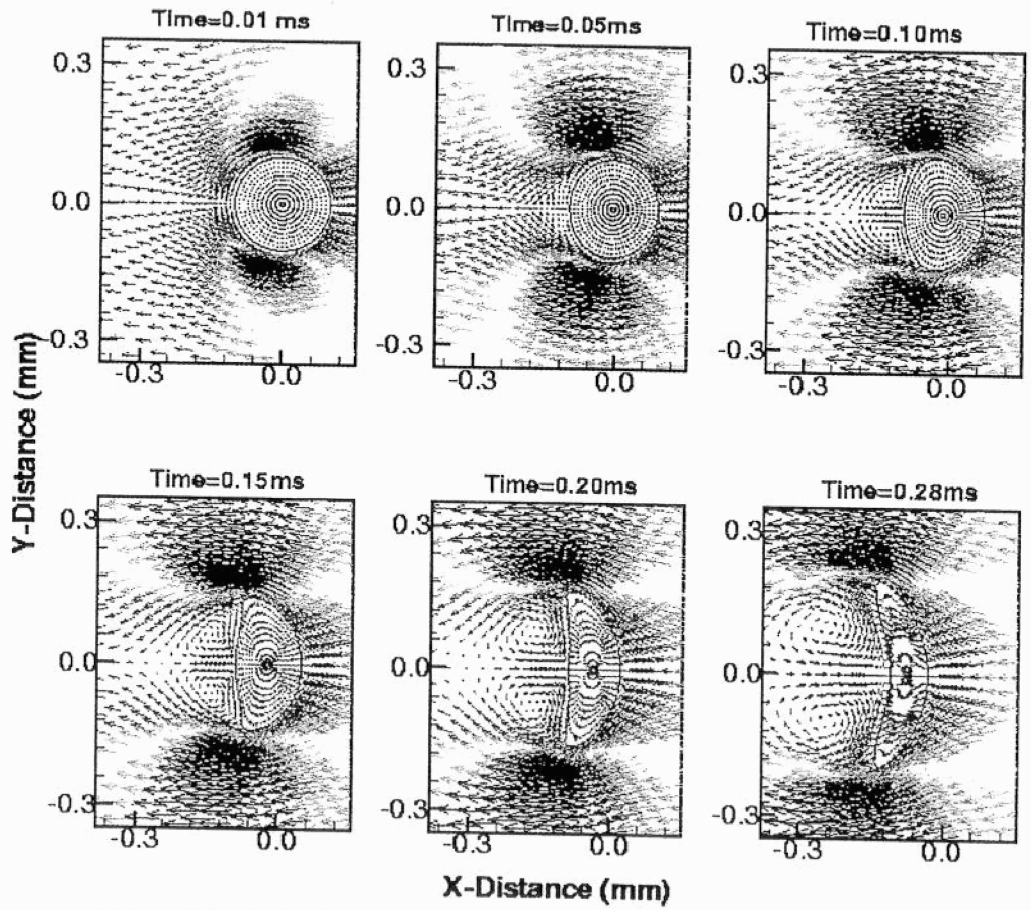
Networking: 9 PCs



Applications

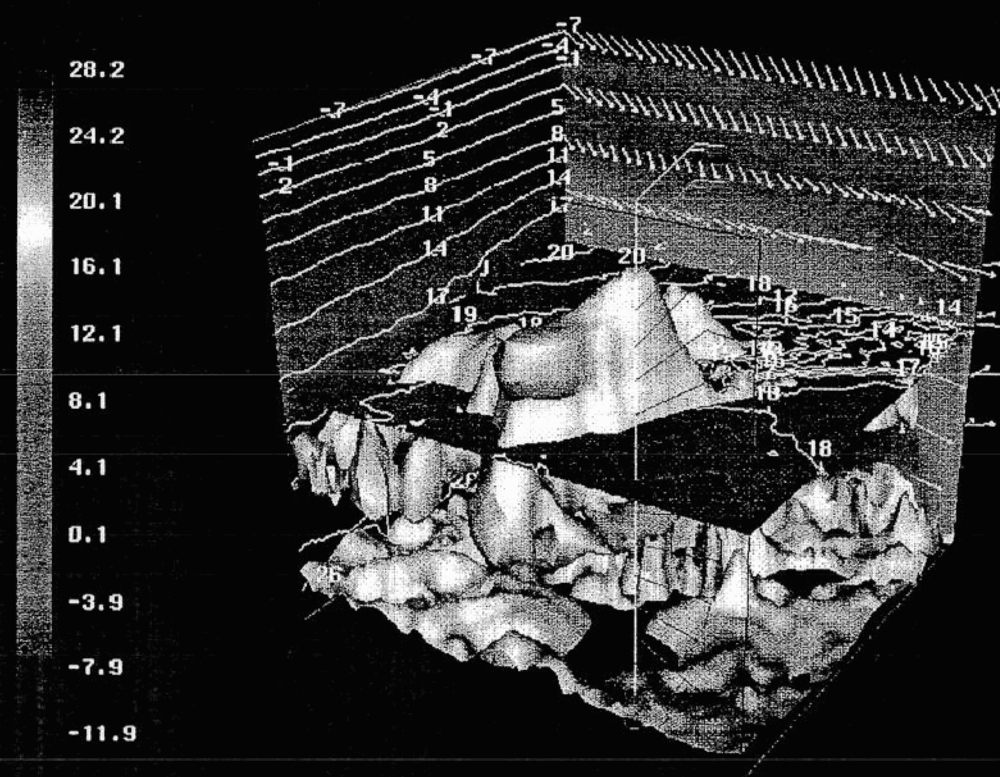
- Parallel Virtual Machine (PVM) Library
- Computational Fluid Dynamics:
  - Grid Generation (Genie ++)
  - Finite Difference Navier-Stokes (FDNS): Chemically Reacting Flows
  - RPLUS: High Speed Propulsion Simulation
  - NPARC and WIND: Generic Aerodynamic Simulation
  - KIVA: Chemically Reacting Flows
  - Scientific Data Visualization (TECPLOT, PLOT-3D)
- Finite Element Analysis: ANSYS

Spray Combustion Simulation: Droplet Dynamics



Velocity Vectors both Inside and Outside Droplet Surface at the Velocity of 4m/s

Scientific Data Visualization: Weather Forecasting

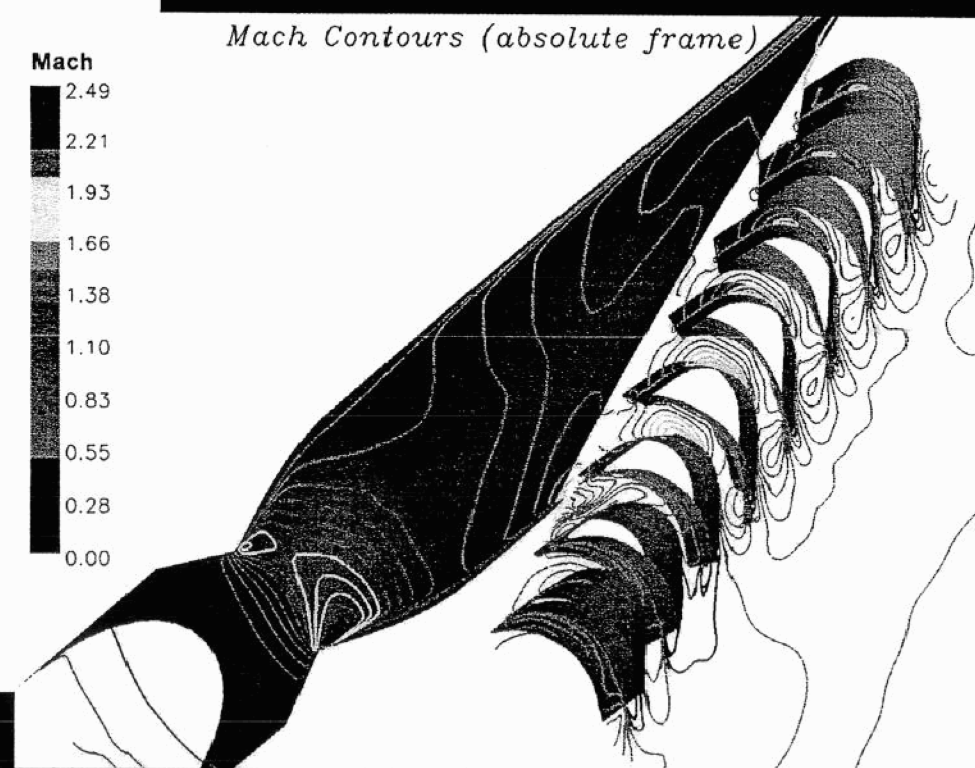


Current Parallel Computing Project using Cluster of PCs

- Develop a low-cost, high-performance parallel computing environment
- Support educational and research work on parallel and distributed computing
- Scalable systems software development to support aerospace research
- Implement state-of-the-art parallel codes

Applications

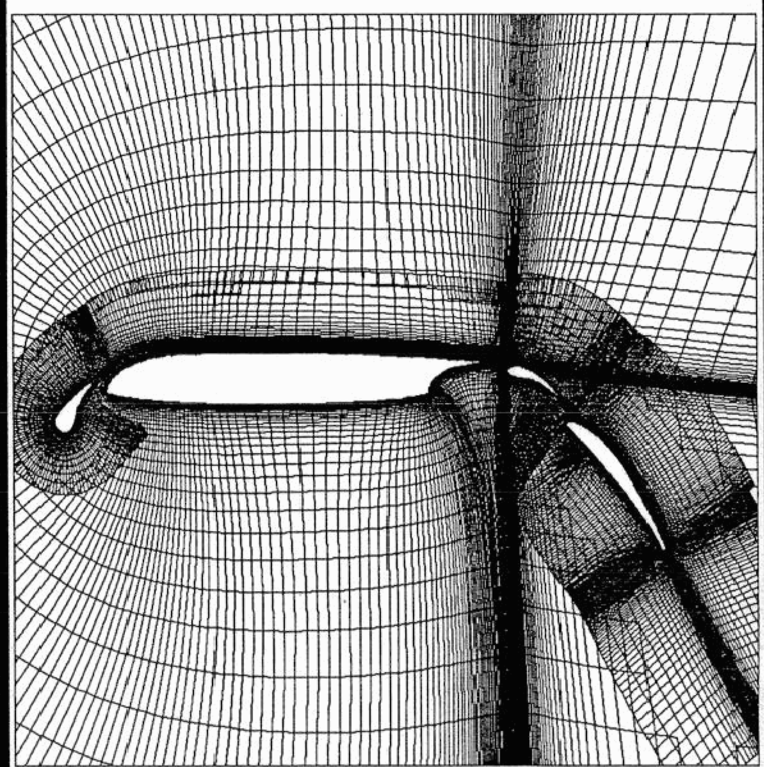
- Turbomachinery: SIMPLEX Turbopump (12 blades, 95 nozzles) using MPI. (Dr. Bruce Vu)



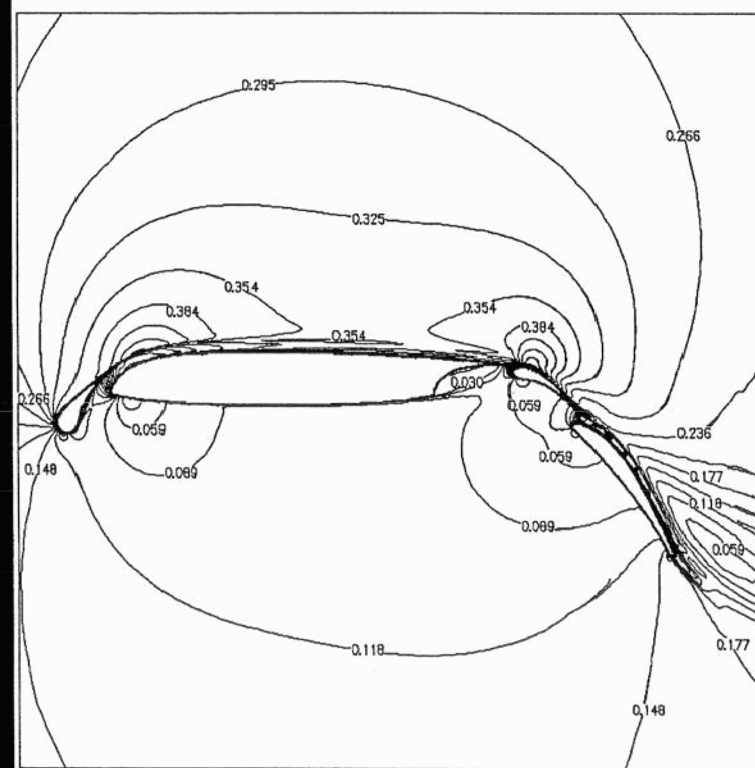
Applications

- Chimera: Multi-Element Airfoils using PVM
  (Dr. Bruce Vu)

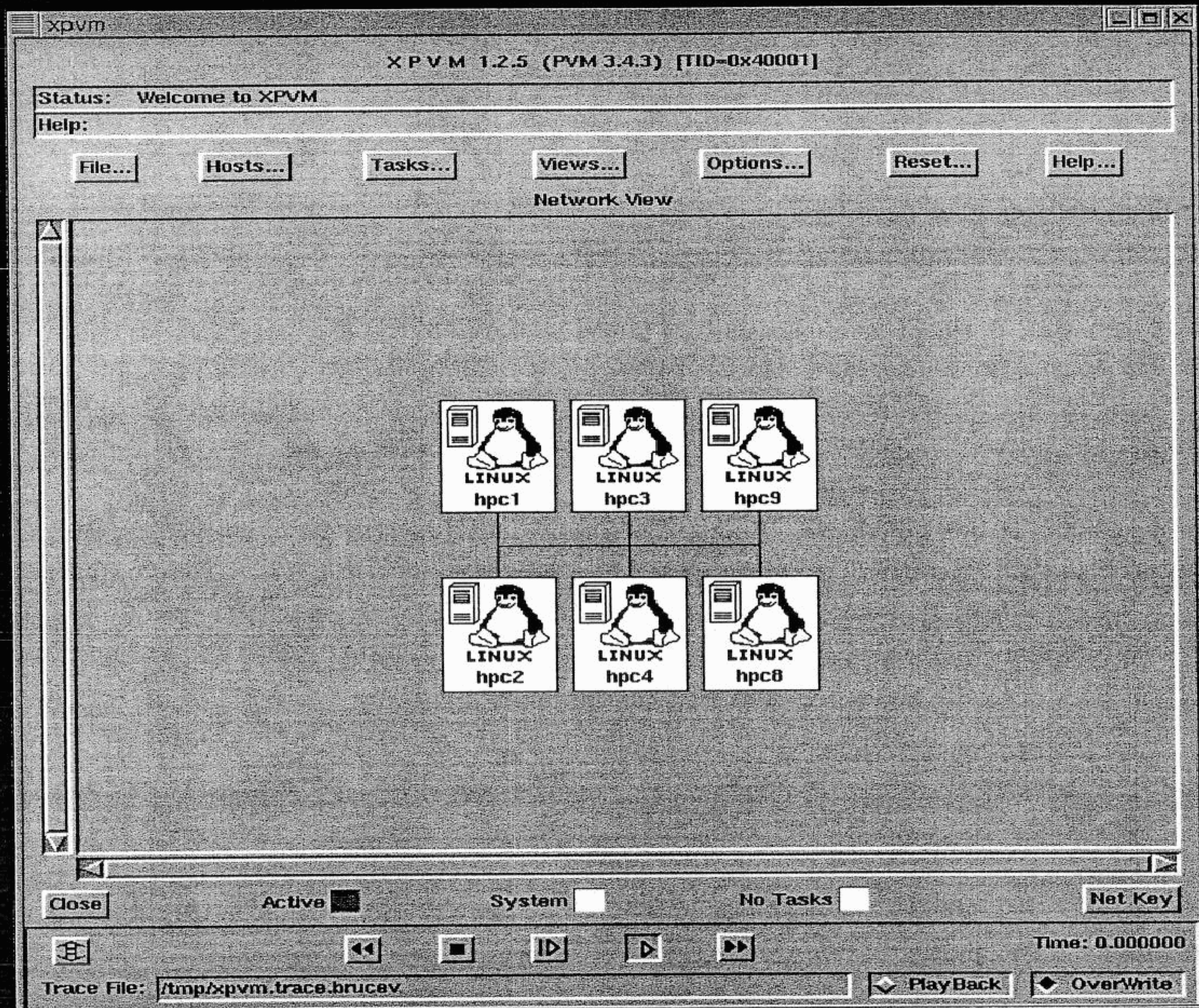
Multiple-Element Airfoil



Mach Contours



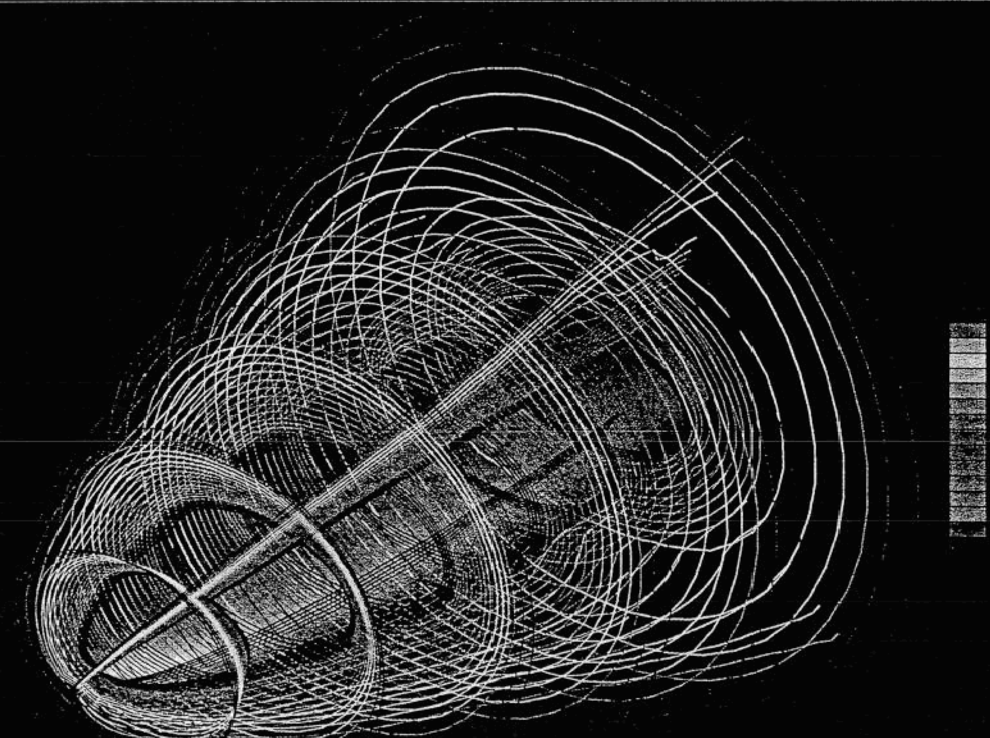
Graphic PVM--HPC Lab



Low-Reynolds Number Hypersonic Aerodynamics

(Dr. Z.T. Deng)

(RPLUS-3D, NPARC-3D, PVM)



CFD Code

(Dr. Z.T. Deng, Dr. R. Rojas-Oviedo)

- RPLUS-2D / 3D:

  Full Navier-Stokes with species transport equations
  in generalized finite volume coordinate system
  Laminar and Turbulent
  Real Gas, Chemically Non-equilibrium Flows
  Robust LU-SW/UP Scheme (Van Leer, Osher)

- ALLSPD-2D / 3D:

  Pre-Conditioning, Multi-phase, Spray
  Chemically non-equilibrium, All Mach number range
  3D Supersonic outflow condition?

CFD Code (Cont.)

- NPARC:

  Excellent for ideal gas wind-tunnel air-breathing engine applications. Full Navier-Stokes, Multi-Blocks
  Thermally perfect gas (Constant Gamma)
  Grid overlapping, Beam-Warming, Complex geometry, Parallel. Algebric turbulent model.

- KIVA-2, KIVA-3:

  3D Chemically reacting flows with spray
  Arbitrary-Lagrangian-Eulerian, 2nd Order

- BURNETT-2D / 3D, CHEMKIN, NASA-SP 273