Final Report for Period: 06/2009 - 08/2009   **Submitted on:** 01/19/2010

Principal Investigator: Yeung, Pui-Kuen .   **Award ID:** 0735157

Organization: GA Tech Res Corp - GIT

Submitted By:

Yeung, Pui-Kuen - Principal Investigator

Title:

NSF Workshop on Cyber-Fluid Dynamics: New Frontiers in Research and Education

Project Participants

Senior Personnel

> **Name:** Yeung, Pui-Kuen
>
> **Worked for more than 160 Hours:**   Yes
>
> **Contribution to Project:**
>
>
> **Name:** Moser, Robert
>
> **Worked for more than 160 Hours:**   No
>
> **Contribution to Project:**
>
>
> **Name:** Plesniak, Michael
>
> **Worked for more than 160 Hours:**   No
>
> **Contribution to Project:**
>
> Prof. Michael Plesniak of Purdue University served as one of
> the discussion leaders at the Workshop and was one of the
> co-authors of the Workshop Report submitted to NSF in December 2007.
>
> **Name:** Meneveau, Charles
>
> **Worked for more than 160 Hours:**   No
>
> **Contribution to Project:**
>
> Prof. Charles Meneveau of The Johns Hopkins University served as
> one of the discussion leaders at the Workshop and was one of the
> co-authors of the Workshop Report submitted to NSF in December 2007.
>
> **Name:** Elghobashi, Said
>
> **Worked for more than 160 Hours:**   No
>
> **Contribution to Project:**
>
> Prof. Said Elghobashi of the University of California, Irvine, served as
> one of the discussion leaders at the Workshop and was one of the
> co-authors of the Workshop Report submitted to NSF in December 2007.
>
> **Name:** Aidum, Cyrus
>
> **Worked for more than 160 Hours:**   No
>
> **Contribution to Project:**
>
> Prof. Cyrus Aidun, of the Georgia Institute of Technology, served as
> one of the discussion leaders at the Workshop and was one of the
> co-authors of the Workshop Report submitted to NSF in December 2007.

Post-doc

Graduate Student

Undergraduate Student

Technician, Programmer

Other Participant

      Name: Valero, Cathy

      Worked for more than 160 Hours: Yes

      Contribution to Project:

      Cathy Valero is the PI's administrative assistant at Georgia Tech.
      She provided administrative support, including hotel contracts,
      catering, printing of program booklet, onsite registration, and
      travel reimbursements for participants. She also traveled to the
      workshop site at NSF.

Research Experience for Undergraduates

Organizational Partners

Other Collaborators or Contacts

We have interacted with the professional society leadership
represented by the American Physical Society, Division of
Fluid Dynamics.

Activities and Findings

Research and Education Activities: (See PDF version submitted by PI at the end of the report)

Findings: (See PDF version submitted by PI at the end of the report)

Training and Development:

Outreach Activities:

The PI has helped a media relations specialist (J.S. Bardi,
of the American Institute of Physics) to plan a press conference
entiled 'Super-computations: space clouds, hurricanes and other
fluid dynamics riddles' at the site of the American Physical
Society March Meeting, in Pittsburgh, PA on March 18, 2009.
This press conference will feature the PI and all five invited
speakers from the technical session 'Fluid Dynamics and Computational
Science'.

Journal Publications

Books or Other One-time Publications

P.K. Yeung, R.D. Moser, M.W. Plesniak, C. Meneveau, S. Elghobashi, C.K. Aidun, "Cyber-Fluid Dynamics

", (2007). Formal submission to NSF, posted electronically, Accepted by NSF Program Director (W.W. Schultz, Fluid Dynamics)
Bibliography: (Final Report to NSF on
NSF Workshop on Cyber-Fluid Dynamics: New Frontiers in Research and Education)

Web/Internet Site

URL(s):
http://www.nsf-cyberfluids.gatech.edu/cybrfd_finalreport.pdf
Description:
This is the formal report of the core workshop activity in this grant.

Other Specific Products

Contributions

Contributions within Discipline:
The Workshop Report has led to a number of actions in response from
the leadership of the American Physical Society, Division of Fluid
Dynamics. For example (as of May 2008) a new Ad-hoc Committee on Cyber-Fluid Dynamics is being formed, and a new sorting category
has been added for the coming Annual APS Fluid Dynamics Meeting
in November 2008.

Contributions to Other Disciplines:
This project has helped promote communication between the fluid dynamics
and national supercomputing resources providers' communities.
The Workshop Report has been sent to the TeraGrid leadership
including the heads of all NSF-supported supercomputing centers.

Contributions to Human Resource Development:

Contributions to Resources for Research and Education:

Contributions Beyond Science and Engineering:

Conference Proceedings

Categories for which nothing is reported:
Organizational Partners
Activities and Findings: Any Training and Development
Any Journal
Any Product
Contributions: To Any Human Resource Development
Contributions: To Any Resources for Research and Education
Contributions: To Any Beyond Science and Engineering
Any Conference

Cyber-Fluid Dynamics

Final Report to the National Science Foundation on

NSF Workshop on Cyber-Fluid Dynamics: New Frontiers in Research and Education

NSF Headquarters, Arlington, VA
July 19-20, 2007
`http://www.nsf-cyberfluids.gatech.edu`

College of Engineering

Organizers:

P.K. Yeung, Georgia Institute of Technology
R.D. Moser, University of Texas at Austin

NSF Program in Fluid Dynamics

(in cooperation with Programs in)
Combustion, Fire and Plasma Systems
Dynamical Systems
Particulate and Multiphase Processes
Interfacial Transport and Thermodynamics

Thermal Transport Processes

Submitted December 21, 2007, by the report co-authors:

P.K. Yeung	Georgia Institute of Technology
R.D. Moser	University of Texas at Austin
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S. Elghobashi	University of California, Irvine
C.K. Aidun	Georgia Institute of Technology

Executive Summary

Major and high-priority investments by NSF in Cyberinfrastructure including future Petascale hardware are promising to greatly accelerate progress in Cyber-enabled Discovery and Innovation for many scientific disciplines, including fluid dynamics, which is of great importance to society, in problems ranging from environmental quality to various biomedical innovations. However, despite having been a prime driver of past HPC advances, fluid dynamicists face substantial challenges in algorithmic readiness for future Petascale platforms, in the sharing and handling of large datasets, and in a scarcity of sponsored support needed especially to develop and sustain new initiatives of a community-wide nature.

The vision behind this 1.5 day workshop held at NSF in July 2007 was to bring together, by invitation, a select but diverse group of leading fluid dynamicists, NSF program officers, and representatives of NSF-funded supercomputer centers, for a synergistic discussion on how best to enhance the impact of advanced cyberinfrastructure for fluid dynamics research and education. The program consisted of select presentations and group or plenary discussion periods focused on the themes of high-performance computing and Cyber activities, turbulence and flow control, complex fluids and multiphysics applications, nano and bio-fluid mechanics, and knowledge discovery and education. NSF's perspectives and future plans were presented by the NSF Assistant Director for Engineering and program directors from the Directorate for Engineering and Office of Cyberinfrastructure. All of the presentations, as well as participants' names and short biographical sketches, are recorded on the conference website, `http://www.nsf-cyberfluids.gatech.edu`, hosted by the Georgia Institute of Technology. The Discussion Leaders were asked to join the workshop organizers to prepare this report, which also includes input from participants via a post-conference questionnaire suggested by the NSF Program Director in Fluid Dynamics.

Discussions at the workshop produced broad consensus on several key issues underlying the community's needs as the era of Petascale computing rapidly approaches. Although large-scale computing has brought many advances to the field, expertise for scaling codes effectively to possibly hundreds of thousands of processors is not widely available, especially for flows with multiphysics content where the mathematical foundations of the subject often cause difficulties often not widely appreciated by practitioners in other disciplines. Training of graduate students who often have little prior programming background is likewise a concern, given the increasingly high level of computer-science expertise that must be mastered. While collaborative research efforts are not uncommon, most in the community do not see a clear path to mechanisms for open-source code development or efficient handling of large datasets which are essential for wide participation. Several reasons were brought forward for the perception that fluid dynamicists have not been using NSF-supported TeraGrid resources at a level commensurate with the magnitude and importance of fluid dynamics problems. One of these is increasing scarcity of funding for research in fundamental fluid dynamics, which provides much of the motivation for use of Cyber resources. This is a situation which (if uncorrected) can imperil the community as a whole, and suggests that the importance of fluid dynamics in many interdisciplinary contexts is not sufficiently well appreciated by the public, funding managers, and reviewers alike.

In view of these observations, we propose several recommendations both to (i) the fluid dynamics community on ways to advance and sustain the discipline in a new era of Cyber opportunities, and (ii) agencies, funding managers, and resource providers on how they can facilitate, encourage, and support the community's efforts.

Recommendations to the Fluid Dynamics Community

We recommend that the community address challenges of large-scale algorithmic scalability aggressively, by drawing from the expertise of top-level computer scientists, while promoting a culture of open communication and community-wide standards so that as many researchers as possible, including students exposed to the national supercomputing landscape, will benefit without duplication of effort. We call on leading data authors and data users in several areas to formulate community agreements on data formats and download or transfer protocols, especially for very large datasets of either computational or experimental origin. Efforts at building virtual organizations incorporating these elements, and more, are highly encouraged. We recommend that the community work more closely, within itself and with NSF program directors, to communicate to a wide audience, including the public, agency officials, and students, the importance of fluid dynamics, both on its own merits and in many interdisciplinary endeavors meeting current areas of national needs. We also urge that the community's primary professional society leadership take an active role in facilitating, guiding and promoting such endeavors from community-minded individuals meeting high standards of scholarship.

Recommendations to NSF, Other Agencies and TeraGrid Resource Providers

We recommend that all major Federal funding agencies examine and strengthen their direct and indirect support for fluid dynamics research, in consideration of the societal importance of the subject, and especially for fundamental research which is the motivator of most large computations helping drive HPC development. Within NSF, we urge that the Fluid Dynamics program be given an immediate and sustained budget increase, with priority given to proposals and community-minded activities designed to allow more researchers to benefit from advanced Cyberinfrastructure. We also recommend that, with help from the community, the Fluid Dynamics program director (and his future successors) continue to be a strong advocate for the subject, at various levels within NSF, including the Office of Cyberinfrastructure, where co-funding of proposals may be appropriate. Interagency dialogs are similarly encouraged. Finally, we recommend that TeraGrid Resource Providers increase their efforts to promote awareness of HPC resources and services available, and that resource allocation committees give greater weight to science impact versus scalability performance, where the challenge varies in different classes of problems.

We expect full adoption of these recommendations will dramatically enable a Cyber-Fluid Dynamics community that will be a leader in using Cyberinfrastructure to maximal benefit, including large-scale computation, dataset handling, and vibrant virtual organizations.

Acronyms

ACI   American Competitiveness Initiative
AFOSR   Air Force Office of Scientific Research
AIChE   American Institute of Chemical Engineers
APS   American Physical Society
ASCI   Advanced Simulation and Computing Initiative (a program of DOE)
ASME   American Society of Mechanical Engineers
CBET   NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems
CDI   Cyber-enabled Discovery and Innovation
CFD   Computational Fluid Dynamics
CFD   Cyber-Fluid Dynamics
CI   Cyberinfrastructure
DFD   Division of Fluid Dynamics (a unit of the APS)
DNS   Direct Numerical Simulation
DOD   U.S Department of Defense
DOE   U.S Department of Energy
EPA   U.S. Environmental Protection Agency
NASA   National Aeronautics and Space Administration
NSF   National Science Foundation
ENG   NSF Directorate for Engineering
HPC   High-performance Computing
LES   Large-eddy Simulation
NIH   National Institutes of Health
OCI   NSF Office of Cyberinfrastructure
ONR   Office of Naval Research
PD   Program Director
PIV   Particle Image Velocimetry
RANS   Reynolds-Averaged Navier-Stokes
VO   Virtual Organization

Acknowledgments

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Contents

1 Introduction, Motivation and Context

Enormous advances in supercomputer power worldwide in the first few years of the 21st Century have been leading to unprecedented opportunities to many fields of science and engineering, such as protein chemistry, astrophysics, earthquake and climate change predictions. Through a number of programs and solicitations (see Appendix A) administered by its Office of Cyberinfrastructure, the National Science Foundation has made investment in Cyberinfrastructure, and more generally the theme of Cyber-enabled Discovery and Innovation (CDI), a priority for at least the next 5 years. In particular, the speed of the fastest supercomputer on the NSF-supported TeraGrid is expected to increase from about 20 Teraflop/s in 2006 to 500 Teraflop/s by December 2007, and likely beyond 10 Petaflop/s by the year 2011, i.e. a factor of 500 within a 5-year time frame. Clearly, this points to a bright future for computational science, in part since such ultra-fast hardware will allow computations at problem sizes not feasible before. However, there are also highly nontrivial challenges such as algorithmic scalability to very large (possibly 10^6) number of processors, long-term archival of Petabyte-sized datasets, and their effective use by the wider research community.

Fluid dynamicists have long been active in High-Performance Computing (HPC), ranging from fundamental studies of turbulence (see, e.g., [1], [2], [3], although the largest calculations to date have been performed outside of the U.S.), to applications in aircraft design, weather prediction, and more recently many important problems in nano- and bio-fluid mechanics. The fluid dynamics community has a healthy tradition of recognizing experiment, theory, and simulation together as essential and inter-dependent branches of scholarly inquiry. However, it is not clear whether many research groups are well prepared to exploit future platforms of hundreds of thousands of processors or more that will will become available in the U.S. within the next few years. Furthermore, compared to some other disciplines (e.g. computational chemistry, or climate modeling), sharing of large datasets between different research groups is often ad-hoc, and sharing of highly developed computer codes is even less common. Since large resource allocations on future high-end computers are likely only for a small number of highly skilled research groups, more collaborative work, e.g. via the "virtual organization" concept currently promoted by NSF, is clearly needed to achieve maximum benefit for all.

Given the context above, and with much encouragement and assistance from the current NSF program director for Fluid Dynamics (W.W. Schultz), we organized an invitation-only workshop at NSF in July 2007, in order to bring together several constituencies for a synergistic discussion on how best to enhance the impact of advanced cyberinfrastructure for fluid dynamics research and education. The majority of attendees are those from the broad fluid dynamics community who have a strong record of commitment in (i) conducting state-of-the-art computations and sharing both data and algorithmic expertise with others, (ii) using simulation data for knowledge discovery, or (iii) enhancing impact via educational and outreach activities. They were joined by several representatives of NSF-supported supercomputer centers, a number of NSF officials from other programs in the CBET Division and the Office of Cyberinfrastructure, as well as the NSF Assistant Director for Engineering.

The *first purpose* of this Report is to document the conduct of the workshop activity, including program content, participant profiles, formal presentations, and group discussion summaries. The *second purpose* is to suggest and help promote collaborative strategies which would help the fluid dynamics community as a whole to be better prepared to fully utilize future advancements of Cyberinfrastructure resources, for both research and education. This

report is prepared by the workshop organizers and breakout group discussion leaders, under a charge from the Fluid Dynamics Program at NSF to provide recommendations based on discussions at the Workshop as well as other forms of input subsequently received from the community. Here we shall interpret the notion of a fluid dynamics community broadly, such that this report should serve as a useful point of reference for not only NSF officials in charge of Fluid Dynamics and related programmatic units, but also the disciplinary leadership in major professional societies, as well as a diverse set of individuals from academia and national laboratories interested in the pursuit of Cyber-enabled discoveries in both fundamental and applied fluid mechanics.

Traditionally, the acronym CFD is taken to represent Computational Fluid Dynamics, which is the development and application of computational methods to fluid dynamic equations, usually in the form of partial differential equations. An underlying theme in our Workshop is to promote the concept of *Cyber-Fluid Dynamics*, which is much broader in scope: encompassing, for example, new challenges in the processing and handling of massive datasets (see [4]), virtual collaborations, and other modes of Cyber-enabled research endeavors, in addition to the conduct of large computations *per se*.

2 Workshop Objectives and Desired Outcomes

Our overall goal was to provide a forum for current leaders in fluid dynamics research and education and Cyberinfrastructure resource management to share ideas, expertise, information, and needs, and to develop collaborative strategies and recommendations that will serve the community as a whole in a broad range of Cyber-enabled endeavors. Decisions on the structure of the Workshop program and selection of participants by invitations were made based on input from NSF and several other individuals, bearing in mind the following objectives of the Workshop activity.

1. *Share expertise and future outlook in advanced computing.* Fluid dynamics currently has a relatively modest presence among the larger user groups on the TeraGrid. Our objective was for leading computational researchers to share their current progress, inform others of data availability, and receive feedback on the types of data needed. We also invited NSF and TeraGrid officials to discuss with Workshop participants resources currently available and projected or desired in the future.

2. *Build a "virtual community" for knowledge discovery.* Although the importance of combined use of theory, experiment, and computation in fluid dynamics research is well accepted, few formal mechanisms exist for sharing large datasets within the community. Our objective was to identify strategies to build and maintain long-term data repositories based on a "virtual community" approach, and to assess the need for funding agencies to support such collaborative efforts.

3. *Promote public awareness, education and outreach.* Wide appreciation for the practical importance and intellectual challenges of fluid mechanics is crucial for sustaining agency investments and recruiting young minds for the long-term health of our discipline. Our objective was to devise educational initiatives drawing on the future promise of Petascale computing, e.g. using scientific visualization, and to help promote computational science as a new field of graduate study.

The desired outcomes of this Workshop can be summarized as consisting of two major aspects. The first is a well-informed research community that is ready and willing to invest time and effort in a collaborative manner to make optimal use of continuing advances in supercomputer power for science discovery, and committed to attracting and training graduate and undergraduate students for these endeavors. The second is an improved funding climate, at NSF and elsewhere, that is necessary to encourage and sustain noew initiatives by our research community, in Cyber-enabled discovery and other complementary approaches in fluid dynamics research.

3 Overview of Program and Participants

A copy of the Workshop Program is included in the Appendix B to this Report. In planning the program an important consideration was to maximize interactions among participants and devote sufficient time for discussion within practical constraints on the workshop length (1.5 days). This required us to limit the number of participants, number of speakers, as well as length of time allowed for most presentations.

The Workshop program began with brief Opening Remarks by P.K. Yeung (Georgia Tech, as Lead Organizer), W.W. Schultz (NSF Program Director for Fluid Dynamics), R.O. Buckius (NSF Assistant Director for Engineering), and J.A. Raper (NSF CBET Division Director). The main portion of the program consisted of five sessions with the themes as indicated below, each followed by a group or plenary discussion period:

Session I. High-performance Computing and Cyber Activities.
NSF's Cyberinfrastructure vision and opportunities, latest developments in architecture, large-scale parallel code development, benchmarking and performance monitoring, database maintenance and access, and scientific visualization.

Session II. Turbulence and Flow Control.
Direct and large-eddy numerical simulation of canonical flows, isotropic turbulence, wall-bounded and free shear flows, control of turbulent boundary layers, intermittency, resolution requirements, mixing and dispersion, flow control strategies and applications, and use of simulation data for theory and modeling.

Session III. Complex fluids and multi-physics applications.
Non-Newtonian fluid mechanics, suspensions, and polymers, multiphase flow, flows with chemical reactions, molecular dynamics simulations, and applications in industrial materials processing.

Session IV. Nano and bio-fluid mechanics.
Microfluids, Lattice Boltzmann methods, fluid mechanics of human circulatory, respiratory, and digestive systems.

Session V. Knowledge discovery and education.
NSF's CDI Vision, Engineering Virtual Organizations (EVO), science gateway issues, web portals, and use of multi-media materials in undergraduate education.

Sessions I and V were central to the rationale for this Workshop, and leadoff presentations were given by NSF Program Directors in charge of Petascale Applications (PetaApps,

nsf07559) and Engineering Virtual Organizations (EVO, nsf07558) solicitations respectively. Other speakers in these sessions included a representative of the TeraGrid resource-provider sites, a researcher who maintains an international numerical simulation database in Europe, and individuals experienced in web-portals, data repositories, scientific visualization, and the analysis of large datasets from highly developed laboratory experiments. Training of graduate students for advanced cyberinfrastructure was also an issue of wide interest.

Sessions II, III and IV were topic sessions focusing on Cyber issues in research areas supported within the Fluid Dynamics Program's portfolio. Speakers were generally selected from the ranks of researchers who either have a reputation for using large-scale computation effectively in studying fundamental flow physics, or are highly familiar with the technical challenges involved in specific classes of problems. Many of these individuals also shared very valuable insights in how the community can work together and compete for financial and cyber resources with a higher degree of success.

Invitations to the Workshop were handled by the PI based on the collective advice and suggestions provided by NSF Program Directors and several key individuals asked to assist in the planning. The primary objective of this invitation process was to assemble a diversified group which covers a wide range of areas of interest and research approaches (e.g., including experimentalists) while also including individuals at different career stages. Attention was also given to NSF's goals of increasing the participation of under-represented groups where appropriate, and to maintain a reasonable degree of balance among different institutions. The process took several weeks to complete but appears to have led to good results. All participants (listed in Appendix C) were asked to supply one-paragraph biographical sketches which were eventually posted on the workshop website.

It is worth noting that a number of other individuals were contacted had expressed strong support for the theme of the Workshop despite being unable to attend. Many of those in fact indicated a strong willingness to be involved in the future for the benefit of our research community at large. Comments and ideas from a wider community beyond the actual attendees have been sought. Likewise, while the size of the workshop was necessarily limited, we also recognize, especially in our follow-up efforts, the activities of other fluid dynamicists (e.g. in atmospheric science, oceanography, applied mathematics) supported by other NSF units.

4   Presentations by NSF and TeraGrid Officials

It is important for the attendees, and the fluid dynamics community at large, to be adequately informed of NSF's perspectives in Cyberinfrastructure investments, and of resources and services available at various TeraGrid sites. We provide below summaries of presentations by several NSF officials and a representative of the TeraGrid.

Dr. Richard Buckius (NSF Assistant Director of Engineering) provided an analysis of NSF investments in separate sub-categories of cyberinfrastructure, and presented data on funding trends from FY 1984 to 2006. He began by noting that the American Competitiveness Initiative [5] calls for doubling over the next 10 years of federal investment in key agencies that support basic research in physical sciences and engineering. He pointed out that many of the Engineering Directorate's programs already support projects relevant to one of the ACI Goals, of advancing modeling and simulation in a broad range of disciplines. Current strengths

are noted in e.g., development and deployment of CI for Virtual Organizations, and the use of CI for large-scale simulation/optimization problems via high-performance computing. Dr. Buckius noted that ENG funding rates have been consistently lower than the NSF average, being at the lowest point in FY 2005, while number of proposals received has been steady or increasing. Multi-investigator awards have been increasingly favored compared to single PI efforts although in the last 2-3 years there is a trend or effort to maintain a balance. Dr, Buckius also pointed out that in the near future NSF plans to invest substantially in the theme of Cyber-Enabled Discovery and Innovation (CDI), which includes sub-areas such as interacting elements, computational experimentation, knowledge extraction, virtual environments, and education in computational discovery.

Dr. Abani Patra (NSF Program Director, Office of Cyberinfrastructure) provided an overview of OCI's programs to accelerate progress in Cyber-enabled Science and Engineering, and encouraged the audience to increase collaborative efforts needed to ensure benefits for many instead of a few. He began by stating that achieving the NSF CI Vision requires synergy between three types of activities, namely (i) creation, deployment and operation of advanced CI; (ii) transformative application to of CI to enhance discovery and learning, and (iii) research to enhance technical and social effectiveness of future CI. NSF is building a portfolio of high-end systems under so-called "Track 1" and "Track 2" competitions with the former expected to be capable of *sustained* performance at 1 Petaflop/s by 2011. Dr. Patra briefly reviewed a number of recently announced software-oriented solicitations, on Petascale software development (nsf07559), Community-based Data Interoperability Networks (nsf07565), Software Development for Cyberinfrastructure (nsf07503), and Strategic Technologies for Cyberinfrastructure (PD 06-7231). Dr. Patra noted that true predictive science will require tight coupling between models and data, but that classical paradigms for science could restrict collaborative endeavors. He suggested the keywords "Engage, Explore, Apply, Share" as the basis of a new paradigm towards the development of community-driven Science Gateways.

Dr. Philip Westmoreland (NSF Program Director for Combustion, Fire and Plasma Systems and of the NSF/ENG Cyberinfrastructure Working Group) spoke on the concepts and uses of Cyberinfrastructure (CI) and Virtual Organizations (VOs). Cyberinfrastructure includes computers, middleware and applications software, Web resources, and the Internet, yet it is more than the sum of its key components. Rather, by understanding the coupling of these resources it provides an infrastructure that enables new approaches to research and development. Dr. Westmoreland then explained that a virtual organization is typically a group of geographically dispersed collaborators engaged in storing, retrieving, analyzing or visualizing data in comparison to theories or models, and working together on a real-time basis using advanced conferencing protocols. References were made to a Cyber-Based Combustion Science workshop held also at NSF in April 2006 (`http://www.nsf-combustion.umd.edu`) and some VO examples activities such as the ongoing Turbulent Premixed Flames (TNF) international workshop (`http://public.ca.sandia.gov/TNF/abstract.html`), Process Informatics Model (`http://www.primekinetics.org`), and the Network for Computational Nanotechnology (`http://www.nanoHUB.org`). Dr. Westmoreland also pointed to the earlier Engineering Virtual Organization solicitation (`http://www.nsf.gov/pubs/2007/nsf07558/nsf07558.htm`) to illustrate NSF's commitment towards promoting these approaches for exploiting CI for both education and research. [Subsequently in September 2007, NSF issued a Foundation-wide solicitation for a five-year, $750 million initiative on Cyber-Enabled Discovery and Innovation (`http://www.nsf.gov/crssprgm/cdi`), which includes VOs as one of the three core themes.]

Dr. Richard Moore (of San Diego Supercomputer Center, and member of TeraGrid Management team) gave an overview of the work of the TeraGrid, which is a network of (currently) 10 NSF-supported Resource Provider sites serving the broad national academic research community. Dr Moore explained the TeraGrid objectives as Deep (science via enabling Tera/Petascale applications), Wide (impact via empowering diverse communities), and Open (cross-site coordination and open partnerships). He gave an abbreviated list of resources available at different sites and indicated that the community can look forward to a lot more on the way, beginning with a new Sun/AMD system that at a peak of 500 Teraflop/s will more than double the total existing capacity by December 2007. (Information on proposal submission for such resources can be found at `https://pops-submit.ci-partnership.org`.) A breakdown of usage of TeraGrid resources by various disciplines was provided, which showed Engineering as apparently under 20%, with Chemical and Transport Systems accounting for about half of this relatively small share of the total. Dr. Moore then mentioned several examples of Science Gateways enabled by TeraGrid member sites which are tailored to meet the computational needs of specific scientific communities. Advanced technologies (e.g., Storage Resource Broker and a global filesystem) are available within the TeraGrid. Several important features of the Network for Earthquake Engineering Simulation (`http://www.nees.org`) were discussed to illustrate capabilities.

Dr. William Schultz (NSF Program Director for Fluid Dynamics) provided some informal but valuable remarks at the close of the Workshop event. As the prime sponsor of this Workshop, he presented the vision of "No CFD'er Left Behind", i.e. the hope that as many researchers as possible in (computational) fluid dynamics be able to benefit substantially from NSF's Cyberinfrastructure investments. He noted that collaborations with computer scientists will often be necessary or fruitful but more cross-talk is needed e.g. in the distinctions between "computer science" and "computational science". Dr. Schultz emphasized that NSF's agenda is open to input or influence from the research community, including the proposal subjects to be encouraged or nurtured. More importantly, he noted that there is a sense that communities in other disciplines have collaborated more effectively, conducted better public outreach, and have been able to obtain funding from a variety of NSF programs including those far from a researcher's own primary area. Dr Schultz advised that proposals that are hypothesis-driven, that give close attention to broader impacts, and provide a balance between modeling and experiments tend to be most successful in panel review. He suggested that the community should work harder on articulating challenges and benefits of their work to society (e.g. by submitting nuggets of research highlights to NSF) and to watch out for future solicitations. Finally he requested that attendees complete a post-conference questionnaire which (at the end) asks each individual what he/she is willing to do for the Cyber-Fluid Dynamics community.

5   Session Summaries and Discussions

We provide session summaries of each of the five topic sessions at the Workshop. Since (in addition to information in Sec. 4) all Abstracts of formal presentations are included in the Appendix D and the presentation files are posted at the workshop website, we focus here mainly on the discussion periods according to notes prepared by the Discussion Leaders. Since some of the issues raised in these discussions were, not surprisingly, not restricted to distinct subject areas (nor to those who specialize in computational approaches), some overlap is expected. Information updates and comments by the report authors are indicated in square brackets.

5.1 High-Performance Computing and Cyber Activities

The following presentations were made in Session I:

1. "Cyberinfrastructure for collaborative and predictive simulations" by Abani K. Patra, NSF (Office of Cyberinfrastructure)

2. "TeraGrid CI resources for CFD research" by Richard L. Moore, San Diego Supercomputer Center

3. "iCFDdatabase: The International CFD database" by Federico Toschi, C.N.R (Italy)

The first two of presentations are explicitly summarized in Sec. 4. The third is about a growing web-portal based in Europe to store and share large datasets in the study of turbulence. It has some of the functional features expected of Virtual Organizations discussed in our Workshop.

The discussion focused on high-performance computing and related issues, including some which arose from the remarks stated during the Opening Session, and from question-and-answer periods following each presentation in Sec. 1. Specifically, the following issues were discussed at length:

Is the fluid dynamics community not a large user of HPC? Although the CFD community has not been getting a very large fraction of NSF-funded HPC resources (TeraGrid), discussions reveal the consensus that it is in fact a major user, on the TeraGrid as well as machines supported by Department of Defense and Department of Energy. Specifically:

- CFD researchers were the pioneers, some researchers have their own clusters and do not need access to publicly-shared HPC facilities.
- Three of the top 20 users of TeraGrid are CFD users. [However, competition from other disciplines for large allocations is very strong, and and there are concerns about the review process.]
- A significant problem is how to handle (store, transfer, visualize) the huge amounts of data that we already generate.

Are CFD codes scaling well, and how can challenges for high scalability be addressed? It was apparent from the discussion (and confirmed by post-conference questionnaire results in Sec. 6) that most practitioners in our community do not have codes readily scalable to the range of $10^4 - 10^6$ processors. Specifically: participants expressed views as follows:

- It is unclear how to solve linear systems on more than 1000 processors. [This comment underscores the fact that not many users have experience in running on such big machines, where new issues in scalability can indeed arise.]
- Depending on the numerical method appropriate to the physical problem at hand, sophisticated pre-conditioners may be necessary.
- Perhaps colleagues in computer science can help develop new methods or algorithms.
- Chemical kinetics in combustion is usually amenable to scale up. [Reacting flow simulations may scale better because more single-processor computation is being done.]

- The astrophysics community (which has interests in fluid dynamics) has developed a community code called FLASH, which is a community code professionally maintained at the University of Chicago. This is a good example for our community.

What are major needs for the Cyber-Fluid Dynamics community? Some of the points listed below also echo those stated in preceding paragraphs.

- To engage in two-way dialog and increase interdisciplinary collaboration with colleagues in computer science and applied mathematics
- To inventory types of solvers and numerical tools
- To identify fundamental roadblocks that prevent or limit scalability
- To develop community-wide resources or codes, such as the FLASH code used in astrophysics, and codes for climate modeling (from NCAR)
- To articulate key problems and benefits to society, as part of effort to promote funding for (computational) science, versus "computer science".
- To identify and articulate Grand Challenge problems which could energize the community and help demonstrate to others the impact of fluid dynamics research on many aspects of society.

How can the fluid dynamics community benefit directly from new NSF Cyberinfrastructure funding? Th discussion here mainly relates to a new NSF solicitation entitled "Cyber-Enabled Discovery and Innovation" (CDI). [The solicitation was not finalized yet at the time of the Workshop; it has since been released publicly in late September 2007.] The solicitation is understood to emphasize three thematic areas of interest to NSF, namely

- From Data to Knowledge
- Understanding Complexity in Natural, Built and Social Systems
- Building Virtual Organizations

It seems that the CFD community is well-poised to respond to the solicitation. For example turbulence researchers face challenges directly related to the explicitly stated thematic areas, e.g. in identifying patterns and structures in massive databases, and simulating and predicting complex stochastic or chaotic systems. [However, since the total number of awards in FY 2008 Foundation-wide is 30, strong competition from other disciplines is expected.]

There have been several recent NSF workshops and panels relevant to the fluid dynamics community. Their recommendations may provide useful insights for us as well. These reports and workshop activities are:

"Report of the National Science Foundation Blue Ribbon Panel on Simulation-Based Engineering Science: Revolutionizing Engineering Science through Simulation", May 2006, J. Tinsley Oden, Chair, University of Texas at Austin.

"Report on the NSF Workshop on Cyber-Based Combustion Science," April 19-20, 2006, [Note several attendees at our Workshop were also present in this past workshop.] Authors: A. Trouv, D.C. Haworth, J.H. Miller, L.K. Su & A. Violi, http://www.nsf-combustion.umd.edu)

"Workshop on Cyberinfrastructure (CI) in Chemical and Biological Process Systems: Impact and Directions, A University-Industry-CI Perspective." September 25-26, 2006, Jim Davis, UCLA.

5.2 Turbulence and Flow Control

The following presentations were made in Session II:

1. "Intermittency, mixing and dispersion in simulations of homogeneous turbulence: the path towards Petascale" by P.K. Yeung (Georgia Tech)

2. "Simulation of wall-bounded turbulence: what more can we learn?" by Robert D. Moser (Univ. Texas at Austin)

3. "Closed-loop flow control: simulation challenges and opportunities" by Tim Colonius (Caltech)

The first two of these described current and possible future uses of large-scale computing for two canonical turbulent flows, namely homogeneous isotropic turbulence and fully-developed turbulent channel flow. The third explored the role of numerical simulation and reduced-order modeling of flow control problems such as drag reduction and mixing enhancement.

Direct numerical simulation (DNS) of turbulent flows has been a prototypical application of large-scale computational fluid dynamics for the past three decades. It has played an increasingly important role in elucidating important physical understanding, facilitating model testing (for LES, RANS, etc), and in developing many flow control strategies. The range of scales that needs to be computed, and hence the number of grid points, is well known to be strong functions of the Reynolds number. With increasing computation power and memory available, higher and higher Reynolds numbers have been achieved. However, serious challenges remain because even at the Reynolds numbers achievable with DNS today, many asymptotic theories still cannot be tested in a satisfactory fashion. And, many practical applications of complex flows or control schemes at high Reynolds numbers cannot yet be computed using DNS. The possibilities for exploiting Petascale computing and beyond seem vast.

The desirability of pursuing cyber fluid dynamics and turbulence simulations on powerful next-generation platforms was beyond doubt to those who participated in this group discussion. Therefore, attention quickly evolved from technical issues associated with simulating turbulent flows and control processes to broader aspects and general challenges of today's funding situation at NSF and what recommendations could be given. The discussion centered on the following themes:

1. Strategies for increasing the turbulence community's participation in HPC and Cyber activities. (Or, what are challenges in effective use of HPC in this area?)

2. What intellectual and strategic arguments can we provide to NSF to help expand the CBET Fluid Dynamics program to a level commensurate to what this existing and developing community clearly requires? This recognizes that fluids and turbulence are in fact still a major player in HPC, but is highly dispersed within other application areas that employ HPC in more recognized fashion (e.g. geosciences, astrophysics).

3. Education and the future: Since fluids and turbulence are major players (although dispersed) in today's most societally relevant fields (environment, energy, homeland defense), it should be fairly straightforward to motivate the next generation of students, especially if targeting broader representation. Further discussion of this important item was postponed to later plenary discussion periods of the workshop.

Strategies for increasing the turbulence community's participation in HPC and Cyber activities

- How to recover the lead that CFD had in the 1980's:

  Front-section placement may still exist, but the label or link to fluid dynamics or turbulence is not well publicized by practitioners. Thus the discipline's broad impact has not received appropriate attention at organizational and institutional levels.

- "Is Turbulence/Fluids really a good HPC flagship application, since strong non-local couplings makes scalability especially challenging?"

  Yes - turbulence simulations very demanding computing applications, and many nontrivial challenges arise in developing highly scalable parallel codes in this area. Attention from the HPC community has increased as a result of a 12288^3 turbulence simulation chosen as one of three target benchmark cases for the planned Track 1 machine funded by NSF. All 5 ASCI Centers supported by DOE have major Turbulence/Fluids components. So, recognition of flagship status actually is already there. What is missing is funding to do the research. Manpower in terms of students and postdoctoral associates of high caliber in this kind of research activity is hence in short supply and difficult to sustain.

- "How will we handle extremely large datasets (12288^3) in the future, when we still have not figured out how to efficiently use and disseminate the 1024^3 data-sets? "

  More research is needed in area of user-friendly accessibility of such datasets ("beyond ftp"). HPC Centers can be quite helpful in this.

- "Is HPC really good/necessary for turbulence research? - Just funding the machine and runs, but without funding the science is insufficient"

  Yes, and it is reasonable to expect that increased recognition of Turbulence/Fluids as a discipline that is a core user/driver of front-line HPC technology should also motivate increased funding for the science. So, this workshop's objectives are moving in the right direction.

Intellectual and strategic arguments to be provided to NSF

What intellectual and strategic can we provide to NSF to help increase CBET fluids program to a level commensurate with what the community clearly requires? Good answers to this question would: (i) enable more funding of fluids and turbulence science in addition to just funding HPC runs, (ii) help alleviate the situation that is leading NSF program director(s) to suggest that the community submit less proposals, (iii) help to push back on the misguided/ill-considered comment sometimes heard that fluid dynamics and turbulence is a "dying field".

The following is a list of thoughts that were presented:

- Organize efforts around large, focused problems (e.g. energy) that appeal more directly to the public.

- Be clear what Petascale HPC turbulence/fluids research will uniquely enable us to do (e.g., compute flow in entire combustor, around aircraft, blood flow in entire human body)

- Many of these arguments for the importance of fluid dynamics research have already been articulated in documents such as the "Fluid Dynamics for National Needs" report [7] prepared by APS-DFD.

- Stress relationship to American Competitiveness Initiative (aero industry, energy, sustainability, etc)

- Formulate clearly that turbulence simulations are an excellent flagship application for the drive "towards Petascale" — a prototypical problem, and a complex, nonlinear and highly coupled system that has important interdisciplinary applications.

- Understand that there are serious challenges ("no one is sure how to do CFD on 10^6 cores") [Other disciplines probably face the same challenge in the future, since no computer of such size exists yet.]

- Understand that there are serious challenges associated with analysis and dissemination tools for large turbulence datasets.

- Stress connections with other communities, where turbulence/fluids-related research is quite healthy (geo, astro, bio). That is, make the case that "they are able to make progress due to contributions done not so long ago by more fundamental turbulence/fluids groups, that were funded adequately in the past but not now". (e.g. Coarse-graining and parameterizations, stochastic tools, CFD algorithms, complexity..)

- Properly redefine "turbulence and fluids research" to be much broader than what detractors often imply.

- US leadership position versus other regions is eroding. (Japan: Earth simulator; China: huge investments in understanding particle transport in boundary layers and sandstorms; Europe: Lagrangian turbulence initiatives, European Turbulence Conference series which is showing impressive growth and quality). We should use this is help build our case for more fluids funding.

- Other communities have a few legacy community codes. But we do not. Perhaps NSF should have a special call for developing such open-source code. Would need to be very large program, likened to an "Academic Fluent" for wide use by our community.

5.3 Complex Fluids and Multi-Physics Applications

The following presentations were made in Session III:

- "Studying the dynamics of heterogeneous continuum systems using DNS" by Gretar Tryggvason (Worcester Polytechnic Institute)

- "Hub-based Petascale collaborations" by Sangtae Kim (Purdue Univ.)

- "Numerical simulations of polymer-turbulence interactions in homogeneous turbulent shear flow of a dilute polymer solution" by Lance R. Collins (Cornell Univ.).

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The first and third speakers in this Session pointed to the importance and challenges of simulating multiphase turbulent flows with bubbles and polymer additives. The second speaker shared his perspectives as a former Director of NSF's CISE Division of Shared Cyberinfrastructure (predecessor of Office of Cyberinfrastructure, see also [6]), and urged that the Cyber-Fluid Dynamics community adopt a new paradigm in research collaborations which would better prepare the community for Petascale computing.

The discussion focused on the high-performance computing of turbulent multiphase and chemically-reacting flows, which include: turbulent flows laden with particles, droplets, bubbles or polymers, turbulent flows of a non-Newtonian fluid, and chemically reacting flows. Some of the major issues considered were:

What are the main distinguishing features of these flows?

Additional complexities compared with classical single-phase turbulence include:

- Governing transport equations and physical laws are needed in addition to Navier-Stokes equations (e.g. particle-fluid and particle-particle interaction forces, chemical reaction rates, polymer stresses, etc.)
- Wider ranges of length- and time-scales than those observed in single-phase turbulent flows (e.g. chemically-reacting liquid sprays)
- Presence of interfaces (discontinuities of properties) between the dispersed phase and the carrier fluid

How much computer power may be needed for these flows at high Reynolds number?

It is clear that the flow features described above necessitate greater computer power requirements than single-phase turbulent flows. For an order-of-magnitude estimate, consider a simple particle-laden turbulent flow of fluid volume of 5×10^{-3} m^3, laden with spherical particles of diameter 50 microns. Assume that the volume fraction of particles is only 10^{-3}. Then the number of particles is 7.6×10^7. Assume also that we have access to a very powerful computer which allows us to solve the 3D Navier-Stokes equations around *a single freely-moving* particle in only *one* CPU second per time step of integrating the governing equations while resolving all the scales of turbulence. Then, for 7.6×10^7 particles, we would need about 2×10^4 CPU hours or 2.4 years for each time step on a single processor. Performing this simulation on a machine with 10^5 processors with excellent algorithm scalability may, however (optimistically) reduce this time to few seconds per time step.

What benefits can Petascale HPC in this area bring?

Successful use of Petascale HPC can produce dramatic progress in:

- *Grand challenge problems with impact on energy saving, alternate fuels, and pollution control.* Example: DNS of chemically-reacting fuel sprays in a practical combustion chamber. The DNS results can then be used to create validated closure models for RANS/LES-SGS.
- *Grand challenge problems with impact on practical chemical processing plants.* Example: DNS of high Reynolds number turbulent flows laden with bubbles or polymers in pipes.
- *Other practical problems.* These include dust storms in deserts or barren landscapes due to deforestation, with adverse effects on optical beam transmission and land erosion.

[Multiphase turbulent boundary layers are very relevant in this context.]

How do we maximize the benefits of Peta-scale HPC simulations?

Some of the ideas below have been noted in Sec. 5.1 or 5.2 already, but are still repeated here for emphasis:

- We need to examine and improve the scalability of the current algorithms for a much larger number of processors (e.g. 10^5). There may be some performance bottlenecks associated with numerical methods used to treat additional terms in the equation of motion.

- We need to engage HPC centers for help in enabling wide dissemination of codes and data.

- We need to work together closely with experimentalists, e.g., they can, from experience, specify boundary conditions and control parameters in ranges which are realistic in applications and can also be computed numerically.

- We need to develop the science of uncertainty estimation for multi-physics problems.

5.4   Nano and Bio-Fluid Mechanics

The following presentations were made in Session IV:

- "Digital human simulation of the human arterial tree on the TeraGrid", by George E. Karniadakis (Brown Univ.)

- "Simulating the multiphysics in microscale flows", by Nadine Aubry (Carnegie-Mellon Univ.)

- "Computational investigations of the couplings between macro-scale and microscale transport of nutrient molecules in the intestines — and a comment on discovery", by James G. Brasseur (Penn State Univ.)

The first speaker provided a detailed description of cross-site simulations conducted simultaneously at five TeraGrid sites and another HPC center in the U.K. The second speaker pointed out the special challenges of computing flows with various phenomena such as the presence of small electrically charged particles. The third speaker described advantages of using lattice-Boltzmann equations in biological problems such as flow in the digestive tract with moving boundaries, and pointed out the challenges of transforming complex scientific datasets into knowledge.

The discussion group recognized that HPC in nano- and bio-fluid mechanics are particularly important considering the rapid growth in these areas and the difficulties with making experimental measurements. Increasing activity is reflected in proposals to NSF and the number of sessions at annual ASME, AIChE, and APS-DFD meetings. The common features of these flow systems are the multiscale multiphysics nature of the problems. To examine the computing needs in these areas, it is more effective to discuss each separately. The bio-fluids area generated substantially more discussion than the nano-fluids area.

Nano-Fluid Mechanics

Fluid mechanics at the nanoscale is fundamental to development of many advances in nanotechnology and subsequent applications. For example, only through HPC one can investigate the underlying physics in convective heat transfer enhancement with nanofluids reported by various investigators. Particulate and multiphase flow in nanoscale channels and passages in various applications pose particular challenges in analysis at the limits of validity of the continuum mechanics where Knudsen number becomes finite. Computations fully bridging the gap from molecular dynamics to continuum mechanics remain unattainable at this time.

The fundamental processes at the nanoscale are not well understood, and coupling between MD and Coupling of MD and continuum simulations needs to be developed. This may require transfer of excessive data between scales with challenging problems in HPC. The methods to couple the scales, especially the transfer of data from macro to micro, remain to be developed. Challenges in the computation of nano-fluid mechanics are often at the fundamental level making the funding sources limited to very few federal agencies.

Bio-Fluid Mechanics

Bio-fluid mechanics with a view towards medical applications is a subject experiencing very rapid growth, with considerable interest within the bioengineering, systems biology and biomedical communities. Flow simulations in the cardiovascular, pulmonary, and digestive systems have become important areas of research. For example, the strong relation between hemodynamic and cardiovascular diseases such as hypertension, arthrosclerosis, and heart disease has created a great need for integrative numerical investigations of the cardiovascular system where transport of blood, biochemical species and cellular response to stress are considered together. Multidisciplinary approach with fluid dynamics simulations coupled to biophysical and biochemical transport spanning the spatial and temporal scales require multiscale/multiphysics/multisystem algorithms and data structures. Recent progress in computational methods and HPC have put within reach major challenges in whole blood simulations including the DNS of deformable red blood cells and large-scale analysis of the integrated cardiovascular system in the human body. These continuing advances are providing potential for breakthroughs in understanding some of the fundamental issues in biological systems. For example, a fundamental technology in predictive medicine that may have great impact is the creation of patient-specific models based on realistic imaging of the vessels and organs and development of predictive modeling tools. Characterization of geometry from various imaging systems and image processing, as well as defining a well-posed and realistic problem with accurate boundary conditions are important requirements for meaningful large-scale simulations.

It has been pointed out at the Workshop that, in contrast to turbulent flow, direct numerical simulation of biotransport problems is in the early stages of development. Computational methods are often "hybrid" in nature and difficult to implement on large parallel systems such as those with 250 processors or more. An important current research need is therefore to developing new approaches for large-scale parallel simulation of integrated bio-fluid transport.

Members of this discussion group are in agreement that an unprecedented opportunity exists in major advances in biosciences and development of devices and methods in clinical applications through integrative understanding of biotransport processes and their consequences

from the molecular to cellular to organ levels. Simulation of biotransport problems with greatest impact involving complex processes are inherently multidisciplinary, requiring not only powerful HPC resources but also collaboration among teams drawing from engineers with varied backgrounds, life scientists, physicists, chemists, computer scientists, mathematicians, and medical scientists and clinicians. Many important biomedical problems can be addressed most effectively by developing integrated models of human physiology across relevant scales bridging from basic understanding to clinical application. Fundamental questions of significant impact for health care can be answered by combination of biotransport with HPC and disease diagnosis, therapy and prevention.

It is worth noting that the 2004 report [8] from the NSF-NIH sponsored workshop on Transport Processes in Biomedical Systems concluded that "the time is right for a national initiative to advance our understanding of biotransport processes in living systems to a new level that will have a major impact on important problems in biology and medicine". The discussion group suggested that an effective strategy would be for NSF and NIH to partner in nurturing the growth and application of biotransport simulations to relevant medical and clinical contexts. HPC resources as well as computational tools funded through NSF jointly with NIH for medical and clinical applications will be essential in enabling a strong national initiative to enhance linkage of scientific development and applications to biology and medicine.

5.5 Knowledge Discovery and Education

Unlike the first four sessions which emphasized technical and scientific issues in fluid flow computations, this Session focused on issues of collaborative activities in science discovery, and on the processing of large datasets from an experimentalist's point of view. The following presentations were made:

- "Virtual organizations as new aids for collaboration", by Philip R. Westmoreland (NSF)

- "Scientific community web sites: what works... and not", by Craig C. Douglas (Univ. of Kentucky & Yale Univ.)

- "eFluids: a high-quality source for data, information, and educational materials in fluid mechanics", by Alexander J. Smits (Princeton Univ.)

- "Visualization methods to advance discovery in fluid dynamics", by Ellen K. Longmire (Univ. of Minnesota)

- "Extreme challenges in turbulence: matching computation to experiment at global scales", by Daniel P. Lathrop (Univ. of Maryland)

The first is summarized in Sec. 4. The second shared successes and pitfalls in organizing and maintaining science community websites. The third is an unique educational and outreach resource that provides a possible model for the Cyber-fluids community. The fourth and the fifth provided important examples of challenges that are common to both simulation and experiment concerning visualization and problems with an extreme range of scales.

We summarize here discussions at two plenary sessions held at the Workshop, at the end of Day 1 and on Day 2 following Session V. Both plenary sessions were planned to provide

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forums for broad cross-cutting issues that arose from various presentation and breakout sessions. Emerging from these discussion were several themes that are distilled and discussed here. Comments made by Workshop attendees generally revolved around the issues of Cyber-enabled discovery and education in support of the core conference theme of Cyber-Fluid Dynamics. It is also useful to think of the role of large-scale computational and communication infrastructure in fluid dynamics knowledge discovery as, broadly, of three types: (1) the generation of information (data) through numerical simulations; (2) the analysis of information (data), regardless of the source; and (3) the distribution and sharing of information, embodied in both data and codes, with a broad fluid dynamics community. All three of these roles were discussed at the Workshop and will be described below.

The use of numerical simulation as a knowledge discovery tool has a long tradition in fluid dynamics, and indeed in the early days of supercomputing on the ILLIAC IV and Cray systems (most notably, at NASA Ames Research Center in the late 1970s), CFD accounted for one of the biggest shares of the resource use. This is not currently the case at NSF-supported HPC centers, which are (subject to an allocation review process) openly available for use by the academic research community. There were a number of possible reasons put forth for this, including (a) the general reduction in funding in fundamental fluid dynamics, (b) the community may not be sufficiently familiar with TeraGrid facilities and policies, (c) that large scale CFD computation is done using resources available through other agencies such as DOD and DOE, and (d) the possibility that fluid dynamics problems have maxed out in computational complexity so that they can be solved on modest and less costly dedicated systems (clusters). The first three of these possibilities probably play a role, but the fourth is more complicated. It is clear from the presentations and discussions at the Workshop that the computational complexity of a wide variety of fluid problems has no upper limit. In the much-discussed case of single-phase homogeneous turbulence, the desire (and need) for ever-larger Reynolds numbers results in very large computational requirements. Likewise complex geometries and additional physics (e.g. multi-phase flows or chemical reactions) also increase CPU expense substantially. The range of fluid dynamics problems that can benefit from increasing levels of computational power (Petascale and even beyond) is apparently very wide.

With increasingly large simulations, or with increasingly sophisticated experimental techniques (e.g. PIV), comes increasing volumes of data to analyze. The real value of this data is that it can be used to answer many more questions than was intended when it was first generated. Thus the knowledge discovery process involves extracting from the simulation or experimental data new diagnostic quantities designed to test specific hypotheses. For very large data sets this poses different computational challenges that are every bit as great as those associated with generating simulation results. As discussed below, the ability to evaluate new diagnostics in such data is most valuable if it is enabled for others in the community (other than the data author).

Making the fruits of our research in fluid dynamics available to the community for knowledge discovery is becoming much more involved than writing a paper. For maximum impact, both simulation and experimental data need to be available to the fluid dynamics community, preferably in "raw" form so that it can be re-analyzed, as necessary. A second way that our fluid dynamics knowledge and computational expertise is expressed is through the codes that we write. These too will have the greatest impact if they are widely shared in the fluid dynamics community. However, there are a number of technical, logistical and cultural issues affecting the sharing of data and simulation codes, that arose during discussions:

- As the semantics of data becomes more complex, the size of data sets gets larger and the sophistication of the analysis becomes greater, using data correctly becomes increasingly difficult. Enabling data users with less expertise in the use of the data than the data author is a challenge that needs to be addressed.

- Datasets coming out of future Petascale computations are likely to be large (perhaps hundreds of Terabytes). Storing and making such data available to the community will be challenging. Moving it around the country is (barring some dramatic advances in the technologies involved) probably not viable, so users will need to process it at the facility where it is stored. Appropriate access will need to be provided.

- Many felt that as a community we were better prepared to share data than codes. It was felt that it was more straightforward to appropriately attribute credit to data authors when their data are used than to code authors when their codes are used. Part of the concern may be that as a research code evolves, its origins may be lost or forgotten. There may also be a concern about how shared codes will be supported or about enabling one's competitors, especially in an environment of limited funding. There is also a potential conflict with the fluid dynamics community's traditions regarding credit for originality and demonstration of independent scholarship by younger researchers, through the development of new data and codes.

- It was also felt that there would be significant benefit to developing and maintaining a community code base for fluid dynamics simulation and research in a variety of situations, which would embody a range of the best algorithms for each situation. This would avoid much duplication of code development effort. Such an academic code base would serve a much different purpose than currently available commercial CFD codes because it would be open source, enabling research and development in algorithms, models etc. Several attendees expressed interest in contributing to such a code base. Clearly such an effort would require funding to develop.

Regarding education in and for Cyber-enabled research, two primary issues were discussed. First is education in the advanced algorithms and programing techniques required to effectively use very large scale resources. It was felt that this aspect was commonly dealt with rather effectively through courses or training workshops offered in such techniques, either academic course or short coursed through computing centers. It seemed that a more serious issue is that students commonly complete undergraduate degrees in engineering without any significant computing or programing experience. Some argued that this was appropriate, since most students will not do software development after completing school. Others pointed out that the algorithmic thinking underlying programing is more generally useful, and thus a meaningful programming experience would be generally valuable. Currently however, most students do not get a meaningful experience by the time they reach graduate school, so that even basic programing techniques need to be learned as part of the graduate school experience.

6 Post-Conference Questionnaire

A two-part post-conference questionnaire was prepared shortly after the Workshop and e-mailed to all invited participants in an electronically editable file format. Participants were

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asked to return the surveys to PI's administrative assistant at Georgia Tech together with their reimbursement materials, or to the Program Director's assistant at NSF. A total of 29 completed surveys were received. Results for the first part of the survey focused on organizational aspects of the Workshop are collected anonymously.

6.1 Conference Feedback

This part of the survey had four questions, each summarized as below.

Question 1 asked participants to rate their satisfaction on a scale of 1 (lowest) to 5 (highest) on the following, for which interpolated median values are noted below:

a.	Clarity of purpose of Workshop	4.2
b.	Pre-conference communications	4.7
c.	Conference room facility	4.2
d.	Catering services	4.2
e.	Conference hotel	4.6
f.	Appropriateness of topics	4.5
g.	Workshop schedule	4.1
h.	Conduct of discussion periods	3.9
i.	Usefulness of workshop website	3.8
j.	Overall degree of satisfaction	4.3

The most significant shortcoming suggested by these numbers was in the conduct of discussion periods, which a number of participants also remarked upon in greater detail in their responses Question 2 below.

Question 2 asked what the respondents liked the *least* about the Workshop. Some of the main points noted were:

1. The general sentiment was that there was insufficient guidance on specific discussion objectives and insufficient time for detailed discussions and development of recommendations. Some also felt the size of the groups were too large to be effective.

2. A different approach in organizing the breakout groups, based on challenges in competing for and using Cyberinfrastructure resources effectively instead of topic areas (Sessions II–IV in the Workshop Agenda) might have allowed better focus on issues of concern to all, such as training of graduate students, low success rate in NSF proposals, and the handling of large datasets.

3. Some respondents also remarked that a small number of presentations seemed to be not very focused on Cyber-issues. More presentations from the computer-science community and from experts sharing expertise in community-building may have been helpful as well.

Question 3 asked what the respondents liked the *most* about the Workshop. Some of the main points noted were:

1. The Workshop generated awareness that fluid dynamics was a founding father of HPC some 20 years ago but for various reasons (e.g. funding) is now taking a back seat to other disciplines, and that we as a community need to change that direction. While exactly "how" to do so is not very clear there is at least general agreement on the motivation to develop a greater presence in and attract more HPC-related support at NSF, in a collaborative manner.

2. Comments received concerning the mix and quality of attendees representing large-scale computing, physical modeling, experimentalists, and computer scientists are generally very positive. Several of the presenters were able to bring refreshing points of view to the audience.

3. Most participants appreciated the opportunity to learn about new NSF Cyber-related opportunities, both from NSF officials first-hand and also from those in the community who have been closely involved in NSF initiatives in the Cyber arena. Information provided concerning TeraGrid resource availability and allocation processes is of general benefit to many of the attendees.

Question 4 asked the respondents to point out any important issues that the Workshop did not address. Some of the main points noted were:

1. The discussions were primarily focused on HPC but a number of other important Cyber-issues such as remote collaboration, archival, processing and visualization of large datasets (both experimental and computational), as well as use of simulation data towards improved modeling, could have been given greater attention.

2. The workshop did not address adequately how we, as a community, should or could organize. There is a suggestion for follow-on group meetings to make recommendations to the fluid dynamics community, including how we value individual intellectual merit versus collaborative endeavors in academia.

3. On the minds of many attendees was certainly the issue of research funding, not just how each individual might have picked up useful ideas, but how to increase funding for fluid dynamics as a whole, both in NSF's core program and elsewhere. More discussions on how fluid mechanics could partner with computer scientists for greater success in competing for prime resources were also desired.

6.2 CFD'er Profiling

The questions asked in this section of the post-conference questionnaire were guided by part of the Closing Remarks presentation by the NSF Fluid Dynamics program director (W.W. Schultz). The main objective is to obtain an approximate idea of what leading members of the community are now currently able to achieve, and to identify ideas and pathways to enable further progress in the field, including collaborative endeavors. A total of 24 responses to this section are available for analysis.

The following observations can be made:

1. About two-thirds of respondents indicated they have been funded by NSF within the last 3 years. Most of these related to the Fluid Dynamics program but some were from other CBET programs (e.g. multiphase flow or combustion), and a smaller number yet were from other Divisions or Directorates at NSF.

2. Except for several who have different backgrounds (experimentalists, resource providers, web portal host, etc) most respondents indicate definite interests in high-performance computation and have received resources from various sites.

3. If we consider 1 billion grid points as an arbitrary cutoff for "large-scale computation", then data from the respondents suggest five (or their close collaborators) have passed this milestone. However, most respondents have a definite interest in "upgrading" in the next 5 years. (In other words, most of them see the potential of Petascale computing platform(s) in the future.)

4. Fortran is the leading primary programming language, followed by C, while use of well-supported software libraries for specific tasks is also common. (It is understood from the discussion periods that the training of students in these high-level programming languages is a widespread concern.)

5. The fraction of respondents who have ever (a) shared their codes with others beside a close co-PI, (b) used codes developed by others with greater computational expertise, or (c) used large datasets provided by others is about two-thirds for all three categories.

6. Less than half of respondents have run large-scale benchmarks. (This may be related to No. 3 above, namely that most respondents have not progressed yet to calculations with thousands of processors.) Only a couple have had experience with competitive "bake-offs".

7. Only a small number (3 or 4) have ever participated in a Fluids-related Wiki or Virtual Organization. (However those who have participated are known to be very active.)

8. With only one or two exceptions, almost all respondents indicated their willingness to (a) contribute their codes to build an "Academic Fluent" type of code collection, as well as start or join a Virtual Organization focusing on fluid dynamics or related disciplines. There were some concerns though with the availability of funding to support or sustain such efforts.

6.3   The Future: Ideas from Participants

A number of respondents also put forth very thoughtful ideas on how the "Cyber-Fluid Dynamics" community can move forward to address present needs and make the best use of future opportunities. We summarize some of the important points as below, in arbitrary order:

1. Some informal working groups can be formed to formulate strategies to advance our field in computer-based science and engineering. These groups can perhaps be convened and/or assisted by the professional societies that have a considerable presence in fluid dynamics research: in particular the Division of Fluid Dynamics (DFD) of the American Physical Society (APS).

2. Some have mentioned their participation as committee members at the International Collaboration for Turbulence Research (ICTR), which is similar to a Virtual Organization, but operates from Europe and is mainly focused on Lagrangian studies of fundamental turbulent flows. We can learn from the ICTR experience, and/or build a separate organization and interact with the ICTR on a regular basis.

3. Similarly, some of the attendees have an active role in the International Computational Fluid Dynamics (iCFD) database of numerical simulation data, hosted in Italy but with datasets originating from various countries. Most of the datasets currently available at the iCDF site are for turbulent flow. A question is whether this is an useful model for specialists in other branches of fluid mechanics.

4. There is a suggestion that (again focusing on turbulence) that codes and data for some representative (canonical) flow geometries should be standardized, archived long-term, and openly shared within the fluid dynamics community.

5. There is a concern that sponsored funding is needed to develop and sustain Fluent-like software repositories for use by the community. There are also a couple of volunteers who have offered to coordinate a new community-wide website.

6. There is a need for better publicity in several forms. For example, high-quality videos are useful for introducing others to our discipline.

7. A small number of respondents also stated their willingness to use their organizational expertise and lessons learned from other fields of science or engineering to help the fluid dynamics community organizer itself better.

8. It is generally agreed that eFluids (`http://www.efluids.com`) is a site that is providing a useful service for the community, especially from an educational point of view. A new Virtual Organization focusing on computations building on eFluids may have many advantages.

9. There are suggestions on how to enhance the public relations image of the fluid dynamics community, including interactions between computation and real-life experimentation. To improve the situation on funding sources the community needs to communicate better with broad audiences on why our discipline is important to society in many multidisciplinary contexts.

10. In order to make shared tools truly useful, some agreement on data formats and programming paradigms may have to be devised, with the hope that most members of the community can be persuaded to adopt recommended standards.

7   Summary and Recommendations

As can be seen from earlier Sections of this Report, the Workshop produced a strong consensus on several issues important to the participation of the fluid dynamic community in current and future uses of Cyberinfrastructure resources supported by NSF and other national funding agencies. Briefly, there is broad agreement on:

- Fluid dynamics is a subject where large-scale computing has brought many advances but the community appears to be not very well prepared for future Petascale computing. Access to resource allocations is modest given the resource needs, and expertise for scaling to possibly hundreds of thousands of processors appears to be found only in a small number of research groups working on specialized problems. Training of students to meet the related computer-science challenges is also a concern.

- Fluid dynamicists have not been as deeply engaged in Cyber-enabled collaborative endeavors as their counterparts in several other disciplines, especially in the sharing of open-source algorithms and the development of standards and conventions essential for wide participation. This can impact the community's success in the coming era of Cyber-enabled Discovery and Innovation. Most participants are willing to collaborative but do not see a clear path to efficient handling of large datasets and especially complex algorithms which may require heavy user support.

- Funding for fundamental fluid dynamics has been in short supply at NSF (resulting in proposal success rates much lower than the NSF average), and also declined sharply at other federal agencies such as DOE and NASA. This situation, if not corrected in the near future, is likely to impair the fluid dynamics community's efforts in adapting to and using future Cyberinfrastructure. It also appears that the importance of fluid dynamics in many interdisciplinary contexts is not sufficiently well appreciated by the public, funding managers and reviewers alike.

In view of these summary observations, we propose several recommendations, to both (i) members of the fluid dynamics community on how they can work to advance and sustain the discipline in a new era of Cyber opportunities, and (ii) agencies, funding managers, and resource providers on how they can facilitate, encourage, and support the community's effort in a number of crucial areas.

These recommendations were formulated in part based on discussions between the event organizers (P.K Yeung, R.D. Moser) and the Group Discussion Leaders at the Workshop (M.W. Plesniak, C. Meneveau, S. Elghobashi, C.K. Aidun). The Vice-Chair of APS-DFD (P.S. Marcus) also participated actively in these discussions. Additional further input and background information was also provided by NSF staff.

7.1 Recommendations to the Fluid Dynamics Community

The coming era of Petascale computing promises to be an exciting frontier that will move at a brisk space and provide great potential for new discovery and modeling techniques in fluid dynamics. In order to fully utilize such opportunities, we recommend that the research community consider the following priorities:

1. *To develop and share expertise for high scalability on future HPC platforms.*

   Many current approaches for parallelizing codes will need to be fundamentally changed for computers with $10^5 - 10^6$ processors. Fluid-mechanical problems are characterized by strong nonlocal couplings which often makes the task of dividing a problem into $10^5 - 10^6$ pieces with reasonably low communication overhead difficult, especially in flows

involving multiphysics content. (Problems solvable by pseudo-spectral schemes may be an exception but are still nontrivial.) We recommend that the community actively engage computer scientists or HPC specialists at NSF-funded TeraGrid sites, to learn about best practices in other fields, and to develop alternative schemes which can scale efficiently up to very large processor counts available in the future. A culture of open communication is needed between those who have gained expertise or experience on large machines and the wider CFD community. We also call for faculty members to be strong voices for academic training in programming, and to provide for their students a higher level of exposure to the national HPC landscape.

2. *To mount wide community efforts on virtual collaborations, databases and HPC codes.*

   While many fluid dynamicists have done outstanding work on difficult problems individually or in small groups, the sheer magnitude of challenges and opportunities in the new age of Cyberinfrastructure dictates a need for more openly collaborative paradigms in pursuing science discovery. Unlike a few other communities which have developed central hubs enabling more rapid progress than otherwise, fluid dynamics also suffers from a lack of accepted community codes and likewise of standards and protocols of handling and sharing of large datasets. We recommend that leading principals in several areas (e.g., turbulence, multiphase flows, biofluid mechanics) work together to identify a small number of HPC-oriented codes as candidates for wide community use, and hence reduce duplication of effort while facilitating progress on new fronts. Community agreements in terms of data formats and download or transfer protocols are also needed, which requires close interactions between data authors and data users, and can benefit from the assistance of national HPC centers. Efforts at building virtual organizations incorporating the elements above, and more, will need to build credibility with the help of highly respected groups in the field. In particular, we urge that the APS-DFD leadership take an active role in guiding and promoting such endeavors for community benefit. Journal editorial boards can also help in developing appropriate guidelines to ensure scholarly quality.

3. *To increase awareness of the subject and make the case for more resources.*

   We recommend that the community, perhaps through the auspices of the APS-DFD leadership, increase efforts to bring to a wide audience the importance of fluid dynamics, on its own merits and in the context of many interdisciplinary endeavors. The effort should include innovative ways of drawing attention to the underappreciated role of our subject in many current areas of National Needs (see [7], a report by J.P. Gollub *et al.*, 2006). It is important that our message be well understood by academic colleagues in other fields, sponsor agency officials, as well as prominent individuals and corporate players in the HPC and Cyber arenas. For example, NSF-supported PIs should respond with greater enthusiasm and effectiveness to calls from from NSF program directors for nuggets of research achievements, and other materials that can help make the case for more resources. We also recommend that leaders in fluids-oriented HPC work closely with existing web portals with an emphasis on education, in order to help excite and recruit bright young minds to our discipline.

It should be understood that success in addressing the issues above will most likely result from, and in fact require, collective efforts by groups of knowledgeable and community-minded individuals committed to promoting the entire field instead of their own specific interests.

7.2 Recommendations to NSF and other Agencies/Providers

The scarcity of research funding for fundamental fluid dynamics [1] (see letter from Hohenberg *et al.* to DOE Undersecretary for Science, in Appendices), which provides much of the motivation behind many large computations, is a factor that limits our current representation in the HPC community. More importantly, new funding is clearly necessary to help initiate and sustain a range of collaborative efforts that a newly energized Cyber-Fluid Dynamics community will likely wish to undertake, with help from the TeraGrid in both expertise and resources.

We make several sets of recommendations as below:

1. *For the NSF Fluid Dynamics Program.*

   A string of highly competent and fair-minded NSF Program Directors in Fluid Dynamics, as well as their review panels, have faced very difficult choices in the face of limited budgets as the proposals they receive increase in quantity and quality. We recommend that the Fluid Dynamics program be given an immediate and sustained budget increase, with emphasis on new funding to support proposals and activities centered around community-minded efforts, including community-wide tools for simulation and data analysis, to bring the benefits of advanced Cyberinfrastructure to as many interested members of the community as possible. The feasibility of small grants to train students in advanced HPC and Cyber techniques or similar supplements to existing grants should be considered. We also recommend that the Fluid Dynamics program director with help from the community as suggested above, continue to be a strong advocate for fundamental fluid dynamics research and education, at the divisional, directorate, and cross-directorate levels within NSF. We also believe the Fluid Dynamics Program should continue to work closely with the Office of Cyberinfrastructure, including co-funding proposals where appropriate. Finally we recommend that advice be sought from OCI program directors on how fluid dynamics can increase its competitiveness compared to other disciplines, in cross-cutting solicitations such as Cyber-enabled Discovery and Innovation (CDI).

2. *For OCI, other NSF Units and other Funding Agencies.*

   The presence and active participation of Program Directors from NSF's OCI and other units in the CBET Division was very encouraging; we hope this signals increasing recognition of fluid dynamics as an important discipline in advanced computation and as an essential element in many other disciplines both within and beyond the CBET division's mission. We recommend that an internal effort be made at NSF to collect data on fluids research supported or jointly supported by programs other than Fluid Dynamics, and to convene a panel of all program directors involved to explore ways in which they can pool resources together to promote the development of Cyber-Fluid Dynamics. We also recommend that a sustained dialog be undertaken with officials at other agencies, including AFOSR, ONR, NIH, DOE, NASA, EPA, etc which do not have a fundamental fluid dynamics program but yet are supporting research on agency-specific problems which rely on knowledge in fluid dynamics. A possible example of desired interagency efforts would be for NSF and NIH to partner in nurturing the growth and application of biotransport simulations to relevant medical and clinical contexts.

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[1] The decline of available funding has been gradual, with reducing support from AFOSR, ONR, DOE, NASA, and has reached such crisis proportions that transcends the usual lamentations that NSF might hear from particular constituencies that try to boost their funding.

3. *For TeraGrid Resource Providers*

Besides operating powerful hardware most of the leading TeraGrid sites provide a range of services, such as strategic consulting, visualization, and science gateway development, that are especially valuable and relevant to the theme of our Cyber-Fluid Dynamics workshop. However, many fluid dynamicists are not very well informed about these services, and some have expressed past dissatisfaction with the resource allocation process as well as a lack of detailed knowledge about reviewers' perspectives. We recommend that the TeraGrid makes a stronger effort to publicize the availability of its resources: e.g., by sending announcement of deadlines to all current NSF grantees or NSF program directors (who may, at their discretion, share the information with their respective subject community). Given the fact that fluid-mechanical problems often pose challenges less evident in other disciplines, a greater emphasis on science merit or impact and less focus on computational scaling in the allocations review process would be very welcome. Finally we recommend that special training for development of science gateways and web portals be made available.

Finally, in the Appendices we include a summary of the "Research in Fluid Dynamics: Meeting National Needs" released by the APS-DFD leadership in April 2006, followed by a letter from Hohenberg, Kadanoff and Langer to the DOE Undersecretary of Science (a similar letter was sent to the NSF Assistant Director for Engineering). Both of these documents underscore the Fluid Dynamics Community's sense of its ability to have major impacts on important national needs in science, technology, and the environment. Although not reflecting latest developments in 2007 [2] the Hohenberg *et al.* letter is indicative of serious concerns about the present and future funding situation in fluid dynamics due to changes that have occurred in several funding agencies in recent years.

Bibliography

[1] R.S. Rogallo & P. Moin (1984). Numerical simulation of turbulent flows. *Annu. Rev. Fluid Mech.* **16**, 99-137.

[2] M. Yokokawa, T. Itakura, A. Uno, T. Ishihara & Y. Kaneda (2002). 16.4-Tflops direct numerical simulation of turbulence by a Fourier spectral method on the Earth Simulator. Proceedings of the *Supercomputing Conference*, Baltimore, November 2002. *See also* Y. Kaneda, Y., T. Ishihara, M. Yokokawa, K. Itakura & A. Uno (2003) Energy dissipation rate and energy spectrum in high resolution direct numerical simulations of turbulence in a periodic box. *Phys. Fluids* **15**, L21-L24.

[3] S. Hoyas & J. Jimenez (2006) Scaling of the velocity fluctuations in turbulent channels up to $Re_\tau = 2003$. *Phys. Fluids* **18**, 011702.

[4] J. Jimenez (2004). Preface. *Annu. Rev. Fluid Mech.* **36**, v.

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[2] While it is not mentioned in the letter, the Mathematics Division and the GEO directorate at NSF also fund fluid dynamics related research. Also, NASA greatly scaled back, but did not eliminate, its fluid dynamics program, especially in microgravity, and has very recently begun increasing external funding in fluid dynamics.

[5] *American Competitiveness Initiative* (2006). White House Domestic Policy Council, Office of Science and Technology Policy. The report is available electronically, at `http://www.ostp.gov/html/ACIBooklet.pdf`.

[6] P.A. Freeman, D.L. Crawford, S. Kim & J.L. Munoz (2005). Cyberinfrastructure for Science and Engineering: Promises and Challenges. *Proc. IEEE*, **93**(3), 682-691.

[7] *Research in Fluid Dynamics: Meeting National Needs* (2006). A Report of the U.S. National Committee on Theoretical and Applied Mechanics, approved by the Executive Committee of the Division of Fluid Dynamics of the American Physical Society. (Authors: J.P. Gollub, H.J. Fernando, M. Gharib, J. Kim, S.B. Pope, A.J. Smits, H.A. Stone.) The report is available electronically, at
`http://www.aps.org/units/dfd/index.html`, or
`http://www7.nationalacademies.org/usnctam/Fluid_Mechanics_II.html`.

[8] Report of the NSF-NIH sponsored workshop on "Transport processes in biomedical systems", Washington, D.C., May 6-7, 2004. The report was prepared by K.R. Diller & G.W. Schmid-Schonbein, and appeared in *Annals of Biomedical Engineeering*, **33**(9), 1136-1141 (2005).

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Appendices

A. Cyber-related Solicitations at NSF, 2006-2008

A list of active hyperlinks to NSF Cyberinfrastructure programs, future plans, solicitations and resources (TeraGrid) is provided at the Workshop webpage. Here we provide a listing of several recent or current Cyber-related solicitations from FY 2006-2008 which may of interest to the fluid dynamics community.

nsf05625	Track 2 High Performance Computing System Acquisition: Towards a Petascale Computing Environment for Science and Engineering (Track 2)
nsf06573	Leadership-Class System Acquisition: Creating a Petascale Computing Environment for Science and Engineering (Track 1)
nsf07558	Engineering Virtual Organization Grants (EVO)
nsf07559	Accelerating Discovery in Science and Engineering through Petascale Simulations and Analysis (PetaApps)
nsf07564	Cyberinfrastructure Training, Education, Advancement and Mentoring for our 21st Century Workforce (CI-TEAM)
nsf07565	Community-based Data Interoperability Networks (INTEROP)
nsf07603	Cyber-Enabled Discovery and Innovation (CDI)
nsf08009	Dear Colleague Letter - Cyberinfrastructure Experiences for Graduate Students (CIEG): Supplements

Most of these solicitations have come to be known by shorter names, which are enclosed in parentheses. More information is readily available from NSF websites, including the homepages of the Office of Cyberinfrastructure and/or Directorate for Engineering. The most recent item (nsf08009) is limited to current awardees of selected divisions and programs (including CBET and Fluid Dynamics) within NSF's Directorate for Engineering.

See also *Cyberinfrastructure Vision for 21st Century Discovery*. A report of the NSF Cyberinfrastructure Council (March 2007).

B. Workshop Agenda

NSF Cyber-Fluid Dynamics Workshop

NSF Headquarters, July 19-20, 2007

Rm 375, Stafford I

Day 1

Continental Breakfast, Available 7:30

Preliminaries

8:30	-	9:05	Welcome and Opening Remarks
			P.K Yeung, Georgia Institute of Technology
			William W. Schultz, NSF Program Director, Fluid Dynamics
			Richard O.Buckius, NSF Assistant Director for Engineering
			Judy A. Raper, NSF CBET Division Director

Session I: High-performance Computing and Cyber Activities
Chair: P.K. Yeung, Georgia Institute of Technology

9:05	-	9:40	Abani K. Patra. NSF (Office of Cyberinfrastructure)
			Cyberinfrastructure for Collaborative and Predictive Simulations
9:40	-	9:58	Richard L. Moore. San Diego Supercomputer Center.
			TeraGrid CI Resources for CFD Research.
9:58	-	10:16	Federico Toschi, C.N.R (Italy)
			iCFDdatabase: The International CFD database

Break

Session II: Turbulence and Flow Control
Chair: Sanjiva K. Lele, Stanford University

10:30	-	10:48	P.K. Yeung, Georgia Institute of Technology
			Intermittency, Mixing and Dispersion in Simulations of
			Homogeneous Turbulence: the Path towards Petascale
10:48	-	11:06	Robert D. Moser, University of Texas at Austin
			Simulation of wall-bounded turbulence: what more can we learn?
11:06	-	11:24	Tim Colonius, California Institute of Technology
			Closed-loop flow control: simulation challenges and opportunities

Break

Breakout Groups in parallel session, 11:40-12:45

I. Discussion Leader: **Michael W. Plesniak, Polytechnic University**
II. Discussion Leader: **Charles Meneveau, Johns Hopkins University**

Lunch (provided): 12:45-14:00

Session III: Complex Fluids and Multi-Physics Applications
Chair: Arnaud Trouve, University of Maryland

14:00	-	14:18	Gretar Tryggvason, Worcester Polytechnic Institute
			Studying the Dynamics of Heterogeneous Continuum Systems using DNS
14:18	-	14:36	Sangtae Kim, Purdue University
			Hub-based Petascale Collaboratories - the new HPC
14:36	-	14:54	Lance R. Collins, Cornell University
			Numerical Simulation of Polymer-Turbulence Interactions in
			Homogeneous Turbulent Shear Flow of a Dilute Polymer Solution

Break

Session IV: Nano and Bio Fluid Mechanics
Chair: Bruce M. Boghosian, Tufts University

15:05	-	15:23	George E. Karniadakis, Brown University
			Teragrid Simulations of the Human Arterial Tree
15:23	-	15:41	Nadine Aubry, Carnegie-Mellon University
			Simulating the Multi-Physics involved in Microscale Flows
15:41	-	15:59	James G. Brasseur, Pennsylvania State University
			Computational Investigations of the Couplings between Macro-scale
			and Micro-scale Transport of Nutrient Molecules in the Intestines

Break

Breakout Groups in parallel session, 16:15-17:20

III. Discussion Leader: **Said E. Elghobashi, University of California at Irvine**
IV. Discussion Leader: **Cyrus K. Aidun, Georgia Institute of Technology**

Plenary Discussion (Sessions I-IV), 17:30-18:30
Discussion Leader: **Robert D. Moser, University of Texas at Austin**

Informal dinner: Matsutake Sushi & Steak Restaurant, 4121 Wilson Boulevard,
Tel. 703-351-8787
Accompanying persons welcome.

Day 2

Continental Breakfast, Available 7:15

Session V: Knowledge Discovery and Education
Chair: James J. Riley, University of Washington

8:15	-	8:45	Phillip R. Westmoreland, NSF (Combustion and Virtual Organizations) Virtual Organizations as New Aids for Collaboration.
8:45	-	9:03	Craig C. Douglas, University of Kentucky & Yale University Scientific Community Web Sites: What Works... and Not
9:03	-	9:21	Alexander J. Smits, Princeton University eFluids: a High-Quality Source for Data, Information, and Educational Materials in Fluid Mechanics
9:21	-	9:39	Ellen K. Longmire, University of Minnesota Visualization Methods to Advance Discovery in Fluid Dynamics
9:39	-	9:57	Daniel P. Lathrop, University of Maryland Extreme Challenges in Turbulence: Matching Computation to Experiment at Global Scales

Break

Plenary Discussion (Sessions V), 10:10-11:10
Discussion Leader: **Robert D. Moser, University of Texas at Austin**

Break

Event Closing and the Future

11:20	-	12:00	Group Reports (Breakout group leaders)
12:00	-	12:20	Follow-Up: NSF and the Fluid Dynamics Community (Schultz)
12:20	-	12:30	Concluding Remarks (Moser/Yeung)

Lunch (provided), 12:30:- (boxed lunches to-go)

Adjourn

C. List of Participants

From the broad fluid dynamics community

Cyrus K. Aidun	Georgia Institute of Technology
Nadine Aubry	Carnegie-Mellon University
Elias Balaras	University of Maryland
Bruce M. Boghosian	Tufts University
James G. Brasseur	Pennsylvania State University
Qin (Jim) Chen	Louisiana State University
Lance R. Collins	Cornell University
Tim Colonius	California Institute of Technology
Stephen de Bruyn Kops	University of Massachusetts, Amhurst
J. Andrzej Domaradzki	University of Southern California
Steven Dong	Purdue University
Craig C. Douglas	University of Kentucky & Yale University
Said E. Elghobashi	University of California, Irvine
Robert T. Fisher	University of Chicago
Rodney O. Fox	Iowa State University
Sharath S. Girimaji	Texas A&M University
Peyman Givi	University of Pittsburgh
Hong G. Im	University of Michigan
George E. Karniadakis	Brown University
John Kim	University of California, Los Angeles
Sangtae Kim	Purdue University
Susan Kurien	Los Alamos National Laboratory
Daniel P. Lathrop	University of Maryland
Sanjiva K. Lele	Stanford University
Ching-Long Lin	University of Iowa
Ellen K. Longmire	University of Minnesota
Krishnan Mahesh	University of Minnesota
Pino Martin	Princeton University
Beverley J. McKeon	California Institute of Technology
Charles Meneveau	The Johns Hopkins University
Robert D. Moser	University of Texas, Austin
Michael W. Plesniak	Polytechnic University
James J. Riley	University of Washington
Alexander J. Smits	Princeton University
Lester K. Su	The Johns Hopkins University
Federico Toschi	C.N.R. (Italy)
Arnaud C. Trouve	University of Maryland
Gretar Tryggvason	Worcester Polytechnic Institute
Dibbons K. Walters	Mississippi State University
P.K. Yeung	Georgia Institute of Technology

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From NSF-supported TeraGrid sites

Richard L. Moore	San Diego Supercomputer Center (SDSC)
Dmitry Pekurovsky	San Diego Supercomputer Center (SDSC)
Rob Pennington	National Center for Supercomputing Applications (NCSA)
Sergiu Sanielevici	Pittsburgh Supercomputing Center (PSC)

From the National Science Foundation

Richard O. Buckius	Assistant Director for Engineering
Marc Ingber	PD, Particulates and Multiphase Processes Program
Stephen P. Meacham	PD, Office of Cyberinfrastructure
Abani K. Patra	PD, Office of Cyberinfrastructure
Judy A. Raper	Director, CBET Division
William W. Schultz	PD, Fluid Dynamics Program
Philip R. Westmoreland	PD, Combustion Fire and Plasma Systems Program and ENG Cyberinfrastructure Working Group

D. Abstracts of Presentations

All presentations are available online at Workshop website (by clicking on name of each presenter in the Agenda).

Abani K. Patra (NSF)
— **"Cyberinfrastructure for Collaborative and Predictive Simulations"**

In this talk we will present an overview of current and future cyberinfrastructure initiatives at NSF/OCI designed to enable modeling and simulations with transformational impact on science. Highlights, strategies and a brief presentation of future possibilities for such initiatives will also be presented. A particular focus of the talk will be the integration of computing, data and human resources in the pursuit of what is often termed "predictive science" facilitated by NSF infrastructure investments.

Richard L. Moore (San Diego Supercomputer Center)
— **"TeraGrid CI Resources for CFD Research"**

We provide an overview of the TeraGrid cyberinfrastructure resources that are available to support the national academic research community, including the CFD community. The CI resources include more than 20 diverse high-end computational systems and will soon be joined by the 500+ TF Ranger system at TACC and subsequent large-scale Track 2 HPC systems. In addition, TeraGrid provides large-scale disk and archival storage resources, visualization systems, data hosting and delivery services, and human expertise in computational science for user applications. We also discuss examples of cyberinfrastructure capabilities that have been established within several examples of virtual science and engineering organizations.

Federico Toschi (C.N.R. Italy)
— **"iCFDdatabase: The International CFD Database"**

The iCFDdatabase (international CFD database) is a database of Computational Fluid Dynamic cases with contributions from different research groups worldwide. The aim of the database is to maximize the scientific outcome of numerical efforts, to provide "classical" reference data for future studies, to setup an unique, centralized reference resource for researchers interested in fluid dynamics. The database is hosted at CINECA (Bologna, Italy), and at present it hosts 3 Terabytes of raw CFD data from 12 different scientific cases. Access to the database both as user or as contributor is open to the whole scientific community. Past experience and future outlook will be discussed.

P.K. Yeung (Georgia Tech)
— **"Intermittency, Mixing, and Dispersion in Simulations of Homogeneous Turbulence: The Path Towards Petascale"**

Tremendous advances in computing power in the 21st Century are enabling the conduct of very-large numerical simulations of turbulence and turbulent mixing, where the general emphasis is to contribute to physical understanding in canonical flow problems that involve an

ever-wider range of scales. In particular, the range of scales resolved is very important in the study of fine-scale intermittency in dissipation and enstrophy fluctuations, of the turbulent mixing of weakly diffusive scalars at high Schmidt number, and of the Reynolds number dependence of Lagrangian statistics that describe turbulent dispersion. We show examples from recent work at 2048³ grid resolution using mainly resources at leading supercomputing sites within the TeraGrid. We also discuss our recent work on algorithmic issues in the light of turbulence on periodic domains as a Grand Challenge model problem in computational science. Successful benchmarking has been performed on 32768 processors on an IBM Blue Gene at IBM Watson Research Center, which is highly encouraging in developments towards true Petascale performance. Finally some future challenges in analyzing and sharing large datasets are briefly addressed.

Robert D. Moser (University of Texas at Austin)
— **"Simulation of Wall-Bounded Turbulence: What More Can We Learn?"**

Since the early DNS of turbulent channel flow by Kim, Moin & Moser in the mid 1980's, there has been an on-going effort to exploit DNS of this simple flow to probe the fundamental character of wall-bounded turbulence. In these twenty years, we have seen an increase in Reynolds number by a factor of 10, to friction Reynolds number of 2000, an increase in domain size by a factor of 12 in area, and an increase in the sophistication of the diagnostics being employed and questions being asked. The scientific results of these efforts have been impressive; for example, the autonomous dynamics of the near-wall viscous layer are now understood, and there has been great progress in sorting out the complexities of the Reynolds number scaling of several important statistical properties of the flow. So, the question arises: what can we still learn from the DNS of channel flow? I argue that the next big opportunity is to determine the asymptotic high Reynolds number dynamics of the log-layer. This would be an accomplishment of the utmost importance, which would enable advances in the manipulation and modeling of wall-bounded turbulence, which have been stalled (I think) due to insufficient understanding of the phenomena. Recent scaling results suggest that friction Reynolds number of about 5000 will be sufficient to plausibly extrapolate to infinite Reynolds number, which should be accessible to DNS in the next several years. Several things will be required to fully explore the high Reynolds number log layer, and these will be described. We appear to be on the verge of a very exciting time in the study of turbulence.

Tim Colonius (California Institute of Technology)
— **"Closed-loop Flow Control: Challenges and Opportunities"**

We will discuss computational challenges and opportunities associated with developing reduced-order models and controllers that can be implemented for real-time closed-loop flow control in applications including drag reduction, separation control, and attenuating flow/acoustic or thermal/acoustic instabilities. Feedback controllers may be developed following either a top-down approach, whereby control is designed around reduced-order models of the flow, or a bottom-up approach whereby control design is directly integrated with the Navier-Stokes equations, or linearizations thereof. In either approach, there are computational challenges beyond accurately simulating the unsteady and or turbulent flow. Similar to optimization techniques, these can include post-processing large amounts of simulation data and solution

of direct and adjoint simulations of the flow for different control inputs. We discuss how these tools from model reduction and control theory are being adapted to enable application to high-dimensional, nonlinear fluid applications. Examples from recent work on controlling cavity oscillations and developing integrated flight/flow control for micro air vehicles will be used to illustrate the issues.

Gretar Tryggvason (Worcester Polytechnic Institute)
— **"Studying the Dynamics of Heterogeneous Continuum Systems Using DNS"**

Systems where continuum models provide an accurate description of the system behavior, but where there is a large difference between the system scale and the smallest continuum scales are found in a wide range of industrial applications as well as in Nature. Multiphase flows, including bubbly flows and boiling, sprays, and solid suspensions, are common examples. Bridging the gap and using our understanding of the small scales to predict the behavior at the system scale is one of the grand challenges of science. Direct Numerical Simulations (DNS) of the evolution of sufficiently small systems so that all continuum scales are fully resolved, yet large enough so that interactions of structures of different scales can take place, are increasingly playing a central role in studies of the dynamics of heterogeneous continuum systems. Recent results for bubbly flows, where DNS have yielded new and unexpected insight into the subtle importance of accurately accounting for bubble deformability, will be used to demonstrate the power of DNS. Examples of other multiphase systems, including boiling, microstructure formation during solidification, chemical reactions, and the electrohydrodynamic behavior of droplet suspensions will also be shown.

Sangtae Kim (Purdue University)
— **"Hub-based Petascale Collaboratories - The New HPC"**

The emergence of cyberinfrastructure as a critical but highly expensive infrastructure for research has created a recursive challenge: preliminary Cyber-investments are needed to form a cohesive social network to organize the community so as to design, build and maintain the shared cyberinfrastructure. The national policy challenge is further confounded by disparities seen across disciplines ranging from the tight-knit social network of the elementary particle (high energy) physicists to the lone scholar paradigm of the fluid dynamicist. This presentation will focus on hub-based collaboratory models suitable for the fluids community given its location on the extreme end of the culture spectrum; special attention will be given to lessons learned from the NIH-sponsored "e coli hub" experience.

Lance R. Collins (Cornell University)
— **"Numerical Simulation of Polymer-Turbulence Interactions in Homogeneous Turbulent Shear Flow of a Dilute Polymer Solution"**

It's been known since the ground-breaking measurements of Toms (1949) that dilute concentrations (parts per million) of polymers in turbulence can reduce the drag on a surface by as much as 80%. Recent direct numerical simulations (DNS) of polymer models, coupled to continuity and the momentum equation (Navier Stokes equation augmented with a polymer stress), replicate much of the experimental phenomenology. Most DNS to date have been based on

the finitely extensible nonlinear elastic model with the closure by Peterlin (FENE-P). We will present a novel numerical algorithm for integrating the FENE-P equation that ensures proper behavior of the conformation tensor used to construct the polymer stress tensor. The algorithm has been implemented in the homogeneous turbulent shear flow code of Rogallo (1981). We will show results from those simulations. We also will discuss the computational challenges of performing simulations that are in some sense "asymptotic" in the key parameters (Reynolds number and Weissenberg number).

George E. Karniadakis (Brown University)
— **"Teragrid Simulations of the Human Arterial Tree"**

Grid computing offers potentially unlimited scalability and is suitable for simulating effectively a wide class of problems in biomechanics. Here I will review the first cross-site simulations performed on the TeraGrid for the human arterial tree and I will discuss some of the mathematical and computational issues involved in stochastic multiscale modeling of integrated biomechanical models, e.g. a full scale model for the human brain vascular network.

Nadine Aubry (Carnegie Mellon University)
P. Singh (New Jersey Institute of Technology)
— **"Simulating the Multi-Physics Involved in Microscale Flows"**

Although the further understanding of micro-fluid dynamics, that is the analysis and control of fluid dynamics in micron-sized devices, is crucial for advancing many microfluidic systems such as laboratory-on-a-chip, it also presents numerous challenges. One of those is the simulation of flows, often multiphase flows, in miniature geometries, specifically when particles are deformable (drops, biological cells, etc.), when the size of the particles is comparable to that of the device or when particle trajectories need to be computed over long time periods to evaluate mixing rates. Another challenge is due to the fact that such flows are difficult to manipulate using mechanical means, and electrical fields are often used for that purpose. In this case, the multi-physics involved needs to be fully accounted for. In this talk, we will present some recent results obtained using various simulation tools, including the direct numerical simulation approach in which the fundamental governing equations are solved simultaneously for the fluid and the particles, as well as for the electric field, without the use of any models.

James G. Brasseur (Pennsylvania State University)
— **"Computational Investigations of the Couplings between Macro-scale and Micro-scale Transport of Nutrient Molecules in the Intestines — and a Comment on Discovery"**

Absorption and secretion of nutrients in the gut (small intestine) occur at the epithelial lining of the gut mucosa. Multitudes of "villi", fingerlike protrusions $\sim 100\ \mu$m in scale, line the mucosal surface. Using multi-scale modeling of the motions of the gut lumen and villi, we are analyzing the coupling of macro-scale mixing driven by the muscularis at the cm scale with micro-scale mixing generated by villi motions at the 100 μm scale. I shall describe the modeling methodology we apply to the macro and micro scale motions in the gut and the coupling between velocity and passive scalar fields on macro-scale and micro-scale grids using

the lattice-Boltzmann framework with moving boundary conditions and passive scalar.

A Comment on "Discovery Environments". One might argue that the science of exploring and transforming scientific data into knowledge and discovery has not kept pace with the technology of generating data. This is of particular concern as we move into the tera and peta generations of data production. We might consider proposing a long term effort for the development of "Discovery Environments," human-computer environments with integrated visual and computational tools for interactive data interrogation to enhance the process of discovery in huge dynamically complex data sets.

Philip R. Westmoreland (NSF)
— **"Virtual Organizations as New Aids for Collaboration"**

Virtual Organizations or VO's (also known as gateways, hubs, and collaboratories) have evolved to the point that they can be extremely valuable for data-rich collaborations. A VO is typically created by a group of individuals whose members and resources may be dispersed globally, yet who function together through the use of cyberinfrastructure (CI). With the access to enabling tools and services, communities can create VO's to facilitate scientific workflows; collaborate on experiments; share information and knowledge; remotely operate instrumentation; run numerical simulations using shared computing resources; dynamically acquire, archive, e-publish, access, mine, analyze, and visualize data; develop new computational models; and deliver unique learning, workforce-development, and innovation tools. Most importantly, each VO design can originate within a community and be explicitly tailored to meet the needs of that specific community. At the same time, to exploit the full power of cyberinfrastructure for a VO's needs, research-domain experts need to collaborate with CI professionals who have expertise in algorithm development, systems operations, and application development. To elaborate on these points, this talk will use examples will be used including PrIMe (primekinetics.org) and the Network for Computational Nanotechnology and its nanoHUB.org portal.

Craig C. Douglas (University of Kentucky & Yale University)
— **"Scientific Community Web Sites: What Works....and Not"**

Community web sites have been common for many years. What works for one scientific community does not necessarily work for any other one. There are specific goals that these sites typically have. Some are simply hyperlinks to other web sites with specific information. Some have extensive tutorials aimed at novices to the field. Others provide portals to software on community based machines. Some even offer community allocations on the TeraGrid and bring new users into the NSF supercomputing community. In this talk, some of the things that work and do not will be discussed based on existing scientific community web sites.

Alexander J. Smits (Princeton University)
— **"eFluids: A High-Quality Source for Data, Information, and Educational Materials in Fluid Mechanics"**

eFluids is a specialty web portal designed to serve as a one-stop web information resource for anyone working in the areas of flow engineering, fluid mechanics research, education and directly related topics. eFluids can play a significant role in fluids research and education

through its many offerings. In research, Data Bases provides links to the principal sources of computational and experimental data compilations. Funding Sources and Key Government Sites help researchers find support for their activities and Technology Transfer helps them find government and industrial partners. Individual Sites helps link together different laboratories and activities world wide. In education, the Gallery of Flow Images and Gallery of Videos can be used to illustrate the wide variety of flow phenomena found in nature. The Gallery of Experiments aims to deliver simple and effective experiments using a minimum of materials and supplies to illustrate the important principles of fluid mechanics. This area is expected to expand significantly under recent NSF funding. The Gallery of Problems provides a source of problems for students in fluid mechanics for use in the classroom or for self-study. Educational Tools and Materials provides an index to sites where educational resources, such as specialized information, instructional material, or computer programs can be found.

Ellen K. Longmire (University of Minnesota)
— **"Visualization Methods to Advance Discovery in Fluid Dynamics"**

As fluid dynamicists, we are interested in understanding the dynamic evolution of key physical mechanisms in three-dimensional flows that evolve in time. This talk will address the development of visualization methods appropriate for interpreting the behavior of turbulent flows. We attempt to identify and examine the evolving behavior of coherent eddies and groups of eddies in turbulent boundary layers. Multivariate visualization methods are developed for dual-plane PIV data, which provides the full velocity gradient tensor in a plane of flow, and for data in three-dimensional volumes from direct numerical simulations. We consider how and why different visual features, such as color, texture, topography and motion, work to convey information efficiently and effectively.

Daniel P. Lathrop (University of Maryland)
— **"Extreme Challenges in Turbulence: Matching Computation to Experiment at Global Scales"**

Turbulent fluid flows in the Earth's atmosphere and core, and in the convective zone of the sun constrain the habitability of the Earth. On time scales from minutes to hundreds of thousands of years those conditions change, in part due to the strongly fluctuating nature of those flows. While this is of no surprise (they are, after all, turbulent), it does affect our ability to understand, model and predict them. Scientific progress is sharply dependent on our ability to numerically model turbulent fluid flows at global scales. In this talk I will address what I see as significant obstacles modeling currently faces. These often depend on the force balances at play, i.e., inertia, rotation, magnetic forces, etc. We now face a scientific state where we still struggle with the nature of turbulent pipe flow (simple geometry and force balance) – the geophysical and astrophysical problems are well beyond that in their complexity and difficulty.

E. "Research in Fluid Dynamics: Meeting National Needs"

We would like draw the attention of those not in the traditional fluid dynamics research community to the report "Research in Fluid Dynamics: Meeting National Needs", which was approved and released by the APS-DFD leadership in April 2006 (see Bibliography for citation details and names of authors). With permission, we provide excerpts from the report below.

The first three paragraphs give a broad introduction of the scope, nature, and relevance of fluid dynamics research for current national needs:

"The science of fluid dynamics describes the motion of liquids and gases and their interaction with solid bodies. It is a broad, interdisciplinary field that touches almost every aspect of our daily lives, and it is central to much of science and engineering. Fluid dynamics impacts defense, homeland security, transportation, manufacturing, medicine, biology, energy and the environment. Predicting the flow of blood in the human body, the behavior of microfluidic devices, the aerodynamic performance of airplanes, cars, and ships, the cooling of electronic components, or the hazards of weather and climate, all require a detailed understanding of fluid dynamics, and therefore substantial research.".

"Fluid dynamics is one of the most challenging and exciting fields of scientific activity simply because of the complexity of the subject and the breadth of the applications. The quest for deeper understanding has inspired numerous advances in applied mathematics, computational physics, and experimental techniques. A central problem is that the governing equations (the Navier-Stokes equations) have no general analytical solution, and computational solutions are challenging. Fluid dynamics is exciting and fruitful today in part because newly available diagnostic methods for experiments and parallel computers for simulations and analysis allow researchers to probe the full complexity of fluid dynamics in all its rich detail".

"The outcomes from this future research will have enormous impact. For instance, they will lead to improved predictions of hurricane landfall and strength by understanding the mechanisms that govern their formation, growth, and interaction with the global weather system. They will speed the development of fusion power by helping to understand and control the instabilities that currently limit the energy densities that are achieved. They will lead to more efficient vehicles, by reducing the friction between the vehicle surface and the surrounding air. They will lead to a new generation of micro-scale devices that will include combustors to replace batteries, advanced flow control devices to cool electronic systems, and labs-on-a-chip to manipulate and interrogate DNA. Already, the number of channels in micro-fluidic devices is growing at a rate faster than the exponential growth in electronic data storage density".

The **Summary** of the report states "*Research in fluid dynamics is expected to have major impacts on important national needs. These include improvements in transportation and energy efficiency, prediction and mitigation of environmental problems, development of novel technologies based on microfluidics, improvements to security and defense, and major contributions to health. Finally, fluid dynamics research makes a large contribution to the training of future engineers and scientists.*"

It can be safely assumed that all members of the fluid dynamics community present at the Workshop are in broad agreement with these statements.
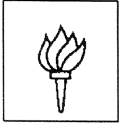
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October 27, 2006

Dr. Raymond Orbach
Under Secretary for Science
U.S. Department of Energy
1000 Independence Avenue SW
Washington, DC 20585

Dear Dr. Orbach,

We are writing to alert you to a crisis in funding for basic research in fluid dynamics. This centrally important and highly interdisciplinary field has recently lost so much financial support that its existence in the US seems to us to be in jeopardy.

The sudden decline in support for research in fluid dynamics is the result of independent adverse developments in all of the major funding agencies:

a) At the NSF, fluid dynamics has fallen into a twilight zone between the physics, materials, and engineering divisions, with no one of these divisions having responsibility for the field as a whole or providing adequate support for young scientists.

b) The DOE has canceled a major program in fluid dynamics on very short notice.

c) NASA has canceled its fluid dynamics program with no notice at all.

d) The DOD has substantially moved away from this area of basic science in its 6.1 and 6.2 programs.

The result of these recent developments is the disappearance of research opportunities in fluid dynamics and in many related areas in which it is essential. Important senior scientists already have left the US and restarted their careers in Europe and Asia. Young scientists have been discouraged from submitting proposals in this area.

We do not believe that this situation is good for the nation at a time when it is engaged in urgent efforts to enhance activities in the basic sciences, with the long-term goal of

improving our competitive position internationally. These efforts have been guided in part by the recent report entitled "Rising Above the Gathering Storm" from the National Academies, which makes the following recommendation (B-1): "Increase the federal investment in long-term basic research... Special attention should be paid to the physical sciences, engineering, mathematics and information sciences, and to the Department of Defense basic-research funding."

We urge the leaders of funding agencies to reexamine their priorities regarding research in fluid dynamics, and to develop a multidisciplinary approach to this field which will serve the national interest.

Specifically, we urge leaders of funding agencies to recognize that:

- Fluid dynamics is at the forefront of research in important conceptual areas such as turbulence, pattern formation, the development of complexity, the limits of scientific prediction, chaos, and more generally in almost every situation in which physical or biological systems are driven away from simple states of equilibrium.

- Research in fluid dynamics has important practical implications, for example, in weather and climate forecasting, the design of chemical processing facilities, drug manufacturing, numerical modeling of complex engineering systems, materials failure, microfluidics, and biofluidics.

- Because most research in fluid dynamics involves only small-scale, but often highly sophisticated instrumentation, this field is ideally suited for training advanced students in designing and carrying out research projects.

- Because fluid dynamics is the essence of a wide variety of familiar phenomena, many of which have great visual appeal, this field provides excellent opportunities for outreach to the general public. It is particularly good for inspiring young students to choose careers in the sciences.

Thus, fluid dynamics is centrally important in a very wide range of the sciences. It has, we believe, been shortchanged almost by accident—but at great potential cost to the nation. We urge you to help remedy this situation.

Sincerely yours,

Pierre Hohenberg (New York University)
Chair Physics Section NAS
pierre.hohenberg@nyu.edu

Leo Kadanoff (University of Chicago)
President Elect, American Physical Society
l-kadanoff@uchicago.edu

James Langer (University of California, Santa Barbara)
Former Vice President, NAS
langer@physics.ucsb.edu

(Affiliations for identification only)

Research Findings

Since this is a workshop organization / community-building project, our findings are focused on observations on the state of our research community, and mainly from the Cyber point of view.

From the CyberFD Workshop, 2007

We begin by quoting excerpts from the Executive Summary of the Final Workshop Report, specifically:

> "Discussions at the workshop produced broad consensus on several key issues underlying the community's needs as the era of Petascale computing rapidly approaches. Although large-scale computing has brought many advances to the field, expertise for scaling codes effectively to possibly hundreds of thousands of processors is not widely available, especially for flows with multiphysics content where the mathematical foundations of the subject often cause difficulties often not widely appreciated by practitioners in other disciplines. Training of graduate students who often have little prior programming background is likewise a concern, given the increasingly high level of computer-science expertise that must be mastered. While collaborative research efforts are not uncommon, most in the community do not see a clear path to mechanisms for open-source code development or efficient handling of large datasets which are essential for wide participation. Several reasons were brought forward for the perception that fluid dynamicists have not been using NSF-supported TeraGrid resources at a level commensurate with the and importance of fluid dynamics problems. One of these is increasing scarcity of funding for research in fundamental fluid dynamics, which provides much of the motivation for use of Cyber resources. This is a situation which (if uncorrected) can imperil the community as a whole, and suggests that the importance of fluid dynamics in many interdisciplinary contexts is not sufficiently well appreciated by the public, funding managers, and reviewers alike."

In view of these observations, the Report Authors proposed several recommendations both to (i) the fluid dynamics community on ways to advance and sustain the discipline in a new era of Cyber opportunities, and (ii) agencies, funding managers, and resource providers on how they can facilitate, encourage, and support the community's efforts. In particular, with minor rephrasing from the prior report, our recommendations to NSF, other funding agencies as well as the TeraGrid resource providers are primarily as follows:

"We recommend that all major Federal funding agencies examine and strengthen their direct and indirect support for fluid dynamics research, in consideration of its societal importance. This is especially true for fundamental research, which is the motivator of most large computations helping drive HPC development. Within NSF, we urge that consideration be given to an immediate and sustained budget increase for the Fluid Dynamics program, with priority for activities designed to benefit from advanced Cyberinfrastructure. We also recommend that, with help from the community, the Fluid Dynamics program director (and his future successors) continue to be a strong advocate for Cyber activities, including co-funding of interdisciplinary proposals as appropriate. Interagency dialogs are similarly encouraged. Finally, we recommend that TeraGrid resource providers increase their efforts to promote awareness of HPC resources and services available, and that resource allocation committees give greater weight to science impact versus HPC scalability performance."

Recent developments and future needs

While most of the observations that we (and the workshop attendees) made in late 2007 remain valid in 2010, we also make a few more recent observations, as below:

1. The lower-than-expected response rate to the Cyber-FD abstracts category initiated at the APS-DFD annual meeting in 2008 is, we believe, not an accurate reflection of the community's interest level, but rather a result of insufficient publicity within our own community, which we need to continue to improve.

2. The need for better publicity outside the fluid dynamics community is even greater. While fluid dynamics is important in numerous other disciplines, awareness of this fact among other scientists and other sponsor agency officials is lagging.

3. To date, the fluid dynamics community has yet to see a strong Virtual Organization effort succeed, say in the context of NSF's Cyber-enabled Discovery and Innovation (CDI) program. The need to adopt and emulate suitable aspects of best practices from other communities (such as nanoscience, earthquake modeling, astronomy, rheology of complex fluids) clearly remains.

4. Community code development and wider access to larger datasets continue to be a challenge. In this context, and in line with a need to learn from communities in other fields of science, it is noteworthy that NSF's Fluid Dynamics program has funded a forthcoming workshop on the *Development of Fluid Mechanics Community Software and Data Resources*, to be held at University of Texas at Austin, in March 2010. The PI of the new workshop as the same as the Co-PI (R.D. Moser) of the workshop that we held in 2007. We look forward to the impact of the forthcoming workshop.

Research Activities

Note: This grant from NSF was to organize a workshop with the objective of bringing together a set of leading members of the fluid dynamics community to explore challenges and opportunities in the new era of Cyber opportunities. The workshop activity was held at NSF Headquarters in July 2007. The list of participants, agenda, and the final workshop project can be found at the URL `http://www.nsf-cyberfluids.gatech.edu` which is posted on the web by the PI's institution (Georgia Tech). Subsequently the grant period was extended to allow remaining funds to be used in support of several follow-up activities deemed to be of benefit to the community. Most, but not all, of these activities took place before the second annual report was submitted in March 2009. We provide below a timeline of the project history and an abbreviated account of the sponsored activities.

While full details of the actual workshop proceedings in 2007 are available in the Final Project Report noted above, for convenience we include the Agenda and the List of Participants as appendices to this document.

Dec. 2006: *project conception*. The idea for holding this workshop was first conceived by Dr. William Schultz, early in his tenure as as Program Director (PD) for Fluid Dynamics at NSF. Dr. Schultz suggested that the PI, as an NSF grantee and major user of NSF-supported supercomputing facilities, take on the task as lead organizer.

Spring 2007: early planning. A series of discussions took place concerning logistical issues decisions such as event date, location, budget, and website development. R.D. Moser (U. Texas at Austin) was recruited as Co-PI. A small informal advisory group with wide interests and exposure in the field was formed to help identify and select potential invitees. with a view for both technical balance and the inclusion of both senior and promising younger members of the community. A number of speakers were contacted early to ensure their interest and availability. The workshop proposal was formally submitted in April 2007.

May-Jun 2007: Attendee and speaker invitations. Upon recommendation by others on the organizing team the PI extended invitations with a wider set of potential participants. Session chairs and group discussion leaders were also selected during this period. Dr. Schultz served as our point of contact with a number of other NSF officials, including the Assistant Director of NSF for Engineering (R. Buckius). The PI also wrote to the heads of several NSF-supported supercomputing centers and invited them to send representatives.

Jul 2007: Workshop was held, July 17-18, at NSF. There were approximately 40 non-NSF participants, including four from the supercomputer centers. NSF's Assistant Director of Engineering, and the CBET Division Director both gave brief remarks, while two other NSF program officers were on the list of speakers. The program spanned 1.5

days and included 5 sessions of 17 formal presentations in total, as well as three group or plenary discussion periods.

Aug 2007: Reimbursements and post-workshop questionnaire. Costs for participant travel and catering, processed by the PI's administrative assistant at Georgia Tech, were both significantly below budgeted amounts, resulting in a surplus that could be used for other activities later. Each participant was asked to complete a questionnaire, which became an useful source of information later used in the workshop report.

Sep-Oct 2007: Report preparation and contacts with professional society leadership. A short one-day meeting was held at NSF for the report authors (consisting of the PI, Co-PI, and four discussion leaders at the workshop) to discuss report preparation. They were joined by NSF staff, including a publicity specialist. as well as the (then) Vice-Chair (P.S. Marcus. UC Berkeley) of the American Physical Society's Division of Fluid Dynamics (APS-DFD).

Nov-Dec 20007: Report preparation and submission. A draft of the Workshop Report was posted on the workshop site shortly before the APS-DFD's annual Fluid Dynamics conference. Attendees were invited to comment. The draft report was also circulated among the APS-DFD's Executive Committee (ExComm) for discussion. The Workshop Report was submitted to Dr. Schultz in late Dec. 2007, on schedule.

May-Jun 2008: Formation of APS-DFD Cyber Fluid Dynamics Ad-hoc Committee. In action responding to recommendations in our Workshop Report, the APS-DFD Executive Committee decided to form an ad-hoc committee, with the PI as Chair. A mission statement was prepared and the committee members were selected based on input from the DFD's leaders and the NSF PD. The initial members thus chosen were J.G. Brasseur (Penn State), G.E. Karniadakis (Brown), J. Koplik (City College, CUNY), B.J. McKeon (Caltech) and M.W. Plesniak (George Washington Univ., and formerly at NSF). *Project funds remaining in our workshop grant were used to support the operation of this committee, including travel and charges for conference calls where applicable.*

Jun-Aug 2008: Initial Committee discussions. Two conference calls were held in this period. Committee members were joined by DFD leadership (P.S. Marcus) and NSF PD (W.W. Schultz). Discussion themes included the need for development of new collaborative tools for Cyber-FD, the need to reach out to other related science communities and funding agencies, as well as the need to increase the visibility of our field. Some of these issues overlap with publicity and media-relations aspects of the DFD's activities, in which two of the committee members (J.G. Brasseur, M.W. Plesniak) have been heavily involved. Two definite action items were to (i) propose a new Cyber-FD category for the DFD annual meeting in Nov. 2008 and (ii) organize a session of invited talks at the APS March Meeting in 2009, jointly with the APS's Division of Computational Physics (DCOMP) in order to highlight the broad value of large computations in fluid dynamics in multi-disciplinary contexts.

Sep-Nov 2008: Continued committee discussions. The committee was alerted by the DFD annual meeting organizers that the number of Cyber-FD abstracts submitted was

low. This points to a need to distinguish between Cyber fluid dynamics from traditional computational fluid dynamics, i.e. to emphasize the broader issues including computational performance, community codes, sharing of large datasets, etc. Discussions took place also on the idea of multidisciplinary workshops that potentially could be funded jointly by Fluid Dynamics with other NSF programs, and an informal meeting was held during the DFD annual meeting. On another front, on behalf of the committee the PI submitted a proposal to the APS for a joint DFD-DCOMP invited session proposal at the 2009 March Meeting. Five highly accomplished speakers were selected, to represent fluid dynamics research in astrophysics, biofluids, combustion, hurricane prediction, and multiphase turbulent flows.

Feb-Apr 2009: 2009 APS March Meeting invited session and publicity. The invited session cited above went well: all the speakers (P. Padoan, UCSD; G.E. Karniadakis, Brown; J.H. Chen, Sandia Livermore; F. Zhang, Penn State; S. Elghobashi, UC Irvine) gave well-prepared and insightful presentations of their latest work, and there was a lot of interesting discussion between the speakers and the audience. The PI was contacted in advance by staff from AIP Media Services (J. Bardi) to hold a press conference to help publicize the session and the speakers' work. Four of the five speakers participated and gave overviews of work in their area suitable for a more general audience; and about 6-8 reporters were in attendance. An article incorporating some of the questions and answers subsequently appeared in the May 2009 issue of *APS News*. In addition, at the suggestion of DFD leadership and with help from the speakers, the PI prepared an article with text and graphics for the DFD Divisional Newsletter of Spring 2009.

Aug 2009: Visit to NSF to meet with new NSF PD and other NSF officials. As PD for NSF's Fluid Dynamics Program, Dr. W.W. Schultz was very closely involved with the Cyber-FD community. Consequently the committee felt it was important that his successor, Dr. H. Henning Winter, who took up his position in late August, be well informed of our past efforts and to be an importance source of valuable advice for us in the future. With adequate travel funds still available, we thus decided to organize a delegation to meet with both outgoing and incoming Fluid Dynamics PDs, with the main purpose being to introduce to the new PD (and other NSF disciplinary staff) the nature of our DFD research community. Since this visit was of a broader scope than Cyber, it was (appropriately) led by and organized in close contact with the DFD leadership (P.S Marcus and A.R. Karagozian, Chair and Vice-Chair for 2009 respectively). Other participants from the committee were J.G. Brasseur, B.J. McKeon, M.W. Plesniak, and P.K Yeung; two additional participants (J.H. Duncan, Maryland; L.M. Walker, CarnegieMellon) were also recruited to ensure broad topic coverage. The outgoing PD (W.W. Schultz) was instrumental in enabling this event and in assembling slides from the participants for use by new PD H.H. Winter. We believe the meeting was a success and has helped promote a working relationship between the new PD and our DFD community.

NSF Cyber-Fluid Dynamics Workshop

NSF Headquarters, July 19-20, 2007

Rm 375, Stafford I

Day 1

Continental Breakfast, Available 7:30

Preliminaries

8:30	-	9:05	Welcome and Opening Remarks
			P.K Yeung, Georgia Institute of Technology
			William W. Schultz, NSF Program Director, Fluid Dynamics
			Richard O.Buckius, NSF Assistant Director for Engineering
			Judy A. Raper, NSF CBET Division Director

Session I: High-performance Computing and Cyber Activities
Chair: P.K. Yeung, Georgia Institute of Technology

9:05	-	9:40	Abani K. Patra. NSF (Office of Cyberinfrastructure)
			Cyberinfrastructure for Collaborative and Predictive Simulations
9:40	-	9:58	Richard L. Moore. San Diego Supercomputer Center.
			TeraGrid CI Resources for CFD Research.
9:58	-	10:16	Federico Toschi, C.N.R (Italy)
			iCFDdatabase: The International CFD database

Break

Session II: Turbulence and Flow Control
Chair: Sanjiva K. Lele, Stanford University

10:30	-	10:48	P.K. Yeung, Georgia Institute of Technology
			Intermittency, Mixing and Dispersion in Simulations of
			Homogeneous Turbulence: the Path towards Petascale
10:48	-	11:06	Robert D. Moser, University of Texas at Austin
			Simulation of wall-bounded turbulence: what more can we learn?
11:06	-	11:24	Tim Colonius, California Institute of Technology
			Closed-loop flow control: simulation challenges and opportunities

Break

Breakout Groups in parallel session, 11:40-12:45

I. Discussion Leader: **Michael W. Plesniak, Polytechnic University**
II. Discussion Leader: **Charles Meneveau, Johns Hopkins University**

Lunch (provided): 12:45-14:00

Session III: Complex Fluids and Multi-Physics Applications
Chair: Arnaud Trouve, University of Maryland

14:00	-	14:18	Gretar Tryggvason, Worcester Polytechnic Institute
			Studying the Dynamics of Heterogeneous Continuum Systems using DNS
14:18	-	14:36	Sangtae Kim, Purdue University
			Hub-based Petascale Collaboratories - the new HPC
14:36	-	14:54	Lance R. Collins, Cornell University
			Numerical Simulation of Polymer-Turbulence Interactions in
			Homogeneous Turbulent Shear Flow of a Dilute Polymer Solution

Break

Session IV: Nano and Bio Fluid Mechanics
Chair: Bruce M. Boghosian, Tufts University

15:05	-	15:23	George E. Karniadakis, Brown University
			Teragrid Simulations of the Human Arterial Tree
15:23	-	15:41	Nadine Aubry, Carnegie-Mellon University
			Simulating the Multi-Physics involved in Microscale Flows
15:41	-	15:59	James G. Brasseur, Pennsylvania State University
			Computational Investigations of the Couplings between Macro-scale
			and Micro-scale Transport of Nutrient Molecules in the Intestines

Break

Breakout Groups in parallel session, 16:15-17:20

III. Discussion Leader: **Said E. Elghobashi, University of California at Irvine**
IV. Discussion Leader: **Cyrus K. Aidun, Georgia Institute of Technology**

Plenary Discussion (Sessions I-IV), 17:30-18:30
Discussion Leader: **Robert D. Moser, University of Texas at Austin**

**Informal dinner: Matsutake Sushi & Steak Restaurant, 4121 Wilson Boulevard,
Tel. 703-351-8787**
Accompanying persons welcome.

Day 2

Continental Breakfast, Available 7:15

Session V: Knowledge Discovery and Education
Chair: James J. Riley, University of Washington

8:15	-	8:45	Phillip R. Westmoreland, NSF (Combustion and Virtual Organizations) Virtual Organizations as New Aids for Collaboration.
8:45	-	9:03	Craig C. Douglas, University of Kentucky & Yale University Scientific Community Web Sites: What Works... and Not
9:03	-	9:21	Alexander J. Smits, Princeton University eFluids: a High-Quality Source for Data, Information, and Educational Materials in Fluid Mechanics
9:21	-	9:39	Ellen K. Longmire, University of Minnesota Visualization Methods to Advance Discovery in Fluid Dynamics
9:39	-	9:57	Daniel P. Lathrop, University of Maryland Extreme Challenges in Turbulence: Matching Computation to Experiment at Global Scales

Break

Plenary Discussion (Sessions V), 10:10-11:10
Discussion Leader: **Robert D. Moser, University of Texas at Austin**

Break

Event Closing and the Future

11:20	-	12:00	Group Reports (Breakout group leaders)
12:00	-	12:20	Follow-Up: NSF and the Fluid Dynamics Community (Schultz)
12:20	-	12:30	Concluding Remarks (Moser/Yeung)

Lunch (provided), 12:30:- (boxed lunches to-go)

Adjourn

Appendix: List of Participants

From the broad fluid dynamics community

(Note: affiliation information as of July 2007)

Cyrus K. Aidun	Georgia Institute of Technology
Nadine Aubry	Carnegie-Mellon University
Elias Balaras	University of Maryland
Bruce M. Boghosian	Tufts University
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