# AN INITIATIVE TO SUPPORT COMPUTATIONAL SCIENCE AT THE UNIVERSITY OF VIRGINIA

**P R E L I M I N A R Y  D R A F T: 7/9/06**

***By the:***
**U.Va. Task Force on Information Technology Infrastructure Supporting Research in Science and Engineering**

## About This Report

This report was developed by the U.Va. Task Force on IT Infrastructure Supporting Research which was created in January 2006. The impetus for this task force originally came from Jim Aylor, Dean of Engineering and Applied Science, in response to perceived shortfalls in the existing infrastructure for computational science. Concurrently, the University Committee for Information Technology established a subcommittee to make recommendations for the support of research computing and to provide information that could be used in the development of the University's capital campaign case statement on information technology. Given the overlapping membership of those two groups they were combined into a single task force whose charge was to develop recommendations on how the University should support information technology needs for research in engineering and the natural sciences.

The Task Force met throughout the Spring 2006 semester on a biweekly basis. In addition an executive committee met weekly to develop further the concepts outlined by the full task force.

The membership of the Task Force is attached. The work of the Task Force led to the formation of a special committee that submitted a $250,000 grant proposal in June 2006 under the NSF CI-TEAM Cyberinfrastructure Workforce Training and Education program.

## Executive Summary

Among the strategic objectives of the University of Virginia are the following goals: (1) Improve the University's core educational mission, (2) attract, retain, and support highly qualified faculty, (3) Develop the University's potential as a research institution together with cutting-edge research programs, (4) promote interdisciplinary collaboration, and (5) develop new modes of learning, teaching, and research. If the University is to fully achieve these objectives it is imperative that a it establish and follow a roadmap to enable computational science and engineering. Computational science is an emerging discipline that will revolutionize how problems are solved. The academic institutions that will emerge as world leaders will be those that recognize the significance of computational science to their strategic goals and act appropriately. This report, developed by the U.Va. Task Force on IT Infrastructure Supporting Research, is the first step toward formulating

an effective strategy for the University of Virginia.

Although it has been customary to think of the needs of computational science in terms of hardware and raw processor power, such a focus overlooks requirements of greater importance: knowledge and expertise. Computational science requires not only discipline specific expertise, but also up-to-date knowledge in areas such as algorithms, programming, optimization, data management, and visualization; more than a single researcher can master.

State of the art computational science will require the collaboration of many skilled people from many disciplines. Such people are currently not widely available, and the training to develop such people is lacking. Graduate and undergraduate curricula remained centered on the research methodologies employed when the faculty were educated, despite the revolutionary changes seen in the last few decades.

Twenty years ago researchers were clearly limited by the available hardware; they could easily devise projects that would exceed the capabilities of the fastest computers. Now the relation is inverted: the capabilities of the most powerful computers easily exceed the average researcher's ability to utilize them in a meaningful way. System capabilities have advanced to the point where remarkable breakthroughs can be made in many fields, but only if the research community is prepared to take advantage of those capabilities.

Many reports have been written by Federal advisory bodies, industry groups and the like attesting to the need for strategic planning in computational science. Many universities have heeded this call and are developing innovative computational science programs in research and education. The Task Force examined these reports and the activities at other academic institutions in developing a series of recommendations for the University of Virginia.

This Task Force Report proposes a series of steps to create a new Initiative in Computational Science and Engineering. This initiative does not address ``commodity'' computing, that is, the basic IT infrastructure; dealing with such infrastructure requirements is a separate issue. Rather the initiative focuses on providing advanced resources that specifically enable breakthrough computational science.

The Task Force felt strongly there is a need to develop a culture of computational science and engineering at the University. More than merely a hardware issue, this will require leadership, a skilled talent pool of experts in the many aspects of computational science, and an organizational structure that permits growth, flexibility and the ability to respond in a timely manner to rapidly changing requirements. In considering all of these concerns and requirements, the Task Force has chosen to frame the goals of this initiative in terms of four categories, with recommendations in each:

**(A) A structure for leadership**

The rapid pace of developments within computational science, the complexities and expense involved in undertaking support for computational science, and the wide range

of disciplines for which computational science is essential, call for strong leadership to coordinate the needs and concerns among the many departments and schools that engage in computational science, and the active participation of the research faculty in planning and policy.

► The Task Force recommends the appointment of a director for research computing (at a senior level, such as an associate vice president) whose responsibilities would include:

** to work with senior university administration to develop and execute a plan for university computational science*
** to promote, develop, and manage external partnerships with other universities and research organizations*
** to oversee the staff of the advanced support team*
** to chair the faculty advisory committee*
** to oversee research policy and resource allocation*

► We also recommend the establishment of a Faculty Advisory Committee for computational science whose purpose would be to provide leadership for and communication and collaboration among the computational science and engineering researchers and the expert community.

**(B) Advanced support for sponsored research**

One of the primary goals of this initiative is to facilitate sponsored research. Many significant future research opportunities will focus on the development of interdisciplinary teams that cut across the traditional school and departmental boundaries and steps should be taken to ensure that the University's proposals will be competitive.

► The Task Force recommends:

** A Grant Development Officer for Computational Science and Engineering should be named. This person would identify appropriate opportunities, work with researchers to assemble teams that can respond to such opportunities, and coordinate the technical aspects and arrange appropriate cost-sharing, resource commitment and other details in the resulting proposal.*

** Seed or development funds be allocated to boot-strap promising new interdisciplinary initiatives and make grant proposals more attractive to funding agencies.*

** Create an environment that encourages and facilitates collaboration, such as to establish a facility where researchers can work together with experts in a resource-rich environment, described below as a center advanced computational science support.*

**(C) Expert support for computational science**

Often discussions of the needs of computational science devolve into discussions of hardware, but that is not the only area of investment needed for computational science.

One of the clear conclusions of the Task Force is that now and in the future the scarce resource will be skilled people. To this end we propose the establishment of the University of Virginia Alliance for Computational Science (UVACS).

A list of the resources that UVACS will coordinate and provide include:

1. *Appropriate access to the appropriate processors, from desktop machines to supercomputers*
2. *Expertise in algorithms and programming*
3. *Use of scientific software and discipline-specific applications*
4. *Networking, including access to very high speed national backbone networks and Grid computing*
5. *Data repositories, data security and access, and data analysis*
6. *Display, including advanced visualization*
7. *Education and training*

This has been previously proposed as a support center for computation in the sciences, although it has not yet been implemented. The Academic Computing Health Sciences (ACHS) center, jointly sponsored by the School of Medicine and ITC, provides a successful example. ACHS supports many small or proof-of-principle projects by core funding, but as projects grow and increase in scope, significant amounts of staff time can be shifted to direct costs. In this manner ongoing funding is leveraged to maintain several times the number of personnel that could otherwise be employed. Thus expert assistance and support for sponsored research permits growth and sustainability of a significant computational science infrastructure.

**(D) Education and training in computational science**

Despite the widespread perception of the importance of and potential for computational science, relatively little has been done to prepare students and researchers for the future. It is imperative that we provide our students with the education and training they will need to be effective researchers, scientists and engineers.

In addition to providing a basic education to our students, the wider benefits of making computational science a part of the graduate and undergraduate curriculum include: improved opportunities for establishing interdisciplinary collaborations, engaging a wider number of researchers in computational activities, improving U.Va.'s visibility and reputation in graduate education and improving graduate recruitment, improve graduate job opportunities, and lay the groundwork for a future degree program in computational science.

While developing a formal curriculum in computational science for our graduate and undergraduate students is a major goal of this initiative, it is also important to develop a less formal program of training for a wider community including students, postdoctoral fellows, and faculty. Thus this initiative should include a regular program of courses, lecture series, mini-courses, and workshops. This would be a "community development" effort, to foster a culture of computational science in the sciences and engineering

Although this Task Force Report does not completely describe a successful University-wide program to support and enable world-class computational science, we do include several specific recommendations to begin to implement the goals outlined above.

The following steps should be taken as soon as possible:

** Identify faculty involved in computational science who could form a core of experts.*
** Form a faculty advisory committee for computational science.*
** Identify a sponsored projects development officer for computational science*
** Identify existing expertise and interest in the core areas of UVACS support, such as visualization. Develop collaborations and communication among existing groups at the University.*
** Appoint a director as soon as possible - there are opportunities to be pursued and there is an immediate need for leadership if we are to achieve the other goals of this initiative.*
** Identify existing expertise within ITC staff who could form the initial core computational group that would become UVACS.*
** Expand and extend existing workshops (presently given by the Research Computing Support Group of ITC) on topics in computational science.*
** Locate a suitable space to site the initial UVACS group*
** Implement the activities of the NSF CI-TEAM proposal for a demonstration project in computational science education.*
** Commence an interdisciplinary seminar series in computational science to build community*
** Integrate these proposed activities into the vision for the Capital Campaign and for the University's long-range planning.*
** Identify components of this initiative that would be suitable for specific funding opportunities within the Capital Campaign.*
** Actively pursue interdisciplinary funding opportunities in computational science and engineering. Identify procedures for providing matching or seed funds in support of sponsored research. Encourage inclusion of direct-cost support for UVACS staff.*

**U.Va. Task Force on Information Technology Infrastructure Supporting Research in Science and Engineering**

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Spring 2006

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