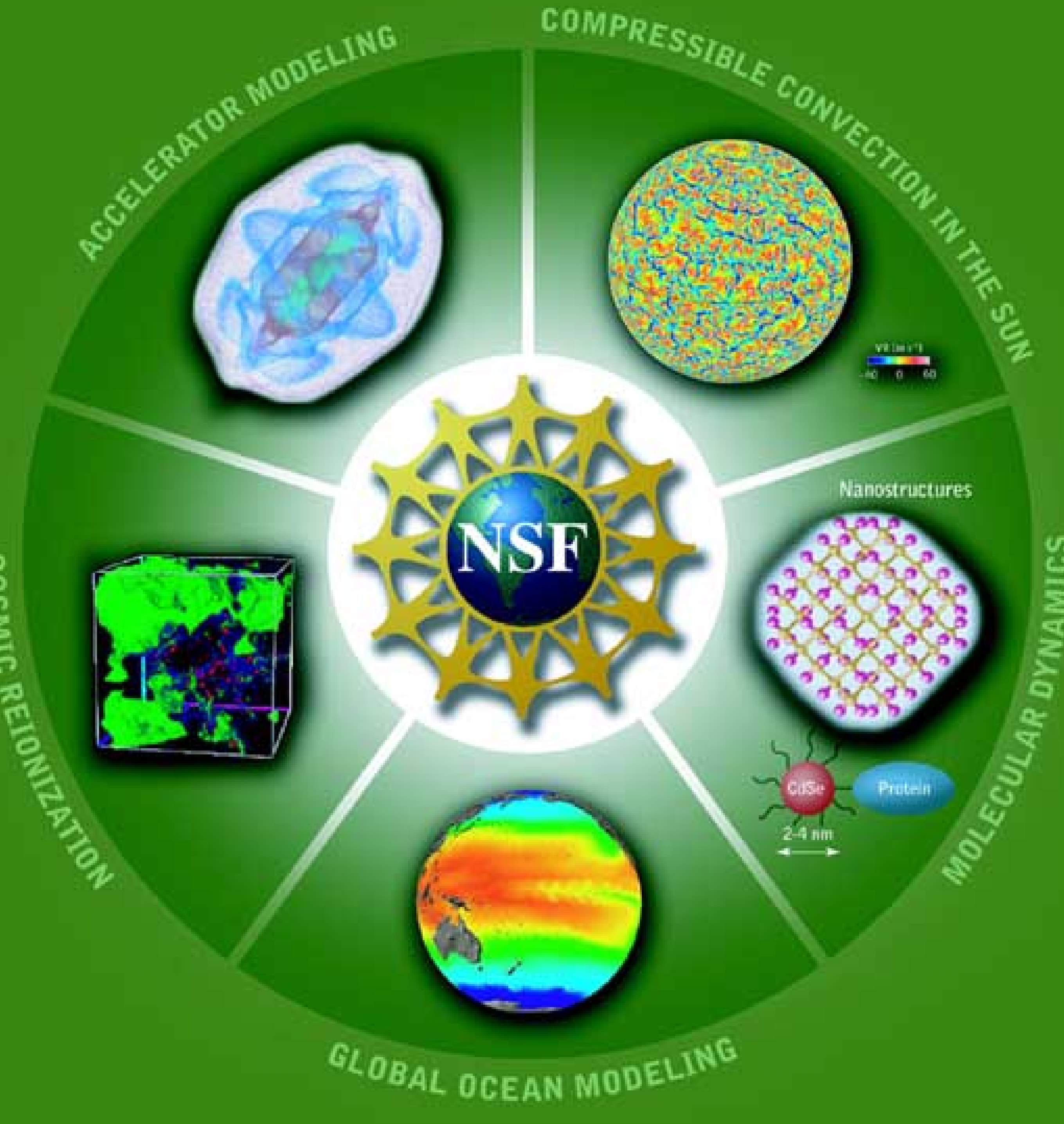
Computation As a Tool for Discovery in Physics

A Report to the
National Science Foundation
by the Steering Committee on
Computational Physics



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A Report to the National Science Foundation by the Steering Committee on Computational Physics

Steering Committee

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The workshop on which this report is based took place on September 11 and 12, 2001, in Arlington, Virginia. The participants were deeply affected by the horrific events on the morning of September 11, but nevertheless made the decision to continue with the meeting. We are deeply grateful to the speakers, who delivered a remarkable set of lectures under extraordinarily stressful circumstances, and to the other participants who energetically contributed to the panels and discussions during two difficult days for the nation.

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EXECUTIVE SUMMARY

The Steering Committee was charged with the task of surveying opportunities and challenges in computational physics, broadly construed. A workshop was held on September 11 and 12, 2001, in which the presenters were asked to represent the state of the computational art in their respective fields and to identify both the outstanding opportunities as well as the barriers to progress in their disciplines. While the workshop could not cover all areas of computational physics that are of interest to the National Science Foundation, the Steering Committee heard many exciting examples of new research directions and problems that are being opened up by the application of modern computational approaches. Some of these examples came from areas that are mature users of computation, such as cosmology, fluid dynamics, plasma physics, and lattice gauge theory. Others came from areas where the use of computation is just coming into prominence or rapidly evolving, such as accelerator design, biophysics, experimental high energy physics, and numerical relativity. All of these research opportunities are in areas that address fundamental scientific questions and/or are of tremendous current societal importance.

The central finding of the committee is that the NSF should create a new program in computational physics, which could serve as an exemplar of similar programs in other NSF directorates. Such a program should support those activities in computational physics that are not adequately addressed by existing programs, placing the NSF in a better position to capitalize on the emerging opportunities in this field. Although the workshop on which this recommendation is based focused on computational physics, it was not constrained by the disciplinary boundaries of the Physics Division. The breadth of opportunity that was demonstrated in the presentations strongly suggests that a new NSF program in this area could be profitably extended to encompass the entire range of disciplines supported by the NSF.

The workshop presentations demonstrated a broad commonality of interests and needs across the entire spectrum of the disciplines represented. In each discipline, there are clear opportunities for discovery and new understanding that are being missed because of the lack of appropriate and focused support for the computational activities of the investigators. Moreover, spectacular advances in the power of computational hardware available to scientists have radically amplified those opportunities, and increased the need for the NSF to address them. The participants in the workshop, and the Steering Committee, also recognized an urgent need for new and strengthened educational programs in computational physics with two components:

1) *training the next generation of computational scientists for academic and industrial careers, and*
2) *integrating computational science into the standard curriculum in physics.*

The NSF should play a leading role for the nation in expanding opportunities at both the undergraduate and graduate levels, and pursuing a new class of educational goals for computational physics. The Steering Committee suspects that similar educational needs exist in the other areas of the Mathematical and Physical Sciences and across other Directorates.

The Committee found that computational investigations in physics are currently supported unevenly and suggests that a new program in computational physics should address the issues of balanced support in two ways:

1) *Software and Hardware* — At all levels, from the desktop to the parallel supercomputer, insufficient attention is being paid to supporting application software development. It is extremely difficult for a principal investigator to find support for the multi-year code development efforts required to fully exploit emerging opportunities in computational physics. Effective support in this area will also make software collaborations in physics more common at every level. The application software issue is particularly acute at the high end of computational resources, where extensive efforts are necessary to develop and optimize applications software for terascale supercomputers. Applications software development provides different challenges than do traditional theoretical studies, and should be one of the distinctive features of the NSF program in computational science. Reflecting its grounding in both theory and experiment, computational science shares attributes of both theoretical and experimental science. The need for substantial support of software development is analogous to support for experimental apparatus.
2) *The Spectrum of Computational Hardware Resources* — At the low end of computational power, the desktop or workstation, current NSF support mechanisms seem to be appropriate. At the highest end, the NSF Partnerships in Advanced Computing Infrastructure (PACI) Program focuses on providing the terascale hardware resources needed by NSF investigators. However, at the mid range, where machines currently consist of tens to a few hundred processors, the level of support seems inadequate. This class of hardware, which can be effectively fielded by university research groups or departments, will play an increasingly important role in research in physics. It should receive particular attention in a new computational physics program.

Another theme which emerged in the workshop discussions is the need for support for closer collaboration between the Physics and Applied Mathematics communities to develop new methods for computational physics. In this century, the challenges of multiple time and length scales in areas as diverse as materials, nanoscience, plasma physics, atmospheric physics, and biophysics have become a new focus of computational research. Meeting those challenges, as well as finding methods that scale well with the number of particles in many-body systems, will likely require new mathematical as well as physical insights.

The support of application software development for tools that are created by the applied mathematics community is an issue for the physics community. An NSF program in computational physics would be most effective if it enabled applied mathematicians to join with physicists as peers in the research enterprise. In this area, again, the Steering Committee suspects that a new program in computational physics might profitably be extended to cover all of the disciplines supported by mathematical or physical sciences at the NSF.

In summary, the committee finds that there is strong impetus for NSF to act now to capture opportunities that have been created over the last decade by the combination of the growth of computing power and the invention of new algorithms and methods. Many of the specific issues that such a program should address are already clear. A new program of effective support for this area can greatly enhance the impact of computation on physics, and enable a range of discoveries in many areas of our field.