

V. CONCLUDING OBSERVATIONS

The central finding of the Steering Committee is that the NSF should create a new program in computational physics. That recommendation and the other principal findings listed in Section II are the main thrust of this report.

However, there are some additional issues that were discussed at the workshop that should inform the establishment of a program in computational physics. The practice of theory and modeling in physics has changed considerably over the past decades, and today computational science shares attributes of both theoretical and experimental science. The need for substantial support of software development is analogous to support for experimental equipment. Theory and modeling now requires its own physical “experimental equipment” as well, in the form of a range of computational hardware from workstations and clusters to supercomputers.

The participants at the workshop agreed that a new program at the NSF should recognize and fund the true costs of software development and maintenance. The scale of modern scientific research software is now frequently so large that it can easily take large teams of scientists and programmers five years or more to develop software for a single problem. The appropriate support of software development is a central issue for theory and modeling in general and is particularly acute for the computational physics community. There was a consensus at the workshop that five-year grants for software development and maintenance should be considered as part of a new program in computational physics.

Finally, the multidisciplinary nature of much computational science and computational physics was apparent at the workshop. Many problems that face us will require breakthroughs in both science and computing to solve them. Multidisciplinary teams of scientists, mathematicians, and computer scientists will be required to attack such problems, and there is now ample evidence of the effectiveness of such teams. There was a clear consensus of the participants that a new program at NSF should also fund these teams, while not neglecting the role of the single principal investigator in computational physics.

The workshop on which this report is based displayed the promise and excitement of computational physics and computational science in general. The promise of the field extends well beyond the areas explicitly covered in this report. No more effective new investment can be made by the National Science Foundation than in a new program in computational physics.