AD-A179 065 SCIENTIFIC COMPUTATIONS IN APPLIED MATHEMATICS PHYSICS CHEMISTRY AND CRYS..(U) PITTSBURGH UNIV PA DEPT OF MATHEMATICS AND STATISTICS W C RHEINBOLDT 10 SEP 85 1/1

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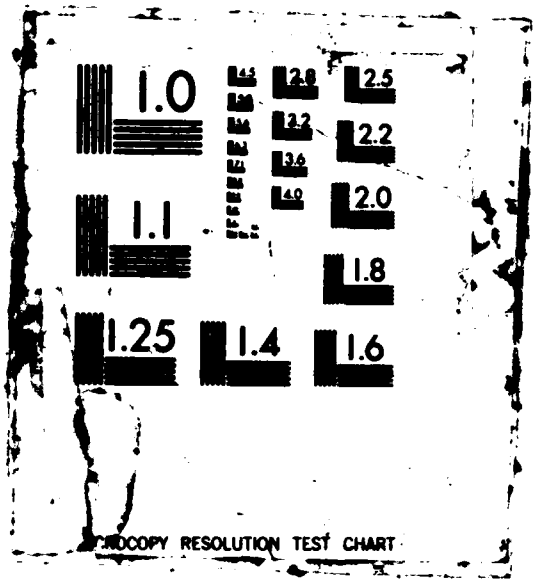
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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

In accordance with this URIP program, the following equipment has been acquired and installed: a FPS-164 MAX scientific computer with 1M words of memory, a matrix algebra accelerator, and FPS-D64 disk subsystem with two drives. The scientific computing facility based on this equipment is now operational It is housed in a specially constructed computer room in close proximity to the four principal departments involved in this activity. From the outset, the facility has been actively used for a range of research projects, including: (1) Methods for the solution of differential/algebraic equations with particular applications to sheet-metal forming and related problems in solid mechanics, (2) Development of computable error estimates of solutions of nonlinear boundary value problems for partial differential equations by finite element techniques, (3) Computational research in crystallography involving principally the determination of three-dimensional structures of biological macromulecules at atomic resolution by x-ray diffraction, (4)Computational methods for solution of parameterized equations with particular emphasis on bifurcation phenomena.

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University of Pittsburgh

FACULTY OF ARTS AND SCIENCES
Department of Mathematics and Statistics

AFOSR-TR 87-0300

September 10, 1985

FINAL REPORT

UNITED STATES AIR FORCE GRANT AFOSR-84-0274 FOR SCIENTIFIC COMPUTATIONS IN APPLIED MATHEMATICS, PHYSICS, CHEMISTRY AND CRYSTALLOGRAPHY

The Grant has been issued under the Department of Defense - University Research Instrumentation Program for 1984/85. In line with the proposal the following equipment has been acquired and installed:

1 FPS-164 MAX Scientific Computer with 1M word of memory,

1 Matrix Algebra Accelerator,

1 FPS-D64 Disk subsystem with two drives
FORTRAN cross compiler, system job executive, Boeing Computer Services Library, and fast matrix solution library.

As outlined in the proposal, the equipment was needed to overcome some of the serious lack of access to sufficiently powerful scientific computing equipment for research efforts in mathematics, physics, chemistry, and crystallography at the University of Pittsburgh. The University recognized that urgent need and decided to augment the funding received under this grant and to establish a more comprehensive scientific computing facility. This facility is now operational and incorporates the following computer equipment:

PITTSBURGH, PA. 15260

1 Gould 32/9780 Dual Processor system,

1 FPS-164 MAX Scientific Computer as outlined above,

1 VAX/VMS 11/750 which serves also as the host for the FPS.

The facility is housed in a specially constructed computer room on the seventh floor of Thackeray Hall on the University's main campus. This location is in close proximity of the four principal departments involved in this activity. The computers are currently accessible from hardwired terminals and over dial-up lines. It will also be connected to the University's new fiber-optic cable network.

The Scientific Computing Facility (SCF) is being operated by the University's Center for Computing and Information Systems under the policy supervision of a Working Group for Scientific Computing which consists of a representative subgroup of the researchers listed in the original proposal for the AFOSR grant. The chairman of this committee is currently Professor W. C. Rheinboldt, the principal investigator of the grant.

From the outset, the facility has been actively used for a range of research projects. We list here only a few representative examples:

Methods for the solution of differential/algebraic equations with particular applications to sheet-metal forming and related problems in solid mechanics.

Development of computable error estimates of solutions of nonlinear boundary value problems for partial differential equations by finite element techniques.

Computational research in crystallography involving principally the determination of three-dimensional structures of biological macromolecules at atomic resolution by x-ray diffraction.

Computational methods for the solution of parameterized equations with particular emphasis on bifurcation phenomena in scientific systems and the determination of singular points.

Computational research on finite difference solutions of time dependent Navier-Stokes equations of compressible fluid flow.

Computational research related to high energy physics problems.

The facility has already proved invaluable in the research work of the proposing interdisciplinary group. It has not only provided a much needed increase in the computing facilities available for scientific computations, but it has stimulated also a much closer cooperation between the members of the group. This increased interaction should prove to be of growing importance in the coming years.

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