PROJECT ADMINISTRATION DATA SHEET

Project No. E-19-651 (R6027-0A0)
Project Director: M. G. White
Sponsor: National Science Foundation

Type Agreement: Grant No. ECS - 8515177

Award Period: From 10/1/85 To 9/30/86

Sponsor Amount:
Estimated: $  
Funded: $  
This Change: $  
Total to Date: $ -0-

Cost Sharing Amount: $ 1,500
Cost Sharing No: E-19-335

Title: Super Computer Use

ADMINISTRATIVE DATA

1) Sponsor Technical Contact:
Frank Huband
National Science Foundation
ENG/ECS
Washington, DC 20550
(202) 357-9618

2) Sponsor Admin/Contractual Matters:
Joe Carrabino
National Science Foundation
DGC/ENG
Washington, DC 20550
(202) 357-9602

Defense Priority Rating: N/A
Military Security Classification: N/A
(or) Company/Industrial Proprietary: N/A

REstrictions
See Attached N/A Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval — Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with N/A

COMMENTS:
This project is for Super Computer Use - no sponsor funds will be expended on this account.

No cost-sharing is required on this project.

COPIES TO:
Project Director
Research Administrative Network
Research Property Management
Accounting

SPONSOR'S I. D. NO.
02-10-2117 85.117

FORM OCA 65-285

Received: 22-2-1985
RETURN: 25-2-1985

GTRC/GTRI Supply Services
Library
Procurement/GTRI Supply Services
Research Communications (OCA)
Research Security Services
Project File
Other A. Jones
GEORGIA INSTITUTE OF TECHNOLOGY

OFFICE OF CONTRACT ADMINISTRATION

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 2/16/87

Project No. E-19-651

Includes Subproject No.(s) N/A

Project Director(s) M. G. White

Sponsor National Science Foundation

Title Super Computer Use

Effective Completion Date: 9/30/86 (Performance) 12/31/86 (Reports)

Grant/Contract Closeout Actions Remaining:

[ ] None
[ ] Final Invoice or Final Fiscal Report
[ ] Closing Documents
[ ] Final Report of Inventions
[ ] Govt. Property Inventory & Related Certificate
[ ] Classified Material Certificate
[ ] Other

Continues Project No. ____________________________ Continued by Project No. ____________________________

COPIES TO:

Project Director
Research Administrative Network
Research Property Management
Accounting
Procurement/EES Supply Services
Research Security Services

Library
GTRI
Research Communications
Project File
Other Ina Lashley
Angela Jones
Russ Embry

Form OCA 60.1028
The grant was a zero budget, computer access time on the Purdue University supercomputer. Before any computing studies were executed at Purdue, we attempted the process of converting our scalar code into vector code using the facilities at the University of Georgia Computing Center. The supercomputer at UGA is very similar to the one at Purdue. The migration of code from our scalar source to the target vector computer code showed less than 10% of the program could be vectorized. The failure to convert the scalar source program could be attributed to a number of "if" statements placed within "do" loops of the source code. This syntax, characteristic of Fortran programming language in the 1960's, is not vectorized by the vector compilers available to us. With only 10% of the source code vectorized, we sought other sources of code to perform the Hückel molecular orbital calculations.

Dr. E. Clementi of IBM's research center in New York was contacted. He is an expert in quantum mechanical calculations and is aware of the many different types of quantum mechanical programs. He suggested that we migrate our Hückel code on the IBM facilities. However, this effort would be unproductive since the resulting target code would run only on parallel processing machines. The Purdue machine is not a parallel processing machine; it is vector processing only. We could not obtain a source code for quantum mechanical calculations, suitable for the Purdue machine. Thus, we terminated any further attempts to use the computer funds provided by the grant.

<table>
<thead>
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<th>ITEM (Check appropriate blocks)</th>
<th>NONE</th>
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<th>PREVIOUSLY FURNISHED SEPARATELY TO PROGRAM</th>
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<td>a. Abstracts of Theses</td>
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<td>c. Data on Scientific Collaborators</td>
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<td>d. Information on Inventions</td>
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<td>e. Technical Description of Project and Results</td>
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<td>f. Other (specify)</td>
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Mark G. White

1/23/87
Final Report
National Science Foundation Grant
for
Supercomputing Time

Georgia Tech Account Number: E - 19 - 651

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