AD-A190 308   MICROVAX NETWORKED COMPUTER SYSTEM(U) PRINCETON UNIV NJ   1/1
              DEPT OF CHEMISTRY H RABITZ DEC 87 AFOSR-TR-87-1958
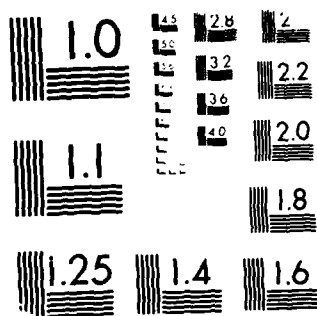   AFOSR-87-0021

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FINAL REPORT

DoD - University Instrumentation Proposal

Microvax Networked Computer System

from

Department of Chemistry, Princeton University

Herschel Rabitz
Herschel Rabitz
Principal Investigator

December 1987

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This final report covers the action taken regarding equipment purchases under Contract AFOSR-87-0021. The funds, totalling $197,286 were for the purpose of purchasing and establishing a network of Microvax computers for research in the area of chemical physics particularly involving dynamics and kinetics phenomena. We have purchased all the original stated items except the line printer and the IBM-PC terminals. These latter items were replaced with the purchase of the extra disk storage deemed important to attain maximal usage from the hardware.

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The overall system network is fully on-line and we are finding that the machines make a significant impact on our research. The design of the networked set of computers linked to the Departmental mainframe Vax is proving to be very effective. Additional experience will be needed to finally establish the optimal mode of system operation but we are already finding considerable speed-up in the rate that computations can be performed. The computers are being especially put to use for studying problems in gas-surface dynamics, molecular collisions and related problems in chemical kinetics. For example, in the case of gas-surface dynamics the system of computers have allowed us to perform extensive wavepacket calculations leading to a deeper understanding of the role of structure in gas-surface interactions. In the case of chemical kinetics we have been able to unravel complex mechanistic details through the use of computational sensitivity analysis. Listed below are several specific recent manuscripts resulting from the use of the Microvax computers.

CURRENT MANUSCRIPTS RESULTING FROM MICROVAX NETWORK

H. Rabitz and M.D. Smooke, Scaling Relations and Self Similarity Conditions in Strongly Coupled Dynamical Systems, J. Phys. Chem., in press.

T-S. Ho and H. Rabitz, Time-dependent Resonance Fluorescence Spectrum of Two-level Atoms: Sensitivity to the Functional Form of the Strong Laser Pumping Fields, Phys. Rev. A, submitted.

A. Peirce, M. Dahleh and H. Rabitz, Optimal Control of Quantum Mechanical Systems: Existence, Numerical Approximation and Applications, Phys. Rev. A, submitted.

A. Peirce and H. Rabitz, Modelling the Effect of Changes in Defect Geometry on Chemically Active Surfaces by the Boundary Element Technique.

A. Peirce and H. Rabitz, An Analysis of the Effect of Defect Structures on Catalytic Surfaces by the Boundary Element Technique.

ITEMS PURCHASED THUSFAR:

Quantity		Model No.	Cost
	Multiuser Microvax		
1	Micro VAX II, 8-user ports, TK50, RD53, 5Mb, world box	DH-630Q3-EA	$ 25310
1	RD53 71 Mb disk drive	RD53A-BA	3483
1	Multiplexer 8 lines	DHV11-M	860
1	Cabinet kit for multiplexer	CK-DHV11-AB	129
1	Micro VMS 8 User license	QZ002-C5	3440
1	Micro VMS 8 User update kit	QZ002-H5	1000
1	VAX Fortran/MicroVMS License	QZ100-UZ	2666
1	VAX Fortran update kit	QZ100-H5	500
1	VAX Pascal/MicroVMS License	QZ126-UZ	2438
1	VAX Pascal update kit	QZ126-H5	500
1	WPS-Plus/VMS License	QZB16-UZ	2850
1	WPS-Plus/VMS update	QZEAM-H5	500
1	LA100 terminal	LA100-BA	1427
1	LN03 A2 Laser Printer	LN03-AA	2272
	Microvax Workstations		
8	VAXstation II VSII/RC VMS 3MB/TK50/RD53 120	SV-LV55N-EK	103166
1	Micro VMS 1 User update kit	Q4001-H5	1000
1	VWS update kit	Q4A96-H5	650
	Archival Storage System		
1	RA81-AA 478 Mb disk drive	RA81-AA	12350
1	UNIBUS disk adapter	UDA50-A	3575
	Installation of RA81/UDA50		1375
	Local Area Network Hardware/Software		
1	DEQNA with cable kit	DEQNA-M	1699
1	DEQNA cabinet	CK-DEQNA-KB	129
2	Local network interconnect	DELNI-AA	2193
1	8 Line Terminal server/cntry	DSRVA-AA	2537
1	DECNET E/N License	QZD04-UZ	542
1	DECNET E/N update kit	QZD04-H5	450
8	DECNET VS E/N License	Q4D04-UZ	3440
1	DECSERVER License	QZ925-UZ	129
1	DECSERVER 100 SPS	TK50QZ295-H5	130

2	Ethernet transmitter	H4005	390
4	Ethernet cable	10MBNE3A-10	260
4	Ethernet cable	20MBNE3A-20	350
4	Ethernet cable	40MBNE3A-40	546
7	Disk Drives with external mounting boxes and cables	RD53-AA	13500
	Shipping and insurance		1500

	Total Expended Funds Thusfar		$ 183786

* The costs include discounts available to Princeton University
  from the Digital Equipment Corporation.

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