

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.

1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE	3. REPORT TYPE AND DATES COVERED	
			FINAL 30 SEP 94 TO 29 MAR 96	
4. TITLE AND SUBTITLE (DURIP94) COMPUTATION AND VISUALIZATION IN NONLINEAR MECHANICS			5. FUNDING NUMBERS F49620-94-1-0460 3484/US 61103D	
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) UNIVERSITY OF MARYLAND INSTITUTE FOR PHYSICAL SCIENCE AND TECHNOLOGY AND DEPARTMENT OF MATHEMATICS COLLEGE PARK, MD 29742			0313	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NM 110 DUNCAN AVE, SUITE B115 BOLLING AFB DC 20332-8080			10. SPONSORING / MONITORING AGENCY REPORT NUMBER F49620-94-1-0460	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION / AVAILABILITY STATEMENT APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) SEE REPORT FOR ABSTRACT				
14. SUBJECT TERMS			15. NUMBER OF PAGES	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT UNCLASSIFIED	18. SECURITY CLASSIFICATION OF THIS PAGE UNCLASSIFIED	19. SECURITY CLASSIFICATION OF ABSTRACT UNCLASSIFIED	20. LIMITATION OF ABSTRACT SAR	

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Final Report DURIP Equipment Award, AFOSR #F49620-94-1-0460

This equipment award was used to purchase high-end computer workstations that have been used to enhance the research conducted under the parent award AFOSR #F49620-95-10198 and the associated AFOSR AASERT award #F49620-93-1-0323. Both strictly computational and high-end visualization equipment was obtained. On the computational side a share of a 40 CPU parallel work-station farm of DEC alpha machines was purchased. The workstation farm is located on campus in the University of Maryland Institute for Advanced Computer Studies (UMIACS) building. As provided by a large NSF infrastructure award to campus, access from my own computer laboratory to the remote super-computer farm facility is via a high-speed (ATM) fiber optic connection. An ATM switch to link all of the workstations in the local lab, is to be installed in the next few weeks. One of the machines to be integrated in this way is the graphics workstation purchased under the DURIP award. That purchase was only made in the last several months. It is a two processor Silicon Graphics Onyx with Infinite Reality Graphics. This is the highest performance graphics currently available from any manufacturer in the world at any price, and was purchased using DURIP funds at a deep academic discount (43%). With the local graphics capabilities and the high speed networking to the CPU farm, we have established a world class high performance computing facility.

The particular equipment purchased was tailored to further my groups research in interactive computation involving path following and multi-parameter continuation, with the computation being steered by the user who monitors the computation in real time using advanced visualization techniques applied to the ensuing bifurcation diagrams. On the software side we are currently integrating and extending the capabilities of two prior codes developed in the lab, namely *MC*² (Multiplier and Constraint Continuation), which was designed to implement interactive multi-parameter continuation on comparatively small problems, and *PCR*, which is a visualization and data-compression post-processor for the one-parameter continuation code *AUTO*. The outcome will be a single code with graphics implemented in OpenGL and Motif, that will allow interactive steering of multi-parameter numerical continuation computations of the solution set of systems of nonlinear two-point boundary value problems, with the visualization running on the local graphics machine, and the computation running on remote high-performance facilities. Because of the speed requirements imposed by interactivity, and the number of individual computations required for multi-parameter continuation such computations have only been made feasible with the hardware provided through the DURIP award. The primary application area within which we are developing our software and computational techniques is the continuum modelling of various macro-molecules. The research on this application is in collaboration with the Materials Lab at WPAFB and is partially supported through an Air Force Phase II SBIR from Wright Labs.