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13. ABSTRACT *(Maximum 200 words)*

In this report we summarize the progress to date, including the implementation of Message Passing Interface (MPI) standard on local supercomputers (Cray and powerful workstations); the development of an integrated simulation environment based on distributive computing; the application of a parallel meolecular-dynamics algorithm; the formation of the research team; and finally, a brief list of research performed in this four-month period.

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TECHNICAL REPORT ON "ADVANCED SIMULATION OF ELECTRONIC MATERIALS: A PARADIGM FOR DISTRIBUTIVE COMPUTING AND SIMULATIONS"

ARO Proposal Number: 34939-MA-SDI
Grant Number: DAAH04-95-1-0651
Period Covered By This Report:
25 September 1995 - 24 January 1996
Principal Investigator: Dr. Xiao-Qian Wang
Grantee Institution: Clark Atlanta University
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The first phase of the project "Advanced Simulation of Electronic Materials: A Paradigm for Distributive Computing and Simulations" was funded for four months (09/25/95-01/24/96.We briefly summarize the progress to date, consistent with the research activities outlined in our original proposal.

(i) Development of an Integrated Simulation Environment Based on Distributive Computing

The proposed research activities are computationally intensive. Fortunately, recent developments at Clark Atlanta University facilitate this work. In response to a DoD Instrumentation Program solicitation, we requested funding for a (low maintenance) high performance supercomputer, the Cray J916, to support ongoing DoD related research. The equipment proposal was awarded in July, 1995. The Cray J916 is now installed and running as a main local supercomputer resource.

The Message Passing Interface (MPI) standard is a new library specification for message-passing, proposed as a standard by a broadly based committee of vendors, implementers, and users. MPI was designed for high performance on both massively parallel machines and on workstation clusters. We have implemented the MPI on the several IBM RISC-6000 workstations (two 590 models and 2 560 models). We also implemented the older version of MPI on the local Cray J916 supercomputer. The implementation of the latest version is in progress, however, there exist machine-compatibility problems for this version. We are in the process of implementing MPI on the two newly arrived IBM RISC-6000 590H workstations. The installation of MPI on these supercomputer and workstations is the first step for an integrated simulation environment based on distributed computing and simulations.

In addition to the local distributive computing environment, we applied massively-parallel Cray-T3d access at Pittsburgh Supercomputing Center and we were granted 2,000 PE/hours resource usage.

(ii) Parallel Molecular-Dynamics Algorithm

As a testbed of the integrated environment for distributive and parallel simulations, we discussed in the proposal the implementation of a parallel molecular dynamics code which uses "pair-functional" potentials to model metals and metal alloys. Specifically, we proposed to follow the recently proposed "force decomposition" method that will allow us to handle systems consisting of millions of atoms.

We have completed the parallel algorithm using the "force matching" method. We have tested the algorithm on the Cray-T3d at the Pittsburgh Supercomputing Center, a massive parallel architecture with 512 nodes. The features of this parallel molecular-dynamics code included *NPT* (fixed number of particle, pressure, or temperature) dynamics, a choice of temperature/pressure controls and boundary conditions, atom and region constraints, and options for dynamics or energy minimization. We plan to port this parallel molecular-dynamics code to the Delta machine at Caltech.

(iii) Research Team

After evaluating more than ten candidates for the postdoctoral research associate position supported by this project, the position is filled by Dr. Miki Nomura, a Ph.D. graduate of the Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign. Her expertise is at high-performance computer simulations of materials. Mr. John Maweu, a minority undergraduate student, is partially supported by this project. In addition to this, Mr. Julian Niles and Mr. Ronald Hickson, minority graduate students (at the Ph.D. and M.S. level, respectively), are participating the research supported by this project.

(iv) Research

Third-order polarizability calculation for C_{60}, C_{70} and C_{84}: Valence electron contributions to the static molecular third-order polarizabilities are calculated for C_{60}, C_{70}, and two stable structures of C_{84} (D_2 and D_{2d}). The method utilized is based on the finite-field approach coupled with semi-empirical polarization calculations on all-valence electrons. An increase in the third-order polarizability contributions is observed for molecular structures, with a reduction in group symmetry, in agreement with recent experimental observations for these fullerenes. (C. E. Moore, B. H. Carderlino, and X. Q. Wang; Results submitted as a *Letter* to *J. Chem. Phys.*; Dr. B. H. Carderino is a professor from Spelman College)

Metallofullerenes: The structural and electronic properties of metallofullerenes, e.g., $Y@C_{82}$, have been studied using first-principles methods. Our study provides a complete analysis of the candidate isomers for the experimentally observed structure. Study of $La@Y_{82}$ and other metallofullerenes are in progress. (X. Q. Wang and J. C. Niles; Results in preparation).

Tight-binding molecular-dynamics of silicon clusters: This work consists of a systematic study of optimal structures and electronic properties of silicon clusters using tight-binding molecular-dynamics method. (R. Hickson and X. Q. Wang, Results in preparation; R. Hickson, M.S. thesis, Clark Atlanta University)

Anisotropic diffusion on hexagonal reconstructed Au(100): We have studied the surface diffusion of adatoms on the hexagonally reconstructed Au(100) surface. Our approach is based on a well-tested many-atom interatomic potential for gold. Our simulation study reveals that the adatoms prefer sitting on top of the unreconstructed second layer atoms, and thus confirms the experimentally observed rectangular shape of adatoms. Our calculation also confirms the experimentally estimated strong anisotropic diffusion of adatoms. (R. Hickson, W. Xu, and X. Q. Wang; Results in preparation)

Electronic structures: We began working on the implementation of discrete wavelet transform to density-functional molecular dynamics algorithm. Currently, we have tested the wavelet transform and inverse wavelet transform, using a set of compactly-supported wavelets developed by Daubechies. The next step is to represent the operators appearing in the Hamiltonian in the wavelet basis. We will apply the wavelet basis to modify a plane-wave based Density-Functional Molecular-Dynamics code: the so-called Car-Parrinello algorithm. (C. J. Tymczak and X. Q. Wang; Abstract to appear in *Bull. Am. Phys. Soc.*)