Final Technical Report
AFOSR Grant F-49620-99-1-0329

Equipment Acquired by Name, Manufacturer, and Cost:

$79,000 toward the purchase of 12-node R-cluster system with twelve 667 MHz Alpha 21264 processors and 4 MB cache from Alta Technology (total cost $123,624).

Special Circumstances:

The equipment purchased deviated somewhat from the original proposal in that it was decided to purchase 12 21264 processor-based Alpha cluster nodes from AltaTech rather than 36 slower 21164 processor-based nodes. The much faster 21264 processors, their larger L2 cache size, and the enhanced communications performance with fewer nodes in the cluster factored into this decision. This change in the equipment list was also based on price/performance considerations and the ease in the administration of a smaller, but faster, cluster. The AFOSR funding was best utilized by this change in the equipment list.

Use of the Equipment:

The research usage of the equipment purchased conforms to that which was described in the original AFOSR proposal. Briefly, the goal of the P.I.'s overall AFOSR-supported research program is to calculate directly from largescale computer simulation the rates of impurity recombination in low temperature high energy density matter (HEDM). In low temperature hydrogen HEDM, quantum effects are very large so our highly specialized quantum molecular dynamics methods are required for these demanding computer simulations. Furthermore, in solids "loaded" with a significant concentration of impurities, the physics behind the recombination dynamics is not well understood. Full scale simulations of the recombination process in such systems are required, and these are now underway on the cluster purchased by the AFOSR grant. The part of the budget ($21,000) to support personnel to aid in the set-up of the cluster and the codes to run on the it was used for Dr. Udo Schmitt, as described in the original proposal.

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13. ABSTRACT *(Maximum 200 words)*
This AFOSR funding was used to acquire local computer resources for dedicated simulations involving novel quantum dynamical studies of impurity recombination dynamics in solid hydrogen systems. Their AFOSR-supported goal is to uncover the factors contributing to the stability of possible high energy density rocket fuels of interest to the Air Force High Energy Density Matter (HEDM) Program.

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