Allocation request

This project is a study of deformation behavior of gold Nano-pyramids. We are pursuing atomistic simulations of the response of these pyramids to compression testing using digital samples containing many millions of atoms. Up to now we could perform simulations with up to a million atoms. These runs in conventional machines take several months to complete.

The problem requires simulations in a powerful massively parallel machine such as system X. Each processor is asked to deal with the response of around 100,000 atoms and the scalability of the problem is excellent. We are using a code that has been repeatedly tested in various parallel systems developed at Sandia National Laboratory (http://www.cs.sandia.gov/~sjplimp/lammps.html).The project is a collaboration with Dr.Diana Farkas from the MSE department and with Professor W. A. Curtin from the Division of Engineering, Brown University and myself. Actual experiments of the pyramid compression are being carried out by Professor W. Gerberich, University of Minnesota. Analysis and interpretation of results will be done by archiving results in a file that will be move onto the CAVE and viewed post mortem using DIVERSE Atomview. When a higher speed network connection is installed between the CAVE and System X it will be possible to run DIVERSE Atomview using computational steering to analysis and interpret results in "real-time" interactively.

The simulations allow detail of the deformation behavior to be studied at the atomic level, and for the first time can approach the scale of the experimental situation relevant to Nano-crystalline materials. The project is currently funded by General Motors at Brown University, but not at Virginia Tech. We are requesting an initial allocation of 100,000 CPU hours, which will allow us to perform about 50 runs with multi-million atom digital samples that will constitute a study of the deformation response that can be compared to the actual experimental results. Once successful, these runs will allow us to obtain specific funding for computing time for this particular project. We also anticipate that these results will lead to a high profile publication which can showcase the power of system X.

Attached is a figure from our preliminary testing. The requested computing time will allow us to take this work to the next level.

Sincerely,

Dr. Ronald D. Kriz,
Associate Professor, Dept: of Engineering Science and Mechanics and
Director, University Visualization and Animation Group,
Virginia Tech.