Mr. Mathew S. Lee wins the OSU Graduate Research Excellence Award for Fall 2002

Mr. Mathew S. Lee is a graduate student in the Mechanical & Aerospace Engineering at Oklahoma State University, Stillwater, Oklahoma. He submitted a thesis on the development of a user-friendly molecular dynamics (MD) simulation system for nanometric cutting and tribology in Fall of 2002 for which he is awarded the Graduate Research Excellence Award. Matt's advisors are Professors Ranga Komanduri and Lionel Raff. In his thesis, Matt used three perspectives, namely, end-user, programmer, and administrator to identify important aspects of the user-friendly system. Documentation is provided from each perspective to enable a researcher to understand and utilize the system efficiently. For the end-user, necessary information on accessing the system to using the simulation software is provided for creating and performing simulations. Default options have been provided in the pre-processing software created to allow for easy implementation of the simulations. Post-processing software created implements animation of the simulations in 2D and 3D. For the programmer, information has been provided on the MDbinfmt library, approaches for coding new simulations, and an introduction on how to apply parallel processing to MD. For the administrator of the user-friendly system, information is given on assembling, installing, and administrating the software system and the workstations. The chief researcher-in-charge can use the documentation provided to handle the computational requirements of researchers using the user-friendly system. Multiple applications were coded before the simulations could be performed. These applications include pre-processing, simulation, and post-processing software. The user-friendly system is aimed at helping the researchers to increase the rate at which MD simulations can be conducted. Clock time is not the only aspect that affects the rate at which simulations can be performed. The users of the system must be familiar with the system and understand how to utilize the system to design, create, and run MD simulations. Two separate parallel processing systems (or Beowulf clusters) were built - one with 8 Digital-alpha workstations and the other with 26 node, 13 dual AMD processors (1.7 GHz per processor) system.