SC99, November 13-19, 1999
Portland, Oregon

Large-scale Normal Coordinate Analysis of Polymer Particles on High Performance Computer*

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ABSTRACT

The spectral and thermal details of polymer particles can be revealed at the atomic level by Normal Coordinate Analysis, a computational method that involves solving a large-scale eigenvalue problem. We report our success in using ARPACK to 1) compute the low frequency modes of several large systems of polymer particles, and 2) to study the density of states and thermal properties of polymer particles. Since the lowest modes (eigenvalues) are tightly clustered, the standard Lanczos algorithm encounters several difficulties. We illustrate how to combine implicitly restarted Lanczos with spectral transformation to effectively extract the desired eigenvalues and eigenvectors. To study the thermal properties of polymers, we must compute the full spectrum of the force matrix. We will demonstrate how this can be done efficiently using ARPACK.

*Research sponsored by the Applied Mathematical Sciences Research Program, Office of Mathematical Information, and Computational Sciences, U.S. Department of Energy under contract DE-AC05-96OR22464 with Lockheed Martin Energy Research Corporation.

**Oak Ridge National Laboratory is managed by Lockheed Martin Energy Research Corporation for the United States Department of Energy under Contract No. DE-AC05-96OR22464.

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