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Mili Shah* (mili@rice.edu), Rice University, CAAM - MS 134, 6100 Main St., Houston, TX 77005, and **Danny C Sorensen**, Rice University, CAAM - MS 134, 6100 Main St, Houston, TX 77005. *Calculating Symmetric Modes of Motion in Molecular Dynamics.*

For many molecules there is an inherent form of symmetry in their structure. However, when the major modes of motion are calculated with the Singular Value Decomposition (SVD), this symmetry is sometimes lost. Enforcing symmetry of the major modes not only preserves the essential symmetric motions of the molecule, but it also averages out some of the random fluctuations that may occur when using the SVD to calculate the major modes. We calculate the *symmetric* modes of motion of a molecule by a process called the Symmetry Preserving Singular Value Decomposition (SPSVD). This process is no more expensive than calculating the regular modes of motion using the SVD and is easily parallelizable. (Received September 13, 2006)