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Normal mode analysis with reduced Hessians for multi-scale modeling techniques AN GHYSELS, University of California - Berkeley, BENJAMIN T. MILLER, National Institues of Health, MICHEL WAROQUIER, Center for Molecular Modeling, BERNARD R. BROOKS, National Institutes of Health — Normal mode analysis is a straight-forward technique to gain insight into the principal motions of molecular systems. Diagonalizing the mass-weighted second derivative matrix (Hessian) results in eigenfrequencies and eigenmodes which indicate the time scale and spatial shape of the vibrations. For large systems, it is often necessary to use Hessians of reduced size in order to limit the required computational resources as well as the amount of information. Methods such as coarse-grained multi-scale models, the Mobile Block Hessian approach, the Vibrational Subsystem Analysis, or the Partial Hessian Vibrational Analysis, focus on specific parts of the spectrum: localized and/or global modes with varying degrees of coupling with the environment. In this presentation, the link between the different approaches will be studied with size-independent metrics and overlap techniques.

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