Implosion-based mapping procedure between all-atom and coarse-grained normal modes

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Dimension reduction is often necessary when attempting to reach longer length and time scales in molecular simulations. It is realized by constraining degrees of freedom or by course-graining the system. When evaluating the accuracy of the dimensional reduction, one encounters a practical challenge: models that have a different number of degrees of freedom yield displacement vectors of different lengths, prohibiting direct comparison.

We have investigated mapping procedures for normal mode analysis, a technique that allows vibrational characterization of a molecule by diagonalizing its mass-weighted Hessian[1]. We review a *horizontal* mapping procedure for the reduced Hessian techniques, which project out degrees of freedom[2]. We then design a *vertical* mapping procedure for the *implosion* of the all-atom (AA) Hessian to a coarse-grained (CG) scale that is based upon Vibrational Subsystem Analysis[3]. Our procedure gives both effective force constants and an effective kinetic tensor.

Next, a series of metrics is developed for comparing frequencies and normal modes across different scales, where special attention is given to proper mass-weighting. These metrics can be categorized as dimension dependent and dimension independent. Frequencies, normal mode vectors, Hessian similarity, and thermal fluctuations all belong to the former group, and require prior mapping for proper evaluation, whereas elastic modulus, shape derivatives, vibrational free energy differences, heat capacity, and projection, are all techniques belonging to the latter group.

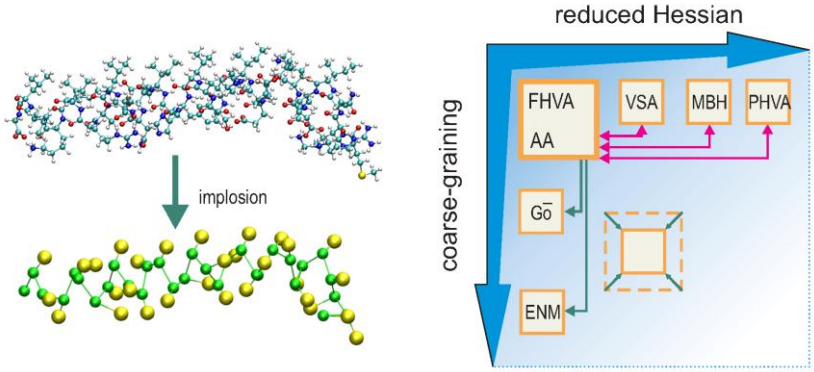

Fig. 1 The normal mode matrices have different sizes because of reduced Hessian techniques or coarse-graining. Comparison of normal modes thus requires *horizontal* or *vertical* mapping, respectively. An *implosion* procedure between the AA and CG scale transforms the vectors to equal length.

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[3] H. Lee Woodcock III, W. Zheng, A. Ghysels, Y. Shao, J. Kong, B.R. Brooks, *J. Chem. Phys.* 129, 214109, 2008