

Integrated Component Mode Synthesis and Dynamic Condensation Simulating Large Protein Dynamics

Jae-In Kim¹, Jeong-Hee Ahn¹, Kilho Eom² and Sungsoo Na¹

Summary

Characterizing dynamic behavior of protein molecules is prerequisite for understanding the biological functions of proteins. Such characterization has been still computationally restricted for large proteins due to large degrees of freedom for Hessian (stiffness) matrix of such proteins. In this article, we address how to computationally solve the large protein dynamics problem by combining the component mode synthesis (CMS) and dynamic condensation (DC). Specifically, CMS allows us to consider the vibration motion of each protein domain instead of whole protein structure, and then the dynamic characteristic of each domain is assembled to provide the insight into dynamics of whole protein structure. It is shown that combined CMS and DC enables us to achieve the fast computation for understanding protein dynamic motion accurately such that the characteristics of low-frequency normal modes obtained by combined CMS and DC is quantitatively comparable to experimental data and/or molecular models. This suggests that combined CMS and DC may allow for gaining insight into dynamics of supramolecules and large structural systems (e.g. lattice dynamics).

¹Department of Mechanical Engineering, Korea University, Seoul 136-701, Republic of Korea

²Nano-Bio Research Center, Korea Institute of Science and Technology (KIST), Seoul 136-791, Republic of Korea

