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Elastic Lattice Models: From Proteins to Diagrid Tall Buildings

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Summary

What do proteins and diagrid tall buildings have in common? Apparently nothing. The former are nanoscopic biological systems, functioning in a complex chemo-physical environment, whose activity is pivotal to carry out a variety of physiological processes. The latter are macroscopic structural systems that are employed nowadays for the design and construction of tall buildings. Nevertheless, in this Thesis, it will be shown that both proteins and diagrid tall buildings can be investigated and modeled by means of the same structural system, the Elastic Lattice Model (ELM). ELMs are spatial structures usually made of springs or bars connected in correspondence of nodes, that can be treated as spherical hinges. In this Thesis, we will use the ELMs to explore a variety of behaviors and features of proteins and diagrids.

In particular, it will be shown that proteins can be efficiently modeled as a network of springs and point masses. Within the framework of modal analysis, these ELMs will be very useful to obtain accurate information regarding protein dynamics and vibrations. Specifically, the low-frequency vibrations extracted from the protein ELMs will be shown to correlate truthfully with the protein biological mechanisms and conformational changes, as well as to provide correct insights on the protein experimental flexibility, as obtained from the experimental B-factors. For this purpose, various modeling approaches will be presented and analyzed. Furthermore, we will see that applying point forces on the protein ELM also provides remarkable insights on protein flexibility. Two novel force application patterns will be reported for this purpose and the results will show that the protein ELMs coupled with the traditional linear static analysis can lead to correct predictions of the protein deformability. Finally, the possible role of geometrical non-linearities will also be investigated within the large-scale conformational changes, which are usually known to exhibit fairly large displacements. From the analyses, it will be shown that these conformational changes often imply curvilinear pathways and possible mechanical non-linearities in the structural response.

Switching to the subject of diagrid tall buildings, the ELMs will then be used to develop a matrix-based method (MBM) for the structural analysis of generic three-dimensional diagrid systems. Based on matrix calculus and the displacements method, the MBM will be applied to perform the structural analysis of diagrids, both alone and coupled with internal cores. The force distribution and the interaction of the external diagrid with the internal resisting element will be studied by inserting the MBM within the General Algorithm (GA), a semi-analytical framework developed few decades ago for the investigation of complex three-dimensional buildings. Furthermore, the MBM will be deeply exploited to investigate the influence of the diagrid geometry on the structural response. Namely, geometrical parameters such as the diagonal inclination, floor shape and building aspect ratio, will be changed in order to obtain information on the lateral and torsional flexibility of the diagrid. From these analysis, it will be shown that different diagrid geometries have a marked effect on the structural response and often a unique solution that allows to optimize all the responses does not exist. For this reason, a novel multi-response optimization will be presented, which makes use, for the first time in this field, of the desirability function approach. Based on the results of the MBM structural analyses, the desirability function will be applied to evaluate the optimal diagrid geometry that simultaneously optimizes the lateral and torsional rigidity, the amount of used material as well as the construction complexity. The outcomes will show that the desirability approach, coupled with the ELM-based MBM, is a simple yet valuable and robust tool for the selection of the optimal diagrid geometry.