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Mechanical and Assembly Units of Viral Capsids Identified via Quasi-Rigid Domain Decomposition GUIDO POLLES, SISSA, GIULIANA INDELICATO, University of York, RAFFAELLO POTESTIO, Max-Planck-Institut für Polymerforschung, Mainz, PAOLO CERMELLI, Universita di Torino, REIDUN TWAROCK, University of York, CRISTIAN MICHELETTI, SISSA — Key steps in a viral life-cycle, such as self-assembly of a protective protein container or in some cases also subsequent maturation events, are governed by the interplay of physico-chemical mechanisms involving various spatial and temporal scales. These salient aspects of a viral life cycle are hence well described and rationalised from a mesoscopic perspective. Accordingly, various experimental and computational efforts have been directed towards identifying the fundamental building blocks that are instrumental for the mechanical response, or constitute the assembly units, of a few specific viral shells. Motivated by these earlier studies we introduce and apply a general and efficient computational scheme for identifying the stable domains of a given viral capsid. The method is based on elastic network models and quasi-rigid domain decomposition. It is first applied to a heterogeneous set of well-characterized viruses (CCMV, MS2, STNV, STMV) for which the known mechanical or assembly domains are correctly identified. The validated method is next applied to other viral particles such as L-A, Pariacoto and polyoma viruses, whose fundamental functional domains are still unknown or debated and for which we formulate verifiable predictions.

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