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Coarse-grained mechanics of viral shells WILLIAM S. KLUG, MELISSA M. GIBBONS, University of California, Los Angeles — We present an approach for creating three-dimensional finite element models of viral capsids from atomic-level structural data (X-ray or cryo-EM). The models capture heterogeneous geometric features and are used in conjunction with three-dimensional nonlinear continuum elasticity to simulate nanoindentation experiments as performed using atomic force microscopy. The method is extremely flexible; able to capture varying levels of detail in the three-dimensional structure. Nanoindentation simulations are presented for several viruses: Hepatitis B, CCMV, HK97, and ϕ29. In addition to purely continuum elastic models a multiscale technique is developed that combines finite-element kinematics with MD energetics such that large-scale deformations are facilitated by a reduction in degrees of freedom. Simulations of these capsid deformation experiments provide a testing ground for the techniques, as well as insight into the strength-determining mechanisms of capsid deformation. These methods can be extended as a framework for modeling other proteins and macromolecular structures in cell biology.

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