Trabajo de master

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How does elasticity affects the binding energy of a biological structure?

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Many biological entities, such like membranes or virus, are formed by small pieces or “modules” which self assembly to create a complex structure. The self assembly process is almost magic, yet quite robust: each module only interacts with its neighbours, with an attractive potential energy, while the entropy helps to bring each piece to its proper place to finally build the ensemble. Cohesion potential energy and entropy are thus essential in the building process. But what about the opposite process of dissasembly? This is a highly relevant biological question, as many virus needs to break up their capsid, formed by proteins, to start the infection. In this TFM work we shall investigate the binding free energy (which contains potential energy and entropy) of the modules of a biological entity. In the limit of completely rigid structure (a wall of bricks) the binding energy of one brick should only depend on the potential energy between neighbouring bricks. In a elastic structure, our hyphotesis is that the entropic component of the binding free energy has a local (from neighbour modules) and a global contribution arising from the elasticity of the whole structure. Does evolution “uses” rigidity to control the virus dissasembly processes depending on the infectious strategy? We will simulate a virus capsid and gradually extract parts of it (the so called pentons). Using Jarzinsky theorem we will numerically evaluate the binding free energy of each part. To achieve more undestanding, we will also consider simplified structure (with connected “spheres”) with different rigidity; to study how does the binding free energy varies with the structure elasticity. Finally we might also consider long structures, like the tobacco virus, where the modules are connected with helical threads, and might lead to spatial correlations in the binding free energy. Another exciting aspect of this TFM is that modelling at Delgado-Buscalioni lab, will be backed up by the experiments with AFM indentation carried out in P.J. de Pablo group.

REFERENCE: Long-Range Cooperative Disassembly and Aging during Adenovirus Uncoating,Natalia Martín-González, Pablo Ibáñez-Freire, Álvaro Ortega-Esteban, Mara Laguna-Castro, Carmen San Martín, Alejandro Valbuena, Rafael Delgado-Buscalioni, and Pedro J. de Pablo. Phys. Rev. X **11**, 021025, 2021

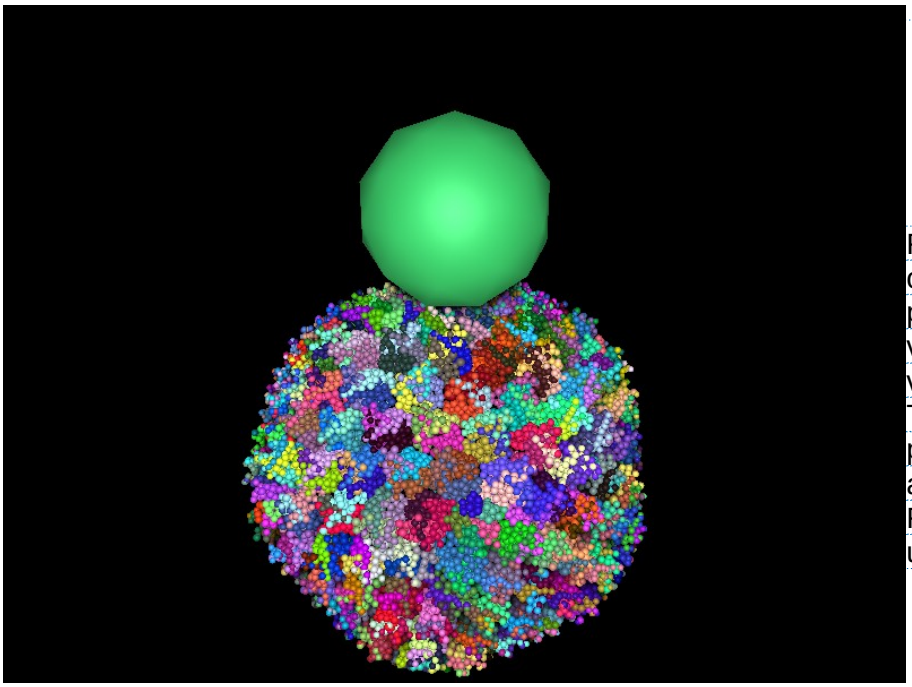

Figure: Computational model of an adenovirus virus being perturbed (compressed) by a virtual AFM tip. This is the virus model we will use in TFM. In performing the computations the student will be assisted by Pablo Ibañez Freire (coder of the model) using the UAMMD code.