Computational biology greatly benefits from approaches such as molecular dynamics simulations. This field is literally exploding with the advent of a continually growing body of large experimental structures and more and more powerful computers. Here I present examples pushing either the time scales or system sizes, reaching experimental structures and more and more powerful approaches such as Atomistic simulations.

Interactive simulations are precious in exploring and generating hypotheses. They introduce human expertise and benefit from the user’s experience and insight. Using a 3D haptic device, molecules can be manipulated with great precision and interactions can be felt in real time via tactile feedback. Below, interactive approaches to study macromolecular structure, flexibility and interactions are shown using interactive molecular dynamics or elastic networks with our own Biospring tool. The latter has been tested in a recent CAPRI round to guide and constrain docking. Macromolecular interactions can be refined via a user-guided set of constraints, interactive deformations and manual assembly steps. Such methods enable expert guided modelling experiments. For the purpose of these simulations, we have developed a freely available software library called MODriver. It facilitates the implementation and application of interactive simulations such that it becomes very easy to render any particle-based molecular simulation or docking engine interactive.