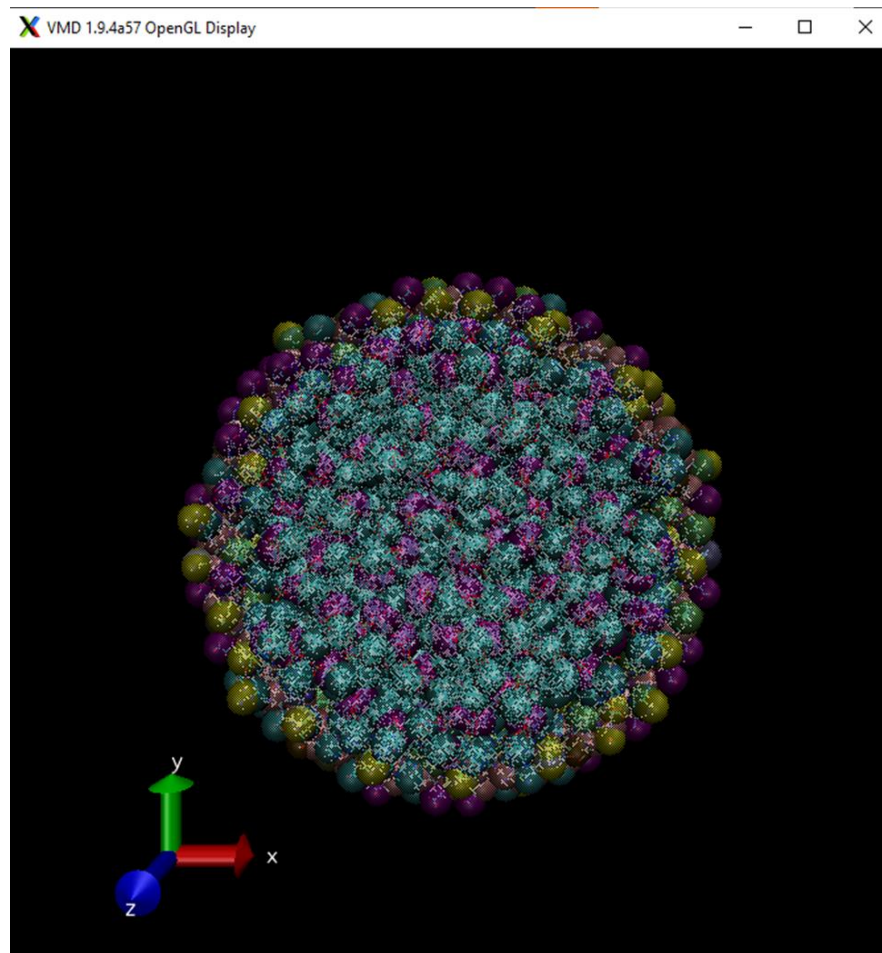


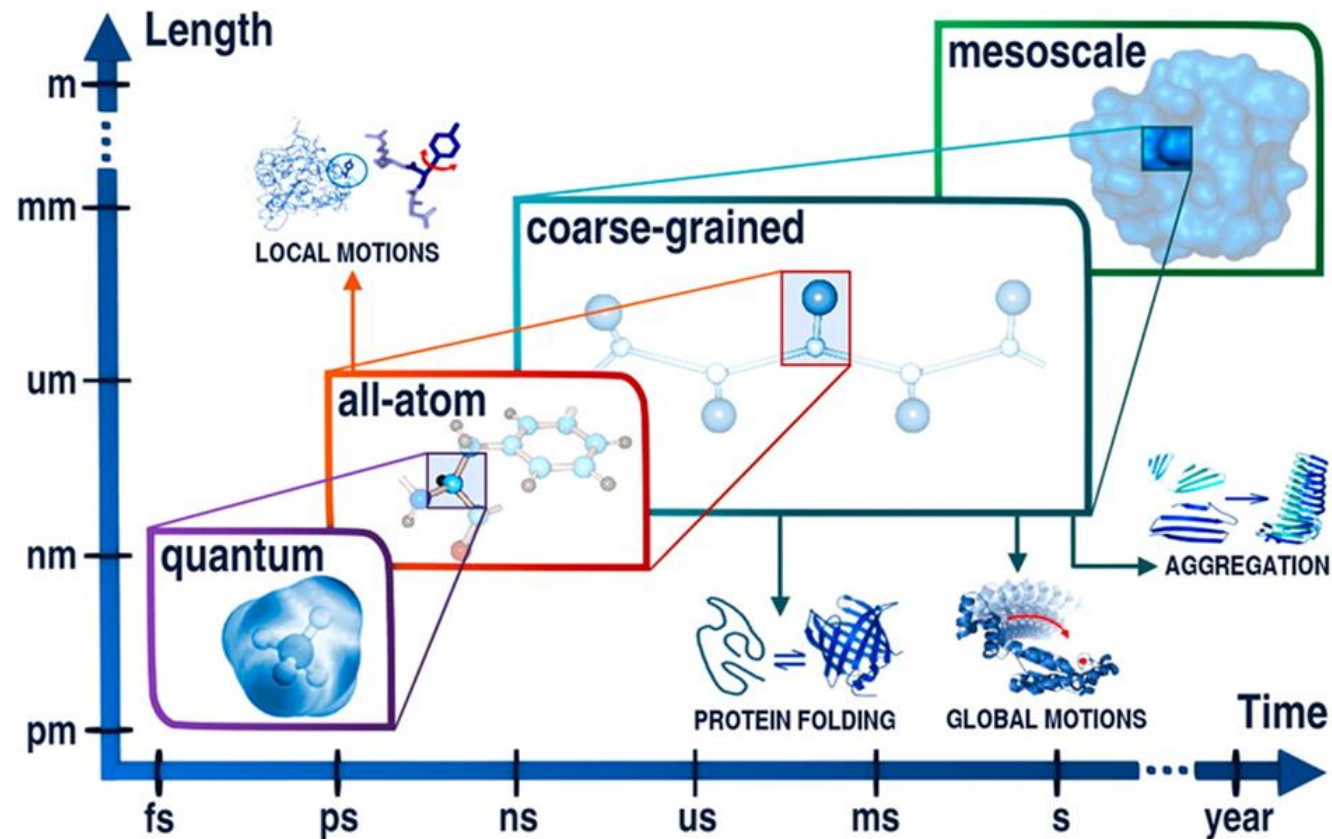
Coarse-grained simulations of dynamic molecular interactions within protein-DNA complex



Presenter: Dr. Draško Tomić

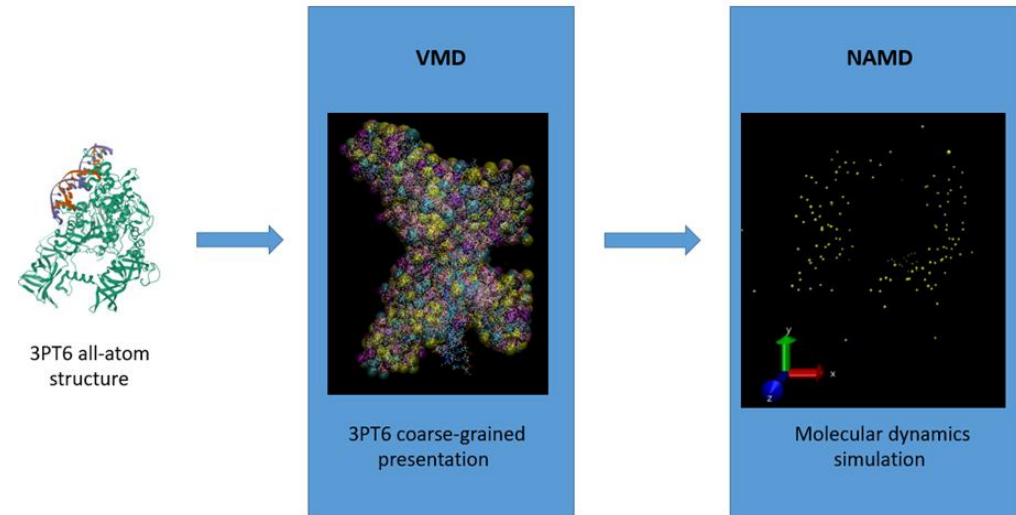
Molecular dynamics challenge

- Biomolecules consist of tens of thousands of atoms, whose correlated motions often have to be calculated in billions of steps of numerical integration to describe the related physiological process.
- DNA molecules are especially challenging due to their high flexibility, strong electric fields, and large variety of potential interactions.
- Consequently, simulations of DNA binding to other molecules can be challenging especially if done on a large time scale. Such simulations require numerous integration steps and approximations that are beyond the reach of today's most powerful computers and algorithms.



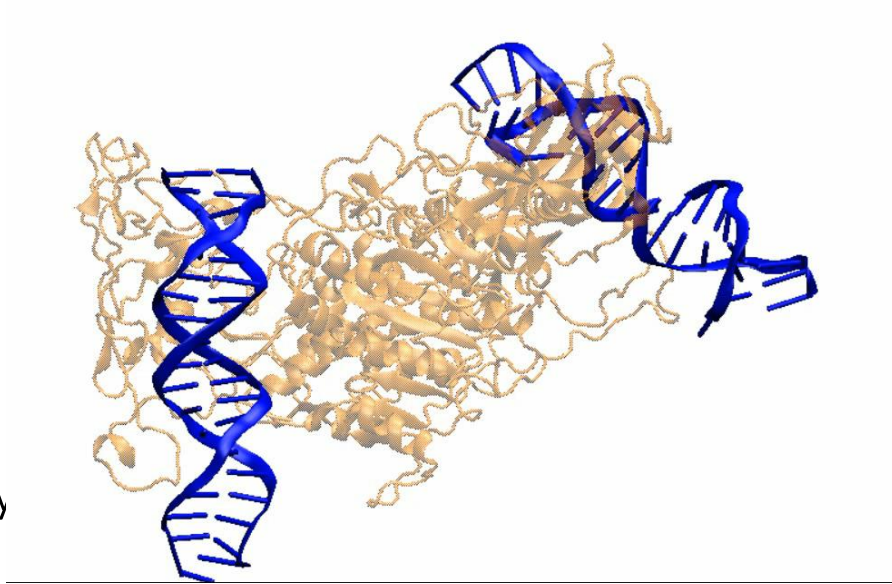
Methods and results

- Our research was conducted on one such structure called 3PT6, which describes DNA in complex with the DNA methyltransferase-1 enzyme.
- A Bura supercomputer at the University of Rijeka running NAMD and VMD multi-scale molecular dynamics programs from the University of Illinois was used for this.
- Results will allow a better understanding of the interaction between DNA and the enzyme DNA methyltransferase, which is still an unsolved challenge.
- A procedure was developed that enables fully automated analysis of any DNA structure on a supercomputer.
- This opens up the possibility of applying the results of our research to other areas, e.g., to increase the accuracy and efficiency of the Vini in silico model of cancer.

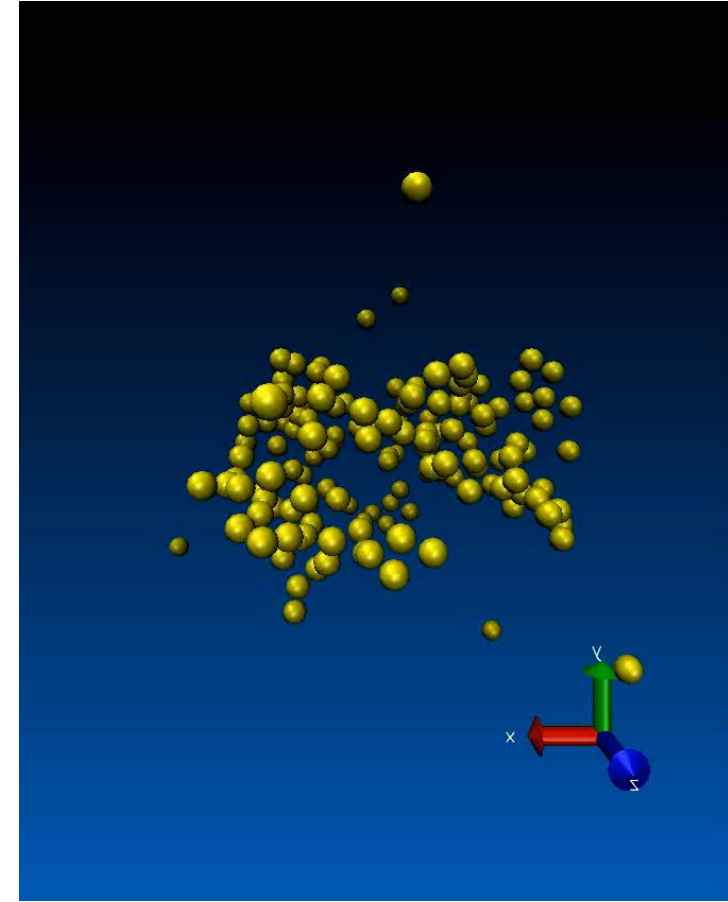


Some final remarks

- According to the available data, coarse-grained simulations of this type have not yet been performed anywhere in the world.
- This research was carried out in collaboration between the Ruđer Bošković Institute and the University of Rijeka.
- Researchers:
Draško Tomić – RBI
Željko Svedružić – UNIRI
Gordan Janeš – UNIRI
- Thank you for attending!



Video 1: 3pt6 all-atom simulation



Video 2: 3pt6 coarse grained simulation