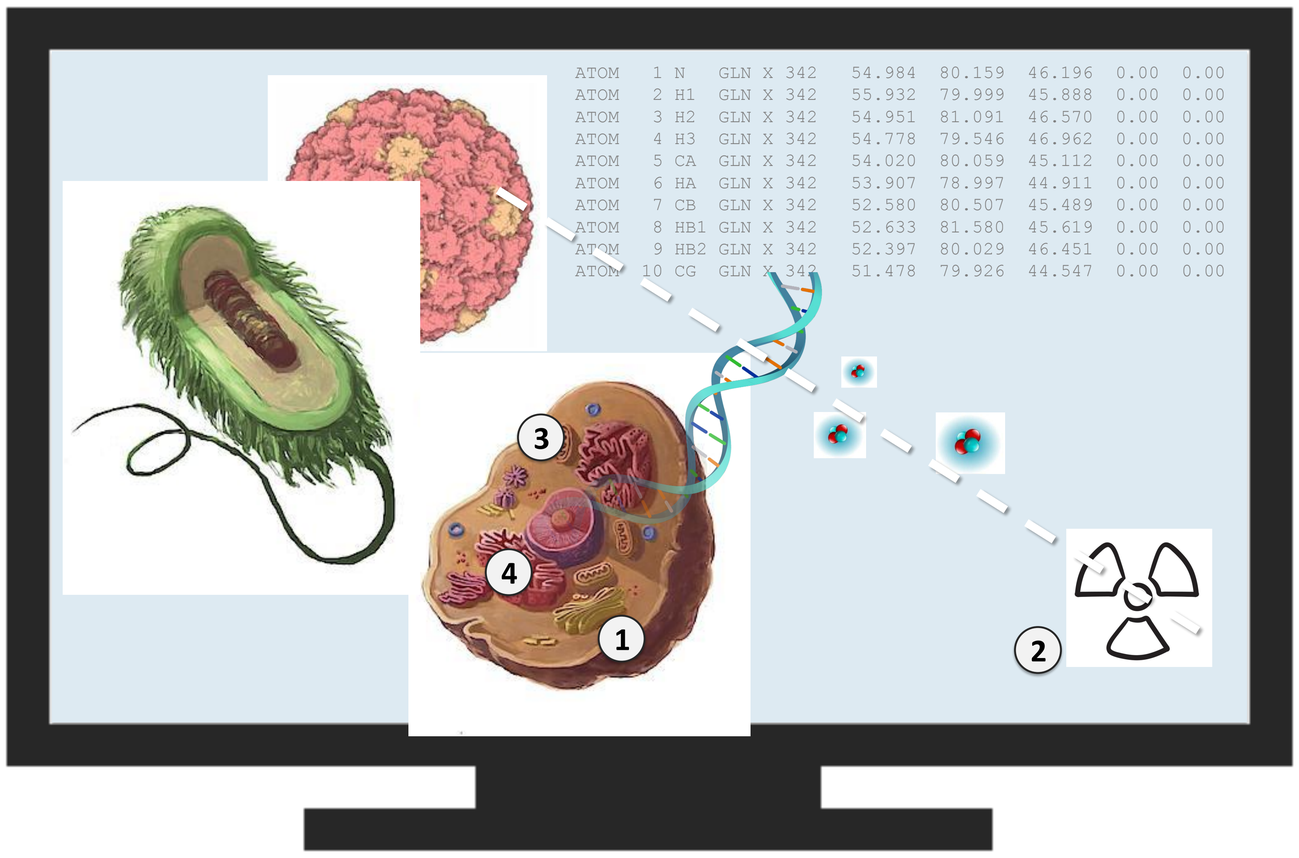
INIZIATIVA SPECIFICA
- BIOPHYS -

BIOPHYS @ TIFPA - FROM THORETICAL PHYSICS TO BIOLOGY (and back)

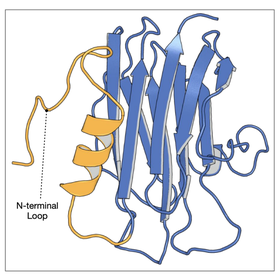
- BIOPHYS **framework**: Characterize the emergent properties of biological systems, from the nano- to the cellular scale, by employing novel methods from *theoretical physics*, the theory of *complex systems* and *advanced computational tools*
- BIOPHYS **objectives**: Develop predictive, testable models to investigate the structure and function of biological factors, e.g., proteins, DNA and RNAs, as well as the states of single cells and their collective behaviour in health and disease
- BIOPHYS@**TIFPA**: Derive a deeper understanding of biology and of the physics of complex systems, starting from specific biology-motivated questions that are interpreted through the lenses of *statistical mechanics*, *field theory*, *computational soft matter physics* and *topology*



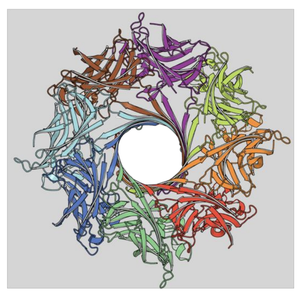
Molecular Dynamics (MD) is a wide-spread *in silico* technique, capable of depicting the behavior of molecular systems at the **nanoscale** - which is hardly accessible by conventional experimental techniques

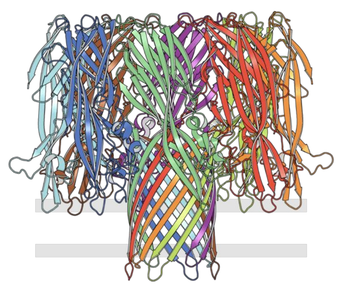
1 - PROTEIN-MEMBRANE COMPLEXES: PORE-FORMING TOXINS (PFTs)

- MD might be employed to detect specific **conformational changes** in a protein structure, e.g. upon interaction with proper substrates and cofactors
- This is the case, for instance, of **pore-forming toxins** (PFTs), capable of «digging» holes within cellular membranes; this process is triggered by a **conformational change upon binding** the membrane



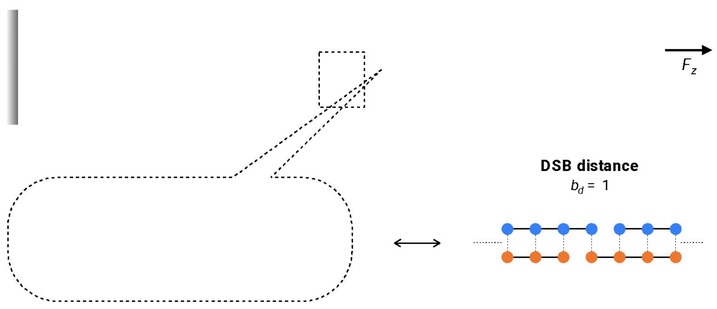
Paternoster et al., in preparation



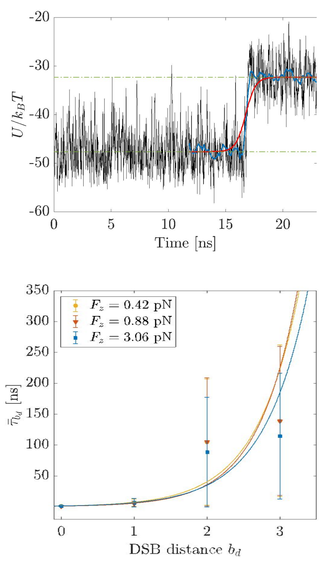


2, 3 - DYNAMICAL CHARACTERIZATION of DNA LESIONS

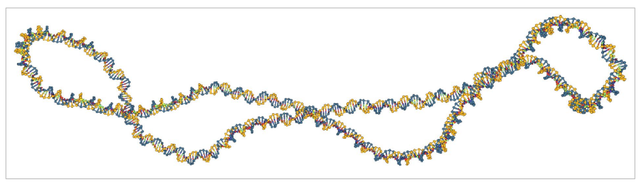
- MD has been successfully employed to describe the evolution of radiation-induced DNA lesions on a variety of systems of both biological and microdosimetric relevance, thereby attempting at bridging the gap between the impact of radiation on DNA and the subsequent cellular outcome



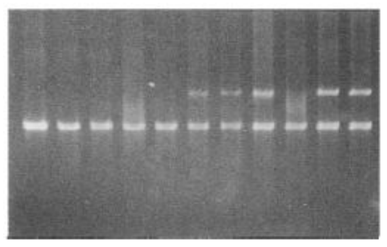
Micheloni et al., Biophysical Journal 2023, 122 (16): 3314-3322



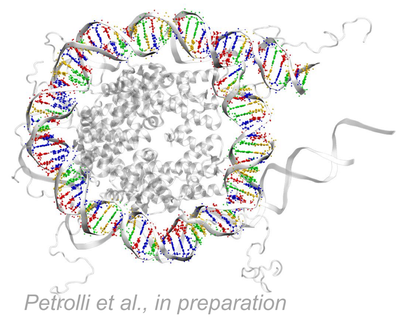
➪ an **optical tweezer-like setup** was employed to determine the characteristic **dynamics** and **rupture times** of a linear DNA filament broken *via* a **double strand break** (i.e. a deleterious lesion of DNA broadly enforced by radiation fields)



Micheloni et al., in preparation



Hanai et al., Int. J. Radiat. Biol. 1998



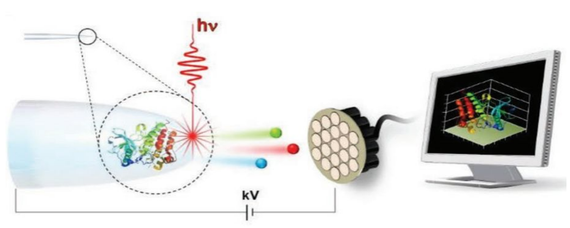
Petrolli et al., in preparation

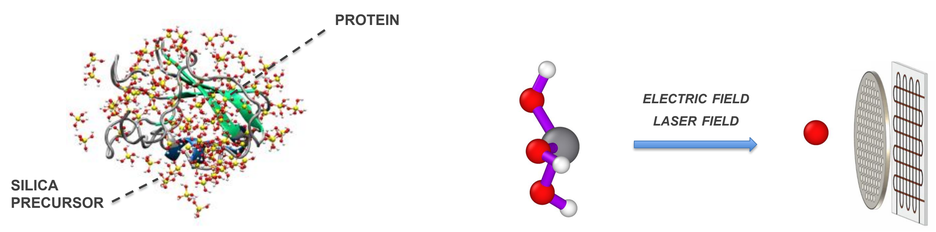
➪ we take advantage of the known (topological, dynamical) properties of complex DNA systems - widely employed in experimental and dosimetric assays - to extract **kinetic insights** on the behavior of **DNA lesions** on **biologically-relevant frameworks** (e.g., chromatin, mitochondrial DNA)

4 - THE MIMOSA PROJECT

- In the FET-open funded project Mimosa, we aim at obtaining a full characterization of a protein material embedded in a silica matrix for subsequent *atomic probe tomography* (APT)
- By employing both *classic MD* and *quantum chemistry* techniques, we have effectively set-up both the **laser ablation** and **silica embedding** stages of the experimental process

Novi Inverardi et al., Biophysica 2023, 3 (2): 276-287; Novi Inverardi, De Tullio et al, in preparation





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