A geometrical DNA model is required to compute radio-induced damages after those three stages.

### Physical stage
- Simulation of the physical interactions at the nanometric scale.

### Physico-chemical stage
- Simulation of the dissociation channels used for the ionized or excited water molecules [3].

### Chemical stage
- Simulation of the radical diffusion as well as their chemical reactions in liquid water [3].

The DnaFabric software

**Software main characteristics**

**Architecture**
- The DnaFabric code is organized in modules that correspond to different fields of expertise.
- Each module contains the files required to define and analyze a hierarchical object of user interest. For example, the module contains the files required to define and analyze a hierarchical object of user interest.

**Scene**
- The Scene module contains the files required to define and analyze a hierarchical object of user interest. For example, the module contains the files required to define and analyze a hierarchical object of user interest.

**Utils**
- The Utils module is based on the Qt library and setups the user interface.

**Run**
- The Run module contains the files required to define and analyze a hierarchical object of user interest. For example, the module contains the files required to define and analyze a hierarchical object of user interest.

**Engines**
- The Engines module allows to run calculations that can interact with a model. Thus, the model can be modified in real-time depending on the evolution of the ongoing calculations — calculation monitoring.

**DnaFabric specifications**
- Work with a list of elements that can be individually accessed: several thousands of billions of objects can be used in a DnaFabric model.
- Such complex models can be visualized thanks to the custom 3D engine included within the DnaFabric modules.
- The Engines module allows to run calculations that can interact with a model. Thus, the model can be modified in real-time depending on the evolution of the ongoing calculations — calculation monitoring.

### Modeling of a human genome in an endothelial cell nucleus

**Construction of a DNA model**
- Using the features provided by DnaFabric, a model describing the DNA from the molecular level to the ultramicro level was created.
- The model is highly adaptable and can be customized to suit the needs of different users. For example, the placement of the voxels described in 4) to build a DNA filament going from a point A to a point B is fully automated.

1. Choose a cell nucleus type: fibroblast, endothelial or lymphocyte.
2. Choose a genome type: male or female. The genome will be randomly generated in a condensed state.
3. Simulate the relaxation of the genome [4] thanks to the Engine module. The resulting genome is in a state corresponding to the G0 phase of the cell cycle.

### The filling of a cell nucleus model with DNA

Any relaxed genome within a cell nucleus can be filled with voxels to add DNA molecules in the nucleus. This filling can be done by two algorithms included in the Engines module of DnaFabric.

1. A loop algorithm that will position the voxels to reproduce the loops performed by the chromosome flaments in each domain (color scheme) of a chromosome.
2. A space-filling algorithm that do not reproduce the loops but focus on maximizing the space occupied by the voxels.

### Conclusion and perspectives

- The DnaFabric software was used to generate data (fibroblast, endothelial and lymphocyte) with condensed and relaxed genomes (male and female).
- The genomes were filled with one continuous chromatid filament per chromosome through the use of voxels and one of the two filling algorithms included in DnaFabric.
- Nucleus with or without filled genomes can be explored in real-time thanks to the 3D engine of DnaFabric.
- Nucleus and genomes can be exported to “.fab2g4dna” files in order to be read by dedicated Geant4 user-applications.
- Using such user-applications, a calculation chain was developed to simulate the calculation, the physical, physico-chemical and chemical stages following the irradiation of a cell nucleus filled with DNA (condensed and filled genome). The calculations are currently ongoing.

### References


