Visualization of biological processes using 3D animation

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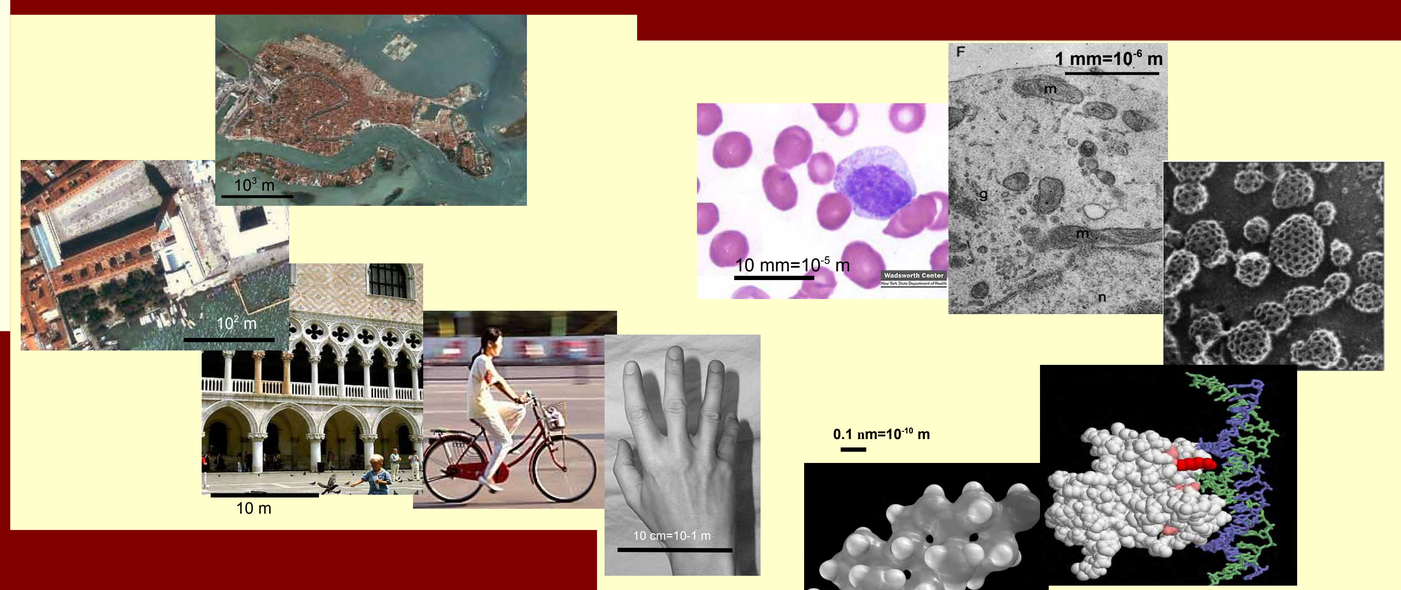
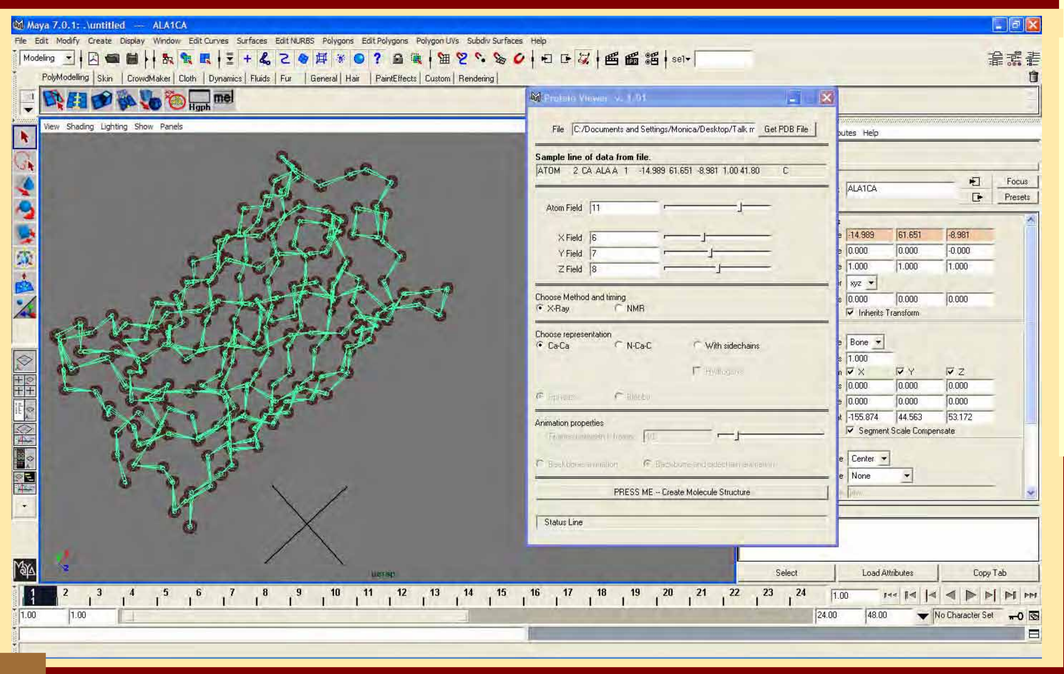
Introduction.
Biological processes are increasingly well known and defined in molecular and structural terms. The state of knowledge is now mature to permit a visualization of many bio-molecules and their interactions in the cellular environment.
In an effort aimed at delivering biological information in a direct, visual way, we have started a project that uses one among the most versatile professional 3D animation programs to represent proteins and other biological molecules. Autodesk-Maya is professional 3D animation and visual effect program developed for the cinema and entertainment industry, which contains the possibility of modelling, animating and adding dynamic features to scenes, before rendering.



Maya-Autodesk.
Maya is one among the most complex 3D animation and Visual Effects programs used in the professional production industry. It contains a vast array of functions, broadly divided in four categories: Modelling, Animation, Dynamics and Rendering.
We have added features that enable dialogue with the scientific database that contains structural information of proteins and other macromolecules of biological interest.
Here is a snapshot of the Maya environment with imported Green Fluorescent Protein, seen as skeleton of alpha carbons, and the interface of our protein viewer program.

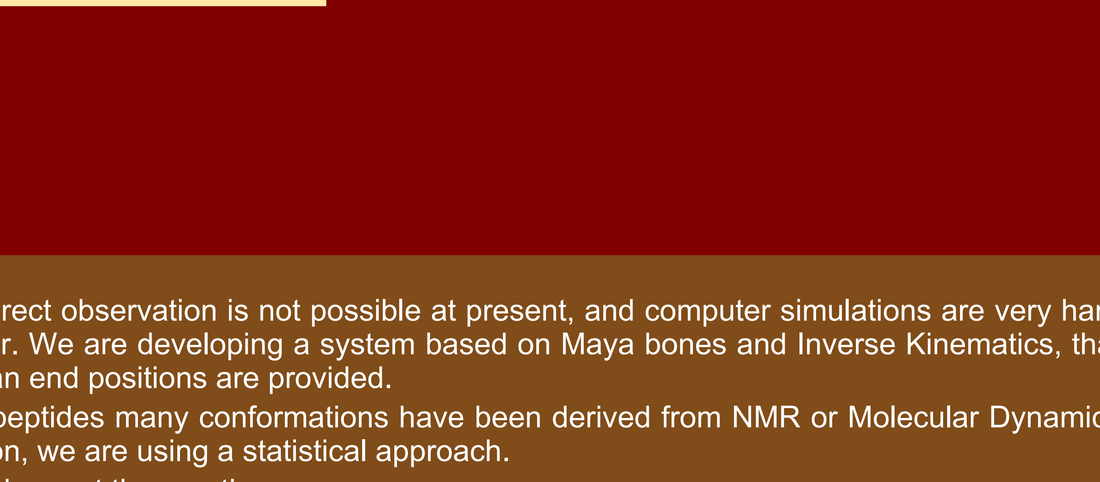


The cellular landscape.
Despite their small size, cells are very complex and articulated structures: a typical T cell is approximately spherical with a diameter of about 10 μm, and contains several components ranging in size from the nanometer (3.4 nm is the diameter of the DNA helix) to few μm (large structures as mitochondria and microtubules).
This is to compare to the relative dimensions of an small packet to that of a city: it is not possible to appreciate features of objects at both scales at the same time.
Any representation of things happening in a cell will have to convey also the idea of different scales.

Importing proteins.
Biological molecules are in essence a collection of atoms connected through atomic bonds.
Our import system uses a library of aminoacids to build the molecule, and assigns to each atom the position retrived from the Protein DataBank file.
Atomic connections are imported as *bones*, a Maya feature that allows movement by rotation at joints, while restricting bending and changes in the lenghth of bones.

Moving proteins.
Exploration of protein motion is still in its infancy: direct observation is not possible at present, and computer simulations are very hard and expensive in term of time and computing power. We are developing a system based on Maya bones and Inverse Kinematics, that can produce organic movements when a start and an end positions are provided.
For an increasing number of small molecules and peptides many conformations have been derived from NMR or Molecular Dynamics studies. To obtain movements from these information, we are using a statistical approach.
Some animations can be seen on our website, or ask me at the meeting.

Testing the system.
Using small molecules whose movements have been studied by Molecular Dynamics simulation, we have tested our motion calculation algorithms.In the three cases studied (Triazine, shown in figure, Bitucarpin and the Alanine Dipeptide), the path calculated with Maya fits with good agreement with the energy landscape.



Rendering moleculess.
The delivery of physico-chemical information through visual clues is one of the major aspects of our research.
Here we report the images of various molecules rendered with different surface features.