BioBlender 2.0 Manual

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1. What is BioBlender

BioBlender is an AddOn, a module that can be used with Blender, with the aim of providing a view of biological, or, better, molecular data according to a set of (visual) codes especially developed, as explained below.
It is based on a series of concepts aimed at showing molecules displaying the features that another molecule would sense. We could say that we try to see molecules with the eyes of other molecules. With this basic idea, we have developed two (for now) elements of a *visual code* which should help our visual and perceptive system to interpret the images in a direct, intuitive way.
Although it is not a rigorous MD tool, BioBlender can also provide some approximate elaboration of protein motion, based on input of two or more conformations for a single protein.

Blender has been selected among the few 3D packages for several reasons: being the only one which is completely Open Source, it allows users, like us and you, to introduce whichever function at any level of its structure. Because it is distributed free of charge, biologists and other experimental scientists might be more prone to 'give it a try', without committing any of the always scarce resources dedicated to research. Blender is supported by a very generous global community that has produced plentiful material to help users, at all levels and in many languages. It will most likely continue to provide help, and BioBlender should make no exception. You, the user, are invited to make use of this material, and to contribute your own, to share with others.

BB2.0 structure

- Main program
- side programs (distributed with BB)
- accessory programs (to be installed by the user)

Graph of BB2.0 structure (?)

2. Install

BioBlender must be installed on Blender, similar to many other AddOns.

In order to have all its functions working properly, BioBlender will need a few other software packages installed, besides Blender:

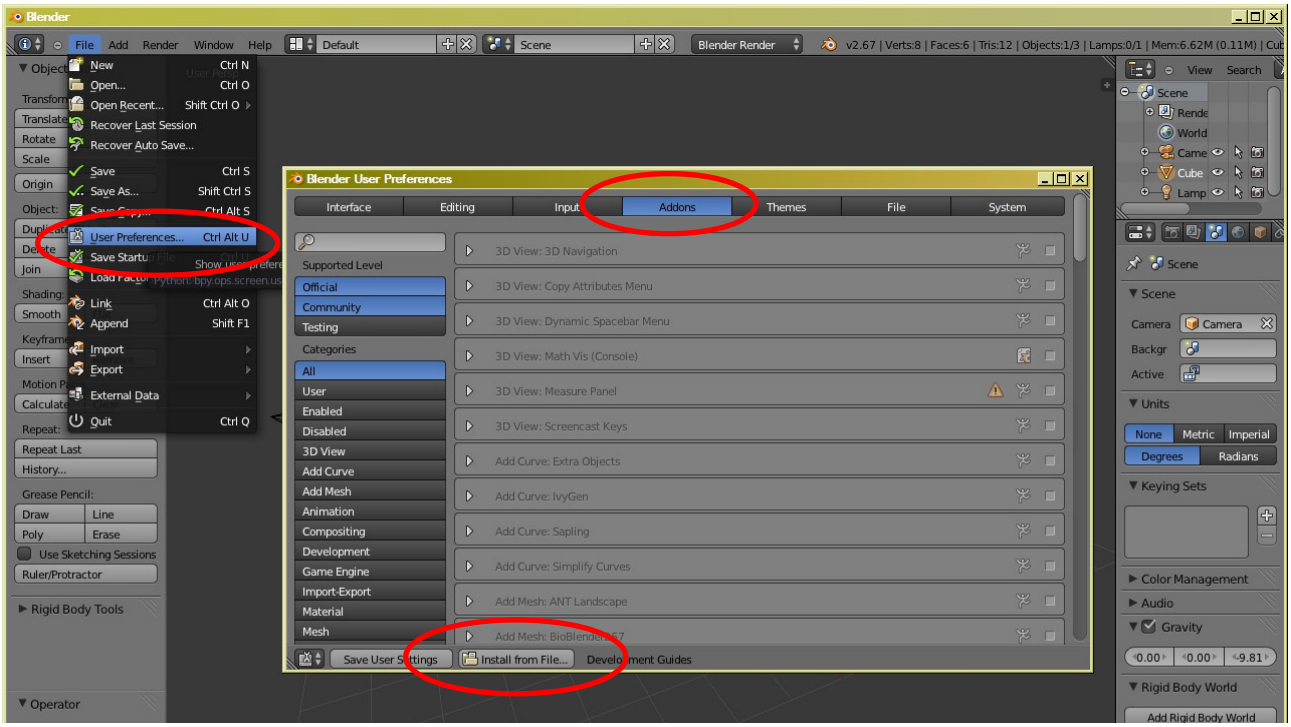
ProDy (used for the NMA option)
PyMOL (necessary for building the molecular surface)
Python 2.7

Once you have installed Blender 2.7 or later

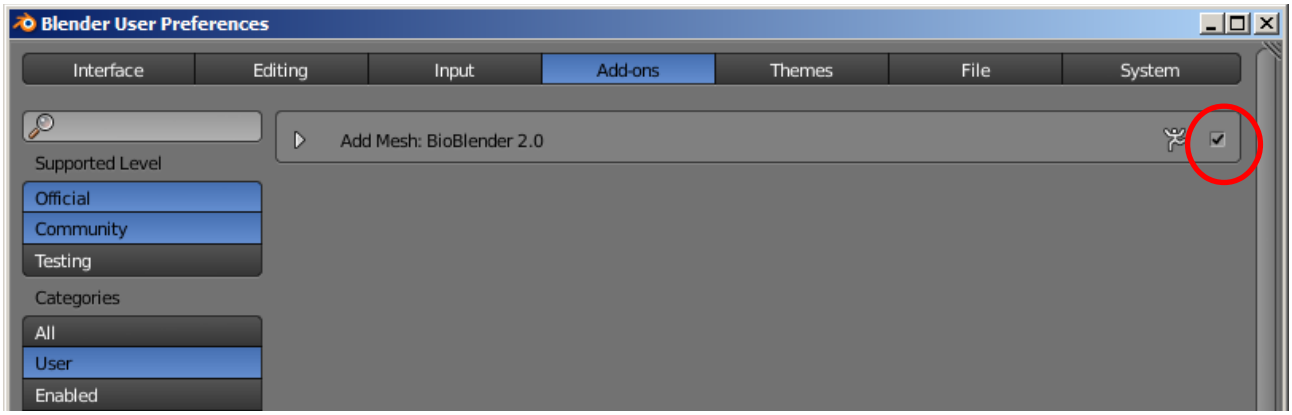
Download BB2.0, and make sure you know where it is. Do not unzip.

Open Blender

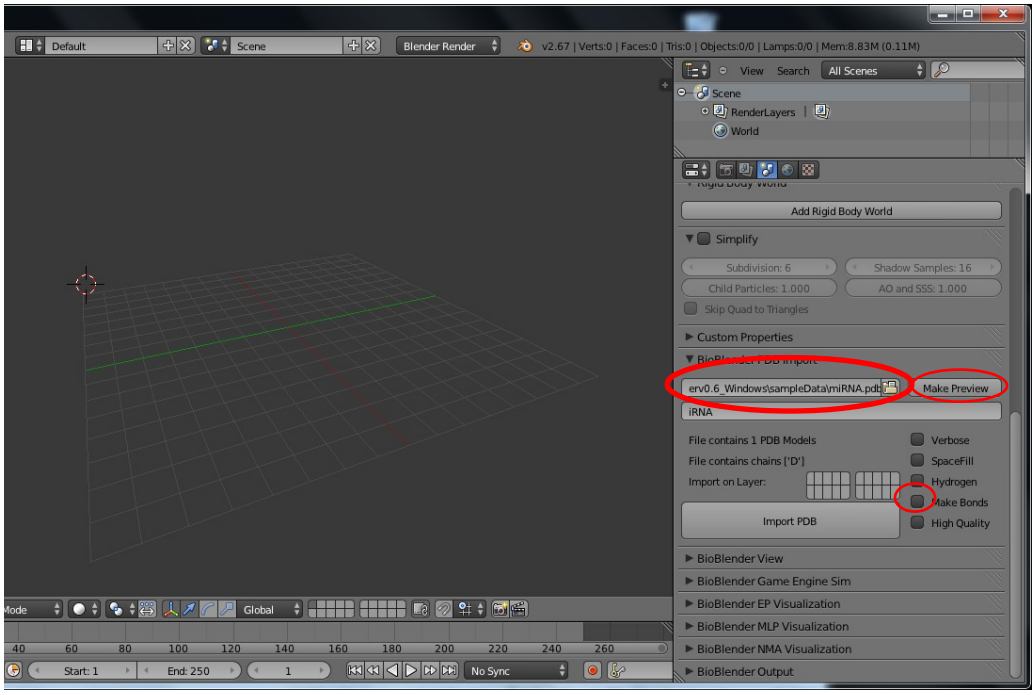
Open the **User Preferences** panel (Ctrl+Alt+U), select tab **Addons**, click **Install from file**.



Locate the zipped BioBlender2.0.zip file, and activate it.



In the Scene panel, the BioBlender functions are now accessible.



(Eliminate from the default scene all object -Cube, Camera and Light- by pressing **a**, **x,** and **Enter.** You may want to save this starting scene, by pressing **Ctrl+u**).

3. Import molecule

3.1 The pdb file

The Protein Data Bank is the central repository for all structural data of molecular biology. It now contains over 100 thousands files, and it is the first source of information for structural and molecular biologists interested in the shape of molecular objects. Most objects are proteins (partial, complex, combined with other molecules etc.), but also nucleic acids, lipids, sugars, and many other small molecules are present, either by themselves, or in combination with one another. Complete information on the PDB and the pdb format can be found on any of the pdb mirror sites, for example here . The relevant features for now are that each atom of the molecule is described with:

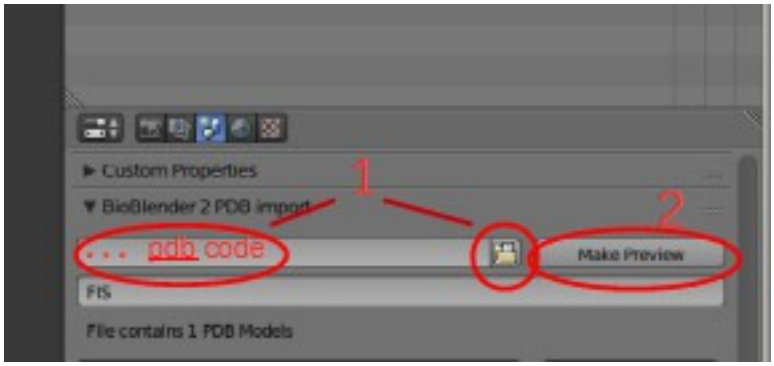
1. a definition (ATOM or HETATM)
2. a (successive) number
3. a name that identify its 'role' (chemical position)
4. the subunit (aminoacid or nucleic acid base)
5. the chain to which it belongs
6. the number of the subunit
7. the three coordinates
    1. x
    2. y
    3. z
8. a temp parameter
9. a R factor
10. the atomic identity of the atom

```
1891  ATOM   3004  C   SER E 105      50.928  44.792 -17.347  1.00 77.36           C
1892  ATOM   3005  O   SER E 105      51.926  45.412 -16.982  1.00 77.64           O
1893  ATOM   3006  CB  SER E 105      49.359  44.854 -15.403  1.00 75.93           C
1894  ATOM   3007  OG  SER E 105      48.117  45.332 -14.916  1.00 76.08           O
1895  ATOM   3008  N   PHE E 106      51.004  43.741 -18.156  1.00 78.96           N
1896  ATOM   3009  CA  PHE E 106      52.307  43.207 -18.556  1.00 80.08           C
1897  ATOM   3010  C   PHE E 106      52.635  43.401 -20.046  1.00 80.75           C
1898  ATOM   3011  O   PHE E 106      53.655  42.906 -20.528  1.00 80.87           O
1899  ATOM   3012  CB  PHE E 106      52.405  41.730 -18.166  1.00 80.15           C
1900  ATOM   3013  CG  PHE E 106      51.880  41.439 -16.787  1.00 80.37           C
1901  ATOM   3014  CD1 PHE E 106      52.536  41.917 -15.666  1.00 80.54           C
1902  ATOM   3015  CD2 PHE E 106      50.724  40.700 -16.612  1.00 80.64           C
1903  ATOM   3016  CE1 PHE E 106      52.053  41.657 -14.397  1.00 80.64           C
1904  ATOM   3017  CE2 PHE E 106      50.237  40.437 -15.346  1.00 80.75           C
1905  ATOM   3018  CZ  PHE E 106      50.902  40.916 -14.238  1.00 80.75           C
1906  ATOM   3019  N   GLY E 107      51.783  44.126 -20.767  1.00 81.32           N
1907  ATOM   3020  CA  GLY E 107      52.049  44.441 -22.171  1.00 81.52           C
1908  ATOM   3021  C   GLY E 107      50.808  44.865 -22.932  1.00 81.58           C
1909  ATOM   3022  O   GLY E 107      50.835  44.993 -24.164  1.00 81.57           O
1910  TER    3023      GLY E 107
1911  HETATM11977  C1  NAG D1052      31.230  39.532 -11.853  1.00 21.18           C
1912  HETATM11978  C2  NAG D1052      30.192  38.448 -11.830  1.00 19.74           C
1913  HETATM11979  C3  NAG D1052      30.240  37.810 -10.469  1.00 19.01           C
1914  HETATM11980  C4  NAG D1052      31.543  37.053 -10.544  1.00 20.97           C
1915  HETATM11981  C5  NAG D1052      32.665  37.954 -11.041  1.00 20.61           C
1916  HETATM11982  C6  NAG D1052      33.826  37.064 -11.421  1.00 20.45           C
1917  HETATM11983  C7  NAG D1052      27.933  39.155 -11.447  1.00 23.78           C
1918  HETATM11984  C8  NAG D1052      26.610  39.567 -12.017  1.00 23.47           C
1919  HETATM11985  N2  NAG D1052      28.905  38.885 -12.296  1.00 22.02           N
1920  HETATM11986  O3  NAG D1052      29.200  36.872 -10.308  1.00 17.79           O
1921  HETATM11987  O4  NAG D1052      31.885  36.521  -9.275  1.00 24.42           O
1922  HETATM11988  O5  NAG D1052      32.332  38.706 -12.183  1.00 21.09           O
1923  HETATM11989  O6  NAG D1052      34.999  37.840 -11.315  1.00 22.18           O
1924  HETATM11990  O7  NAG D1052      28.090  39.061 -10.238  1.00 26.44           O
1925  HETATM11991  C1  NAG D1078      21.249  83.555 -29.714  1.00 25.25           C
```

Plenty of other information is present in the pdb file, as well as in the website of the protein Data bank, and users are encouraged to peruse these sources.
Molecular structure is defined as the atomic position (atomic coordinates) of the atoms that compose the molecule.

3.2 Atoms and bonds
In biological molecules, it is extremely rare (but not unheard of) to find an isolated atom. The vast majority are combined (linked by chemical bonds) in large groups that ca reach up to hundreds of thousands atoms. Luckily, scientists have been able to decode the 'building blocks' of such large molecules, which are typically made up of few tens of atoms (*aminoacids*, such as Alanine, Serine, Glutammate etc., *nucleic acids*, such as Adenine, Guanine, etc, *sugars*, such as glucose, ribose etc, *lipids*, and others).
The bonds that link the atoms one to another can be roughly assimilated to rigid body joints: they have some degree of freedom, but quite limited. This feature makes it possible to use the Blender Game Engine to approximately simulate their behavior. We will see in Chapter 5 how BioBledner deals with molecular motion.
The activity of proteins is such because their atoms change position while staying linked.

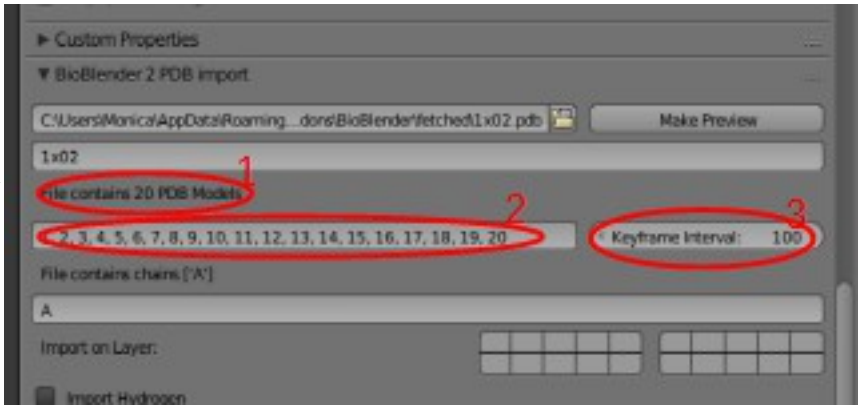
3.3 BioBlender Import
1. Select a PDB file (1), either using the 4 letter code (for PDB.org fetch), or browse in your own files.



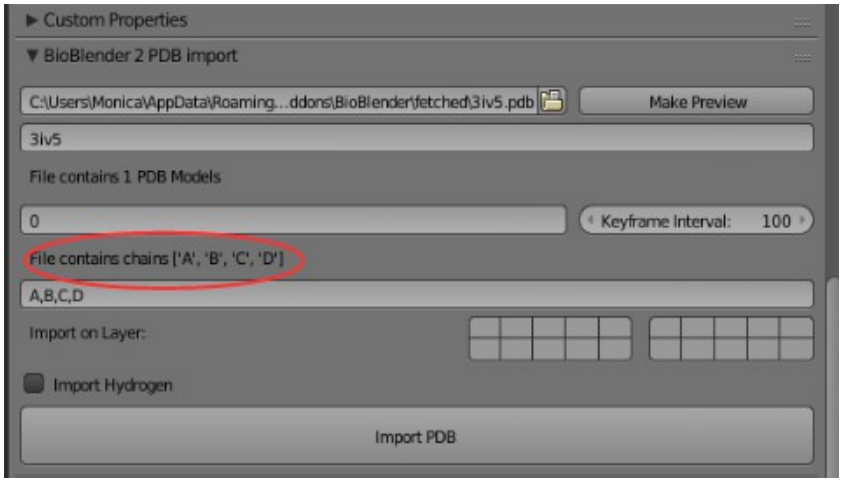
2. Click **Make Preview**, so that BioBlender can access the file, and prompt you with relevant options;

Next, consider one or more of the following situations that may apply:

- if your file is an NMR collection, BB will recognize how many models are present (1), and prompt you to select which models (2) to import (up to 100), in which order, and how separate (how many frames between each model 3).



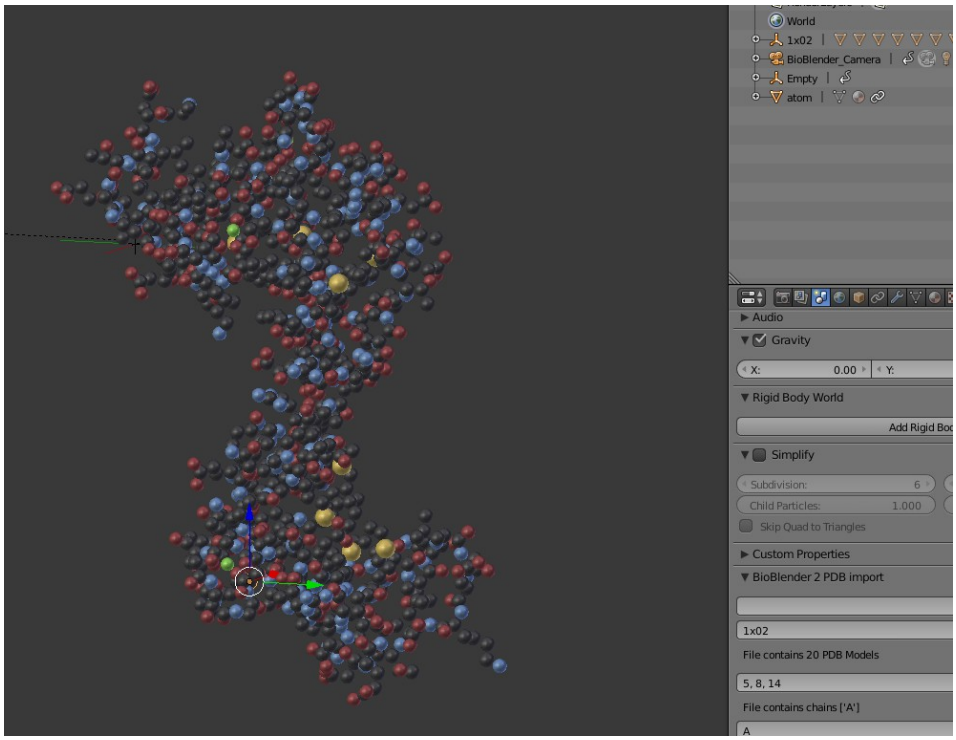
- if your file contains only one model (e.g. X-ray), with 1 or more chains, BioBlender will prompt you to select which chains to import (default is ALL). In this case, the file contains 4 chians: 2 monomers of the DNA binding protein fis (A and B) and the 2 DNA strands (C and D). If you want to see it inBioBlender, you probably know what is in the pdb file; if you don't, you willl have to check it by reading inside.



- if you wish to use the NMA feature (calculated by ProDy, wich must be installed in the computer independently), select the NMA parameters now, before importing. In case of NMR, ProDy will calculate NMA for the first Model in the NMR file.

- consider the opportunity of importing Hydrogens (if they are present at all in the file pdb): the default option is NOT. Including H will make the system very heavy, will significantly prolong the import time, and usually do not add much useful information. They are important when considering water interactions.

Now everything is set to **Import PDB**.
This may take few seconds to a minute or so, depending on the size and complexity of your molecule. Together with the molecule, BioBlender adds to the scene a set of lights and a camera. Press 0 to get a view form the camera, and adjust according to your need.



In the 3D viewport, your molecule is built as atoms.
In the Outliner there is a new Empty object,with the name of the PDB file (or its last 4 letters), and with all atoms as children of the Empty

To be continued...