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:

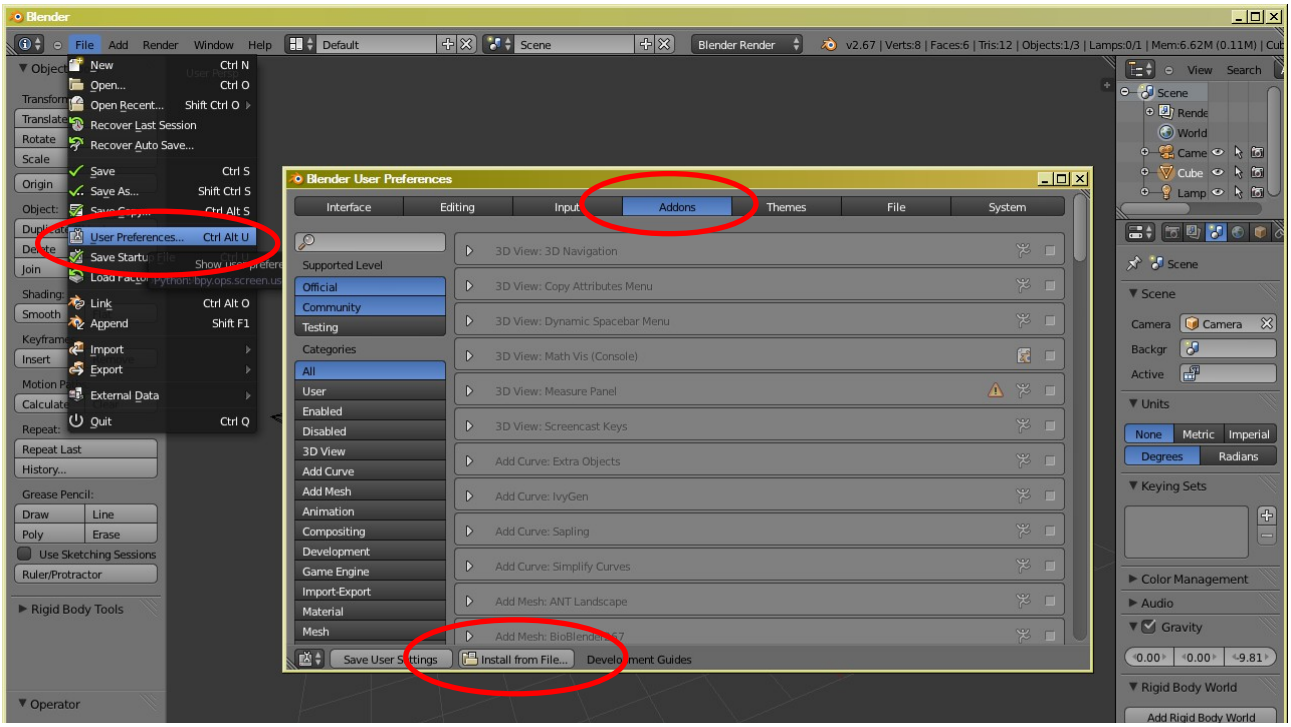
ProDy (used for the NMA option)
PyMOL (necessary for building the molecular surface)
Python 2.7

Once you have installed Blender 2.7 or later

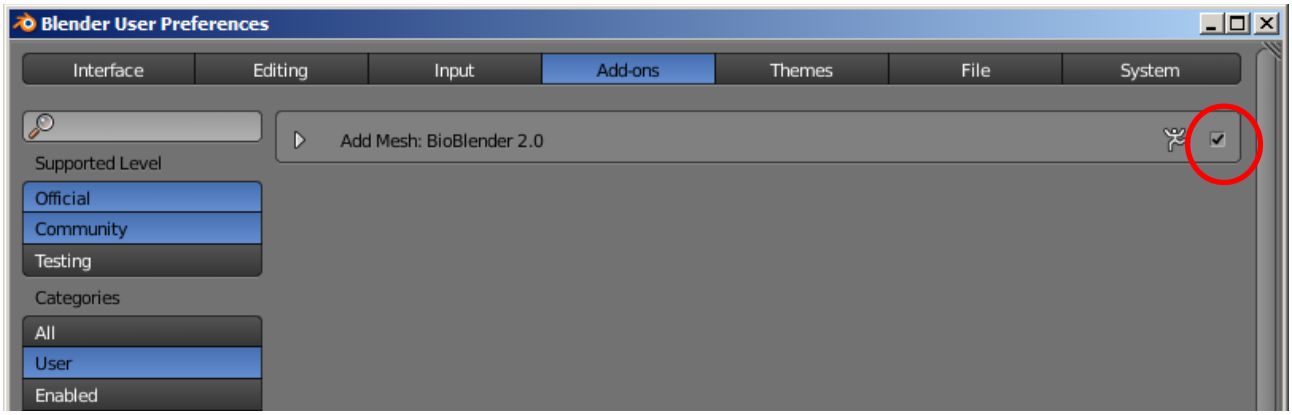
Download BB2.0, and make sure you know where it is. Do not unzip.

Open Blender

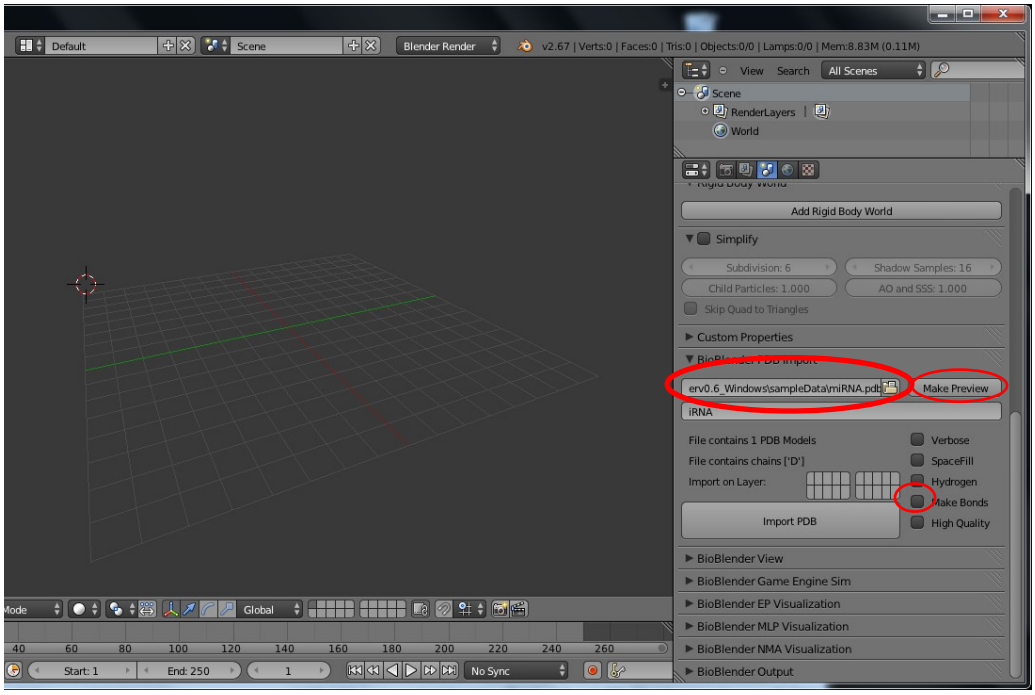
Open the **User Preferences** panel (Ctrl+Alt+U), select tab **Addons**, click **Install from file**.



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

Select a PDB file, either using the 4 letter code (for PDB.org fetch), or browse in your own files. Click **Make Preview**, so that BioBlender can access the file, and provide relevant options:

- if your file is an NMR collection, BB will prompt you to select which models to import (up to 100), in which order, and how separate (how many frames between each model).
You may wish to activate the **Make Bonds**, to enable the creation of rigid body joints as chemical bonds, for more accurate animation when using the Game Engine (see below).

- 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).

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

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.