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**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación

MD Setup Workflow installation

with



BioExcel Building Blocks

**PATC Simulation Environment for Life Sciences,
BSC 2023**

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The team



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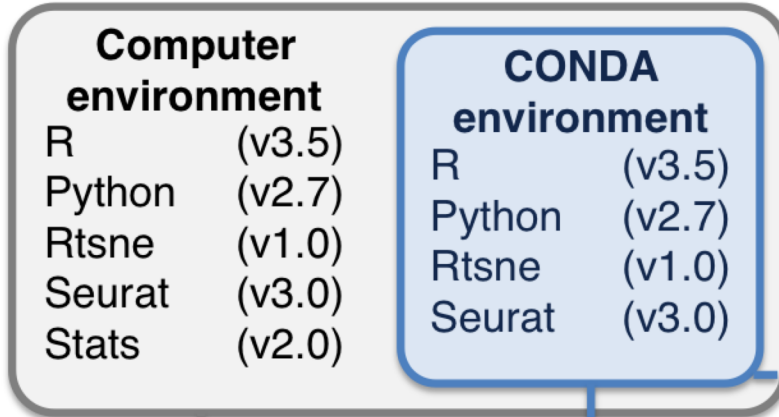
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Person #1



Run Sauron

Results!

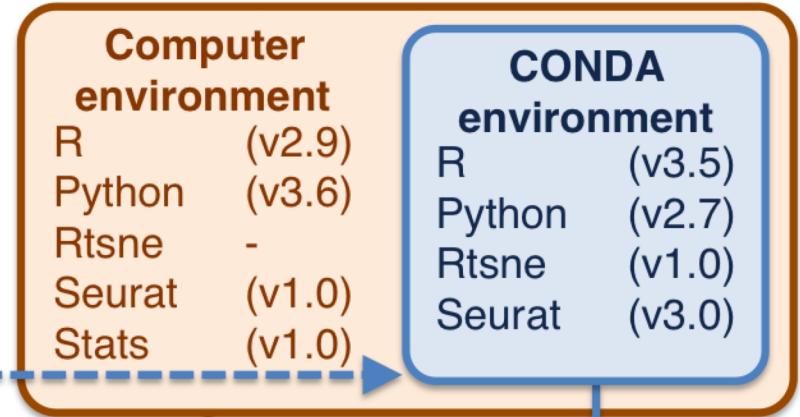


Run Sauron

Results!



Person #2



Run Sauron

ERROR ! ❌

Rtsne missing!
Seurat not v3.0!
You need R v3.2!

Run Sauron

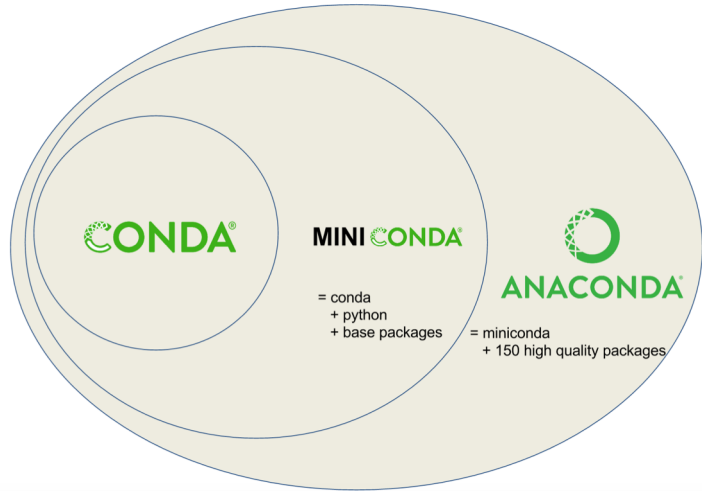
Results!



Protein MD Setup – Anaconda installation

<https://www.anaconda.com/>

Environment manager: all package dependencies are taken care of at the time of download.



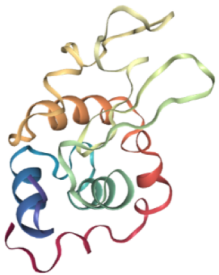
The screenshot shows the Biobb website interface. At the top, the logo 'biobb' is displayed next to the URL <http://mmb.irbbarcelona.org/biobb>. A navigation menu includes 'Home', 'Availability', 'Documentation', 'Workflows', and 'About'. A dropdown menu is open under 'Availability', showing options: 'Launch', 'Download & Install', 'Tutorials', and 'Release Notes'. Below the navigation, there are three large buttons for installation: 'Install in Mac OS' (with a Mac OS logo), 'Install in Ubuntu' (with the Ubuntu logo), and 'Install in Windows 10 (WSL)' (with the Windows logo and a small Ubuntu logo).

Protein MD Setup - Tutorial

<http://mmb.irbbarcelona.org/biobb/workflows>

GROMACS PROTEIN MD SETUP

2022.3



This tutorial aims to illustrate the process of setting up a simulation system containing a protein, step by step, using the BioExcel Building Blocks library (biobb). The particular example used is the Lysozyme protein (PDB code 1AKI).

WorkflowHub Jupyter Notebook CWL Python Galaxy

Launch Jupyter Notebook * Galaxy BioBB Workflows

View tutorial Open GitHub repository Open documentation

gmx md protein

(*) Binder for biobb is a small installation and to promote fair use of our resources, one user is allowed to run only one notebook server at a time. Launching a new notebook server should stop the previous one. Users cannot see the notebooks run by other users, but please avoid entering secret data to the notebooks.

Protein MD Setup – Tutorial installation

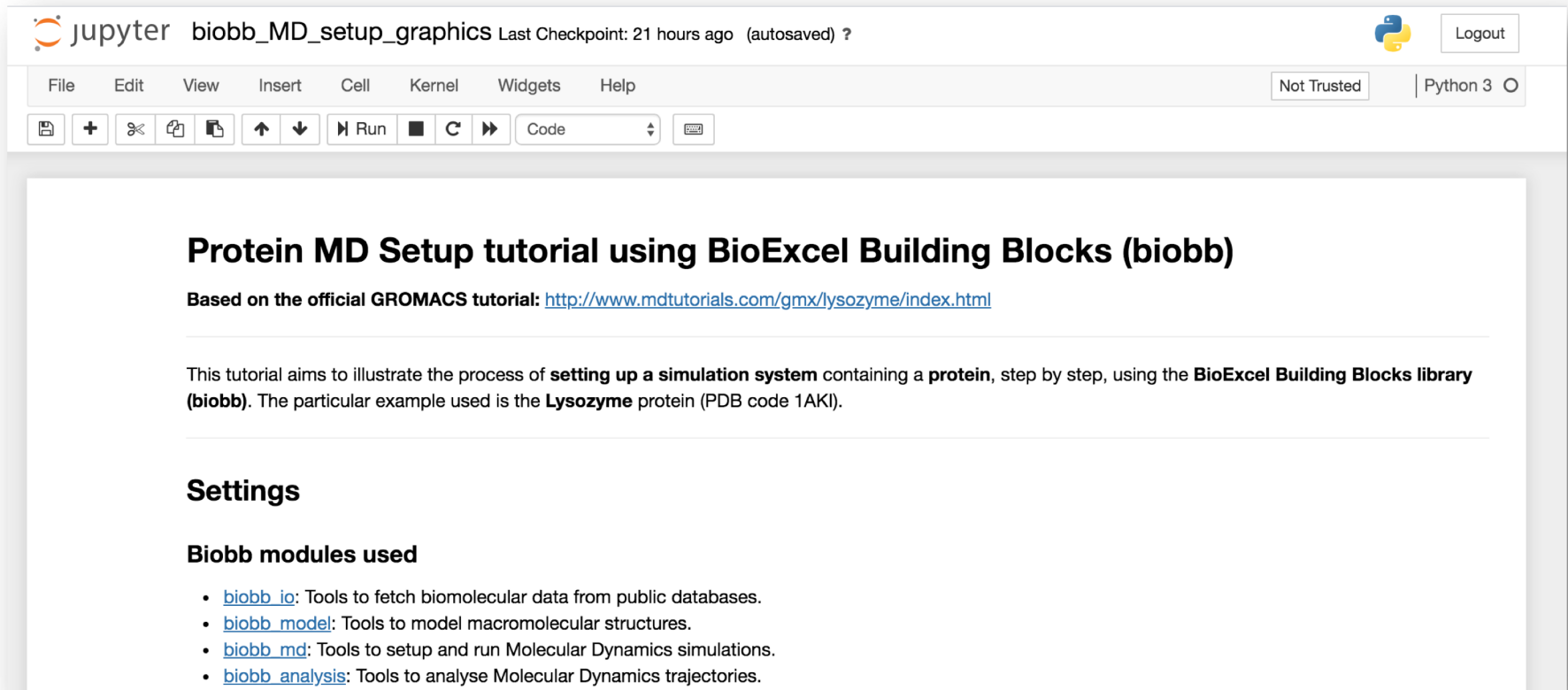
Conda Installation and Launch


```
git clone https://github.com/bioexcel/biobb_wf_md_setup.git
cd biobb_wf_md_setup
conda env create -f conda_env/environment.yml
conda activate biobb_GMX_MDsetup_tutorial
jupyter nbextension enable python-markdown/main
jupyter-notebook biobb_wf_md_setup/notebooks/biobb_MDsetup_tutorial.ipynb
```



Protein MD Setup – Jupyter Notebook

jupyter-notebook biobb_wf_md_setup/notebooks/biobb_MDsetup_tutorial.ipynb



jupyter biobb_MD_setup_graphics Last Checkpoint: 21 hours ago (autosaved) ?  Logout

File Edit View Insert Cell Kernel Widgets Help Not Trusted Python 3

Run Code

Protein MD Setup tutorial using BioExcel Building Blocks (biobb)

Based on the official GROMACS tutorial: <http://www.mdtutorials.com/gmx/lysozyme/index.html>

This tutorial aims to illustrate the process of **setting up a simulation system** containing a **protein**, step by step, using the **BioExcel Building Blocks library (biobb)**. The particular example used is the **Lysozyme** protein (PDB code 1AKI).

Settings

Biobb modules used

- [biobb_io](#): Tools to fetch biomolecular data from public databases.
- [biobb_model](#): Tools to model macromolecular structures.
- [biobb_md](#): Tools to setup and run Molecular Dynamics simulations.
- [biobb_analysis](#): Tools to analyse Molecular Dynamics trajectories.