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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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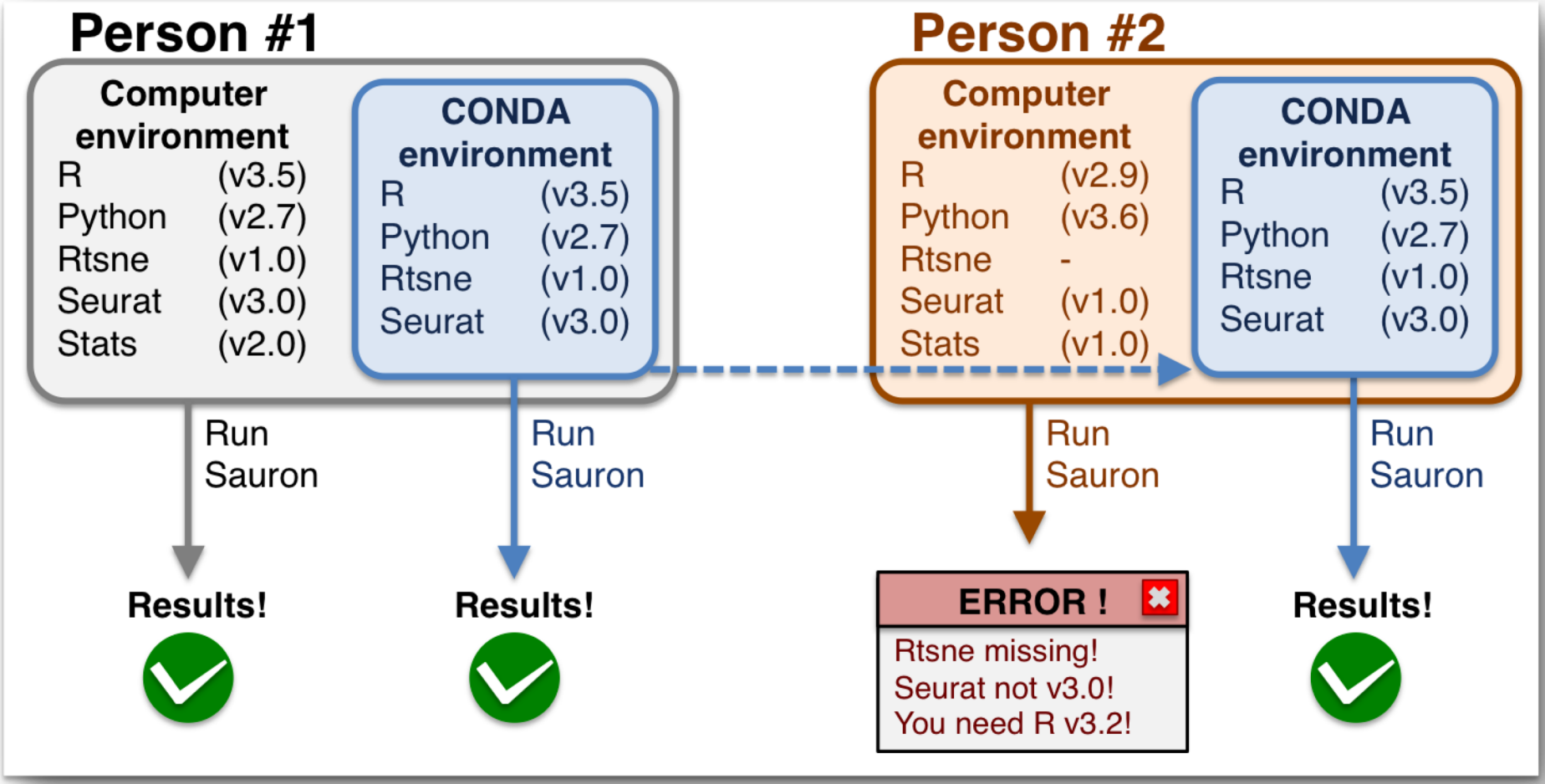
Conda Packaging System

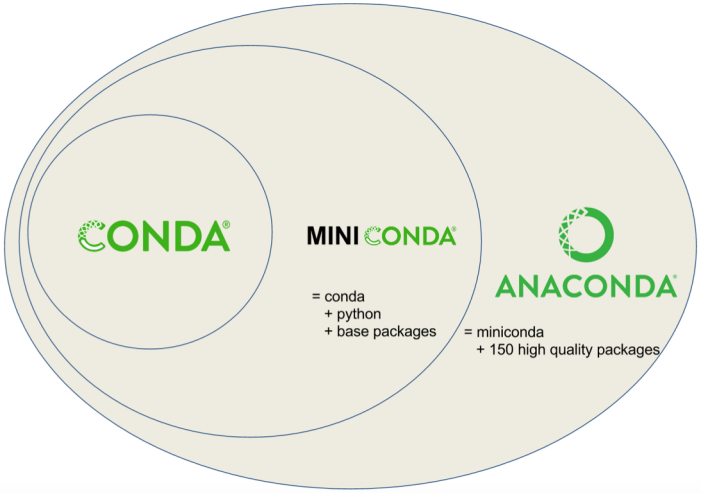
https://nbisweden.github.io/

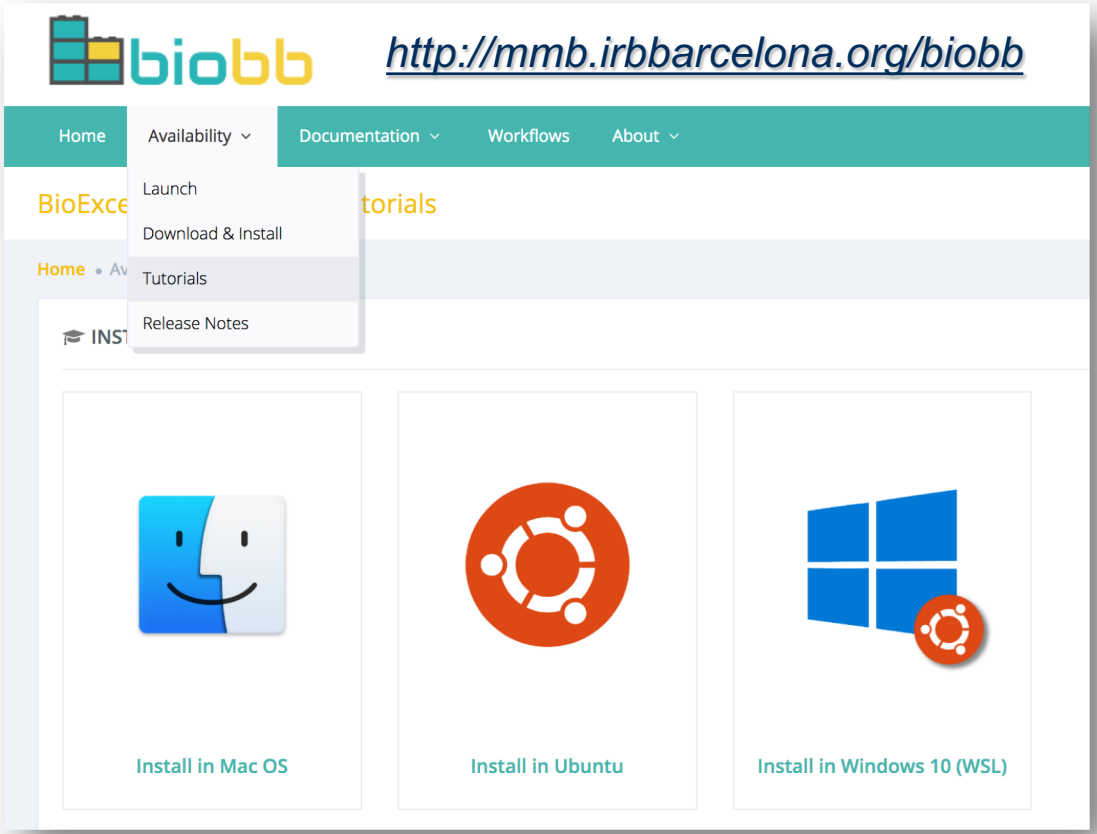


Protein MD Setup – Anaconda installation

https://www.anaconda.com/

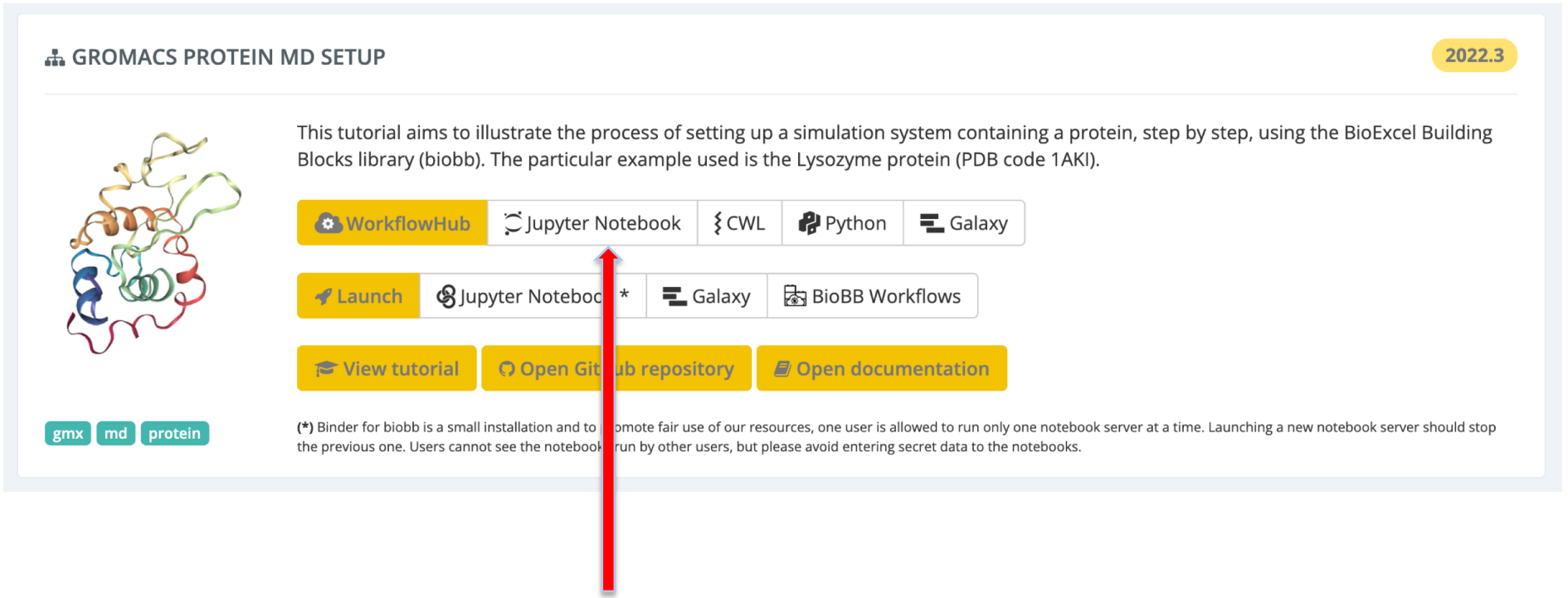
Environment manager: all package dependencies are taken care of at the time of download.





Protein MD Setup - Tutorial

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



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