

# Installing MD analysis packages w/ conda

- `conda create --name mdanalysis`
- `conda activate mdanalysis`
- `conda config --add channels conda-forge`
- `conda install jupyter pandas mdanalysis pymbar`
  - jupyter - for interactive coding notebooks
  - pandas - for data analysis
  - mdanalysis - for loading and analyzing MD trajectories
  - pymbar - for calculating free energies. also contains equilibration detection.
- If you want to try Markov State Models, you may need to downgrade python first
  - `conda install python=3.7`
  - `conda install pyemma`
    - pyemma - for Markov state models

# **Dimensionality reduction with principal component analysis**