

## PyModSim

FASTA sequence

1.

Structure Prediction  
AlphaFold

PDB AlphaFold DB

AlphaFold Model

2.

Model Refinement  
MODELLER

PDB External

Refined Model

3.

Membrane Positioning  
PPM

Homology Model

## PyMemDyn

Protein Model(s)

PDB Ligands

PDB Cofactors

PDB Model

1.

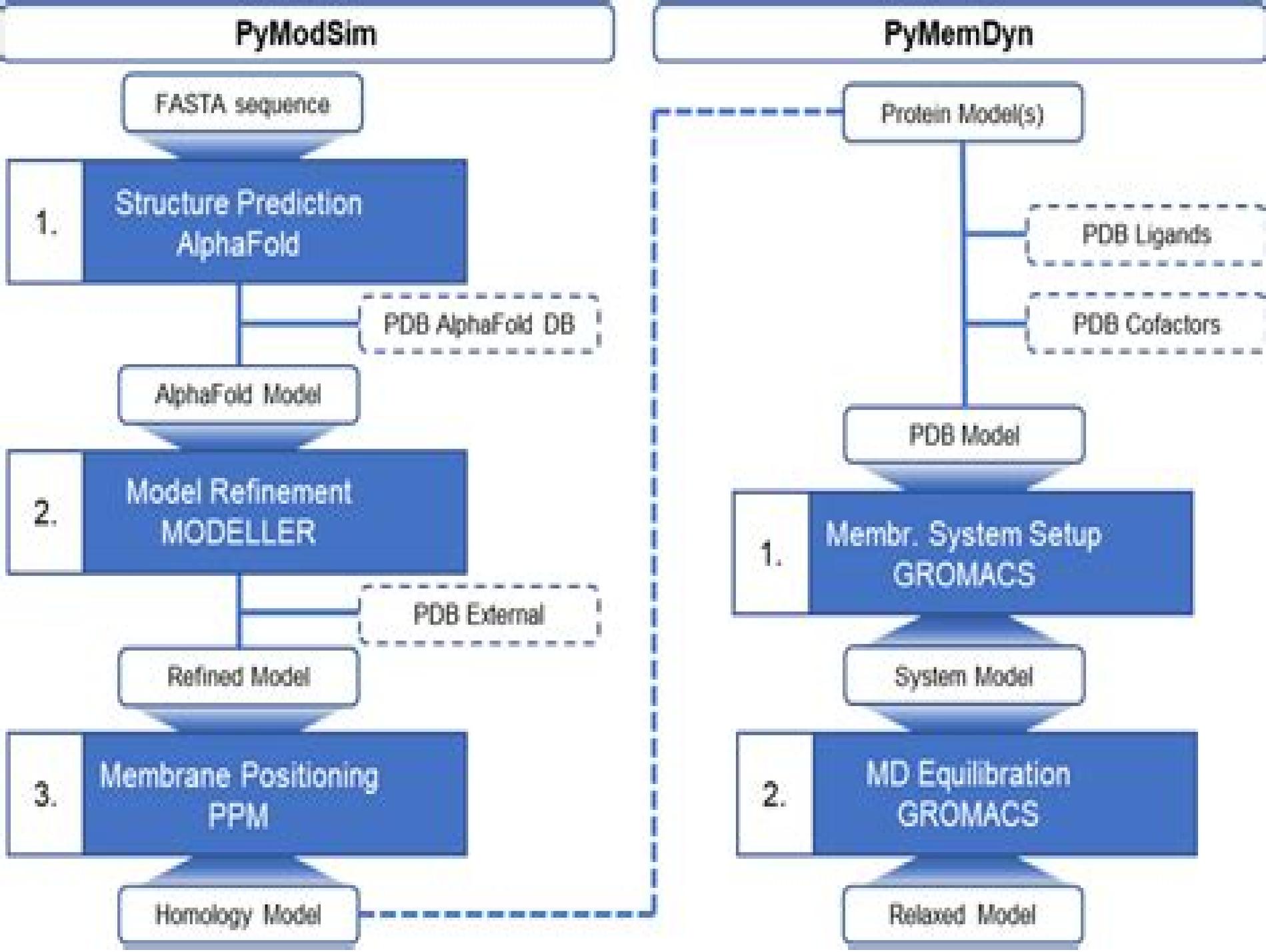
Membr. System Setup  
GROMACS

System Model

2.

MD Equilibration  
GROMACS

Relaxed Model



# Modsim Iii A Tutorial

**Yicheng Fang**



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