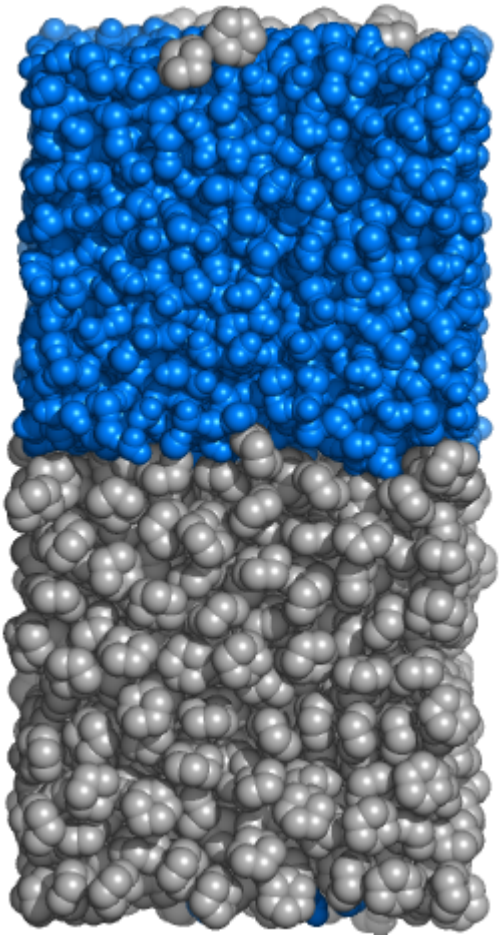
Example 2: Biphasic Systems

Example 2: Building Biphasic Systems

Studay system

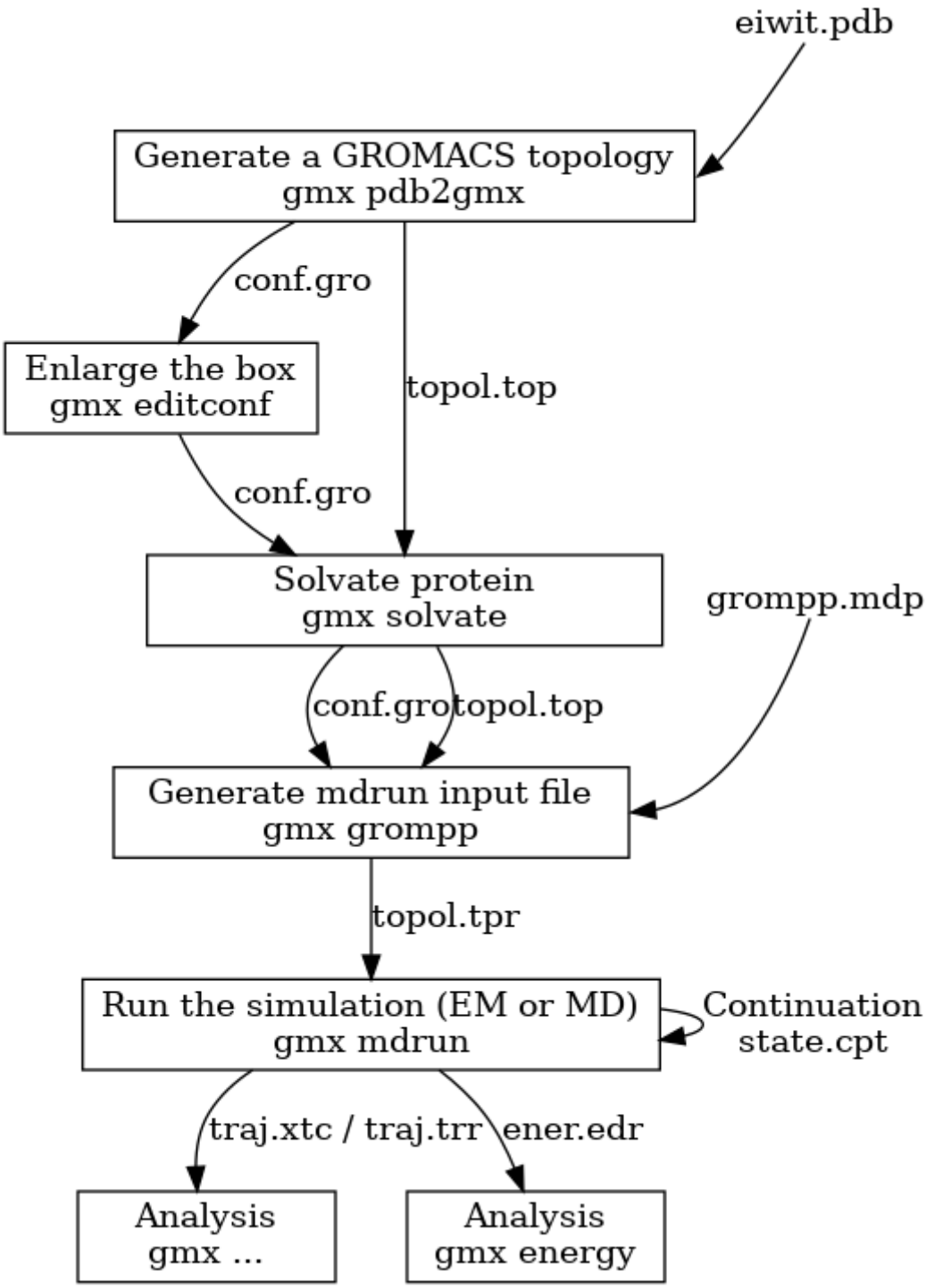


The original tutorial was to make a heterogeneous biphasic system composed of hydrophobic (cyclohexane) and hydrophilic (water) layers.

Here we are going to use benzene to replace cyclohexane as a demostration of how to use CHARMM-GUI to make a new ligand.

As we covered before, Gromacs simulations require two starting input files for a structure:

- Coordinate file: this can be a Protein Data Bank pdb file, or Gromacs
- Toplogy file: this can be a Gromacs top file



Prepare benzene with CHARMM-GUI

Register a Charmm-GUI account

Go to https://charmm-gui.org/ and register an account.

Model a molecule

Go to Ligand Reader and Modeler to search or create a molecule.

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