Prerequisites:

1. You must install the Ubuntu operating system in order to install and use Gromacs tool to do molecular dynamics simulation analysis.

Prerequisite Terminologies:

In order to have a better understanding of the main topic, you should have the basic concept of the following terms:

- Molecular Dynamics Simulation
- GROMACS tool
- Pre-processing of the protein structure
- Construction of topology file for simulation
- Defining a Solvent box for simulation

Introduction:

Molecular dynamics (MD) is a computer simulation method for analyzing the physical movements of atoms and molecules. GROMACS is a versatile package to perform molecular dynamics. After creating a solvent box for simulation, the next phase in molecular dynamic simulation is to apply solvation. The

GROMACS program ‘solvate’ can be used to apply the solvation within the protein structure and to solvate the solute configuration. Following are the basic options of the solvate tool:

- ❏ Option to specify input files:
  - ❏ **-cp** (protein.gro) (Optional) - Structural file.
  - ❏ **-cs** (spc216.gro) (Library) - Structural file.
- ❏ Options to specify input/output files:
  - ❏ **-p** (topol.top) (Optional) - Topology file.
- ❏ Options to specify output files:
  - ❏ **-o** (output.gro) - Structural file.

Steps:

- Open the terminal and call the ‘gmx’ and call the solvate tool within the gmx followed by the protein configuration file, solvent configuration file, topology file and the output file name (i.e: solvate.gro), as follows:

  gmx solvate -cp protein_newbox.gro -cs spc216.gro -o solvate.gro -p topol.top

  - Here, the ‘protein_newbox.gro’ file is the protein configuration file which contains the solvent box with the centered protein structure.
  - ‘spc216.gro’ is the solvent configuration file which comes by default when you install the GROMACS tool. As we are utilizing water as the solvent so you can use this solvent configuration file.
  - ‘topol.top’ is the topology file. This file is necessary because water molecules that are being added in the solvent box, that information will be incorporated into

the topology file as it is the most prime file in the molecular dynamic simulation.
    - ‘solvate.gro’ is the output file which will have the solvation information for the simulation.
- Run the above command and it’ll generate the solvation file for molecular dynamic simulation analysis.
- Open the ‘solvate.gro’ file within the PyMol to visualize it. [You can now visualize the solvent box around the protein structure.]

Summary:

In this video tutorial, we learned about the GROMACS program ‘solvate’ and its options. We also got to know how to apply solvation or to put solvate in the solvent box in which the protein structure is available as centered using the solvate tool.