Simulation protocol to obtain open pore i-v characteristics of graphene nanopore.
Explained below is a step by step procedure, with all relevent simulation parameters, to configure graphene nanopore membrane in NAMD and calculate i-v characteristics.

1. A 96Å $\times$ 96Å graphene membrane with a pore diameter = 3 nm is constructed using the following protocol: The lattice points $\vec{r}_{\rm mn}$ for the graphene membrane are given by, $\vec{r}_{\rm mn}$ = m $\vec{a}_1$ + n $\vec{a}_2$, m, n $\in$ $\mathbb{Z}$, where 2-D lattice vectors $\vec{a}_1 = \left(\frac{\sqrt{3}}{2}a, \frac{a}{2}\right)$ and $\vec{a}_2 = \left(\frac{\sqrt{3}}{2}a, -\frac{a}{2}\right)$, here $a = \sqrt{3} \times a_{\rm C-C}$ = 2.46 Å and $a_{\rm C-C}$ is the distance between two carbon atoms, namely, 1.42 Å. Each unit cell for graphene has two atoms, one at $\vec{r}_{\rm mn}$ and one at $\vec{r}_{\rm mn}$ + (a, 0). The pore is constructed by removing atoms whose coordinates satisfy the condition $x^2 + y^2 \leq d^2$, where d (=3nm) is the diameter of the pore. The parameters for carbon atoms of graphene were those of type CA in the CHARMM27 force field. The psf file is generated using PSFGEN. The graphene membrane has geometrical center located at (0,0). In the simulations the outer edge of graphene membrane is fixed by using fixed atom constraints of NAMD, the following atoms were fixed, the tcl selection for the constraint atom is (resname GRP is the resname for graphene)

   ```
   set sel [atomselect top "resname GRP
   and {x > 35 or x < -35 or y > 35 or y < -35}"]
   ```

2. The above graphene membrane is solvated by padding water $\pm$75Å the z$-$ direction. The system is ionized with 1M KCL (corresponds to 1613 K^+ and 1613 Cl^- atoms), the size of the system is 126,308 atoms. The solvation and ionization can be trivially performed using VMD plugins *Add Solvation box* and *Add Ions*. The water model used is TIP3P and parameter for ions are from CHARMM27.
3. The system is minimized for 4000 steps and then heated to 295 K in 4000 steps.
4. A 0.5 ns simulation under NPT ensemble followed by 1.5 ns NVT ensemble was performed to equilibriate the system. The NPT simulation was done using Nosé-Hoover Langevin piston pressure control at 1 bar. Langevin dynamics was used to control temperature. A damping of 0.2/ps is used on graphene atoms and water (non-hydrogen atoms). Note we do not apply langevin bias to the ions as applying Langevin forces to the ions, whose motion due to the electric field we are trying to measure, could lead to a subtle bias in the current. This can be achieved by using a langevin pdb file in NAMD thermostat section, with the following rules

   ```
   set all [atomselect top all]
   $all set beta 0
   set sel [atomselect top "water and name OH2"]
   ```

```
$sel set beta 0.2
set sel [atomselect top "resname GRP"]
$sel set beta 0.2
```

5. An electric field $E = -23 \times \frac{V_0}{L_Z}$ Kcal/Mol Åe, is applied along the z-direction, where $V_0 = 3.0$ V and $L_z = 135$ Å. Note the L_z that is used is the value the system relaxes to after the equilibriation. A 7 ns simulation is performed under the constant e-Field.
6. The total ionic current $I(t)$ is computed using

$$I(t) = \frac{1}{\Delta t L_z} \sum_{i=1}^{N} q_i \big[z_i(t + \Delta t) - z_i(t) \big], \tag{1}$$

   where the sum runs over all ions, Δt was chosen to be 50 ps and z_i and q_i are the z coordinate and charge of ion i, respectively. L_z represents the system dimension in the z-direction.

7. PME parameters used

```
PME                 on
PMEGridSizeX        96
PMEGridSizeY        96
PMEGridSizeZ        256
```

8. Integration parameters

```
timestep            1.0
nonbondedFreq       2
fullElectFrequency  4
stepspercycle       20
```

9. cuttoffs etc.,

```
exclude             scaled1-4
1-4scaling          1.0
cutoff              12.
switching           on
switchdist          10.
pairlistdist        13.5
```

One must be aware that diffusion and transport properties of ions are very sensitive to the cutoffs, switching distances, water model and force field itself.

The following two articles shed more insight into this

1) N. Modi, P. R. Singh, K. R. Mahendran, R. Schulz, M. Winterhalter, and U. Kleinekathofer, Probing the Transport of Ionic Liquids in Aqueous Solution Through Nanopores, J. Phys. Chem. Lett. 2, 2331-2336 (2011)

2)David B. Wells, Swati Bhattacharya, Rogan Carr, Christopher Maffeo, Anthony Ho, Jeffrey Comer, and Aleksei Aksimentiev. Optimization of the molecular dynamics method for simulations of DNA and ion transport through biological nanopores. In Nanopore-based technology: single molecule characterization and DNA sequencing. Humana Press, 2011.

Also, interesting may be a similar study on open pore characteristics using Gromacs (with NaCl)
Ion transport through a graphene nanopore G Hu, M Mao, S Ghosal - Nanotechnology, 2012