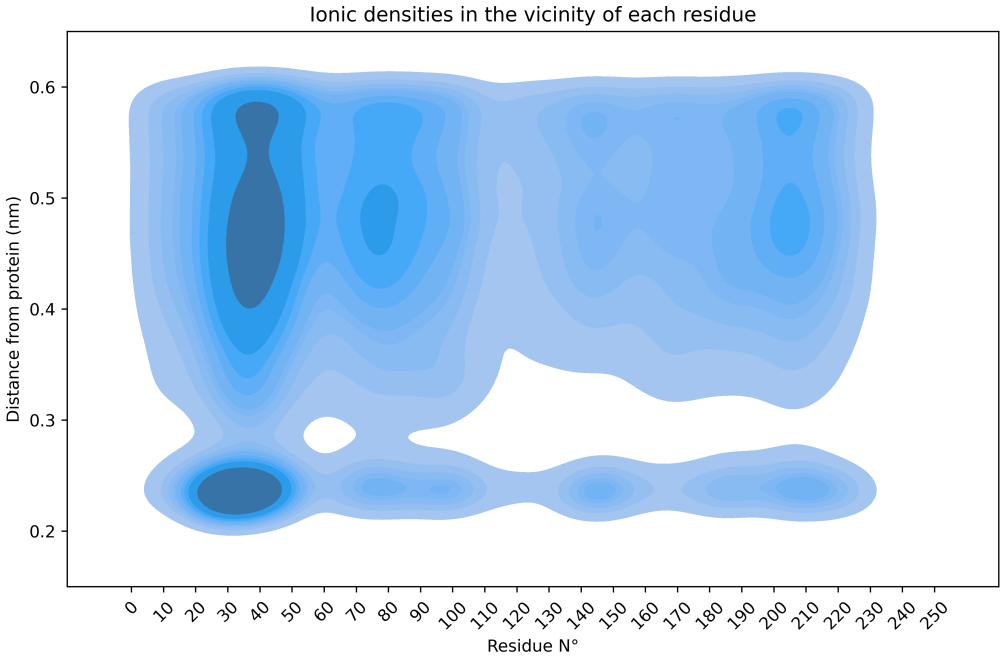

Ionic Density Map generator

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Public access: https://github.com/Eddy-Barraud/IDM

Requirements : numpy pandas matplotlib seaborn mdtraj

This app is converting pairdist XVG files to Ionic Density Maps (IDM). The python script is using Seaborn and MDTraj libraries.

IDM represents the normalized probability to find an ion at a given distance of each protein residue along the simulation time.

1. Generate with GROMACS a pairdist XVG file using a command like the one below :

```
gmx pairdist -f 12.npt_9.xtc -s 12.npt_9.tpr -n index.ndx -refgrouping res -selgrouping all -o 12.npt_9.pairdist.xvg
```

When asked, enter the protein group number, then a group with ions (Na, NaW, Na-Cl, etc...)

2. Then, generate a topology file of that system, named **sys.gro** (IMPORTANT), using a command like below :

```
gmx editconf -f 12.npt_9.gro -n index.ndx -o sys.gro
```

When asked, enter a group that contains the protein AND the ions, i.e., a group containing the two groups entered at step 1.

3. Copy the 12.npt_9.pairdist.xvg and the sys.gro files to the same folder as the app IDM.Gen.exe

4. Run the script.

```
python IonicDensityMap.py
```

It will convert each XVG file to a map named filename.density.png, only is the map file is not already present.

Another file, named filename.mindist.png, is created, it corresponds to a heatmap of the minimum distance between each residue and any of the ions across time.