Ionic Density Map generator

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Public access: https://github.com/eddydu44/IDM

This app is converting pairdist XVG files to Ionic Density Maps (IDM). The python script behind the app 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. Execute the app.

It will convert each XVG file to a map named filename.density.png

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 accross time.