Here is a sample workflow to get my data points.

Now I will structure all elements of the workflow to optimize into into the best code possible.

```
Creating initial structure gel_ionization_interface.py
                    │
                    ▼
Running Lammps equilibration `lammps -in 1_equil.lammps`
                    │
                    ▼
Running Lammps simulation `lammps -in sim.lammps`
        │               │               │
        ▼               ▼               ▼
Creating lammps    Creating PBS    Creating bash
    files              file          run files
        │               │               │
        └───────────────┼───────────────┘
                        ▼
                Analyzing results
        │                       │
        ▼                       │
Electrostatic Potential         │
        │                       │
        ▼                       │
Create VMD file to get          │
electrostatic profile           │
        │                       │
        ▼                       │
Create .sh script for           │
batch run                       │
        │                       │
        ▼                       │
Run VMD script on the           │
supercomputer                   │
        │                       ▼
        ▼                  Profile info
    Get .dx file       │       │       │
        │              ▼       ▼       ▼
        ▼          Density  Pressure  Energy
Convert .dx file       │       │       │
into csv               │       │       │
        │              │       │       │
        └──────────────┴───────┴───────┘
                        ▼
Convert dump files -with multiframe info- into csv file with ave profile + std
                        │
                        ▼
Run analysis of ave profile curves and convert into steps
                │               │
                ▼               ▼
          plot results    save into csv file for replotting
```