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Model.py part 2

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Outline of model.py

- main　　>主程式
  - packmol　　>建pdb
  - autopsf　　>建結、加水、加離子
  - **charmm2lmp >建立給lammps的data檔**
  - **createTWCC >把國網需要的檔案全部丟到一個資料夾方便上傳**

本次模擬用的力場

- CHARMM36m
- MacKerell Lab (umaryland.edu)

本次模擬用的力場

- CgenFF
- Generalized CHARMM

- ATOM
- BOND
- ANGLE
- DIHEDRAL
- IP
- NBFIX

WHY LAMMPS

- LAMMPS Molecular Dynamics Simulator
- Very, very flexible and straight forward
- What does the files mentioned earlier relate to LAMMPS?

How to run LAMMPS?

- **Data file**: The atoms, bonding and parameters
- **Input file**: The setup and variable used in simulations

Software comparison

In most cases, only 2 files are required in LAMMPS

However, How to convert **pdb+psf+top+par** into a **single data file**?

Requirements	GROMACS	LAMMPS
Atoms	Pdb /Gro file	**Data file**
Structure	Psf, itp, top file	**Data file**
Parameters	Itp files	**Data files**
Input variables	Mdp files	**Input files**

CHARMM2LMP

- perl **charmm2lammps.pl** 1_25 5_ionzied **-**cmap charmm36
- Error?
- topo readlammpsdata xxx.data

快速丟國網

- input file
- bash file

Details

- Structure in main function
- What do other arguments mean?

python model.py 1 1 100(water) 10(NaCl)

- Packmol
- psf
- solvate(xxxxx,boxsize)
- delete water(n_water=**110(+22*KEMA)**)
- ionize(substitute water -> ion , SOD CLA)

- KEMA 自带-22e
- 如果 1KEMA　0 NaCl
- ionized(MA=22 CLA=0)

- 如果 1KEMA　10 NaCl
- ionized(NA=32 CLA=10)

Next week

- How we create the input alpha-keratin fragments?
- How we revise the topology file (dictionary) and the parameter files?