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Model.py part 1

Computational Mechanics and Intelligence Lab
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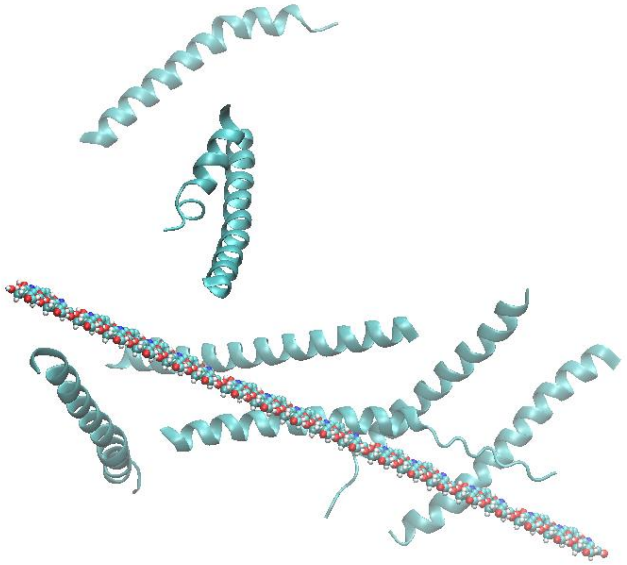
Outline of model.py

- 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

課題一：如何把分子組成一個系統？

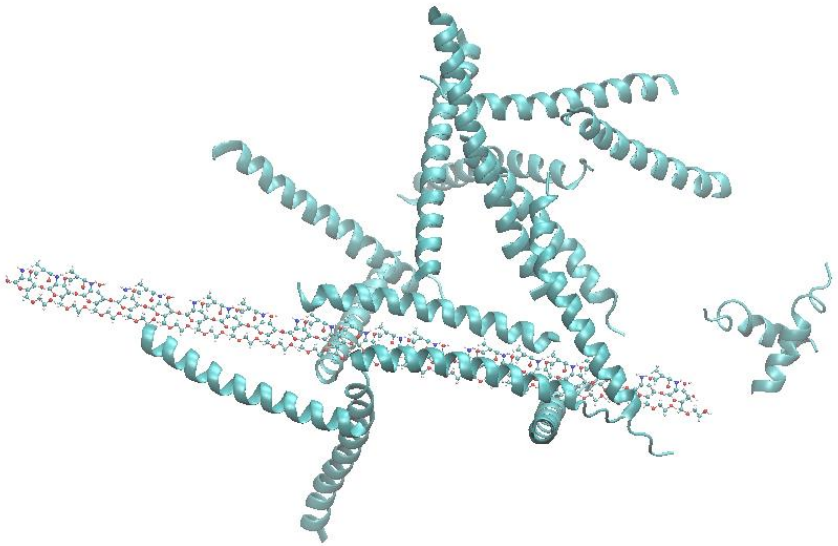
python model.py 1 1 10 8 100 0 0

1組KEMA(8條)+1條GCMA



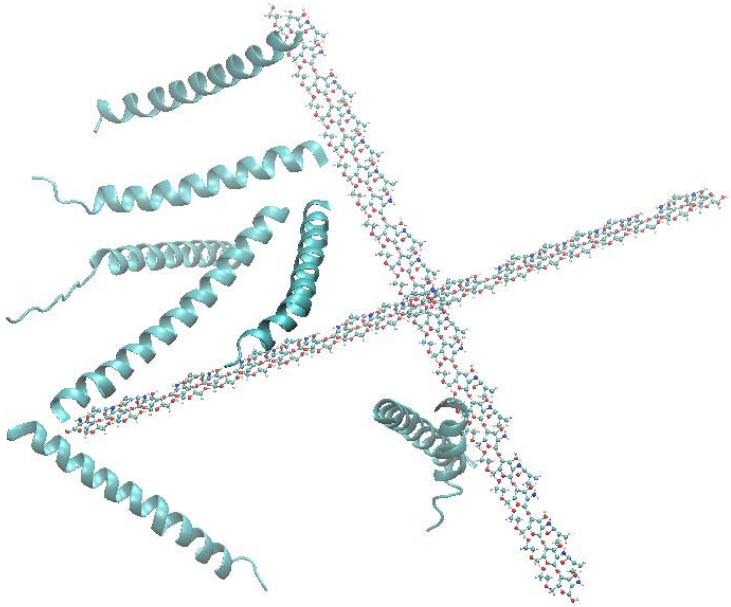
python model.py 2 1 10 8 100 0 0

2組KEMA(16條)+1條GCMA



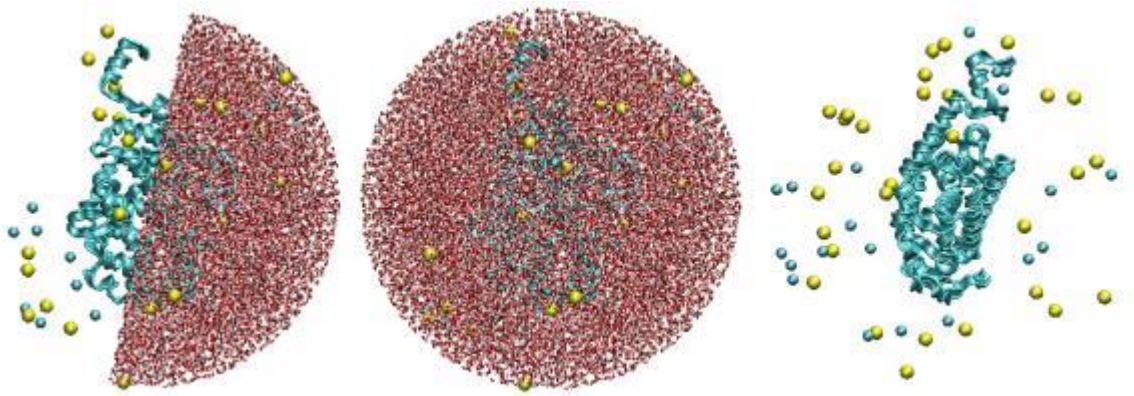
python model.py 1 2 10 8 100 0 0

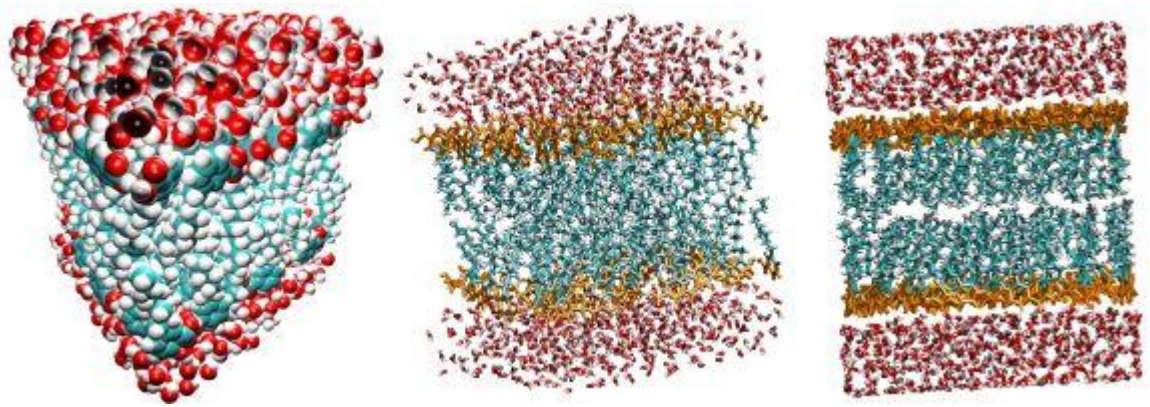
1組KEMA(8條)+2條GCMA



Packmol

- Download: [Packmol - Initial configurations for Molecular Dynamics (unicamp.br)]
- 把**PDB file**組成想要的樣子



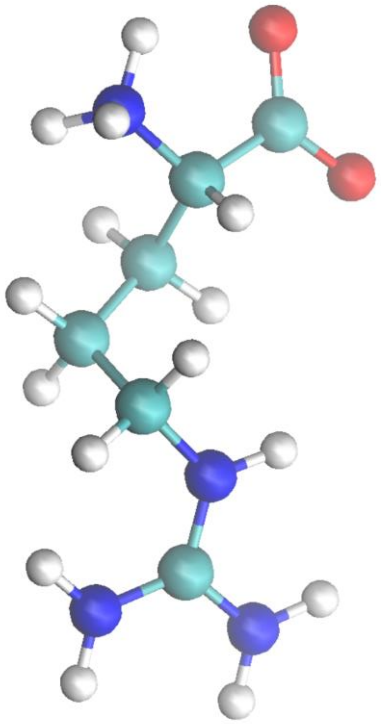


PDB file: Protein Data Bank：內含原子座標的文字檔

第幾顆原子　　胺基酸縮寫　　x,y,z座標

ATOM	819	N	LYS	98	7.807	-0.822	-11.638	1.00	0.00	A
ATOM	820	H	LYS	98	7.307	-0.460	-10.874	1.00	0.00	A
ATOM	821	CA	LYS	98	8.308	0.098	-12.642	1.00	0.00	A
ATOM	822	CB	LYS	98	7.138	0.725	-13.402	1.00	0.00	A
ATOM	823	CG	LYS	98	7.567	1.607	-14.566	1.00	0.00	A
ATOM	824	CD	LYS	98	6.366	2.334	-15.146	1.00	0.00	A
ATOM	825	CE	LYS	98	6.783	3.373	-16.182	1.00	0.00	A
ATOM	826	NZ	LYS	98	7.635	4.399	-15.602	1.00	0.00	A
ATOM	827	HZ1	LYS	98	7.791	5.167	-16.280	1.00	0.00	A
ATOM	828	HZ2	LYS	98	8.579	4.009	-15.328	1.00	0.00	A
ATOM	829	HZ3	LYS	98	7.206	4.789	-14.726	1.00	0.00	A
ATOM	830	C	LYS	98	9.171	1.164	-11.976	1.00	0.00	A
ATOM	831	O	LYS	98	10.385	1.168	-12.179	1.00	0.00	A

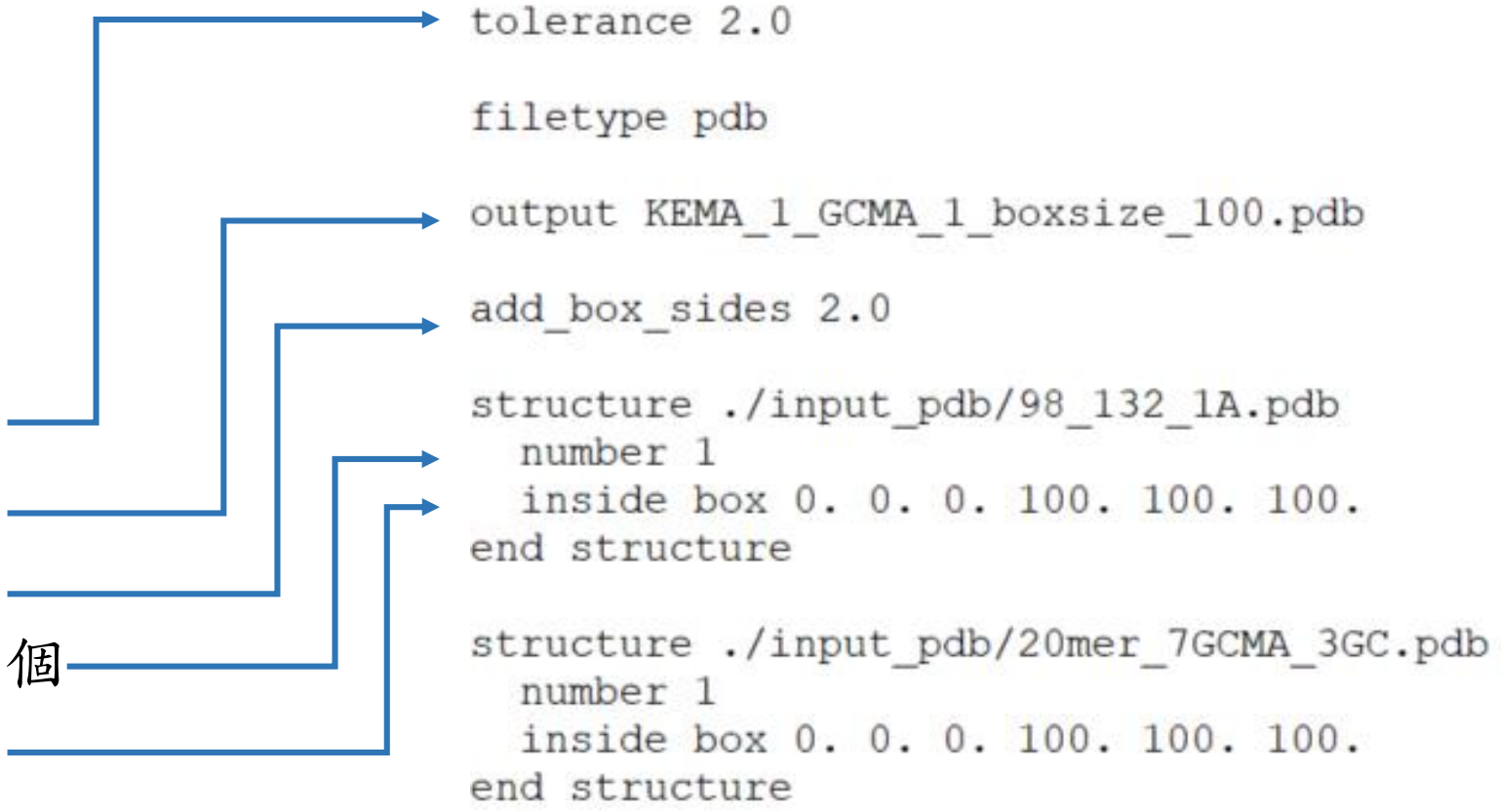
碳氫氧或其他　　第幾個胺基酸



實作: 1 KEMA+ 1 GCMA

- packmol < input.inp

- input.inp:
  - 每個分子之間距離多少
  - 輸出的檔案叫甚麼明子
  - 盒子外面要再擴大嗎
  - 要放哪些分子、分別幾個
  - 盒子多大



If Success:

```
 Initial approximation is a solution. Nothing to do.

 Solution written to file: KEMA_1_GCMA_1_boxsize_100.pdb

################################################################################

                            Success!
          Final objective function value: .39727E-02
          Maximum violation of target distance:   0.000000
          Maximum violation of the constraints: .18606E-02

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          Please cite this work if Packmol was useful:

        L. Martinez, R. Andrade, E. G. Birgin, J. M. Martinez,
      PACKMOL: A package for building initial configurations for
               molecular dynamics simulations.
       Journal of Computational Chemistry, 30:2157-2164,2009.

################################################################################

  Running time:    9.37500000E-02  seconds.

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```
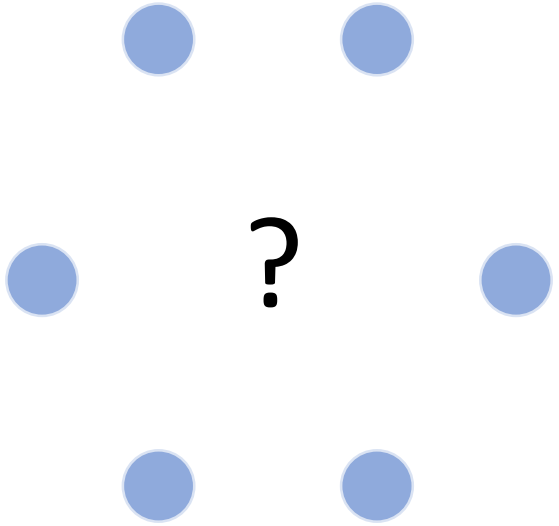
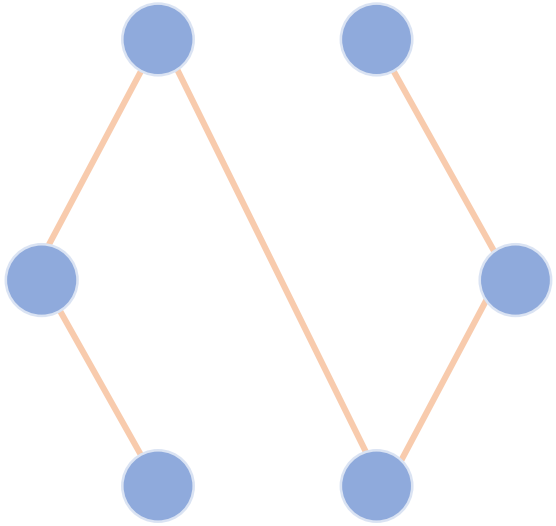
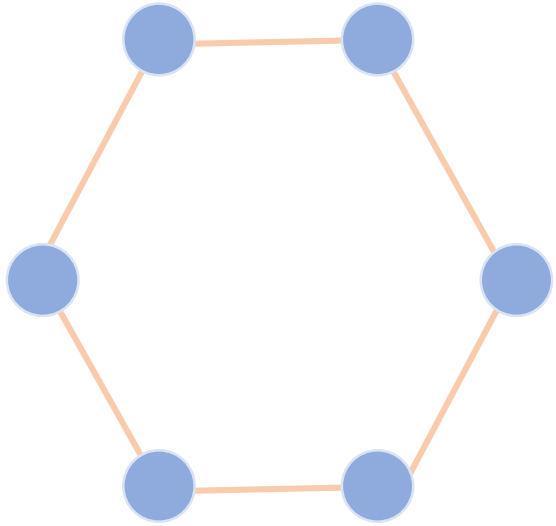

課題二：有原子座標，要如何連接他們？



From PDB only



Assumption 1



Assumption 2

PSF file: Protein Structure

- bond：預設兩個為一鍵結
- angle：預設3個為一個鍵角
- dihedral/improper：預設4個為一個二面角

```
1403 !NBOND: bonds
     1           5           2           1           3           1           4           1

2530 !NTHETA: angles
     1           5           6           1           5          23           2           1           5

3630 !NPHI: dihedrals
     1           5           7          10           1           5           7           8
```

PSF generator: VMD tool

課題三：如何加水？如何刪水？

- 加水：solvate
- 刪水：Python實作

課題四：如何加離子？

自動化目的

- 方便快速建模

目標

python model.py [nK] [nG] [boxsize] [nwater] [nNaCl]

->建立一個資料夾 名字是：KEMA_nK_GCMA_nG_water_nwater_NaCl_nNaCl

->把建好的模型存入該資料夾，最後輸出out.pdb, out.psf