Семинар 11: Использование пакета SOP-GPU

1 О программном пакете SOP-GPU

Пакет SOP-GPU, где SOP обозначает модель самоорганизующегося полимера (Self Organized Polymer), реализованная на графическом процессоре (GPU) – это научный программный пакет для проведения симуляций динамики Ланжевена процессов механического или температурного развертывания белков и механического сдавливания больших биомолекулярных систем в пределах экспериментальной временной шкалы от миллисекунды до секунды. Пакет SOP-GPU использует приближенное представление белков на основе C_α-углерода (coarse-grained) в сочетании с вычислительной мощностью современных графических процессоров (ГП).

2 Конфигурационный файл для эквилибрации системы

```
# GPU parameters
device 0 # GPU device system ID
block_size 256 # Block size on a GPU


# Topology limitations
max_covalent 4 # Maximum number of covalent bonds per residue
max_native 256 # Maximum number of native contacts per residue
max_pairs 256 # Maximum number of repulsive pairs per residue
```

```
max_possiblePairs 512 # Maximum number of repulsive pairs per residue


# Protein name
name ww_6 # Name, assigned to the protein
stage equil # Simulation stage

# Input system
topology  topologies/<name>.top # Topology file
coordinates     structures/<name>.pdb # Initial coordinates PDB
# (generated by 'sop-top')

# Force field
temperature 0.6  # System temperature in kcal/mol (0.6 ~ 300K)
zeta 50.0 # Water friction
R_limit 2.0 # FENE potential parameter (R0)
kspring_cov 20.0 # Covalent spring coeffitient
a 3.8 # Repulsive LJ radius
el 1.0 # Repulsive LJ Energy scale

# Verlet list generation
pairs_cutoff 20.0 # Verlet list cut-off
pairs_freq 1000 # Frequency of generating Verlet list

# Simulations
numsteps 1000000 # Total number of steps
timestep 0.08 # Timestep
seed 1119726 # Random seed (actual seed is constructed from this and run number)
```

```
firstrun 1 # Run number (i.e. number of trajectory)
runnum 100 # Number of trajectories to run simultaneously

# Output
reffilename  <name>.ref.pdb # Referance pdb to load into VMD
outputtiming 10000 # Frequency of printing out data
outputname dat/<name>_<run>_<stage>.dat # Filename mask for energy file
dcdfreq 10000 # Frequency of saving output and
# coordinates into dcd file
DCDfile dcd/<name>_<run>_<stage>.dcd # Filename mask for dcd file
restartfreq 100000 # Frequency of saving restart
# coordinates and parameters
restartname  output/<name>_<run>_restart # Name of restart files (extensions
# .pdb and .conf will be added)
finalcoord structures/<name>_<run>_<stage>_final.pdb # Filename mask for final
# coordinates file
```

3 Конфигурационный файл для силовой денатурации

```
# GPU parameters
device 0 # GPU device system ID
block_size 256 # Block size on a GPU

# Topology limitations
max_covalent 4 # Maximum number of covalent bonds per residue
max_native 256 # Maximum number of native contacts per residue
```

```
max_pairs 256 # Maximum number of repulsive pairs per residue
max_possiblePairs 512 # Maximum number of repulsive pairs per residue

# Protein name
name ww_6 # Name, assigned to the protein
stage pull # Simulation stage

# Input system
topology  topologies/<name>.top # Topology file
coordinates     structures/<name>_<run>_equil_final.pdb # Initial coordinates
# (final coordinates of equilibrium simulations)

# Force field
temperature 0.6  # System temperature in kcal/mol (0.6 ~ 300K)
zeta 50.0 # Water friction
R_limit 2.0 # FENE potential parameter (R0)
kspring_cov 20.0 # Covalent spring coeffitient
a 3.8 # Repulsive LJ radius
el 1.0 # Repulsive LJ Energy scale

# Verlet list generation
pairs_cutoff 20.0 # Verlet list cut-off
pairs_freq 1000 # Frequency of generating Verlet list

# Pulling
fixed_beads 1 # Number of fixed beads.
fixed1 0 # First fixed bead (to fix more beads, add 'fixed2',
# 'fixed3'... and change the 'fixed_beads')
```

```
pulled_beads  1 # Number of beads being pulled
pulled1 231 # Fist pulled bead (same story as with fixed)
deltax 0.0005 # Pulling speed in A per pairs_freq
k_trans 0.05 # Cantilever spring constant
pullDirection endToEnd # Direction of pulling
pullOutput pull/<name>_<run>_<stage>.dat # Pulling output file

# End to end
fixedEnd <fixed1># First end to compute end-to-end distance
pulledEnd <pulled1># Second end to compute end-to-end distance

# Simulations
numsteps 3000000000 # Total number of steps
timestep 0.08 # Timestep
seed 1119726 # Random seed (actual seed is
# constructed from this and run number)
firstrun 1 # Run number (i.e. number of trajectory)
runnum 100 # Number of trajectories to run simultaneously

# Output
reffilename  <name>.ref.pdb # Referance pdb to load into VMD
outputtiming 10000 # Frequency of printing out data
outputname dat/<name>_<run>_<stage>.dat # Filename mask for energy file
dcdfreq 10000 # Frequency of saving output and
# coordinates into dcd file
DCDfile dcd/<name>_<run>_<stage>.dcd # Filename mask for dcd file
restartfreq 100000 # Frequency of saving restart
# coordinates and parameters
```

```
restartname  output/<name>_<run>_restart # Name of restart files
# (extensions will be added)
finalcoord structures/<name>_<run>_<stage>_final.pdb # Filename mask for
# final coordinates file
```