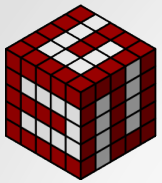

GENESIS

Generalized-ensemble simulation system

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GENESIS tutorial 3
REMD

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II. How to do other types of REMD?

- ✓ Pressure REMD
- ✓ Surface-tension REMD
- ✓ Hamiltonian REMD (Replica-exchange umbrella sampling)
- ✓ 2D-REMD (T-REMD/H-REMD)

Basic usage

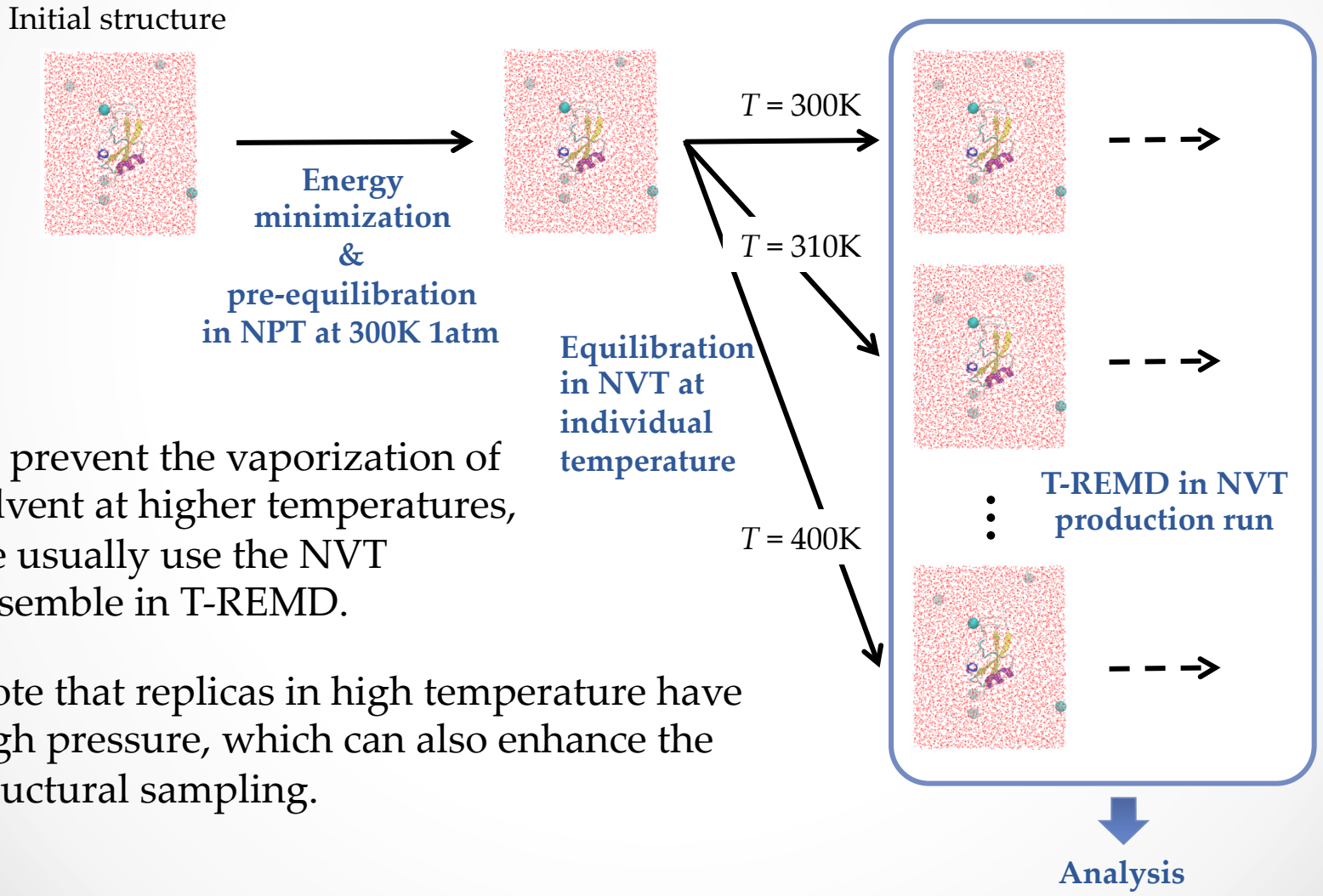
In this tutorial, we use not only `spdyn` but also `analysis tools` in the install directory.

```
# enter the login node
$ ssh -l userXX riken.eastus.cloudapp.azure.com

# enter a computational node (n001-n017)
$ ssh nXXX

# Run spdyn using hybrid MPI/OpenMP
# Note that each node has 24 CPU cores
$ export OMP_NUM_THREADS=3
$ mpirun –np 8 /home2/data/genesis/bin.CPU.dp/spdyn INP

# Run analysis tools (do not use mpirun)
$ /home2/data/genesis/bin.CPU.dp/some_analysis INP
```

Part I

Temperature REMD simulation of alanine tripeptide in water

Overall flow of T-REMD simulations

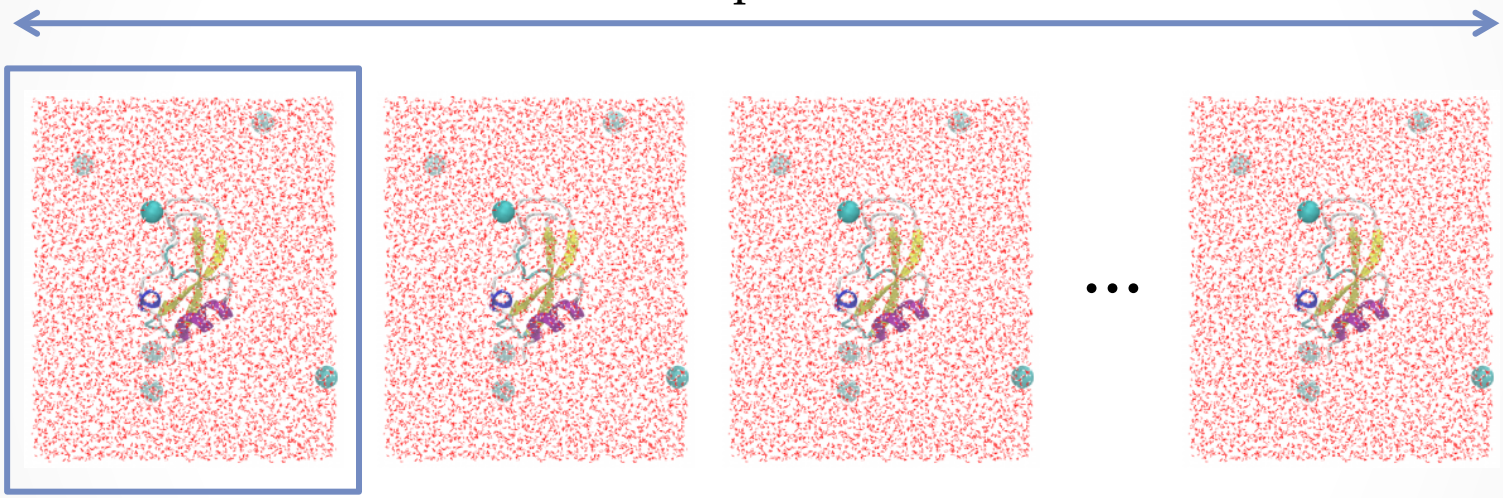


- To prevent the vaporization of solvent at higher temperatures, we usually use the NVT ensemble in T-REMD.
- Note that replicas in high temperature have high pressure, which can also enhance the structural sampling.

How many CPU cores we need?

Now, we want to use *m* CPU cores in one replica and *n* replicas in total.

n replicas



m CPU cores
= # of MPI processors × # of OpenMP threads

We need *m* × *n* CPU cores in total to perform REMD in GENESIS

In this tutorial, we use **6 replicas** due to limitation of the available CPUs.
(1 replica = 4 CPUs with 1 OpenMP thread)

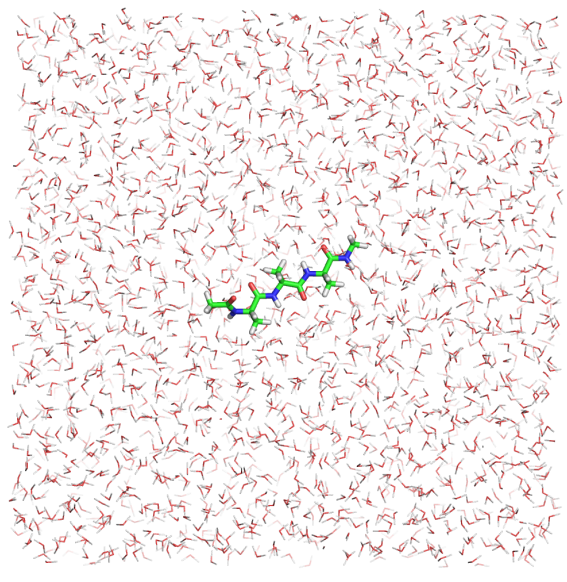
Preparation

```
$ cd Tutorial_3
$ ls
Part1 Part2

$ cd Part1
$ ls
0_setup       2_pre-equilibration  4_production
1_minimize    3_equilibration      5_analysis
```

In Part I, we will change the directory
from 0_setup to 5_analysis step by step

Step0. Preparation of the initial structure

Our target system: Alanine tripeptide in TIP3P water



Number of protein atoms: 42
Number of water molecules: 9250

We use CHARMM C36 force field

```
# change directory
$ cd 0_setup

$ ls
top_all36_prot.rtf      wbox.pdb
par_all36_prot.prm      wbox.psf
toppar_water_ions.str
```

PDB, PSF, Parameter and topology files are already prepared.

Step1. Energy minimization

We carry out 5,000-steps energy minimization with the steepest descent method, where the positional restraints are applied on the protein heavy atoms.

```
[INPUT]
topfile = ../0_setup/top_all36_prot.rtf     # topology file
parfile = ../0_setup/par_all36_prot.prm     # parameter file
strfile = ../0_setup/toppar_water_ions.str  # stream file
psffile = ../0_setup/wbox.psf               # protein structure file
pdbfile = ../0_setup/wbox.pdb               # PDB file
reffile = ../0_setup/wbox.pdb               # PDB file for restraints

[OUTPUT]
dcdfile    = step1.dcd      # DCD trajectory file
rstfile    = step1.rst      # restart file

[MINIMIZE]
method           = SD       # Steepest descent method
nsteps           = 5000     # number of minimization steps
eneout_period    =  100     # energy output period
crdout_period    =  100     # coordinates output period
rstout_period    = 5000     # restart output period

[SELECTION]
group1           = sid:PROA and heavy

[RESTRAINTS]
nfunctions       = 1        # number of functions
function1        = POSI     # restraint function type
direction1       = ALL      # direction
constant1        = 1.0      # force constant
select_index1    = 1        # restrained groups
```

Step2. Pre-equilibration

NVT MD with posres ➔ NPT MD with posres ➔ NPT MD without posres

```
[INPUT]
rstfile = ../1_minimize/step1.rst

[OUTPUT]
dcdfile   = step2.1.dcd
rstfile   = step2.1.rst

[DYNAMICS]
integrator     = LEAP
nsteps         =  5000

[ENSEMBLE]
ensemble       = NVT
tpcontrol      = LANGEVIN
temperature    = 300.00

[SELECTION]
group1         = sid:PROA and heavy

[RESTRAINTS]
nfunctions     = 1
function1      = POSI
direction1     = ALL
constant1      = 1.0
select_index1 = 1
```

```
[INPUT]
rstfile = step2.1.rst

[OUTPUT]
dcdfile   = step2.2.dcd
rstfile   = step2.2.rst

[DYNAMICS]
integrator     = LEAP
nsteps         =  5000

[ENSEMBLE]
ensemble       = NPT
tpcontrol      = LANGEVIN
temperature    = 300.00
pressure       = 1.0
isotropy       = ISO

[SELECTION]
group1         = sid:PROA and heavy

[RESTRAINTS]
nfunctions     = 1
function1      = POSI
direction1     = ALL
constant1      = 1.0
select_index1 = 1
```

```
[INPUT]
rstfile = step2.2.rst

[OUTPUT]
dcdfile   = step2.3.dcd
rstfile   = step2.3.rst

[DYNAMICS]
integrator     = LEAP
nsteps         =  5000

[ENSEMBLE]
ensemble       = NPT
tpcontrol      = LANGEVIN
temperature    = 300.00
pressure       = 1.0
isotropy       = ISO
```

We gradually equilibrate the system by vanishing the restrains and switching the ensembles.

Step3. Equilibration at each temperature

At Step3, we can use the REMD module in GENESIS, where **REMD without replica exchange** is performed.

```
[INPUT]
rstfile = ../2_pre-equilibration/step2.3.rst

[OUTPUT]
dcdfile  = step3_rep{}.dcd
rstfile  = step3_rep{}.rst
remfile  = step3_rep{}.rem
logfile  = step3_rep{}.log

[ENERGY]
forcefield        = CHARMM
electrostatic     = PME
switchdist        = 10.0
cutoffdist        = 12.0
pairlistdist      = 13.5

[DYNAMICS]
integrator        = LEAP
nsteps            = 5000
timestep          = 0.002
eneout_period     =    10
crdout_period     =   100
rstout_period     =  5000

[CONSTRAINTS]
rigid_bond        = YES     # use SHAKE/SETTLE
```

Replica index is automatically inserted into {} of the output filename.

```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00

[REMD]
dimension         =
exchange_period   = 0  # no parameter exchange
type1             =
nreplica1         =
parameters1       =
```

- In GENESIS, REMD can be achieved by just adding the [REMD] section in the control file for a conventional MD.

Let's edit the [REMD] section!

Prepare replica temperatures

We prepare temperatures to be used in REMD by utilizing the temperature generator server (http://folding.bmc.uu.se/remd/)

Exchange probability of 0.2-0.3 is supposed to realize efficient structural sampling in REMD.

Exchange probability:	0.2	Tolerance:	1e-4
Lower temperature limit:	300	Upper temperature limit:	500
Number of water molecules:	9250	Constraints in water:	Rigid
Number of protein atoms:	42	Constraints in the protein:	Bonds to hydrogens only
Hydrogens in protein:	All H	Virtual sites in protein:	None
Simulation type:	NPT		

Submit Clear

We use SETTLE and SHAKE for bond constraint

The estimated temperatures are
300.00, 301.81, …, …, 501.46 (90 replicas!)

➔ **We select first 6 temperatures in this tutorial.**

Control file for equilibration

```
[INPUT]
rstfile = ../2_pre-equilibration/step2.3.rst

[OUTPUT]
dcdfile   = step3_rep{}.dcd
rstfile   = step3_rep{}.rst
remfile   = step3_rep{}.rem
logfile   = step3_rep{}.log

[ENERGY]
forcefield        = CHARMM
electrostatic     = PME
switchdist        = 10.0
cutoffdist        = 12.0
pairlistdist      = 13.5

[DYNAMICS]
integrator        = LEAP
nsteps            = 5000
timestep          = 0.002
eneout_period     =    10
crdout_period     =   100
rstout_period     =  5000

[CONSTRAINTS]
rigid_bond        = YES
```

```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00

[REMD]
dimension         = 1
exchange_period   = 0   # no parameter exchange
type1             = temperature
nreplica1         = 6
parameters1       = 300.00 302.53 305.09  ¥
                    307.65 310.24 312.85
```

Submitting a job

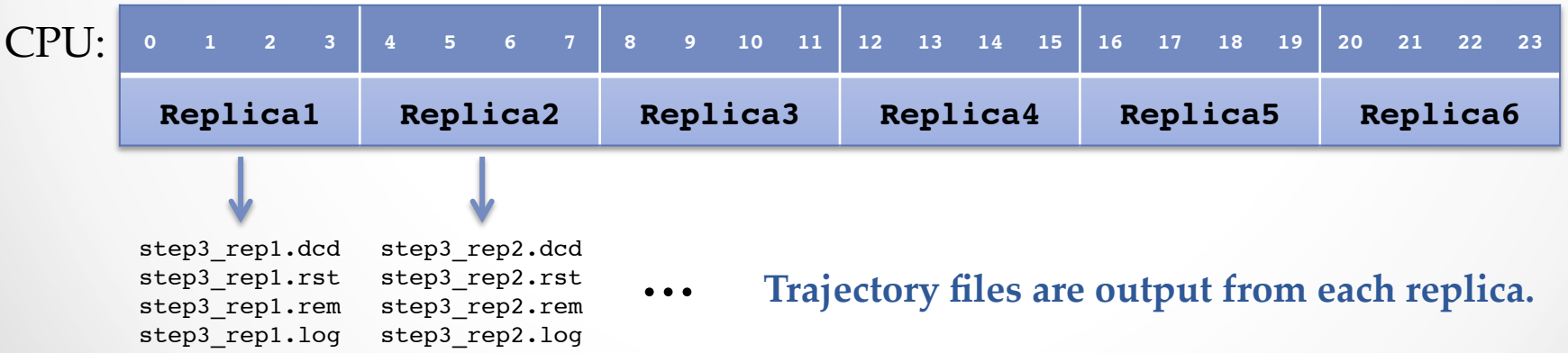
In GENESIS, number of CPU cores per replica is automatically determined by dividing total number of CPU cores by total number of replicas.

$$N_{\text{CPUs/replica}} = N_{\text{total CPUs}} / N_{\text{replicas}}$$

specified by a command

specified in the control file

```
$ export OMP_NUM_THREADS=1
$ mpirun –np 24 /home2/data/genesis/bin.CPU.dp/spdyn step3.inp
```



Trajectory files are output from each replica.

Let's submit a job!

Step4. Production run of REMD

To perform a production run, we just modify the previous control file for the equilibration run.

```
[INPUT]
rstfile = ../3_equilibration/step3_rep{}.rst

[OUTPUT]
dcdfile   = step4_rep{}.dcd
rstfile   = step4_rep{}.rst
remfile   = step4_rep{}.rem
logfile   = step4_rep{}.log

[ENERGY]
forcefield        = CHARMM
electrostatic     = PME
switchdist        = 10.0
cutoffdist        = 12.0
pairlistdist      = 13.5

[DYNAMICS]
integrator        = LEAP
nsteps            = 5000
timestep          = 0.002
eneout_period     =    10
crdout_period     =   100
rstout_period     =  5000

[CONSTRAINTS]
rigid_bond        = YES
```

```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00

[REMD]
dimension         = 1
exchange_period   = 500
type1             = temperature
nreplica1         = 6
parameters1       = 300.00 302.53 305.09  ¥
                    307.65 310.24 312.85
```

In this example, replica exchange is attempted every 500 steps.

Let's edit [REMD] section and submit a production job!

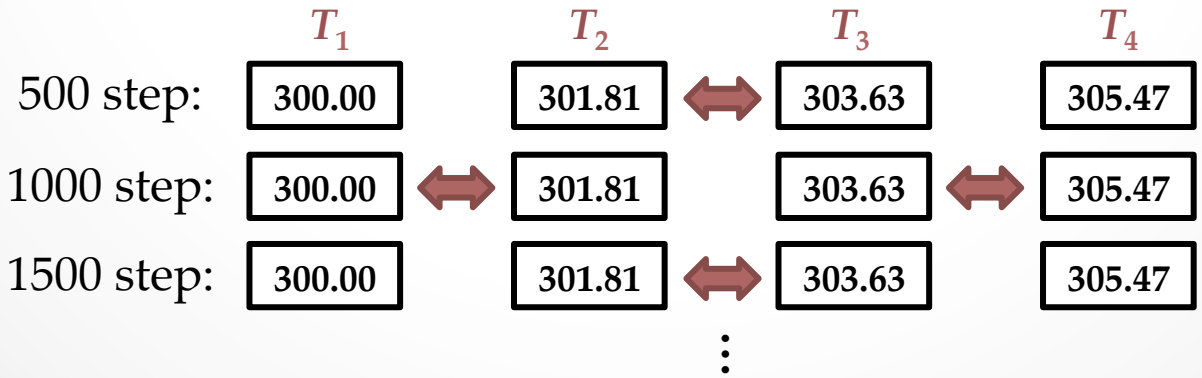
log information

```
REMD> Step:         500   Dimension:     1   ExchangePattern:     2
  Replica      ExchangeTrial              AcceptanceRatio       Before        After
        1           1 >     0   N            0 /         0     300.000      300.000
        2           2 >     3   A            1 /         1     301.810      303.630
        3           3 >     2   A            1 /         1     303.630      301.810
        4           4 >     0   N            0 /         0     305.470      305.470
Parameter     :    300.000   303.630   301.810   305.470
RepIDtoParmID:           1         3         2         4
ParmIDtoRepID:           1         3         2         4
```

T_2-T_3, T_4-T_5, T_6-T_7,… pairs

```
REMD> Step:        1000   Dimension:     1   ExchangePattern:     1
  Replica      ExchangeTrial              AcceptanceRatio       Before        After
        1           1 >     2   A            1 /         1     300.000      301.810
        2           3 >     4   R            0 /         1     303.630      303.630
        3           2 >     1   A            1 /         1     301.810      300.000
        4           4 >     3   R            0 /         1     305.470      305.470
Parameter     :    301.810   303.630   300.000   305.470
RepIDtoParmID:           2         3         1         4
ParmIDtoRepID:           3         1         2         4
```

T_1-T_2, T_3-T_4, T_5-T_6,… pairs



log information

```
REMD> Step:         500   Dimension:     1   ExchangePattern:     2
  Replica      ExchangeTrial                 AcceptanceRatio       Before        After
        1          1 >      0   N              0 /          0     300.000      300.000
        2          2 >      3   A              1 /          1     301.810      303.630
        3          3 >      2   A              1 /          1     303.630      301.810
        4          4 >      0   N              0 /          0     305.470      305.470
Parameter    :    300.000   303.630   301.810   305.470
RepIDtoParmID:          1         3         2         4
ParmIDtoRepID:          1         3         2         4
```

```
REMD> Step:        1000   Dimension:     1   ExchangePattern:     1
  Replica      ExchangeTrial                 AcceptanceRatio       Before        After
        1          1 >      2   A              1 /          1     300.000      301.810
        2          3 >      4   R              0 /          1     303.630      303.630
        3          2 >      1   A              1 /          1     301.810      300.000
        4          4 >      3   R              0 /          1     305.470      305.470
Parameter    :    301.810   303.630   300.000   305.470
RepIDtoParmID:          2         3         1         4
ParmIDtoRepID:          3         1         2         4
```

After long REMD run, “Acceptance ratio” will get close to the value that was specified in the REMD temperature generator.

log information

```
REMD> Step:         500   Dimension:     1   ExchangePattern:     2
  Replica      ExchangeTrial              AcceptanceRatio       Before        After
        1          1 >      0   N            0 /          0     300.000      300.000
        2          2 >      3   A            1 /          1     301.810      303.630
        3          3 >      2   A            1 /          1     303.630      301.810
        4          4 >      0   N            0 /          0     305.470      305.470
Parameter     :    300.000   303.630   301.810   305.470
RepIDtoParmID:           1         3         2         4
ParmIDtoRepID:           1         3         2         4
```

Permutation function

```
REMD> Step:        1000   Dimension:     1   ExchangePattern:     1
  Replica      ExchangeTrial              AcceptanceRatio       Before        After
        1          1 >      2   A            1 /          1     300.000      301.810
        2          3 >      4   R            0 /          1     303.630      303.630
        3          2 >      1   A            1 /          1     301.810      300.000
        4          4 >      3   R            0 /          1     305.470      305.470
Parameter     :    301.810   303.630   300.000   305.470
RepIDtoParmID:           2         3         1         4
ParmIDtoRepID:           3         1         2         4
```

$f(T_1) = \text{Replica3}$ $\qquad$ $f^{-1}(\text{Replica3}) = T_1$

Eq (5) in the Sugita & Okamoto paper:
Chem. Phys. Lett., 314 (1999) 141–151

$$\begin{cases} i = i(m) & \equiv f(m), \\ m = m(i) & \equiv f^{-1}(i), \end{cases}$$

Analyze log information 1

Time courses of the replica index which has T_1 = 300K:

```
$ cd ~/Part1/5_analysis/1_replica_index

$ grep "ParmIDtoRepID:" ../../4_production/log > replica_id.log

$ gnuplot
gnuplot> set terminal x11
gnuplot> plot [][0:7] 'replica_id.log' u 0:2
```

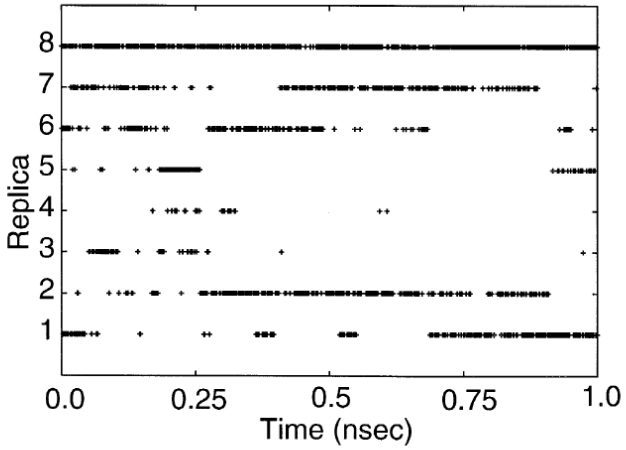


Fig. 1. Time series of replica exchange at T = 200 K.

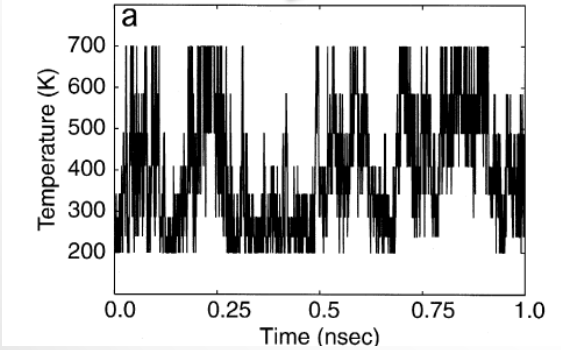
`gnuplot` is installed in the login node only! To display the plot data by gnuplot, login the node with –X option.

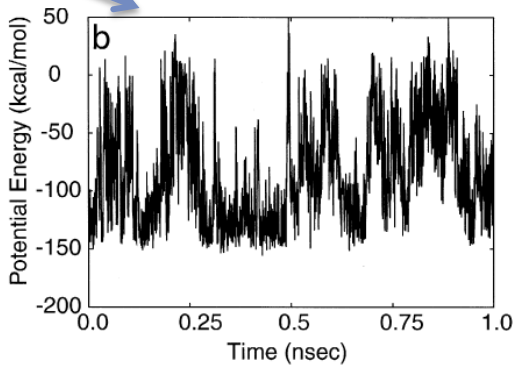
(ref) Sugita & Okamoto
Chem. Phys. Lett., 314 (1999) 141–151

Analyze log information 2

Time courses of the temperature and potential energy in Replica 1

```
$ cd ~/Part1/5_analysis/2_temperature_energy

$ grep "Parameter    :" ../../4_production/log > parameter.log

$ grep “INFO:” ../../4_production/step4_rep1.log > rep1.log

$ gnuplot
gnuplot> set terminal x11
gnuplot> plot ‘parameter.log’ u 0:3 with lines
gnuplot> plot ‘rep1.log’ u 3:5 with lines
```





(ref) Sugita & Okamoto
Chem. Phys. Lett., 314 (1999) 141–151

Output files

In the REMD simulations, the following files are generated from each replica.

- ✓ `step4_repX.dcd:` Coordinates trajectory
- ✓ `step4_repX.rem:` Parameter index
- ✓ `step4_repX.log:` Energy log in each replica
- ✓ `step4_repX.rst:` Restart file including the last coordinates, velocities, replica parameter index, etc.

Note that dcdfile and energy logfile contain "mixed coordinates and energies at different temperatures"

➔ We need to sort the information by temperature to analyze the trajectories at the focusing temperature.

Sorting the coordinates (4 replicas case)

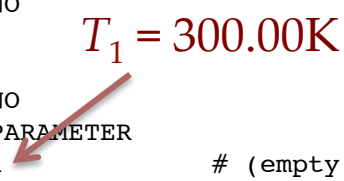
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
Replica 1	dcdfile			T_1					T_2					T_3						T_4					T_4	
	remfile	1				2					3					4					4						3
Replica 2	dcdfile			T_2					T_1					T_1					T_2					T_3	
	remfile	2				1					1					2					3						4
Replica 3	dcdfile			T_3					T_4					T_4					T_3					T_2	
	remfile	3				4					4					3					2						1
Replica 4	dcdfile			T_4					T_3					T_2					T_1					T_1	
	remfile	4				3					2					1					1						2

Sorting by T_1

		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
	dcdfile			T_1					T_1					T_1						T_1					T_1	

Convert REMD trajectory

```
[INPUT]
psffile = ../0_setup/wbox.psf                 # protein structure file
reffile = ../0_setup/wbox.pdb                 # PDB file
dcdfile = ../4_production/step4_rep{}.dcd     # DCD trajectory file
remfile = ../4_production/step4_rep{}.rem     # replica exchange ID file

[OUTPUT]
pdbfile = step4.pdb                           # output PDB file
trjfile = step4_parm{}.dcd                    # output trajectory file

[SELECTION]
group1  = all

[FITTING]
fitting_method = NO

[OPTION]
check_only     = NO
convert_type   = PARAMETER
convert_ids    = 1              # (empty = all)
dcd_md_period  = 100            # coordinates output period
trjout_format  = DCD            # (PDB/DCD)
trjout_type    = COOR+BOX       # (COOR/COOR+BOX)
trjout_atom    = 1              # output atom selection
pbc_correct    = NO             # (wrap molecules)
```




```
$ cd ~/Part1/5_analysis/3_remd_convert
$ /home2/data/genesis/bin.CPU.dp/remd_convert INP > log
```

Further analysis

After the trajectory is converted, we analyze the trajectories in more details, for example,

- End-to-end distance of the peptide
- Dihedral angle of the backbone atoms
- Principal component analysis
- Free energy profile

Part II

Other REMD simulations

REMD functions in GENESIS

In Part I,
we learned how to perform Temperature REMD in the NVT ensemble

GENESIS can employ various types of REMD methods:

- Temperature REMD in the NPT ensemble
- Pressure REMD in the NPT ensemble
- Surface-tension REMD in the NPγT ensemble (for biomembranes)
- Hamiltonian REMD (restraint potential exchange)
- 2D-REMD (T-REMD/P-REMD)
- 2D-REMD (T-REMD/H-REMD)

In Part II, we learn how to edit the control file for various type of REMD in GENESIS.

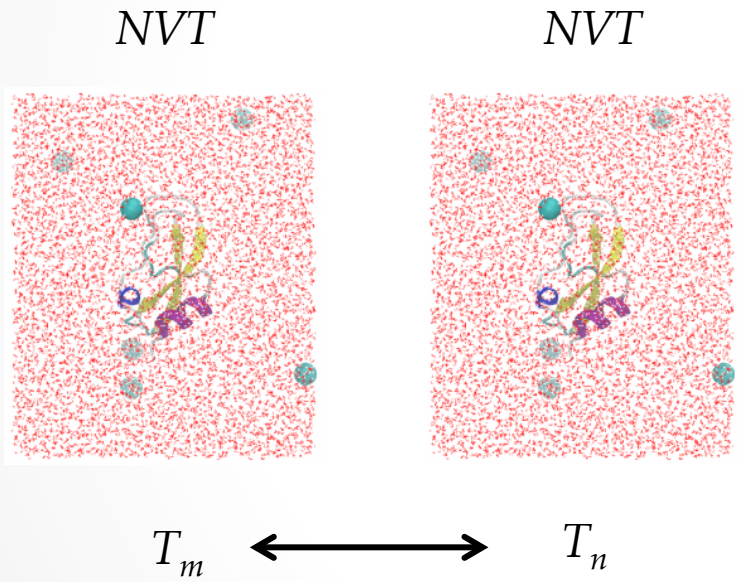
Preparation

```
$ cd Tutorial_3
$ ls
Part1 Part2

$ cd Part2
$ ls
Example     Practice2   Practice4   Practice6
Practice1   Practice3   Practice5   Practice7
```

In Part II, we will change the directory
from Practice1 to Practice7 step by step.
(Difficulty is gradually increased!)

Example

Temperature REMD in the NVT ensemble (Tutorial I)
using 4 replicas with T = 300, 310, 320, 330K

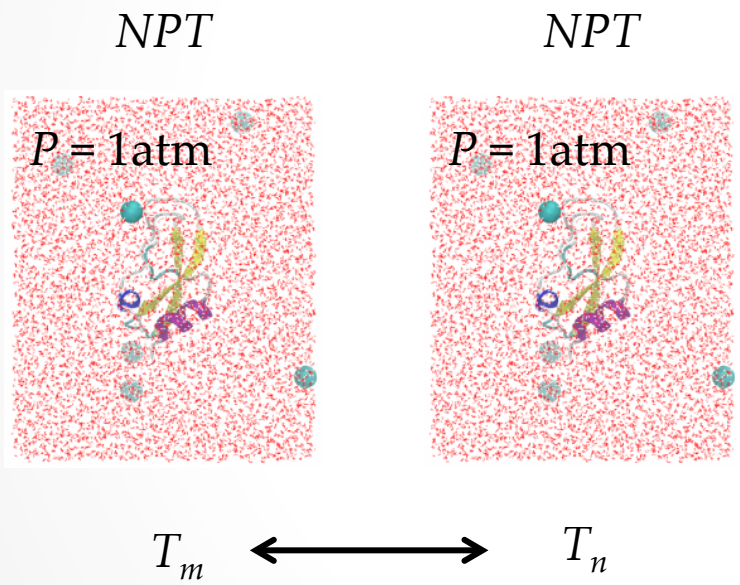



```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN

[REMD]
dimension         = 1
exchange_period   = 500
type1             = temperature
nreplica1         = 4
parameters1       = 300.0 310.0 320.0 330.0
```

Level: ★☆☆☆☆

Practice 1

Temperature REMD in the NPT ensemble at P = 1atm
(isotropic pressure coupling) using 4 replicas with T = 300, 310, 320, 330K




```
[ENSEMBLE]
ensemble          = ____
tpcontrol         = LANGEVIN
________          = _
________          = ___

[REMD]
dimension         = 1
exchange_period   = 1000
type1             = temperature
nreplica1         = 4
parameters1       = 300.0 310.0 320.0 330.0
```

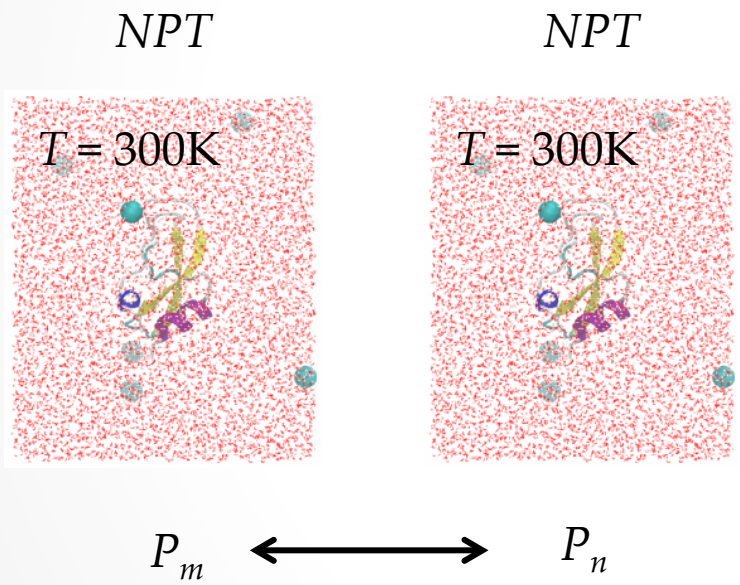
Hints:

- [ENSEMBLE] section is modified
- Step2.2 and 2.3 in Part I
- See User manual p.42-44

Level: ★★☆☆☆

Practice 2

Pressure REMD in the NPT ensemble at T = 300K
(isotropic pressure coupling) using 4 replicas with P = 1, 10, 100, 1000atm




```
[ENSEMBLE]
ensemble          = ___
tpcontrol         = LANGEVIN
___________       = ___
________          = ___

[REMD]
dimension         = 1
exchange_period   = 500
type1             = _________
nreplica1         = 4
parameters1       = ___ ___ ___ ___
```

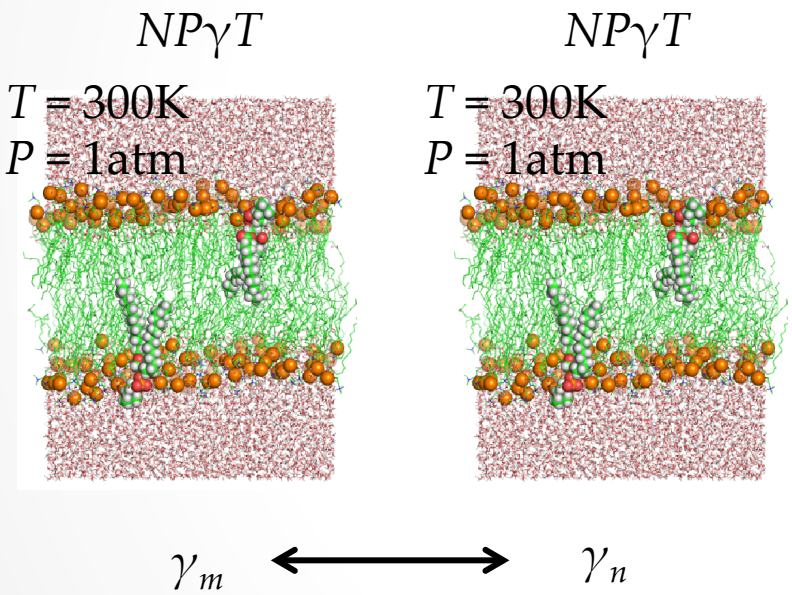
Hints:

- [ENSEMBLE] and [REMD] sections should be modified
- Step2.2 and 2.3 in Part I
- See User manual P.54

Level: ★★☆☆☆

Practice 3

Surface-tension REMD in the NPγT ensemble at T = 300K and P_n = 1atm (semi-isotropic pressure coupling) using 5 replicas with γ = -10, -5, 0, 5, 10dyn/cm




```
[ENSEMBLE]
ensemble          = ____
tpcontrol         = LANGEVIN
________          = ___
________          = _
________          = ________

[REMD]
dimension         = 1
exchange_period   = 500
type1             = _____
nreplica1         = 5
parameters1       = ___ ___ ___ ___ ___
```

Level: ★★★☆☆

Practice 4

Two-dimensional T-REMD/P-REMD

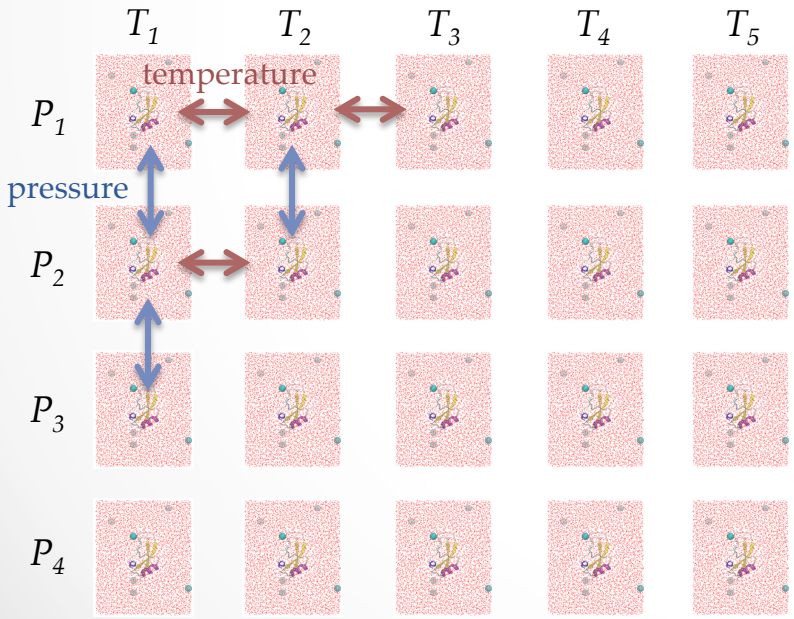
Temperature:

300, 310, 320, 330, 340K (5 replicas)

Pressure:

1, 10, 100, 1000atm (4 replicas) isotropic pressure coupling

5 x 4 = 20 replicas in total

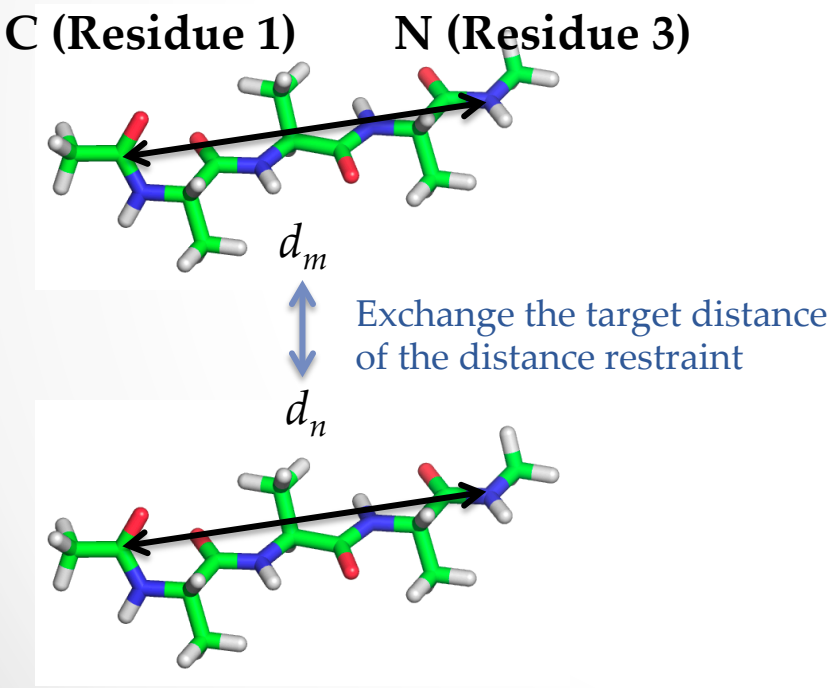



```
[ENSEMBLE]
ensemble          = ____
tpcontrol         = LANGEVIN

[REMD]
dimension         =
exchange_period   = 500
type1             =
nreplica1         =
parameters1       =

?
```

Level: ★★★★☆

Practice 5

Restraint-potential REMD (REUS) in the NVT ensemble using 4 replicas, where we apply distance restraints (3, 4, 5, and 6 Å with k = 10 kcal/mol/Å^2) between C atom in Residue 1 and N atom in Residue 3




```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00

[SELECTION]
group1            = an:__ and _________
group2            = an:__ and _________

[RESTRAINTS]
nfunctions        = 1
function1         = DIST
select_index1     = 1 2
constant1         = ___ ___ ___ ___
reference1        = ___ ___ ___ ___

[REMD]
dimension         = 1
exchange_period   = 500
type1             = ____________
nreplica1         = 4
rest_function1    = _
```

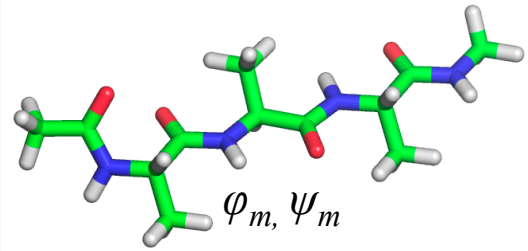
Common to conventional MD with distance restraint

Level: ★★★★★

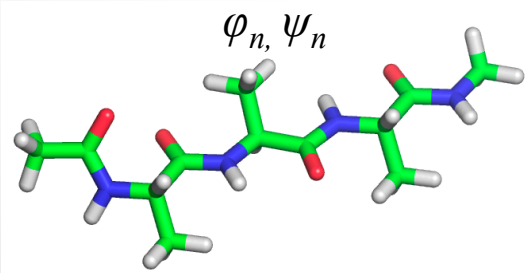
Practice 6

Restraint-potential REMD (REUS) in the NVT ensemble using 4 replicas, where we apply dihedral angle restraints on φ and ψ of Residue 2
(φ,ψ) = (180, 180), (170, 170), (160, 160), (150, 150) with k = 10 kcal/mol/Å^2

φ =C-N-CA-C
ψ =N-CA-C-N



Exchange the target two dihedral angles




```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00

[SELECTION]
group1            = an:__ and ________
  :                         :

[RESTRAINTS]
nfunctions        = _
function1         = ____
select_index1     = 1 2 3 4
constant1         = ___ ___ ___ ___
reference1        = ___ ___ ___ ___
function2         = ____
select_index2     = 2 3 4 5
constant2         = ___ ___ ___ ___
reference2        = ___ ___ ___ ___

[REMD]
dimension         = 1
exchange_period   = 500
type1             = ___________
nreplica1         = 4
rest_function1    = _ _
```

Level: ★★★★★

Practice 7

Two-dimensional T-REMD/REUS in the NVT ensemble

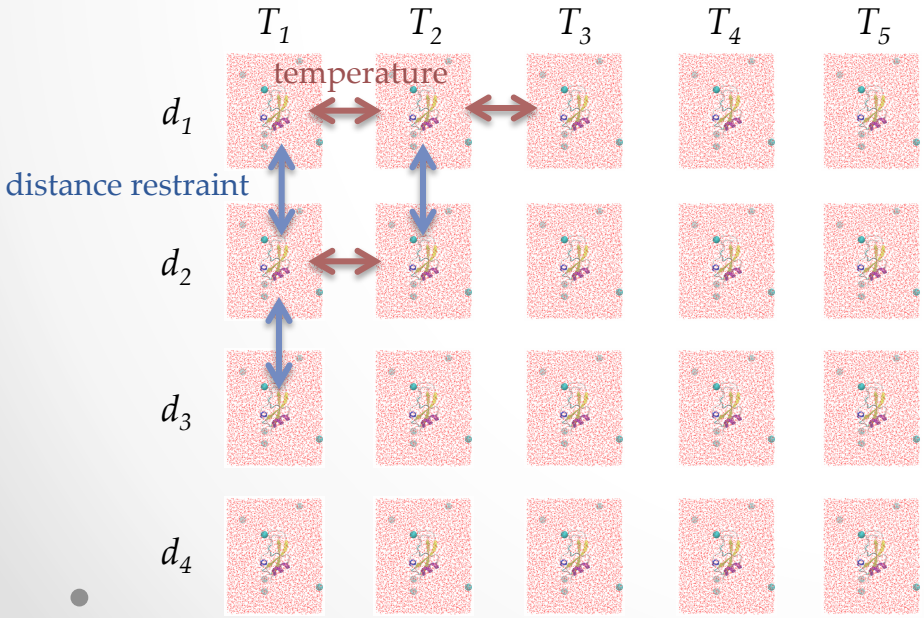
Temperature:

300, 310, 320, 330, 340K

Restraints:

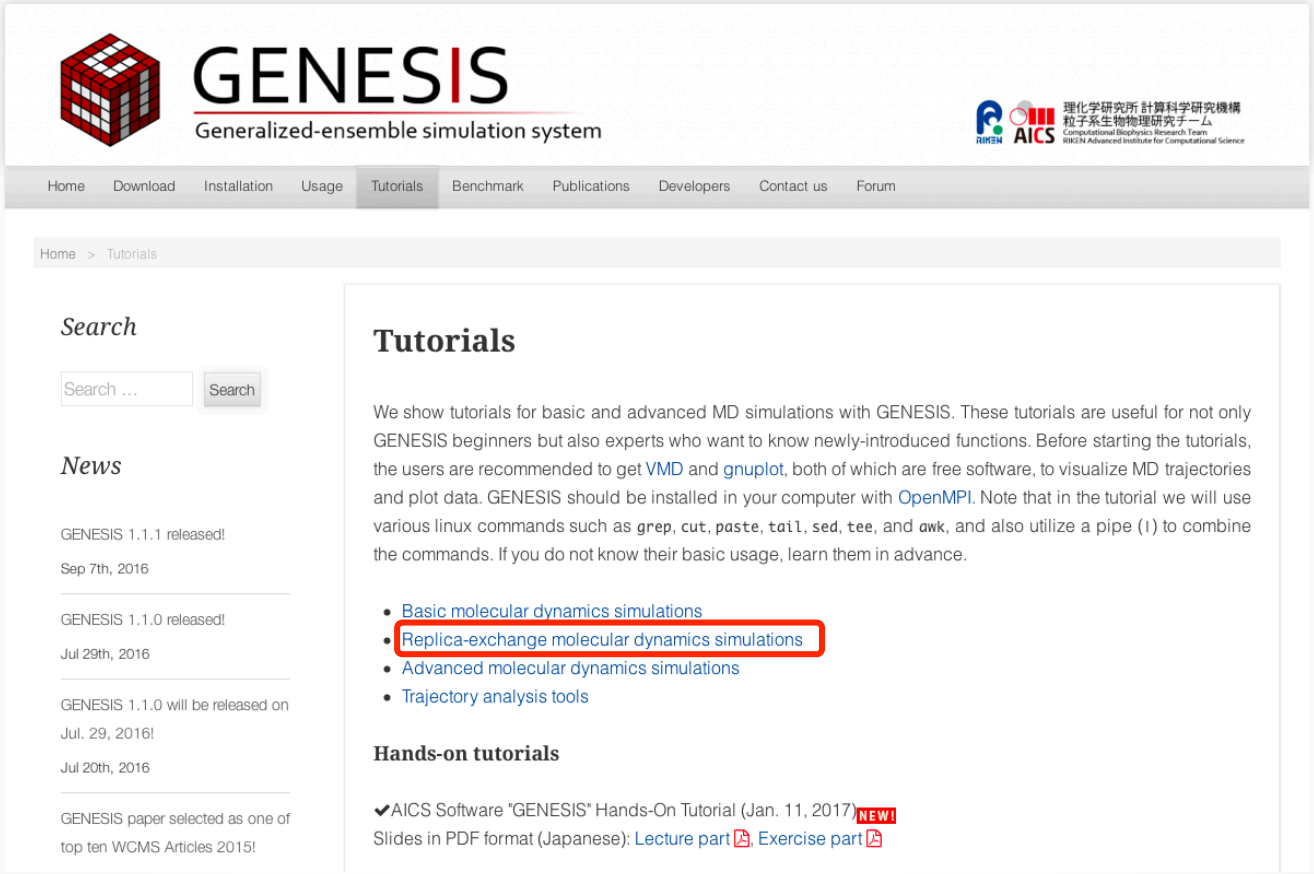
distance restraints (3, 4, 5, and 6 Å with k = 10 kcal/mol/Å^2)
between Cα atoms (atom name `CA`)
in Residue No. 1 and 3

5 x 4 = 20 replicas in total




```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00

Hint: Practice 4 + Practice 5
```

References


GENESIS
Generalized-ensemble simulation system
理化学研究所 計算科学研究機構
粒子系生物物理研究チーム
Computational Biophysics Research Team
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GENESIS 1.1.1 released!
Sep 7th, 2016
GENESIS 1.1.0 released!
Jul 29th, 2016
GENESIS 1.1.0 will be released on Jul. 29, 2016!
Jul 20th, 2016
GENESIS paper selected as one of top ten WCMS Articles 2015!
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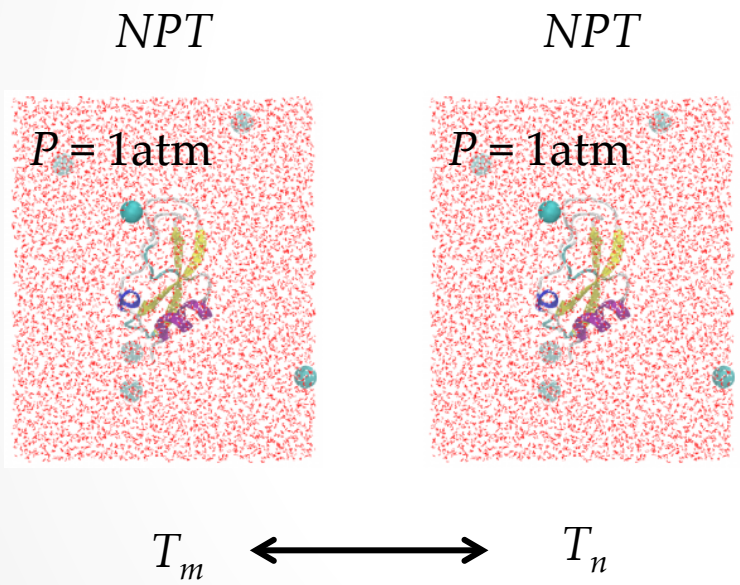
We show tutorials for basic and advanced MD simulations with GENESIS. These tutorials are useful for not only GENESIS beginners but also experts who want to know newly-introduced functions. Before starting the tutorials, the users are recommended to get VMD and gnuplot, both of which are free software, to visualize MD trajectories and plot data. GENESIS should be installed in your computer with OpenMPI. Note that in the tutorial we will use various linux commands such as grep, cut, paste, tail, sed, tee, and awk, and also utilize a pipe (|) to combine the commands. If you do not know their basic usage, learn them in advance.
Basic molecular dynamics simulations
Replica-exchange molecular dynamics simulations
Advanced molecular dynamics simulations
Trajectory analysis tools
Hands-on tutorials
✔AICS Software "GENESIS" Hands-On Tutorial (Jan. 11, 2017) NEW!
Slides in PDF format (Japanese): Lecture part, Exercise part

Appendix

Level: ★☆☆☆☆

Practice 1

Temperature REMD in the NPT ensemble at P = 1atm
(isotropic pressure coupling) using 4 replicas with T = 300, 310, 320, 330K




```
[ENSEMBLE]
ensemble          = NPT
tpcontrol         = LANGEVIN
pressure          = 1
isotropy          = ISO

[REMD]
dimension         = 1
exchange_period   = 1000
type1             = temperature
nreplica1         = 4
parameters1       = 300.0 310.0 320.0 330.0
```

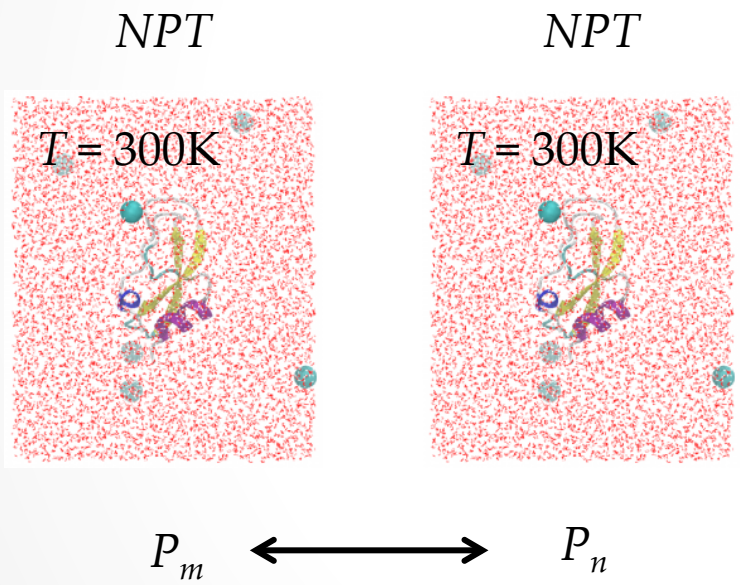
Hints:

- [ENSEMBLE] section is modified
- Step2.2 and 2.3 in Part I
- See User manual p.42-44

Level: ★★☆☆☆

Practice 2

Pressure REMD in the NPT ensemble at T = 300K
(isotropic pressure coupling) using 4 replicas with P = 1, 10, 100, 1000atm




```
[ENSEMBLE]
ensemble          = NPT
tpcontrol         = LANGEVIN
temperature       = 300
isotropy          = ISO

[REMD]
dimension         = 1
exchange_period   = 500
type1             = pressure
nreplica1         = 4
parameters1       = 1 10 100 1000
```

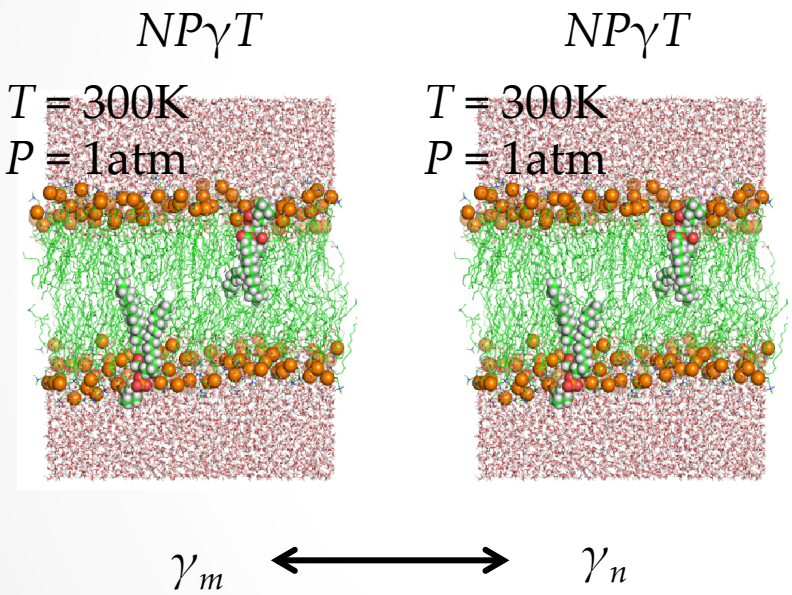
Hints:

- [ENSEMBLE] and [REMD] sections should be modified
- Step2.2 and 2.3 in Part I
- See User manual P.54

Level: ★★☆☆☆

Practice 3

Surface-tension REMD in the NPγT ensemble at T = 300K and P_n = 1atm (semi-isotropic pressure coupling) using 5 replicas with γ = -10, -5, 0, 5, 10dyn/cm




```
[ENSEMBLE]
ensemble          = NPgT
tpcontrol         = LANGEVIN
temperature       = 300
pressure          = 1
isotropy          = SEMI-ISO

[REMD]
dimension         = 1
exchange_period   = 500
type1             = GAMMA
nreplica1         = 5
parameters1       = -10 -5 0 5 10
```

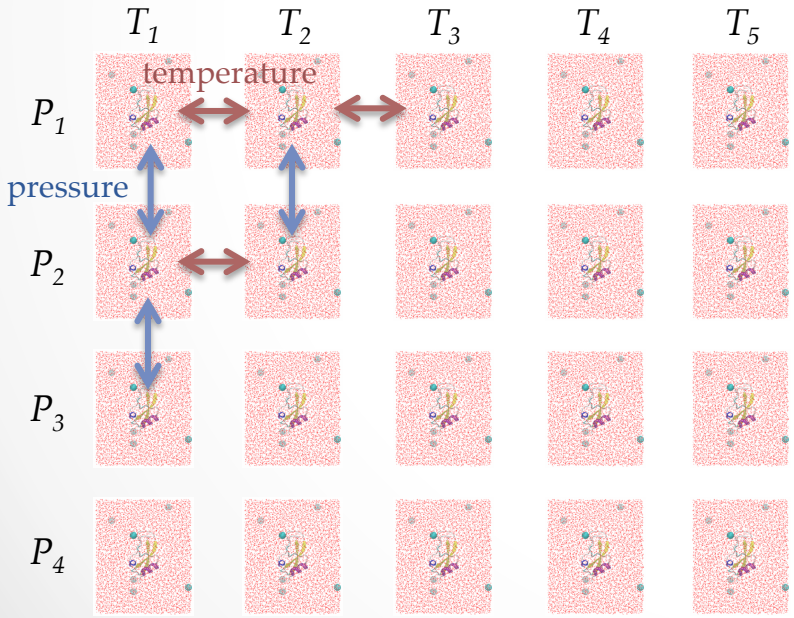
Level: ★★★☆☆

Practice 4

Two-dimensional T-REMD/P-REMD

Temperature:
300, 310, 320, 330, 340K (5 replicas)
Pressure:
1, 10, 100, 1000atm (4 replicas) isotropic pressure coupling

5 x 4 = 20 replicas in total



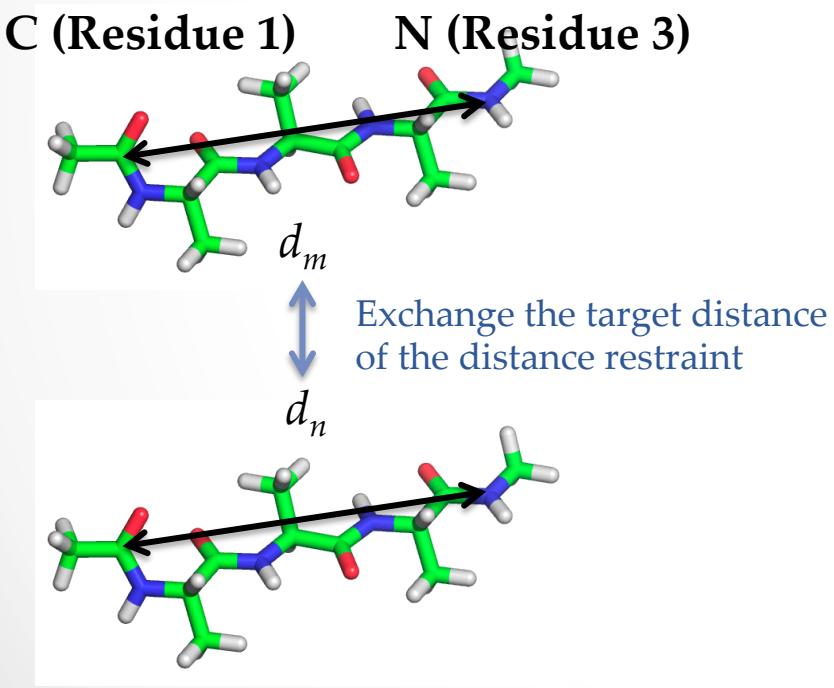

```
[ENSEMBLE]
ensemble          = NPT
tpcontrol         = LANGEVIN

[REMD]
dimension         = 2
exchange_period   = 500
type1             = temperature
nreplica1         = 5
parameters1       = 300 310 320 330 340
type2             = pressure
nreplica2         = 4
parameters2       = 1 10 100 1000
```

Level: ★★★★☆

Practice 5

Restraint-potential REMD (REUS) in the NVT ensemble using 4 replicas, where we apply distance restraints (3, 4, 5, and 6 Å with k = 10 kcal/mol/Å^2) between C atom in Residue 1 and N atom in Residue 3




```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00

[SELECTION]
group1            = an:C and rno:1
group2            = an:N and rno:3

[RESTRAINTS]
nfunctions        = 1
function1         = DIST
select_index1     = 1 2
constant1         = 10 10 10 10
reference1        =  3  4  5  6

[REMD]
dimension         = 1
exchange_period   = 500
type1             = RESTRAINT
nreplica1         = 4
rest_function1    = 1
```

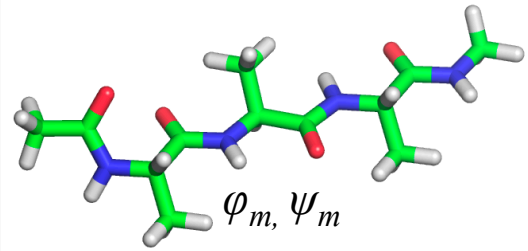
Common to conventional MD with distance restraint

Level: ★★★★★

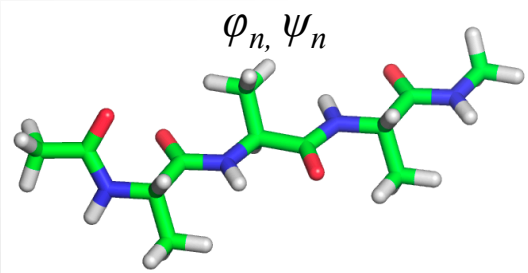
Practice 6

Restraint-potential REMD (REUS) in the NVT ensemble using 4 replicas, where we apply dihedral angle restraints on φ and ψ of Residue 2
(φ,ψ) = (180, 180), (170, 170), (160, 160), (150, 150) with k = 10 kcal/mol/Å^2

φ =C-N-CA-C
ψ =N-CA-C-N



Exchange the target two dihedral angles




```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00
[SELECTION]
group1            = an:C  and rno:1
group2            = an:N  and rno:2
group3            = an:CA and rno:2
group4            = an:C  and rno:2
group5            = an:N  and rno:3

[RESTRAINTS]
nfunctions        = 2
function1         = DIHED
select_index1     = 1 2 3 4
constant1         =  10  10  10  10
reference1        = 180 170 160 150
function2         = DIHED
select_index2     = 2 3 4 5
constant2         =  10  10  10  10
reference2        = 180 170 160 150

[REMD]
dimension         = 1
exchange_period   = 500
type1             = RESTRAINT
nreplica1         = 4
rest_function1    = 1 2
```

Level: ★★★★★

Practice 7

Two-dimensional T-REMD/REUS in the NVT ensemble

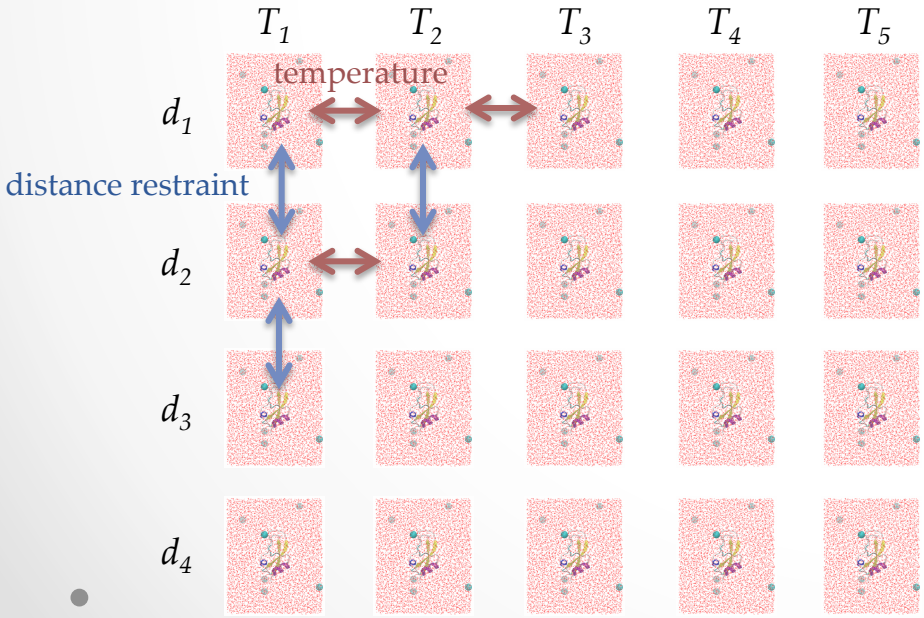
Temperature:

300, 310, 320, 330, 340K

Restraints:

distance restraints (3, 4, 5, and 6 Å with k = 10 kcal/mol/Å^2)
between Cα atoms (atom name `CA`)
in Residue No. 1 and 3

5 x 4 = 20 replicas in total




```
[ENSEMBLE]
ensemble          = NVT
tpcontrol         = LANGEVIN
temperature       = 300.00

[SELECTION]
group1            = an:CA and rno:1
group2            = an:CA and rno:3

[RESTRAINTS]
nfunctions        = 1
function1         = DIST
select_index1     = 1 2
constant1         = 10 10 10 10
reference1        =  3  4  5  6

[REMD]
dimension         = 2
exchange_period   = 500
type1             = temperature
nreplica1         = 5
parameters1       = 300 310 320 330 340
type2             = RESTRAINT
nreplica2         = 4
rest_function2    = 1
```