Brief user guide of GENESIS2.0beta

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This brief user guide assumes that the user is familiar to GENESIS1.X.

1. How to obtain

You can obtain the program from https://github.com/genesis-release-r-ccs/genesis-2.0.

2. How to compile

You can do the following procedure

```
$autoreconf
$./configure –enable-single
$make
```

According to hardware platform, you can write additional options when running configure.

1) Fugaku

```
$./configure –enable-single –host=Fugaku
```

2) Intel KNL (Here I assume that the login node and calculation node have different hardware architecture)

```
$./configure –enable-single –with-simd=MIC-AVX512
```

3) GPU

```
$./configure –enable-gpu –with-cuda={your path of CUDA library}
```

Unlike GENESIS1.X, the default FORTRAN/C compilers are ‘mpiifort’ and ‘mpiicc”, respectively. If there is no such compilers, then the program will next search for “mpif90” and “mpicc”. If there are both “mpiifort” and “mpif90” and you want to use “mpif90”, please define FC=mpif90.

3. New control input in GENESIS2.0beta

1) [ENERGY] section

- **nonbond_kernel** *AUTOSELECT / GENERIC / KGENERIC / FUGAKU / INTELKNL / GPU*

AUTOSELECT is the default. To test the energy result, you can define other kernels. The main reason of this is not to compile many times just for test of kernels. In the case of GPU, please remember that you should compile with gpu option.

- **PME_scheme** *AUTOSELECT / OPT_1DALLTOALL / NOOPT_1DALLTOALL / OPT_2DALLTOALL / NOOPT_2DALLTOALL*

AUTOSELECT is the default. As a default, it compares four schemes and choose the best one. If you want to use large grid spacing with higher PME spline order, we recommend *OPT_1DALLTALL* or *OPT_2DALLTOALL.*

2) [DYNAMICS] section

The maximum time step can be used is 3.5 fs with RESPA. In this case you can define long-range electrostatic / pairlist update / thermostat update / barostat update as following:

```
[DYNAMICS]
integrator         =  VRES
timestep           =  0.0035
elec_long_period   =     2
nbupdate_period    =     6
thermostat_period  =    6
barostat_period     =    6
```

It should be noted that, hydrogen mass repartitioning (HMR) scheme should be used to avoid constraint error. To do this, please write

```
hydrogen_mr      = YES
hmr_target       = solute
hmr_ratio        = 3.0
hmr_ratio_xh1    = 2.0
```

Here, “hydrogen_mr” means the usage of HMR. “hmr_target=solute” means HMR not for water molecules. If you write “hmr_ratio=3.0”, mass of hydrogen atoms multiplied by three whereas

the mass of bonded heavy atom is decreased to conserve the total mass. “hmr_ratio_xh1=2.0” is recommended when there are ring structures. Please note that you don’t need to change mass in the psf or prmtop file. You can change the mass during MD simulation just by writing above things in the control input.

3) [ENSEMBLE] section

In the [ENSEBLE] section, please write “group_tp = yes”. This option considers XHn group as one particle when calculating temperature and pressure values. It accelerates the overall speed by avoiding iteration procedure in thermostat and barostat.

4) [BOUNDARY] section

In the [BOUNDARY] section, “cell_size_buffer” key is added in GENESIS2.0beta. In SPDYN, the minimum cell size is determined as (pairlistdist+2.0)/2. Cell size is again increased such that the cell number in each dimension is divisible by the domain number. In some cases, the cell size could be less than (pairlistdist+2.0)/2 during NPT MD simulations, which can make the MD simulation unreliable. In GENESIS1.X, “0.6” is added as buffer to avoid such a problem. However, in some cases, such buffer values can slow down the MD speed. In addition, we don’t need to add the buffer value if the cell size is greater than (pairlistdist+2.0)/2.given the domain number. In this case, you can define the buffer value according to your purpose. Default is same as GAT, so you can skip using this if you are not sure of the relationship between box size and domain numbers.