GENESIS
Generalized-ensemble simulation system

GENESIS Hands-on Part 2-2:

High performance computation with GENESIS

Jaewoon Jung
RIKEN Center for Computational Science
2024/07/01

IUPAB2024 Hands-on Training Program CHARMM-GUI/GENESIS MD Tutorial

Schedule of GENESIS parts (6/30-7/2)

06/30 Part1	
13:30 – 15:00	GENESIS basics and GENESIS on Fugaku (Kobayashi) Lecture
	Hands-on tutorial on Fugaku

07/01 Part 2	
14:30 – 15:30	Coarse-grained simulations in GENESIS (Tan)
15:30 – 16:30	High-performance computation with GENESIS (Jung)

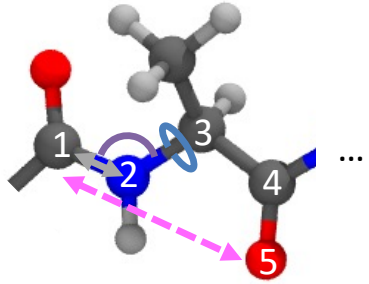
07/02 Part 3	
13:30 – 15:00	Generalized-ensemble simulations using GENESIS (Ito)

Contents

- Decision of Nonbonded interaction scheme
- Large time step integration with Hydrogen Mass Repartitioning
- Others

Force calculation for biological systems

Force can be divided into bonding and nonbonding interactions.



...

Hydrogen: Light Gray
Carbon: Dark Gray
Oxygen: Red
Nitrogen: Blue

$$E_{\text{potential}} = \sum_{\text{bonds}} k_b(b - b_0)^2$$ **Bond** (ex. 1-2, 2-3, …)

$$+ \sum_{\text{angles}} k_\theta(\theta - \theta_0)^2$$ **Angle** (ex. 1-2-3, 2-3-4,..)

$$+ \sum_{\text{dihedrals}} k_\varphi[1 + cos(n\varphi - \delta)]$$ **Dihedral** (ex. 1-2-3-4, …)

Bonding
O(***N***)

$$+ \sum_{\substack{\text{non-bonded} \\ \text{pairs}}} \left[\varepsilon_{ij}^{min} \left\{ \left(\frac{R_{ij}^{\min}}{r_{ij}} \right)^{12} - \left(\frac{R_{ij}^{\min}}{r_{ij}} \right)^{6} \right\} + \frac{q_i q_j}{r_{ij}} \right]$$

Nonbonding
O(N^2)

van der Waals (ex. 1-5, …) :

Coulomb (ex. 1-5, …) :

Nonbonded interactions

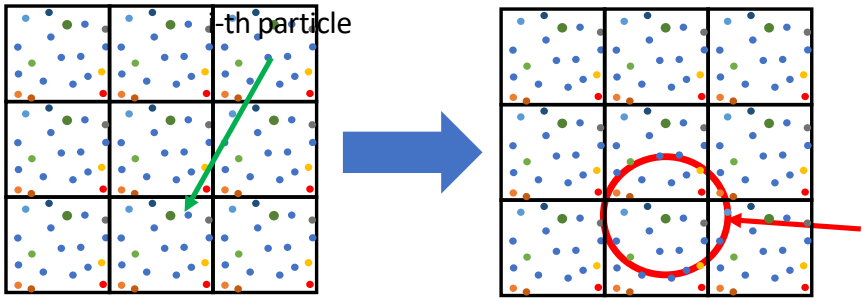
- Nonbonded interactions (Coulomb + vdW) are the main **bottleneck** of simulations.
- Nonbonded interactions are divided into those of real space with cutoff-distance and reciprocal lattice space.

Real space calculation

$$\sum_{ij,\mathbf{n}}\left[\varepsilon_{ij}^{min}\left\{\left(\frac{R_{ij}^{\min}}{r_{ij,\mathbf{n}}}\right)^{12}-\left(\frac{R_{ij}^{\min}}{r_{ij,\mathbf{n}}}\right)^{6}\right\}+\frac{q_iq_j}{r_{ij,\mathbf{n}}}\right]\rightarrow\sum_{\substack{ij,\mathbf{n}\\ r_{ij}<R_c}}\left[\varepsilon_{ij}^{min}\left\{\left(\frac{R_{ij}^{\min}}{r_{ij,\mathbf{n}}}\right)^{12}-\left(\frac{R_{ij}^{\min}}{r_{ij,\mathbf{n}}}\right)^{6}\right\}+\frac{q_iq_j\mathrm{erfc}(\alpha r_{ij,\mathbf{n}})}{r_{ij,\mathbf{n}}}\right]$$

$$\frac{1}{2\pi V}\sum_{\mathbf{k}\neq\mathbf{0}}\frac{\exp(-\pi^2\mathbf{k}^2/\alpha^2)}{\mathbf{k}^2}|S(\mathbf{k})|^2-\frac{\alpha}{\sqrt{\pi}}\sum_{i=1}^{N}q_i^2$$

Reciprocal space calculation



Range of *j*-th particle that interacts with *i*-th particle

Nonbonded interaction kernels in GENESIS

- In GENESIS, there are four interaction kernels for real space nonbonded interaction.

  1. Generic 2. Fugaku 3. Intel 4. GPU

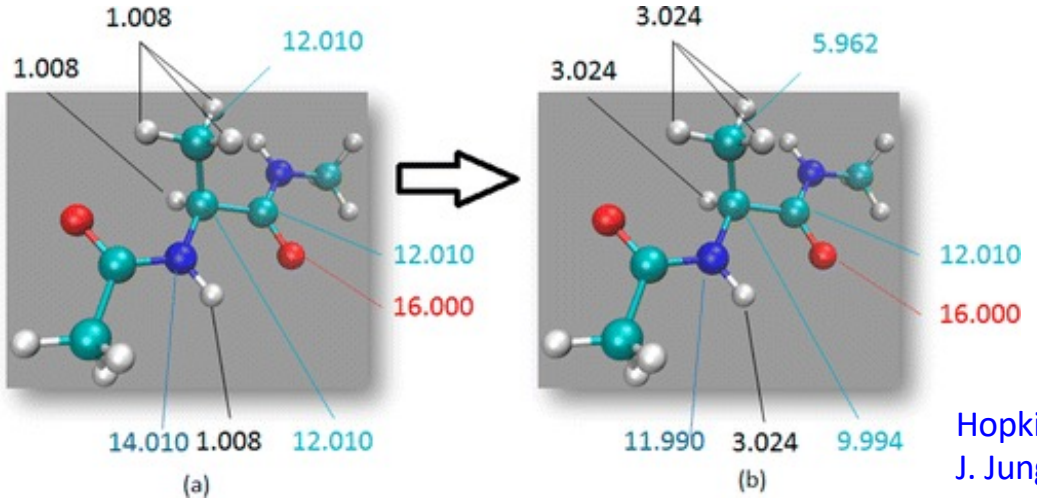
- Please choose the best calculation kernel from MD with small simulation time (We will do at this time).

- We also have four reciprocal space calculation schemes.
- Reciprocal space calculation scheme is decided by GENESIS by executing each scheme before starting MD.

Contents

- Decision of Nonbonded interaction scheme
- Large time step integration with Hydrogen Mass Repartitioning
- Others

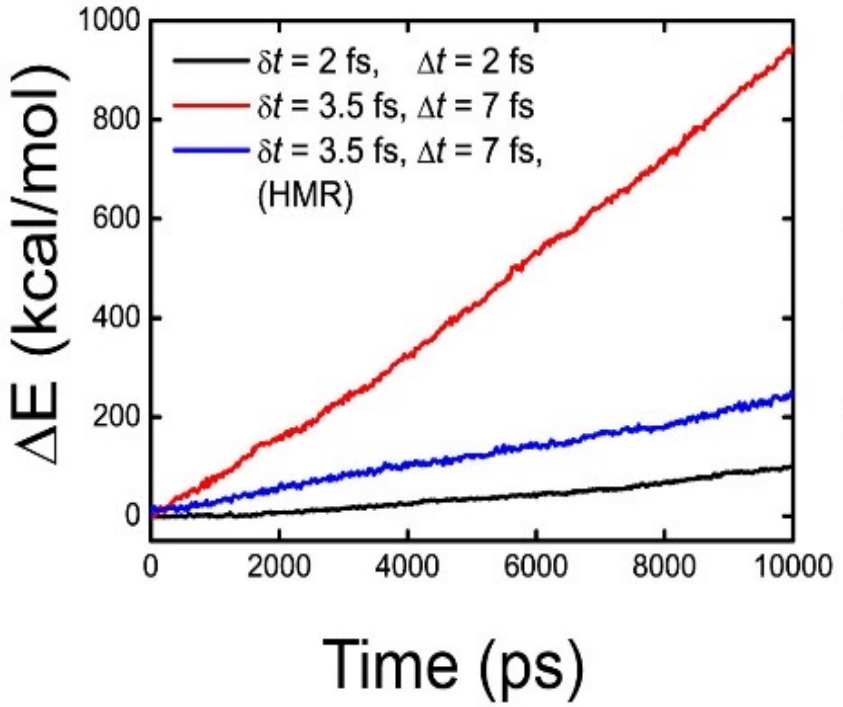
Hydrogen Mass Repartitioning (HMR) scheme



Hopkins *et al.*, JCTC. **11**, 1864 (2015))
J. Jung *et al.*, JCTC. **17**, 5312 (2021))

- Increase the mass of hydrogen atoms while reducing the mass of heavy atoms such that the total mass of one hydrogen group is not changed.
- With the HMR scheme, we can avoid the problem of SHAKE/RATTLE error by reducing the displacement of hydrogen atoms.
- We increase the mass of the hydrogen atoms three times.

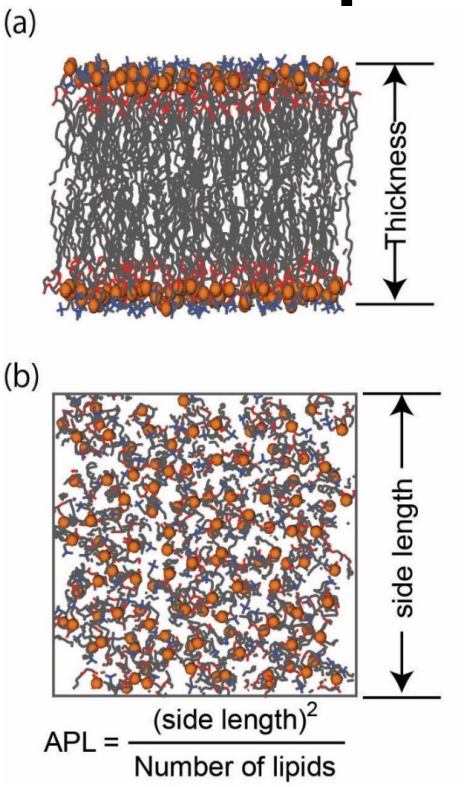
HMR increases the stability (example of energy drift)

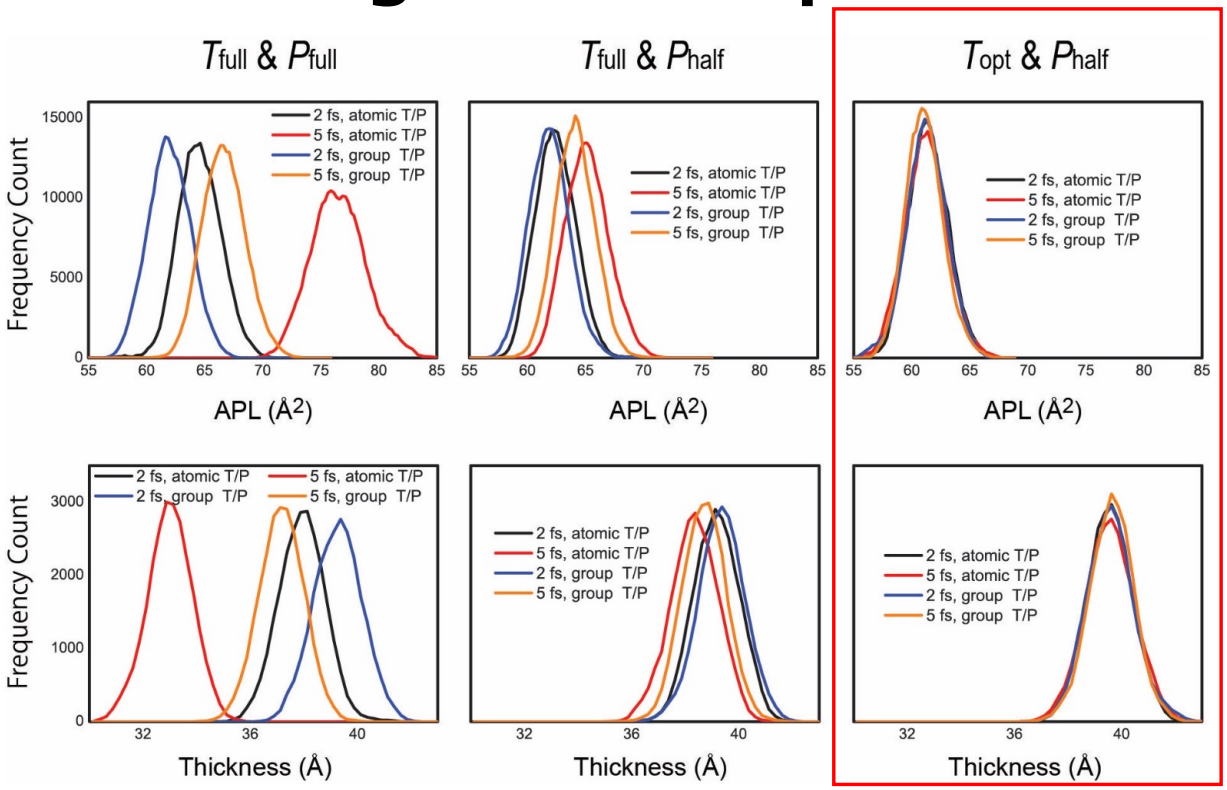


- HMR reduces the energy drift and increases the overall stability.

J. Jung *et al.*, JCTC. **17**, 5312 (2021))

Accurate temperature/pressure evaluation is important for large time step!!





Conventional temperature and pressure evaluation

Accurate temperature and pressure evaluation in GENESIS

J. Jung *et al*., JCTC, **15**, 84 (2019))
J. Jung et al., JCP, 153, 234115

Contents

- Decision of Nonbonded interaction scheme
- Large time step integration with Hydrogen Mass Repartitioning
- Others

Multiple time step integration

We can reduce the computational cost by skipping slow motion force every other step