B-15 Development of replica-permutation method in the isothermal-isobaric ensemble

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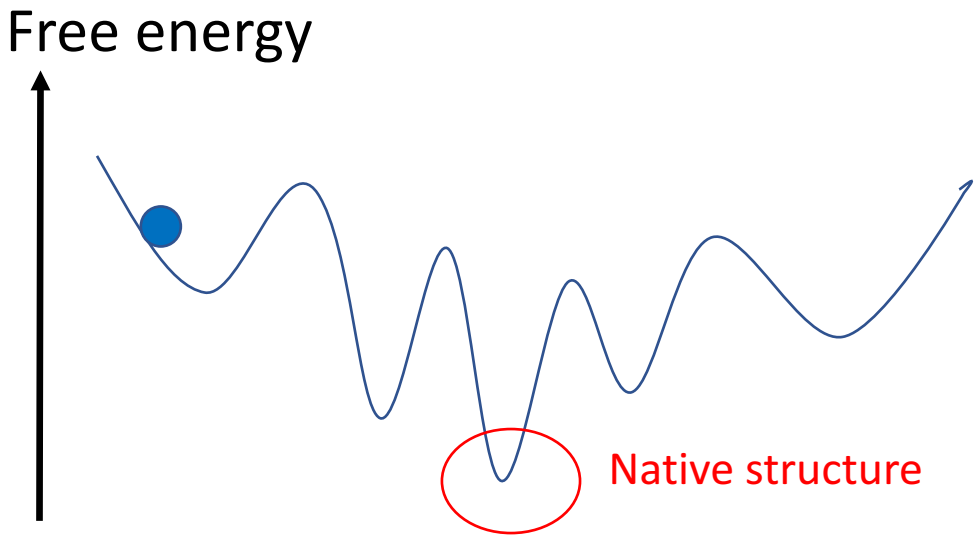
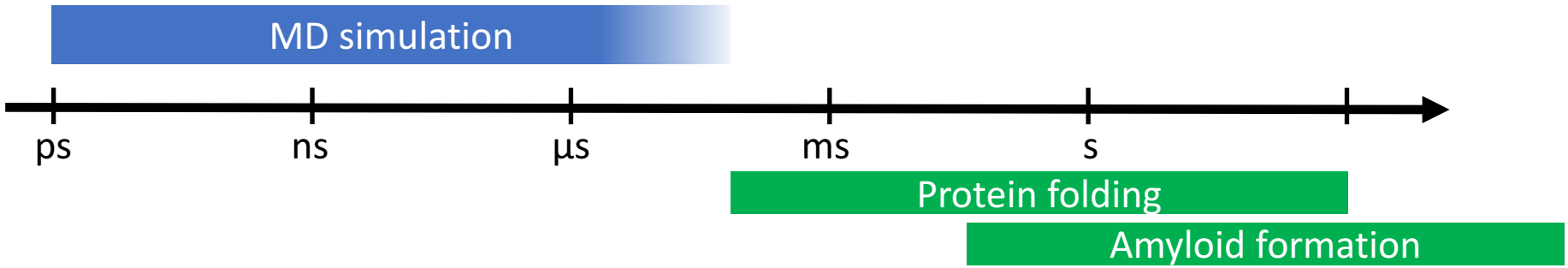
Back ground:

Molecular dynamics simulation for biomolecules

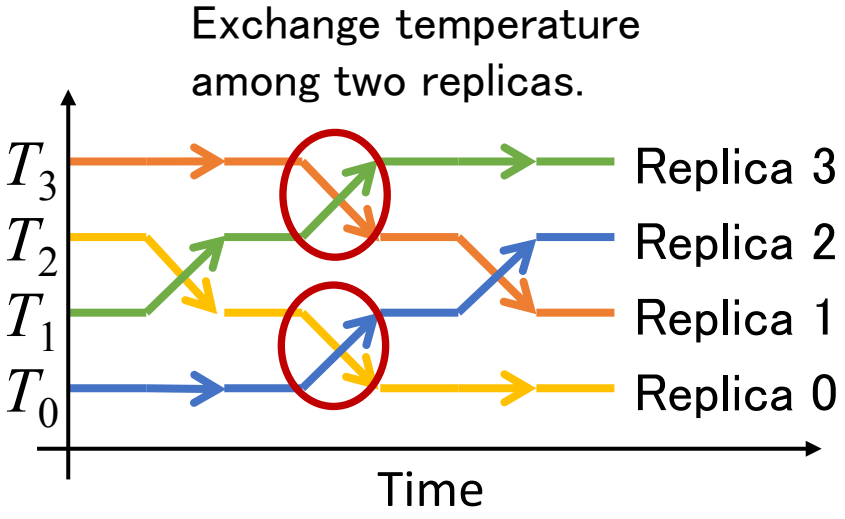


It is difficult to simulate protein folding and amyloid formation by using conventional MD.

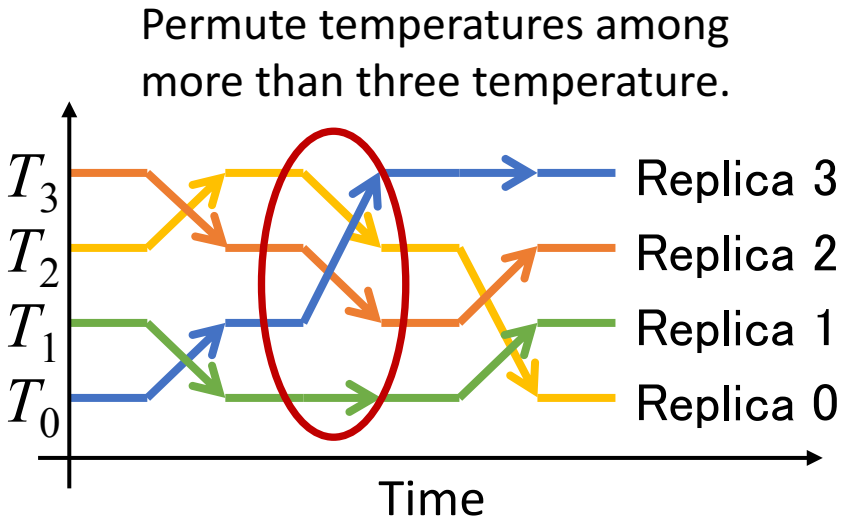


Background: Replica-permutation method

Replica-exchange method



Replica-permutation method



Replica-permutation method

- ✓ Better alternative to the Replica-exchange method.
  - → Efficient conformational sampling.
  - → Better convergence of amount of statistics.
- ✓ Highly parallelized algorithm.

Isothermal–Isobaric Replica–Permutation Method

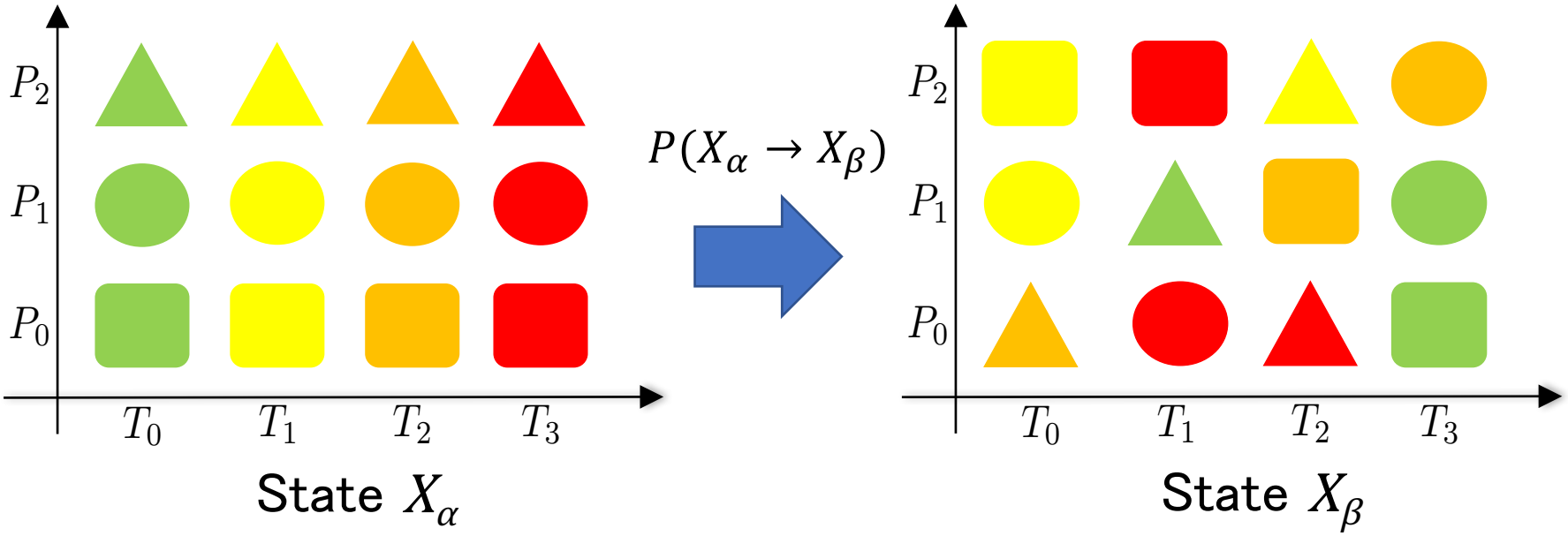
Step 0 : Let's consider M_0 temperatures T_{m0} and M_1 pressures P_{m1}.

→ The total number of replicas is $M = M_0 \times M_1$.

Step 1 : Carry out MD/MC simulation in *NPT* ensemble.

Step 2 : Permute temperature and pressure.

(That is, transition from state X_α to state X_β.)



M. Yamauchi, H. Okumura, *J. Chem. Phys.* **147** 184107 (2017).

Comparison of sampling efficiency

■ Tunneling events

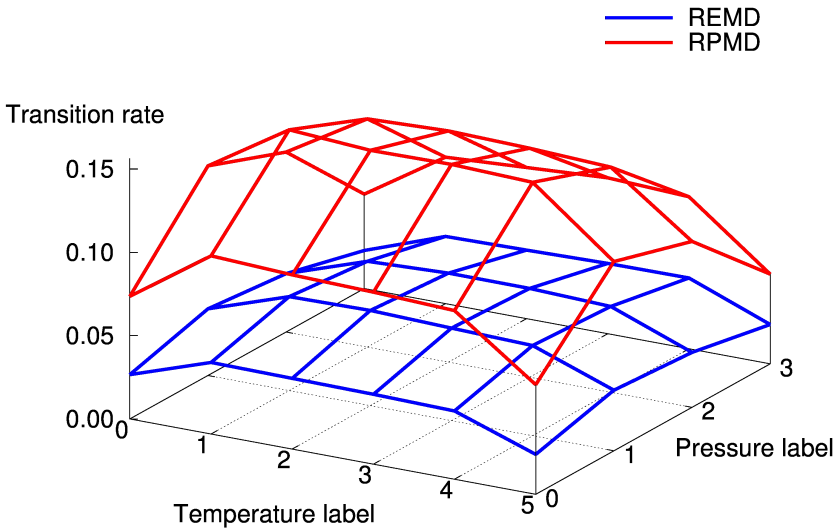
	RPMD	REMD
T	64 ± 1 ×2	34 ± 1
P	146 ± 2 ×4	37 ± 1

In both *T* and *P* spaces,

Replica-permutation method

> Replica-exchange method

■ Transition rate of parameter label



Transition rate:

Replica-permutation method

> Replica-exchange method

→ More efficient sampling is realized.

Summary

1. We developed the isothermal–isobaric replica–permutation method.

2. This method is more efficient than the isothermal–isobaric replica–exchange method.
    - The number of tunneling events.
    - Transition probability of parameter label.