# On the infinite swapping limit for parallel tempering

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If the underlying distribution $\pi$ is unimodal, the sampling is straightforward and the associated numerical results are reliable.

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Note that the higher the temperature, the "flatter" the distribution, the less likely for the Markov chain to get stuck at local minima of $V$.

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MC for $\pi_\tau$ $(\tau > 1)$ results in easier movement among local minima of $V(\theta)$.

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Minimization algorithm: sample Markov chain under small $\tau$.
However, small $\tau$ results in less mobility, the chain more easily get stuck in local minima of $f$.

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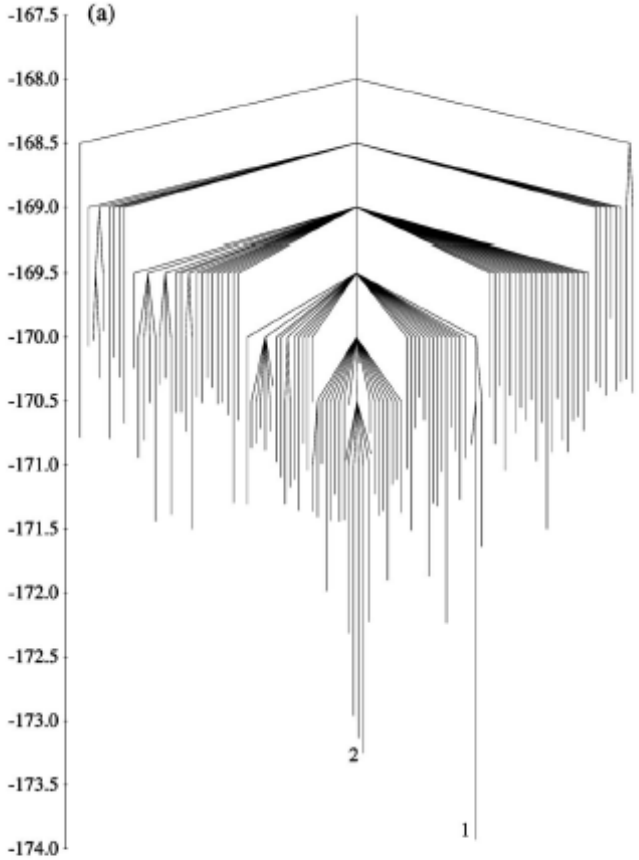
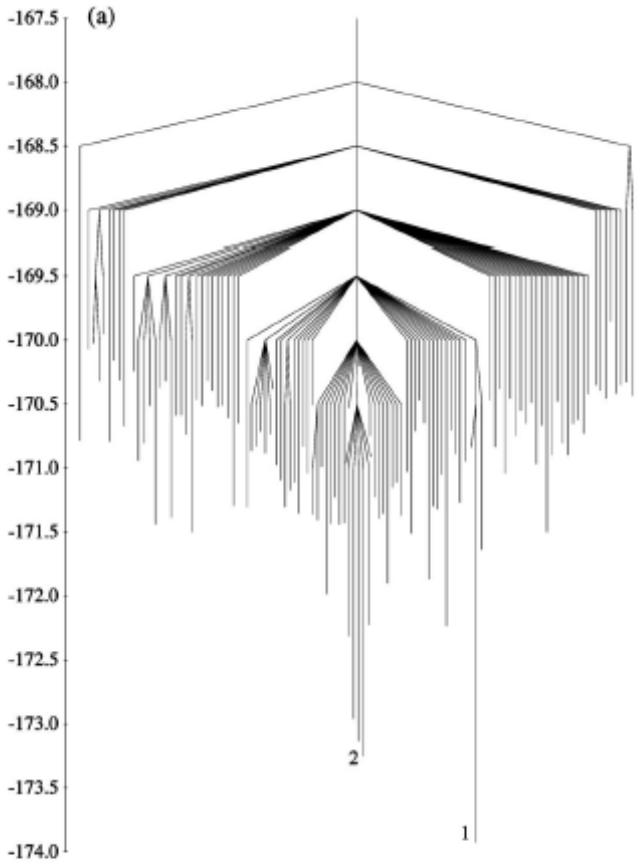
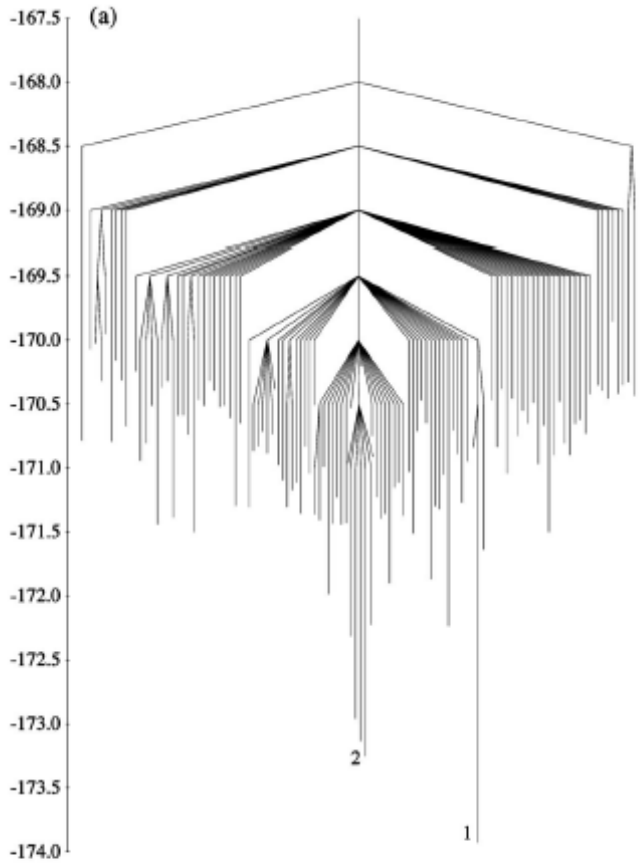
An example of such is the Lennard-Jones cluster of 38 atoms. This potential has $\approx 10^{14}$ local minima. The lowest 150 and their "connectivity" graph are as in the figure (taken from Doyle, Miller & Wales, JCP, 1999).






Global minimum only discovered 10+ years ago.




Global minimum only discovered 10+ years ago. Focus on overcoming rare-event sampling issues.

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5. Concluding remarks

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$$\frac{1}{T}\int_0^T f(X(t))dt \to \int_{\mathbb{R}^d} f(x)\pi(dx)?$$

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**$2^{nd}$ eigenvalue.** Consider the transition kernel

$$p(dx, T, x_0) = \mathbb{P}\{X(T) \in dx | X(0) = x_0\}.$$

Under mild conditions the exponential rate of convergence

$$p(dx, T, x_0) \to \pi(dx)$$

is determined by the sub-dominant eigenvalue of the operator corresponding to $X$. Used to characterize "efficiency" of the corresponding Monte Carlo.

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**Asymptotic variance.** Also a popular quantity for comparing efficiency of algorithms, but is a property of the algorithm once one is already at equilibrium. Also does not properly reflect the time averaging.

**Large deviation rate.** We will use the LD rate $I$, where a larger rate implies faster convergence.

# A representative example

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Compute the average potential energy and other functionals with respect to a Gibbs measure of the form

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- Simulations are done using a discrete time model.

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with $W_1$ and $W_2$ independent. Now introduce *swaps* (Swendsen, Geyer), i.e., $X_1^a$ and $X_2^a$ *exchange locations* with state dependent intensity

$$ag(x_1, x_2) \doteq a\left(1 \wedge \frac{\pi_{\tau_1}(x_2)\,\pi_{\tau_2}(x_1)}{\pi_{\tau_1}(x_1)\,\pi_{\tau_2}(x_2)}\right),$$

with $a > 0$, as the "swap rate."

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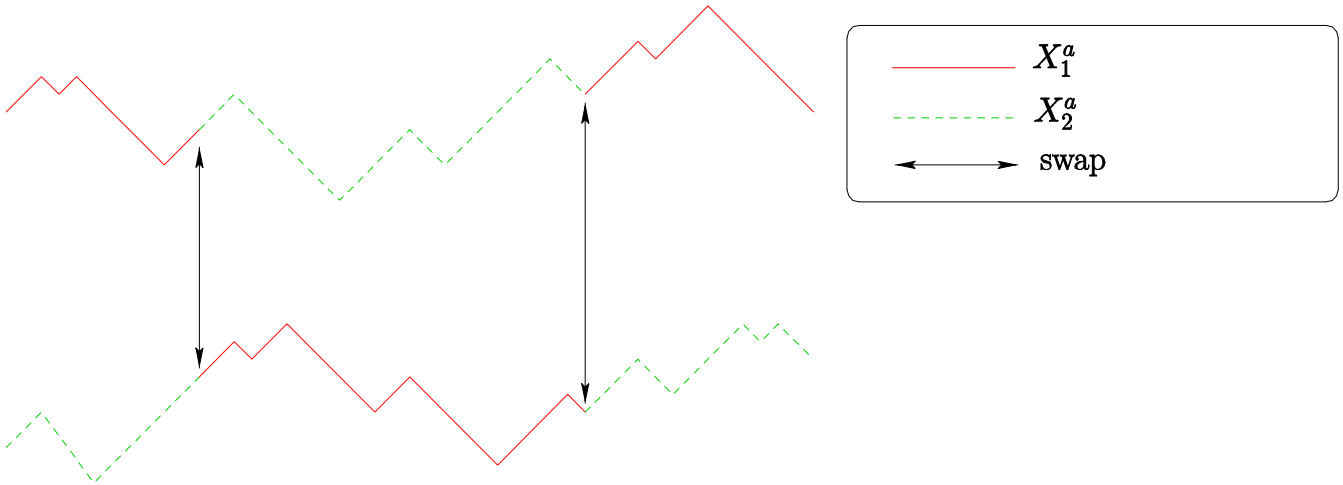

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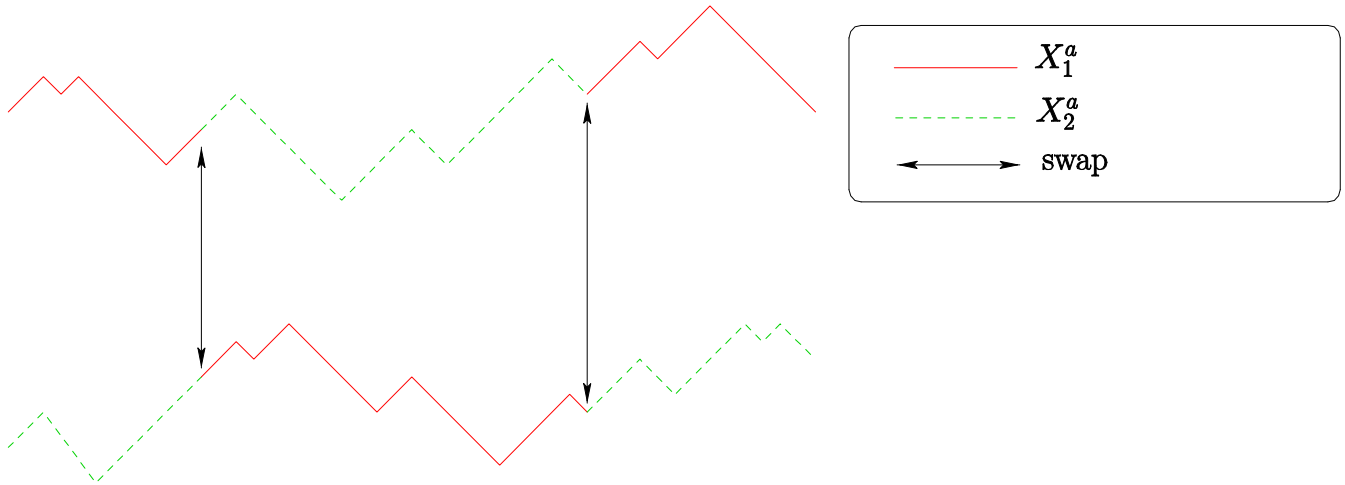


One can check (detailed balance condition): with this swapping intensity, invariant distribution of the joint process

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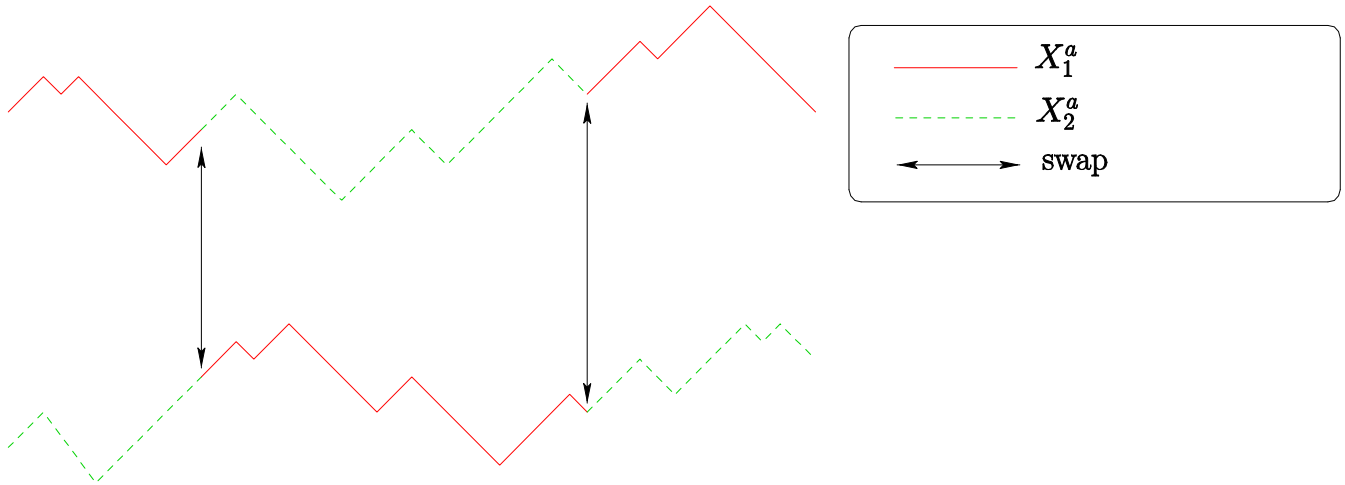


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3. Swapping enables information flow from high temperatures to low temperatures.

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To achieve maximum rate of convergence, we choose $a$ such that $I^a$ is the largest possible.

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$$J_1(\nu) = 0 \text{ iff } \theta(x_2, x_1) = \theta(x_1, x_2) \ \nu\text{-a.s.}$$

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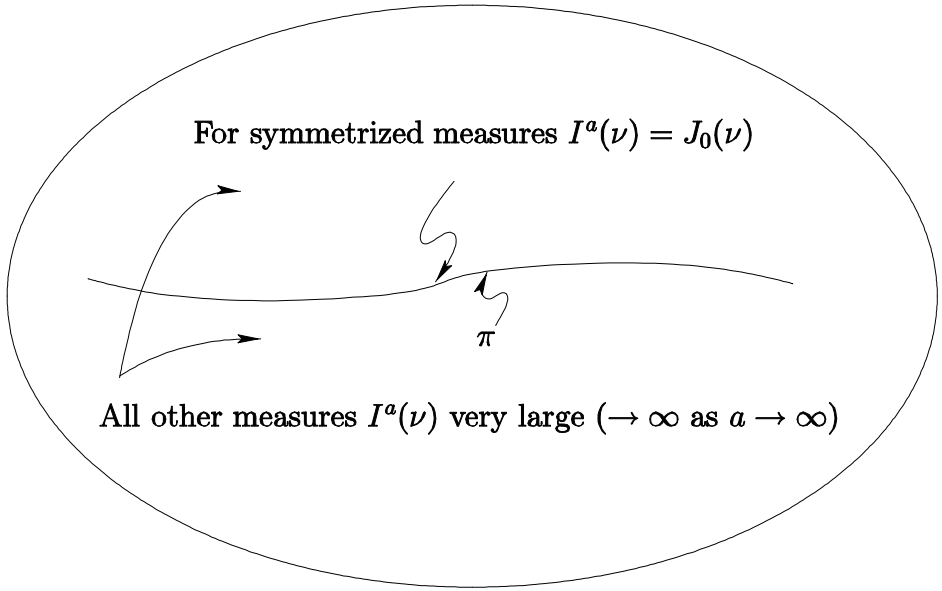

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**An alternative perspective:** rather than swap particles, swap temperatures, and use "weighted" empirical measure.

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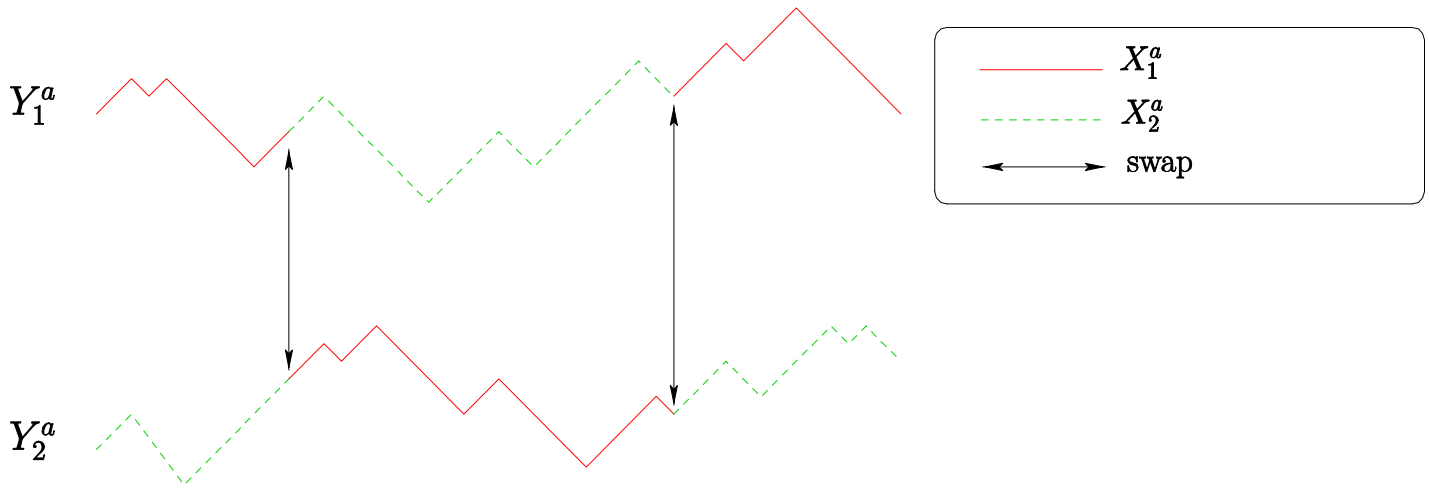

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Ergodic theory $\eta_T^a \to \pi$ . $(Y_1^a, Y_2^a, \eta_T^a)$ admits a well defined weak limit $a \to \infty$. Define state dependent weight

$$\begin{aligned}
\rho_1(x_1, x_2) &\doteq \frac{\pi_{\tau_1}(x_1)\,\pi_{\tau_2}(x_2)}{\pi_{\tau_1}(x_1)\,\pi_{\tau_2}(x_2) + \pi_{\tau_1}(x_2)\,\pi_{\tau_2}(x_1)}, \\
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\end{aligned}$$

# Infinite swapping limit (cont'd)

The triple has following weak limit

$$dY_1 = -\nabla V(Y_1)dt + \sqrt{2\tau_1\rho_1(Y_1, Y_2) + 2\tau_2\rho_2(Y_1, Y_2)}dW_1$$
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$$\lim_{a\to\infty} I^a(\nu) = I^\infty(\nu) \doteq \begin{cases} J_0(\nu) & \text{if } \theta(x_1, x_2) = \theta(x_2, x_1) \\ \infty & \text{otherwise} \end{cases}$$

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- Need for computational feasibility leads to *partial infinite swapping*.

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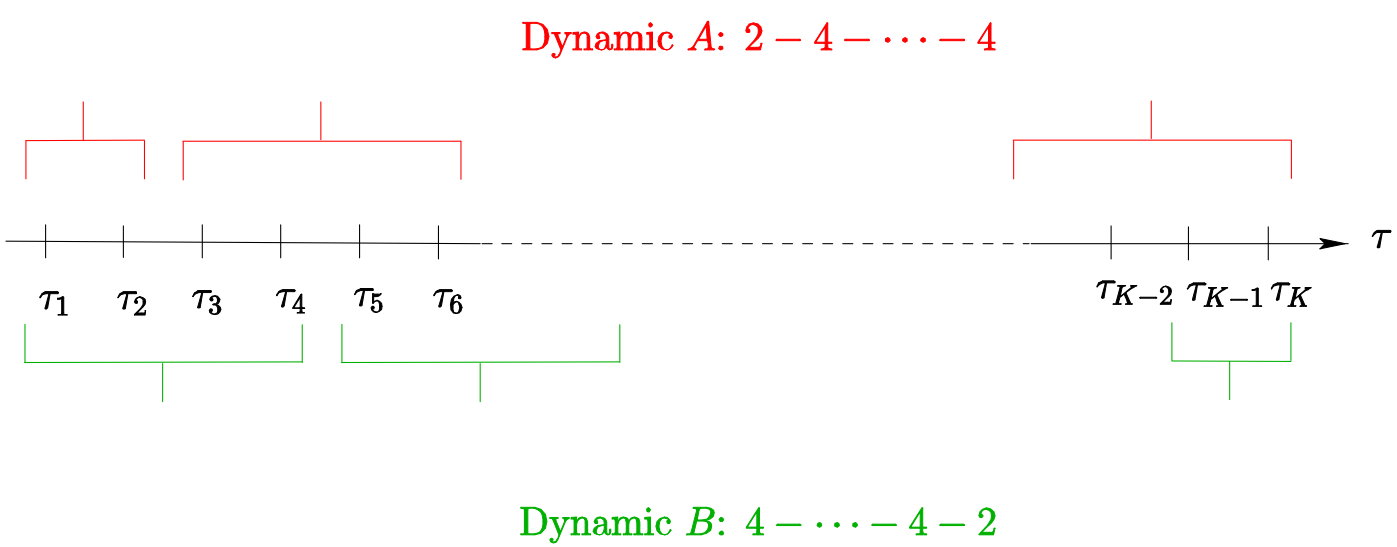
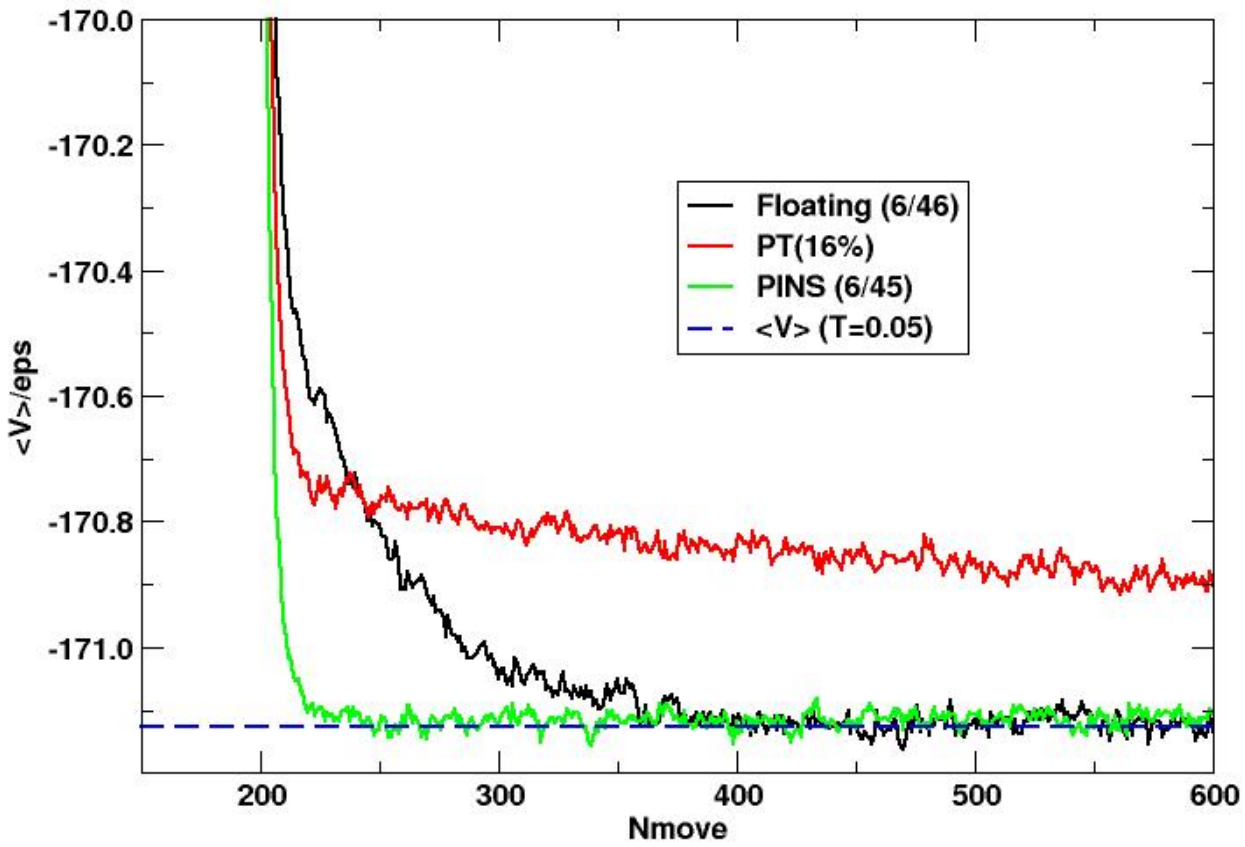
Examples are Dynamics $A$ and $B$ in figure:



# Comparison of PINS and PT

Relaxation study of convergence to equilibrium for LJ-38: parallel tempering versus partial infinite swapping, only lowest temperature illustrated.



# Concluding remarks

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- Mathematical paper: "On the infinite swapping limit for parallel tempering", Dupuis, Liu, Plattner and Doll, to be appeared in SIAM J. on MMS
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- Selection of "best" subgroups for partial infinite swapping approximations.
- Better quantitative understanding of rate of marginals such as $I_1^\infty(\gamma)$
- Application to other problems such as function minimization.