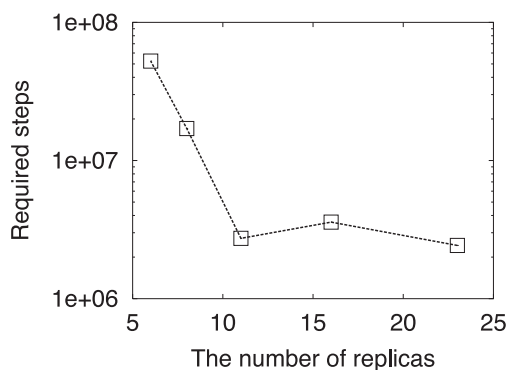


Replica-Exchange Molecular Dynamics Toolkit

We have developed a toolkit to generate replica-exchange method programs suitable for solving the multiple-minima problem. The toolkit was designed as an object-oriented framework containing a set of C++ abstract classes whose subclasses enable one to incorporate an arbitrary force field implementation, and to use various functionalities. The efficiency of the toolkit was evaluated by generating new variants of simulation programs which implement the CHARMM force field. It was shown that the toolkit not only reduces the total computational cost but parallelizes the simulation at an efficiency that was relatively linear with the number of CPUs.



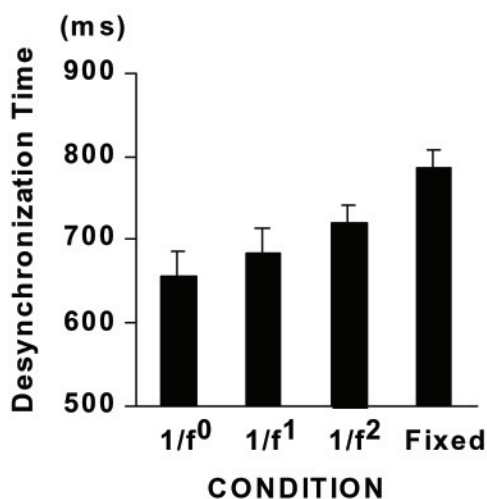
Number of required conformations to decrease the error of heat capacity to less than 0.01 kcal/mol · K is shown as a function of the number of replicas

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The Effect of $1/f^n$ Fluctuation in Inter-stimulus Intervals on the Elicitation of a GO/NO-GO Response

We studied the relationship between a $1/f^n$ fluctuation in the inter-stimulus interval (ISI) and the elicitation of a magnetoencephalographic (MEG) GO/NO-GO response. The ISI times of the tone pulses were given by three types of fluctuation, $1/f^0$, $1/f^1$, and $1/f^2$, and with a fixed interval. The RMS values of the mismatch field (MMF) ($F(3/24)=10.94$; $p=0.0001$) and the duration time of beta band desynchronization (BBD) of the left occipital area sensors (CH75/76) for the NO-GO response ($F(3/24)=6.43$; $p=0.0024$) were significantly increased correlated with the fluctuation exponent. The temporal ordering within the stimulus was reflected in the activity of the BBD.



Relationship between the exponent of fluctuation and the desynchronization time in the beta band of the left occipital area channel CH75/76 for the NO-GO response. Each point is the mean with SE bar for 9 normal adults

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