A new type of dynamical behavior of a multistable system is reported. We found that a simple non-equilibrium system can reduce its effective temperature autonomously at a global minimum if the residual frustration at the global minimum is sufficiently small. This highlights an unexpected feature of non-equilibrium multistable systems.

How can one escape from a labyrinth? The question is important not only for a game player but also for a researcher of multistable systems. Evolution of complex systems sometimes obeys an optimization process of a kind of “energy” function. Since the landscape of the energy is in general multistable, the harm of trap at local minima prevents the system from reaching a global minimum. A conventional way to escape from local minima is to make thermal fluctuation in such systems, and the relaxation process under thermal fluctuations has been extensively studied.

However, there is a dilemma in regard to the barrier crossing probability in a multistable potential and the stationary probability distribution of the system: High temperature fluctuations make a barrier crossing between basins of multistable potential easy. However, unfortunately, high temperature fluctuations also make the mean energy over a probability distribution increase. The simulated annealing method, which is a strategy to lead a system to a global minimum by gradually decreasing the temperature of the thermal fluctuation, was introduced to avoid the dilemma and was successfully applied to several fields such as image restoration, protein folding, neural networks and so on. However, the method seems somewhat unnatural and inconvenient for physical processes for two reasons: 1) one must “control” the temperature of a system gradually, because the convergence to a global minimum is guaranteed when one spends an infinite time decreasing the temperature; 2) the system never stops even if the system passes the global minimum state as long as the temperature is finite. This implies that the dilemma cannot be solved essentially even by the “simulated annealing” method.

Although the simulated annealing method is a kind of relaxation process, one should remember the fact that the method is based on equilibrium statistical mechanics because it uses the Boltzmann distribution, which is realized for the system with detailed balance, in its process. Therefore, we conjectured that the dilemma might be solved in a non-equilibrium condition. The conjecture is partially motivated by Levinthal’s paradox that a protein is folded from its initial structure much quicker than the exhaustive sampling. We report in this paper a preliminary example of a solution of the dilemma by numerical simulation of a simple model.

One finds that the “energy” of a multistable system is generally composed of
plural competitive constraints or interactions each of which is relatively simple, and the competition results in frustration in the system. The global minimum is, thereby, the state where such constraints are mostly satisfied: the frustration is expected to be minimal there. An interesting example of this competitive dynamics can be found in on-line learning process of neural networks. Radons et al. reported\(^8\) that an effective temperature of parameter fluctuations caused by a probabilistic successive pattern input in a learning process by backpropagation can decrease autonomously at a global minimum under condition that all constraints (patterns) can be perfectly satisfied at a global minimum.\(^9\) The condition is called “perfectly trainable”, which is approximately satisfied for a network with a sufficiently large number of neurons.\(^10\)

The autonomous decrease of fluctuation was also found in the learning process of chaotic time series by a conventional feedforward neural network\(^11\) and in the learning by the neural network with coupled oscillators.\(^12\) Recent study of on-line learning by neural networks indicates that non-thermal fluctuation due to the successive change of the local potential (error) is important not only for escape from local minima but also for an acceleration of a relaxation process even without local minima.\(^13\) This requires a clear understanding of the effect of non-thermal fluctuations due to fluctuating potentials.

Dynamics which autonomously change the effective temperature are quite interesting from the viewpoint of relaxation processes in non-equilibrium conditions. However, the discussion above was limited for learning by neural networks, and dynamical analysis of a “perfectly trainable” system has not been carried out due to their high-dimensionality and their complex structures. To investigate the autonomous, annealing-like dynamics clearly, we find a minimal model which satisfies the following conditions: 1) Each partial potential (constraint) term, \(V_i(x)\), is expressed in a positive definite, differentiable function so that a zero value state corresponds to a frustration-free state; 2) global potential, \(V(x)\), is a linear sum of the constraints; 3) the dynamics obey a plain relaxation (gradient descent) process of a dissipative particle under time-dependent potentials; 4) the system has small residual frustration in a global minimum state; 5) the functional form of the partial potential is selected to make the residual frustration of the global minimum small in order to demonstrate typical self-annealing dynamics; 6) the amplitudes of the partial potentials fluctuate in order to make non-equilibrium fluctuations.

A dynamics which satisfy these conditions is realized by the following:

\[
x_{n+1} = x_n - \Delta t \frac{\partial V_{pn}(x)}{\partial x} |_{x=x_n},
\]

where a global potential is \(V(x)=1/N \sum_{i=1}^{N} V_i(x)\); the partial potential with index \(i\) is \(V_i(x) = (1 - \cos(a_i x + \delta_i))/2\) [for \(-10 \leq x \leq 10\), otherwise \(V_i(x) = \infty\)]; the coefficients \(a_i\) and \(\delta_i\) are arbitrary constants; \(p_n\) is the index of the partial potential at discrete time \(n\), which is chosen randomly from the partial potential indices, \(\{1, 2, 3, ..., N\}\); and \(\Delta t\) is a constant. It should be noted that local minima of the global potential are not attributed to one of the local minima of the partial potential, but are attributed to the result of interference of all partial potentials, which is consistent with general multistable systems. The multistability of the partial potential is not unnatural at
least for learning by neural networks, because there are generally multiple available solutions in the systems. The “energy” landscape discussed here is multistable and has a global minimum near \( x=0 \) when the phase shift coefficient, \( |\delta_i| \), is small enough. The pre-factor \( 1/N \) in the potential is only for normalization.

It should be noted that the dynamics of Eq. (1) correspond to an extreme example of the self-annealing dynamics that the amplitudes of partial potentials fluctuate independently: only one potential is alive each time step in this extreme case. However, the result is not essentially altered when plural partial potentials are alive, whereas the non-equilibrium effect is weakened in this case. It should also be noted that the central result is the same for continuous time dynamics with slowly varying amplitudes of partial potentials with time scale of \( \Delta t \). The dynamics coincide with a plain relaxation process of a “quenched” global potential in the limit \( \Delta t \to 0 \), because the system “feels” an average potential. Therefore, the finiteness of the parameter, \( \Delta t \), is essential for the “non-equilibrium” dynamics.

We find that the present system has a “self-annealing”\(^{14}\) ability that fluctuations in phase space decrease at a global minimum \textit{autonomously} if the amplitudes of constraints (partial potentials) fluctuate as in Eq. (1). First we show the most ideal case that the system is in a frustration-free state at a global minimum, which is realized by setting all the coefficients, \( \delta_i \), to be zero. Figure 1 shows that the motion of the system started in a basin of a local minimum stops suddenly when the system reaches a global minimum state, a typical exam-

![Temporal evolution of the self-annealing dynamics in the most ideal case.](https://example.com/figure1)

**Fig. 1.** Temporal evolution of the self-annealing dynamics in the most ideal case. a) Landscape of a total potential energy, \( V(x) \), where the number, \( N \), of partial potentials is 10. The coefficients, \( a_i \), are chosen as: \{1, 1.38, 2.75, 1.96, 1.27, 1.64, 1.42, 2.29, 2.47, 2.72\} for demonstration. The coefficients, \( \delta_i \), are chosen as zero in order to stabilize the global minimum state perfectly. b) Typical trajectories of a phase space and a total energy.
Fig. 2. Temporal evolution of the conventional Langevin equation subject to random noise (Eq. (2)), where $\xi_n$ is a uniform random number, $r_n$, $|r_n|<0.5$. Typical trajectories of a phase space and a total energy are shown. The potentials used are the same as in Fig. 1.

Fig. 3. Temporal evolution of the self-annealing dynamics in the less ideal case. a) Landscape of a total potential energy. The number, $N$, of partial potentials and the coefficients, $a_i$, are chosen as in Fig. 1. The coefficients, $\delta_i$, are chosen as: $\{-0.7, 0.2, -0.2, 0.1, -0.6, 0.3, -0.5, 0.1, -0.3, 0.2\}$ respectively corresponding to $\{a_i\}$ in Fig. 1. b) Typical trajectories of a phase space and a total energy.

Example of the "self-annealing dynamics". It should be emphasized that the frustration is not reduced much at a local minimum, in contrast with the global minimum state. These dynamics are qualitatively different from conventional dynamics (Langevin equation) subject to thermal noise (Fig. 2):

$$x_{n+1} = x_n - \Delta t \frac{\partial V(x)}{\partial x} |_{x=x_n} + \xi_n, \quad (2)$$

where $\xi$ is a probabilistic random noise with zero mean. This observation of the self-annealing dynamics is understandable because the perfectly global minimum condition ($V=0$) implies that each of the partial potentials is simulta-
neously minimized at the global minimum \( V' = 0 \), while the local minimum condition \( \frac{\partial V}{\partial x} = 0 \) does not imply stability at a local minimum for all partial potentials \( \exists i : \frac{\partial V_i}{\partial x} \neq 0 ; \text{ or } \frac{\partial^2 V_i}{\partial x^2} < 0 \).

The discussion above may seem too ideal, since the perfect minimum condition, \( V(x) = 0 \), must be assumed at a global minimum state. Next, we discuss the case that the perfect minimum condition is not satisfied even in a global minimum state (Fig. 3(a)). The situation is realized when some of the partial potentials, \( V_i \), are not minimized at the global minimum, due to the finite values of \( \delta_i \). As shown in Fig. 3(b), numerical simulation shows that the system never stops at a global minimum; however, the system can reduce its activity (fluctuation of the system) when it reaches a global minimum and can be stabilized enough to stay in the global minimum. The stability of a system at the global minimum state in the present potential is guaranteed if the following inequality is satisfied: \( \Delta t \cdot \max |a_i| < \min |(\pi - \delta_i)/a_i - \delta_i/a_i| \), which is derived from the worst condition that a particle cannot be transferred to the next basin of any partial potential by an overshooting of the largest potential gradient of partial potentials. The inequality roughly explains the stability at a global minimum: increase of \( \Delta t \), \( |a_i| \) and \( |\delta_i| \) breaks the stability at a global minimum. Because an increase of \( |\delta_i| \) from zero increases the residual frustration at a global minimum, the "self-annealing" dynamics works less effectively if residual frustration at a global minimum is not small.

We showed in this paper that an autonomous, annealing-like dynamics ("self-annealing dynamics") is possible in a non-equilibrium multistable system where the residual frustration at a global minimum is sufficiently small: The self-annealing dynamics has a unique property as to the convergence toward a global minimum, in contrast with simulated annealing: the system under self-annealing dynamics decreases its effective temperature by itself suddenly when the system reaches a global minimum. Non-equilibrium multistable systems can be qualitatively different from equilibrium multistable systems of which fluctuation is characterized by thermal temperature. In general multistable systems, the global minimum is the state, by definition, where each interaction is mostly satisfied on average; which implies that the frustration of the system is expected to be mostly solved in a global minimum state.\(^{15}\) Therefore, the present simulation suggests that other non-equilibrium systems with different forms of interactions (constraints) may have the possibility of showing self-annealing dynamics.

In many-body systems with exchange interactions, the global potential is conventionally composed of pairs of elements with coupling coefficients, where a spin glass system is a prototype. In conventional solid state material, it is usually assumed that the exchange interaction is fixed as known in "quenched" systems. In such quenched systems, the self-annealing dynamics does not appear. However, we conjecture that some many body systems such as biological systems which are far from equilibrium conditions might show self-annealing dynamics, since the exchange interaction may fluctuate in such systems. We also expect that the self-annealing dynamics might be useful for optimization problems where the energy (or error) function of the problem is made by the composition of multiple constraints: successive evolution of the system under the presentation of a partial constraint can produce the self-annealing
dynamics. Studies of such realizations are under way.

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