

Simulation Science

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Abstract

The strategy of Simulation Science at NIFS is described. In contrast with the strategy of the Santa Fe Institute where an artificial rule is given to a personal computer and a pattern evolution governed by the rule is obtained to apply it to the sort of real world phenomenon, our strategy is such that big simulations are carried out for various complex phenomena in the real world by a world-largest supercomputer at hand to extract a global rule common to complex systems with different many-body interacting forces. Having once obtained such a universal rule, then one may be able to predict how a complex system evolves globally.

Keywords:

simulation science, science of complexity, Santa Fe Institute, self-organization

1. Beyond the Age of Nonlinear Solver

Creating a new paradigm beyond the Modern Science is highly invoked. The Modern Science has been governing the fundamental thought of human beings for more than three hundreds years since Descartes and Newton. In doing Science, one breaks a piece out of the whole and defines its boundary definitely, thereby the outside world being considered as a known and unaffected background. Any consistent back reaction to the outside world is ignored, not because we are not interested in it but simply because we do not have a clear paradigm to include it.

The most successful and reliable tool that human beings have invented for comprehending the universe is the mathematics. Mathematics has convinced us, after three hundred years exploration, that at least non-human (non-living) phenomena are reasonably to be comprehended. However, any single identity or phenomenon in nature cannot stand as it is, but is slightly or deeply related to numerous other agencies that existed or happened in the past through highly tangled causal chains. In Modern Science, any tiny interactions, when so judged compared with other

interactions at an arbitrary instantaneous moment, are thrown into trash cans, despite the fact that we are concerned with the long time evolution. It may happen, though, that the larger (linear) growth rate modes can be stabilized in a rather short time scale by mutual mode coupling effects among those modes or by changing the background structure, while smaller growth rate modes keep growing, though slowly, without being affected much by the nonlinear stabilization of the larger modes. Then it becomes quite possible that an initially tiny growth rate mode eventually becomes the ruler of the world of interest and reigns it. Of course, this new world could after some time be destroyed by other modes. Such a change of the ruler might continue forever.

In nature there are uncountable number of events that cannot be explained by the conventional perturbational treatment introducing small parameters. Nature is not that simple. Most phenomena in nature change repeatedly their spatio-temporal behaviors in rather instantaneous fashions, no matter how the system may be considered to be well represented by a small parameter expansion at an arbitrary moment and

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position. Biological evaluation is such a typical example.

In the meantime, computer appeared, and it now becomes possible to solve any individual complex phenomenon by it. Therefore, the present day computer may well be called the age of "Nonlinear Solver". However as far as we are satisfied only with solving a seemingly complex single phenomenon, computer simulation would act only as a passive role in Science and never open up a new paradigm of Science. The ability of "supercomputer" has currently grown up so that almost any highly tangled phenomena, now called "complex phenomena", can individually be solved. It is now time to go beyond this simple passive stage as the age of Nonlinear Solver, and certainly this can now be done. In this paper proposed is a new scientific methodology for the 21st century that would go beyond the age of Nonlinear Solver. This new age of computer simulation may well be called the age of "Simulation Science".

2. The Strategy of Simulation Science

The Santa Fe Institute is now widely known as the Center of Excellence that challenges the Complexity [1].

《The Santa Fe Strategy for Complexity》

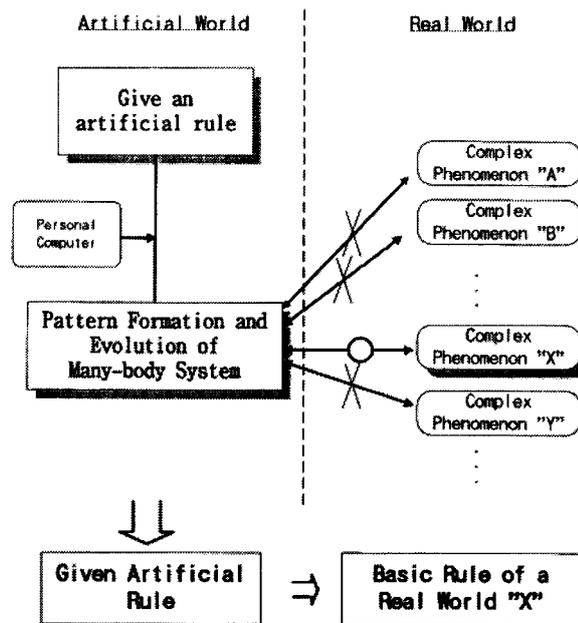


Fig. 1 The Santa Fe Institute Strategy towards the Science of Complexity.

The strategy is the following. First, one gives a simple artificial rule that might govern the behavior of an artificial complex system and simulates its evolution according to the artificial rule by, say, a personal computer. Secondly, one compares the spatial or temporal pattern obtained by the simulation with that occurring in the real world. Then, one hypothesizes that the given artificial rule be the rule of the real world (see, Fig.1) .

In contrast with this approach, our strategy of Simulation Science takes an opposite way in the sense that we directly deal with complex phenomena happening in the real world [2-5]. By fully utilizing advanced technologies such as a supercomputer and periphery visualization devices, we reveal the dynamical evolutions of various complex phenomena of which governing laws are already disclosed by the Modern Science. Then we seek for a universal rule commonly appearing among the revealed complex phenomena and construct a working hypothesis on how order is created in a many-body system, i.e., a self-organization hypothesis. Having this working hypothesis in mind, we

< Strategy of "Simulation Science" >

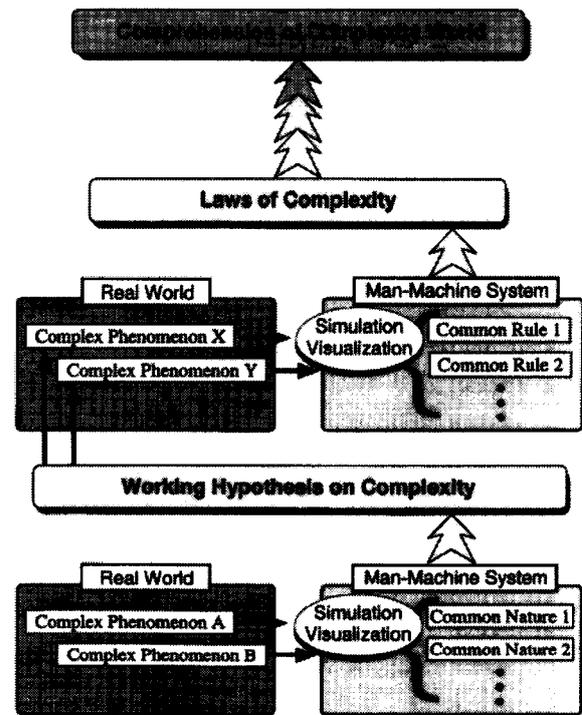


Fig. 2 The NIFS Strategy towards the Science of Complexity (Simulation Science).

predict certain behaviors for other many-body systems with different interaction forces with the hope to endorse or upgrade it. Repeating this process, we hope that the hypothesis will eventually be sublimated into a universal law governing the behaviors of many-body systems (see, Fig.2).

3. Self-Organization Hypothesis

We make a working hypothesis that "openness" and "nonlinearity" are the fundamentals of complexity. Openness implies that the system is subject to "excitation" from an external world and "exhaust" into an external world. Subject to an external excitation, a nonlinear system is non-equilibrated, unless the equilibration rate of the system such as the diffusion rate is large enough. When the non-equilibration goes beyond a certain threshold, the system suffers from deformation (instability). As the deformation grows, the deformation (potential) energy stored by acting against the restoring force to the original structure also grows. Usually a complex system allows discrete structures corresponding to the largeness of excitation energy. Therefore, the deformation of the original structure can not last unlimitedly, but eventually exceeds the bound of the deformation (catastrophic or bifurcation point) and goes into a new state.

Here we turn our eyes to the "exhaust". Excitation is the principal agency of causing self-organization. On the other hand, the exhaust appears to be passive in self-organization. However, it actually plays an important role. In fact, disorderliness or superfluity is inevitably created during the process of order creation. If the disorderliness (so-called entropy in the equilibrium dynamics) is kept in the system, the discreteness may be obscured or may happen to disappear. Thus, it is said that expulsion of disorderliness from the system is largely influential on self-organization.

4. Self-Organization Scenario

Since the scenario is given elsewhere [2-5], we will only present the summary of the simulation results which endorse the scenario. In this work we will not be interested in the spatial pattern itself because it is dependent upon details of the nonlinearity of the system. In other words, the pattern is by large an internal feature. Instead, we are more concerned with the universality irrespective of nonlinearity of the system, or the type of nonlinear interactions such as the long range force or the short range force.

First, we shall examine two extreme cases of

external excitation, namely, sudden excitation and continuous excitation. For various examples where the interaction forces (nonlinearity) are different, we have performed simulations.

Two typical dynamical evolutions for sudden excitation are shown in Fig.3, which represent the stepwise relaxation toward the minimum energy state [6,7]. Also, shown in Fig. 4 are five examples for continuous excitation which exhibit intermittent burst-like evolutions [8-11].

The final examples, Fig.5, shows how the exhaust of disorderliness reflects upon the self-organized structure [11].

Finally, we note that the production rate of disorderliness is maximized when order is most actively

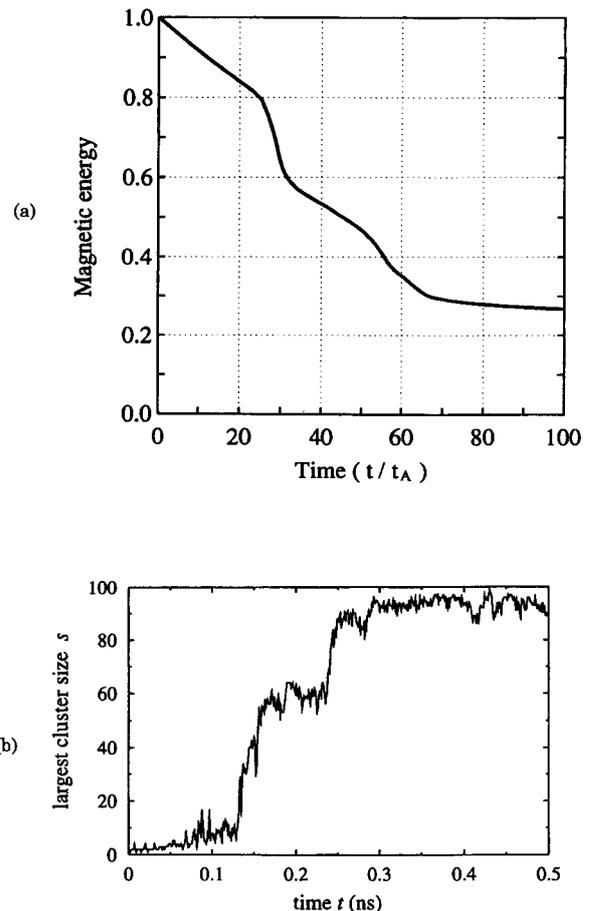


Fig. 3 Stepwise relaxation towards the minimum energy state for a sudden excitation: (a) magnetohydrodynamic self-organization when the system is suddenly excited to a higher energy level [6], (b) polymer crystallization when the heat bath temperature is suddenly decreased [7].

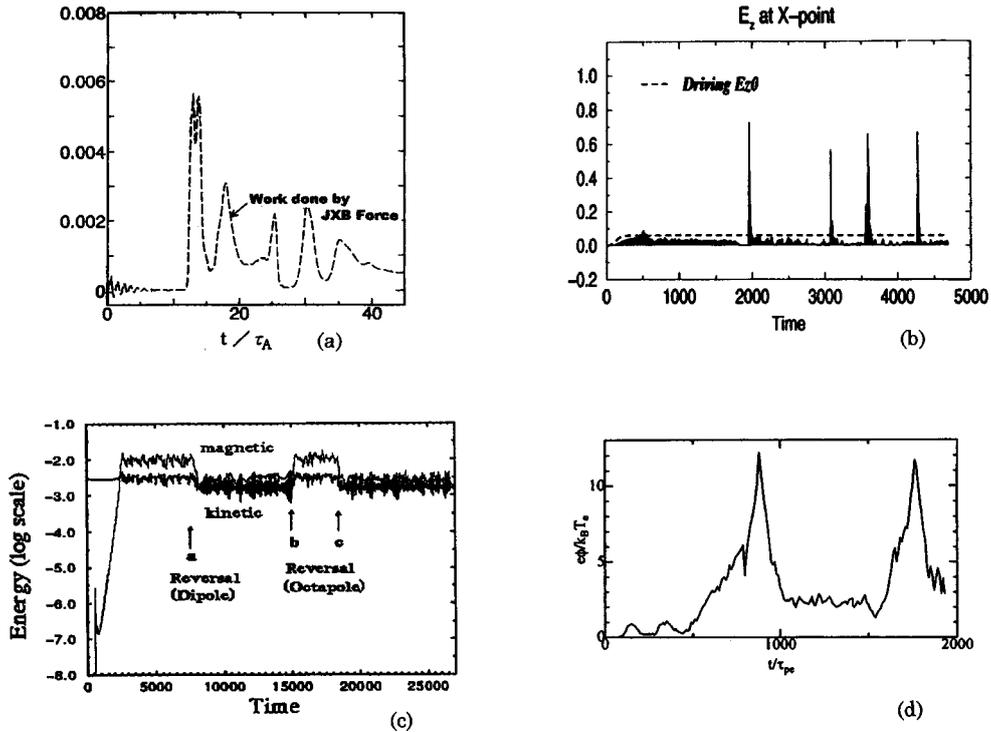


Fig. 4 Intermittent self-adaptive excursions between local maxima and local minima for a continuous excitation: (a) Topological transitions of a continuously twisted flux tube [8], (b) energy releases of a continuously driven magnetic reconnection [9], (c) dipole and octapole reversals of a dynamo problem [10], and (d) formations of giant (super) double layers in a current driven plasma system [11].

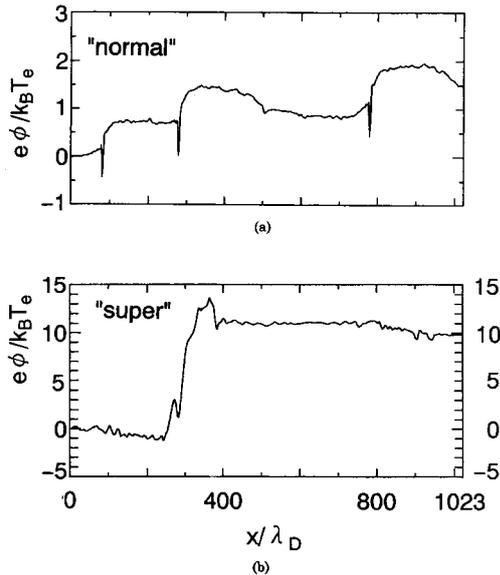


Fig. 5 Difference in the self-organized structure between the disorderliness-reserved system and disorderliness-expulsed system for double layer formation [11]: (a) double layer for the disorderliness-reserved case and (b) giant double layer for the disorderliness-expulsed case.

created, though the quantitative evidences are omitted here because of the limit of space.

5. Summary

We have presented our strategy of opening up a new paradigm for the 21st Century Science by means of advanced supercomputer and visualization technologies, which we name "Simulation Science".

One important successful output derived from this strategy was demonstrated. A universal rule is derived that self-organization evolves in an intermittent fashion for a continuous excitation from an external world, while it relaxes towards a minimum energy state in a stepwise fashion for a sudden excitation. It is also demonstrated that depending upon whether disorderliness is expelled or not, the self-organized structure exhibits a qualitatively different one.

Acknowledgements

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