Classical mechanics, complexity and the methodology

Kuiying Deng

Research on complexity has exploded in recent years, despite the lack of mature theoretical and computational tools. By refining the concepts from complex systems and classical mechanics, here we propose that the methodology developed in classical mechanics over the last four centuries, together with those from other disciplines, might once again nurture the new science of complexity in the coming years.

It is safe to say that the science of mechanics might be the oldest branch of modern science, and it has been playing an irreplaceable role in the development of humankind[1]. However, with the trend of research in complexity arising in recent years[2], which involves almost all branches of natural science[3,4], classical mechanics, as the embodiment of simplicity or reductionism, is gradually fading out of interest of the scientific community, despite its great success in engineering such as NASA's New Frontiers program[5]. Here we propose that, just as the development of relativity theory and quantum mechanics in the 20th century[6], the methodology developed in classical mechanics over the last four centuries, together with those from other disciplines, might once again nurture the new science of complexity in the coming years.

Definition of complex systems

Complexity, the study of complex systems, is a new perspective totally different from traditional reductionism that has long dominated the scientific community. Synthesizing diverse definitions in the literature[4], we define the complex system as one in which two or more distinct agents interact in such a way that its global patterns of behaviour would be reconstructed if any important agents or interactions were removed or significantly changed. In this definition, the following considerations are essential.

(i) Two or more agents. Despite the fact that the literature defines a complex system as consisting of a large number of agents, in our opinion two is enough for complexity. Just as the school of a multitude of fish can amazingly swim in a donut-like shape[3], the double pendulum consisting of two simple pendulums is also not simple; it can exhibit complex chaotic behaviour[7].

(ii) Identical or distinct agents. In stark contrast to emphasizing the complex system consisting of identical or similar multiple agents[8], in our opinion each agent has a different role to play in defining the system[2]. Even originally identical agents finally evolve to be different. For example, the blue-streak cleaner wrasse (*Labroides dimidiatus*) lives in groups consisting of one male and multiple females with a rigid hierarchy. When the male dies or leaves, the top-ranking female changes sex to a male and takes over the harem[9].

(iii) Stability and susceptibility of patterns. The characteristic feature of the complex system is that some patterns emerge due to the collective behaviour of all individual agents that interact with each other[3,8]. However, what patterns are is, to a large extent, based on people's subjective observations. Here we emphasize that patterns should be time-independent and stable under different environments despite the versatility of responses of the system. On the other hand, the removal of any important agent or interaction would cause the reconstruction of patterns of the system, unless they are replaced with other agents or interactions.

The interactions between these considerations result in a complex system, and, roughly put, the definition of a complex system itself could be loosely considered as a complex system. But what is a pattern and how do we describe it are not mentioned in this definition; and they are still challenging.

The recognition of patterns is closely related to modelling levels that are extensively encountered in dealing with complex systems. A scale-free hierarchical architecture exists in living cells[10]. Finite groups have intrinsic structures of levels consisting of simple groups[4]. A pattern pertaining to a certain level usually vanishes in a lower level, despite the converse being true in some special cases such as fractals.

The process of formation of patterns from lower levels by interactions between agents is called emergence. Unpredictability of the emergent patterns is the essential feature of complex systems evolving, and the aim of complexity research is to understand the underlying basic rules, that is, determinism in the midst of chaos[4]. But where the boundary between levels lies, and how to quantitatively measure complexity, are still ambiguous[3,4].

The controversy between emergentists and reductionists has already lasted for decades, especially in the community of physics. Traditional reductionists devote themselves to constructing the theory of everything, whereas emergentists advocate the end of reductionism[11]. The prediction and exploration of the cosmic microwave radiation in the second half of the last century are the triumph both of cosmology and reductionism[12]. Here we prefer to believe that complexity and simplicity are two perspectives of the complex system. They are mutually reinforcing and need to be explored by emergentists and reductionists working together.

Background from structural dynamics

In the last four centuries, the science of classical mechanics has developed rich tools to deal with complex mechanical systems. Not only is the turbulent flow in fluid dynamics a perfect example of complexity, but two main theoretical views widely adopted in complexity research, Eulerian and Lagrangian, also actually originated from fluid dynamics[3]. In particular, the subject matter of analytical mechanics and structural dynamics is to study the dynamical behaviour of the complex mechanical system consisting of many particles and components that are linked to each other[6,13].

One of the foundations of analytical mechanics is Hamilton's principle, which is equivalent to Newton's laws in nature.

Instead of dealing with interacting forces between components, Hamilton's principle adopts the concept of action function

$$I = \int_{t_1}^{t_2} L(q,\dot{q},t)\mathrm{d}t, \quad (1)$$

to describe the state of a dynamical system, where q is the vector of generalized coordinates, and $L(q,\dot{q},t)$ is the Lagrangian defined as the kinetic energy of a system minus its potential energy. Hamilton's principle states that the real path, out of all virtual paths satisfying both the start and end constraints, makes the variation of the action function vanish[11]. That is, the real path of the system satisfies

$$\delta I = 0. \quad (2)$$

Classical mechanics adopts the concept of degree of freedom (DOF) to describe the complexity of the mechanical system. Discrete systems such as a mass-spring system have finite DOFs, whereas continuous systems such as a beam or a plate have infinite DOFs. For the discrete holonomic system, the number of DOFs is equal to that of generalized coordinates. The ordinary and partial differential equations governing the dynamical behaviour of the former and the latter respectively, can be derived from Hamilton's principle.

The response of a mechanical system can be extended in the modal space by the normal mode analysis technique. In other words, the response can be expressed as the linear sum of time-independent natural modes. That is

$$x(t) = \sum_{i=1}^{n} c_i(t)\xi_i, \quad (3)$$

where n is the number of DOFs, $c_i(t)$ are time-dependent weighted coefficients, and ξ_i are time-independent normal modes, which are the natural features of the system whenever it bears external forces or not.

The system has different responses corresponding to different external environments, but its normal modes remain unvaried[14]. Hence the normal modes of a dynamical system are actually the emergent patterns describing its collective behaviour, according to the definition of the complex system, which emerge from components interacting with each other. One crucial feature of normal modes is that they would not change with external forces, whereas they would be reconstructed if any important components or interactions are removed or significantly changed.

The Rayleigh–Ritz method can greatly reduce the complexity of dealing with the mechanical system by assuming the lowest several modes when computing its dynamical responses. That is, it is assumed that

$$x(t) \approx \hat{x}(t) = \sum_{i=1}^{\hat{n}} c_i(t)\hat{\xi}_i \quad (4)$$

where $\hat{n} \ll n$, and $\hat{\xi}_i$ are assumed modes. The more similar the assumed modes $\hat{\xi}_i$ are to the actual ones ξ_i, the higher the accuracy of computation is. However, the difficulty of assuming proper modes increases with the increasing complexity of the system. Then the finite element method (FEM) greatly extends its capability as a substitute.

Instead of assuming the global modes of the system, FEM hypothetically breaks the system into many small pieces called finite elements, and then computes the responses of the system by assuming the shape functions of those finite elements, which are far simple compared to the global modes of the system. Usually linear shape functions are enough to satisfy the accuracy requirements in engineering applications. It is easily implemented to enhance the accuracy of computations either by increasing the number of finite elements or by increasing the order of shape functions. Commercial software of FEM analysis such as Nastran and Ansys are widely used in engineering.

In face of the increasing complexity of modern mechanical systems such as huge airplanes and launch vehicles, several substructure synthesis techniques have been developed, such as component-mode synthesis and branch-mode analysis. The dynamic characteristics of the system are gained by integrating together the lowest several modes of its substructures, which are relatively simple and can be analysed by FEM. These techniques dramatically reduce the number of DOFs of the system without losing its important physical characteristics. One especially valuable feature is that there is no need to recalculate the whole structure when any substructure is redesigned.

In terms of complexity theory, we can sum up as follows how classical mechanics deals with the complexity of mechanical systems. The nonlinear modes of substructures emerge from a large number of finite elements with linear shape functions, while the global complex modes of the system emerge from those of two or more substructures. Finite elements, substructures and the system form three intrinsic levels of dealing with the dynamic behaviour of complex mechanical systems (Figure 1). More importantly, the time-dependent responses of the system emerge as the linear sum of their time-independent

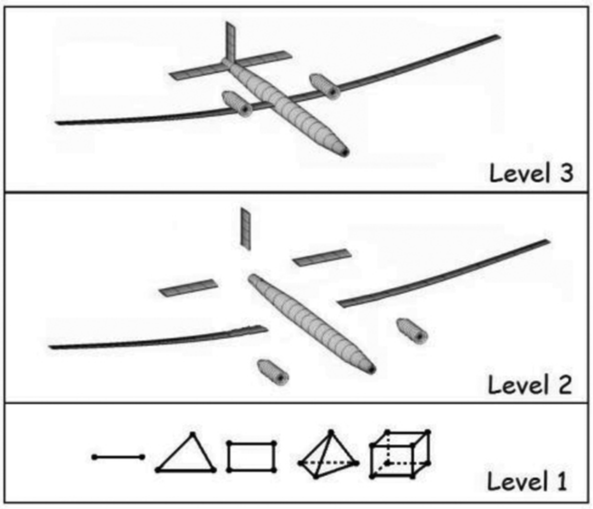

Figure 1. Levels of analysis of an airplane in structural dynamics. Level 1: finite elements; level 2: substructures; and level 3: the system. (Note: the finite element model of the airplane is from http://aerospace.engin.umich.edu/research/structure.html).

normal modes, and the responses can be well approximated by the linear sum of several lowest assumed modes, the number of which is far less than that of DOFs of the system itself.

The methodology

At present, two important methods of conducting research on complexity are complex networks[15] and game theory[16]. The former studies different topological structures of interactions between agents by tools from graph theory, such as small-world networks and scale-free networks[17]. The latter studies strategic interactions between self-interested agents, considered to be a promising framework of integrating many branches of social and natural sciences[18]. The evolution of cooperation among self-interested agents, one of the far-reaching areas related to complexity, has already attracted broad interests across disciplines lately[19], much work of which is based on game theory and complex networks[20]. Research shows that topological structures have an indispensable effect on the evolution of cooperation in the society of humans or animals[21].

The theory of complex networks studies how the topology of complex systems is formed. Scale-free networks form by two mechanisms of growth and preferential attachment. The small-world feature and the power law distribution of degrees of nodes can be considered as emergent patterns of the network[17,22]. Despite the fact that they do not sufficiently reveal how the topology of networks evolves in the real world, network theory paves the way for handling complexity in a sense[2].

Game theory considers adaption of agents to each other. As its extension, evolutionary game dynamics incorporates the principles of natural selection[23], while Darwinian dynamics constructs a fitness-generating function (G-function) approach to continuous-trait evolutionary games, which allows for simultaneous consideration of population dynamics and strategy dynamics[24]. Nevertheless, an important feature of complex systems, adaption to environments, has not attracted much attention, which might be a promising research topic[25].

However, due to lack of proper mathematical tools, current research in complexity is, in large part, conducted by computer simulations. Based on the above discussion, we propose that structural dynamics might assist in research on the dynamical behaviour of complex systems with a total set of theoretical and computational tools, if at least the following considerations could be incorporated.

(i) Modelling levels and emergence. It is especially important to choose proper levels to model emergent patterns. Do not model bulldozers with quarks[26]. It is unnecessary to model a living organism starting from carbon, hydrogen, oxygen and nitrogen. In our opinion, it may be appropriate that the process of modelling starts from the level just lower by one than the level we concern. FEM shows that nonlinear dynamic responses at the higher level can emerge sufficiently from linear elements at the lower level.

(ii) Memory and stability. Different agents play different roles in the complex system. There must exist special agents responsible for the memory of patterns, which is important for the stability of a system. The memory of artificial neural networks is ruined once any link between neurons is destroyed[27], whereas the human brain allocating special areas to store memory shows sufficient stability. One of the characteristic features of computers is the separation of software and hardware[3], which makes software live forever in theory.

(iii) Agent intelligence and interactions. Patterns emerging from interactions should develop some kind of function or intelligence. The stronger the relations between agents, the smarter the complex system should be. Relations between agents are actually some kind of constraints to activities of self-interested agents[3]. The intelligence of individual agents should decrease with relations between them getting stronger. In the prisoner's dilemma, each agent has two choices of cooperation or defection, but if they are closely related, such as in the setting of siblings or couples, then cooperation is the only rational strategy corresponding to the much stronger relations between them; as a result, two agents as a unit gain maximum payoff[25,28].

Outlook

In fact, classical mechanics does not go out of date, noting that the special theory of relativity is an extension of it, and how much closely similar the fundamental equations of quantum mechanics are to those of analytical mechanics[6]. Since 1980s, the normal mode analysis has been widely applied in the dynamic analysis of protein macro-molecules, a kind of typical complex system, to explain their slow, large-amplitude motions, which are essential for the functions of proteins[29]. The component-mode synthesis methods have been applied in the study of molecular biology[30]. Both methods also originated from structural dynamics, and unexpectedly they are brought to deal with complexity in biology.

What we already know usually contributes much to the understanding of novel and complex phenomena. In our opinion, the future development of complexity theory would no doubt benefit much from the rich and effective theoretical tools developed in classical mechanics, especially in analytical mechanics and structural dynamics which deal with complex mechanical systems.

1. Mach, E., *The Science of Mechanics: A Critical and Historical Account of its Development*, Open Court Publishing Co., Chicago, 1907.
2. Barabási, A.-L., *Nature Phys*., 2005, **1**, 68–70.
3. Koch, C. and Laurent, G., *Science*, 1999, **284**, 96–98; Parrish, J. K. and Edelstein-Keshet, L., *Science*, 1999, **284**, 99–101.
4. Rind, D., *Science*, 1999, **284**, 105–107; Whitesides, G. M. and Ismagilov, R. F., *Science*, 1999, **284**, 89–92; Pearce, N. and Merletti, F., *Epidemiology*, 2006, **35**, 515–519; Foote, R., *Science*, 2007, **318**, 410–412.
5. Baker, J., *Science*, 2007, **318**, 215; Krupp, N., *Science*, 2007, **318**, 216–217.
6. Johns, O. D., *Analytical Mechanics for Relativity Theory and Quantum Mechanics*, Oxford University Press, New York, 2005.
7. Stachowiak, T. and Okada, T., *Chaos, Solitons Fractals*, 2006, **29**, 417–422.
8. Vicsek, T., *Nature*, 2001, **411**, 421.
9. Robertson, D. R., *Science*, 1972, **177**, 1007–1009.
10. Oltvai, Z. N. and Barabási, A.-L., *Science*, 2002, **298**, 763–764.
11. Anderson, P. W., *Science*, 1972, **177**, 393–396; Laughlin, R. B. and Pines, D., *Proc. Natl. Acad. Sci. USA*, 2000, **97**, 28–31.
12. Wolfenstein, L., *Proc. Natl. Acad. Sci. USA*, 2003, **100**, 5001–5003.
13. Meirovitch, L., *Computational Methods in Structural Dynamics*, Sijthoff & Noordhoff, Maryland, 1980.

14. Gladwel, G. M. L., *Proc. R. Soc. London, Ser. A*, 1985, **401**, 299–315.
15. Strogatz, S. H., *Nature*, 2001, **410**, 268–276; Newman, M. E. J., *SIAM Rev*., 2003, **45**, 167–256.
16. von Neumann, J. and Morgenstern, O., *Theory of Games and Economic Behavior*, Princeton University Press, Princeton, New Jersey, 1944; Deng, K., Ph D dissertation, Peking University, Beijing, 2012.
17. Watts, D. J. and Strogatz, S. H., *Nature*, 1998, **393**, 440–442; Barabási, A.-L. and Albert, R., *Science*, 1999, **286**, 509–512.
18. Binmore, K. G., *Playing for Real: A Text on Game Theory*, Oxford University Press, New York, 2007.
19. Pennisi, E., *Science*, 2005, **309**, 93–93; Pennisi, E., *Science*, 2009, **325**, 1196–1199.
20. Nowak, M. A., *Science*, 2006, **314**, 1560–1563; Boyd, R., Gintis, H. and Bowles, S., *Science*, 2010, **328**, 617–620; Gintis, H., *J. Theor. Biol*., 2000, **206**, 169–179; Deng, K., Gintis, H. and Chu, T., *J. Theor. Biol*., 2011, **268**, 141–145; Deng, K., Li, Z. and Chu, T., In Proceedings of the 15th IEEE International Conference on Engineering of Complex Computer Systems, Oxford, 2010, pp. 296–301; Deng, K., Li, Z., Kurokawa, S. and Chu, T., *Theor. Popul. Biol*., 2012, **81**, 284–291; Hauser, O. P., Rand, D. G., Peysakhovich, A. and Nowak, M. A., *Nature*, 2014, **511**, 220–223; Stewart, A. J. and Plotkin, J. B., *Proc. Natl. Acad. Sci. USA*, 2014, **111**, 17558–17563.
21. Hauert, C. and Doebeli, M., *Nature*, 2004, **284**, 87–89; Lieberman, E., Hauert, C. and Nowak, M. A., *Nature*, 2005, **433**, 312–316; Ohtsuki, H., Hauert, C., Lieberman, E. and Nowak, M. A., *Nature*, 2006, **441**, 502–505.
22. Deng, K. and Huang, Y., *Curr. Sci*., 2013, **105**, 755–756.
23. Nowak, M. A., *Evolutionary Dynamics: Exploring the Equations of Life*, Belknap Press of Harvard University Press, Cambridge, Mass., 2006.
24. Vincent, T. L. and Brown, J. S., *Evolutionary Game Theory, Natural Selection, and Darwinian Dynamics*, Cambridge University Press, Cambridge, UK, 2005; Brown, J. S. and Vincent, T. L., *Proc. R. Soc. London, Ser. B*, 2008, **275**, 1985–1994; Deng, K. and Chu, T., *PLoS ONE*, 2011, **6**, e25496/1–9.
25. Deng, K. and Chu, T., *PLoS ONE*, 2011, **6**, e19014/1–9; Deng, K., Presented at the 27th International Conference on Game Theory, New York, 2016.
26. Goldenfeld, N. and Kadanoff, L. P., *Science*, 1999, **284**, 87–89.
27. Haykin, S. S., *Neural Networks: A Comprehensive Foundation*, Prentice Hall, New Jersey, 1999.
28. Axelrod, R. and Hamilton, W. D., *Science*, 1981, **211**, 1390–1396; Deng, K. and Chu, T., *Int. Econ. Lett*., 2013, **2**, 30–41.
29. Levitt, M., Sander, C. and Stern, P. S., *J. Mol. Biol*., 1985, **181**, 423–447; Alexandrov, V. *et al*., *Protein Sci*., 2005, **14**, 633–643.
30. Ming, D., Kong, Y., Wu, Y. and Ma, J., *Proc. Natl. Acad. Sci. USA*, 2003, **100**, 104–109.

ACKNOWLEDGEMENT. This work was supported by the recruitment programme of excellent talents of Hebei University (No. 2014-304).

Kuiying Deng is in the Department of Engineering Mechanics, Hebei University, Baoding 071002, China, and State Key Laboratory for Turbulence and Complex Systems, College of Engineering, Peking University, Beijing 100871, China.
e-mail: RossDeng@pku.edu.cn