



Views & Comments

Exploring the Logic and Landscape of the Knowledge System: Multilevel Structures, Each Multiscaled with Complexity at the Mesoscale

Jinghai Li

Vice President of International Council for Science

State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China

1. Breaking habitual thinking patterns

Breaking the patterns of habitual thinking is crucial in order to welcome a new revolution of science and technology (S&T) and to realize a new paradigm of scientific research. We are facing a new era for S&T, in which there are more opportunities than challenges. However, this new era calls for governments and scientific communities to recognize that the most important issue might be something other than discussions of investment and rewards.

Contemporary science achieved remarkable progress in the 20th century, contributing to the expansion of knowledge and human capability in sustainable development. As science continues to expand in both temporal and spatial dimensions, it has given rise to many new technologies. In particular, the development of energy, materials, information, and biological technologies has fundamentally changed the production mode and lifestyle of human beings, and promoted civilization.

On the other hand, people have gradually come to realize that, while new challenges in human sustainable development demand solutions, some problems in nature, engineering, social science, and humanity itself cannot be solved based on currently available knowledge. Reductionism focuses on details at smaller and smaller scales, while holism emphasizes global behaviors. Bridging these two perspectives is still not possible. As a result, it is difficult to establish correlations between different levels of a system or between different scales on the same level, severely limiting human capability in sustainable development and presenting challenges to both natural and social science.

Meanwhile, the progress of information technology and the explosive expansion of knowledge are propelling the possible emergence of a new scientific research paradigm [1]. Transdisciplinarity [2–5] and the integration of different disciplines are believed to be the main path [3] to new breakthroughs. Contemporary science is becoming more and more open and globalized. At such a time, when opportunities are greater than challenges, all countries around the world have promulgated various key research programs, reconstructed their national innovation systems, and placed increasing expectations on contributions from S&T. A new S&T revolution is being widely anticipated.

Scientific communities in all countries are appealing to their governments to increase S&T investment, and in turn, govern-

ments are more eager than ever to see rewards from their investment. Therefore, relationships among governments, industries, universities, and research institutions are drawing more and more attention from all levels of society, and seem even more complicated than the science itself.

Increasing S&T investment and promoting coordination between governments, industries, universities, and research institutions are certainly important. However, has this single-minded focus detracted attention from other issues that may have a greater influence on the evolution of S&T? This author posits that the evolution of S&T itself is being widely overlooked and may play a more critical role in responding to global challenges, accelerating scientific progresses, and creating a new scientific research paradigm than is currently acknowledged. For example:

- The knowledge system and its missing links: Can we sort out the logical relationship and architecture of scientific knowledge on the basis of current understandings, so as to optimize the layout of modern S&T and further identify the missing links in the knowledge system?
- Actions driving a new paradigm: Facing the waves of big data, open access to knowledge, and globalization of scientific research, how do we rationally guide and drive the formation and development of a new scientific research paradigm, as opposed to passively waiting for its appearance?

In addition, understanding the logic and structure of the knowledge system and the resulting shift in scientific research paradigms will pose a series of new requirements in the structure and management of innovation systems and education systems in all countries. This paper breaks away from habitual thinking and attempts to explore these questions.

2. Clarifying the logic and structure of the contemporary knowledge system

The logic and structure of the contemporary knowledge system should be systematically clarified, with the logic and structure of scientific knowledge and applied technology as well as the relationship between them becoming the basis for the layout of the research and development (R&D) and educational systems. By clarifying the structure and logic of the knowledge system, all the disciplines and fields of S&T can be organized into a logical land-

scape. Such an organization will promote transdisciplinarity and the integration of different disciplines, greatly enhance the efficiency of scientific research, and accelerate the progress of S&T.

The research objects of all disciplines and fields include the physical world, chemical science, life science, social science, and many others. These objects have logical relationships with each other; therefore, the knowledge and technologies arising from them should follow the same structure and logic.

However, the current layout of disciplines and fields is not based on this inherent structure and logic; rather, it evolved gradually from the classification of specific problems of interest under the condition of very limited human understanding and probably under the irrational influence of accidental or human factors. When viewed objectively, the current layout lacks a systematic consideration of the entire knowledge system. For example, basic disciplines include math, physics, chemistry, astronomy, geoscience, and biology, each of which has been further divided into various sub-disciplines. Applied fields include energy, materials, information, the environment, and so forth, each of which has been further divided into a number of sub-fields. Such divisions and sub-divisions give rise to many crossover disciplines and fields—that is, interdisciplines. Statistics show that there are currently about 8530 definable disciplines and fields [2]. Since there is no systematic logic connecting all these disciplines and fields, it is difficult to clearly see the intrinsic relationships among different aspects of knowledge. In addition, although the detailed classification of disciplines, fields, and their branches certainly has a positive influence on the initial stages of their development, it can imperceptibly lead to isolation between disciplines and fields in later stages of development. Such isolation is not conducive to seamless transdisciplinarity and integration; hence, it presents barriers to the future development of S&T.

Therefore, we have every reason to ask the following questions: What are the logical relationships among various disciplines? Are there any rules among the various aspects of knowledge that have already been accumulated? Is it possible to break the present classification of disciplines and fields and sketch out a better layout of S&T according to the logical relationships of existing knowledge? Are there any missing links in the current knowledge system? If yes, do they constitute bottleneck problems in the development of modern S&T? All of these questions need

serious consideration at present, and may be more important than the debate on investment and rewards.

Clarifying the logical relationships among different disciplines and fields, based on the current accumulation of knowledge in S&T, is not only conducive to the development and organization of scientific research institutions, but also facilitative to transdisciplinarity [3] and the achievement of a seamless integration of related disciplines, ultimately minimizing repetition and promoting cooperation. Meanwhile, it will greatly promote the reconstruction of the education system and the cultivation of transdisciplinary talents. In this sense, the structure and logic of the knowledge system should meet the following criteria:

- Similarity: The logic and structure of the scientific knowledge system should be consistent with those of the research objects from which knowledge originates.
- Universality: Maximum effort should be made to extract common principles and to reduce any repetition and fragmentation in the knowledge system, thereby fostering transdisciplinarity and integration.
- Adaptability: The hierarchical logic and structure of research objects and the knowledge system should be organically unified with major socioeconomic needs so as to cope with global challenges more scientifically under the full support of the knowledge system.

3. The multilevel, multiscale attributes and mesoscale complexity of the knowledge system

More attention should be paid to the multilevel, multiscale attributes and mesoscale complexity of the knowledge system. The hierarchical structures of the physical world and of humanity itself, as well as the logical relationships therein, manifest as a multilevel architecture, and each level manifests as a multiscale structure. It is the core task for contemporary science to establish the relationships among the different scales on each level and the correlation among different levels. The mesoscale structure on each level is the key to achieving this core task. Therefore, “multilevel,” “multiscale,” and “mesoscale” attributes will be the prominent characteristics of a reasonable knowledge system.

The research objects of S&T, listed in Fig. 1, include: the **physical world**, the **chemical science** developed during the processes

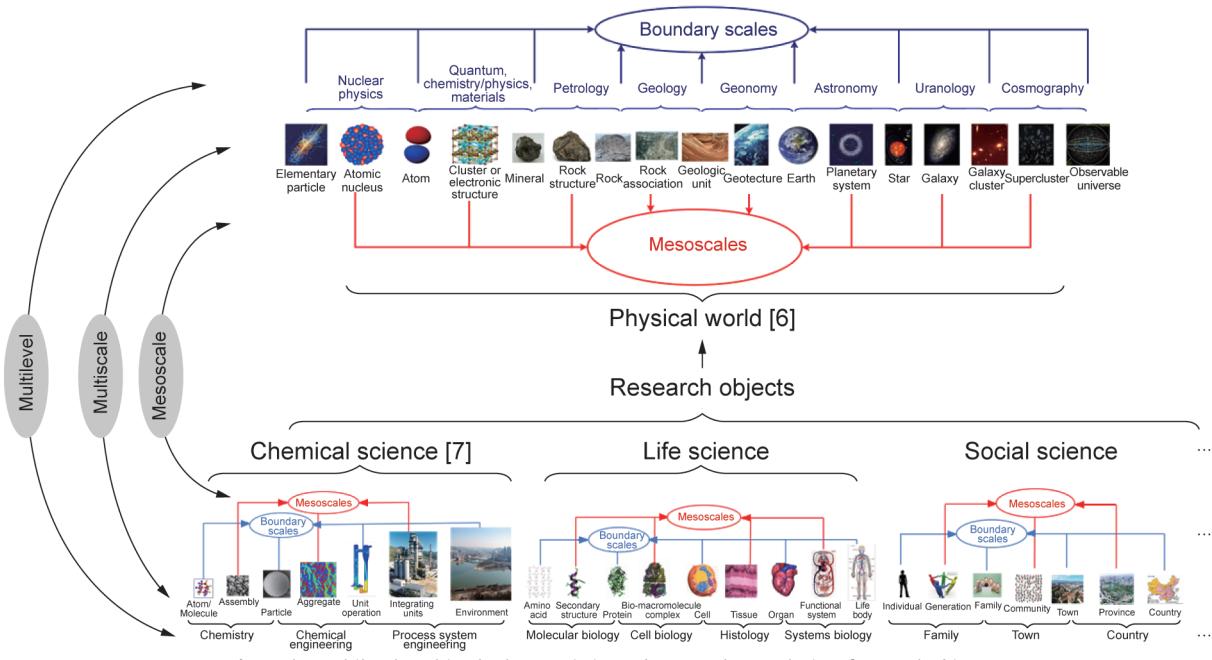


Fig. 1. The multilevel, multiscale characteristics and mesoscale complexity of research objects.

of human activities in production, the **life science** developed during the process of humanity coming to understand itself, and **social science** devoted to understanding human behaviors.

The prefix “meso” originates from the ancient Greek word *mesos*, meaning “middle” or “in between.” When studying problems or processes, it is common to consider a “system” as consisting of a large number of “elements.” The system is also subject to influences at a boundary defined between the system domain and its surroundings. The mesoscale here is not an absolute physical dimension of size, but a relative concept to describe phenomena and processes that manifest between element scales and system scales. These mesoscales could be at different levels of the physical world and in different physical dimensions [7]. The mesoscopic scale traditionally discussed in physics is just one mesoscale between the molecular scale and bulk material scale [8].

Traditional methods focus on the element scale and system scale on each level, while the dynamic heterogeneous structures that the mesoscale phenomena between elements and systems manifest are the common challenge of all fields. It should be noted that mesoscale processes are not only field-dependent, but also level-specific within a field, as described in Fig. 1; this characteristic gives rise to the complexity inherent in mesoscale problems.

3.1. The physical world

Under the Big Bang hypothesis, the elementary particles that were formed in the initial expansion aggregate into different atoms in an extremely non-equilibrium dynamic process; these different atoms further aggregate into molecules and macroscopic materials or minerals. Different minerals constitute rocks, and rocks constitute geological units, which further constitute the earth and all kinds of celestial bodies, and so on, through to the universe. Therefore, there are multilevel, multiscale structures between elementary particles and the universe. Historical development of knowledge gives rise to different disciplines at different levels that are difficult to integrate. On the one hand, this is a natural reflection of the nature of the knowledge system; on the other hand, this multilevel nature leads to isolation between levels. The object of a “system” for a discipline is an “element” to its contiguous discipline, and vice versa. Therefore, the terms and methods for the same research object, particularly at boundary scales, may vary greatly in different disciplines, leading to isolation between disciplines. This has long been a problem in S&T, and one on which insufficient effort has been focused, even though the problem has been recognized.

3.2. Chemical science

Chemical science also manifests multilevel and multiscale characteristics. As research goes deeper, our understanding of the multilevel and multiscale characteristics of chemical science grows clearer and clearer. The process of material transformation involves three levels: material, reactor, and environment [7]. These levels respectively correspond to the different phases of material processing R&D, that is, material innovation, process equipment R&D, and system integration. Specifically, each level contains the element scale, mesoscale, and system scale. Although the research content and objects on the three levels are entirely different, resulting in different sub-disciplines, they have the following attributes in common: ① The three levels all have multiscale characteristics; ② the boundary scales involved in the three levels (i.e., atom/molecule, particle, unit equipment, and ecological environment) have been deeply explored in traditional studies, leading to the formation of the different disciplines of

chemistry, chemical engineering, and process system engineering; and ③ the mesoscale problems between the two boundary scales on each of the three levels are very poorly understood, and form bottlenecks in material innovation, process equipment scale-up, and system integration. These issues have become focal problems in chemical science and engineering R&D, and are preventing further breakthroughs toward the goal of sustainable development.

3.3. Life science

The life system also manifests as classic multilevel, multiscale, and mesoscale structures, and the research objects, contents, and methods differ on different levels. All four levels show multiscale characteristics: the bio-macromolecular level includes amino acids and nucleotides, secondary structures and proteins; the cellular level includes bio-macromolecules such as proteins, super molecular machines or sub-cellular organelles formed by many molecules (including bio-macromolecules and other molecules), and cells; the organ level consists of cells, tissues, and functional organs; and the living entity level is composed of organs, functional systems (such as the digestive system, blood system, and nervous system), and the complete living entity. The boundary scales involved in the four levels—that is, the elementary molecules, bio-macromolecules, cells, organs, and living entity—have been explored deeply in traditional theoretical research, leading to the formation of different disciplines: molecular biology, cellular biology, histology, and systems biology. However, the mesoscale problems between the two boundary scales on each of the four levels are very poorly understood, resulting in bottleneck problems in non-coding ribonucleic acid (RNA) and dynamic protein structure, organelle regulation, and tissue and functional systems, respectively. These have become the unresolved focal problems in modern biological and medical R&D, breakthroughs of which will lead to revolutionary progress in life science.

3.4. Social science

Social science is a major category of academic disciplines, concerned with society and the relationships among individuals within a society [9]. It also features multiple levels, such as family, town, country, and so on, multiple scales on each level, and mesoscale complexities within each level. That is, the collective phenomena at each level are also the most challenging problems in respective sub-branches of this field, although this premise will not be elaborated in this article.

3.5. The common attribute of the four categories of science

The above four categories of research objects, also shown in Fig. 1, are only representative selections of scientific research. In fact, many other research objects exist that are not in the form of visible objects, but which also show multilevel, multiscale characteristics and mesoscale complexity, such as the nervous and cognitive system, linguistic logic and structure, and so forth. Regardless of the specific research objects, the common attribute for the four categories of science is prominent: All possess multilevel systems, and each level is multiscaled, with mesoscale complexity between the unit scale and the system scale.

Recent studies suggest that mesoscale problems on multiple levels have become a common, great challenge for realizing the quantification of all levels and the correlation between different levels [6–8,10,11]. Although all mesoscale problems manifest diversity and complexity, they are likely to meet a common principle governing their common natures, such as heterogeneity,

dynamics and phase separation, and so forth. A branch of modern science usually takes one level as its research object. The fusion and integration of different levels is still very difficult. On a single level (or sub-discipline), modern science pays more attention to its element and system scales, yet insufficient attention to its mesoscale problem standing between element and system. As a result, researchers have to adopt average approaches to treat the mesoscale heterogeneity. Thus, there emerges a science of complexity that attempts to link microscale with macroscale. However, the science of complexity does not pay sufficient attention to the mesoscale problems on different levels, nor does it recognize the missing scientific principle common for all mesoscales. This is the fundamental reason and driving force as to why the concept of mesoscience is proposed [6–8,10,11].

4. Integrating the knowledge and technological systems into a single landscape

The knowledge system and the technological system could be integrated into a single landscape. Generally speaking, the structure and logic of all applied fields involve the same scientific knowledge category; the only difference lies in the manifestation of the problems solved by using the knowledge. Therefore, all applied fields also possess multilevel, multiscale, and mesoscale characteristics, and can be integrated with the knowledge system into a single unified logic landscape.

Specific technological or applied fields are all developed based on the above levels of knowledge, and in the course of development, they provide concrete evidence for identifying common rules in the knowledge system. Therefore, the increasingly blurry boundary between science and technology is exactly a result of this attribute.

According to the similarity of the involved research content, we can preliminarily merge the main technical research related to sustainable development, such as energy, materials, information, earth systems and climate, life and health, agriculture, space, and so forth, into the multilevel knowledge system. (There are, of course, other ways of classification, but they do not affect our analysis of the relationship between knowledge and technological fields.) Every field involves the above multilevel, multiscale knowledge in its development, and is different from every other field only in the objective of application. Here, the engineering

level is much more diverse than other levels, with respect to different fields.

However, due to limited understanding, studies on common basic scientific problems are referred to as “fundamental research,” and studies on applying knowledge to solve concrete problems are referred to as “applied research.” It seems that such a classification is neither conducive to the transdisciplinarity of different fields, nor conducive to the integration of different knowledge sub-systems. It is believed that with increased understanding of the knowledge system, such differentiations will gradually fade away.

Based on the discussion in the above two sections, and taking into consideration the multilevel, multiscale attributes of existing knowledge and nature, we can come up with the relationship between the knowledge system and the applied fields; that is, the layout or landscape of S&T, as shown in Fig. 2. The concentric circles in this diagram refer to knowledge, which involves multiple levels including elementary particles, molecules/atoms, materials, engineering, geosciences, space, astronomy, and the universe. The lines radiating out from the center refer to fields where knowledge is applied, and traverse all levels of knowledge for each field. The center of the diagram refers to the tools, theories, methods, and knowledge commonly used for all R&D activities, such as mathematics, mechanics, system science, and so forth. Organizing scientific research according to the structure and logic outlined in Fig. 2 is expected to raise the efficiency of innovation systems, making the organization of research activities more rational. Of course, Fig. 2 is certainly not a complete picture, but merely a rough frame that needs further improvement. However, although different people may suggest different organizational schemes, the landscape described in Fig. 2 should not vary much.

5. Closing gaps in the existing knowledge system

Gaps in the existing knowledge system should be closed. The mesoscale problems at all levels are common missing links in the knowledge system and, in particular, may follow a common principle. The discovery and confirmation of this principle will induce revolutionary progress in S&T.

In the above multilevel knowledge system, researchers are usually more concerned with the element and the system on each level (i.e., boundary scales), and with how multiple elements

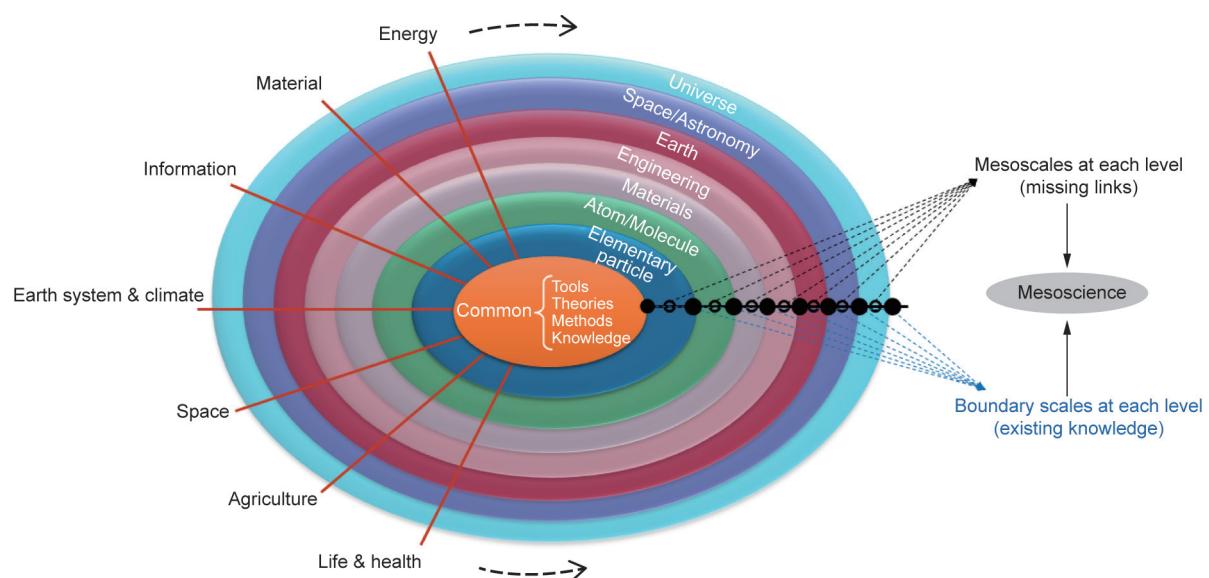


Fig. 2. Conceptual model of the landscape of science and technology.

constitute a system, in an attempt to correlate element behaviors with system behaviors. Such level-specific understanding gradually leads to the formation of various sub-disciplines. However, researchers have gradually come to realize that the element behaviors on each level are relatively simple and can be described with existing knowledge, while the interaction among elements, which largely determines the attributes of the system on the same level (i.e., the element for its neighboring level), is very complicated and cannot be solved by traditional theories and methods. The mesoscale problems are usually approached merely according to experimental phenomena or based on assumptions: Statistical mechanics hypothesizes the distribution function, fluid hydrodynamics hypothesizes the constitutive equation, and astronomy even speculates average parameters over numerous stars and galaxies. Neglecting the mesoscale processes and their governing principles has created a missing link in modern scientific knowledge and a serious obstacle preventing S&T from further development. For example, many problems in engineering still rely on average treatment without considering mesoscale structures; similarly, many forms of engineering software for computing turbulence, chemical processes, weather, and climate tend to coarse-grain parameters within computational grids according to empirical parameters or assumptions. Some disciplines have not even realized the importance of mesoscales, even though they have been working on such scales. Much of the research with the multiscale concept pays attention to element scales and system scales without emphasizing mesoscales, neglecting the important governing rules there. This situation has changed in recent years, but the focus on mesoscales is not yet sufficient. The seamless integration of knowledge on different levels is even more difficult. In addition, in a complete process, a boundary scale between two neighboring levels is subject to both levels of processes, which are dependent on the respective mesoscales at the corresponding levels. Therefore, it is clear that a boundary scale between two levels can be completely resolved only when the two mesoscales involved are understood. That is, the traditional knowledge on boundary scales also needs to be upgraded in relation to the mesoscale effects.

In recent years, the concept of mesoscience has brought attention to this issue. More importantly, it has led to the assertion that the mesoscale problems on different levels for different fields may follow a common physical principle and be formulated by a unified mathematical framework [6,8]. Once this concept is confirmed and developed into a transdisciplinary science, the

missing links in the existing knowledge system will be filled, forcefully driving the advancement and integration of all disciplines. Therefore, mesoscience could be a common frontier of all disciplines and fields that is worth great attention across the whole spectrum of S&T, and which should belong to the knowledge category at the center of Fig. 2.

Progress has been made in chemical engineering [6,7,10–12], from a specific mesoscale modeling for gas-solid systems (the so-called energy-minimization multiscale (EMMS) model) to a general principle of compromise in competition between dominant mechanisms (the EMMS principle). It is believed that all mesoscale problems or processes are dominated jointly by at least two mechanisms. Here, we consider Mechanism A = extremum 1 and Mechanism B = extremum 2, jointly governing the system behavior, as a general case in order to simplify later discussion. The A- and B-dominated states coexist in an alternating manner with respect to both time and space [6]. Therefore, the variational criterion for the system can be physically expressed as compromise in competition between dominant mechanisms, and can be mathematically formulated into a multi-objective variational problem, that is, the EMMS principle [6–8]:

Structural variables:

$$\mathbf{X} = \{x_1, x_2, \dots, x_n\}$$

Compromise between competing mechanisms:

$$\text{Extremalizing } \begin{pmatrix} A(\mathbf{X}) \\ B(\mathbf{X}) \end{pmatrix}$$

Subject to conservation laws:

$$F_i(\mathbf{X}) = 0, i = 1, 2, \dots, m \quad (m < n)$$

In changing the extent of the relative dominance of B over A, three regimes occur successively, as shown in Fig. 3 for gas-solid fluidization, and are characterized by distinct structures:

- A-dominated: If A = extremum 1 plays a dominant role while B = extremum 2 is suppressed, the steady state of the system is exclusively A-dominated, while B has no influence on the structure of the system.
- A-B compromise in competition: With increasing dominance of B = extremum 2 over A = extremum 1, there is a critical condition at which A loses its absolute dominance over B and has to compromise with B. This leads to the alternate appearance of a B-dominated state and an A-dominated state (not necessarily fully dominated, depending on the

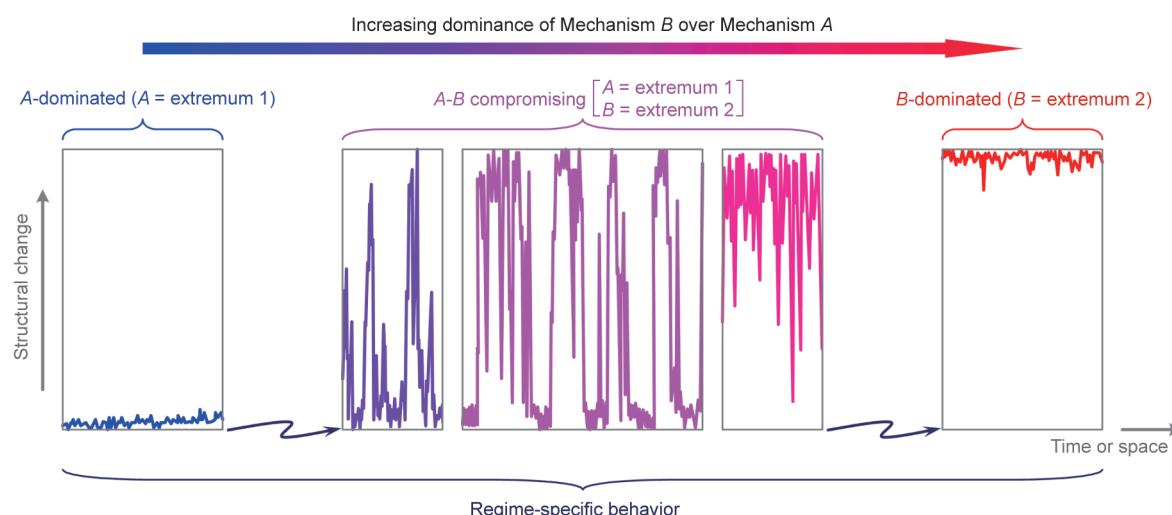


Fig. 3. Three regimes occur successively with changing the relative dominance of Mechanism B over Mechanism A.

relative dominance between these two mechanisms [13], as shown in Fig. 3) with respect to time and space, giving rise to the complexity of dynamic changes at the mesoscale of a system.

- *B*-dominated: When the dominance of *B* reaches another critical value, *A* will be completely suppressed while *B* is fully realized so that the system becomes exclusively *B*-dominated.

Although more complexity and diversity of regime transitions may occur with changing relative dominance between different mechanisms for various systems in different fields, the above-discussed three-regime feature seems to be general. This regime-specific nature, plus the field- and level-dependent difference, gives rise to complexity in looking for a common principle for mesoscale phenomena [13].

To confirm and extend the generality of the EMMS principle, transdisciplinarity is needed for different disciplines in order to look for more evidence for the generality of the principle of compromise in competition. That is, the level-specific nature should be clarified by studying different systems at different levels, while the regime-specific nature needs to be confirmed in various systems by changing operating conditions. As long as progress is made in this aspect, mesoscience will be established, and mesoscale problems in different fields will be resolved, resulting in revolutionary progress in different fields with respect to theory, computation, and experiments, as proposed in Fig. 4.

Since the complexity and diversity of the real world always occurs at mesoscales, it is natural for theories, experiments, and computations to all focus on mesoscale phenomena, as shown in Fig. 4. Firstly, theory should be established to express the principle of compromise in competition at mesoscales and to formulate multiscale dynamic structures via multi-objective variational approaches. With increasing evidence from concrete

problems, mesoscience may be developed as a transdisciplinary science. Secondly, experiments will generate multiscale data, and mesoscience approaches could be used to identify the dominant mechanisms behind these data and to model such data with mesoscale modeling, which would also hopefully give evidence for the generality of mesoscience. Thirdly, computation will be based on mesoscience in establishing multiscale modeling, in constructing both software and hardware [11] through realizing the logical and structural similarity between them in order to realize the so-called virtual reality. If mesoscience is developed, as expected, a new paradigm of scientific research will be enabled, in which mesoscience will play an important role not only in revealing mechanisms behind phenomena, but also in upgrading the predictability of modeling and in speeding up computation to realize virtual reality [14].

6. Deducing the common principle of mesoscience

The common principle of mesoscience may have to be deduced by studying concrete mesoscale problems, while keeping generality in mind; that is, by looking from specificity to generality. The essence of most challenges we face nowadays is rooted in mesoscale complexity. Due to the diversity of such complexity, it may not be practical to directly formulate a general theory for mesoscales. Instead, more evidence for the common principle of mesoscience should be deduced from the study of concrete problems.

According to the above analysis, and considering the current frontiers and challenges in various fields, the problems below can be taken as typical examples of mesoscale problems, among many others. The application of the concept of mesoscience, as described in Fig. 4, will accelerate the solution of these problems. Furthermore, breakthroughs in understanding these problems will drive major progress in corresponding disciplines and fields,

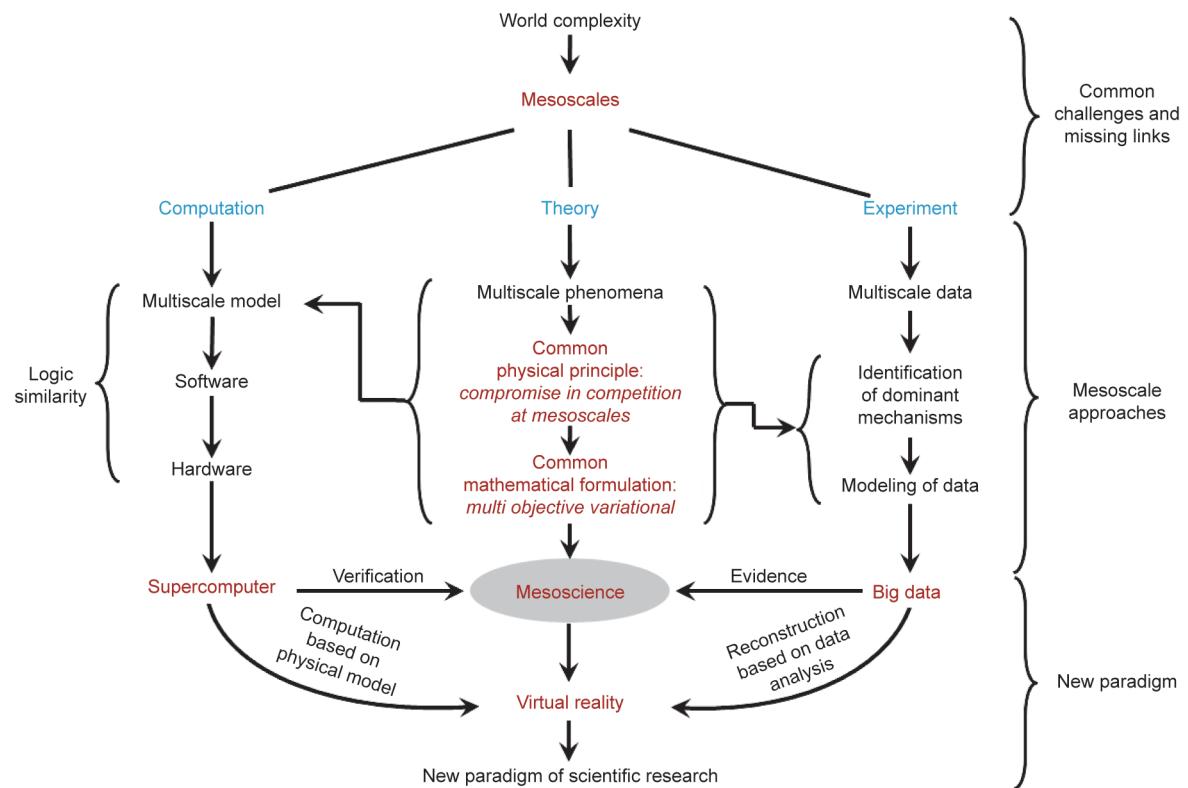


Fig. 4. Relationship between big data, supercomputing, mesoscience, virtual reality, and the path to a new paradigm of science and technology (modified from Ref. [3]).

which will in turn provide concrete examples, and hence, evidence for the universality of mesoscience. Some of typical mesoscale problems include:

- Revealing the intrinsic mechanisms of photovoltaic process, photosynthetic phenomenon, and catalysis to revolutionize the technology of sustainable energy resources and materials, and provide a solution for dealing with climate change and realizing sustainable development;
- Understanding mesoscale problems on the levels of three-dimensional dynamic protein structure and intracellular dynamic processes in order to greatly propel the revolution of life and health science forward;
- Understanding the complex systems of turbulence, weather, climate, engineering dynamic systems, astronomy, and the universe in order to greatly enhance human capacity for sustainable development, and increase our ability to understand nature and prevent disasters;
- Understanding the multilevel, multiscale information transmitting and processing mechanisms of the nervous system in order to propel progress in cognition, brain, computing, and intelligence sciences;
- Revealing the mechanism and design of superconductors, energy (heat, electricity) storage, quantum materials, and functional materials in order to lead to major breakthroughs in energy, information, and materials fields;
- Quantifying material design, rational synthesis, and the smart large-scale production of various materials in order to accelerate the modernization process of industries, especially the manufacturing industry; and
- Applying the mesoscale concept to supercomputing, big data, and virtual reality in order to greatly enhance people's ability to understand nature, cause major changes in the mode of scientific research and development, and further revolutionize our production mode and lifestyle.

In addition, new breakthroughs in the mesoscale problems on the two extreme levels shown in Fig. 2 (e.g., quantum mechanics on the smallest extremum and evolution rules of the universe on the largest extremum) will fundamentally deepen human understanding of the physical world.

Solving these problems from different fields with the concept of mesoscience will promote the development of transdisciplinarity in a rational, three-pronged manner, as shown in Fig. 5:

- **Transdisciplinarity approach 1: Across different levels of sub-disciplines in the same discipline.** The mesoscience concept discussed here was proposed in studying mesoscale problems at different levels (sub-disciplines) of chemical science [7,8], such as interfacial and material structures at the material level; dynamic heterogeneity of gas-solid systems, gas-liquid systems, and turbulence at the reactor level; and process synthesis superstructures [15] at the environmental level.
- **Transdisciplinarity approach 2: Across different disciplines.** Studying the challenging problems listed above involves many different fields. For example, in the nervous system, dynamic changes at mesoscales of different levels are expected to follow the same governing rule as those in complex flows, correlated electron systems, protein structures, and catalysis, all of which are possibly related to the principle of compromise in competition between different dominant mechanisms.
- **Transdisciplinarity approach 3: Across global issues that are common for all disciplines.** Transdisciplinarity can be extended to the study of common global issues for all fields, such as big data, supercomputing, and virtual reality, as discussed in Fig. 4.

If these three transdisciplinarity approaches can be explored jointly by different disciplines and fields, we will see an entirely different landscape of S&T based on sharing common principles

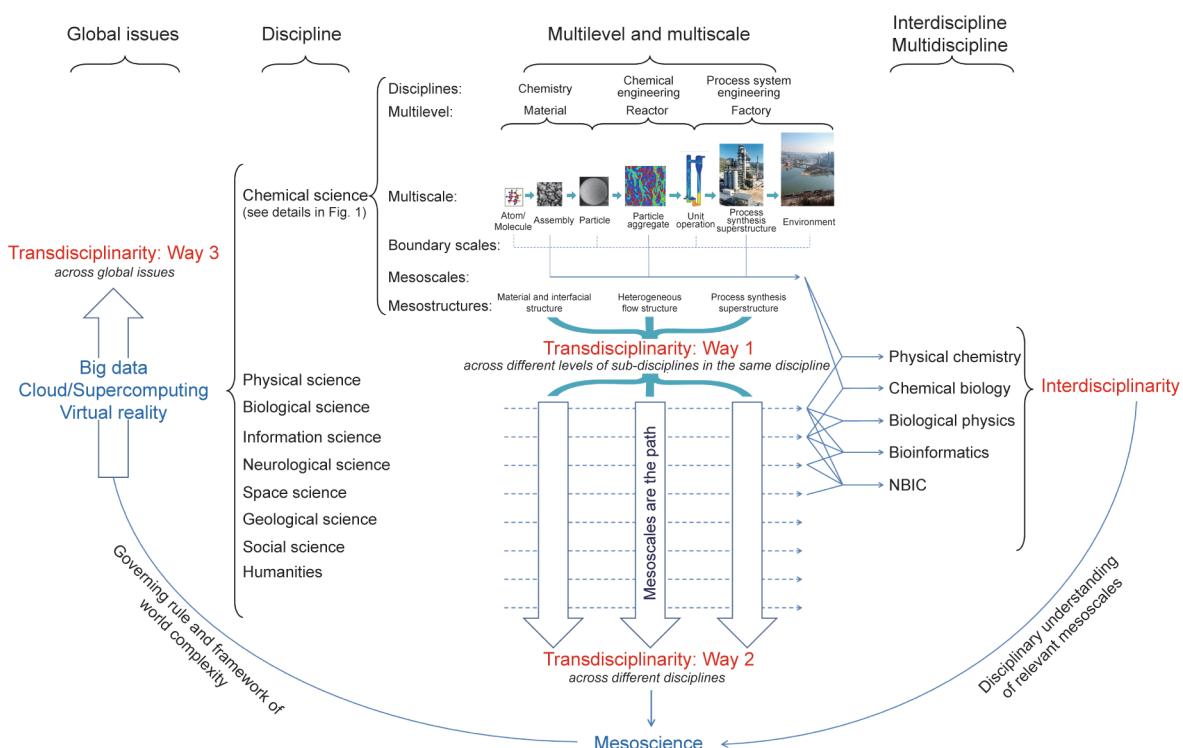


Fig. 5. Transdisciplinarity in three approaches: across different levels of sub-disciplines in the same discipline, across different disciplines, and across global issues (from Ref. [3] with modifications). NBIC stands for nanotechnology, biotechnology, information technology, and cognitive science.

at mesoscales. This statement may be risky; however, it does at least deserve attention and exploratory effort.

The strategy of the EMMS principle of compromise in competition for mesoscience (described in Section 5) is different from the strategy followed by thermodynamics which tries to establish a single variational function to define the steady states of systems.

In fact, as long as two or more dominant mechanisms are involved (i.e., the A-B compromise regime discussed in Section 5 and Fig. 3), it is very difficult to directly deduce a single variational criterion, due to the conflict of "interest" between different dominant mechanisms. Compromise in competition between two variational functions featuring two different mechanisms (likely related to different dissipative processes) has to be taken into account. This might be the reason why it is so difficult to define a single general variational criterion [16] in nonlinear and non-equilibrium thermodynamics for dissipative structures [17], leading to many debates [18] among researchers.

From the EMMS principle, the generality of which has been confirmed in many systems [6,8,11], we would further predict that these debates mentioned above is due to a neglect of the principle of compromise in competition and the regime-specific nature of the variational criteria, as shown in Section 5 and Fig. 3, although more evidence is needed to clarify this deduction. That is, both the minimum [19] and the maximum [20] of dissipation, governing different dominant mechanisms, are involved in shaping the structures of complex systems, as evidenced in turbulent flow [21,22], gas-solid fluidization [12,13], and the reaction-diffusion process [23] detailed in Ref. [13]. Both can occur in the same system, but only in the A-B compromising regime shown in Fig. 3 and in the form of alternate realization of their respective extremal tendencies at the same time but in different locations, or at the same location but at different times. For the A-dominated and the B-dominated regimes, however, a single function (i.e., either minimum dissipation or maximum dissipation) could be used, since the dissipative process in either of these two cases is single-mechanism dominated.

From the evidence currently available, it can be predicted that the debate mentioned above will be clarified by considering the compromise in competition between different dominant mechanisms corresponding to different variational criteria and their regime-specific nature. This means that a single variational criterion in term of total dissipation (entropy production) is likely impossible in the A-B compromising regime. Such a vital issue has not received attention. One of the tasks for mesoscience is to address this problem, as detailed in Ref. [13]. Another question to be justified is: To what extent can this kind of generality be applied? A mesoscience program has been launched by the Nature Science Foundation of China (NSFC) to finance researchers from different fields [24,25]. The theme of the program is to collect more evidence and explore the generality of the EMMS principle of compromise in competition in different aspects, such as the principle itself and the variational criteria.

7. A case study of planning research in energy technology

Currently, research in energy is probably organized on the basis of energy categories, such as nuclear, renewable, and fossil energy. In future, an energy research complex should be comprehensively and transdisciplinarily designed according to the logic of the knowledge system, so that the key technologies and common scientific issues for the whole field can be identified and used as the basis for organizing teams, establishing divisions, and creating platforms.

Energy is one of the most essential factors for social and eco-

nomic sustainable development; however, its use gives rise to the global challenge of climate change. Naturally, energy has been taken as the mission for most governmental and industrial R&D organizations. The efficiency of energy research is very much related to the capability of humans in sustainable development. Rational planning and organization of R&D activities in these organizations are essential for efficient research activities that enable the occurrence of the so-called revolution in energy. However, it is a fact that research activities worldwide in the energy field have been organized without a consideration of the logic and structure of the knowledge system; and that as a result, transdisciplinarity is difficult to implement, due to limitations in organizational and managerial reasoning. For example, nuclear energy, renewable energy, and fossil fuels are usually studied separately in different labs, and are developed in almost an isolated way from each other. Even worse, they are studied and developed by totally different disciplines, with a neglect of the common knowledge and complementary nature that they inherently share with each other. This situation should be changed in future, as we discuss new revolutions of S&T, explore new paradigms of scientific research, and cope with global challenges.

With the structure and logic of the knowledge system in mind, Fig. 6 proposes a preliminary design of an energy research complex that is engaged in nuclear, renewable, and fossil fuel energies. That is, the following procedure should be followed when organizing research in the energy field.

- Forming specific teams: The most challenging scientific problems for each category of energy at different levels should be identified, such as nuclear, renewables, and fossil fuels, so that specific research teams can be organized to focus on these category-specific issues.
- Creating interdisciplinary divisions: The relationship between specific problems for different energies at the same level should be analyzed in order to identify common scientific issues, so as to organize more general research divisions at the same level, but for different energies—that is, interdisciplinary divisions.
- Creating transdisciplinary centers: Common challenges at different levels should be looked for, such as mesoscale problems, which indicate the most important research focus. This calls for a division for studying general problems in the energy field—that is, a transdisciplinary center.
- Establishing common platforms: Common platforms should be established for different teams and divisions, with an emphasis on the global capability of theory, experiment, and computation.

Such a hierarchical design of an energy research complex might be expected to minimize the repetition of research, and to maximize the interaction between different teams and divisions, resulting in an extremely high R&D capability. Of course, governance consistent with this design is also critical to reach this goal.

8. The formation of a new scientific research paradigm

Guidance should be provided for the formation of a new scientific research paradigm. Clarification of the logic and structure in the knowledge system will lead to changes in theories, methods, tools, and ways of thinking. Propelled by information technology and data science, this paradigm shift will, in turn, cause fundamental changes in the future scientific research mode. How to cope with these changes is another critical question that requires attention from the scientific community, the government, and all stakeholders.

(1) Changes induced by information technology: With the de-

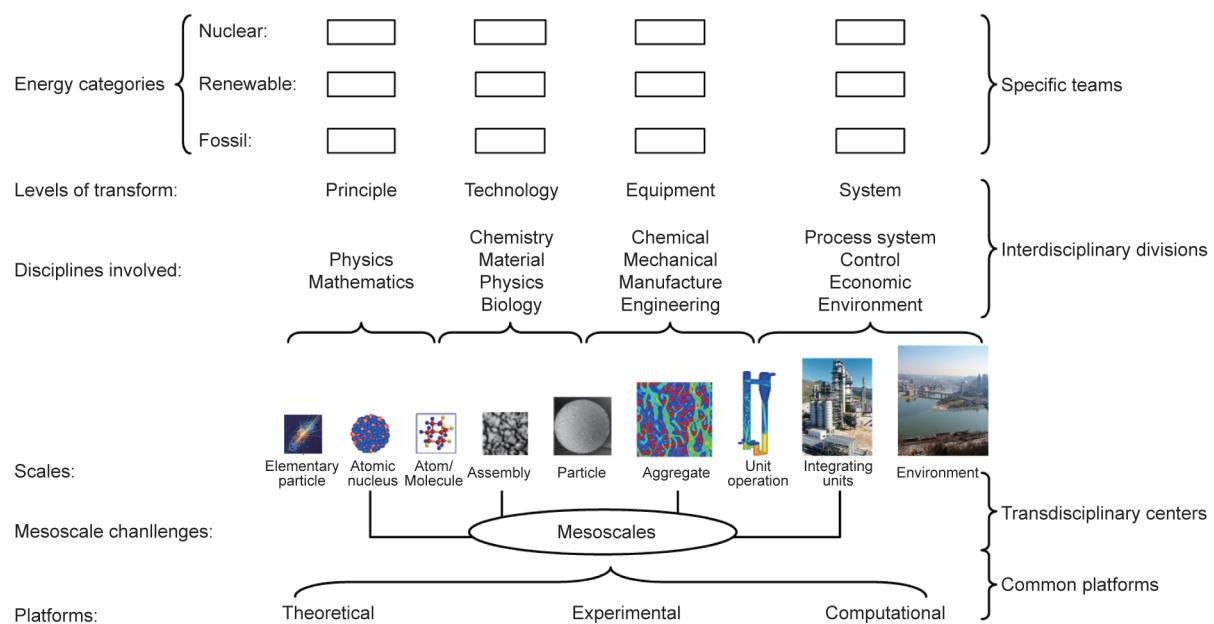


Fig. 6. Planning a comprehensive energy research complex while considering the logic and structure of the knowledge system.

development of information technology and the rising wave of big data, a new paradigm of scientific research is on the way [1]. This process is accompanied by the rapid development of openness and globalization in science. Open access (OA) and various new modes of publishing and communication will give rise to revolutionary changes in the environment of scientific research. Yet, the question of how to rationally guide this revolution is currently a major challenge to scientific research management. For example, although OA is surely conducive to the sharing of new knowledge, how should OA develop in a healthy fashion, in order to avoid an “over-commercialization” of knowledge that prevents its dissemination? What regulations should be established to ensure that OA benefits humanity? As another example, information technology is surely very important in the reform of how knowledge is disseminated; but how do we ensure the quality of knowledge and the order of knowledge dissemination? How do we ensure a timely acquisition of reliable knowledge from massive data? As a third example, big data is considered very likely to reshape the mode of scientific research [1]; but what is the scientific principle behind big data? This question requires the full consideration of the S&T community. Such questions are numerous and need global regulations to standardize them. Just as the patent system was gradually established in the process of technological development, new global agreements and joint actions are necessary to guide the development of a new scientific research paradigm.

(2) Changes induced by breakthroughs in research methods, theories, and technologies: Considering the structure and logic of the knowledge system, as discussed above, and the missing links regarding mesoscales, research methods, theories, and tools should result in corresponding changes. These changes will be important characteristics of the new scientific research paradigm, and will need some disciplinary recombination. For example, the mesoscale structure tends to show spatiotemporal dynamics and highly heterogeneous attributes, featuring a coupling of order and disorder. This coupling poses a great challenge for measurement and experimental techniques, since high resolution, in both time and space, is required. Measurement of the three-dimensional dynamic structures of protein, the collective movement of electrons in materials, and the law of mesoscale signal transduction

on each level of the nervous system, and so forth, will all be important parts of future scientific research. Fundamental changes will take place in research methods as well. Present research methods dominated by analysis, deduction, and determinism will continue to give way to numerical and graphical simulations and other non-deterministic methods. Virtual reality will also become an important means of research. Some traditional theories based on static state, linearity, and equilibrium will be replaced by dynamic, nonlinear, non-equilibrium, and system theories that center on mesoscale structure. Breakthroughs in mesoscale problems on different levels will make it possible to integrate and fuse different levels of knowledge, leading to transdisciplinarity of different disciplines. Research institutions and organizations should be reorganized systematically to adopt the logic of the knowledge system. All of these changes will probably be trends in future development.

We should be fully prepared for the changes in the modes of scientific research and thinking that will be caused by transformation in these two aspects, in order to rationally prevent conventional thinking from hindering development and to guide S&T to develop in a healthy and rapid manner.

9. Conclusions

The concerted efforts of all stakeholders are needed in order to effect the necessary changes. Complete understanding of the structure and logic of the knowledge system and the changes in the scientific research environment will lead to the gradual formation of a new layout of S&T and a new scientific research paradigm. This paradigm will be one of the characteristics of S&T in the 21st century. However, it calls for intentional joint efforts; otherwise, this process could be very slow due to our inertia in thinking. The purpose of this paper is to remind the global community that the advancement of this process requires the joint efforts of all disciplines as well as firm support from governments. Dissolving disciplinary boundaries, appreciating new thoughts, and so forth, require an open mind and impetus from the S&T community, the government, and all international science organizations. The attitudes of all parties toward these changes will

largely determine the occurrence of a new S&T revolution, and the formation of a new scientific research paradigm, which are essential for open and global science, where “open” refers not only to accessing knowledge, but also to the way of thinking, and “global” refers not only to space, but also to transdisciplinarity in all sciences, as a whole landscape! Natural sciences, humanities, and social sciences will be unified, to some extent, through the common path of mesoscales, with increasing understanding of possible common principles. All parties concerned should fully recognize this point. Only in this way can humanity respond effectively to the challenges of globalization.

In addition, these changes will call for a reformation of national innovation systems, education systems, and scientific research management modes in all countries. All governments should actively adapt to these changes, make necessary adjustments in their national innovation systems, and optimize the scale and structure of their S&T systems. At the global level, international science organizations should consider the relationships among the innovation systems of all nations and even the establishment of a global innovation system—or, at least, cooperation among different nations in the context of “open and global science.” This is the only way we can effectively enhance the efficiency and capacity of the innovation system, and ensure the rapid development of S&T under the condition of a limited increase in scientific research investment. This paradigm shift is probably much more important than merely demanding investment and pursuing rewards from investment in S&T.

Finally, this author wants to emphasize that we are in an era of fast changes. The capability and flexibility to adapt to these changes will be crucial in speeding up the development of S&T and thereby addressing global challenges. Scientific communities, industries, governments, and, in particular, international organizations with the capability and responsibility of raising a global voice in science, should make this paradigm shift a priority in their work!

Acknowledgements

The author would like to thank the colleagues at the EMMS Group for their long term cooperation and contribution previously on the EMMS model and now on mesoscience. Sincere thanks should be extended to Profs. Ying Hu, Xiaoye Cao, and Jiaofeng Pan for their reading the first draft in Chinese and giving suggestions, to Profs. Zhongxian Zhao, Zhizhen Wang, Jianzhong Xu, Yuntai Chen, and Wei Li for their time and discussion at a group discussion on the draft. Specially, I would like to thank Mr. Zhengyu Wang, Mr. Yan Zhuang, Ms. Kai Feng, and Drs. Wenlai Huang, Xiaowei Wang, and Jian Wang for their help in English and figures. Particularly, the author would thank Dr. Angela Welch for polishing English. The financial support of Natural Science Foundation of China (NSFC) (91334000) on the mesoscience program,

entitled “Mechanism and Manipulation at Mesoscales of Multiphase Reaction Systems,” is highly appreciated.

References

- [1] Hey T, Tansley S, Tolle K, editors. *The fourth paradigm: data-intensive scientific discovery*. Redmond: Microsoft Research; 2009.
- [2] United Nations Educational, Scientific and Cultural Organization, Division of Philosophy and Ethics. *Transdisciplinarity: stimulating synergies, integrating knowledge*. Paris: United Nations Educational, Scientific and Cultural Organization; 1998.
- [3] Li J. Mesoscales: the path to transdisciplinarity. *Chem Eng J* 2015;277:112–5.
- [4] Nicolescu B, editor. *Transdisciplinarity: theory and practice*. New York: Hampton Press; 2008.
- [5] Liu Z. *Modern disciplinary sciences*. Hangzhou: Zhejiang Education Press; 1998. Chinese.
- [6] Li J, Ge W, Wang W, Yang N, Liu X, Wang L, et al. From multiscale modeling to meso-science: a chemical engineering perspective. Berlin: Springer; 2013.
- [7] Li J, Ge W, Kwaak M. Meso-scale phenomena from compromise—a common challenge, not only for chemical engineering. 2009. arXiv:0912.5407.
- [8] Li J. Approaching virtual process engineering with exploring mesoscience. *Chem Eng J* 2015;278:541–55.
- [9] Social science [Internet]. San Francisco: Wikimedia Foundation, Inc. [cited 2016 Jun 21]. Available from: https://en.wikipedia.org/wiki/social_science.
- [10] Li J, Huang W. Towards mesoscience: the principle of compromise in competition. Berlin: Springer; 2014.
- [11] Ge W, Wang W, Yang N, Li J, Kwaak M, Chen F, et al. Meso-scale oriented simulation towards virtual process engineering (VPE)—The EMMS Paradigm. *Chem Eng Sci* 2011;66(19):4426–58.
- [12] Li J, Zhang J, Ge W, Liu X. Multi-scale methodology for complex systems. *Chem Eng Sci* 2004;59(8–9):1687–700.
- [13] Li J, Ge W, Wang W, Yang N, Wang J, Huang W. Focusing on mesoscales: from the energy-minimization multiscale model to mesoscience. *Curr Opin Chem Eng* 2016;13:10–23.
- [14] Guo L, Li Z, Li J, Liu X, Lu B, Meng F, et al. Harnessing the power of virtual reality. *Chem Eng Prog* 2012;108(7):28–33.
- [15] Floudas CA, Niziolek AM, Onel O, Matthews LR. Multi-scale systems engineering for energy and the environment: challenges and opportunities. *AIChE J* 2016;62(3):602–23.
- [16] Gage DH, Schiffer M, Kline SJ, Reynolds WC. The non-existence of a general thermokinetic variational principle. In: Donnelly RJ, Herman R, Prigogine I, editors *Non-equilibrium thermodynamics variational techniques and stability*. Chicago: University of Chicago press; 1966. p. 283–6.
- [17] Nicolis G, Prigogine I. Self-organization in nonequilibrium systems: from dissipative structures to order through fluctuations. New York: Wiley; 1977.
- [18] Martyushev LM. Entropy and entropy production: old misconceptions and new breakthroughs. *Entropy (Basel)* 2013;15(4):1152–70.
- [19] Prigogine I. *Introduction to thermodynamics of irreversible processes*. 3rd ed. New York: John Wiley & Sons Ltd.; 1968.
- [20] Ziegler H. *An introduction to thermomechanics*. Amsterdam: North-Holland Publishing Company; 1983.
- [21] Li J, Zhang Z, Ge W, Sun Q, Yuan J. A simple variational criterion for turbulent flow in pipe. *Chem Eng Sci* 1999;54(8):1151–54.
- [22] Wang L, Qiu X, Zhang L, Li J. Turbulence originating from the compromise-in-competition between viscosity and inertia. *Chem Eng J* 2016;300:83–97.
- [23] Huang W, Li J. Compromise between minimization and maximization of entropy production in reversible Gray-Scott model. *Chem Eng Sci* 2016. In press. <http://dx.doi.org/10.1016/j.ces.2016.08.022>.
- [24] NSFC initiates the major research plan on meso-science [Internet]. Beijing: Bureau of International Cooperation, NSFC; c2007 [updated 2012 Sep 13; cited 2016 Jun 21]. Available from: <http://www.nsfc.gov.cn/publish/portal1/tab158/info39251.htm>.
- [25] Li J, Hu Y, Yuan Q. Mesoscience: exploring old problems from a new angle. *Scientia Sinica (Chimica)* 2014;44(3):277–81. Chinese.