REVIEW ARTICLES

Multiscale coupling: challenges and opportunities*

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Abstract Multiscale coupling is ubiquitous in nature and attracts broad interests of scientists from mathematicians, physicists, machinists, chemists to biologists. However, much less attention has been paid to its intrinsic implication. In this paper, multiscale coupling is introduced by studying two typical examples in classic mechanics: fluid turbulence and solid failure. The nature of multiscale coupling in the two examples lies in their physical diversities and strong coupling over wide-range scales. The theories of dynamical system and statistical mechanics provide fundamental methods for the multiscale coupling problems. The diverse multiscale couplings call for unified approaches and might expedite new concepts, theories and disciplines.

Keywords: multiscale coupling, statistical mechanics, fluid turbulence, solid failure.

Space-time scales characterize physical phenomena in nature[1]. For example, fluid turbulence is characterized by various eddies of different scales and solid failure by various damages of different scales. Studies on physical phenomena are usually carried out on different scales and even marked by scales themselves. For example, the space-time scales of astronomy are often described by the units of year and light year, and microbiology by minute and micrometer. While the scientific research in last century focused on the extreme scales such as cosmos and quantum, the scientific research in the 21st century might focus more on the body scales.

Multiscale couplings characterize the complexity of physical phenomena in nature[2~4]. Multiscale coupling phenomena exhibit the interplay of coherent structures and random fluctuations on different scales due to their interactions. In fluid turbulence, the interactions of different eddies over a wide range lead to a complex flow pattern; in solid failure, the interactions of microdamages on different scales result in macroscale damages via intermediate cracks. The complete deterministic methods do not work for the multiscale coupling problems due to their random fluctuations, and the complete stochastic methods do not work either due to their deterministic coherent structures. A possibly workable approach is to choose suitable statistics on coherent structures. However, the choice of the suitable statistics is dependent on the understanding of the nature of multiscale coupling. Therefore, multiscale coupling becomes a new challenge in the 21st century.

The multiscale couplings have different implications in different disciplines at different stages. The multiscale couplings problems of our interests lie in the diversity and coupling of different physics on different scales. The diversity is characterized by the multiple physical mechanisms on different scales, and the coupling between the physical mechanisms on different scales determines the global behaviors. The diversity and coupling act as the two sides of a golden coin and both of them take effects simultaneously.

The dynamical system theory and statistical mechanics provide fundamental tools for multiscale coupling problems. In classic mechanics, the dynamical systems at a single scale can be constructed using the Newton laws. If there is no coupling, the dynamical system can fully describe the physics on one scale and the remaining work is to solve the dynamical equations. In this sense problem-solving is very straightforward. In an equilibrium state, the coupling can be treated based on the principle of equal probability: the

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behaviors on macro-scales are statistical averaging on microscales with a given probability density function (pdf). All results are obtained from the statistical averaging. In principle, such multiscale coupling problems are not difficult. However, many multiscale coupling problems are non-equilibrium and nonlinear. The couplings among different scales are strong and/or very sensitive so that they cannot be treated by either statistical averaging or small perturbation. They have to be treated as strong coupling. In the case of sensitive coupling, some random perturbations on small scales could be extremely amplified through the nonlinear processes, leading to intensive responses on large scales. Statistical mechanics provides a startpoint for such problems. However, workable theories and approaches are still under development. They are new challenges and also new opportunities to our research.

Two typical examples on multiscale coupling are fluid turbulence and solid failure, which are also the unsolved problems in classic mechanics.

1 Fluid turbulence

Fluid turbulence exhibits complex flow patterns of various eddies over wide-range scales. These eddies have different physical mechanisms and are strongly coupled. In the last century, the physics of eddies on different scales were presumed to be self-similar so that the similarity solutions could be obtained; and the couplings among different scale eddies were presumed to be weak so that the perturbed solutions could be obtained. It is the similarity and perturbation methods that solve such difficult problems as the boundary layer in aeronautics and aerospace, which led to a golden time for classic mechanics. However, the problems in turbulence that we have today are completely different from the previous ones. Today's problems are the strong couplings of different physics on different scales so the similarity and perturbation methods do not work at all. Therefore, new theoretical approaches and numerical methods for diverse physics and strong coupling have to be developed.

Statistic mechanics serves as a useful tool for multiscale modeling in turbulence[5~7]. Generally, the statistical description of turbulence can be achieved by moment and pdf approaches[8]. However, the moment approach has difficulty in dealing with nonlinearity and the pdf approach has difficulty in dealing with spatial coupling. Both of them need some phenomenological assumption. The assumptions have to be justified. Mapping closure approximation (MCA)[9] is a new deductive approach that can treat the spatial coupling by successive approximation without any *ad hoc* assumptions. In the MCA approach, no assumption on the form of coupling is needed. An unknown form of coupling between different scales is treated as the one mapped from a known form of coupling and the mapping is completely determined by the dynamics. The difference of MCA from the previous mapping closures approach[10,11] lies in its nature of successive approximation in the sense of successively larger joint pdfs. The MAC approach has been developed for turbulent mixing[12].

Most numerical simulations work for a certain range of scales. Direct numerical simulations can resolve all scales of interests but it is prohibitively expensive for engineering problems[13]; Reynolds average methods can only resolve the averaged motion. When modeling the effects of all other scales on averaged motions, such models are difficult to construct[14]; in large-eddy simulations (LES), the motion of large scales is calculated while the effects of the motion of small scales on larger scales are modeled[15,16]. Since motions of small scales in turbulence are universal to some extent, the modeling can be constructed. However, turbulent motions cannot be simply decomposed into large and small scales. It is well-known that the scales in turbulence are over a wide range and the motions at different scale ranges might be physically different. In order to take these different physical mechanisms at different scale ranges into account, multiscale LES (MLES)[17,18] is being developed: the velocity fields are decomposed into multiple components corresponding to different scales. The different scales are corresponding to different physics. Different physics on different scales require different subgrid scale models. The LES equations with different subgrid scale models need different numerical schemes and grids. The MLES approach has been used to calculate time correlations of turbulence velocity fields[19].

The research on turbulence modeling has made a great progress, especially on individual problems of interest. However, there are still many complaints on it: can we have a universal model that can be used for all of the turbulence problems? Unfortunately, the universal model for turbulence does not exist. If one insists that the universal model does exist, the universal model for turbulence is just the Navier-Stokes equation itself. All of the turbulence models are some simplifications of Navier-Stokes equation so they lose some properties. Thus, the turbulence models cannot recover all properties of Navier-Stokes equation and are not universal. In other words, all of the turbulence models should be the approximate representations of turbulence while Navier-Stokes equation is admitted to be fully the representations of turbulence. The mission of turbulence modeling is to develop the approximate representations of turbulence for some relevant physics of interest. In this sense, turbulence is a research topic more than an unresolved problem. Turbulence modeling is the source of creative thoughts for the multiscale coupling problems.

2 Solid failure

The living environment of human beings is substantially supported by solid media. Solid failure occurs in almost every aspect of human life, including all fields of engineering and the most severe natural events, e. g. the earthquakes and the avalanches. Solid failure has been a typically difficult problem from the 20th century to the 21st century due to its incredible complexity[20]. For example, the difficulty of the failure prediction of solid media is related to its two complex characteristics: (1) the solid failure exhibits catastrophe transitions and the precursory features of catastrophe are difficult to observe; (2) the catastrophe of systems macroscopically identical may display different behaviors from sample to sample. In other words, the catastrophe has some uncertainty, and it is insufficient to represent the catastrophe only by its macroscopically average properties. The underlying mechanism of the above-mentioned complexity can be attributed to the multiscale coupling. The evolution of solid failure relates to a wide range of space-time scales[21,22]. In order to deal with solid failure, we have to develop new theories based on non-equilibrium statistical mechanics[23,24] instead of the fracture mechanics dealing with a single macroscopic crack. In fact, the failure usually appears as a trans-scale process from accumulation of a great number of microdamages and a series of nonlinear inverse cascade to macroscopic catastrophe. During the nonlinear evolution, some disordered details on small scales can be strongly amplified and become significantly effective on large scales, so the catastrophe behavior would be affected. Because it is impossible to identify the disordered details on all of smaller scales, the catastrophe displays uncertainty[25]. This is the so called trans-scale sensitivity.

A possible strategy for catastrophe prediction is to search for the universality of catastrophe. We have made some progress in the following two aspects.

Statistical mesoscopic damage mechanics[26~29] is a statistical theory linking mesoscopic and macroscopic scales about damage evolution in multiscale heterogeneous media. Based on the statistical mesoscopic damage mechanics, a function called dynamical function of damage can be derived. The macroscopic damage evolution is governed by the dynamical function of damage. In particular, a transition point from random damage to damage localization can be determined. The damage localization is an important precursor of catastrophe. In such a formulation, several dimensionless parameters linking mesoscopic and macroscopic scales of space and time play an essential role.

Another common precursor of catastrophe is the critical sensitivity[30], which implies that the response of a system to external controlled parameters becomes significantly sensitive as approaching its catastrophe transition point. From statistical analysis based on mesoscopic dynamical models, we propose the concept of critical sensitivity, which is the result of damage cascade from mesoscopic to macroscopic scales.

Both the damage localization and the critical sensitivity, revealed in the trans-scale formulation linking mesoscopic and macroscopic scales, are typical multiscale phenomena. They might be universal and observable, so they may give some clues to catastrophe prediction. This case implies that the multiscale coupling theory on solid failure need to be developed.

Multiscale couplings in fluid turbulence and solid failure share the fundamental concepts, methods and theories, although fluid turbulence and solid failure are completely different in their physical mechanisms. Both of them are non-equilibrium and nonlinear with strong couplings among different scales. Either perturbation or similarity method cannot be applied to those cases. They are trans-scale sensitive so that some local fluctuations on some scale can induce a global catastrophe. Therefore, the multiscale coupling is a new challenge that specially calls for multidiscipline investigations.

There is no universal approach available so far for the multiscale coupling problems, while progress has been made individually in some of these problems. At least, no universal approach is available until successful non-equilibrium theory for statistical physics appears. However, successes in some individual multiscale coupling problems might induce a unified approach for some kind of multiscale problems. Unified approaches might be initiated from the intersection of different disciplines. That is to say, similar approaches that are successfully applied to different multiscale coupling problems might provide new opportunities for the unified approach for physical problems of strong coupling. Just as the unification of the electronics and magnets in the form of Maxwell equation in the 18th century, and of biology and molecular science in the molecular biology in the 20th century, the unification of different concepts, approaches and theories in diverse multiscale couplings might plant the roots for new disciplines. In addition to the unification of statistical physics, fluid turbulence and solid failure, the new roots for multiscale couplings lie in the unification of statistical mechanics with soft matters and continuum mechanics; with life science such as gene sequence and protein, with quasi-continuum mechanics for atomic interactions at nano/micro scales. In fact, we have to deal with a variety of complex phenomena. The origins of complex phenomena lie in the multi-physical interaction on multiscales. In such problems, decoupling does not work at all. Therefore, multiscale coupling is a typically difficult problem of wide interest in mathematics, physics, mechanics and life science.

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