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Multiscale coupling in complex mechanical systems

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Abstract

Multiscale coupling attracts broad interests from mechanics, physics and chemistry to biology. The diversity and coupling of physics at different scales are two essential features of multiscale problems in far-from-equilibrium systems. The two features present fundamental difficulties and are great challenges to multiscale modeling and simulation. The theory of dynamical system and statistical mechanics provide fundamental tools for the multiscale coupling problems. The paper presents some closed multiscale formulations, e.g., the mapping closure approximation, multiscale large-eddy simulation and statistical mesoscopic damage mechanics, for two typical multiscale coupling problems in mechanics, that is, turbulence in fluids and failure in solids. It is pointed that developing a tractable, closed nonequilibrium statistical theory may be an effective approach to deal with the multiscale coupling problems. Some common characteristics of the statistical theory are discussed.

Keywords: Multiscale coupling; Solid mechanics; Fluid mechanics; Materials failure; Turbulence; Nonlinear dynamics

1. Introduction

In the past several years, there has been an explosive growth of interest in the multiscale coupling problems (Glimm and Sharp, 1997; Phillips, 2001; Kwauk and Li, 2000; He et al., 2003). Generally speaking, the multiscale problems can be categorized into three classes: related to equilibrium, near equilibrium, and far-from-equilibrium cases. At present, a great challenge of multiscale problems is the multiscale coupling effects in far from equilibrium systems. The traditional approaches are insufficient for such problems.

For a far from equilibrium system, the multiscale coupling problems present the following characteristics:

(1) There may be several active scales spanning very wide ranges of space and time (Barenblatt, 1979). For example, in materials failure, the atomic bonds in solid materials are at the scale of angstroms (10^{-10} m) and may break at femtoseconds (10^{-15} s), while the resulting fracture is at the scale of the whole size of the sample and may take seconds or hours (Bazant and Chen, 1997). Vortical structures in the atmosphere may range from meters to thousands of kilometers, while the viscous dissipation of the vortices appears at the mean free path of molecular.
(2) The physical mechanisms or the dynamics may differ on different scales (Bai et al., 2002a). It is well known that universal similarity has made some success in multiscale problems, e.g., the similar solutions in mechanics and the power-law behaviors in critical phenomena. However, the universal similarity gets rooted in self-similarity in physics at various scales, and this is questionable in cases of physics diversity. More importantly, for far from equilibrium systems, the dynamics usually display strong nonlinearity, and the dynamical nonlinearity plays an essential role in multiscale evolution.
(3) The multiscale coupling is usually strong and/or sensitive (Xia et al., 1997). It is inappropriate to deal with an isolated scale of interest and eliminate all other scales. The perturbation method suitable for weak coupling condition also fails in dealing with strong coupling effects. In addition, the mean field approximation cannot be directly applied to the case with sensitive multiscale coupling. Furthermore, for an equilibrium state, the statistical mechanics is a successful

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theory dealing with the coupling between microscopic and macroscopic scales. The basic postulate of this approach is the principle of equal probability. However, for far from equilibrium state, the principle of equal probability fails, and there is no simple statistical relationship between microscopic and macroscopic scales.

The diversity and coupling of physics at various scales are two essential features of multiscale problems in far from equilibrium systems. Hence, the vital key to multiscale problems is to characterize the coupling effects between different physics on various scales. In addition, in engineering and natural media, there inevitably exists disordered heterogeneity. The coupling between dynamical nonlinearity and the disordered heterogeneity at multiscales makes the problem much more complex.

In recent years, great efforts have been made to characterize the coupling effects in complex multiscale systems. Several new approaches have been presented and developed (Bai et al., 2002a; Phillips, 2001; He and Rubinstein, 2003; Hughes et al., 2001). In this paper, we introduce these methods for two typical multiscale coupling examples in classic mechanics: fluid turbulence and solid failure. It is well-known that both fluid turbulence and solid failure are most difficult problems in mechanics. The richness of complexity in these phenomena is mainly rooted in the multiscale coupling effect. The characteristics and mechanisms in these systems are very much different, and at present, it seems difficult to construct a unified theoretical framework for these problems. However, there might be some common points, which are noticeable and valuable to us if we want to establish a theoretical framework for problems with multiscale coupling effects.

2. Multiscale coupling in turbulence

Fluid turbulence exhibits complex flow patterns of different scale eddies. These eddies are involved in different physics at different scales and might be coupled strongly with each other. Traditionally, turbulence modeling and simulation are constructed over one single scale range and thus have some limitations. For example, the turbulence models responsible for energy dissipation at small scales may completely fail in intermittency. Therefore, multiscale modeling and simulation are necessary to be developed.

The diverse physics and strong coupling present two fundamental difficulties for turbulence multiscale modeling and simulation. First, the diversity excludes the existence of scale-similarity solutions so that the classic similarity method does not work at all. More complicated is that there exist chaotic motions at small eddies which interplay with coherent structures at large eddies. The interactions of chaotic motions over an extensive scale range are the core of nonlinear dynamics. Second, the strong coupling requires inclusion of the physical effects at other scales. The inclusion can be taken neither as a small perturbation due to the coupling intensity, nor as a simple averaging since there is no scale separation.

The statistical–mechanical treatment of multiscale coupling is a useful approach for turbulence multiscale modeling and simulation. The reason for it will be explained later. We will introduce our recent work aligned in this direction: mapping closure approximation approach and multiscale large-eddy simulation. The goal for the efforts is to develop such multiscale models and simulation approaches for both theoretical analysis and numerical calculation so that models can (1) express the significant physics of interest without reference to the full detail of Navier–Stokes turbulence; (2) be theoretically tractable and numerically implementable in compact forms and (3) can be formulated in a deductive fashion from Navier–Stokes equation without any empirical assumption.

2.1. Mapping closure approximation

The statistical description of turbulence can be generally achieved by the moment and probability density function (PDF) approaches (Pope, 1991). However, the moment approach is difficult with nonlinearity and the PDF approach is difficult with spatial coupling. Both of them need to introduce some phenomenological assumptions. The assumptions have to be justified. Mapping closure approximation (MCA) (He and Rubinstein, 2003) 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 made. 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 between MCA and the previous mapping closures approach (Chen et al., 1989; Pope, 1991) lies in its nature of successive approximation in the sense of successively larger joint PDFs. The MAC approach has been typically developed for the advection–diffusion-reaction equations (He and Zhang, 2004).

We consider the simple case of a reactive scalar advected by a stochastic velocity field:

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = \Gamma \nabla^2 \varphi + Q(\varphi), \tag{1}$$

where the velocity field $\mathbf{u}$ obeys $\nabla \cdot \mathbf{u} = 0$ and is independent of the scalar field. Without loss of generality, it may be prescribed as a known homogeneous and isotropic Gaussian field. Γ is a molecular diffusivity, $Q(\varphi)$ mimics a one-species chemical reaction.

In the MCA approach, the scalar field is mapped from a known random field by a mapping function

$$\varphi(\mathbf{x}, t) = X(\theta(\mathbf{x}, t), t). \tag{2}$$

Here, the known random field $\theta(\mathbf{x},t)$ is taken as a Gaussian reference field. Its one- and two-point joint PDFs are defined by

$$g_1(\eta)=\frac{1}{\sqrt{2\pi}}\exp\left[-\frac{\eta^2}{2}\right], \tag{3}$$

$$g_2(\eta_1,\eta_2,r,t)\equiv g_1(\eta_1,\eta_2,\rho(r,t)) =\frac{1}{2\pi\sqrt{1-\rho^2}}\exp\left[-\frac{\eta_1^2+\eta_2^2-2\rho\eta_1\eta_2}{2(1-\rho^2)}\right], \tag{4}$$

where

$$\rho(r,t)=\frac{\langle\theta(\mathbf{x},t)\theta(\mathbf{x}+\mathbf{r},t)\rangle}{\langle\theta^2(\mathbf{x},t)\rangle}. \tag{5}$$

Here r is the magnitude of separation vector $\mathbf{r}$. The mapping function is required to represent the one- and two-point joint PDFs of the scalar φ via the following equations:

$$f_1(\psi,t)=g_1(\eta)\left[\frac{\partial X(\eta,t)}{\partial\eta}\right]^{-1}, \tag{6}$$

$$f_2(\psi_1,\psi_2,r,t)=g_2(\eta_1,\eta_2,r,t)\left[\frac{\partial X(\eta_1,t)}{\partial\eta_1}\frac{\partial X(\eta_2,t)}{\partial\eta_2}\right]^{-1}. \tag{7}$$

In the classic mapping closure approach (Chen et al., 1989; Pope, 1991), the mapping function X is only required to represent the one-point PDF of the scalar φ via Eq. (6). Differentiating Eq. (6) with respect to t yields

$$\frac{\partial f_1}{\partial t}+\frac{\partial}{\partial\psi}\left[f_1\frac{\partial X}{\partial t}\right]=0. \tag{8}$$

Meanwhile, the transport equation for the one-point PDF, $f_1(\psi,t)$, can be derived by the test function method (Kimura and Kraichnan, 1993) as

$$\frac{\partial f_1}{\partial t}+\frac{\partial}{\partial\psi}[f_1\langle\Gamma\nabla^2\varphi+Q(\varphi)|\psi\rangle]=0. \tag{9}$$

Thus, comparing Eqs. (8) and (9), substituting (2) and using the Gaussian regression on conditional moments, the transport equation for the mapping function (2) becomes

$$\frac{\partial X}{\partial t}=-C\rho''(0,t)\Gamma\left[\frac{\partial^2 X}{\partial\eta^2}-\eta\frac{\partial X}{\partial\eta}\right]+Q(X). \tag{10}$$

It is easily shown from the Gaussianity Eqs. (3) and (4) that $\langle(\nabla\theta)^2\rangle=-C\rho''(0,t)$, where $C=2$ for a two-dimensional physical space and $C=3$ for a three-dimensional physical space. Eq. (10) has been obtained in (Chen et al., 1989), where $-C\rho''(0,t)$ is represented by the variance $\langle(\nabla\theta)^2\rangle$. However, the correlation $\rho(r,t)$ in Eq. (10) still remains to be unknown and has to be input externally. For example, it is set using the results from direct numerical simulation in Chen et al. (1989). Therefore, Eq. (10) is unclosed.

The two-point correlation $\rho(r,t)$ cannot be obtained from the one-point PDF $g_1(\eta)$. Rather, it has to be calculated from the two-point joint PDF $g_2(\eta_1,\eta_2,r,t)$. Hence, we propose to invoke the two-point joint PDF (Eq. (4)), which is not used in the classic mapping closure approach. By differentiating Eq. (7) with respect to t, we obtain

$$\frac{\partial f_2}{\partial t}+\frac{\partial}{\partial\psi_1}\left[f_2\frac{\partial X_1}{\partial t}\right]+\frac{\partial}{\partial\psi_2}\left[f_2\frac{\partial X_2}{\partial t}\right]=\frac{f_2}{g_2}\frac{\partial g_2}{\partial t}. \tag{11}$$

The transport equation for the two-point joint PDF f_2 derived from the test function method (Kimura and Kraichnan, 1993) has the form

$$\frac{\partial f_2}{\partial t}+\nabla_r\cdot[f_2\langle(u_2-u_1)|\psi_1,\psi_2\rangle] =-\frac{\partial}{\partial\psi_1}[f_2\langle\Gamma\nabla^2\varphi_1+Q(\varphi_1)|\psi_1,\psi_2\rangle] -\frac{\partial}{\partial\psi_2}[f_2\langle\Gamma\nabla^2\varphi_2+Q(\varphi_2)|\psi_1,\psi_2\rangle]. \tag{12}$$

Subtracting Eq. (11) from Eq. (12) leads to

$$\frac{f_2}{g_2}\frac{\partial f_2}{\partial t}+\nabla_r\cdot[f_2\langle(u_2-u_1)|\psi_1,\psi_2\rangle] =\frac{\partial}{\partial\psi_1}[f_2H_1]+\frac{\partial}{\partial\psi_2}[f_2H_2], \tag{13}$$

where

$$H_k=\Gamma\langle\nabla^2\varphi_k|\psi_k\rangle-\Gamma\langle\nabla^2\varphi_k|\psi_1,\psi_2\rangle. \tag{14}$$

Multiplying Eq. (13) by ψ_1 and ψ_2 and then taking the mean with substitution of Eqs. (2), (4) and (7), we obtain the transport equation for $\rho(r,t)$ as follows:

$$\frac{\partial\rho(r,t)}{\partial t}+\nabla_r\cdot\langle(\mathbf{u}_2-\mathbf{u}_1)X_1X_2\rangle\left\langle\frac{\partial X_1}{\partial\eta_1}\frac{\partial X_2}{\partial\eta_2}\right\rangle^{-1} =2\Gamma\left[\rho''(r,t)+\frac{\rho'(r,t)}{r}-C\rho(r,t)\rho''(0,t) +\rho'^2(r,t)\left\langle\frac{\partial^2 X_1}{\partial\eta_1^2}\frac{\partial^2 X_2}{\partial\eta_2^2}\right\rangle\left\langle\frac{\partial X_1}{\partial\eta_1}\frac{\partial X_2}{\partial\eta_2}\right\rangle^{-1}\right], \tag{15}$$

where the Gaussian regression is again used. Eqs. (10) and (15) form a closed system for the mapping function, where Eq. (10) describes the evolution of the shape of the mapping function and Eq. (15) specifies the rate at which the mapping function evolves. Numerical simulations verify the validity of the MCA models.

A formal representation for N-point joint PDFs f_N can be also obtained using the mapping function (Eq. (2)) and the N-point joint PDF g_N of reference field:

$$f_N(\psi_1,\ldots,\psi_N,t)=g_N(\psi_1,\ldots,\psi_N,t)\cdot\left[\frac{\partial X_1}{\partial\eta_1}\cdots\frac{\partial X_2}{\partial\eta_2}\right]^{-1}, \tag{16}$$

where the reference field may not be Gaussian. Eq. (16) forms a MCA hierarchy for the PDFs representations. If the reference field is nonGaussian, the hierarchy represents a successive approximation of the MCA approach to statistics of scalar fields. In particular, the second equation with $N=2$ are responsible for two-point correlations and the following-up equations with $N>2$ for the N-point correlations. If the reference field is Gaussian, the approximation is automatically truncated since the N-point PDFs of Gaussian random field is completely determined by its two-point joint PDF. In this sense, the MCA approach for Gaussian reference fields used in this paper is self-contained. The mapping equations could be derived from the governing equations, for example, Eqs. (10) and (15) are derived from the scalar equations. As soon as the solutions of the mapping equations are obtained, the statistics of the unknown random fields can be calculated via Eqs. (6) and (7). In this approach, the multiscale properties of the unknown random fields are represented by the known Gaussian random fields via the nonlinear mapping. The Gaussian random fields may be chosen as multiscale fields, such as their energy spectra have several compact peaks. Therefore, the strong coupling of different scales are represented by nonlinear mapping of scale interaction in multiscale Gaussain random fields. Since the PDF approach could treat nonlinearity exactly, the MCA approach is able to treat the strong coupling of scales.

2.2. Multiscale large-eddy simulation

Numerical simulations resolve some ranges of scales due to its nature of discritization. Direct numerical simulations resolve all scales of interests but it is prohibitively expensive for engineering problems; Reynolds average methods only resolve the averaged motion modeling the effects of all other scales on averaged motions. Such kind of models are difficult to construct due to modeling all other scales; involved in large-eddy simulations (LES), the motion of large scales are calculated while the effects of the motion of small scales on larger scales are modeled. Since the 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 account for these different physics at different scale ranges, multiscale LES (MLES) is being developed: the velocity fields are decomposed into multiple components corresponding to different scales. The different scales are corresponding to different physics. The different physics at different scales require different subgrid scale models. The LES equations with different subgrid scale models need different numerical schemes and grids.

Multiscale method has a long history and different implications. The different implications lead to different numerical implementations and thus produce different results. In the MLES developed by Hughes et al. (2001), turbulence models are confined to small scales but not applied to large scales. The MLES method can be understood as follows: the solutions of Navier–Stokes equation are decomposed into resolved and unresolved parts, where the resolved ones are numerically calculated on grids and the unresolved parts are discarded under the grids. Further, the resolved solutions are partitioned into two parts: large and small scales. In classic LES method, subgrid scale models are applied to the resolved parts of both large and small scales in order to account for the effects of unresolved scales on all of resolved scales; in Hughes's MLES method, the subgrid-scale models are only applied to the small-scale parts and the effects of unresolved scales on the large scales are ignored. The reason for it is that small scales are mostly responsible for energy dissipation so that the eddy viscosity coefficients are dominantly large at small scales and negligibly small at large scales. The MLES method leads to better predictions on the statistics related with energy (He et al., 2002b).

We suggest applying two different subgrid-scale models to large and small scales. The multiscale LES approach could be described and the governing equation of Navier–Stokes fields can be written in Fourier space as follows:

$$\left(\frac{\partial}{\partial t}+\nu k^2\right)u_i(\vec{k},t) = -\frac{i}{2}M_{\mathrm{imn}}(\vec{k},\vec{p},\vec{q})u_{\mathrm{m}}(\vec{p},t)u_{\mathrm{n}}(\vec{q},t)+f_i(\vec{k},t), \quad (17)$$

where M is a project operator and f a large-scale random forcing. The velocity field could be divided into two groups: the resolved velocity field u^R and the unresolved one u^U. The resolved velocity field is further partitioned into the large-scale part u^l and the small-scale part u^s. Their governing equation for the large and small scale parts are, respectively,

$$\left(\frac{\partial}{\partial t}+\nu k^2\right)u_i^l(\vec{k},t) = -\frac{i}{2}\underset{p,q\in u^R}{M_{\mathrm{imn}}}(\vec{k},\vec{p},\vec{q})u_{\mathrm{m}}^l(\vec{p},t)u_{\mathrm{n}}^l(\vec{q},t) + f_i(\vec{k},t)+M^l_{p,q\notin U^R}, \quad (18)$$

$$\left(\frac{\partial}{\partial t}+\nu k^2\right)u_i^s(\vec{k},t) = -\frac{i}{2}\underset{p,q\in u^R}{M_{\mathrm{imn}}}(\vec{k},\vec{p},\vec{q})u_{\mathrm{m}}^s(\vec{p},t)u_{\mathrm{n}}^s(\vec{q},t)+M^s_{p,q\notin U^R}, \quad (19)$$

where $M^l_{p,q\notin U^R}$ and $M^s_{p,q\notin U^R}$ are the large-scale and small-scale parts that interact with unresolved scales. In the usual LES approach, they are modeled using the same SGS models. In the multiscale approach (Hughes et al., 2001), the first one is ignored and the second one is modeled. Although the effects of unresolved scales on large scales can be negligible in terms of energy balance, the effects have to be recovered based on the relevant physics of the unresolved scales, such as random backscatters. Our approach is to develop different SGS models for those two different parts. A significant example is time correlations with its application to aero-acoustics. The LES with the subgrid-scale models responsible for energy balance overpredicts decorrelation time scale (He et al., 2002a). The overprediction could be remedied by application of random forcing model to large scales. The multiscale large eddy simulation method could be generalized to multiple partitions of the resolved solution in company with application of multiscale subgrid scale models. The challenge is to develop the multiscale subgrid scale models for relevant physics in partitioned ranges of scales.

3. Multiscale coupling in solid failure

Our previous studies show that the failure of heterogeneous brittle media under loading has three phases on different scales (Bai et al., 1994; Xia et al., 2000):

(1) globally stable accumulation of microdamage;
(2) damage localization; and
(3) catastrophic rupture.

The microdamage is on an intermediate scale between microscopic and macroscopic, named mesoscopic scale. Obviously, the accumulation of microdamage occurs at mesoscopic scale, the damage localization occurs at locally macroscopic scale, and the catastrophic rupture occurs at globally macroscopic scale. In addition, the physics of the three phases are different: the accumulation of microdamage results from nucleation, extension and coalescence of microdamages; the damage localization is relevant to the evolution mode of damage pattern dynamics and the rupture concerning catastrophe transition. Generally, the dynamics of these physical processes is nonlinear.

It is observed that the damage and rupture in disordered heterogeneous brittle media displays catastrophe transition, sample specificity and trans-scale sensitivity (Bai et al., 2002b; Xia et al., 1996; Xia et al., 2002; Zhang et al., 2004). These features signify that the different scales involved in material failure are strongly and sensitively coupled. Actually, the whole process of damage and rupture appears as an inverse cascade from smaller scales to larger scales and eventually to global scale of the system. During such a process, the effects of some disordered structures at mesoscopic scales can be amplified significantly due to dynamical nonlinearity, and become important at local macroscopic scales, which lead to sample specificity of catastrophe transition. Therefore, catastrophe transition, sample specificity, and trans-scale sensitivity can be attributed to the coupling effects between the dynamical nonlinearity and the disordered heterogeneity on multiscales.

The physics diversity and strong coupling between multiscales and multiphysics are two fundamental difficulties in the problem of solid failure. In addition, these difficulties can be greatly enhanced by the dynamic nonlinearity and the disordered heterogeneity on multiscales. These difficulties make the popular similarity and perturbation methods unfit. Then, what is the suitable approach to this problem?

3.1. Statistical mesoscopic damage mechanics

In principle, the problem of solid failure can be represented by a statistical approach linking microscopic scale and macroscopic scale. However, it is difficult to represent nonequilibrium statistical evolution in a statistical approach linking microscopic and macroscopic scales due to the huge span of the scale. In addition, there are no simple direct connections between microscopic and macroscopic features in the process. Furthermore, a noticeable feature in the problem is the richness of structures and processes at mesoscopic scale. These mesoscale structures, such as grains, microcracks, etc. play significant role in the problem. Hence, a rational approach is to select the intermediate but essential scale between macroscopic and microscopic scales, namely mesoscopic scales, and to develop a statistical approach linking mesoscopic and macroscopic scales. Such a theory is called statistical mesoscopic damage mechanics. Statistical mesoscopic damage mechanics can be constructed based on various mesoscopic representations, e.g., mesoscopic damage representation (Bai et al., 2002a; Wang et al., 2002), and mesoscopic unit representation (Zhang et al., 2004). In this paper, we introduce the framework based on mesoscopic unit representation, which is called driven nonlinear threshold model.

In the driven nonlinear threshold model (Rundle et al., 2000; Xia et al., 2000; Zhang et al., 2004), it is assumed that a macroscopic representative element (at $\mathbf{x}$) is comprised of a great number of mesoscopic units, which are characterized by their broken threshold. The mesoscopic units are assumed to be statistically identical, and their threshold σ_c follows a statistical distribution function. The macroscopic representative element is subjected to nominal driving force $\sigma_0(\mathbf{x}, t)$, which is adopted as macroscopic, external parameter. When a unit breaks, it will be excluded from the distribution function. So, we introduce a time-dependent distribution function of intact units $\varphi(\sigma_c, \mathbf{x}, t)$ with initial condition

$$\varphi(\sigma_c, \mathbf{x}, t = 0) = h(\sigma_c, \mathbf{x}). \tag{20}$$

By applying local mean field approximation to the macroscopic representative element, we obtain the relationship between the true driving force and the nominal driving force:

$$\sigma(\mathbf{x}, t) = \frac{\sigma_0(\mathbf{x}, t)}{1 - D(\mathbf{x}, t)}, \tag{21}$$

where D is continuum damage defined as

$$D(\mathbf{x}, t) = 1 - \int_0^\infty \varphi(\sigma_c, \mathbf{x}, t)\, \mathrm{d}\sigma_c. \tag{22}$$

It is noticeable that the behavior of an individual macroscopic representative element does not display sample specificity owing to the mean field approximation.

The evolution of distribution function $\varphi(\sigma_c, \mathbf{x}, t)$ is suggested to be governed by an equation based on damage relaxation model (the velocity of the macroscopic representative element is neglected):

$$\frac{\partial \varphi(\sigma_c, \mathbf{x}, t)}{\partial t} = -\frac{\varphi(\sigma_c, \mathbf{x}, t)}{\tau}, \tag{23}$$

where τ is the characteristic time of damage relaxation. Generally speaking, τ is a function of the true driving force $\sigma(\mathbf{x}, t)$ and the threshold σ_c of mesoscopic units, $\tau = \tau(\sigma_c, \sigma(\mathbf{x}, t))$. Integrating Eq. (23) and substituting the definition of continuum damage (Eq. (22)) in the obtained equation, we obtain the evolution equation of continuum damage:

$$\begin{aligned}\frac{\partial D(\mathbf{x}, t)}{\partial t} &= f = -\int_0^\infty \frac{\partial \varphi(\sigma_c, \mathbf{x}, t)}{\partial t}\, \mathrm{d}\sigma_c \\ &= \int_0^\infty \frac{\varphi(\sigma_c, \mathbf{x}, t)}{\tau(\sigma_c, \sigma(\mathbf{x}, t))}\, \mathrm{d}\sigma_c,\end{aligned} \tag{24}$$

where f is the dynamic function of damage (DFD), the agent linking mesoscopic damage relaxation and macroscopic damage evolution.

To establish a closed, complete formulation, Eq. (24) should be associated with traditional, macroscopic equations of continuum, momentum, and energy, as well as constitutive relationship. This is a formulation of intrinsically trans-scale closure. However, it is worth noticing that in the constitutive relationship, the effects of microdamage should be taken into account as a reduction in the elastic modulus:

$$E(\mathbf{x}, t) = E_0(\mathbf{x})(1 - D(\mathbf{x}, t)), \tag{25}$$

where E_0 is the intact elastic modulus, and E the effective elastic modulus of damaged media. In addition, the stress appearing in traditional macroscopic equations is nominal stress denoted by $\sigma_0(\mathbf{x}, t)$, while the stress in mesoscopic dynamics equation (Eq. (24)) is the true driving stress $\sigma(\mathbf{x}, t)$.

With the above-mentioned formulation, we investigated the role of multiscale coupling in damage evolution and failure, in particular, at two transition points: the localization transition and the catastrophe transition. In Section 3.2, we derive a criterion to damage localization transition. In Section 3.3, we present a common precursor of catastrophic rupture called critical sensitivity, which may give a clue to prediction of catastrophe transition. In Section 3.4, the energy dissipation during damage and failure is discussed.

3.2. Damage localization

Localization is one of the typical characteristics in complex phenomena. Damage localization is defined as the formation of damage pattern that some heavily damaged local areas are surrounded by lightly damaged areas (Bai et al., 2002a,b). In particular, damage localization refers to the transition of damage evolution mode from randomly and statistically homogeneous damage to inhomogeneous damage. The damage localization can be represented by statistical mesoscopic damage mechanics.

There are three characteristic scales in the formulation of statistical mesoscopic damage mechanics: the scale of mesoscopic damage, the scale of macroscopic, representative element and the scale of the sample, i.e., the global scale. It is interesting that the damage localization is concerning an emerging new scale: the scale of localization, which is an uncertain scale between representative element scale and global scale. This can be attributed to pattern formation or self-organization phenomenon.

In order to demonstrate the mechanism of damage localization, i.e., how the localization scale emerges between representative scale and global scale, we introduce a closed approximation at macroscopic scale. In other words, we introduce an approximate model of dynamical function of damage expressed by merely macroscopic variables:

$$f = f(D(\mathbf{x}, t), \sigma_0(\mathbf{x}, t)). \tag{26}$$

For simplicity, let us consider one-dimensional state. Thus, the continuum damage field equation (Eq. (24)) becomes

$$\frac{\partial D(x, t)}{\partial t} = f(D(x, t), \sigma_0(x, t)), \tag{27}$$

where x is the one-dimensional coordinate of the macroscopic representative element.

In the area with $D \neq 0$, $\partial D/\partial x \neq 0$, the condition of the appearance of damage localization can be represented as

$$\frac{\dfrac{\partial \frac{\partial D}{\partial x}}{\partial t}}{\dfrac{\partial D}{\partial x}} \geqslant \frac{\partial D/\partial t}{D} \quad \text{or} \quad \frac{\partial}{\partial t}\left(\frac{\partial D/\partial x}{D}\right) \geqslant 0. \tag{28}$$

Eq. (28) means that the relative in-homogeneity of continuum damage enhances with time.

From Eqs. (27) and (28), the criterion of damage localization is expressed by

$$f_D \geqslant \frac{f}{D} - f_{\sigma_0}\frac{\sigma_{0x}}{D_x}, \tag{29}$$

where $f_D = \partial f/\partial D$, $f_{\sigma_0} = \partial f/\partial \sigma_0$, $\sigma_{0x} = \partial \sigma_0/\partial x$ and $D_x = \partial D/\partial x$.

In the simple case with uniform nominal stress $\sigma_{0x} = 0$, the criterion of damage localization becomes

$$f_D \geqslant \frac{f}{D}. \tag{30}$$

From $f_D = f/D$, a threshold continuum damage D_L can be obtained, and the damage localization will appear when $D \geqslant D_L$. In this case, the damage localization results from the amplification of pre-existing statistical fluctuations at small scales, and hence, displays uncertainty macroscopically. That is to say, in macroscopically identical samples under identical macroscopic loading, the locations, scales and degrees of damage localization may be very different from sample to sample.

3.3. Critical sensitivity

The sample-specific catastrophe is the other typical characteristic in complex phenomena. This leads to difficulty in the catastrophe prediction. A possible strategy is to seek common features in the vicinity of catastrophe, which may give some clues to catastrophe prediction.

Critical sensitivity may be a common feature of catastrophe in multiscale heterogeneous brittle media (Xia et al., 2002; Zhang et al., 2004). The critical sensitivity means that, in heterogeneous brittle media, the response of the system to controlled parameters, like external loading, may become significantly sensitive as the system approaches its catastrophe transition point.

Let us consider the case of monotonic, quasi-static loading. For simplicity, we neglect the position dependence of all macroscopic variables, and adopt the global mean field approximation. In this case, the only controlled parameter is the nominal stress σ_0 and the continuum damage is determined by the nominal driving force $D = D(\sigma_0)$, which satisfies the following equation:

$$D(\sigma_0) = \int_0^{\frac{\sigma_0}{1-D(\sigma_0)}} h(\sigma_c)\, \mathrm{d}\sigma_c. \tag{31}$$

Denoting damage-induced cumulative energy release by $Q(\sigma_0)$, we define the response to external loading as

$$R(\sigma_0) = \frac{\mathrm{d}Q(\sigma_0)}{\mathrm{d}\sigma_0} \tag{32}$$

and the sensitivity is measured by

$$S(\sigma_0) = \frac{\sigma_0}{R(\sigma_0)} \frac{\mathrm{d}R(\sigma_0)}{\mathrm{d}\sigma_0}. \tag{33}$$

The catastrophe is defined by that infinitesimal increase of controlled parameter induces finite response, i.e., the catastrophe transition point $\sigma_0 = \sigma_{0\mathrm{f}}$ satisfies the following condition:

$$\frac{\mathrm{d}D(\sigma_0)}{\mathrm{d}\sigma_0} = \infty \quad \text{or} \quad R(\sigma_0) = \infty. \tag{34}$$

We will denote the damage fraction at catastrophe transition point by D_c. For $\sigma_0 < \sigma_{0\mathrm{f}}$, the equilibrium state of the system evolves continuously with increasing σ_0 and $D(\sigma_{0\mathrm{f}}) < D_\mathrm{c}$. This is the phase of stable accumulation of damage. However, at $\sigma_0 = \sigma_{0\mathrm{f}}$, the equilibrium state jumps to global failure state ($D = 1$) displaying catastrophe transition, i.e. the system falls into a situation of self-sustained catastrophic failure.

If the initial distribution function is assumed to be a Weibull distribution function

$$h(\sigma_c) = \frac{m}{\eta}\left(\frac{\sigma_c}{\eta}\right)^{m-1} \exp\left(-\left(\frac{\sigma_c}{\eta}\right)^m\right), \tag{35}$$

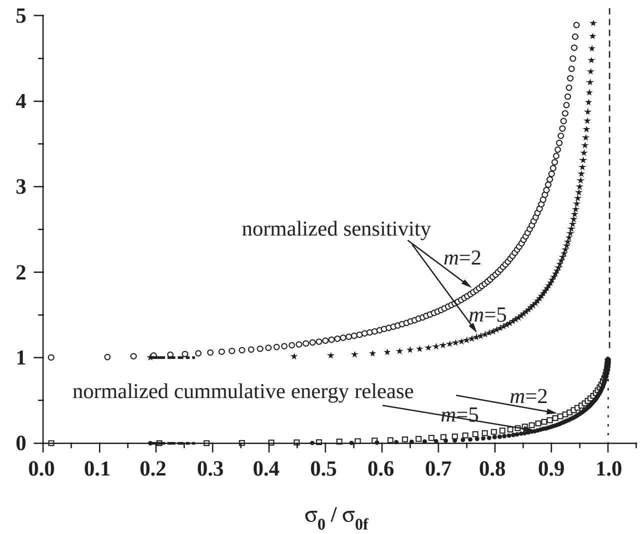

Fig. 1. Cumulative energy release and critical sensitivity in driven nonlinear threshold systems in the case of quasi-static loading based on mean field approximation and damage relaxation model (Zhang et al., 2003).

where m is the Weibull modulus and we take $\eta = 1$. The catastrophe appears at $\sigma_{0\mathrm{f}} = (me)^{-1/m}$ and $D_\mathrm{c} = 1 - \mathrm{e}^{-1/m}$ (Zhang et al., 2004). As the nominal driving force σ_0 approaches $\sigma_{0\mathrm{f}}$, the sensitivity $S(\sigma_0)$ increases significantly ($\lim_{\sigma_0 \to \sigma_{0\mathrm{f}}} S(\sigma_0) = \infty$, see Fig. 1) suggesting the critical sensitivity.

For the case with time-dependent nominal driving force $\sigma_0(t)$, the distribution function $f(\sigma_c, t)$ can be solved from Eqs. (20)–(23). The energy release rate is proportional to

$$R(t) = \frac{\sigma_0^2(t)}{(1-D(t))^2} \frac{\mathrm{d}D(t)}{\mathrm{d}t}, \tag{36}$$

where

$$D(t) = 1 - \int_0^\infty \varphi(\sigma_c, t)\, \mathrm{d}\sigma_c. \tag{37}$$

The sensitivity of response of the system to nominal driving force can be measured by

$$S(t) = \frac{\sigma_0(t)}{R(t)} \frac{\mathrm{d}R(t)/\mathrm{d}t}{\mathrm{d}\sigma_0(t)/\mathrm{d}t}. \tag{38}$$

In Eq. (38), there are two characteristic time scales in the model: the characteristic times of damage relaxation and external loading, respectively. The evolution behavior is determined by the ratio of two time scales reflecting the coupling and competition of the loading and the relaxation processes. The results (Xia et al., 2002) show that the behavior of the system may be very different from that in the quasi-static loading case, but the sensitivity also increases significantly prior to catastrophe suggesting the critical sensitivity of catastrophe, as shown in Fig. 2.

Taking the damage-induced stress fluctuations and stress re-distribution into account, we also investigated the catastrophe behavior in macroscopically identical samples with

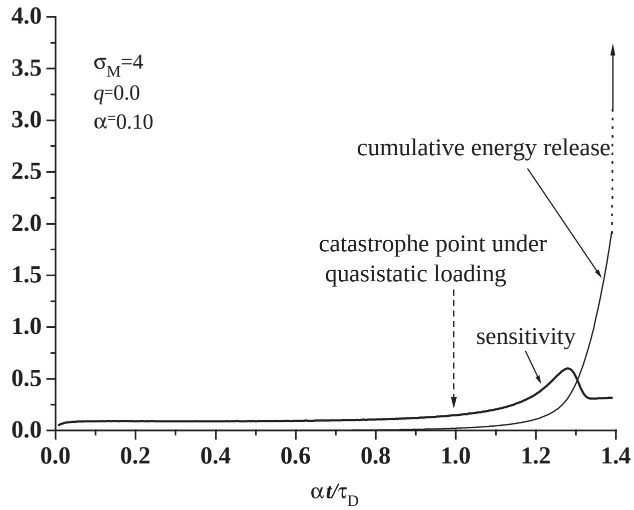

Fig. 2. Cumulative energy release and sensitivity in the case of time-dependent nominal driving force $\sigma_0(t) = \alpha(\sigma_{0f}/\tau_0)t$ (Zhang et al., 2003).

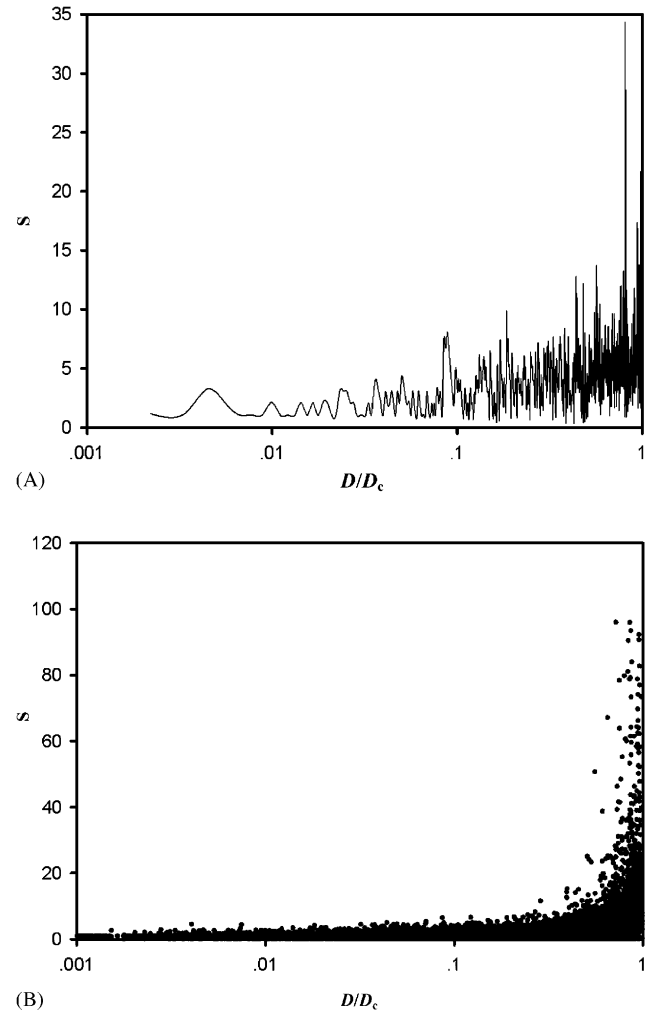

Fig. 3. Critical sensitivity based on numerical simulations (Xia et al., 2002) (A) simulation result of a single sample and (B) simulation result of 200 samples.

the driven nonlinear threshold model. The numerical results show that the catastrophe transition point and the time series of sensitivity are different from sample to sample (Fig. 3). However, all of the samples present critical sensitivity, i.e., the sensitivity increases significantly prior to catastrophe. At the catastrophe transition point, the system falls into a situation of self-sustained failure. Meanwhile, correlation scale of stress fluctuations increases from the scale of mesoscopic heterogeneity to macroscopic scale. Such a behavior is named the trans-scale fluctuations (Bai et al., 2002a,b; Xia et al., 2002). The damage-induced stress redistribution is the main dynamical nonlinearity in the damage and rupture phenomena. The trans-scale fluctuations mean that the stress fluctuations resulting from damage-induced stress redistribution display dynamical coupling between multiscales.

The failure prediction is one of the greatest scientific, technological and societal concerns. In multiscale heterogeneous brittle media, the multiscale coupling results in sample-specific catastrophe. This implies that the failure is sensitively dependent on the details of disordered heterogeneity on multiscales, which leads to difficulties in failure prediction. Based on a closed multiscale formulation for damage evolution, the statistical mesoscopic damage mechanics, we found that the damage localization and the critical sensitivity may be common precursory features of catastrophe in multiscale heterogeneous brittle media. To monitor these precursors may give some clues to catastrophe prediction.

3.4. Energy dissipation

Energy dissipation, or energy release, is an important aspect in damage and failure of solids (see Figs. 1 and 2). From the point of view of energy dissipation, the damage accumulation corresponds to energy dissipation at smaller scales (mesoscopic scales) and the catastrophic rupture corresponds to energy dissipation at very much larger scales (macroscopic or global scales). In Section 3.3, we defined the sensitivity based on damage-induced energy release. It is noticeable that as a precursory feature of catastrophe, the critical sensitivity implies an essential, trans-scale correlation, i.e., the correlation between energy dissipations at smaller and much larger scales. The underlying mechanism is trans-scale, dynamical coupling: the sensitivity reflects the effect of inverse cascade of energy release from smaller scales to larger scales, and, as catastrophe transition point is approached the inverse cascade of energy release at mesoscopic scales triggers the catastrophic energy release.

Now we consider the case of quasi-static, monotonic loading. Based on mean-field approximations (21), (22) and (25) and assuming that the threshold of mesoscopic units follows Weibull distribution function (35), the cumulative input work $W(\varepsilon)$ and the cumulative energy release $Q(\varepsilon)$ are expressed by

$$W(\varepsilon) = \int_0^{\varepsilon} \sigma_0 \, d\varepsilon = E_0 \int_0^{\varepsilon} \varepsilon \exp(-\varepsilon^m) \, d\varepsilon \tag{39}$$

and

$$Q(\varepsilon) = W(\varepsilon) - \tfrac{1}{2} E_0 \varepsilon^2 \exp(-\varepsilon^m) = E_0 \int_0^{\varepsilon} \varepsilon \exp(-\varepsilon^m) \, d\varepsilon - \frac{1}{2} E_0 \varepsilon^2 \exp(-\varepsilon^m), \tag{40}$$

respectively, where ε denotes the strain expressed by the unit with $\eta = 1$. Defining energy dissipation coefficient

$$\lambda = \frac{Q}{W}, \tag{41}$$

we obtain

$$\lambda(\varepsilon) = 1 - \frac{\frac{1}{2} \varepsilon^2 \exp(-\varepsilon^m)}{\int_0^{\varepsilon} \varepsilon \exp(-\varepsilon^m) \, d\varepsilon}. \tag{42}$$

It is interesting to note that the energy dissipation coefficient λ is independent of the initial elastic modulus E_0, a macroscopically averaging parameter, and is only dependent on the Weibull modulus m, which characterizes the diversity of unit threshold at mesoscopic scales, i.e., mesoscopic heterogeneity.

4. Discussions

The physical diversity and strong coupling between multiscales and multi-physics are two fundamental difficulties for multiscale coupling problems in far from equilibrium systems. These difficulties can be compounded by the dynamic nonlinearity and the disordered heterogeneity on multiscales. The classic similarity method and perturbation method do not work at all for these problems. In this paper, we present some methods for two typical multiscale coupling problems in mechanics: turbulence in fluids and failure in solids. The characteristics and mechanisms in these systems are very much different, and at present, it seems difficult to construct a unified theoretical framework for these problems. However, they might share the common points, which are noticeable.

(1) Nonequilibrium statistical theory based on nonlinear dynamics may be an effective approach to most multiscale coupling problems. The number of degrees of freedom at smaller scale is much higher than that at larger scale. Furthermore, the disorder and stochasticity may play important roles in the problems. So, the statistical theory is the first choice to link different scales. For far from equilibrium systems, simple relationship between microscopic scale and macroscopic scale, such as the principle of equal probability in equilibrium state, is no longer available. Therefore, it is necessary to introduce various statistical evolution models.

(2) To choose suitable scale range, reasonable representation and the relevant dynamical model is very important for the derivation of a closed multiscale formulation, which should be tractable but reflect the main physical mechanism. In principle, the multiscale coupling problems can be represented by a statistical approach linking microscopic scale and macroscopic scale. However, it is difficult to represent nonequilibrium statistical evolution in a statistical approach linking microscopic and macroscopic scales due to the huge span of the scales. A possible approach is to select several intermediate and essential scales between macroscopic and microscopic scales. The elementary objects at the intermediate scales are really the systems with huge degrees of freedom. However, in a tractable framework, we have to select a few most important collective degrees of freedom to characterize the elementary objects at the intermediate scales. As the scale range and the representation are chosen, we have to construct the relevant dynamic models at various scales and the coupling model linking different scales.

(3) In multiscale coupling problems, strong interactions among multi-physics at different scales usually exist. Therefore, joint probability density functions and correlation functions, like the BBGKY hierarchy in traditional statistical physics, have to be introduced into theoretical formulation. This makes the formulation untractable. It becomes necessary to introduce proper approximation at some level based on their dynamics. The mapping closure approximation approach is a new development in this direction.

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