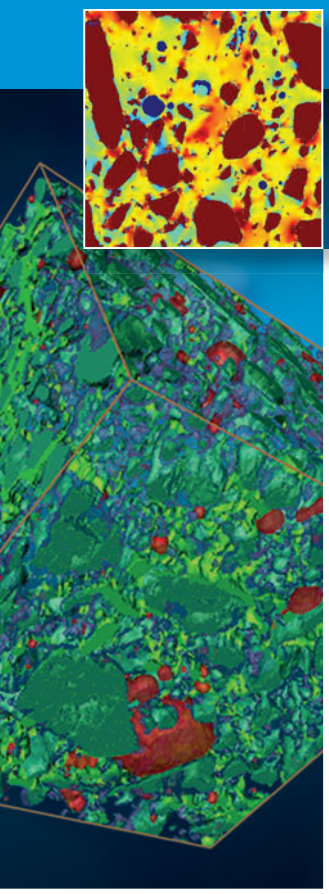


Multiscale modeling of microstructure–property relations

M.G.D. Geers and J. Yvonnet

The recent decades have seen significant progress in linking the mechanical performance of materials to their underlying microstructure. This article presents an overview of some of these achievements, trends, and challenges. Attention is given to methods initially developed for micromechanics and their gradual evolution toward powerful multiscale methods. Various methods have been proposed for bridging scales in mechanics of materials, all aiming for efficiency and accuracy. Computational homogenization is one of these powerful approaches, now used systematically for the assessment of structure–property relations. Novel solution methods and model reduction techniques provide tools to speed up the structure–property analysis, whereby large-scale computations have been made possible. Truly fast analyses of microstructures may be expected in the near future.

Introduction

"Building an airplane atom by atom" or "making a steel from scratch" are statements that are still unrealistic, even though they challenge and stimulate scientific developments. Materials science and mechanics of materials, focusing on different length scales and applications, coexisted as different disciplines for many decades. Yet, the sustained development of novel multiscale methods and computational solution strategies as well as growing computational power, are gradually conglomerating both fields.

The gap between the scale of atoms and the properties of an engineering material used in a macroscopic application entails different length scales, time scales, substructures at these different scales, and a large degree of complexity in the evolving structure, energetics, and dynamics across these scales. For these reasons, it remains strictly unrealistic to build engineering structures from the bottom up. Tackling the intrinsic relation between microstructure (at each of the scales) with scales revealing engineering properties requires appropriate methods that properly handle scale transitions and complexity in a sufficiently accurate manner.[1] It is with this objective in mind that multiscale methods have emerged over the years and are gaining systematic importance, both in materials science and various engineering disciplines.

Providing a complete overview of all single-scale models, solution methods, and associated scale couplings is obviously not a feasible task. This article, therefore, focuses on mechanical properties of engineering materials. Selected important methods that address (some) of the (spatial) scale transitions will be highlighted. "Unraveling complexity" thereby constitutes the common thrust forward.

Micromechanics of materials—From microstructure to properties

Microstructures are typically characterized through the spatial distribution of different phases with distinct properties and interfaces. Provided the properties of each of the single phases are adequately understood and characterized, the composite behavior of the resulting "mixture" can be determined. Early developments in this direction date back to the classical rule of mixtures (Voigt, 1887) and the upper and lower bounds defined by Reuss/Taylor[2] and Sachs.[3] The use of composites in past decades as novel engineering materials triggered novel insights and models, all aiming to predict the mechanical behavior of heterogeneous microstructures as if they were replaced by an "equivalent homogeneous continuum." This resulted in the term "homogenization," which has been used in this sense since then. The analytical solutions for an ellipsoidal-shaped inclusion in a matrix by Eshelby[4] and the many contributions by Hill[5] established "micromechanics" as a true discipline. An overview of the field of continuum micromechanics can be found in the survey provided by Zaoui.[6]

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Homogenization theories for heterogeneous microstructures have been developed since the 1950s. Many of them rely on a geometrical simplification of the underlying microstructure. In the first decades, attention was mainly given to elastic heterogeneous solids. The first extensions toward nonlinear material behavior emerged through the work of Kröner,[7] Hill,[5] Hutchinson,[8] and many others. As a result, we now have access to a plethora of homogenization techniques dealing with various kinds of microstructural behavior, such as plasticity, elasto-viscoplasticity, porous materials, polycrystals, and fiber-matrix systems. The main goal in most of these theories is to identify a closed-form constitutive equation that defines the relationship between material response (i.e., the stress state) and its excitation (i.e., deformation or strain).

These simplified homogenization theories have served, to a great extent, in the understanding of materials at the engineering level. However, there are some intrinsic limitations to these theories that have triggered and nurtured the development of more powerful multiscale methods, including (1) the geometrical simplifications adopted (microstructures were considerably idealized); (2) the limitations in complexity regarding the behavior of each of the individual phases; (3) the treatment of interfaces, which are considered to be perfect or entirely debonded, whereas the physical reality is considerably more complex; and (4) overlooked microstructural defects that are inherent to all microstructures.

Multiscale approaches for structure–property relations

Brief overview of multiscale methods

The number of models developed at single scales is huge, ranging from density functional theory at the smallest scales, molecular dynamics at the atomic scale, and (semi-) discrete models, such as discrete dislocation plasticity, microstructural lattice models, continuum microstructural models, and continuum macroscopic models at larger and continuum scales. Each of these approaches aims to tackle the response of the considered material (or phase) at a given spatial scale and often also at a given temporal scale.

A microstructure, however, is a complex geometrical arrangement of different phases and interfaces. Linking the properties at the engineering scale (typically the scale of the device or component, which may range from micrometers to meters) to the microstructural scale inevitably requires a two-scale approach (or more, if needed). This is what characterizes a "multiscale" model.

Based on the nature and geometry of the scale of the heterogeneities, different types of multiscale methods can be distinguished.[9–12] Emphasis here is on spatial multiscale approaches seeking the effective macroscopic response of statistically representative volume elements (RVEs) of the underlying microstructure. The RVE is typically a sample volume element of material that is large enough to represent the statistical fluctuations in the microstructure and hence capture the effective (averaged) mechanical properties. From the perspective of the underlying problem formulation, one can distinguish between:

- Concurrent methods—where both scales are simultaneously addressed, generally using different methodologies, for different scales, in different parts of the problem domain.[11]
- Hierarchical methods—where different scales are hierarchically coupled in the same part of a domain (e.g., computational homogenization).
- Hybrid methods—revealing a hybrid coupling scheme between the scales (e.g., generalized finite elements,[13] quasi-continuum approach,[14] multigrid methods,[15] and the variational multiscale method).[16]

The underlying solution procedure for each of the multiscale problems can be either (1) parallel (solving both scales monolithically), (2) serial or sequential (data passing between the scales), or (3) coupled or decoupled (using coupled online computations or decoupled offline computations).

The versatility of a multiscale method obviously depends on the assumptions made and the accuracy of the descriptions used at the underlying fine scales. Multiscale mechanics have evolved toward a methodology that naturally fills the gap within materials science, where the physics, synthesis, and material characterization of single phases and microstructures are a key concern. In the mechanics community, advanced nonlinear continuum models of detailed microstructures are being developed. In computational materials science,[17,18] various examples exist that unravel microscale mechanisms using analyses at the nanoscale (including Monte Carlo methods for statistical analyses). In this context, computational materials science and computational multiscale micromechanics have gradually started to merge.

Among the various multiscale methods developed, this article will touch upon one method in particular, computational homogenization, and also briefly report on some of the other methods. It should be noted that this mainly concerns the spatial multiscale problem. Many of the single-scale models make use of vastly different time scales (or loading rates), and incorporating them is possible if either no temporal scale transition is used (i.e., the fast microstructural fluctuations are fully resolved) or a time scale separation applies (i.e., fast fluctuations can be eliminated from the slow ones).

Computational homogenization

Homogenization of microstructures substitutes microstructural complexity by an equivalent homogeneous continuum. For this purpose, RVEs or representative unit cells are used.

In order to "homogenize" a microstructure, a scale separation principle must be adopted, implying that the relevant microscales are much smaller than the characteristic fluctuation scale in the macroscopic strain field. Many homogenization techniques have been developed, including composites,[19] materials revealing size effects,[20] and random physically nonlinear materials.[21] Several asymptotic (or mathematical) homogenization approaches for nonlinear material behavior have been proposed and developed as well.[22]

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Computational homogenization is a powerful method to extract the macroscopic behavior on the basis of an underlying microstructural RVE. The method consists of a coupled solution of two nested boundary value problems, one at each scale. **Figure 1** shows the elementary principles of the method for a mechanical homogenization problem. The deformation (strain) at the macroscopic scale is transferred to the microscale using deformation averaging, through which appropriate boundary conditions can be constructed. The solution of the microscale boundary value problem results in the macroscopic stress and tangent operators (derivatives of the stress tensor with respect to the strain or deformation tensor) using the energy consistency (Hill-Mandel) condition linking both scales. With the resulting macroscopic stress–strain behavior, a macroscale equilibrium problem can be solved (if needed).

If the finite element method (FEM) is used to solve the boundary value problems at both scales, the method is also referred to as the FE^2 method.[23] The strength of this method is that it works for arbitrarily nonlinear behavior, including microstructural evolution at the microscale. The quality of the results depend on the modeling approximations made at the fine scale. There are no additional approximations at the coarse (macroscopic) scale. The basic (first-order) method is now well established.[24–28]

The computational homogenization scheme has been extended in various directions: higher-order continua[29] (to address size effects); damage and localization;[30] thermomechanics;[31] substructured shells;[32] cohesive interfaces;[33] electromagnetics; diffusion; sintering; heat flow, contact, and friction;[34] and wave propagation in solids.[35] In terms of materials, applications can be found for metals, textiles, cellular and porous materials, composites, granular materials, soft matter, bone, and Li-ion batteries.

This method is powerful and accurate, and therefore, used often as a reference solution for other more simplified homogenization schemes. However, it comes with a high computational cost, which limits its applicability for many applications involving complex microstructures. To address this, appropriate algorithms have been developed to speed up multiscale simulations of this type, as discussed further in this article.

Examples of structure–property relations

Copper-rubber interface delamination in stretchable electronics

An example of the application of the computational homogenization method concerns the analysis of copper-rubber interfaces, used in most stretchable electronics applications.[36–38] These interfaces typically fail as a result of rubber fibrillation at the rough copper interface (fibrils, attached to the copper, which are drawn from the rubber upon delamination). Even though the intrinsic microscale adhesion between copper and rubber polydimethylsiloxane is only in the range of 1 J/m^2, macroscopic peel tests report a work of separation of up to 1000 J/m^2 or more. **Figure 2** illustrates the various contributions underlying this gap, ranging from fibril stretching, dynamical energy release in the fibrils and their bulk footings, and the interactions between neighboring fibrils.

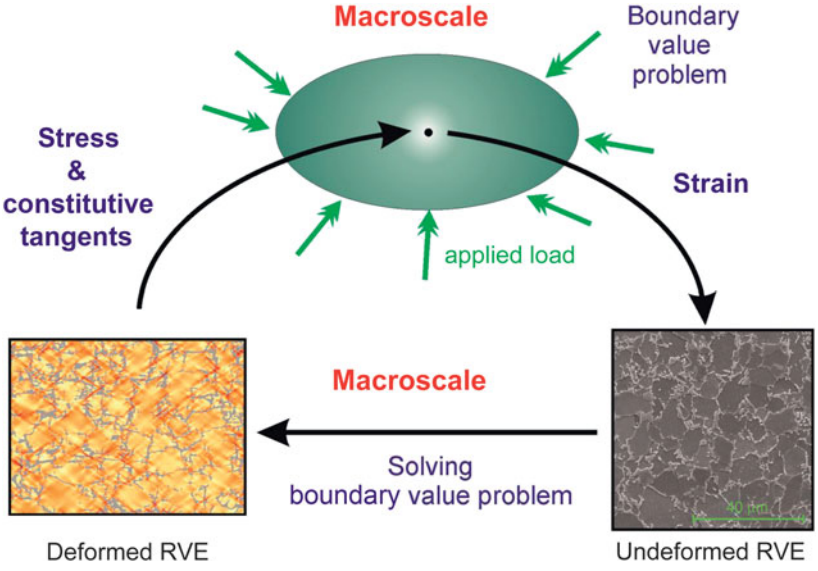


Figure 1. Computational homogenization is one of the most powerful methods to extract properties from a microstructure. (Top) The strain from the macroscale is passed to (bottom right) a representative volume element (RVE); (bottom, right to left) the microscale boundary value problem is solved; (bottom left) the average stress and constitutive tangents are extracted from the solution and passed (top) to the macroscale; the microscale problem shown here is a dual-phase steel loaded in 10% pure shear, solved with a fast Fourier-based solution technique. The deformed RVE highlights the equivalent plastic strain in the ferrite matrix phase.

Advanced dislocation-based plasticity models

The plasticity of metals, ranging from the atomic scale via individual dislocations to collective dislocation motion toward macroscale plasticity, has been the subject of multiscale analysis for many years.[1] **Figure 3** illustrates the characteristic couplings between the scales. For metal plasticity, two recent structure–property modeling approaches are emphasized.

Kooiman et al.[39–42] analyzed the coarse graining of the collective behavior of dislocations using the general equation for the non-equilibrium reversible-irreversible coupling scheme.[43] One of the key results of this work,[42] highlighted in Figure 3 (bottom plots), is that the macroscopic relation between applied mechanical load and dislocation flux is nonlinear (power law), whereas the input relation between load and dislocation velocity at the microscale is linear. This constitutes an emergent phenomenon, which is shown to be dominant over other contributions. Note that this method also properly handles the time-scale transition,[42] which is one of the grand challenges in multiscale modeling.

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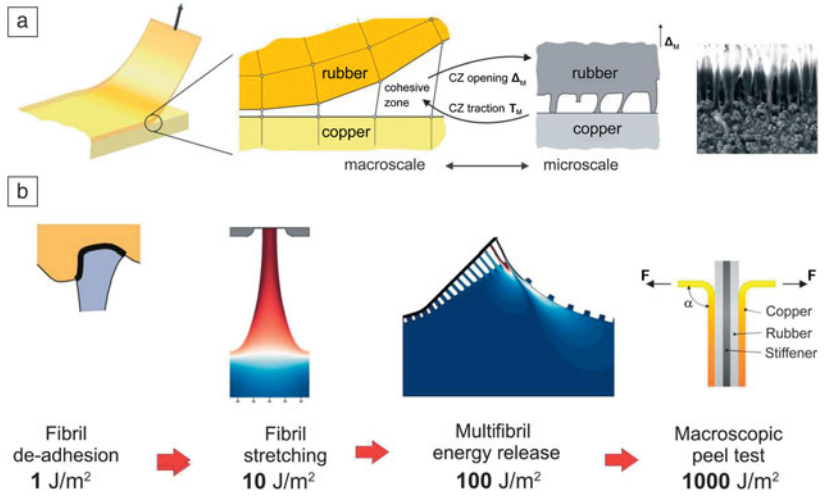


Figure 2. (a) Computational homogenization applied to a copper-rubber interface problem, from left to right: the delaminating interface at the macroscale; the macroscale cohesive zone (CZ) interfacial model, computing the traction vector ($\mathbf{T}_M$) from the interfacial opening vector Δ_M; the microscale model with individual fibrils; and a micrograph of the real fibrils. (b) Energetic contributions to the macroscopic work of separation across the scales, from left to right: adhesion energy at the level of a single fibril; stretch energy of a fibril; energy release in the rubber upon fibril fracture or de-adhesion; and macroscopic work of separation in a peel test under an applied force **F** and an angle α.[37,38]

The plasticity of metallic interfaces (e.g., grain and phase boundaries) is indicated in Figure 3 as well. This is a highly complex problem, since gliding dislocations interact with the grain-boundary defect structure, giving rise to dislocation pile-ups, dislocation absorption, transmission, and nucleation events. Van Beers et al.[44–47] proposed a thermodynamically consistent model for interface plasticity inspired by the results from atomistic simulations and discrete dislocation plasticity results. This model accounts for the grain-boundary energy and defect structure, as well the defect redistribution within the grain boundary upon absorbing dislocations in the grain boundary.

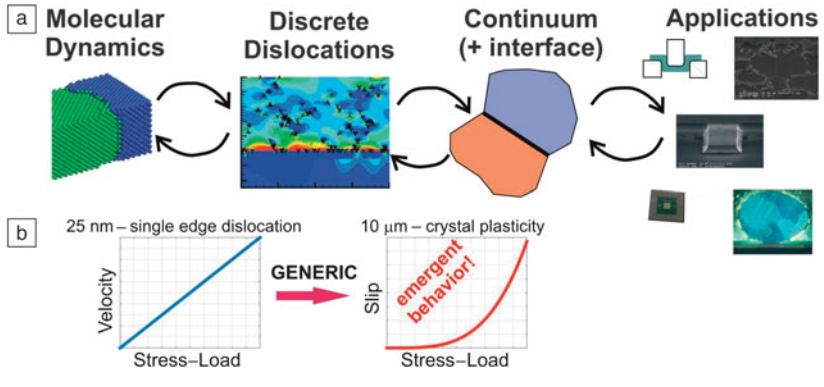


Figure 3. Multiscale analysis of metals, from dislocations to crystal plasticity. (a) Scales and models involved, from left to right: atomistic scale, molecular dynamics; dislocation scale, discrete dislocation dynamics; single-crystal scale, crystal plasticity; application scale, continuum plasticity models. (b) (Left) The collective behavior of individual dislocations (linear velocity–stress profile) leads to (right) emergent contributions at the crystal continuum level (power-law slip–stress profile).[42]

Reducing computational costs in multiscale materials modeling

New methodologies for fast microstructural calculations on RVE

To model realistic microstructural RVEs in two dimensions[48] or three dimensions, efficient methods must be developed to reduce the costs related to fine-scale computations. Three-dimensional (3D) models are required in situations where two-dimensional (2D) models fall short, for example, for glass-fiber fibrous composites with nonparallel directions[49] or in complex morphologies, such as those encountered in cementitious[49] and polycrystalline materials. The main difficulty in taking complex 3D microstructural geometries into account is to define efficient high-resolution methods, especially when the microstructure is obtained from experimental microtomography images.

The fast Fourier transform (FFT) method[26,50–52] is a fast numerical technique to solve the mechanical problem in the RVE. This image-based numerical method does not require prior meshing (finite element discretization), (i.e., partitioning the domain into simple geometrical subdomains), allowing handling of arbitrary (possibly evolving) microstructural geometries. Equilibrium and heat-flux conservation are, in particular, treated in the Fourier domain, assuming spatial periodicity of fields, even though the geometry is not itself periodic. Altendorf et al.[49] used FFT to study the local and effective properties of complex glass-fiber composites with high resolution. Escoda et al.[53] used FFT to compute both local and effective stress fields in 3D high-resolution models (constructed from 3D gray-level images containing up to 735^3 voxels) of mortar material microstructure (see **Figure 4**).

Lavergne et al.[54] investigated the effect of the aggregate morphology on the viscoelastic effective behavior of concrete using FFT. Chen et al.[55] investigated the combined effects of mechanical loading and recrystallization in 3D polycrystals using combined FFT and phase-field modeling. Such studies allow the determination of the parameters in the microstructure that have an influence on the lifetime of the material. Yvonnet[56] developed a modified FFT method operating in the real-space domain only, to avoid the alternate Fourier-space–real-space evaluation of the different operators and to facilitate parallelization.

A critical comparison between several methods for solving RVE problems with complex microstructures was provided in a recent review.[57] Using a benchmark problem, classical discretization techniques, the eXtended Finite

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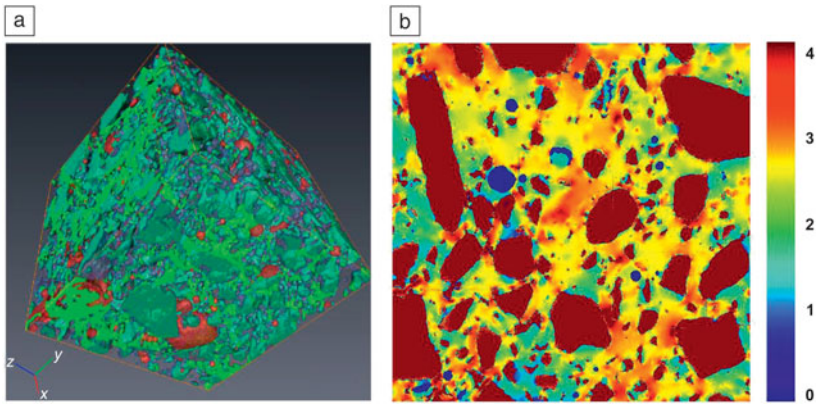


Figure 4. (a) 3D view of a mortar microstructure, voids in red, aggregates in other colors, and transparent matrix. The displayed volume measures 1.25 × 1.25 × 1.25 cm^3. (b) 2D section of the normalized mean stress component $\sigma_m/[E_m\langle\varepsilon\rangle]$ at high contrasts of elastic properties in the mortar microstructure of (a) loaded with an average volumetric strain $\langle\varepsilon\rangle$. σ_m, E_m denote the local hydrostatic stress and Young's modulus, respectively. The resolution is 25 μm/voxel. Reproduced with permission from Reference 53. © 2011 Elsevier.

Element method[58,59] (for modeling interfaces in regular meshes), classical FEM with regular meshes and smoothed properties,[60] and the FFT methods were compared in terms of the resulting computational efficiency and accuracy. In particular, it was shown that the FFT method is the most efficient method for fine models in the absence of discontinuities such as cracks or imperfectly bounded interfaces, while the eXtended Finite Element method can provide an adequate accuracy even for coarse models by accurately describing the discontinuities at the interfaces.

Reducing computational costs in nonlinear coupled simulations at two scales

One of the main challenges of computational homogenization is the computational complexity involved in solving boundary value problems at two (or more) scales. Of particular interest are predictive multiscale methods, which include both the aforementioned realistic microstructures, and in addition, the macroscopic engineering scale with its loading conditions. These simulations can become extremely costly given the large number of degrees of freedom involved. Recent approaches aim to alleviate the computational complexity in two-scale simulations using parallel implementation strategies, reduced-order modeling, and decoupled approaches.

Parallelization of computational homogenization[23,26,28] relies on the distribution of the numerous local microscale boundary value problems, typically evaluated at the integration points of the discretized macroscopic structure, over many processors (cores). Nguyen et al.[61] introduced a parallel implementation of the FE^2 method for multiscale failure with multiphysics coupling for concrete. Ladevèze et al.[62] developed a domain-decomposition-like method to solve heterogeneous composite problems. In this context, the domain was decomposed into substructures and interfaces, and the so-called LATIN (Large Time INcrement) method was used to solve the two-scale problem. This technique involves a space–time decomposition of the fields in tandem with a special iterative solver involving a global linear problem and local nonlinear problems over the structure of interest. Fritzen et al.[63] proposed massively parallelizing FE^2 methods with graphical processing units. These specialized electronic circuits, originally designed to accelerate the display of images, were used to reduce the costs of multilevel techniques and gain several orders of magnitude computational cost reduction. Mosby and Matouš[64] developed massively parallel computing strategies to solve huge multiscale problems, the largest involving a total of 28.1 billion nonlinear equations solved on 393,216 computing cores. An example of their work is shown in **Figure 5**.

Introducing model reduction in FE^2 methods was first initiated for hyperelastic composites to study the effects of reinforcements in rubbers,[65] where the proper orthogonal decomposition (POD)[66] technique was used to reduce local computations. POD is used for extracting correlations from arbitrary sets of data and determining the most relevant set of modes for an evolving system. These modes consist of linearly independent fields (e.g., displacement fields) that characterize the evolution of the system. Local computations were reduced by projecting local fields on a POD basis, then reducing the large sets of nonlinear equations of microstructural calculations.[65]

Hernández et al.[67] proposed a POD reduced-basis multiscale method with an interpolatory integration scheme that overcomes ill-posedeness problems (corresponding to nonuniqueness of the solution) in model reduction techniques of multiscale damage problems by embedding the gradient of the POD modes. Wen and Zabaras[68] proposed a POD multiscale method for stochastic FE^2 problems. Sparks and Oskay[69] proposed a method for identification of optimal reduced-order models for inelastic and failure response of heterogeneous materials, employing the eigendeformation-based reduced-order homogenization approach. Halabi et al.[70] recently replaced POD-parametrization of local fields in FE^2 by proper generalized decomposition[71] tensor product approximations to reduce costs related to offline computations.

Dvorak[72] initiated another important nonlinear micromechanical homogenization method, mainly applied to elasto-viscoplastic materials and metal-matrix composites, known as the transformation field analysis (TFA). In order to properly reproduce the local heterogeneous fields, nonuniform transformation analysis (NFTA)[73,74] was developed. In this method, anelastic modes are extracted from snapshots of nonlinear simulations using POD. Fritzen et al.[75] proposed an extended NTFA method and presented a comparative study between their

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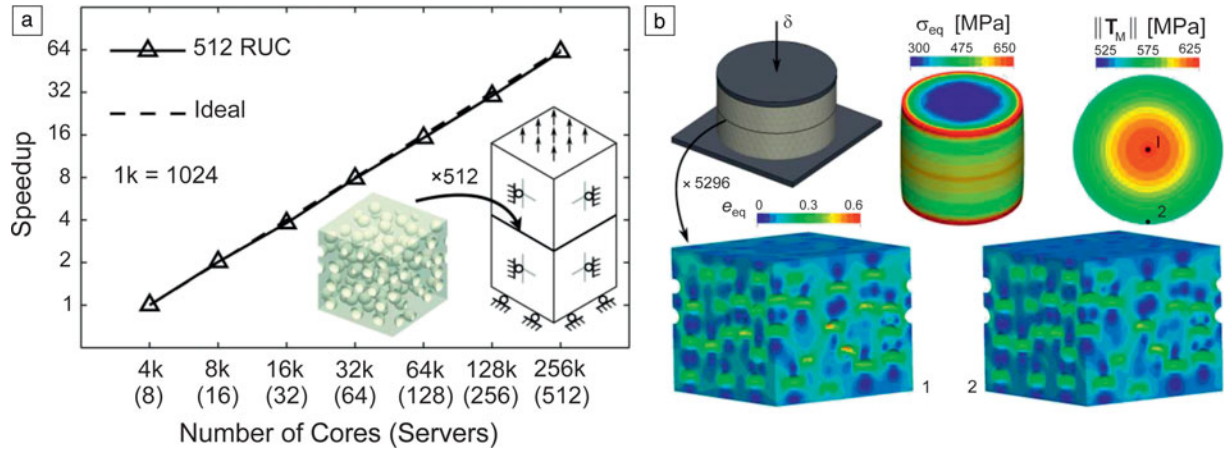


Figure 5. Computational speedup of a hierarchically parallel multiscale solver. (a) The macroscale is discretized with 17.5k finite elements and 9.8k nonlinear degrees of freedom (DOFs) and is computed using 32 cores. Each of the 512 representative unit cells (RUCs) are discretized with 1.46M finite elements and 773k nonlinear DOFs, and is computed using 512 cores. The complete multiscale simulation contains 747M finite elements and 396M DOFs. (b) (Bottom) The 1 and 2 strain plots are associated with the corresponding 1 and 2 points located on the (upper right) mid-plane of the structure. This figure illustrates the drastic computational time reduction enabled by parallel computations in nonlinear multiscale modeling. Reproduced with permission from Reference 64. © 2016 IOP Publishing. Note: δ, applied displacement; σ_{eq}, equivalent stress; $\mathbf{T}_M$, traction vector; e_{eq}, equivalent strain.

method and NTFA, showing the limitations of classical NTFA and the more general character of their technique to handle arbitrary elasto-viscoplastic behaviors with rate dependency.

A last and promising class of methods is decoupled nonlinear homogenization methods. First a set of offline calculations is performed. Then, techniques are developed to construct "*a posteriori*" the effective behavior based on these calculations. Local calculations are no longer required, which reduces the cost of coupled multiscale simulations by several orders of magnitude.[76] A first natural choice is to identify functional forms of the macroscopic constitutive equations:[77] Numerical material tests are conducted on a unit cell to identify material parameters of the assumed constitutive law. This methodology implies "guessing" the form of the equation describing the effective behavior, which is not obvious in a general nonlinear context and for arbitrary (anisotropic) microstructures.

To overcome this issue, database methods were developed[77–80] to compute the response of nonlinear composites using an interpolation technique in a higher dimensional space from a prior set of databases composed of numerical evaluations of the quantities of interest (e.g., the effective energy of the RVE under various loads) computed from offline nonlinear calculations on the RVE. The obtained database can be compressed using tensor product approximations to accelerate macroscopic behavior evaluation during the structural (online) calculations.[81] Such methods enabled the solution of one of the first nonlinear multiscale stochastic problems.[82,83] Another promising development is the use of neural networks in nonlinear multiscale methods[84] to construct fully decoupled approaches, where neural networks are employed to define the complex mapping between both macroscopic loading and microstructural parameters and the effective response of the RVE.

Concluding remarks

While this article mainly focused on spatial multiscale methods and computational homogenization in particular, two additional points must be addressed. The first concerns the propagation of uncertainties across the scales. This topic constitutes an emerging area of interest in computational homogenization.[85,86] The second point concerns the temporal multiscale problem. As previously emphasized, algorithms either deal with a scale transition only in space (using equal time scales), or with time scales that fully separate. Multiscale methods studying phenomena modeled at different time scales generally require proper separation of time scales.[43] The rigorous coupling between spatial and temporal scales in a multiscale setting is one of the open challenges.

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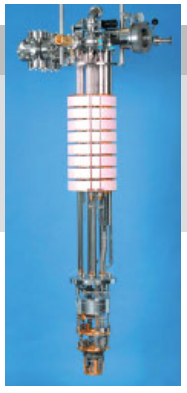
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