REVIEW ARTICLE | INSIGHT
https://doi.org/10.1038/s41563-020-00913-0

nature materials

Mesoscopic and multiscale modelling in materials

Jacob Fish[1]✉, Gregory J. Wagner[2] and Sinan Keten[2]

The concept of multiscale modelling has emerged over the last few decades to describe procedures that seek to simulate continuum-scale behaviour using information gleaned from computational models of finer scales in the system, rather than resorting to empirical constitutive models. A large number of such methods have been developed, taking a range of approaches to bridging across multiple length and time scales. Here we introduce some of the key concepts of multiscale modelling and present a sampling of methods from across several categories of models, including techniques developed in recent years that integrate new fields such as machine learning and material design.

Multiscale modelling is a concept that influences many fields, but its impact on material modelling over the past few decades has been particularly noteworthy. Multiscale modelling concerns the derivation of equations, parameters or simulation algorithms that describe behaviour at a given length scale on the basis of the physics at a finer scale, provided that the fine-scale physics and structure are better understood than those at a coarser scale. The fine scale may include electrons, atoms, molecules and their assemblies, or mesoscale structures such as phases or grains. This contrasts with the conventional phenomenological paradigm, which describes material behaviour directly at a coarser scale relevant for analysis and design and is much more reliant on available experimental data rather than on physics. Perhaps an equally important objective of multiscale models is the ability to map a continuum-scale description such as deformation or temperature field onto smaller-scale features, such as the relative positions and velocities of atoms or grains. While providing a link between fine and coarse scales using tools of statistical mechanics may be trivial for homogeneous materials and simple properties, the undertaking becomes challenging for heterogeneous systems, particularly for describing large deformation and failure of materials, which often involve history-dependent mechanisms. Resolution of these complicated issues has drawn many minds to this deep and alluring topic. Numerous past reviews[1–4] have discussed the advantages that can be achieved by this kind of multiscale approach. It is believed that multiscale computations will play a critical role in future nanotechnology and materials genome research[5].

The goal of this Review is to introduce some of the key concepts, to survey the current landscape in multiscale modelling and to highlight recent advances and some important and promising areas for future research. We summarize work developed during the current era of growth in multiscale modelling, including ideas formulated in the 1990s and 2000s that continue to influence the shape of the field, and give examples of recent contributions that assimilate new areas such as machine learning and material design into the multiscale domain. Our review focuses on models of the mechanical and thermomechanical performance of solids, since these models provide a convenient through-line for tracing development of multiscale theory, but many concepts discussed can be extended to multiscale predictions of electrical, magnetic and chemical properties of complex materials.

Development of multiscale modelling

The development of many multiscale models begins with the recognition that a given assumption, such as the use of a particular constitutive equation, is inadequate for some important range of material response. The mathematical description of material behaviour consists of two types of equation: those that directly reflect physical laws, and those that do not. For example, equilibrium and kinematical equations represent conservation of quantities such as mass, momentum and energy. Conversely, constitutive equations are material specific and cannot usually be derived directly, including all parameters, from physical laws. Linear constitutive models may be easily quantified experimentally, but this is by no means the case for nonlinear, anisotropic or history-dependent materials. In practice, however, a few constitutive law parameters are believed to 'capture' different failure mechanisms observed in experiments—an approach known as phenomenological modelling. It describes empirical relationships of observations, which are consistent with fundamental theory but are not directly derived from it. Alternatively, constitutive equations or field quantities may be derived from finer scales, where physical phenomena are believed to be better understood than the emergent coarse-scale behaviour. This alternative is the focus of this Review.

Challenges in multiscale modelling. The decision to pursue a multiscale approach involves a trade-off between increased model fidelity with the added complexity, and corresponding reduction in precision and increase in uncertainty, that a multiscale simulation brings. An appropriate guiding principle for assessing the need for finer scales is Occam's razor: simplicity is preferred, complexity only when necessary. The use of any multiscale approach, then, has to be carefully weighed on a case-by-case basis. Another consideration is purely computational, arising because of the existence of multiple spatial and temporal scales. Consider, for instance, the Airbus A380 depicted in Box 1.

It is tempting to start at the ab initio scale and to upscale, scale after scale, all the way to the product scale. This, unfortunately, is not realistic due to the enormous computational complexity involved. As an illustration, consider just two continuum scales of the above structural problem (coarse and fine) having n integration points, N load increments at a coarse scale and I average iterations at both scales. The total number of linear solves of the unit cell problem is thus nNI^2—a formidable computational cost when dealing with large numbers of unit cells and when the size (number of degrees of freedom) of these unit cells is substantial. Each additional scale brings further multiplicative increases.

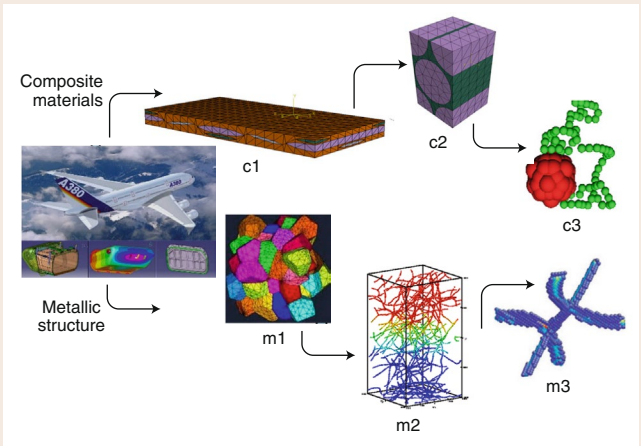
The computational complexity of deducing continuum models directly from atomistics is even greater. Deterministic atomistic-level computations can model systems up to the order of several billions of atoms for timescales of the order of nanoseconds, but this remains orders of magnitude below continuum length and time scales (usually in millimetres and milliseconds). Continuum-level simulations may be applicable at these larger scales, but at the expense of explicit

[1]Columbia University, New York, NY, USA. [2]Northwestern University, Evanston, IL, USA. ✉e-mail: fishj@columbia.edu

Box 1 | Multiple scales in the Airbus A380

Airbus 380: 53 m long with a wingspan of 80 m and height of 24 m. It consists of hundreds of thousands of structural components and many more structural details. In the fuselage alone there are more than 750,000 holes and cutouts. In addition to various structural scales, there are numerous material scales. At the coarsest material scales, the composites portion of the fuselage consists of laminate and woven/textile composite scales; at the intermediate scale is a tow or yarn, which consists of a bundle of fibres; finally, there are one or more discrete scales, including atomistic and ab initio (quantum) scales. The metal portion of the aeroplane consists of a polycrystalline scale, a single-crystal scale that considers dislocation density, a discrete dislocation scale and finally atomistic and ab initio (not shown) scales.

Composite material—c1, woven composite architecture; c2, tow microstructure; c3, molecular structure of polymer resin. Metallic structure—m1, polycrystal; m2, dislocations; m3, atomistic structure. Figure reproduced with permission from ref. [3], Wiley.



atomistic resolution. Addressing this tyranny of scales requires the introduction of efficient and accurate methods to distil information and transfer between scales, or the judicious use of fine-scale information only in isolated parts of the domain while prescribing formulations that couple to surrounding scales. Most modern multiscale simulation approaches make use of one or both of these strategies.

Foundations and historical development. Multiscale science and engineering is a relatively new discipline but has its precursors in various approximation theories that relate macroscale or mean behaviour to atomistic scales. One such foundational concept is the Cauchy–Born rule[6], which allows the mapping of macroscale deformations to the displacements of the atoms resulting in stretching or compression of chemical bonds. The Cauchy–Born rule states that, for simple crystal structures, the positions of the atoms within the lattice follow the average strain of the medium. Once we define the interatomic potential describing the lattice bond interactions, minimization of the potential energy defines the ground-state crystal configuration, and the geometric mapping between continuum strains and atomic movements enables us to use the atomistically determined strain-energy density to calculate the macroscopic stress–strain relationship. Given its generic nature, the Cauchy–Born rule has been applied to many different material systems, and can even be used to describe nonlinear elastic behaviour at large deformations[7]. Applications include computation of material constants such as bulk compressibility for Bravais lattices[6], and prediction of the properties of various nanomaterials such as carbon nanostructures[7]. Despite its usefulness, the Cauchy–Born rule has a number of limitations. Because of the affine deformation assumption, it is not possible to accurately capture failure mechanisms in materials that exhibit softening and localization. The reliance only on interatomic potentials to compute strain-energy density works well when enthalpic contributions are dominant over entropy, but fails for systems where configurational entropy changes substantially with applied deformation, or when the minimum-energy configuration of the system deviates from those prescribed by the macroscale deformation gradient as the system deforms[8]. Despite these shortcomings, the Cauchy–Born rule and subsequent developments based on it, such as quasicontinuum (QC) methods, have been foundational for the development of multiscale methods for studying the mechanics of materials.

Other approximation theories have also helped lay the groundwork for multiscale simulations. The Cauchy–Born rule is itself analogous to the Voigt approximation[9], which assumes that the fine-scale strain in a representative volume element (RVE) coincides with that on the macroscale; the related so-called constant stress hypothesis is identified with Reuss[10]. Transformation field analysis[11] and reduced order homogenization[12,13] assume uniformity of inelastic deformation (eigenstrains) over heterogeneous microphases. Mathematical homogenization theory based on the multiple-scale asymptotic expansion[14] assumes scale separation, whereas its engineering counterpart based on the so-called Hill–Mandel macrohomogeneity condition[15] assumes equivalency between the internal virtual work at an RVE level and that of the overall coarse-scale fields.

Development of multiscale simulation technology as it exists today was spurred by a number of other innovation triggers from the mathematics, physics and computer science communities. These include statistical mechanics[16], quantum mechanics[17], homogenization theory[14,18,19] and its various modern variants (ABC[20], GFEM[21], MSFEM[22], HMM[23], VMS[24], MEPU[25], GMH[26–28]) and linear algebra (for example multigrid[29], domain decomposition[30] and global–local[31]). Another fascinating discovery was a homogenization-based multigrid[32–36], which takes advantage of the fact that heterogeneous systems are highly oscillatory, and therefore an oscillatory response can be effectively captured by solving a local problem using computationally inexpensive relaxation methods, while a smooth response can be resolved by solving a much smaller homogenized coarse-scale problem.

Categorization and qualification of multiscale methods

A categorization scheme for multiscale methods, and representative examples, are summarized in Table 1. To organize our discussion, we follow previous reviews of multiscale methods by dividing multiscale approaches into two main categories: upscaling and resolved-scale methods. Since various multiscale methods were conceived in different scientific communities, there has been a proliferation of definitions. For instance, upscaling methods have also been referred to as hierarchical, information-passing or computational homogenization-like methods; resolved-scale methods have also been described as concurrent, global–local and scale-bridging methods. (We avoid the term 'concurrent' in this setting because it seems to be used in different ways by various practitioners: some simply to indicate simultaneity[37], as the non-technical definition of the word implies; others to specify strong, two-way coupling[38]; still others to include all resolved-scale approaches[39].) Different terminologies are also used to describe various scales. For example, the fine scale may (depending on the problem) be coined as a microscale, unresolvable scale, subgrid scale, atomistic scale or discrete scale; the coarse scale may be called the macroscale, resolvable scale, continuum scale or component scale. Here we will simply

Table 1 | Summary of multiscale computational methods and representative examples

Category		Key features	Examples and applications
Upscaling methods	Maths based (homogenization)	• Identical (or similar) physics models applied at both scales • Interscale coupling based on asymptotic theory, wavelets or macrohomogeneity conditions • RVE or unit cell to compute effective properties	Wavelet-based methods[41–44]; metamaterials[146,147]; acoustics[146]; composites[12,13,19,26,27]; multiphysics[148,103]; stochastic methods[134,135]; wave propagation[104]
	Physics based	• Different physics models applied at multiple scales • Upscaling based on physical principals and insight	Mechanics of carbon nanostructure[70]; interface/interphase effects in polymer composites[69,124]; self-assembly and phase separation in soft materials and biomolecular systems[72 73,74].
	Data driven	• Macroscale response inferred through machine learning or automated model order reduction • Training data obtained from offline fine-scale simulations • Closed-form description of interscale dependence not required	Plasticity in composites[79]; granular materials[78]; plasticity damage in glass[77]; turbulent flow[149]
Resolved-scale methods	Domain decomposition	• Separate physics models and discretization schemes used in different spatial domains • Multiple scales simulated concurrently • Coupling strategy emphasizes bridging at spatial interfaces (overlap or handshake) • Useful when fine scale is important in small subregion of problem	Atomistic-to-continuum coupling[80–85]; fracture and crack tip behaviour[81,150]; nanoindentation[151]; dislocations[80]; heat transfer[90]; architected materials[147]
	Multigrid	• Separate physics models and discretization schemes used in different spatial domains • Multiple scales simulated concurrently • Coupling strategy emphasizes interscale operators (restriction and prolongation) • Solution algorithms similar to iterative multigrid matrix solvers	Convergence studies[32]; diffusion problems[35]; structural composites[33,34]; high-energy ball-milled materials[97]; atomistic-to-continuum linking[152]; shell–solid linking[153]

refer to the two scales as the fine and the coarse scale. For more than two scales, we will refer to the additional scales as mesoscales. We also point out that the majority of multiscale methods address multiple length scales, and such methods are the focus of this section.

In upscaling methods, the fine-scale response is approximated or idealized, and only its average effect is captured. In the resolved-scale approaches, fine- and coarse-scale responses are resolved in different parts of the problem domain simultaneously, and information between scales is exchanged at the interface. In an important subclass of resolved-scale methods, which we here refer to as multigrid methods, the overall and high-frequency responses are also linked via interscale transfer operators derived from homogenization or similar theoretical approaches.

Upscaling-based multiscale methods. Upscaling methods, which link discrete scales (electronic structure, atomistic, coarse-grained atomistic), continuum scales (material constituents and component scales) or combinations of the two may further be classified into the following three subcategories: (1) maths-based methods, where coarser scale equations are mathematically derived, typically using multiple-scale asymptotic methods, multiresolution methods and various enrichment schemes; (2) physics-based methods, where governing equations at each scale are postulated directly, but their structure and properties are upscaled using physical principles, including coarse-grained molecular dynamics (MD), dislocation dynamics, phase field, cellular automata and so on, where a coarser-scale model is derived using physical principles; (3) data-driven methods, where coarse-scale or reduced-order models are constructed from large numbers of fine-scale simulations using machine learning or similar artificial-intelligence approaches.

An alternative subcategorization of upscaling methods is based on the flow of information, which can be either one or two way. Two-way upscaling methods possess a feedback loop that continuously evolves the fine-scale model and updates the coarse-scale model appropriately. One-way upscaling methods derive the

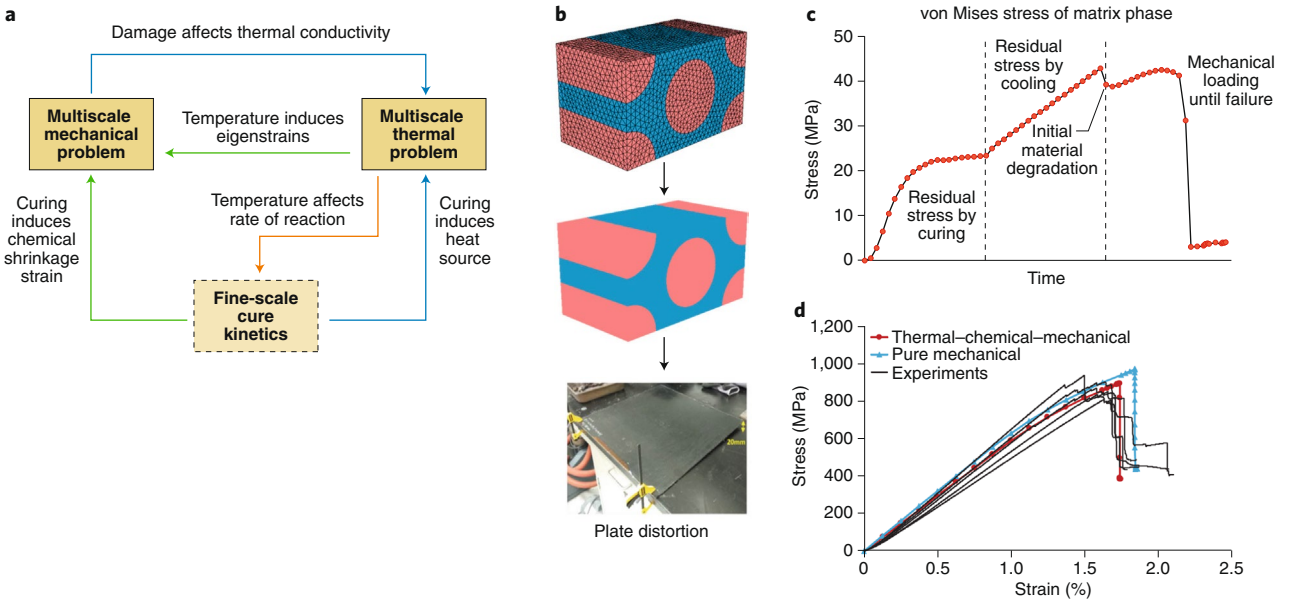


Fig. 1 | Modelling the effects of manufacturing on performance of composites. a, Coupling of chemothermomechanical processes at multiple spatial scales. **b**, Model reduction and mathematical upscaling. **c**, Predicted residual stresses induced by manufacturing. **d**, Model validation at a component level. Credit: adapted with permission from ref. [68], Wiley

coarse-scale constitutive model from a priori fine-scale data. Upscaling methods that fall into the former subcategory include nonlinear computational homogenization, while those in the latter category include computational homogenization with microconstituents in a linear elastic regime, as well as various coarse-graining approaches.

We distinguish between upscaling of continua, which is based on the methods of continuum mechanics, and upscaling of discrete media, where fine-scale phases are governed by motion of atoms as described by MD. At a continuum scale, heterogeneous materials consist of clearly distinguishable phases that show different mechanical and transport material properties, whereas at an atomistic scale they are governed by interatomic potentials. The premise of upscaling is that the governing equations and material structure at a fine (continuum or discrete) scale are well understood, or at least better understood than those at the coarse scale. Under this premise, upscaling provides a framework by which well defined fine-scale equations are used to deduce coarse-scale equations. The benefit of upscaling is that the behaviour of materials can be determined with limited testing and calibration of the coarse-scale model.

Upscaling of continua can be used to predict the full anisotropic properties and behaviours of heterogeneous materials, which are often difficult to evaluate experimentally or model phenomenologically. In addition to describing the overall behaviour of heterogeneous materials, upscaling can provide local fields in a process known as localization or postprocessing. This information is notably important in understanding and predicting material damage and failure.

Deriving continuum equations from atomistics is more challenging. While the mechanical description can be explicitly derived from atomistics (as has been successfully demonstrated using techniques described throughout this section), the thermal process can only be accounted for phenomenologically in the form of a heat transfer equation. The mechanism for heat transfer depends on the material system. In gases, for example, heat is transferred by direct collisions between molecules, while in non-metallic solids, such as ceramics, the energy carriers are lattice vibrations (phonons). In metals, heat transfer is primarily through electron transport. This implies that for metals the base mathematical model that describes the motion of atomic nuclei does not contain sufficient information for development of a complete phenomenological model of heat transfer. Quantum-mechanical considerations, or at least approximations of heat transfer that include non-phononic mechanisms[40], are unavoidable in this case.

Maths-based upscaling methods. Homogenization of continua is the study of partial differential equations with rapidly oscillating periodic coefficients. The process of replacing an equation having oscillatory coefficients, particularly in space, with one having homogeneous (uniform) coefficients is known as upscaling of continua or simply upscaling. The effective properties are calculated by solving a fine-scale problem over the RVE or unit-cell domain, which is defined to be of large enough size to be statistically representative of the heterogeneous medium. The link between the coarse- and fine-scale equations can be established using either (1) multiple-scale asymptotic methods or (2) the so-called Hill–Mandel macrohomogeneity condition[15].

The basic limitation of these methods is that they assume scale separation. An alternative homogenization strategy is based on multiresolution analysis[41–44], which considers transition between two adjacent scales explicitly, a procedure that may then be repeated recursively over multiple scales. The key element in multiresolution analysis is wavelets, which are an alternative basis set that has significant advantages over conventional finite elements. The solution resolution can be systematically enhanced in specific regions in space and time, particularly where the solution varies rapidly, through the addition of high-resolution wavelets to the basis set. This can be repeated for multiple spatial or temporal scales without causing numerical instabilities. The coarse-scale solution can be obtained by recursively condensing out the fine-scale solutions and by approximating the corresponding Schur complements for computational efficiency. The remarkable property of multiresolution analysis is that the computational expense of the equation solution scales linearly with the number of basis functions, even for non-homogeneous resolution. This linear scaling stems from the sparsity of the differential operator matrix and the fact that the resulting algebraic system can be effectively solved using multigrid methods.

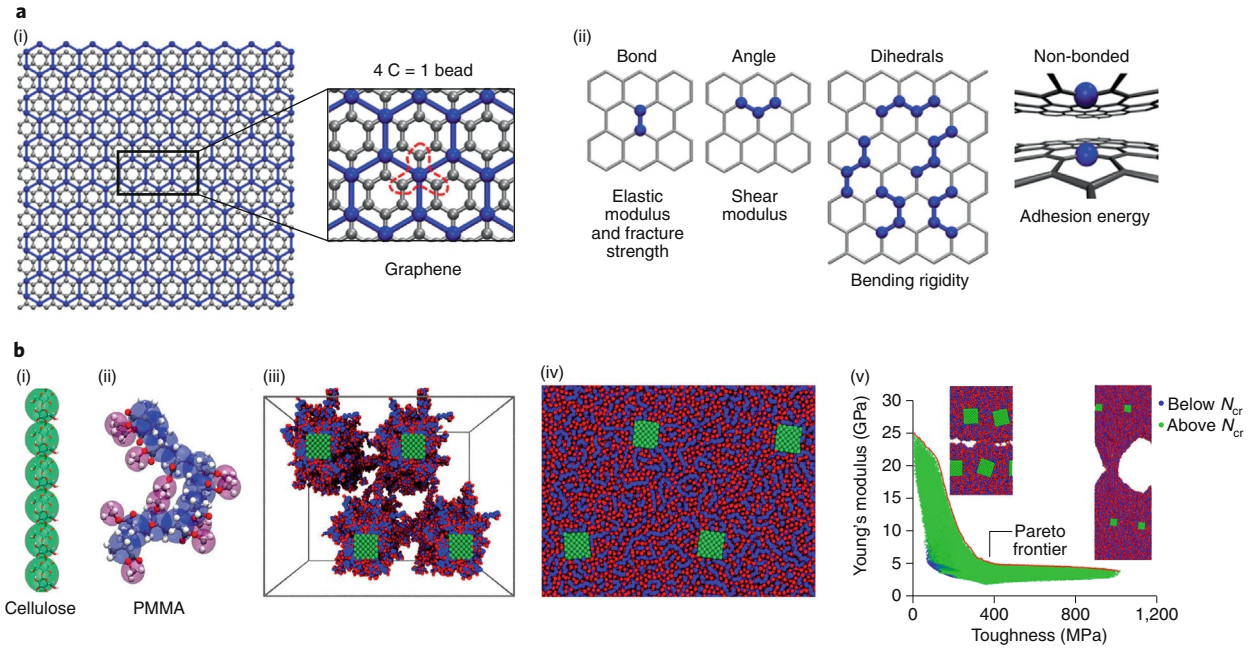


Fig. 2 | Physics-based upscaling approaches for coarse graining of MD. a, Strain-energy mapping approach shown for graphene, where four carbon atoms map onto a single coarse-grained bead (i) and potential parameters are selected to match specific mechanical properties that stem from different strain-energy contributions computed via all-atom MD or density functional theory. (ii) Typical interaction terms used in a coarse-grained model. For example, elastic moduli and tensile strength can be used to calibrate coarse-grained bond parameters, shear and bending energies can be used to parameterize angle and dihedrals, and adhesion energy can be used to tune non-bonded terms. The coarse-grained model can then be used to study various graphitic assemblies and nanocomposites at larger length and time scales. **b**, Modelling polymer nanocomposites using coarse-grained MD on the basis of Boltzmann inversion and energy renormalization concepts, coupled with machine learning. In this case, cellulose nanocrystals (i) grafted with poly(methyl methacrylate) (PMMA) (ii) form a nanocomposite through self-assembly (iii,iv). Each coarse-grained bead represents a group of united atoms at the monomer scale with parameters derived from all-atom MD probability distributions and dynamics data. Assembled structures are tested mechanically to generate datasets to train metamodels, which then can rapidly populate material design charts (v). In this case, simulations combined with a Gaussian process metamodel allow rapid exploration of the molecular design parameters such as grafting density and graft length. The design chart can be used to discover composite variables (that is, N_{cr}, critical chain length) that govern the mechanical performance of polymer-grafted nanoparticle assemblies. Credit: panel **a** reproduced with permission from ref. [70], Elsevier; panel **b** adapted with permission from ref. [124], American Chemical Society

Considerable success has been also reported using a finite-element basis at multiple scales as an alternative to wavelets[22–25], as well as using wavelets as resolved-scale methods.

The RVE problem is driven by the coarse-scale field gradient or strain. Once the RVE boundary value problem subjected to periodic (or essential, natural) boundary conditions is analysed, the coarse-scale flux or stress is obtained by averaging the corresponding fine-scale field.

For problems where the coarse-scale field varies rapidly over the RVE domain, the coarse-scale field gradient or strain is no longer constant over the RVE domain, and consequently the input–output relation should be stated in terms of higher-order fields[45–48].

For nonlinear history-dependent problems, upscaling methods for atomistic or continuum media would have had little practical impact due to the enormous computational complexity involved. Thus, reduced-order models have been actively studied. Some important reduced-order methods include the Voronoi cell method[49], spectral method[50], network approximation method[51], fast Fourier transforms[52], mesh-free reproducing kernel particle method[53], finite-volume direct-averaging micromechanics[54], transformation field analysis[11,55], methods of cells[56], methods based on control theory including balanced truncation[57,58], optimal Hankel norm approximation[59], proper orthogonal decomposition[60,61], data-driven-based reduced-order methods[62–65], reduced-order homogenization methods for two scales[12] and more than two scales[13], and non-uniform transformation field methods[66,67]. Figure 1 presents an illustration of the mathematical upscaling and model reduction in polymer-based composites[68].

Physics-based upscaling methods. Physics-based approaches in multiscale analysis typically try to capture specific physical phenomena at the right resolution with greater computational efficiency. Here we focus our attention on systems that emphasize discrete-to-discrete mapping. We emphasize that physics-based models typically also involve mathematical or statistical analysis, but additionally require a physical assumption or model upon which the parameterizations are built. A classic example of such models is systematically coarse-grained MD simulations, where data from all-atom MD trajectories is utilized to develop a model with fewer degrees of freedom and simpler interatomic potentials that can be more quickly computed. Underlying groups of atoms are represented with superatoms or coarse-grained beads that interact with each other via effective potentials, but the specifics vary depending on the material system being modelled. These methods map the discrete atomic scale to a coarser discrete (rather than continuum) description; such a discrete-to-discrete mapping is desired for cases such as polymeric, polycrystalline and biological materials where capturing the shape and size of finite building blocks that make up the matter is important. An example of such a scenario could be cases where the discrete nature of a polymeric chain needs to be captured to describe chain conformations and dynamics in larger-scale thin films in a chemistry-specific fashion[69]. Currently, the largest debate on this type of coarse graining is how one should determine the effective interactions, for instance those between beads representing monomers or united atomic groups in a polymeric system. In single-crystal systems, strain-energy mapping (Fig. 2a) is a simple

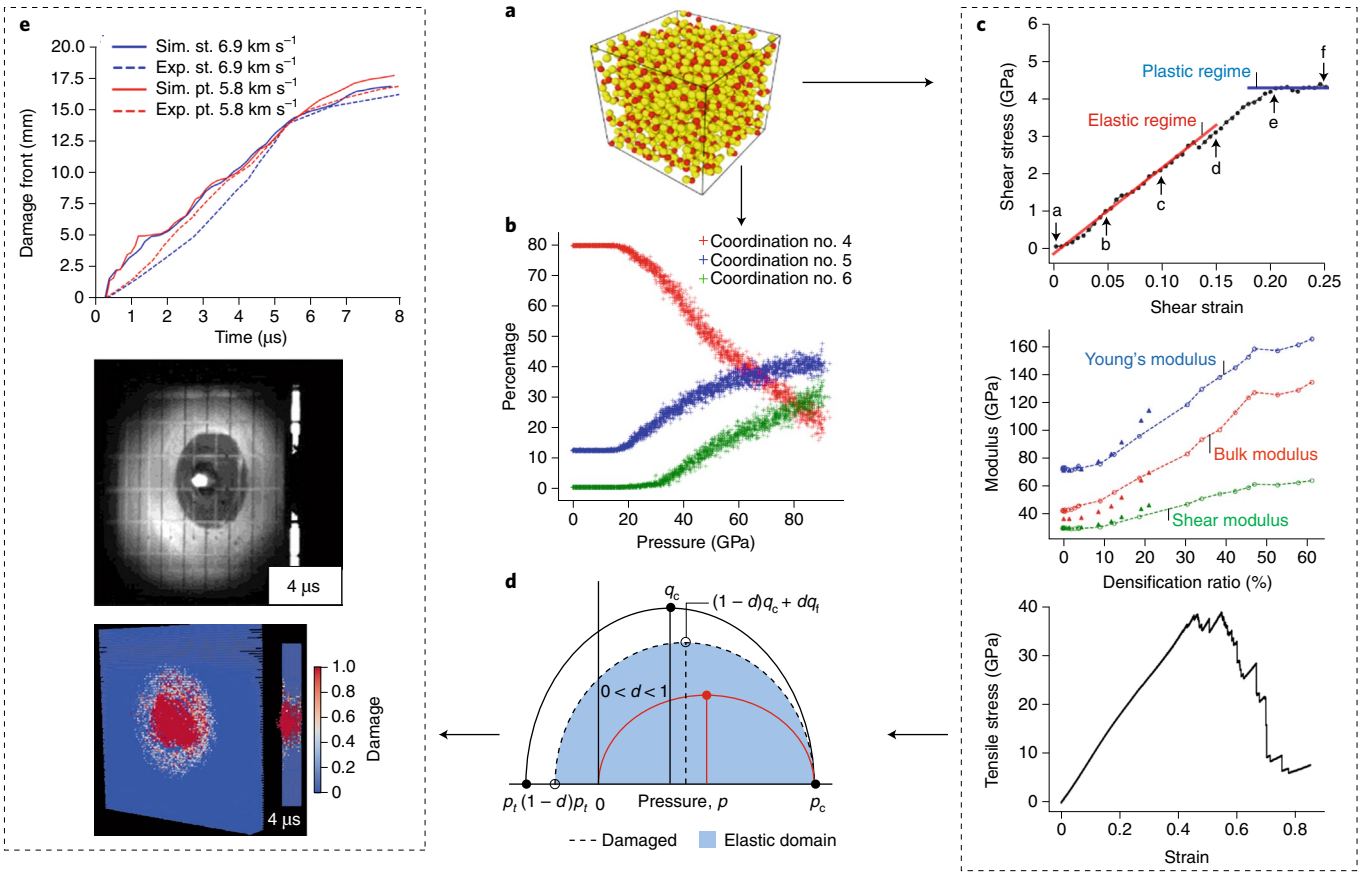


Fig. 3 | Data-driven model for high-pressure densification of silica glass. a, Construction of silica-glass atomistic unit cell using a melt–quench approach. **b**, Verification of molecular structure. **c**, Construction of the training set. **d**, Neural network training of continuum-coupled-state-based plasticity–damage model. **e**, Validation: hypervelocity impact experiment versus peridynamics simulation. st., steel; pt., platinum. Credit: adapted with permission from ref. [77], Springer

approach used to create an equivalent lattice system that has the same bulk mechanical response as the atomistic system[70]. This approach is useful for single-crystal, ideal systems without defects, but often does not capture all dynamical and mechanical properties accurately; for instance, local energy minima or configurations arising from the finer degrees of freedom may be missed. In polycrystalline materials and metals, physical features such as grains occur at intermediate scales, while defects still may emerge at the atomic scale. Methods such as discrete dislocation dynamics have been employed to efficiently predict complex physics in such systems at multiple length scales[71].

For amorphous materials such as polymers and other soft matter, approaches to coarse graining typically involve bottom-up methods such as matching the free energy or the potential of mean force[72], or capturing certain bulk properties of the material by parameterizing interactions empirically in a top-down fashion[73,74]. Capturing entropic contributions to intermolecular interactions remains challenging for these systems. A popular approach examines obtaining probability distributions of atomic positions, using the Boltzmann probability distribution to obtain an initial estimate of potential parameters, and then iteratively refining these terms to realize different structural states with correct probabilities (Fig. 2b). This method, called iterative Boltzmann inversion, has gained traction particularly in the polymer community, and is generally an excellent starting point for systematic coarse graining[75]. The lost degrees of freedom and their associated configurational entropy cause issues in capturing dynamics at different temperatures, but this can be partly alleviated by renormalizing the cohesive-energy parameters as demonstrated for glass-formers at a wide range of temperatures[76].

Data-driven upscaling methods. Lacking a closed-form constitutive model, a fruitful direction is to develop a surrogate model for the fine-scale problem, possibly informed by precomputed ('offline') fine-scale simulations. Because of the potentially large number of input parameters necessary to capture the relevant macroscale variables as well as the microscale state, especially for time- or history-dependent problems, data-driven techniques may be the ideal approach to capturing the response of the system. Recent interest in this strategy has grown concurrently with the explosion of development in machine learning and related methods for pattern detection, dimensionality reduction, model building and decision making. The structures of many of these techniques are already familiar to computational material modellers—for example, artificial neural networks (ANNs) provide a powerful version of what modellers will recognize as nonlinear curve fitting—but efficient new algorithms combined with increasing availability of large computational resources allow the development of relationships between datasets unobtainable from physical insight alone.

Some recent examples demonstrate the potential of such approaches. An ANN-based upscaled continuum model, trained using MD simulations on an RVE, has been demonstrated for hypervelocity impact on silica-glass windscreens in space vehicles[77] (Fig. 3). Deep reinforcement learning has been used to develop data-driven constitutive relationships of traction–separation laws in granular materials[78]. In this approach, results of

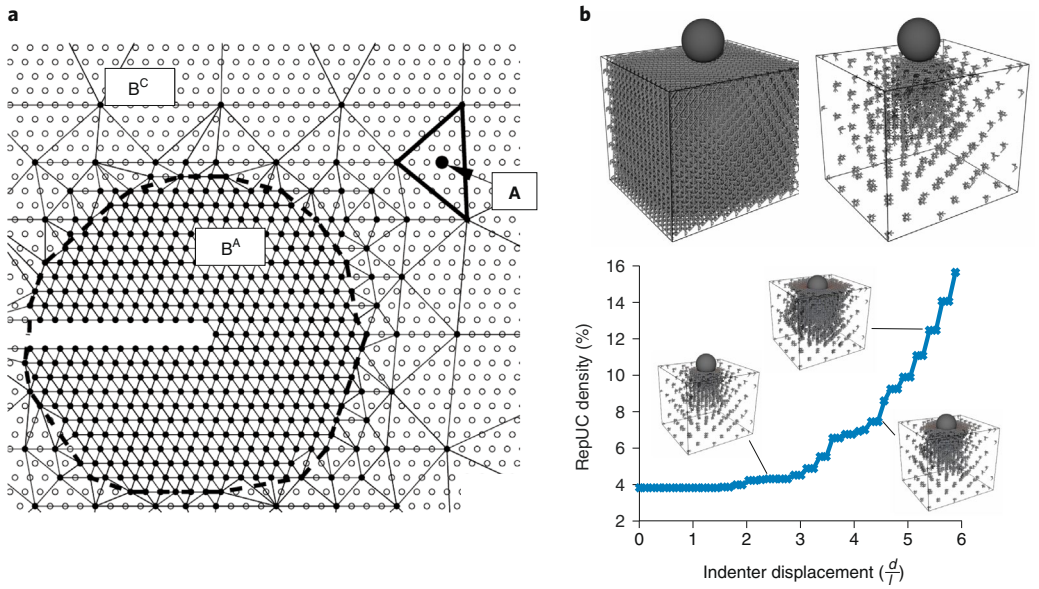


Fig. 4 | QC modelling of atomistic and continuum lattice systems. a, 2D Atomistic–continuum system coupled through the QC method[86]. The fully refined atomistic region (B^A) uses atomic forces computed from a standard interatomic potential. In the continuum region (B^C), only selected atoms (black circles at the nodes of triangular elements) are directly simulated, while energies of the remaining atoms (open circles) are calculated according to the Cauchy–Born rule. Displacements of non-represented atoms, for example A, are given by linear interpolation on the triangular elements bounded by the represented atoms. **b**, QC representation of a truss lattice[92], in which model size is reduced by representing only selected unit cells analogous to the QC methodology (top). QC simulation of indentation of the system uses adaptive refinement to modify the representation (bottom). RepUC, representative unit cell; *d*, indentation depth; *l*, lattice beam length. Credit: panels reproduced with permission from: **a**, ref. [86], IOP; **b**, ref. [92], Elsevier

discrete-element-method simulations of RVEs at the fine scale are used to train an ANN relating macroscale stress and displacement to a list of internal variables such as porosity and coordination number; the deep reinforcement learning finds the optimal relationship between variables that characterizes the complex material response. In yet another approach, the self-consistent clustering analysis method[79] enables efficient simulation of plastic deformation on RVEs for materials with complex microstructure. This method uses a set of offline, linear elastic simulations of an RVE, and then uses a *k*-means clustering to categorize computational cells on the basis of their response; the basic hypothesis is that cells that have similar elastic responses will also have similar behaviours under plastic loading, and can be grouped into superelements with constant response. The result is a vastly accelerated microscale simulation that is efficient enough to use at every macroscale integration point in a multiscale-coupled model.

Resolved-scale methods. A number of methods involve the direct simulation of fine-scale behaviour, but only in a localized region. The main difference between the two subcategories of resolved-scale methods is in the emphasis on interfacial information transfers in physical space (for domain decomposition) versus interscale transfer operations (for multigrid methods). Both methods are particularly attractive for multiscale material systems either when scale separation does not exist or when the quantities of interest are at a fine scale, for example crack propagation. The two types of method discussed herein assume that the fine-scale model including its geometry is known either from direct measurements or from reconstruction in a portion of a problem domain.

Domain-decomposition-based methods. An attractive strategy for reducing the cost of a fine-scale simulation (such as an MD computation) is to limit the fine-scale representation to a small subregion of the full domain, while using a less computationally demanding coarse-scale representation for the remaining material. This approach is of course most useful when the coarse-scale representation loses validity only in a small part of the domain. For problems in solids, this is typically true near defects such as dislocations, crack tips, grain boundaries and surfaces. In these cases, a simple (possibly nonlinear and/or anisotropic) elasticity model may be used away from the defects, while a full atomistic representation is needed near the defects. This allows fine-scale quantities of interest, such as dislocation energies or crack tip behaviour, to be queried with molecular precision, while macroscale loading and other boundary conditions are efficiently carried by the continuum.

The most well known such approach, and one of the first, is the QC method[80], which couples an MD region with a surrounding finite-element representation through a one-to-one match between atoms and finite-element nodes at the interface (Fig. 4a). A Cauchy–Born constitutive model is used in the continuum to make the regions consistent. Related techniques[81–85] vary the form of the interface, but most appeal either to a partitioning of the total system energy between the two domains or a matching of forces across the boundary to formally derive the coupled system equations; a benchmarking study[86] showed that energy-based methods with a correction included for so-called 'ghost-force' errors[87] led to a good combination of accuracy and efficiency. Although the original QC method was developed for static systems, extensions have been made to dynamics, including systems at finite temperature accounting for vibrational energy modes[88,89] and the transfer of heat across the interface for non-equilibrium systems[90,40]. An interesting recent extension of QC methods is to multiscale architectured materials[91,92], for which the microstructures considered are periodic networks of trusses, beams or plates rather than atomic lattices (Fig. 4b).

In time-dependent problems, a commonly encountered artefact of the coupling is the internal reflection of vibrational waves within the fine-scale subdomain. This phenomenon arises when the energy in the fine scales cannot be accurately represented in the coarse-scale domain, and thus cannot pass through the fine/coarse interface. Methods to remove these reflections include the inclusion of

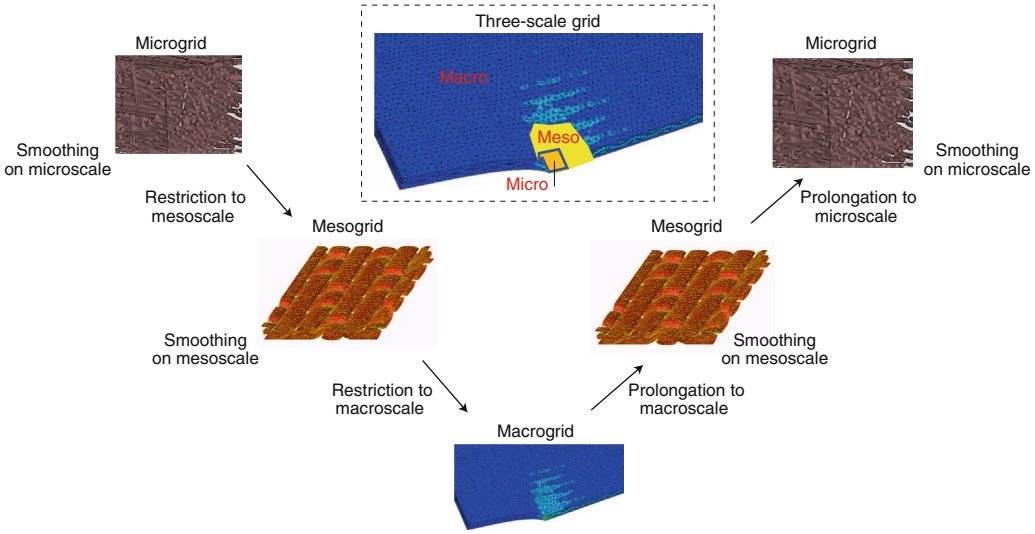


Fig. 5 | Schematic showing a single multigrid V cycle consisting of three scales. In the first half of the cycle, solution relaxations are recursively ('smoothing') carried out at each scale, and residuals are passed (restricted) to the coarser scales through appropriate restriction operators. A full direct solution is then computed on the coarsest (macro) scale, and displacements are recursively prolongated and smoothed onto the finer-scale meshes.

carefully defined absorbing boundary conditions based on a generalized Langevin equation[83,93], or a perfectly matched layer[94]. Another difficulty, more commonly confronted in domain-decomposed fluid systems, is the handling of mass flux across the interface, requiring that new atoms be inserted in a dense system without artificially disturbing the total energy. Successful approaches typically combine algorithms for particle insertion (such as the USHER algorithm[95]) with overlap regions that allow equilibration of the two representations near the interface[96].

Multigrid-based multiscale methods. Multigrid-based methods achieve a similar goal to domain decomposition but approach the problem from a different direction by first carefully defining the interscale operations, and only then systematically dropping the unneeded fine scales where possible. The basic idea of the multigrid-based multiscale method is an iterative approach between scales. A three-scale process that includes fibrous microstructure, woven macrostructure and composite macrostructure is illustrated in Fig. 5 and Box 2. It has been shown[32] on a linear elastic model problem that the spectral radius r, which measures reduction of error in a single cycle, can be made very small for problems with a large difference in properties between microconstituents. For instance, for carbon-fibre-reinforced polymer matrix composites with modulus ratio in excess of 100, the spectral radius is of the order of 10^{-2} and the iterative process converges in just three cycles up to a tolerance of 10^{-5}. This contrasts with homogeneous materials, where the error in each cycle reduces by a factor of 3 only. A similar trend has also been observed for a complex nonlinear problem[34].

As in multiresolution upscaling methods, the interscale treatment in multigrid methods has parallels with techniques used in image processing[97] that can be used to construct restriction and prolongation operators.

Multiple temporal scales

While the majority of multiscale methods discussed thus far target problems with multiple spatial scales, multiple timescales are prevalent in many materials systems and may pose even greater simulation challenges. In molecular systems, the separation between the atomic vibration timescale and the frequency of diffusion processes, such as atom hops, may allow the use of transition-state theory to develop temporal multiscale methods. When the frequencies of all possible transitions are known, the kinetic Monte Carlo method[98] can be used to advance the system in time. More often, transitions must be determined through numerical exploration of the local potential-energy surface[99] or other dynamic approaches to cataloguing events and their frequencies[100–102].

Beyond the atomic length scale, other physical processes inherently take place at multiple temporal scales. For instance, fatigue of materials is a multi-timescale phenomenon because the cyclic load period is typically of the order of seconds, while the lifetime of a component may exceed years. Simultaneous consideration of atomistic and continuum scales at a finite temperature is characterized by a fast timescale of atomistic vibrations and much slower evolution of continuum processes. Finally, consideration of coupled physics, such as thermochemomechanical processes, introduces multiple temporal scales due to different characteristic timescales of these processes.

One temporal multiscale modelling approach that has been used for wave propagation, fatigue and atomistic homogenization problems is based on multiple-scale asymptotic expansions in both time and space[26,27,103–105]. Another type of model relies on time integration of the coarse-scale variables using temporal derivatives that are computed from short-burst fine-scale simulations. This approach is epitomized by the equation-free model[106], in the sense that the governing equations for the coarse-scale variables are unknown and unneeded. At each coarse-scale time step in this method, the fine scale is simulated for long enough to extract a rate of change in the coarse-scale state, which is then extrapolated over a potentially much longer time step. In practice, the effectiveness of this approach depends strongly on the feasibility of initializing fine scales conditioned on a given coarse state (the lifting operation), yet consistent with the correct dynamics of the full system. One strategy is to allow the fine-scale system to relax to a slow manifold before extracting coarse dynamics, but this is predicated on a clear separation of fast and slow scales. Progress in this and similar methods requires research on accurate and efficient lifting operators for specific applications. For example, inclusion of two-point correlation functions and careful control of intermediate-scale components are needed to achieve acceleration of kinetic Monte Carlo simulations of evolution of crystal surfaces[107]. A promising direction in the development of lifting operators is the use of machine-learning techniques to generate realistic representative samples of microstructural configurations, such as the use of

Box 2 | A three-scale process

In step 1, known as relaxation or smoothing in multigrid literature, a fine-scale model (at either continuum or atomistic scale) is constructed on a portion of a problem domain where fine-scale resolution is required, and checked to determine if the fine-scale governing equations are satisfied. If so, the solution is considered to be converged. Otherwise, the fine-scale problem domain is divided into possibly overlapping subdomains. On each subdomain, a local discretized problem is solved by subjecting the boundary nodes (or atoms) of each local subdomain to the boundary solution obtained from postprocessing in step 2.

In step 2, the discretized fine-scale solution obtained after relaxation is inserted into the fine-scale system of equations, and the fine-scale residual is computed. The fine-scale residual is applied as an external load onto the coarse-scale mesh, and the coarse-scale residual computed. This step is known as restriction. For more than two scales, the mesoscale solution(s) are recursively approximated by relaxation, similarly to step 1, and then restricted (step 2) to the coarser scales until the coarsest scale of interest is reached.

In step 3, the coarse-scale solution is computed using a coarse mesh with homogenized material properties obtained from upscaling. This process is referred to as coarse-grid correction.

In step 4, the fine-scale solution is reconstructed by postprocessing using a prolongation operator that links the fine- and coarse-scale solutions at an RVE level and then smoothed by relaxation; this prolongation operator is derived from homogenization theory and is likely to be different from, and superior to, the classical linear interpolation operator. For more than two scales, this process is recursively repeated until the finest-scale equilibrium is reached. The iterative process is repeated until the residual on the finest scale vanishes.

generative adversarial networks, which train paired generative and discriminative modules to produce microstructures on the basis of low-dimensional descriptors[108,109].

Methods that combine multiple-temporal- and spatial-scale approaches have also been introduced. Hyperdynamics[110] augments the interatomic potential of the system with a bias potential to increase the frequency of transition events, and has been used together with an atomistic-to-continuum coupling method to model crack propagation[111]. In the 'hyper-QC' method[112,113], hyperdynamics is combined with the finite-temperature QC method ('hot-QC') to demonstrate speed-ups as high as 10,000 for simulation of nanoindentation of thin films[113].

Multiscale materials design and analysis

Multiscale simulation methods provide a powerful tool for efficient design of new materials, especially when combined with material property databases. However, the uncertainties inherent in both computations and measurements, and their complex interaction across scales, lead to a need for improved approaches to understanding error and uncertainty.

ICME and materials databases. Historically, significant advances in multiscale modelling of materials came through the metals research community, particularly with advances in modelling of complex multicomponent alloys using integrated computational tools. The advent of accurate density functional theory calculations and CALPHAD (calculation of phase diagrams) tools catapulted metallurgical advances forwards over the past few decades[114]. Widespread community adoption of these capabilities has resulted in many success stories for materials design. A notable example is the in silico design of high-performance alloys for aircraft landing gear-steels[115], which demonstrated the importance of multiscale methods for discovering new materials that can withstand extreme mechanical and chemical environments. Designed by QuesTek Innovations, Ferrium S53 was the first computationally designed and qualified alloy to reach flight stage, combining seemingly disparate properties such as corrosion resistance without toxic cadmium coating, high stress-corrosion cracking resistance and very high strength. Integrated computational materials engineering (ICME) and the Materials Genome Initiative (MGI) efforts catalysed the implementation of multiscale methods in a wide array of applications spanning polymers, ceramics, biomolecular materials and electronic materials. This has resulted in a plethora of software and databases such as the Open Quantum Materials Database (OQMD)[116] and the Materials Project[117] for many aspects of materials engineering including structure predictions, thermodynamic calculations and prediction of phase diagrams[118].

A particular challenge in the soft-materials community is the integration of various databases that are geared towards a subset of material properties, such as glass-transition temperature, chi parameter and other metrics relevant for mechanical behaviour. In this context, developments such as the Materials Data Facility[119] catalysed by MGI may facilitate greater community participation and integration, by offering the flexibility to store materials data of any size, and from any source.

Machine-learning techniques are gaining traction in the materials research community, where now the ability to carry out high-throughput calculations is paving the way for developing both physics-based and data-driven relationships that accelerate materials design[120]. Apart from aforementioned successes in the metals community, materials genome and informatics approaches are being employed in amorphous materials. A notable example is the combination of physics-based models with ANNs and empirical models for the design of ultrastrong glass[121]. Applications of machine-learning techniques are also emerging in soft matter, for instance for the design of dielectrics[122]. Data-driven and machine learning tools are widely sought after for multiphasic or multicomponent materials where the design space is typically very large, such as polymer nanocomposites. A preliminary step is building experimental databases of material parameters such as the NanoMine data resource[123]. Physics-based multiscale methods can also generate input datasets for data-driven design. For example, a recent study utilized Gaussian process metamodels informed from systematically coarse-grained MD simulations to discover optimal mechanical properties of polymer-grafted nanoparticle assemblies. Once trained and validated, such surrogate models can be used to generate new data points by interpolating simulated outcomes very rapidly, while sensitivity analyses easily reveal parameters that matter the most[124] (Fig. 3b). Approaches that combine machine learning with physics-based multiscale models are anticipated to accelerate materials discovery in the upcoming era of materials informatics.

Uncertainty quantification. One major hurdle in successful utilization of multiscale methods is uncertainty quantification (UQ) of nonlinear behaviour of fine-scale phases and its effect on the coarse-scale quantities of interest. The challenge is to quantify the dominant input uncertainties and propagate them. Error and uncertainty in simulation results can arise from a number of sources, including the incomplete knowledge (epistemic uncertainty) of the modelled physics and associated parameters such as material properties and problem geometry, as well as the inherent randomness (aleatoric uncertainty) in the values of many of these parameters. Multiscale simulations bring further complexity, as the effects of errors propagate across models and scales; paucity of experimental data at finer scales in particular limits the precision of multiscale models. An important area of research is statistical UQ for multiscale

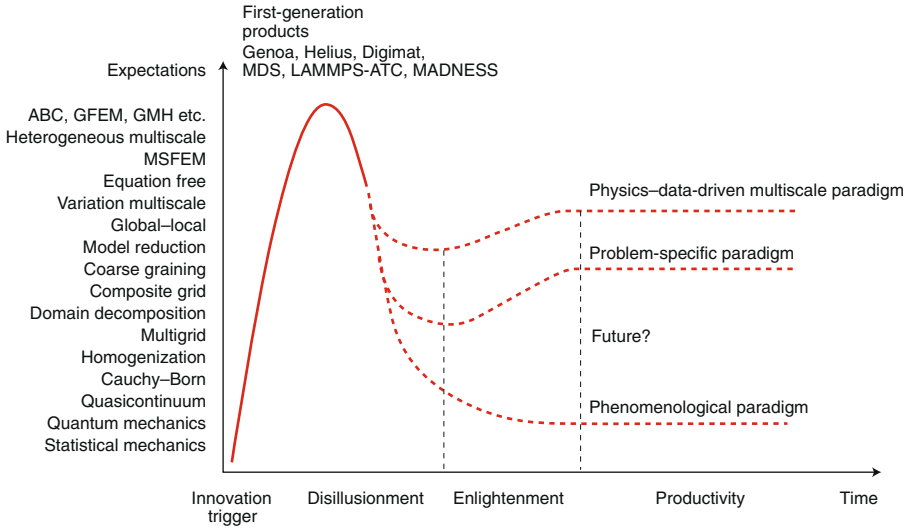


Fig. 6 | Gartner cycle for multiscale science and engineering. Potential paradigms of choice (multiscale versus phenomenological) are shown as possible future paths. After its initial growth spurred by the various innovation triggers mentioned in the introduction, interest and activity in multiscale simulation expanded through the 1990s and early 2000s. Any hopes for simple resolutions to the complexity of multiscale problems were eventually dashed, and no single method or simulation framework has been found that can be universally applied across all types of material system and application. However, the wake of this storm of initial activity has left the field with a range of well researched approaches, as described in this Review, that each have strengths for specific classes of problems.

methods, with a relatively small number of examples of rigorous UQ applied to the propagation of error in upscaling methods[125–128] and domain-decomposed atomistic-to-continuum approaches[129]. A discussion of UQ principles and their application to multiscale systems is provided in previous reviews.[130] As those authors point out, multiscale simulations have the effect of transforming epistemic uncertainty in coarse-scale parameters (for example, the parameters in a continuum plasticity model) into aleatoric uncertainty arising from the randomness of the fine scales (for example, the atomic structure of a polycrystal); epistemic uncertainty at the fine scale can be reduced by averaging over ensembles of fine-scale realizations. However, fine-scale models incur additional epistemic uncertainty of their own, such as the parameters in an interatomic potential. The development of approaches to calculate these effects on overall uncertainty is an important area for research.

Continued development of multiscale modelling requires the integration of multiscale methods with UQ. Various stochastic multiscale approaches can be categorized according to the specific multiscale strategy and stochastic methodology. A straightforward method is Monte Carlo simulation of uncertainty; however, this approach is often prohibitively expensive, since a large number of samples (each one a full system calculation) are required for reasonable accuracy. A commonly used more efficient method is the Galerkin polynomial chaos method, which shows exponential convergence with respect to the polynomial order[131]. Among non-intrusive approaches that are more efficient than Monte Carlo sampling are a non-intrusive version of polynomial chaos[132], the stochastic collocation method[133], which has been applied to multiscale problems[134], and the perturbation-based homogenization approach[135].

For random microstructures, an important part of UQ is microstructure characterization and reconstruction[136,137], including greyscale image binarization, point-correlation and cluster-correlation characterization, and the simulated annealing algorithm for microstructure reconstruction.

Outlook and directions

Like many new technologies, multiscale modelling appears to obey Amara's law: the effects of an innovation are typically overestimated in the short term and underestimated in the long term. This pattern

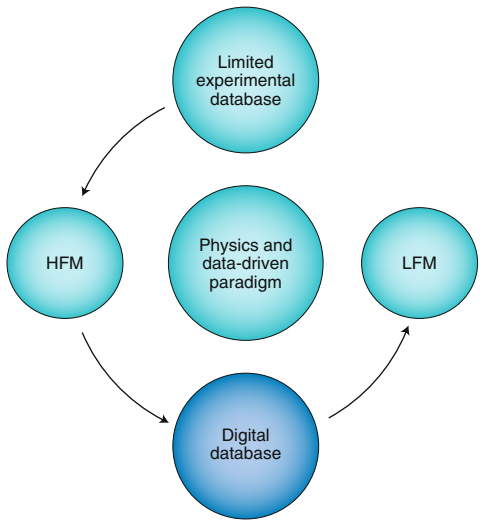


Fig. 7 | A single level of the multilevel directly computable physics framework. A limited experimental database is employed to construct an HFM. The HFM generates a digital database to complement limited experimental data. An LFM is conceived from the digital/experimental database using machine-learning search in a space constrained by conservation laws on the model, upscaling framework and approximations introduced by model reduction. The LFM is deployed for scientific discovery or engineering design. The process is multilevel, where the LFM may serve as an HFM at the next level. Credit: adapted with permission from from ref. [64], Wiley

is also exemplified by the Gartner hype cycle (Fig. 6). One of the most promising directions that may further propel the field of multiscale science and engineering appears to be the harnessing of machine learning and other artificial-intelligence approaches for linking scales. The distillation of numerous fine-scale simulations, each involving extremely large numbers of degrees of freedom, into models describing coarse-scale behaviour seems to be a natural task for such data-driven methods. Often overlooked is the role that artificial

intelligence may have in the reverse process: the initialization of fine-scale configurations, consistent with a given coarse-scale state, that represent a realistic ensemble and whose simulation can be used to determine the mean behaviour. The development of computational methods that combine physical principles (such as conservation of mass, momentum and energy) with data-driven constitutive models is a burgeoning topic in the field of computational science[138,139].

Figure 7 depicts a possible new multiscale paradigm that combines physics and data-driven approaches. By this approach a high-fidelity multiscale model is conceived at a finer scale, such as an electronic, molecular or finer continuum scale, typically characterized by a prohibitive computational complexity, but a fairly well understood mathematical model with narrow parameter design space. The rationale for utilizing a high-fidelity model (HFM) at this initial stage is that despite its formidable computational complexity it can be formulated with relative ease on the basis of the limited and often non-existent experimental data set. Next, given an extensive digital database subsequently generated by the HFM, the primary objective then becomes the construction of a low-fidelity model (LFM) using machine learning in a space constrained by conservation laws at a coarser scale, boundary and initial conditions, and physics- or maths-based upscaling laws that may or may not employ scale-separation principles. The HFM can then be further coarsened in the multilevel framework and ultimately deployed for scientific discovery or engineering design.

The potential impact of multiscale science and engineering on the practicing world, in both engineering and scientific discovery communities, is yet to be determined. After all, despite the impressive innovation triggers depicted in Fig. 6 that culminated in the first generation of multiscale software (for example Genoa[140], Helius[141], Digimat[142], MDS[143], LAMMPS-ATC[144], MADNESS[145]), these packages so far have been able to capture only a tiny fraction of the engineering design and scientific discovery market. Will the conventional phenomenological paradigm, which is simple but strongly reliant on available experimental data, remain the norm? Or will the multiscale paradigm, perhaps in combination with data-driven approaches, surpass it to become the method of choice in engineering design and scientific discovery? It is likely that the answer lies somewhere in between, where the choice between phenomenology and the mathematical rigour provided by multiscale models remains problem dependent. We believe that further progress towards fulfilling the promise of multiscale science and engineering requires not only the continued development of its mathematical, physical, computational and data-driven aspects, but crucially its applicability to broader societal needs beyond those traditionally of interest to the academic community.

Received: 8 October 2019; Accepted: 9 December 2020;
Published online: 27 May 2021

References

1. Curtin, W. A. & Miller, R. E. Atomistic/continuum coupling in computational materials science. *Model. Simul. Mater. Sci. Eng.* **11**, R33–R68 (2003).
2. Fish, J. Bridging the scales in nano engineering and science. *J. Nanoparticle Res.* **8**, 577–594 (2006).
3. Fish, J. *Practical Multiscaling* (Wiley, 2014).
4. Ghosh, S. & Dimiduk, D. (eds). *Computational Methods for Microstructure–Property Relationships* (Springer, 2011).
5. National Science and Technology Council CoT *National Nanotechnology Initiative* Supplement to the President's FY 2004 Budget (2003).
6. Ericksen, J. L. On the Cauchy–Born rule. *Math. Mech. Solids* **13**, 199–220 (2008).
7. Arroyo, M. & Belytschko, T. Finite crystal elasticity of carbon nanotubes based on the exponential Cauchy–Born rule. *Phys. Rev. B* **69**, 115415 (2004).
8. Friesecke, G. & Theil, F. Validity and failure of the Cauchy–Born hypothesis in a two-dimensional mass–spring lattice. *J. Nonlinear Sci.* **12**, 445–478 (2002).
9. Voigt, W. Ueber die Beziehung zwischen den beiden Elasticitätsconstanten isotroper Körper. *Ann. Phys. (Leipzig)* **274**, 573–587 (1889).
10. Reuss, A. Account of the liquid limit of mixed crystals on the basis of the plasticity condition for single crystal. *Z. Angew. Math. Mech.* **9**, 49–58 (1929).
11. Dvorak, G. J. & Benveniste, Y. On transformation strains and uniform-fields in multiphase elastic media. *Proc. R. Soc. A* **437**, 291–310 (1992).
12. Oskay, C. & Fish, J. Eigendeformation-based reduced order homogenization for failure analysis of heterogeneous materials. *Comput. Methods Appl. Mech. Eng.* **196**, 1216–1243 (2007).
13. Yuan, Z. & Fish, J. Multiple scale eigendeformation-based reduced order homogenization. *Comput. Methods Appl. Mech. Eng.* **198**, 2016–2038 (2009).
14. Bakhvalov, N. S. & Panasenko, G. P. *Homogenisation: Averaging Processes in Periodic Media: Mathematical Problems in the Mechanics of Composite Materials* (Kluwer, 1989).
15. Hill, R. Elastic properties of reinforced solids: some theoretical principles. *J. Mech. Phys. Solids* **11**, 357–372 (1963).
16. Tolman, R. C. *The Principles of Statistical Mechanics* (Clarendon, 1938).
17. Dirac, P. A. M. *The Principles of Quantum Mechanics* 4th edn (Clarendon, 1958).
18. Sanchez-Palencia, E. *Non-Homogenous Media and Vibration Theory* (Springer, 1980).
19. Suquet, P. M. in *Homogenization Techniques for Composite Media* (eds Sanchez-Palencia, E. & Zaoui, A.) 193–279 (Lecture Notes in Physics Vol. 272, Springer, 1985).
20. Elkhodary, K. I., Greene, M. S., Tang, S., Belytschko, T. & Liu, W. K. Archetype-blending continuum theory. *Comput. Methods Appl. Mech. Eng.* **254**, 309–333 (2013).
21. Duarte, C. A., Babuska, I. & Oden, J. T. Generalized finite element methods for three-dimensional structural mechanics problems. *Comput. Struct.* **77**, 215–232 (2000).
22. Hou, T. Y. & Wu, X. H. A multiscale finite element method for elliptic problems in composite materials and porous media. *J. Comput. Phys.* **134**, 169–189 (1997).
23. Weinan, E., Engquist, B. & Huang, Z. Y. Heterogeneous multiscale method: a general methodology for multiscale modeling. *Phys. Rev. B* **67**, 092101 (2003).
24. Hughes, T. J. R. Multiscale phenomena: Green's functions, the Dirichlet-to-Neumann formulation, subgrid scale models, bubbles and the origins of stabilized methods. *Comput. Methods Appl. Mech. Eng.* **127**, 387–401 (1995).
25. Fish, J. & Yuan, Z. Multiscale enrichment based on partition of unity. *Int. J. Numer. Methods Eng.* **62**, 1341–1359 (2005).
26. Chen, W. & Fish, J. A generalized space–time mathematical homogenization theory for bridging atomistic and continuum scales. *Int. J. Numer. Methods Eng.* **67**, 253–271 (2006).
27. Fish, J., Chen, W. & Li, R. G. Generalized mathematical homogenization of atomistic media at finite temperatures in three dimensions. *Comput. Methods Appl. Mech. Eng.* **196**, 908–922 (2007).
28. Li, A. Q., Li, R. G. & Fish, J. Generalized mathematical homogenization: from theory to practice. *Comput. Methods Appl. Mech. Eng.* **197**, 3225–3248 (2008).
29. Fedorenko, R. P. A relaxation method for solving elliptic difference equations. *USSR Comput. Math. Math. Phys.* **1**, 1092–1096 (1962).
30. Schwarz, H. A. Ueber einige Abbildungsaufgaben. *J. Reine Angew. Math.* **1869**, 105 (1869).
31. Mote, C. D. Global–local finite element. *Int. J. Numer. Methods Eng.* **3**, 565–574 (1971).
32. Fish, J. & Belsky, V. Multigrid method for periodic heterogeneous media part 1: convergence studies for one-dimensional case. *Comput. Methods Appl. Mech. Eng.* **126**, 1–16 (1995).
33. Fish, J. & Belsky, V. Multigrid method for periodic heterogeneous media. II. Multiscale modeling and quality control in multidimensional case. *Comput. Methods Appl. Mech. Eng.* **126**, 17–38 (1995).
34. Miehe, C. & Bayreuther, C. G. On multiscale FE analyses of heterogeneous structures: from homogenization to multigrid solvers. *Int. J. Numer. Methods Eng.* **71**, 1135–1180 (2007).
35. Knapek, S. Matrix-dependent multigrid homogenization for diffusion problems. *SIAM J. Sci. Comput.* **20**, 515–533 (1998).
36. Moulton, J. D., Dendy, J. E. & Hyman, J. M. The black box multigrid numerical homogenization algorithm. *J. Comput. Phys.* **142**, 80–108 (1998).
37. Tadmor, E. B. & Miller, R. E. *Modeling Materials: Continuum, Atomistic, and Multiscale Techniques* (Cambridge Univ. Press, 2011).
38. Liu, W. K., Karpov, E. G., Zhang, S. & Park, H. S. An introduction to computational nanomechanics and materials. *Comput. Methods Appl. Mech. Eng.* **193**, 1529–1578 (2004).
39. Oden, J. T., Prudhomme, S., Romkes, A. & Buaman, P. Multi-scale modeling of physical phenomena: adaptive control of models. *SIAM J. Sci. Comput.* **28**, 2359–2389 (2006).
40. Jones, R. E., Templeton, J. A., Wagner, G. J., Olmsted, D. & Modine, N. A. Electron transport enhanced molecular dynamics for metals and semi-metals. *Int. J. Numer. Methods Eng.* **83**, 940–967 (2010).

41. Mallat, S. G. A theory for multiresolution signal decomposition—the wavelet representation. *IEEE Trans. Pattern Anal. Mach. Intell.* **11**, 674–693 (1989).
42. Beylkin, G. & Coult, N. A multiresolution strategy for reduction of elliptic PDEs and eigenvalue problems. *Appl. Comput. Harmon. Anal.* **5**, 129–155 (1998).
43. Gilbert, A. C. A comparison of multiresolution and classical one-dimensional homogenization schemes. *Appl. Comput. Harmon. Anal.* **5**, 1–35 (1998).
44. Mehraeen, S. & Chen, J. S. Wavelet Galerkin method in multi-scale homogenization of heterogeneous media. *Int. J. Numer. Methods Eng.* **66**, 381–403 (2006).
45. Geers, M. G. D., Kouznetsova, V. G. & Brekelmans, W. A. M. Multi-scale computational homogenization: trends and challenges. *J. Comput. Appl. Math.* **234**, 2175–2182 (2010).
46. Fish, J. & Kuznetsov, S. Computational continua. *Int. J. Numer. Methods Eng.* **84**, 774–802 (2010).
47. Allaire, G. & Habibi, Z. Second order corrector in the homogenization of a conductive–radiative heat transfer problem. *Discret. Contin. Dyn. Syst. B* **18**, 1–36 (2013).
48. Saeb, S., Steinmann, P. & Javili, A. Aspects of computational homogenization at finite deformations: a unifying review from Reuss' to Voigt's bound. *Appl. Mech. Rev.* **68** (2016).
49. Ghosh, S. & Moorthy, S. Elastic–plastic analysis of arbitrary heterogeneous materials with the Voronoi-cell finite-element method. *Comput. Methods Appl. Mech. Eng.* **121**, 373–409 (1995).
50. Aboudi, J. A continuum theory for fiber-reinforced elastic–viscoplastic composites. *Int. J. Eng. Sci.* **20**, 605–621 (1982).
51. Berlyand, L. & Kolpakov, A. Network approximation in the limit of small interparticle distance of the effective properties of a high-contrast random dispersed composite. *Arch. Ration. Mech. Anal.* **159**, 179–227 (2001).
52. Moulinec, H. & Suquet, P. A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Comput. Methods Appl. Mech. Eng.* **157**, 69–94 (1998).
53. Chen, J. S., Pan, C., Wu, C. T. & Liu, W. K. Reproducing kernel particle methods for large deformation analysis of nonlinear structures. *Comput. Methods Appl. Mech. Eng.* **139**, 195–229 (1996).
54. Cavalcante, M. A. A., Khatam, H. & Pindera, M. J. Homogenization of elastic–plastic periodic materials by FVDAM and FEM approaches—an assessment. *Composites B* **42**, 1713–1730 (2011).
55. Dvorak, G. J. On uniform fields in heterogeneous media. *Proc. R. Soc. A* **431**, 89–110 (1990).
56. Paley, M. & Aboudi, J. Micromechanical analysis of composites by the generalized cells model. *Mech. Mater.* **14**, 127–139 (1992).
57. Moore, B. C. Principal component analysis in linear-systems—controllability, observability, and model-reduction. *IEEE Trans. Autom. Control* **26**, 17–32 (1981).
58. Green, M. A relative error bound for balanced stochastic truncation. *IEEE Trans. Autom. Control* **33**, 961–965 (1988).
59. Glover, K. All optimal Hankel-norm approximations of linear-multivariable systems and their L_∞ error bounds. *Int. J. Control* **39**, 1115–1193 (1984).
60. Krysl, P., Lall, S. & Marsden, J. E. Dimensional model reduction in non-linear finite element dynamics of solids and structures. *Int. J. Numer. Methods Eng.* **51**, 479–504 (2001).
61. Yvonnet, J. & He, Q. C. The reduced model multiscale method (R3M) for the non-linear homogenization of hyperelastic media at finite strains. *J. Comput. Phys.* **223**, 341–368 (2007).
62. Le, B. A., Yvonnet, J. & He, Q. C. Computational homogenization of nonlinear elastic materials using neural networks. *Int. J. Numer. Methods Eng.* **104**, 1061–1084 (2015).
63. Bhattacharjee, S. & Matous, K. A nonlinear manifold-based reduced order model for multiscale analysis of heterogeneous hyperelastic materials. *J. Comput. Phys.* **313**, 635–653 (2016).
64. Fish, J., Yuan, Z. F. & Kumar, R. Computational certification under limited experiments. *Int. J. Numer. Methods Eng.* **114**, 172–195 (2018).
65. Wang, Y., Cheung, S. W., Chung, E. T., Efendiev, Y. & Wang, M. Deep multiscale model learning. *J. Comp. Phys* **406**, 109071 (2020).
66. Michel, J. C. & Suquet, P. Computational analysis of nonlinear composite structures using the nonuniform transformation field analysis. *Comput. Methods Appl. Mech. Eng.* **193**, 5477–5502 (2004).
67. Fritzen, F. & Bohlke, T. Nonuniform transformation field analysis of materials with morphological anisotropy. *Compos. Sci. Technol.* **71**, 433–442 (2011).
68. Yuan, Z. F., Aitharaju, V. & Fish, J. A coupled thermo-chemo-mechanical reduced-order multiscale model for predicting process-induced distortions, residual stresses, and strength. *Int. J. Numer. Methods Eng.* **121**, 1440–1455 (2019).
69. Hsu, D. D., Xia, W., Song, J. & Keten, S. Glass-transition and side-chain dynamics in thin films: explaining dissimilar free surface effects for polystyrene vs poly(methyl methacrylate). *ACS Macro Lett.* **5**, 481–486 (2016).
70. Ruiz, L., Xia, W., Meng, Z. & Keten, S. A coarse-grained model for the mechanical behavior of multi-layer graphene. *Carbon* **82**, 103–115 (2015).
71. Bulatov, V. & Cai, W. *Computer Simulations of Dislocations* Vol. 3 (Oxford Univ. Press, 2006).
72. Noid, W. G. et al. The multiscale coarse-graining method. I. A rigorous bridge between atomistic and coarse-grained models. *J. Chem. Phys.* **128**, 244114 (2008).
73. Groot, R. D. & Warren, P. B. Dissipative particle dynamics: bridging the gap between atomistic and mesoscopic simulation. *J. Chem. Phys.* **107**, 4423–4435 (1997).
74. Marrink, S. J., Risselada, H. J., Yefimov, S., Tieleman, D. P. & de Vries, A. H. The MARTINI force field: coarse grained model for biomolecular simulations. *J. Phys. Chem. B* **111**, 7812–7824 (2007).
75. Reith, D., Pütz, M. & Müller-Plathe, F. Deriving effective mesoscale potentials from atomistic simulations. *J. Comput. Chem.* **24**, 1624–1636 (2003).
76. Xia, W. et al. Energy renormalization for coarse-graining polymers having different segmental structures. *Sci. Adv.* **5**, eaav4683 (2019).
77. Xu, W. T., Jiao, Y. & Fish, J. An atomistically-informed multiplicative hyper-elasto-plasticity-damage model for high-pressure induced densification of silica glass. *Comput. Mech.* **66**, 155–187 (2020).
78. Wang, K. & Sun, W. C. Meta-modeling game for deriving theory-consistent, microstructure-based traction–separation laws via deep reinforcement learning. *Comput. Methods Appl. Mech. Eng.* **346**, 216–241 (2019).
79. Liu, Z., Bessa, M. A. & Liu, W. K. Self-consistent clustering analysis: an efficient multi-scale scheme for inelastic heterogeneous materials. *Comput. Methods Appl. Mech. Eng.* **306**, 319–341 (2016).
80. Tadmor, E. B., Ortiz, M. & Phillips, R. Quasicontinuum analysis of defects in solids. *Philos. Mag. A* **73**, 1529–1563 (1996).
81. Kohlhoff, S., Gumbsch, P. & Fischmeister, H. F. Crack propagation in b.c.c. crystals studied with a combined finite-element and atomistic model. *Philos. Mag. A* **64**, 851–878 (1991).
82. Xiao, S. P. & Belytschko, T. A bridging domain method for coupling continua with molecular dynamics. *Comput. Methods Appl. Mech. Eng.* **193**, 1645–1669 (2004).
83. Wagner, G. J. & Liu, W. K. Coupling of atomistic and continuum simulations using a bridging scale decomposition. *J. Comput. Phys.* **190**, 249–274 (2003).
84. Rudd, R. E. & Broughton, J. Q. Concurrent coupling of length scales in solid state systems. *Phys. Status Solidi b* **217**, 251–291 (2000).
85. Badia, S. et al. A force-based blending model for atomistic-to-continuum coupling. *Int. J. Multiscale Comput. Eng.* **5**, 387–406 (2007).
86. Miller, R. E. & Tadmor, E. B. A unified framework and performance benchmark of fourteen multiscale atomistic/continuum coupling methods. *Model. Simul. Mater. Sci. Eng.* **17**, 053001 (2009).
87. Luskin, M. & Ortner, C. Atomistic-to-continuum coupling. *Acta Numer.* **22**, 397–508 (2013).
88. Dupuy, L. M., Tadmor, E. B., Miller, R. E. & Phillips, R. Finite-temperature quasicontinuum: molecular dynamics without all the atoms. *Phys. Rev. Lett.* **95**, 060202 (2005).
89. Tadmor, E. B., Legoll, F., Kim, W. K., Dupuy, L. M. & Miller, R. E. Finite-temperature quasi-continuum. *Appl. Mech. Rev.* **65**, 10803–10803 (2013).
90. Wagner, G. J., Jones, R. E., Templeton, J. A. & Parks, M. L. An atomistic-to-continuum coupling method for heat transfer in solids. *Comput. Methods Appl. Mech. Eng.* **197**, 3351–3365 (2008).
91. Beex, L. A. A., Peerlings, R. H. J. & Geers, M. G. D. A multiscale quasicontinuum method for lattice models with bond failure and fiber sliding. *Comput. Methods Appl. Mech. Eng.* **269**, 108–122 (2014).
92. Phlipot, G. P. & Kochmann, D. M. A quasicontinuum theory for the nonlinear mechanical response of general periodic truss lattices. *J. Mech. Phys. Solids* **124**, 758–780 (2019).
93. Cai, W., de Koning, M., Bulatov, V. V. & Yip, S. Minimizing boundary reflections in coupled-domain simulations. *Phys. Rev. Lett.* **85**, 3213–3216 (2000).
94. Li, S., Liu, X., Agrawal, A. & To, A. C. Perfectly matched multiscale simulations for discrete lattice systems: extension to multiple dimensions. *Phys. Rev. B* **74**, 045418 (2006).
95. Delgado-Buscalioni, R. & Coveney, P. V. USHER: an algorithm for particle insertion in dense fluids. *J. Chem. Phys.* **119**, 978–987 (2003).
96. Guo, L., Chen, S. & Robbins, M. O. Multi-scale simulation method for electroosmotic flows. *Eur. Phys. J. Spec. Top.* **225**, 1551–1582 (2016).
97. Yushu, D. & Matouš, K. The image-based multiscale multigrid solver, preconditioner, and reduced order model. *J. Comput. Phys.* **406**, 109165–109165 (2020).
98. Voter A. F. in *Radiation Effects in Solids* (eds Sickafus, K. E. et al.) (NATO Science Series Vol. 235, Springer, 2007).
99. Henkelman, G. & Jonsson, H. Long time scale kinetic Monte Carlo simulations without lattice approximation and predefined event table. *J. Chem. Phys.* **115**, 9657–9666 (2001).

100. Voter, A. F. Parallel replica method for dynamics of infrequent events. *Phys. Rev. B* **57**, 13985–13988 (1998).
101. Sorensen, M. R. & Voter, A. F. Temperature-accelerated dynamics for simulation of infrequent events. *J. Chem. Phys.* **112**, 9599–9606 (2000).
102. Voter, A. F., Montalenti, F. & Germann, T. C. Extending the time scale in atomistic simulation of materials. *Annu. Rev. Mater. Res.* **32**, 321–346 (2002).
103. Yu, Q. & Fish, J. Multiscale asymptotic homogenization for multiphysics problems with multiple spatial and temporal scales: a coupled thermo-viscoelastic example problem. *Int. J. Solids Struct.* **39**, 6429–6452 (2002).
104. Chen, W. & Fish, J. A dispersive model for wave propagation in periodic heterogeneous media based on homogenization with multiple spatial and temporal scales. *J. Appl. Mech.* **68**, 153–161 (2000).
105. Oskay, C. & Fish, J. Fatigue life prediction using 2-scale temporal asymptotic homogenization. *Int. J. Numer. Methods Eng.* **61**, 329–359 (2004).
106. Kevrekidis, I. G. & Samaey, G. Equation-free multiscale computation: algorithms and applications. *Annu. Rev. Phys. Chem.* **60**, 321–344 (2009).
107. Wagner, G. J., Zhou, X. & Plimpton, S. J. Equation-free accelerated simulations of the morphological relaxation of crystal surfaces. *Int. J. Multiscale Comput. Eng.* **8**, 423–439 (2010).
108. Mosser, L., Dubrule, O. & Blunt, M. J. Reconstruction of three-dimensional porous media using generative adversarial neural networks. *Phys. Rev. E* **96**, 043309 (2017).
109. Yang, Z. et al. Microstructural materials design via deep adversarial learning methodology. *J. Mech. Design* **140**, 111416 (2018).
110. Voter, A. F. A method for accelerating the molecular dynamics simulation of infrequent events. *J. Chem. Phys.* **106**, 4665–4677 (1997).
111. Chakraborty, S. & Ghosh, S. Hyperdynamics accelerated concurrent atomistic–continuum model for developing crack propagation models in elastic crystalline materials. *Comput. Mater. Sci.* **154**, 212–224 (2018).
112. Kim, W. K., Luskin, M., Perez, D., Voter, A. F. & Tadmor, E. B. Hyper-QC: an accelerated finite-temperature quasicontinuum method using hyperdynamics. *J. Mech. Phys. Solids* **63**, 94–112 (2014).
113. Kim, W. K. & Tadmor, E. B. Accelerated quasicontinuum: a practical perspective on hyper-QC with application to nanoindentation. *Philos. Mag.* **97**, 2284–2316 (2017).
114. Saunders, N. & Miodownik A. P. *CALPHAD (Calculation of Phase Diagrams): a Comprehensive Guide* (Elsevier, 1998).
115. Olson, G. B. & Kuehmann, C. Materials genomics: from CALPHAD to flight. *Scr. Mater.* **70**, 25–30 (2014).
116. Saal, J. E., Kirklin, S., Aykol, M., Meredig, B. & Wolverton, C. Materials design and discovery with high-throughput density functional theory: the Open Quantum Materials Database (OQMD). *JOM* **65**, 1501–1509 (2013).
117. Jain, A. et al. Commentary: The Materials Project: a materials genome approach to accelerating materials innovation. *APL Mater.* **1**, 011002 (2013).
118. de Pablo, J. J. et al. New frontiers for the Materials Genome Initiative. *NPJ Comput. Mater.* **5**, 41 (2019).
119. Blaiszik, B. et al. The Materials Data Facility: data services to advance materials science research. *JOM* **68**, 2045–2052 (2016).
120. Butler, K. T., Davies, D. W., Cartwright, H., Isayev, O. & Walsh, A. Machine learning for molecular and materials science. *Nature* **559**, 547–555 (2018).
121. Mauro, J. C., Tandia, A., Vargheese, K. D., Mauro, Y. Z. & Smedskjaer, M. M. Accelerating the design of functional glasses through modeling. *Chem. Mater.* **28**, 4267–4277 (2016).
122. Ramprasad, R., Batra, R., Pilania, G., Mannodi-Kanakkithodi, A. & Kim, C. Machine learning in materials informatics: recent applications and prospects. *NPJ Comput. Mater.* **3**, 54 (2017).
123. Zhao, H. et al. Perspective: NanoMine: a material genome approach for polymer nanocomposites analysis and design. *APL Mater.* **4**, 053204 (2016).
124. Hansoge, N. K. et al. Materials by design for stiff and tough hairy nanoparticle assemblies. *ACS Nano* **12**, 7946–7958 (2018).
125. Koslowski, M. & Strachan, A. Uncertainty propagation in a multiscale model of nanocrystalline plasticity. *Reliab. Eng. Syst. Saf.* **96**, 1161–1170 (2011).
126. Kouchmeshky, B. & Zabaras, N. Microstructure model reduction and uncertainty quantification in multiscale deformation processes. *Comput. Mater. Sci.* **48**, 213–227 (2010).
127. Bostanabad, R. et al. Uncertainty quantification in multiscale simulation of woven fiber composites. *Comput. Methods Appl. Mech. Eng.* **338**, 506–532 (2018).
128. Mehrez, L., Fish, J., Aitharaju, V., Rodgers, W. R. & Ghanem, R. A PCE-based multiscale framework for the characterization of uncertainties in complex systems. *Comput. Mech.* **61**, 219–236 (2018).
129. Salloum, M. & Templeton, J. Inference and uncertainty propagation of atomistically informed continuum constitutive laws, part 2: generalized continuum models based on Gaussian processes. *Int. J. Uncertain. Quantif.* **4**, 171–184 (2013).
130. Chernatynskiy, A., Phillpot, S. R. & LeSar, R. Uncertainty quantification in multiscale simulation of materials: a prospective. *Annu. Rev. Mater. Res.* **43**, 157–182 (2013).
131. Ghanem, R. & Spanos, P. D. *Stochastic Finite Elements: a Spectral Approach* (Springer, 1991).
132. Reagan, M. T., Najm, H. N., Ghanem, R. G. & Knio, O. M. Uncertainty quantification in reacting-flow simulations through non-intrusive spectral projection. *Combust. Flame* **132**, 545–555 (2003).
133. Mathelin, L., Hussaini, M. Y. & Zang, T. A. Stochastic approaches to uncertainty quantification in CFD simulations. *Numer. Algorithms* **38**, 209–236 (2005).
134. Fish, J. & Wu, W. A nonintrusive stochastic multiscale solver. *Int. J. Numer. Methods Eng.* **88**, 862–879 (2011).
135. Kaminski, M. & Kleiber, M. Perturbation based stochastic finite element method for homogenization of two-phase elastic composites. *Comput. Struct.* **78**, 811–826 (2000).
136. Liu, Y., Greene, M. S., Chen, W., Dikin, D. A. & Liu, W. K. Computational microstructure characterization and reconstruction for stochastic multiscale material design. *Computer-Aided Des.* **45**, 65–76 (2013).
137. Lee, H., Brandyberry, M., Tudor, A. & Matous, K. Three-dimensional reconstruction of statistically optimal unit cells of polydisperse particulate composites from microtomography. *Phys. Rev. E* **80**, 061301 (2009).
138. Kirchdoerfer, T. & Ortiz, M. Data-driven computational mechanics. *Comput. Methods Appl. Mech. Eng.* **304**, 81–101 (2016).
139. Raissi, M., Perdikaris, P. & Karniadakis, G. E. Physics-informed neural networks: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comput. Phys.* **378**, 686–707 (2019).
140. AlphaSTAR http://www.alphastarcorp.com
141. Autodesk: Helius Composite https://www.autodesk.com/products/helius-composite/overview
142. Xstream https://www.e-xstream.com
143. Altair Multiscale-Designer https://altairhyperworks.com/product/Multiscale-Designer
144. Templeton, J. A., Jones, R. E., Lee, J. W., Zimmerman, J. A. & Wong, B. M. A long-range electric field solver for molecular dynamics based on atomistic-to-continuum modeling. *J. Chem. Theory Comput.* **7**, 1736–1749 (2011).
145. Harrison R. J. et al. MADNESS: a multiresolution, adaptive numerical environment for scientific simulation. *SIAM J. Sci. Comput.* **38**, S123–S142 (2015).
146. Sridhar, A., Kouznetsova, V. G. & Geers, M. G. D. Homogenization of locally resonant acoustic metamaterials towards an emergent enriched continuum. *Comput. Mech.* **57**, 423–435 (2016).
147. Kochmann, D. M., Hopkins, J. B. & Valdevit, L. Multiscale modeling and optimization of the mechanics of hierarchical metamaterials. *MRS Bull.* **44**, 773–781 (2019).
148. Özdemir, I., Brekelmans, W. A. M. & Geers, M. G. D. Computational homogenization for heat conduction in heterogeneous solids. *Int. J. Numer. Methods Eng.* **73**, 185–204 (2008).
149. Ling, J., Kurzawski, A. & Templeton, J. Reynolds averaged turbulence modelling using deep neural networks with embedded invariance. *J. Fluid Mech.* **807**, 155–166 (2016).
150. Nair, A. K., Warner, D. H., Hennig, R. G. & Curtin, W. A. Coupling quantum and continuum scales to predict crack tip dislocation nucleation. *Scr. Mater.* **63**, 1212–1215 (2010).
151. Smith, G. S., Tadmor, E. B., Bernstein, N. & Kaxiras, E. Multiscale simulations of silicon nanoindentation. *Acta Mater.* **49**, 4089–4101 (2001).
152. Fish, J. & Chen, W. Discrete-to-continuum bridging based on multigrid principles. *Comput. Methods Appl. Mech. Eng.* **193**, 1693–1711 (2004).
153. Fish, J., Suvorov, A. & Belsky, V. Hierarchical composite grid method for global–local analysis of laminated composite shells. *Appl. Numer. Math.* **23**, 241–258 (1997).

Competing interests

The authors declare no competing interests.

Additional information

Correspondence should be addressed to J.F.