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Bridging the scales in nano engineering and science

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Abstract

This review article describes various multiscale approaches, development of which was spurred by the emergence of nanotechnology. The multiscale approaches are grouped into two main categories: information-passing and concurrent. In the concurrent multiscale methods both, the discrete and continuum scales are simultaneously resolved, whereas in the information-passing schemes, the discrete scale is modelled and its gross response is infused into the continuum scale. Most of the information-passing approaches provide sublinear computational complexity, (i.e., scales sublinearly with the cost of solving a fine scale problem), but the quantities of interest are limited to or defined only on the coarse scale. The issues of appropriate scale selection and uncertainty quantification are also reviewed.

Introduction

The need for new simulation technologies

Consider two engines depicted in Figure 1. The size of the jet engine shown in Figure 1a is of order of meters; continuum description by means of partial differential equations prevails, and consequently, it is appropriate to use discretization methods such as finite elements or finite differences. On the other hand, the rotary motor in Figure 1b has a diameter of 30 nm. It drives *Salmonella* and *E. coli* bacteria by rotating at around 20,000 rpm, at energy consumption of around 10^{-16} W and with energy conversion efficiency close to 100% (Namba, 2004).

This remarkably efficient nano-engine does not obey continuum principles because it is simply too small; continuum description does not account for predominant surface effects that would result in too stiff behaviour. On the other hand, a brute force approach of modelling the rotary motor entirely on atomistic scale would necessitate billions of unknowns and consideration of time scales on the order of 10^{-15} s.

This suggests a multiscale computational paradigm where important atomistic features could be captured at a fraction of computational cost required by atomistic simulation of the entire system (Rudd & Broughton, 1998).

Examples and qualification of multiscale methods

A modelling and simulation approach is termed multiscale if it is capable of resolving certain quantities of interest with a significantly lower cost than solving the corresponding fine-scale system. Schematically, a multiscale method has to satisfy

the so-called Accuracy and Cost Requirements (ACR) test:

$$\text{Error in quantities of interest} < \text{tol}$$

$$\frac{\text{Cost of multiscale solver}}{\text{Cost of fine scale solver}} \ll 1$$

This review article focuses on two categories of multiscale approaches: information-passing and concurrent. In the information-passing multiscale approach (see Section 2), the discrete scale is modelled and its gross response is infused into continuum (or discrete coarse-grained) scale, whereas in the concurrent approach (see Section 3), both, the discrete and continuum scales (or coarse-grained) are simultaneously resolved. The issue of quantification of modelling errors introduced due to introduction of coarser scales is discussed in Section 4.

To motivate the need for the two scale-bridging technologies, we consider several applications. First, is a nanomachine depicted in Figure 2. The device is about 50 microns across or half of the typical human hair thickness. The size of the device does not allow accurate representation of processes in the contact region by continuum material description, which can be derived from

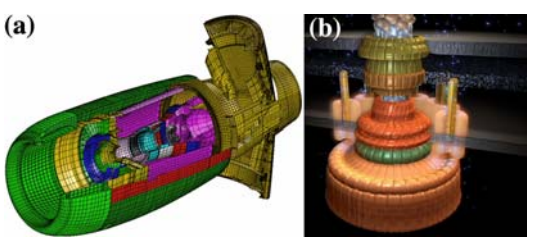

Figure 1. (a) macro-engine, (b) nano-engine.

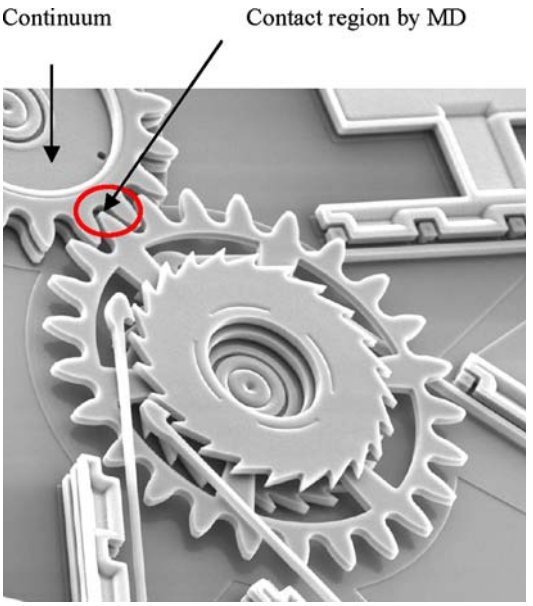

Figure 2. A photograph of a nanomachine developed at Sandia made by a scanning electron microscope. The nanomachine is used to drive a microscopic mirror.

one of the information-passing approaches (see Section 2). In these critical regions, discrete representation must be considered instead, giving rise to the concurrent modelling (see Section 3) (Figures 3 and 4).

Similar scale bridging technologies are needed for modelling of nanonwires (Liang & Zhou, 2004; Park & Zimmerman, 2005), nanobelts, nanohelixes and nanorings (Wang, 2004; Wang et al., 2004; Kulkarni et al., 2005). Atomistic modelling of these nano-components have recently allowed the discovery of a novel shape memory effect and the

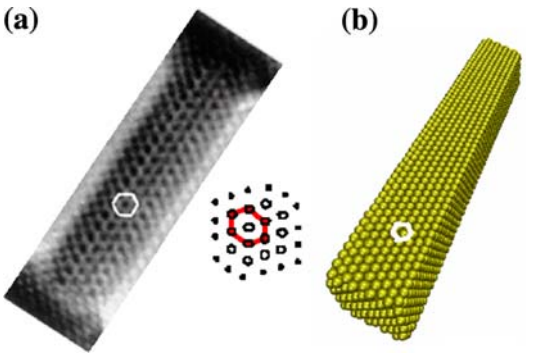

Figure 3. Physical (a) and computational (b) models of nanowires (Liang & Zhou, 2004).

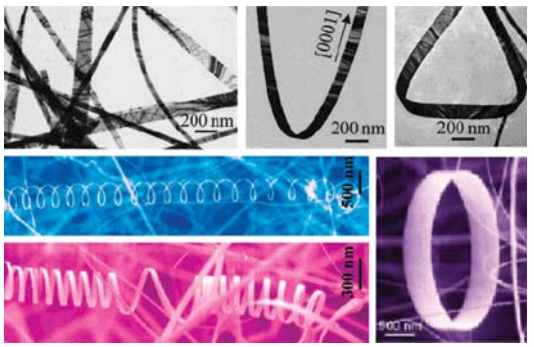

Figure 4. Nanobelts, nanohelixes and nanorings (Wang, 2004; Wang et al., 2004).

ability of recovering elongations of up to 50% under tensile loading and unloading as opposed to 5–8% typical for most bulk shape memory alloys. Interestingly, this phenomenon only exists at the nanometer scale and is associated with a reversible crystallographic lattice reorientation driven by the high surface-stress-induced internal stresses at the nanoscale. It is strongly size- and temperature-dependent. Multiscale issues involve continuum thermomechanical modelling and coupling of atomistic and continuum descriptions (Liang & Zhou, 2005). These capabilities are needed to design stronger, defect-resistant nanostructures, as advanced sensors, and as high strength structural reinforcing materials.

Another important phenomenon which requires fine scale (atomistic) resolution in the vicinity of free surfaces and coarse-grained modelling in the interior is a process of wetting and spreading (Heine et al., 2005). In applications involving liquid state transport at the nano scale, traditional hydrodynamic theories for wetting kinetics are no longer valid as surface tension effects become dominant. Studying this length scale of liquids wetting solids via experiment is met with a number of difficulties and a great benefit can be derived from the information-passing and concurrent multiscale modelling of this phenomenon (Webb et al., 2005) (Figure 5).

To this end, we focus on the qualification of multiscale methods. Loosely speaking, the information-passing multiscale approach is likely to pass the so-called ACR test provided that:

(i) the quantities of interest are limited to or defined only on the coarse scale (provided that this quantities are computable from the fine scale), and
(ii) special features of the fine scale problem, such as scale separation and self-similarity, are taken advantage of.

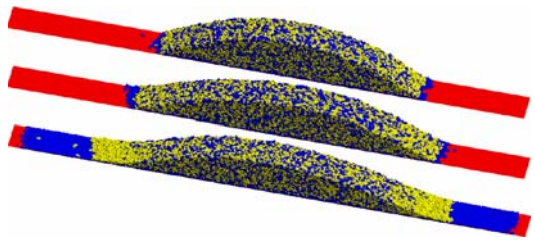

Figure 5. Molecular dynamics simulations to reveal the spreading mechanism for binary polymer droplets (Heine et al., 2005).

On the other hand, for the concurrent multiscale approach to pass the ACR test, the following conditions must be satisfied:

(i) the interface (or interphase) between the fine and coarse scales should be properly engineered (see Section 3), and
(iia) the information-passing multiscale approach of choice should serve as an adequate mechanism for capturing the lower frequency response of the fine-scale system, or alternatively,
(iib) the fine scale model should be limited to a small part of the computational domain.

The ACR condition (iia) represents a stronger requirement typically satisfied by multigrid-based concurrent methods (see Section 3.3), but not by domain bridging (Section 3.1) or local enrichment (Section 3.2) concurrent methods. It is important to note that even though concurrent approaches may pass the ACR test, their computational cost will typically exceed that of the information-passing methods. Nevertheless, they offer a distinct advantage over the information-passing methods by virtue of being able to resolve fine scale details in critical regions. Therefore, concurrent multiscale approaches are typically pursued when the fine scale information is either necessary, or if not resolved, may pollute significant errors on the coarse scale information of interest.

For complementary reading we refer to an excellent review articles (Ghoniem & Cho, 2002; Curtin & Miller, 2003; Aubry et al., 2004; Chong, 2004; Liu et al., 2004; McVeigh et al., 2006).

The importance of simulation to nanotechnology

The potential impact of multiscale science and engineering on nanotechnology has been realized by a number of government agencies. The FY2004 National Nanotechnology Bill authorizing $3.7 billion over the next four years which among others calls for 'urgent need for theory, modelling, large-scale computer simulation, and new design tools in order to understand, control, and accelerate (nanotechnology) development' (Marburger et al., 2004). Lead by Roco (Roco, 2000), NSF announced a multiple-year program (NSF, 2001) on collaborative research in the area of nanoscale science and engineering, which among others calls for 'computation and information technology.' NSF Blue Ribbon Panel on Simulation-Based Engineering Science (SBES) identified scale bridging as a major barrier (Oden et al., 2006).

NSF, NIH, NASA and DOE have joined to announce the 'Interagency Opportunities in Multi-Scale Modelling in Biomedical, Biological and Behavioural Sciences'. The recent $8.5 million DOE program on 'Multiscale Mathematics Research and Education', calls for research and education "in applied mathematics needed to break through the current barriers in our understanding of complex physical processes that occur on a wide range of interacting length- and time-scales."

In 2004 alone, DOE has organized three workshops on multiscale mathematics with emphasis on discrete to continuum scale bridging. Over a similar period, NSF co-sponsored four workshops on multiscale modelling. Strong interest in academic community lead to the introduction of two interdisciplinary multiscale journals: the SIAM Multiscale Modelling and Simulation Journal (SIAM), and the Int. J. for Multiscale Computational Engineering (Begell).

Information-passing multiscale methods

In the information-passing multiscale methods, calculations at finer scale, and of high-computational complexity, are used to evaluate certain quantities for use in a more approximate or phenomenological computational methodology at a longer length/time scale. This type of scale bridging is also known as sequential, serial or parameter-passing. For nonlinear problems, fine and coarse scale models are two-way coupled, i.e., the information continuously flows between the scales.

In this section we review several information-passing bridging technique including: the Force field calibration method, which constructs effective interatomic potentials and eliminates the need for explicitly tracing the evolution of electronic structure; the Generalized Mathematical Homogenization (GMH) theory (Fish & Schwob, 2003; Fish et al., 2005; Chen & Fish, 2006; Fish & Chen, 2006a), which constructs an equivalent continuum description directly from molecular dynamics (MD) equations; the Quasicontinuum method (Tadmor et al., 1996), which can be viewed as an engineering counterpart of the mathematical homogenization; the Multiscale Enrichment based on the Partition of Unity (MEPU) method (Fish & Yuan, 2005), which gives rise to the enriched coarse grained formulation; the Heterogeneous Multiscale Method (HMM) (E et al., 2003), which provides equivalent coarse scale integrands; the Variational Multiscale Method (VMS) (Hughes, 1995), which can be viewed as an equivalent coarse scale element builder; the Coarse-Grained Molecular Dynamics (CGMD) (Rudd & Broughton, 1998), which derives effective Hamiltonian for the coarse-grained problem; the Discontinuous Galerkin (DG) Method (Hou & Wu, 1997), which constructs discontinuous enrichment; the equation-free method (EFM) (Kevrekidis et al., 2004), which makes no assumption on the response of the coarse scale problem; proper orthogonal decomposition (POD) which generates a set of "snapshots" on the fine scale to create a reduced-space basis; the Kinetic Monte Carlo (KMC) and atomistically informed Dislocation Dynamics (DD) methods, which bridge diverse scales by calibrating certain KMC and DD parameters from molecular dynamics or quantum mechanics calculations.

Force field calibration

On the subnanometer scale, the evolution of the electronic structure is tracked using quantum mechanical models based on the density-functional theory (DFT) (Parr & Yang, 1989). Higher level quantum chemical calculation and explicit Van der Waals interaction parameter can be used to describe interactions for weakly bound systems (Wu et al., 2001), and Car-Parinello molecular dynamics (Car & Parrinello, 1985) to study

dynamical evolution of systems. Relatively small systems (10,000 atoms) can be modelled by these methods. Quantum simulations are typically five to six orders of magnitude more computational demanding than classical molecular dynamics methods. Alternative methods to model electronic structure in systems containing millions of atoms have been demonstrated using empirical tight binding. Recent research efforts (Aidun, 2005) are focussing on developing information-passing multiscale methods that construct effective interatomic potentials aimed at eliminating the need for explicitly tracing the evolution of electronic structure (Brenner, 1990; van Duin et al., 2001). These types of methods have the potential of modelling systems of up to 100s of millions of atoms (few 100 nm). For instance in van Duin et al. (2001), a general bond-order-dependent potential in which the van der Waals and Coulomb forces are included from the beginning and the dissociation and reaction curves are derived from QC calculations. An accurate description of quantum phenomena such as resonance, unsaturated valences in radical systems and chemical reactions have been obtained. While van Duin et al. (2001) was restricted to hydrocarbons, the framework developed is valid for any molecular system of any class of compounds (Strachan et al., 2003).

Generalized Mathematical Homogenization (GMH) theory

In the GMH approach a multiple scale space–time asymptotic expansion is employed to approximate the displacement field

$$\mathbf{u}(\mathbf{x},\mathbf{y},\tau,t,s_i)=\mathbf{u}^0+\varepsilon\mathbf{u}^1\ldots \tag{1}$$

where $\mathbf{x}$ is a differentiable continuum coordinate; $\mathbf{y}=\mathbf{x}/\varepsilon$ the discrete coordinate denoting position of atoms in a unit cell and $0<\varepsilon\ll 1$; τ the fast time coordinate, which tracks vibration of atoms for finite temperature applications; t the usual time coordinate; s_i the slow time coordinates, which from the physics point of view capture dispersion effects, whereas from the mathematics point of view eliminate secularity of asymptotic expansions. We first outline the O(1) GMH theory without consideration of slow time scales.

The primary objective of GMH is to construct continuum equations directly from Molecular Dynamics (MD) equations

$$m_i(\mathbf{Y}_i)\mathbf{u}_i(\mathbf{X}_i,\mathbf{Y}_i,t,\tau)=\frac{1}{\varepsilon}\sum_{j\neq i}\mathbf{f}_{ij}(\mathbf{x}_{ij}) \tag{2}$$

where $\mathbf{f}_{ij}$, $\mathbf{x}_{ij}$ are the interatomic force and the radius vector between atoms i and j, respectively; and m_i is the mass of atom i. Capital and lower case letters denote initial and current positions of atoms, respectively. In Eq. (2) for simplicity pairwise interatomic potential is considered, which may be inadequate for solids. Expanding $\mathbf{x}_{ij}=\varepsilon\mathbf{x}_{ij}^0+\varepsilon^2\mathbf{x}_{ij}^1+\cdots$ in asymptotic sequence and the force field $\mathbf{f}_{ij}$ in Taylor's series expansion around the leading order term $\varepsilon\mathbf{x}_{ij}^0$ yields a set of coupled continuum-atomistic governing equations:

(i) Fine scale equation:

$$\frac{m_i}{\varepsilon}\frac{\partial^2\mathbf{u}^1}{\partial\tau^2}=\sum_{j(\neq i)}\mathbf{f}_{ij}\times\left\{\left(\mathbf{F}(\mathbf{u}^0)\cdot\left[\mathbf{X}_{ij}+\varepsilon\left(\mathbf{u}^1(\mathbf{x}_j)-\mathbf{u}^1(\mathbf{x}_i)\right)\right]\right\}$$

subjected to the deformation gradient $\mathbf{F}(\mathbf{u}^0)$ and temperature T obtained from the continuum equations.

(ii) Coarse scale mechanical equation

$$\rho_0\frac{\partial^2\mathbf{u}^0(\mathbf{X},t)}{\partial t^2}-\nabla_{\mathbf{X}}\cdot\langle\mathbf{P}\rangle=0$$

$$\mathbf{P}(\mathbf{X},t,\tau)=\frac{1}{2\Theta}\sum_{i=1}^{n}\sum_{j\neq i}[\mathbf{f}_{ij}\otimes\mathbf{X}_{ij}]$$

(ii) Heat flow (coarse scale) equation

$$C\frac{\partial\langle T\rangle}{\partial t}-\nabla_{\mathbf{X}}\cdot\langle\mathbf{q}(\mathbf{X},t,\tau)\rangle=-2\langle\mathbf{P}\rangle:\nabla_{\mathbf{X}}\frac{\partial\mathbf{u}^0(\mathbf{X},t)}{\partial t}$$

$$\mathbf{q}(\mathbf{X},t,\tau)=\frac{1}{2\Theta}\sum_{i=1}^{n}\sum_{j\neq i}\left[\left(2\frac{\partial\mathbf{u}^0}{\partial t}+\frac{\partial\mathbf{u}_i^1}{\partial\tau}\right)\cdot(\mathbf{f}_{ij}\otimes\mathbf{X}_{ij})\right]$$

where $\mathbf{P}$ and $\mathbf{q}$ are the First Piola–Kirchhoff stress tensor and thermal flux vector, respectively; T the temperature; ρ the density; Θ the volume of the atomistic unit cell; $\nabla_X\cdot()$ the divergence operator with respect to the initial coordinates; $\mathbf{X}_{ij}$ the initial separation between atoms i and j.

The temporal averaging operator is defined as

$$\langle \chi(\tau) \rangle = \frac{1}{\tau_0} \int_0^{\tau_0} \chi(\tau) d\tau$$

where τ_0 is a characteristic time period of the function $\chi(\tau)$.

It can be seen that the First Piola–Kirchoff stress derived from the O(1) GMH theory coincides with the mechanical term in the virial stress formula (Irving & Kirkwood, 1950; Hardy, 1982 among others). For more details on the O(1) GMH theory and its numerical implementation see Fish et al. (2005) and Fish and Chen (2006a).

The motivation for introduction of slow time scales was given in Fish and Chen (2001), where it has been shown that in absence of slow time scales the scaling parameter $\varepsilon = O(\sqrt{\bar{t}})$ becomes time dependent, where $\bar{t}$ is the normalized time coordinate. Consequently, as $\bar{t} \to \infty$ the asymptotic expansion becomes no longer uniformly valid.

Higher order GMH theory incorporating slow time scales leads to the nonlocal continuum description (Fish et al., 2002a, b; Fish & Schwob, 2003). Alternatively, a close form solution for slow time scales can be obtained leading to an algebraic system of equations with a single time scale (Chen & Fish, 2006). Extension of the GMH theory to finite temperatures using fast time scales has been given in Fish et al. (2005) and Fish and Chen (2006a).

Figure 6 compares the GMH, with the spatial homogenization approach developed in Chung (2004) and molecular dynamics simulation for wave propagation in a layered lattice structure (Chen & Fish, 2006). It can be seen that the GMH theory offers a comparable accuracy to MD simulation despite significant cost reduction.

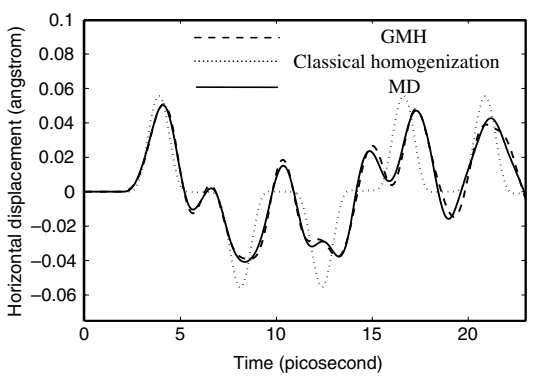

Figure 6. Comparison of GMH with classical (spatial) homogenization and molecular dynamics (MD) simulations.

To this end we note that for the GMH approach to be valid both the temporal and spatial scales have to be separable. For instance, if the essential events of the faster fine scale model occur on the same time scales as the details of processes computed using the slower coarse model, then the time scales cannot be separated. Likewise, if the wavelength of the travelling signal is of the order of magnitude of the fine scale features, then the spatial scales cannot be separated.

Quasicontinuum

Quasicontinuum is a continuum description where constitutive equations are constructed directly from atomistics rather than from a phenomenological constitutive model. The atomistically informed constitutive model is adequate as long as continuum fields are slowly varying over a unit cell domain. In its original form (Tadmor et al., 1996) the quasicontinuum method was formulated for simple Bravais crystals assuming uniform deformation of atoms. In a more general case with heterogeneous interatomic potentials, a unit cell problem has to be solved instead (Tadmor et al., 1999). In this more general scenario, the quasicontinuum resembles GMH and as such it can be viewed as an engineering counterpart of the mathematical theory. Note that both the "engineering" and mathematical homogenization methods involve solution of an atomistic unit cell problem and subsequently feeding the continuum problem with effective properties.

Multiscale enrichment based on the partition of unity

Multiscale enrichment based on partition of unity (MEPU) (Fish & Yuan, 2005) is a synthesis of the generalized mathematical homogenization (Chen & Fish, 2006) and partition of unity (Babuska et al., 1994; Melenk & Babuska, 1996; Moes et al., 1999) methods. MEPU can be used to enrich the coarse scale continuum description or the coarse-grained discrete formulations. It is primarily intended to extend the range of applicability of the mathematical homogenization theory to problems where scale separation may not be valid, such as in the

case of nonperiodic solutions or problems where the coarse solution may rapidly vary over the domain of a unit cell.

MEPU belongs to the category of methods employing hierarchical decomposition of the approximation space in the form of

$$\mathbf{u} = \mathbf{u}^{\mathrm{c}} + \mathbf{u}^{\mathrm{f}} \tag{3}$$

where $\mathbf{u}^{\mathrm{c}}$ and $\mathbf{u}^{\mathrm{f}}$ are the coarse and fine scale solutions, respectively. Note that in GMH $\mathbf{u}^{\mathrm{c}} = \mathbf{u}^{0}(\mathbf{x})$ and $\mathbf{u}^{\mathrm{f}} \approx \varepsilon \mathbf{u}^{1}(\mathbf{x}, \mathbf{y})$. In MEPU, on the other hand,

$$\mathbf{u} = \sum \mathbf{N}(\mathbf{x})\mathbf{d} + \sum \mathbf{H}(\mathbf{x})\mathbf{N}(\mathbf{x})\mathbf{a} \tag{4}$$

where **N** are the coarse scale element shape functions; **H**(**x**) the influence function obtained from the unit cell solution; **d, a** the nodal and enrichment degrees-of-freedom, respectively. The influence functions can be either discrete (obtained from the atomistic unit cell) or continuous. MEPU allows consideration of nonperiodic fields by associating different unit cells with different Gauss points in the coarse scale elements.

To reduce the computational cost, homogenization-like integration scheme is devised. By this approach the value of a function at a Gauss point of a coarse scale element is replaced by an average computed over a unit cell domain centred at a Gauss point. It has been proved that the accuracy of the homogenization-like integration scheme is of order $O(1/n)$ where n is a number of unit cells in the coarse scale element domain.

Figure 7 depicts a molecular model of a polymer subjected to uniform macroscopic fields. The polymer has been modelled using a single MEPU element with nine degrees of freedom per node (Fish & Yuan 2005). The error in the L_2 norm of displacements was 2% compared to the 9% using quasicontinuum method.

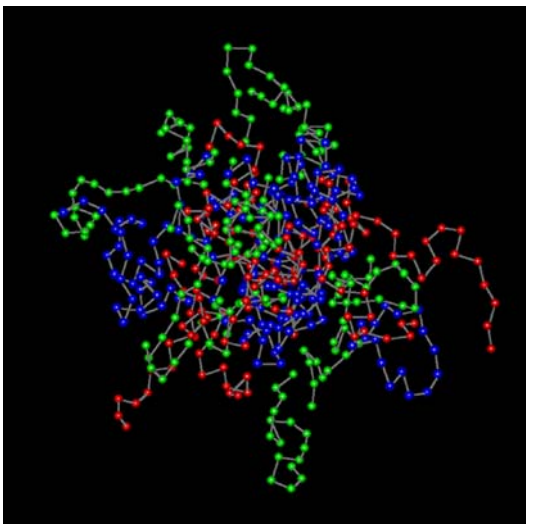

Figure 7. MD model of a polymer.

Variational multiscale method

The variational multiscale method (VMS) was originally developed for enriching continuum solutions with fine scale continuum description. Most common implementation of the method assumes the fine scale enrichment $\mathbf{u}^{\mathrm{f}}$ to be a residual free bubble vanishing on the coarse scale element boundaries. By this assumption the enrichment functions can be condensed out on the element level to give *effective coarse scale elements* as opposed to *effective fields or material properties* in the GMH approach. Alternatively, a better accuracy can be obtained by enforcing enrichment functions to vanish on the element boundaries in the weak sense.

VMS can be easily extended to enriching coarse grained descriptions. In this scenario the coarse grained description which amounts to interpolating the solution between the representative atoms, (element nodes in Figure 8) can be enriched using the kinematics of individual atoms in the areas where such enrichment in necessary. Since positions of atoms may not coincide with coarse scale element boundaries, homogeneous boundary condition of atoms residing in the close vicinity to the element boundaries can be enforced (weakly on in the strong sense) as shown in Figure 8.

Heterogeneous multiscale method

The basic idea of the heterogeneous multiscale method (HMM) is to approximate the coarse scale integrands by data computed from the auxiliary fine scale problem (E et al., 2003). The auxiliary fine scale problem is an atomistic cell subjected to boundary conditions extracted from the coarse scale solution. HMM can be viewed as a methodology for constructing *effective integrands* based on the fine scale data as opposed to effective elements in VMS.

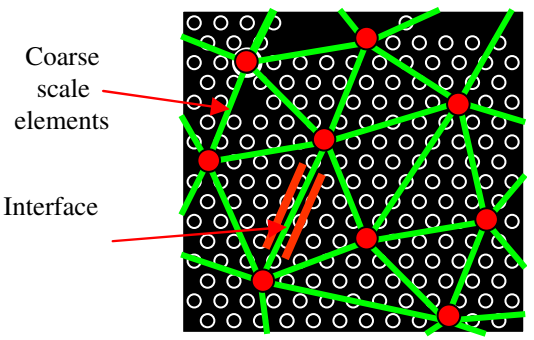

Figure 8. VMS for enriching coarse grained models.

Coarse-grained molecular dynamics

The coarse-grained molecular dynamics (CGMD) (Rudd & Broughton, 1998; Rudd, 2004) method constructs coarse grained Hamilton's equations from MD equations under fixed thermodynamic conditions.

The representative atoms, (similar to those employed in the quasicontinuum method) are enforced to preserve an average position and momenta of the fine scale atoms

$$\mathbf{u}^{\mathrm{c}}(t) = \mathbf{R}\mathbf{u}^{\mathrm{f}}(t) \quad \mathbf{p}^{\mathrm{c}}(t) = \mathbf{R}\mathbf{p}^{\mathrm{f}}(t) \tag{5}$$

where $\mathbf{R}$ is weighting or restriction operator, $\mathbf{p}^{\mathrm{c}}$, $\mathbf{p}^{\mathrm{f}}$ are the momenta at the coarse and fine scales, respectively. The coarse-grained Hamiltonian, H^{c}, is defined as the classical canonical ensemble average of the molecular dynamics Hamiltonian H^{f} in the displacement-momenta space subjected to the restriction constraint (5)

$$H^{\mathrm{C}} = \frac{1}{Z}\int \Delta P H^{\mathrm{f}} dp^{\mathrm{f}} du^{\mathrm{f}} \tag{6}$$

where $P = \exp(-H^{\mathrm{f}}/k_{\mathrm{B}}T)$ is the probability function, T the temperature, H^{f} the fine scale Hamiltonian, k_{B} the Boltzman constant, Δ enforces constraints in (5) and Z is the partition function.

Discontinuous Galerkin (DG) method

The so-called multiscale finite element method (MsFEM) developed by Hou and Wu (1997) belongs to the category of discontinuous Galerkin methods. In the MsFEM the displacement field is approximated as $\mathbf{u} = \mathbf{u}^0(x) + \varepsilon\,\mathbf{H}\,(x)\boldsymbol{\varepsilon}^{\theta}(x)$, which closely resembles the method of mathematical homogenization, but introduces no multiple spatial coordinates and thus results in C^{-1} continuous approximation of the solution. The oversampling idea of Babuska and Osborn (1983) is used to control the errors resulting from the discontinuity.

Equation free method

In the equation free method (EFM) the fine scale problem is evolved at some sampling points in the coarse scale domain. These sampling points are represented by an atomistic unit cell. Unlike in the aforementioned information-passing methods (with exception of GMH where the coarse scale problem is derived) the coarse problem is assumed to be unknown in EFM. Once the solution in two subsequent time steps on the fine scale is computed and then restricted to the coarse scale $\mathbf{u}^{\mathrm{c}}(t) = \mathbf{R}\mathbf{u}^{\mathrm{f}}(t)$ and $\mathbf{u}^{\mathrm{c}}(t+\delta t) = \mathbf{R}\mathbf{u}^{\mathrm{c}}(t+\delta t)$ then the coarse scale solution at $t + \triangle t (\triangle t \gg \delta t)$ is obtained by projective integration or extrapolation in time domain. The fine-to-coarse scale operators are well defined, but the definition of the information flow from the coarse to the fine scale remains to be the main challenge. This type of formulation may be attractive for complex biosystems whose coarse scale behaviour is often unknown.

Model reduction

The proper orthogonal decomposition (POD) (Lumley, 1967) widely used in fluid dynamics community is closely related to EFM. POD generates a set of "snapshots" on the fine scale to create a reduced-space basis, onto which the fine scale equations are projected to predict the evolution on the coarse scale.

An alternative model reduction approach aimed at bridging a continuum property of interest and the molecular dynamics model has been developed in Hurst and Wen (2005). The balanced truncation model reduction approach used in the context of linearized nonequilibrium molecular dynamics (NEMD) equations has been applied to compute shear viscosity. The input/output pair selected was the shear stress and shear strain rate. The reduced order model has been found to correctly identify the dominant mode identical to that of continuum model as well as the shear viscosity.

For a review article on application of model reduction methods to large scale semi-discrete system we refer to Gressick et al. (2005).

KMC-based information-passing methods

Most of the aforementioned multiscale approaches with exception of EFM and GMH deal with bridging spatial scales. Linking diverse time scales is even more challenging. For instance, to capture the dynamics of atomistic vibrations, the time step should be of the order of femtoseconds, whereas the residence time of an adatom between hops is of the order of microseconds. This 'time gap' can be addressed using Kinetic Monte Carlo (KMC) based methods. The basic idea of this approach is summarized below.

Let the probability of finding a system in state σ_i at time t to be denoted as $P(\sigma_i, t)$ and the rate of transitions from σ_i to σ_{i+1} to be $W(\sigma_i, \sigma_{i+1})$. KMC is an algorithm that solves for the probability function $P(\sigma_i, t)$ such that

$$\frac{\partial P}{\partial t} = \sum (P(\sigma_i, t) W(\sigma_i, \sigma_{i+1}) - P(\sigma_{i+1}, t) W(\sigma_{i+1}, \sigma_i))$$

The rate of transition can be expressed as a product of an attempt rate and the probability of success per attempt, which is taken as an exponential of the energy barrier to the process. The attempt rate for event i is defined as

$$r_i = \mu_i \exp(-E_i / k_B T) \tag{7}$$

where μ_i is a frequency prefactor expressed in terms of a vibrational frequency for surface processes (Grujicic et al., 2003; Johnson et al., 2003; Picu, 2003) and E_i is the free energy barrier. KMC falls into the category of information-passing methods because the frequency prefactor and the energy barrier can be calculated from molecular dynamics or quantum mechanics simulations.

Atomistically informed dislocation dynamics

In many nanotechnology applications involving thin films or coatings dislocation-interface interactions are very important. The dislocations can be considered as the basic elements of a grain-size model in which their interactions are determined by a combination of linear elasticity and atomistic simulations. A general dislocation dynamics (DD) approach for computing elastic field of arbitrary dislocation loops in anisotropic multilayer thin films has been given in Cuitino (1997) and Ghoniem (2004). Atomistically informed DD approach can be viewed as an information-passing scheme where the underlying properties of dislocations, such as the strength of a dislocation junction or the cross-slip probability are 'imported' from the atomistic simulations of elementary dislocation processes (Moriarty et al., 2002).

Concurrent multiscale methods

In this section we present a class of multiscale approaches for systems, whose behaviour depends on physics at multiple scales. Friction and fracture are among many problems (see Section 1.2) falling into this category. In fracture, the crack tip bond breaking can be described with a quantum-mechanical model of bonding, while the rest of the sample is described with empirical potentials. In friction, it might be necessary to describe the surface interaction using quantum-chemical approaches while using continuum elasticity to simulate the contact forces. For these types of problems, multiple scales have to be simultaneously resolved in different portions of the problem domain. Multiscale methods based on the concurrent resolution of multiple scales are often coined as embedded, concurrent, integrated or hand-shaking multiscale methods. Various domain bridging methods (Broughton et al., 1999; Belytschko & Xiao, 2003; Miller, 2003; Wagner et al., 2004), multigrid methods (Fish & Belsky, 1995a, b; Moulton et al., 1998; Knapek 1999; Datta et al., 2004; Fish & Chen, 2004; Waisman & Fish, 2006) and local enrichment methods (Fish & Markolefas, 1992; Fish et al., 1994; Moes et al., 1999; Strouboulis et al., 2001; Wagner & Liu, 2003; Fish & Yuan, 2005) are used to communicate the information between the subdomains represented by different mathematical models.

An important aspect of concurrent methods is matching condition at the interface between different mathematical models. For instance, at the MD/continuum interface, MD generates phonons which are not represented in the continuum region and hence might be reflected at the continuum/MD interface. Formulation of absorbing inter-

faces include damping (Broughton et al., 1999), Langevin equation (Wagner & Liu, 2003), precomputing exact absorbing boundary conditions for harmonic potentials (Cai et al., 2000), approximating exact absorbing boundary conditions and calibrating coefficients to minimize reflection (E & Huang, 2001), matching the properties of continuum and MD at the interface (Muralidharan et al., 2003), and bridging domain method (Belytschko & Xiao, 2003; Ben Dhia & Rateau, 2005). By refining the finite element mesh to atomistic scale at the interface (Broughton et al., 1999), the issue of phonon reflection can be circumvented. A review of various interface formulations can be found in Curtin and Miller (Miller, 2003). For concurrent bridging between discrete dislocations and continuum region we refer to Shilkrot et al. (2002).

Another important aspect of concurrent bridging is building temporal interfaces. For example, in a typical atomistic-continuum problem the time scale for integrating MD equations is dictated by the interatomic spacing and highly heterogeneous interatomic connections. At the continuum scale, the time step could be much larger primarily because the stiff connections have been homogenized out and the spacing between the discrete points (for instance, FE nodes) could be substantially larger. Temporal interfaces can be built using various multi-time-step methods (Smolinski et al., 1988) and local enrichment functions in time domain (Bottasso, 2002), whereas the space–time interfaces can be constructed using the space–time DG method (Sobh et al., 2000). The multi-step technique developed in Belytschko and Xiao (2003) preserves stability of time integrators and at the same time minimizes spurious reflections from the interfaces.

In the remainder of this section we outline the basic ideas of the domain bridging (Section 3.1), local enrichment (Section 3.2), and multigrid (Section 3.3) based concurrent multiscale methods common to several aforementioned approaches. We emphasize that the above multiscale methods are concerned with a concurrent bridging of dissimilar mathematical models representing different scales, as opposed to the classical domain decomposition, multigrid and enrichment methods, which are primarily concerned with efficient solution of a single scale mathematically similar models.

In the domain bridging based concurrent multiscale (DBCM) approach, the fine Ω^{f} and coarse Ω^{c} scale subdomains could be either overlapping or coexistent as shown in Figure 9. The interface, Γ, could be the same or lower dimensional manifold. In the multigrid based concurrent multiscale (MGCM) and the local enrichment based concurrent multiscale (LECM) approaches the subdomains are coexisting (Figure 9a). The interface, $\Gamma \subset \Omega^{\mathrm{f}}$, is a subdomain in Ω^{f} defined to be in the close vicinity to the boundary $\partial\Gamma$ as shown in Figure 9a. It could be the same or lower dimensional manifold, in which case $\Gamma = \partial\Gamma$.

Domain bridging based concurrent multiscale method

Consider a conservative system consisting of continuum (c) – discrete (f) subdomains (Figure 9b). Let $\mathbf{p}_i^{\mathrm{f}}$, $\mathbf{u}_i^{\mathrm{f}}$ be the momenta and displacements of atom i, and $\dot{\mathbf{u}}^{\mathrm{c}}(x), \mathbf{u}^{\mathrm{c}}(x)$ be the velocities and displacements of the continuum. The Hamiltonian that weakly satisfies compatibility between the discrete and continuum regions at the interface Γ is defined as

$$
\begin{aligned}
H = & \int_{\Omega^{\mathrm{C}}} \alpha^{\mathrm{c}} \left[\frac{1}{2} \rho \dot{\mathbf{u}}^{\mathrm{CT}} \dot{\mathbf{u}}^{\mathrm{c}} + w^{\mathrm{c}}\left(\mathbf{u}^{\mathrm{C}}\right) \right] d\Omega^{\mathrm{C}} \\
& + \sum_{i,j \neq i} \alpha^{\mathrm{f}} \left[\frac{\mathbf{p}_i^{\mathrm{f}} \cdot \mathbf{p}_i^{\mathrm{f}}}{2m^{\mathrm{f}}} + w^{\mathrm{f}}\left(\mathbf{u}_i^{\mathrm{f}}, \mathbf{u}_j^{\mathrm{f}}\right) \right] \\
& + \int_{\Gamma} \lambda(x) \left[\delta\left(\mathbf{u}^{\mathrm{C}}(x) - \mathbf{u}_i^{\mathrm{f}}\right) \right] d\Gamma
\end{aligned}
$$

where $\alpha^{\mathrm{C}} + \alpha^{\mathrm{f}} = 1$ is enforced so that the energy would not count twice; $\alpha^{\mathrm{C}} = 1$ on $\Omega^{\mathrm{C}} - \Gamma$ in case of

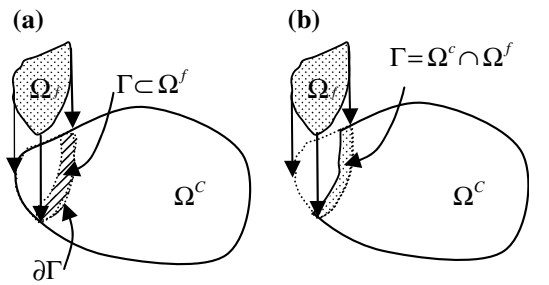

Figure 9. (a) coexisting domains and (b) overlapping domains.

overlapping subdomains and $\Omega^C - \Omega^f$ in case of coexisting subdomains; in both cases $\alpha^f = 1$ on $\Omega^f - \Gamma$. δ is a delta function; the atomistic region is defined over $x_i^f \in \Omega^f$; $w^C(x), w^f(\mathbf{u}_i^f, \mathbf{u}_j^f)$ are the continuum internal energy and the pairwise interaction of the atoms (for simplicity considered here), respectively.

In Belytschko and Xiao (2003) the overlapping subdomains were considered with α^C, α^f to vary linearly on Γ and compatibility enforced in a strong form. In Broughton et al. (1999) an overlapping subdomains were considered with $\alpha^C = \alpha^f = 0.5$. The Arlequin method (Ben Dhia & Rateau, 2005) was applied to bridge between continuum scales only.

The domain bridging method has been applied to link discrete scales: quantum mechanics and molecular dynamics descriptions in (Adhikari et al., 2004). The so-called hybrid QM/MM scheme has been used to study the interaction of acetone with carbon nanotubes as shown in Figure 10.

In Figure 10 the acetone molecule and few atoms on carbon nanotube (shown as ball and stick) are included using full quantum mechanical scheme while rest of the system (shown as sticks) are modelled using semi-classical PM3 method.

The above formulation can be extended to more than two scales. For instance, in Broughton et al. (1999) the computational domain was decomposed into three parts: a continuum region discretized with finite elements, an atomistic region modelled by molecular dynamics, and a quantum mechanical region where the tight binding model is used to model bond breaking.

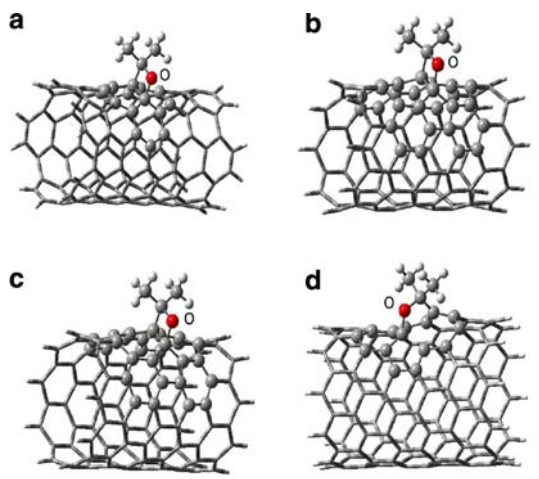

Figure 10. Snap shots of acetone-nanotube structure during chemical reaction using QM/MM method (Adhikari et al., 2004).

Local enrichment based concurrent multiscale method

The local enrichment based concurrent multiscale (LECM) method employs hierarchical decomposition of the form given in Eq. (3). For the enrichment scheme to be qualified in the LECM category, the enrichment function must have *local supports* and has to be *complete*, i.e., in the limit as the approximation of $\mathbf{u}^f$ is enriched it converges to the fine scale description. For instance, in one of the VMS variants (Hughes 1995), in the limit as $\mathbf{u}^f$ is locally enriched the method does not converge to the fine scale description because there is no refinement on coarse scale element boundaries. Examples of complete enrichment spaces can be found in Fish and Markolefas (1992), Fish et al. (1994), Strouboulis et al. (2001) and Fish and Yuan (2005), but such complete enrichment spaces cannot be locally condensed out.

The resulting Hamiltonian in LECM is given by

$$H = \sum_{i \subset \Omega} w^f\left(\mathbf{u}^C(x_i) + \alpha \mathbf{u}_i^f\right) + \sum_{i \subset \Omega} \frac{1}{2} m \left(\dot{\mathbf{u}}^C(x_i) + \alpha \dot{\mathbf{u}}_i^f\right)^T \left(\dot{\mathbf{u}}^C(x_i) + \alpha \dot{\mathbf{u}}_i^f\right) + \sum_{i \subset \Gamma} \lambda(x_i) \mathbf{u}_i^f$$

where $\alpha = 1$ on Ω^f and $\alpha = 0$ elsewhere. In the above $\mathbf{u}^C$ is a coarse grained model, such as quasicontinuum, defined on the entire problem domain $\Omega^C = \Omega$. w^f is a pairwise interaction of the atoms.

LECM offers the advantage inherent to hierarchical methods, including the ease of solution enrichment and *a posteriori* model error estimation. But unlike DBCM, which uses dissimilar mathematical models, LECM is limited to similar mathematical models at different scales.

A variant of the LECM method has been recently developed by Wagner and Liu (2003). In the so-called bridging scale method, atomistic description is superimposed onto a continuous finite element mesh in the critical regions. The displacement field is decomposed as

$$\mathbf{u} = \mathbf{N}\mathbf{d} + (\mathbf{I} - \mathbf{P})\mathbf{q}$$

where $\mathbf{P}$ is the projection operator defined to minimized the mass-weighted square of the error between the fine and coarse scale descriptions.

Generalization of the bridging scale to three dimensions, including the numerical calculation of the molecular dynamics boundary condition was developed in (Park et al., 2005a, b).

Multigrid based concurrent multiscale method

The motivation for use of multigrid ideas for multiscale problems was given in Fish and Belsky (1995a, b). To convey the basic ideas, consider a one-dimensional two-scale elliptic problem

$$\frac{d}{dx}\left(K(x)\frac{du}{dx}\right) + b(x) = 0$$
$$x \in (0, L) \quad u(0) = u(L) = 0$$

with oscillatory periodic piecewise constant coefficients K_1, K_2 and 0.5 volume fraction.

The above equation is discretized with $2(m-1)$ elements – each element possessing constant coefficients. The eigenvalues can be computed in a closed form:

$$\lambda^k = \frac{\frac{4\tilde{K}}{h}\sin^2\left(k\frac{\pi}{2m}\right)}{1 + \sqrt{1 - q\sin^2\left(k\frac{\pi}{2m}\right)}},$$
$$\lambda^{2m-k} = \frac{\frac{4\tilde{K}}{h}\sin^2\left(k\frac{\pi}{2m}\right)}{1 - \sqrt{1 - q\sin^2\left(k\frac{\pi}{2m}\right)}}$$

where $1 \leq k < m$; $2h$ the unit cell size; $\tilde{K}$ the overall coefficients and q the ratio between geometric and arithmetic averages of the coefficients given as:

$$\tilde{K} = \frac{2K_1K_2}{K_1 + K_2}, \quad \sqrt{q} = \frac{\sqrt{K_1K_2}}{(K_1 + K_2)/2}$$

Note that in many applications of interest and in particular those described at the atomistic scale $K_1 \gg K_2$ or $K_2 \gg K_1$ or $0 < q \ll 1$. Consequently, the eigenvalues are clustered at the two ends of the spectrum, with one half being O(1) and the other half being $O(1/q)$. More importantly, the O(1) eigenvalues are identical to those obtained by the problem with homogenized coefficients. This character of the spectrum suggests a computational strategy based on the philosophy of multilevel methods. In such a multilevel strategy smoother is designated to capture the higher frequency response of the fine scale model represented by a linear combination of the $O(1/q)$ eigenmodes. The auxiliary coarse model is then engineered to effectively capture the remaining lower frequency response of the fine scale problem. For a periodic heterogeneous medium, such an auxiliary coarse model coincides with the boundary value problem with homogenized coefficients as evidenced by the identical eigenvalues. The resulting multiscale prolongation Q operator is given by

$$Q = Q^{\mathrm{C}} + Q^{\mathrm{f}} \tag{8}$$

where Q^{C}, Q^{f} are the classical (smooth) prolongation and the fine scale correction obtained from the discretization of the influence functions, respectively. The rate of convergence of the multigrid process for the two-scale problem is governed by .(Fish & Belsky, 1995a, b):

$$\|e_{i+1}\| = q\|e_i\|/(4 + q) \tag{9}$$

where $\|e_{i+1}\|$ is the norm of error in iteration $i+1$. For example, if either K_1/K_2 or K_2/K_1, is 100, then the two-scale process converges in three iterations up to the tolerance of 10^{-5}.

In principle, any information-passing approach described in Section 2 can be used as an auxiliary coarse model to capture the lower frequency response of the fine scale problem. The multiscale prolongation depends on the choice of the information-passing approach.

To this end we describe the application of multigrid ideas to bridging diverse time scales. The space–time variational multigrid method developed in Waisman and Fish (2006) is aimed at bridging between atomistic scale and either coarse grained discrete or continuum scales. The method consists of the wave-form relaxation scheme aimed at capturing the high frequency response of the atomistic vibrations and the coarse scale solution in space and time intended to resolve smooth features of the discrete medium. The waveform relaxation (Miekkala & Nevanlinna, 1987; Giladi & Keller, 2002) decomposes the system into very small subsystem (for instance, atom-by-atom decomposition) which can be integrated in parallel

and take advantage of unstructured time integrators. The waveform relaxation can be also interpreted as atom-by-atom minimization of MD Hamiltonian.

Then a coarse model correction at a certain time step $u^{\mathrm{f}} + Qe^{\mathrm{C}}$ can be calculated from the Hamilton principle on the subspace of coarse scale functions

$$H(\mathbf{e}^{\mathrm{c}}) = \sum w^{\mathrm{f}}\left(\mathbf{u}^{\mathrm{f}} + Q\mathbf{e}^{\mathrm{c}}\right) + \sum \frac{1}{2} m\left(\dot{\mathbf{u}}^{\mathrm{f}} + Q\mathbf{e}^{\mathrm{c}}\right)^{\mathrm{T}}\left(\dot{\mathbf{u}}^{\mathrm{f}} + Q\mathbf{e}^{\mathrm{c}}\right) \rightarrow \min_{\mathbf{e}^{\mathrm{c}}}$$

The method has been used to simulate a polymer structure shown in Figure 7 and compared to the classical explicit integration. Significant speed-ups have been observed in particular on parallel machines. These results show that as the number of processors increases, the speed-up factor between the MG and velocity-verlet methods increases. The main reason for the increase in the speed-up factor is due to reduced processors communication. In the case of standard explicit or implicit methods processors are communicating after every time step. However, in the MG and WR case the communication between processors only takes place at the end of each window.

The coarse scale model was constructed using aggregation method (Fish & Belsky, 1997), where each polymer chain was defined as an aggregate (Figure 11).

The rate of convergence on a model problem with harmonic potentials has been studied in Fish and Chen (2004). A multiscale filter (Fish & Qu, 2000; Qu & Fish, 2000; Waisman et al., 2004) is needed for indefinite systems, such as those arising from chemical reactions or breakage of interatomic connections. For related wave-form relaxation multigrid methods (Horton & Vandewalle, 1995).

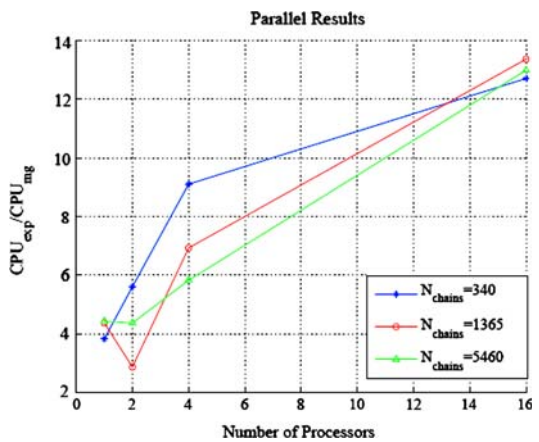

Figure 11. Comparison of Explicit and space–time multigrid methods on a parallel machine.

A posteriori model error estimation

In devising a rigorous discrete-to-continuum scale-bridging framework, one of the main barriers is increased uncertainty/complexity introduced by discrete scales as illustrated in Figure 12.

As a guiding principle for assessing the need for finer scales, it is appropriate to recall the statement made by Einstein, who stated that "the model used should be the simplest one possible, but not simpler." The optimal multiscale model has to be carefully weighted on case-by-case basis. For example, in case of metal matrix composites (MMC) with almost periodic arrangement of fibers, introducing finer scales might be advantageous since the bulk material typically does not follow normality rules and developing a phenomenological coarse scale constitutive model might be challenging at best. The behaviour of each phase is well understood and obtaining the overall response of the material from its fine scale constituents can be obtained using homogenization. On the other hand, in brittle ceramics composites (CMC), the microcracks are often randomly distributed and characterization of their interface properties is difficult. In this case, the use of fine scale models may not be desirable.

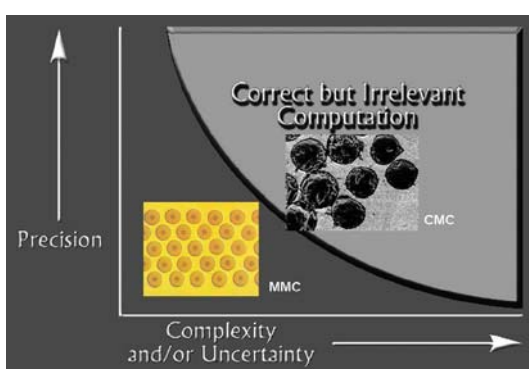

Figure 12. Reduced precision due to increase in uncertainty and/or complexity.

Ensuring reliability of multiscale modelling and simulation tools is one the key ingredients of modern engineering and science. The fundamental building block are: (i) formulation of a hierarchy of multiscale models, and (ii) *a posterior* model error estimation including uncertainty quantification.

In the remainder of this section, we focus on the aforementioned two issues.

Hierarchy of multiscale models

Hierarchical models are a sequence of mathematical models, which include increasingly more sophisticated effects, represented by finer scales in the present context. The most-comprehensive member of the sequence is based on the "first principles", such as Density Functional Theory, which evaluates the system energies by tracing the ground states of the electrons. The modelling error associated with any other member of the sequence is assessed by comparing it to the most-sophisticated member of the hierarchical sequence. A member of the sequence is considered to be admissibly accurate if the modelling error in the data of interest is sufficiently small. The goal is to identify an optimal member of the sequence, which is both admissibly accurate and computationally least expensive.

Hierarchical models differ in at least three respects: (i) spatial and temporal scale at which they are represented, (ii) model interaction, and (iii) the ability to account for uncertainty. Model error control for continuum descriptions must also consider multiphysics errors arising from simplified considerations of multifield interactions. Loosely speaking, a member of the sequence is considered to be admissibly accurate if the modelling error in the data of interest is sufficiently small. The goal is to identify an optimal member of the sequence that is admissibly accurate and most efficient to solve.

Since the exact solution of the most comprehensive model is usually not computationally feasible, the challenge is compute a posteriori error estimates.

Model error estimates

An error estimate of a particular model in a hierarchy can be obtained by comparison to higher level members (often solved approximately). For example, the error of the continuum or discrete coarse-grained model can be estimated based on the magnitude of field gradients. The error of the KMC model is largely dictated by the accuracy of the individual rates and assumptions regarding separation of time scales. The error in molecular mechanics models can be determined by comparison with DFT calculations. In these cases, errors also arise from the statistical variation of the simulation cell, artificial boundary and/or initial conditions, and are associated with the cell size and simulation time scales. The error introduced by multiscale asymptotic methods can be estimated by comparing the magnitude of the terms neglected in the asymptotic sequence to those taken into account and by the magnitude secular terms (Fish et al., 1994). The error associated with coupling of physical processes can be obtained using the Green's function approach.

An alternative approach, which estimates modelling errors in so-called quantities of interest has been developed in Oden et al. (2005). Upper and lower bounds of modelling errors in local quantities of interest for this class of problems were developed in Oden and Vemaganti (2000) and model adaptivity based on the so-called Goals algorithm was first presented in Vemaganti and Oden (2001). These methods are closely related to those of the systems control theory, including balance truncation and optimal Hankel norm approximation (Antoulas et al., 2004).

Modelling errors are often formulated as inequality constraints to reflect the uncertainty in the parameters of the system at the relevant scales to make the model selection criterion aware of the sensitivity of the hierarchy of models to their associated uncertainties.

The error due to uncertainty can be estimated by the statistical sampling of data and numerical experiments (Ghanem & Pellissetti, 2002; Sakamoto & Ghanem, 2002). The quality of a predictive model is dependent on the quality of the model, the data used in its calibration, and its numerical and statistical discretization. The model synthesizes the variability in material properties at different scales into physics-based stochastic processes.

Stochastic approaches to multiscale modelling and propagation of uncertainty for scale and multiphysics coupling have begun to receive

attention. Deterministic variability at a finer scale is modelled at a coarser scale as a random character of the coarse-scale behaviour. These methods, which rely on the integration of wavelet multi-resolution analysis with spectral decompositions of stochastic processes, were developed for linking similar models defined at different scales (Ghanem & Shi, 2002). An extension to resolutions involving multi-physics approximations is a significant nascent research area. Polynomial chaos decompositions that permit the encapsulation of uncertainty into a computationally tractable form play a significant role in this context. Most other representations of uncertainty have focused on computing statistical norms of the stochastic quantities (Kleiber & Tran, 1992).

Closing remarks

The state-of-the-art information-passing and concurrent multiscale approaches were reviewed. Out of over 100 articles referenced more than 50% were published in the last four years. Many of the multiscale methods reviewed are still at their embryonic stage of development. Comparative study of various multiscale methods presented and in particular those that emerged in the past few years is very scarce at best. The primary goal of this article is to give the reader a brief account of rapidly emerging modelling and simulation technologies that we believe will eventually become an equal partner to experimentation. The article is not intended to serve as an optimal method selector. Yet, certain general trends that can be used as a guiding principle are emerging. These guidelines are summarized below.

- The choice between an information-passing and a concurrent method depends on computational resources available and quantities of interest. For instance, if only ensemble averages are of interest, the accuracy provided by an information passing method is generally sufficient. A counter example is an evolution and growth of defects, which necessitates utilization of one of the concurrent multiscale methods.
- When coarse scale equations are unknown, the analyst can either bypass their construction using EFM (Kevrekidis et al., 2004) or by deriving coarse scale equations from the fine scale using GMH (Fish & Schwob, 2003; Fish et al., 2005; Chen & Fish, 2006; Fish & Chen, 2006b).
- The choice between multigrid-based and domain decomposition-based concurrent approaches typically depends on the size of a fine scale region. When the size of a fine scale region is negligible compared to the entire problem domain, domain decomposition-based approaches will typically suffice. Otherwise, the use of multigrid-based concurrent approaches should be pursued provided that an efficient coarse grid can be constructed.
- With exception of EFM-, GMH- and KMC-based approaches, the rest of multiscale approaches presented directly address the issue of spatial scale bridging only. Nevertheless, any coarse graining method in space typically increases the stable time step, and therefore indirectly, is multiscale in time.
- Because of increase in uncertainty at the finer scale ensuring reliability of multiscale simulations poses the main challenge. Hierarchical modelling strategy by which a sequence of mathematical models with increasingly more sophisticated effects is used for model verification, offers one of the most promising venues to address the issue of reliability.

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