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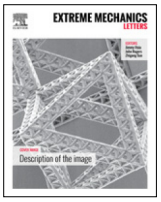

Computational homogenization at extreme scales

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ABSTRACT

Multi-scale simulations at extreme scales in terms of both physical length scales and computational resources are presented. In this letter, we introduce a hierarchically parallel computational homogenization solver that employs hundreds of thousands of computing cores and resolves $\mathcal{O}(10^5)$ in material length scales (from $\mathcal{O}$(cm) to $\mathcal{O}$(100 nm)). Simulations of this kind are important in understanding the multi-scale essence of many natural and synthetically made materials. Thus, we present a simulation consisting of 53.8 Billion finite elements with 28.1 Billion nonlinear equations that is solved on 393,216 computing cores (786,432 threads). The excellent parallel performance of the computational homogenization solver is demonstrated by a strong scaling test from 4,096 to 262,144 cores. A fully coupled multi-scale damage simulation shows a complex crack profile at the micro-scale and the macroscopic crack tunneling phenomenon. Such large and predictive simulations are an important step towards *Virtual Materials Testing* and can aid in development of new material formulations with extreme properties. Furthermore, the high computational efficiency of our computational homogenization solver holds great promise for utilizing the next generation of exascale parallel computing platforms that are expected to accelerate computations through orders of magnitude increase in parallelism rather than speed of each processor.

1. Introduction

The societal and economic pressure for improved performance of engineered systems has placed great emphasis on development of materials with extreme properties and their application in extreme environments. For example, development of advanced high strength multiphase steels [1] for improved automotive crash worthiness, structured materials [2] and meta-materials [3], fiber/particle reinforced polymeric composites [4,5] with wide application from aerospace to consumer sports equipment, and multi-functional systems such as self-healing [6] or electrically conductive adhesives [7] has become reality. In many cases, these advanced materials are multi-scale in nature, and accurately predicting their response is essential for improved design and safety assessment.

Of particular interest to this letter are predictive multi-scale simulations of these complex heterogeneous materials in typical mechanical systems. In such engineering analysis and optimal design, phenomenological constitutive models of heterogeneous materials may prove insufficient. Thus, detailed simulations that include microstructural effects and relevant micro-scale physics are required. Direct numerical modeling (DNM), which captures all of the relevant physics and length scales in a single simulation, is an accurate method for predicting the *in situ* multi-scale behavior of heterogeneous materials. However, even for small structures, these simulations can become extremely large as the required numerical resolution leads to a large number of degrees of freedom (DOFs). Such large simulations remain intractable, even for today's

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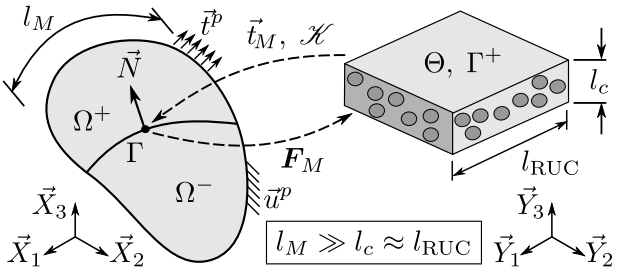

Fig. 1. Schematic of the multi-scale kinematics for heterogeneous interfaces with a comparison of length-scales.

supercomputers [8]. Moreover, the parallel algorithmic complexity of such computations mitigates the potential improvements gained on high-performance computing (HPC) systems [9–11]. On the other hand, computational homogenization (CH) [12–14] provides an alternative highly accurate modeling strategy with reduced computational requirements. However, until recently [12], CH has frequently been regarded as impractical or limited to small theoretical examples.

In this letter, we present extreme scale simulations (in terms of both physical scales and computing resources) using a hierarchically parallel CH solver [12] that enables the efficient computation of large realistic engineering problems. In particular, we focus on failure of heterogeneous interfaces such as adhesive layers. For the first time, fully-coupled multi-scale simulations are used to predict important fracture properties, such as toughness and crack speed, from the material behavior of the individual micro-scale constituents in the 3D finite strain regime.

In addition, we show the solver's ability to efficiently compute the fully coupled nonlinear multi-scale response of structures with resolution from $\mathcal{O}$(cm) to $\mathcal{O}$(100 nm), containing 53.8 Billion finite elements and 28.1 Billion nonlinear equations. Furthermore, we demonstrate ideal computational strong scaling performance of the hierarchically parallel solver using up to 262,144 computing cores. The ability to compute such large problems is an important step towards predictive simulations and the *Virtual Materials Testing* paradigm. In addition, future exascale HPC resources are expected to accelerate computations through orders of magnitude increase in parallelism rather than increasing the speed of each processor [15–18]. Therefore, the high scalability of CH makes it a promising approach to efficiently use future exascale HPC resources for scientific investigation and discovery.

2. Computational homogenization for interfaces

Before we proceed to extreme scale computations, we review the CH theory and its implementation [19,20,12] for completeness of the presentation. The CH of heterogeneous interfaces is shown schematically in Fig. 1, where two bodies (adherends) denoted as $\Omega^{\pm}$ are separated by a heterogeneous layer with thickness l_c. The layer is collapsed to an interface, Γ, and a representative unit cell (RUC, Θ) is locally attached to each material point on the interface. The RUC contains all of the micro-scale complexity in terms of both structure and constitutive behavior. Under applied load, the deformation of the macro-scale adherends, $\Omega^{\pm}$, is described by the deformation gradient, $\boldsymbol{F} = \boldsymbol{I} + \vec{\nabla}_{\vec{X}}\vec{u}$, where $\vec{u}$ are the macro-scale displacements. The deformation of a macroscopic point on the interface, Γ, is described by the deformation gradient, $\boldsymbol{F}_M = \boldsymbol{I} + \frac{1}{l_c}[\![\vec{u}]\!] \otimes \vec{N}$, where $\vec{N}$ is the normal to the interface (see Fig. 1) and $[\![\vec{u}]\!] = \vec{u}^+ - \vec{u}^-$ is the opening displacement of the interface. The deformation within the microstructure is a function of both macro- and micro-variables, with $\boldsymbol{F} = \boldsymbol{F}_M + \vec{\nabla}_{\vec{Y}}\vec{w}$, where $\vec{w}$ are the micro-scale displacement fluctuations.

The weak form of macro-scale equilibrium neglecting inertia and body forces is given by

$$\int_{\Omega^{\pm}} \boldsymbol{S}_M : \left[\boldsymbol{F}^T \vec{\nabla}_{\vec{X}} \delta\vec{u}\right]^{\mathrm{sym}} \mathrm{d}\Omega^{\pm} + \int_{\Gamma} \vec{t}_M \cdot [\![\delta\vec{u}]\!]\, \mathrm{d}A - \int_{\partial\Omega^t} \vec{t}^p \cdot \delta\vec{u}\, \mathrm{d}A = 0. \tag{1}$$

In Eq. (1), $\boldsymbol{S}_M$ is the second Piola–Kirchhoff stress given by a known constitutive model for the adherends, while $\vec{t}_M$ is the macro-scale traction vector across the interface that is computationally derived from the RUC as described in the sequel.

The Hill–Mandel condition for interfaces is given by [19,12,20]

$$\inf_{[\![\vec{u}]\!]} \psi([\![\vec{u}]\!]) = \inf_{[\![\vec{u}]\!]} \inf_{\vec{w}} \frac{l_c}{|\Theta|} \int_{\Theta} W_m(\boldsymbol{F}_M + \vec{\nabla}_{\vec{Y}}\vec{w})\, \mathrm{d}\Theta, \tag{2}$$

which relates the unknown macro-scale traction–separation potential, ψ, to the average known micro-scale strain energy density, W_m. Taking variations of Eq. (2) with respect to the macro-scale and micro-scale variables leads to

$$\frac{l_c}{|\Theta|} \int_{\Theta} \boldsymbol{S}_m : \left[\boldsymbol{F}^T \vec{\nabla}_{\vec{Y}} \delta\vec{w}\right]^{\mathrm{sym}} \mathrm{d}\Theta = 0, \tag{3}$$

$$\vec{t}_M = \frac{1}{|\Theta|}\left[\int_{\Theta} \boldsymbol{F}\boldsymbol{S}_m\, \mathrm{d}\Theta\right] \cdot \vec{N}. \tag{4}$$

Eq. (3) is the weak form of micro-scale equilibrium, and Eq. (4) is the closure equation for the macro-scale traction vector across the interface employed in Eq. (1). In Eqs. (3)–(4), $\boldsymbol{S}_m = 2\,\partial W_m/\partial \boldsymbol{C}$ where $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$. Note that in this work, we make use of semi-periodic micro-scale boundary conditions ($\vec{w} = \vec{0}\ \forall \vec{Y} \in \Gamma^{\pm}$ and $\vec{w}^+ = \vec{w}^-\ \forall \vec{Y} \in \partial\Theta^{\pm}$) and our RUCs are periodic in the $\vec{Y}_{1,2}$-directions (see Fig. 1). Other admissible boundary conditions are discussed in [20].