Multiscale Computations: Boom or Bust

by
Jacob Fish

Multiscale Science and Engineering Center
Rensselaer Polytechnic Institute

"... approaches that integrate more than one such technique (...molecular simulations, continuum-based models, etc.) will play an important role in this effort."

The rationale for multiscale computations

Consider a textbook boundary value problem, which consists of equilibrium, kinematical, and constitutive equations together with essential and natural boundary conditions. These equations can be classified into two categories: those that directly follow from physical laws and those that don't. Wikipedia [1] defines "a constitutive equation as a relation between two physical quantities that is specific to a material or substance, and does *not follow directly from physical law*. It is combined with other equations (equilibrium and kinematical equations) that do represent physical laws to solve some physical problem."

In other words, it is convenient to label all that we do not know about the boundary value problem as a constitutive law (originally coined by Walter Noll in 1954), and designate an experimentalist to quantify the constitutive law parameters. While for linear elastic materials this is a trivial exercise, this is not the case for anisotropic history-dependent materials well into their nonlinear regime. In theory, if material response is history-dependent, one would need infinite number of experiments to quantify its response. In practice, however, one defines a hand-full of constitutive law parameters that are believed to "capture" various failure mechanism observed experimentally. This is known as *phenomenological modeling,* which relates several different empirical observations of phenomena to each other, in a way that is consistent with fundamental theory, but is not directly derived from it**.**

An alternative is to derive constitutive equations (or directly field quantities) from finer scale(s), at the scale where established laws of physics are better understood. The enormous gains that can be accrued by this approach have been reported in numerous articles [2 - 7]. Multiscale computations have been identified (see page 14 in [8]) as one of the areas critical to future nanotechnology advances. The FY2004 $3.7-billion-dollar National Nanotechnology Bill (page 14 in [7]) states that: "approaches that integrate more than one such technique (…molecular simulations, continuum-based models, etc.) will play an important role in this effort."

One of the main barriers of such a multiscale approach is increased uncertainty/complexity introduced by finer scales as illustrated in *Fig. 1*. 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 use of multiscale approach 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 multiscale approach may not be desirable.

The hype and the reality

Multiscale Science and Engineering is relatively new field and as most new technologies it begins with *naive euphoria* (see Fig. 2) when inventor(s) are usually submersed in the ideas themselves and often tend to overpromise, in part to generate funds to continue their work. Hype is a natural

handmaiden to overpromise, and most technologies build rapidly to a peak of hype [9].

For instance, early expert systems success led to inflated claims and unrealistic expectations. The field did not grow as rapidly as investors had been led to expect, and this translated into disillusionment. Back in 1981 Feigenbaum et al. [10] reckoned that while artificial intelligence (AI) was already 25-years old, it "was a gangly and arrogant youth, yearning for a maturity that was nowhere evident." Interestingly, today you can purchase the hardcover AI handbook [9] for as much as $0.73 on Amazon. Multiscale computations had their share of overpromise, such as inflated claims of designing drugs atom-by-atom [11] or reliable design of Boeing 787 from first principles [12] just to mention a few.

Following this *naïve euphoria* (*see Fig.2*), there is almost always an over-reaction to ideas that are not fully developed, and this inevitably leads to a crash, followed by a period of wallowing in the depths of cynicism. Many new technologies evolve to this point, and then fade away. The ones that survive do so because industry (or perhaps someone else) finds a "good use" (= true user benefit) for this new technology.

Towards the "good use" at Rensselaer

At Rensselaer over the past six years we became increasingly interested in transitioning multiscale technologies to industry and government. The Multiscale Design System (MDS), schematically illustrated in *Fig. 3*, is a product of such a "good us". The MDS has been originally developed for design of high-temperature engine components (CMC airfoil in the Joint Strike Fighter) and lightweight structural components in automotive and aerospace industries.

The system shown in *Fig. 3* consists of the following modules and technologies:

a. ***Mathematical upscaling*:** derivation of coarse-scale equations from fine-scale equations using non linear mathematical homogenization theory [13 - 17].

b. ***Computational upscaling****:* reducing the complexity of solving a fine-scale problem to a manageable size that can be adapted based on available computational resources and error estimates in the quantities of interest [18]. The model reduction approach adopted in [17] is based on the concept of eigenstrains [19].

"Multiscale computations had their share of overpromise, such as inflated claims of designing drugs atom-by-atom or reliable design of Boeing 787 from first principles ..."

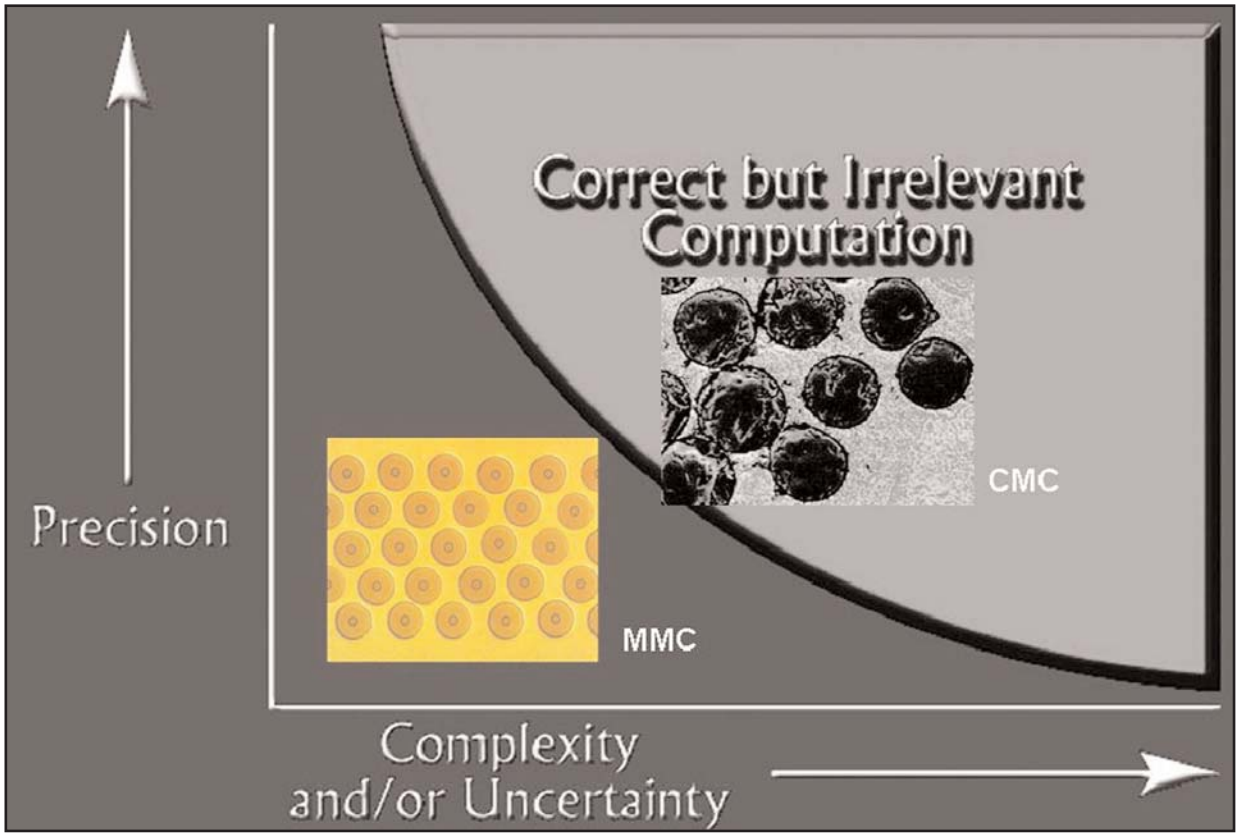

Figure 1:
Reduced precision due to increase in uncertainty and/or complexity

c. ***Model calibration:***
solving an inverse problem for constitutive parameters (interfaces, fibers/tows, matrix) by minimizing the error between experimental data at coupon [20] and fine-scale (nanoindentation tests [21]).

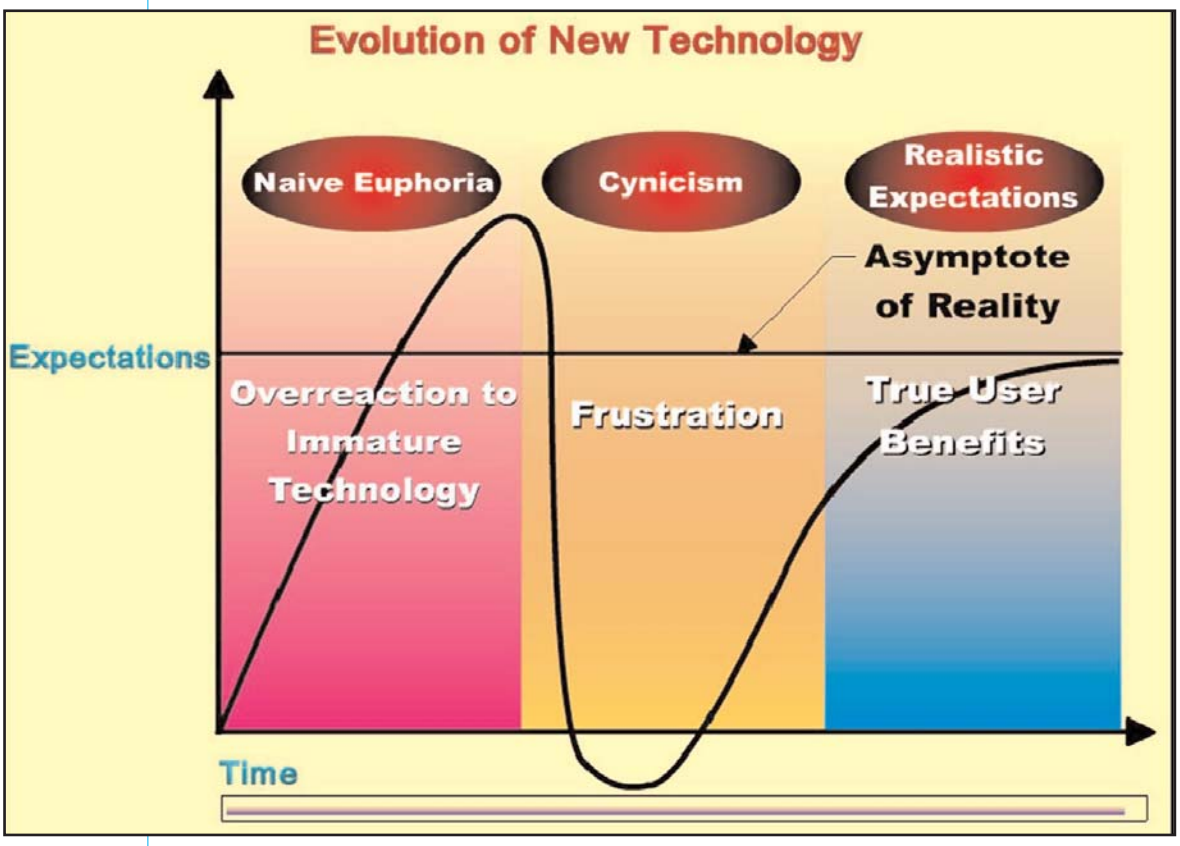

Figure 2:
Evolution of New Technology

Another variant of MDS (*Fig. 3*) for design of components made of nanostructured materials is currently under development at Rensselaer. In this variant, the fine scale model is at the atomistic scale. The coarse scale equations (coupled thermo-mechanical equations of continuum) are systematically derived (upscaled) using the Generalized Mathematical Homogenization [22, 23]. The Proper Orthogonal Decomposition (POD) combined with the space-time multilevel method [24] are employed for systematic model reduction, to capture the critical modes of dislocation motion.

Rensselaer is among the first universities to recognize that a systematic multiscale theory combined with intensive technology transfer effort would propel the Institute's initiatives in biotechnology, nanotechnology, energy, and microelectronics. Last year Rensselaer established its Multiscale Science and Engineering Center (MSEC) [25] involving 60 faculty from 10 departments.

"What would the properties of materials be if we could really arrange the atoms the way we want them?" "

Closing remarks

The ultimate question is whether computational mechanics community is ready to take upon the 49-year old challenge [26] posed by Nobel Prize Laureate Richard Feynman, who stated: "What would the properties of materials be if we could really arrange the atoms the way we want them?" More broadly stated, what is the likelihood that in foreseeable future we will able to engineer optimal system behavior by manipulating fine-scale features? The author of this article believes that progress towards fulfilling the promise of multiscale science and engineering hinges not only on its development as a discipline, concerned with understanding and integration of mathematical, computational, and domain expertise sciences, but more so with its ability to meet broader societal needs beyond those of interest to academic community. After all, as compelling as the finite element theory is, the future of the field may have been in douby, if it has not been embraced by practitioners. ●

References

[1] http://www.wikipedia.org/

[2] *Curtin, W.A. and R.E. Miller*, **Atomistic/continuum coupling in computational materials science**, Modeling and Simulation in Materials Science and Engineering. 11(3)(2003)R33-R68.

[3] *Fish, J.*, **Bridging the scales in nano engineering and science**, Journal of Nanoparticle Research. 8 (2006) 577-594.

[4] *Fish, J.*, ed. **Bridging the Scales in Science and Engineering**. Oxford University Press, 2007.

[5] *Ghoniem, N.M. and K. Cho*, **The emerging role of multiscale modeling in nano- and micro-mechanics of materials**, Modeling in Engineering and Sciences. 3 (2) (2002) 147-173.

[6] *Liu, W.K., E.G. Karpov, and et. al.*, **An introduction to computational nanomechanics and materials**, Computer Methods in Applied Mechanics and Engineering. 193 (2004) 1529-1578.

[7] *Khare R, Mielke SL, Paci JT, Zhang SL, Ballarini R, Schatz GC, Belytschko T,* **Coupled quantum mechanical/molecular mechanical modeling of the fracture of defective carbon nanotubes and graphene sheets**, Physical Review B. 75 (7) (2007) Art. No. 075412.

[8] **National Nanotechnology Initiative**. Supplement to the President's FY 2004 Budget. National Science and Technology Council Committee on Technology.

[9] *J. Bezdek*, **Fuzzy Models-What Are They, and Why?**, IEEE Trans. Fuzzy Sys., 1, 1-5 (1993)

[10] *Avron Barr (Author), Paul R. Cohen (Author), Edward A. Feigenbaum (Editor).* **The Handbook of Artificial Intelligence**, Volume IV (Paperback), Addison-Wesley (C) (January 1990).

[11] Fortune Magazine, October 5, 1981.

[12] Private communications

[13] *Terada, K. and N. Kikuchi,* **Nonlinear homogeniza-tion method for practical applications**, in Computa-tional Methods in Micromechanics, S. Ghosh and M. Ostoja-Starzewski, Editors. 1995, ASME. p. 1-16.

[14] *Fish, J., K. Shek, M. Pandheeradi, and M.S. Shephard*, **Computational Plasticity for Composite Structures Based on Mathematical Homogenization: Theory and Practice.** Computer Methods in Applied Mechanics and Engineering, 1997. 148: p. 53-73.

[15] *Kouznetsova, V., W.-A. Brekelmans, and F.P.-T. Baaijens*, **An approach to micro-macro modeling of heterogeneous materials.** Computational Mechanics, 2001. 27: p. 37-48

[16] *Yuan, Z. and J. Fish,* **Towards Realization of Computational Homogenization in Practice**. International Journal for Numerical Methods in Engineering, 2007. in print

[17] *Ghosh, S., K. Lee, and S. Moorthy*, **Two scale analysis of heterogeneous elasticplastic materials with as-ymptotic homogenization and Voronoi cell finite ele-ment model.** Computer Methods in Applied Mechan-ics and Engineering, 1996. 132: p. 63-116

[18] *Oskay, C. and J. Fish*, **Eigendeformation-Based Reduced Order Homogenization**. Computer Methods in Applied Mechanics and Engineering, 2007. 196: p. 1216-1243

[19] *Mura, T.*, **Micromechanics of Defects in Solids**. 1987, Dordrecht: Martinus Nijhoff

[20] *Botkin, M., N. Johnos, E. Zywicz, and S. Simunovic*, **Crashworthiness Simulation of Composite Automotive Structures**, in Proceedings of 13th Annual Engineer-ing Soc. of Adv. Comp. Technology. 1988: Detroit.

[21] *Kumar, R., W.M. Cross, L. Kjerengtroen, and J.J. Kellar*, **Fiber Bias in Nanoindentation of Polymer Matrix Composites**. Composite Interfaces, 2004. 11(5/6): p. 431-440.

[22] *J. Fish, W. Chen, R. Li*, **"Generalized mathematical homogenization of atomistic media at finite temperatures in three dimensions,"** Comp. Meth. Appl. Mech. Engng., Vol. 196, pp. 908-922, (2007)

[23] *A. Li, R. Li and J. Fish*, **"Generalized Mathematical Homogenization: From Theory to Practice,"** to appear in Comp. Meth. Appl. Mech. Engng. (2007).

[24] *H. Waisman and J. Fish*, **"Space-time multigrid method for molecular dynamics simulations,"** Comp. Meth. Appl. Mech. Engng., Volume 195, Issues 44-47, pp. 6542-6559, (2006)

[25] http://msec.rpi.edu/

[26] *Feynman, R.P.,* **There's Plenty of Room at the Bottomt** in 29th Annual Meeting of the American Physical So-ciety. 1959: California Institute of Technology.

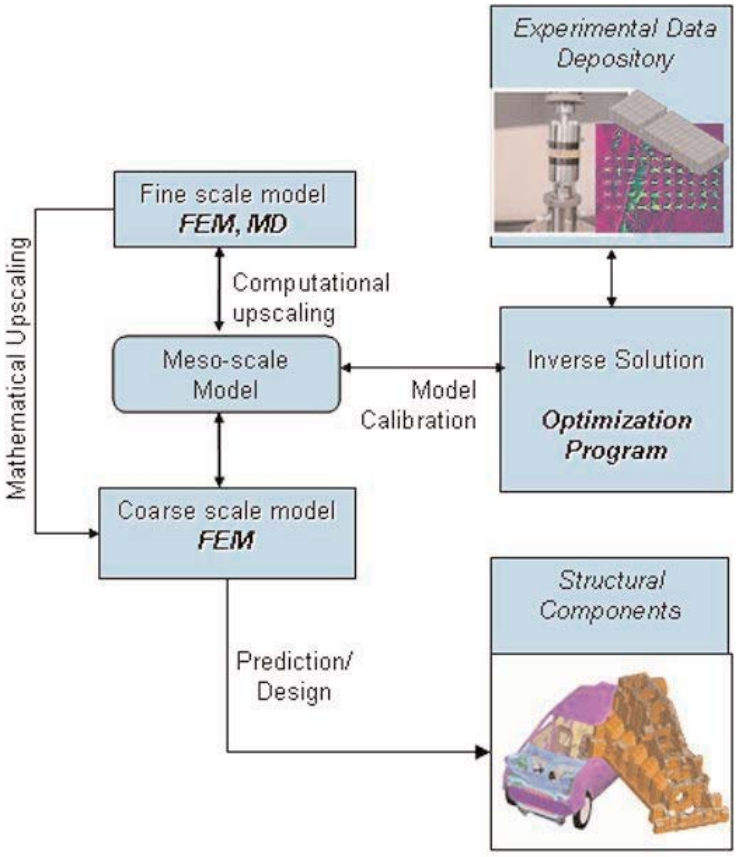

Figure 3: *A prototype of MDS developed at Rensselaer*