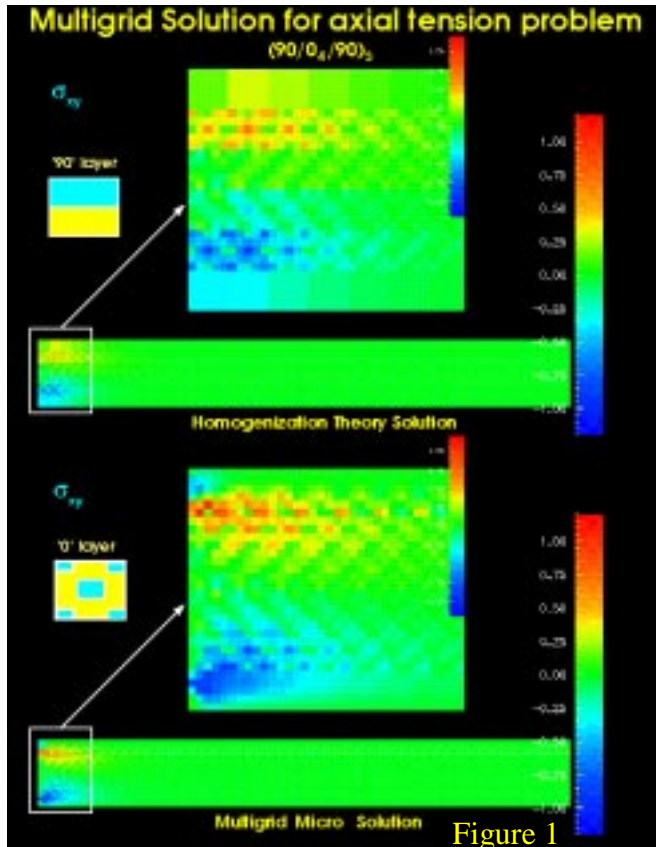


# HOLISTIC APPROACH FOR PROBLEMS IN HETEROGENEOUS MEDIA

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In analyzing composite structures it is common practice to carry out distinct levels of analysis corresponding to different length scales: (i) macroscale (structural level), (ii) mesoscale (laminate level), and (iii) microscale (the level of microconstituents). On the structural level structural components are treated discretely, while individual plies are not recognized, except in determining the stiffness of the shell. On the laminate level, individual plies are treated discretely, while microconstituents are treated collectively as a homogenized medium. The ply properties can be determined experimentally, or they can be predicted from micromechanics. For micromechanical analysis individual phases (matrix, fiber and their interphases) are treated discretely, while the atomic scale is not recognized. These steps comprise a sequence of interdependent analyses in the sense that the output from one level is used as input to the next level, where constitutive laws serve as bridging mechanisms between the scales. It is important to note that any level of analysis is

currently performed totally independent of others provided that the required input data is available, perhaps from the experiment. There is no doubt, that this approach reflects a compromise aimed at bridging the length scales in excess of six orders of magnitude. The obvious question arises as to the validity limits of such a step-by-step procedure. Let us examine, if there is a need for a coupled approach that will consider phenomena simultaneously at several different scales? And if the answer is positive, is the current status of software and hardware tools mature enough for such coupled multiscale considerations?

Let us first address the first issue. Figure 1 depicts the shear stress distribution in the axial tension problem in a  $(90/0_4/90)_s$  laminate. Results are shown for one quarter of the plate cross section in the  $xy$  plane. The lines of symmetry are at the bottom and on the right hand side of the cross section. The uniform tension load is applied normal to the  $xy$  plane. The zoomed area of shear stress distribution in the close vicinity to the free edge is also shown.

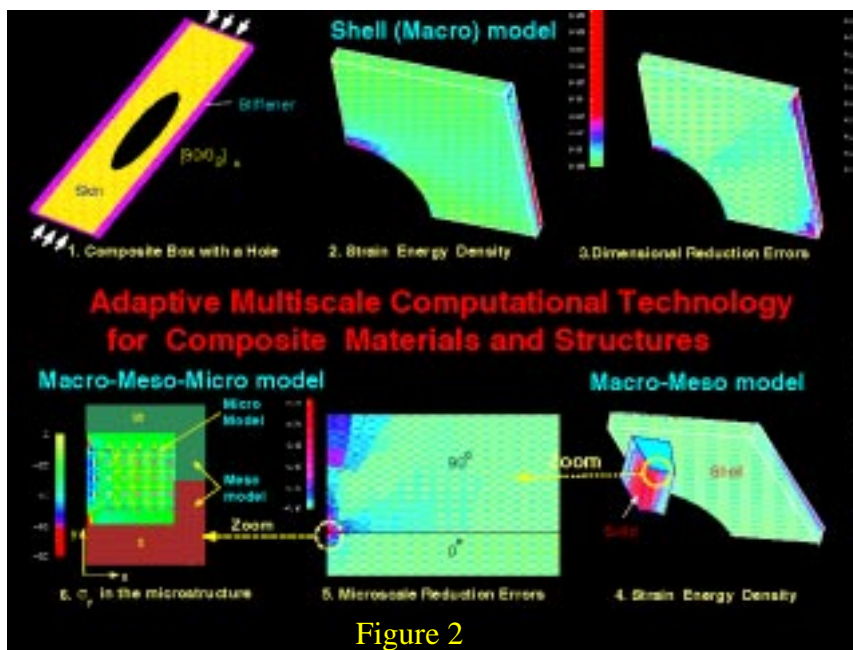
Results of the classical step-by-step procedure based on the homogenization theory are compared to the reference solution where the size of finite elements is of the same order of magnitude as that of material heterogeneity. It can be seen that a classical step-by-step procedure predicts accurate shear

stress distribution except for the close vicinity to the free edge, where it significantly underestimates maximum stress values, and along the entire interface between the two dissimilar layers. The reference solution shows oscillatory shear stresses developed along the entire interface, while the solution based on the classical step-by-step approach shows no such stress concentration. The magnitude of these oscillatory shear stresses is roughly 1/3 of the maximum shear stresses developed at the interface, but even so, these interface shear stresses may significantly affect the propagation of the delamination crack emanating from the free edge.

The coupling between the scales is even more profound in woven or textile composites. A typical unit cell size for a woven microstructure ranges from 3mm for plane weaves to more than 10mm for 3D woven composites. Thus the unit cell size for textile or woven composites could be of the same order of magnitude as the small geometrical feature, such holes and cutouts, in the macrostructure.

Recent theoretical and numerical studies conducted at Rensselaer ([2], see also [8]) have shown that in the areas of high gradients, primarily developed in the boundary layers at free edges and interfaces, the classical uncoupled step-by-step procedure may lead to poor predictions of local fields, since it assumes uniformity of macroscopic fields over the unit cell domain.

The simulation of the evolution of failure processes in heterogeneous media poses an even greater obstacle to the classical step-by-step approach. Reliable simulations of failure processes in heterogeneous media emanating from the smallest scale, such as microvoid nucleation at a particle-matrix interface, and followed by their coalescence and structural failure, require revitalization of classical bridging mechanisms between various modeling levels.



With the substantial increase in computing power and advances in computational technology, it is now feasible to use more sophisticated mathematical models and more refined discrete models, which would be able to account for close interaction between several different scales. In devising such an optimal computational model, it is appropriate to recall the statement made by Einstein, “*The model used should be the simplest one possible, but not simpler.*” The approach described in this article advocates to start from a *simpler* model perhaps based on the

classical step-by-step approach, which may or may not adequately simulate the response, and then adaptively refine both the mathematical and numerical models to permit coupled multiscale considerations, whenever and wherever these are needed, until the *simplest possible model* is obtained. We will refer to such a modeling strategy as the *holistic approach* to emphasize the coupled interaction between the modeling levels.

To address the question regarding the maturity of existing hardware and software tools needed for such holistic considerations, we demonstrate the application of the holistic approach by analyzing a typical aerospace component as shown in Figure 2.

The adaptive strategy starts by employing classical *Discretization Error* indicators and adaptively refining the finite element mesh on the macromechanical (shell) level to ensure accurate Macro-solutions. Subsequently, *Dimensional Reduction Error* ([1], [6], [7]) indicators identify the areas where the most critical interlaminar behavior takes place, and consequently, a more sophisticated discrete layer model is placed there. Fast iterative solvers based on the multigrid technology with special inter-scale connection operators [3], [4] are used to solve a coupled two-scale Macro-Meso model. Once the phenomena of interest on the Macro-Meso levels have been accurately resolved, *Microscale Reduction Error* ([2], [8]) indicators are used to identify the location of critical microprocesses and consequently, a micro-mesh is placed there. The three-scale coupled Macro-Meso-Micro model is again solved using a three-scale multigrid process [3]. Finally, *Discretization Error* indicators and adaptive refinement strategy are employed simultaneously at three different scales to ensure reliable multiscale simulations.

The three-scale model described in Figure 2 contains over 1,000,000 degrees-of-freedom. The estimated CPU time for solving it with conventional solvers based on skyline storage is over 700 hours on a single processor SPARCstation 10/51, which essentially makes the model obsolete from the practical point of view. Using a special purpose multigrid technology for heterogeneous media [3], the same problem has been solved in less than 16 hours on a single processor SPARCstation 10/51, turning it into a practically an overnight job.

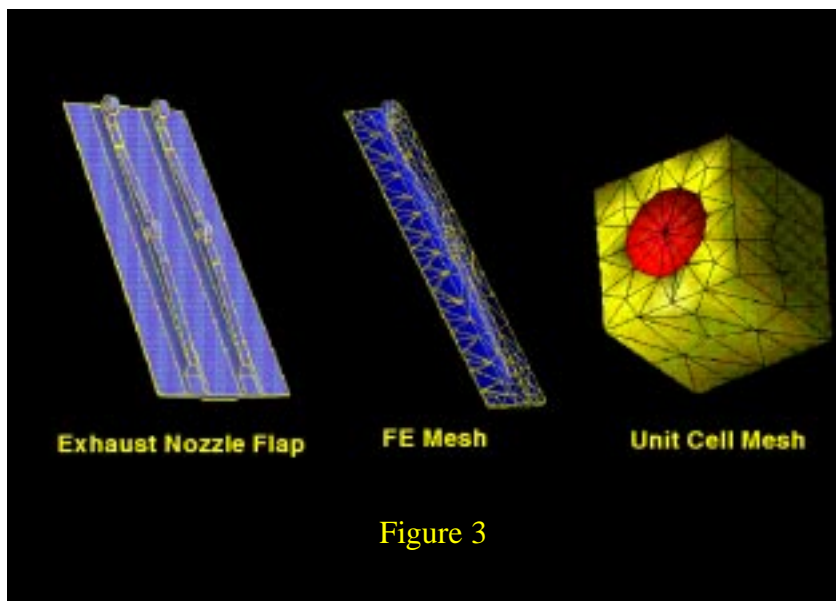


Figure 3

The computational challenge of solving nonlinear heterogeneous systems is even greater. The solution of large scale history-dependent nonlinear systems that provides an accurate resolution of local fields is not feasible even by means of the classical uncoupled step-by-step approach. While for linear problems a unit cell problem has to be solved only once, for nonlinear history dependent systems it has to be solved at every increment and for each integration point. Moreover, history data has to be updated at a number of inte-

gration points equal to the product of integration points at all modeling scales considered. To illustrate the computational complexity involved we consider elasto-plastic analysis of the two-scale composite flap problem shown in Figure 3. The macrostructure is discretized with 788 tetrahedral elements (993 unknowns), whereas microstructure is discretized with 98 elements in fiber domain and 253 elements in the matrix domain. The CPU time on SPARC 10/51 for this problem is approximately 8 hours, as opposed to 10 seconds if metal plasticity is used instead, which means that 99.7% of CPU time is spent on constitutive equations. This raises the question whether the observation made by Hill 30 years earlier stating that "... for nonlinear systems the computations needed to establish any constitutive law are formidable indeed..." is still valid today.

Recently, a novel modeling scheme based on mathematical homogenization theory with eigenstrains [5] and a rapid postprocessing procedure enabled to solve large scale structural systems in heterogeneous media at a cost comparable to problems in homogeneous media without significantly compromising on solution accuracy. This work [5] represents a major breakthrough in the realm,

where modeling schemes are either too simple to provide reliable solutions for difficult problems or too complex due to the computational complexity involved.

In the next few paragraphs I will briefly summarize essential features of the holistic approach, including: (i) idealization error estimators aimed at quantifying the quality of numerical and mathematical models in heterogeneous media and steering construction of the multiscale computational models, (ii) multigrid technology with mechanism-based inter-scale transfer operators aimed at super-convergent solution of the multiscale computational models, (iii) mathematical homogenization theory with eigenstrains and rapid postprocessing scheme with variational history recovery, and (iv) system identification for in-situ characterization of phases and their interfaces. Discussion on limitations of the present approach and future research directions conclude this note.

### **Idealization error estimators**

Idealization error estimators for laminated composite shell structures are aimed to quantify two sources of modeling errors and to address the following issues:

i. What are the regions within the problem domain where the macromechanical description (shell model), which is the most inexpensive modeling capability, is insufficient, i.e., where the shell model introduces unacceptable errors with respect to a more comprehensive ply-by-ply (mesomechanical) model. Dimensional Reduction error (DRE) estimators should be able to identify not only the precise location within the plane of the shell, but also the layers within the laminate where the use of mesomechanical description may result in unacceptable errors of interlaminar stresses.

One such approach [1] is based on approximation of the dimensional reduction error as a linear combination of Co functions in the auxiliary *mesomechanical* finite element mesh which can accurately represent the kinematics of individual plies. For other approaches see [6] and [7].

ii. Enriching the fundamental kinematics of the equivalent single-layer (macro) model with a discrete-layer (meso) model in the vicinity of the most critical layers enables to model various failure modes on the lamina level such as delamination. Unfortunately, in many cases the mechanism that causes failure is at a much smaller scale - the scale of microconstituents. A common computational rationale today is to investigate various microprocesses that may lead to a progressive failure by considering a unit cell or a representative volume problem. The mechanisms that allow us to do so are the classical assumptions of periodicity and uniformity of macroscopic fields. However, in the areas of high stress concentration, which are of critical interest to the analyst, periodicity assumptions are not valid, and thus the application of conventional homogenization techniques in the “hot spots” may lead to poor predictions of local fields.

The adequacy (or lack of it) of the homogenization theory can be assessed on the basis of the uniform validity of n-scale asymptotic expansion [2], which serves as a basis of the mathematical homogenization theory. The asymptotic expansion is considered to be uniformly valid if the terms in the asymptotic sequence are rapidly decreasing. Thus, the quality of the homogenization can be assessed on the basis of the relative magnitude of the first term neglected by the classical theory compared to those taken into account. An alternative approach has been developed in [8].

A closed form expression of idealization error estimators associated with the Microscale Reduction [2] shows that there are four major factors affecting the homogenization errors: (i) The size of the unit cell, (ii) the Dundars mismatch parameter between the phases, (iii) the volume fraction, (iv) the strain gradients on the macro-scale.



## Mathematical homogenization theory with eigenstrains and rapid postprocessing scheme with variational history recovery

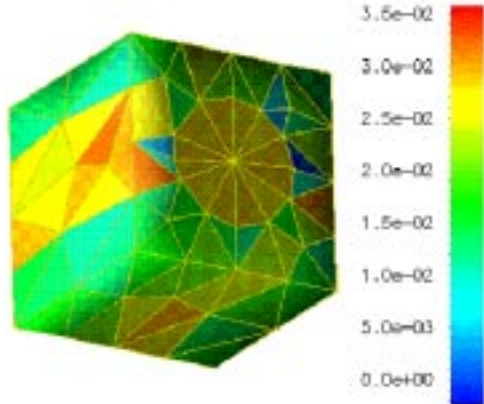


Figure 4

In reference [5] the classical mathematical homogenization theory for heterogeneous medium has been generalized to account for eigenstrains. Starting from the double scale asymptotic expansion for displacements and eigenstrains a close form expression relating arbitrary eigenstrains to the mechanical fields in the phases has been derived. Subsequently, the overall structural response is computed using averaging scheme by which phase concentration factors are computed in the average sense for each phase, i.e. history data is updated only at two/three points (fiber and matrix/ interphase) in the microstructure, one for each phase. Macroscopic history data is stored in

the data base and then subjected in the postprocessing stage onto the unit cell in the critical location identified by microscale reduction error indicators.

For the flap problem considered in Figure 3 the CPU time for the averaging scheme with variational micro-history recovery is only 30 seconds on SPARC 10/51 as opposed to 8 hours using classical mathematical homogenization theory. Figure 4 shows that the maximum error in the microstress in the unit cell located in the critical region is only 3% in comparison to the classical mathematical homogenization theory.

## Fast iterative solvers for a heterogeneous medium

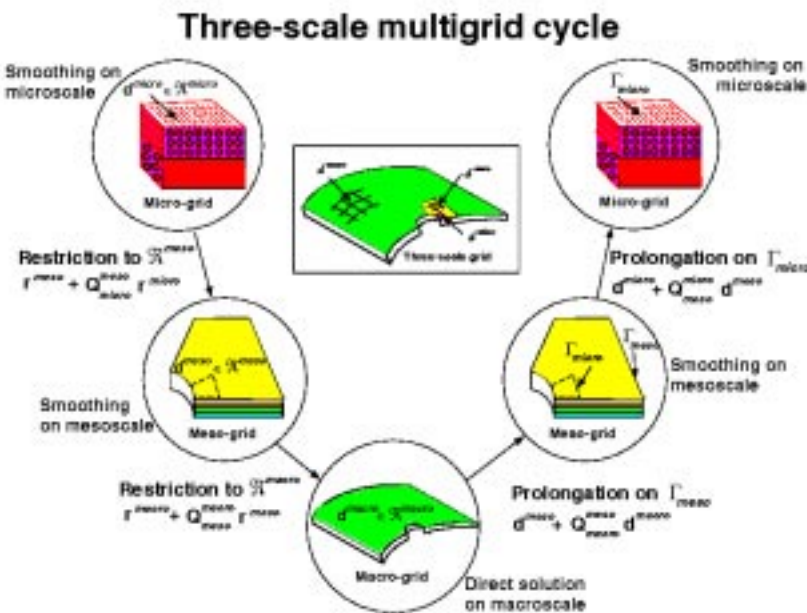


Figure 5

The multigrid technology with special inter-scale connection operators has been found to possess superconvergent characteristics for the periodic heterogeneous medium [3], [4]. The V-cycle with a minimum number of levels equal to the number of scales considered (Figure 5) starts by performing several smoothing iterations on the micro-scale in the regions identified by MRE indicators. Consequently, the higher frequency modes of error are damped out immediately. The remaining part of the solution error is smooth, and hence, can be effectively eliminated on the

auxiliary coarse mesh. It has been found [3], [4] that the finite element mesh on the meso-scale (ply level) serves as a perfect mechanism for capturing the lower frequency response on the micro-scale. Therefore, the residual in the finite element mesh on the micro-scale is restricted to the meso-scale,

while the smooth part of the solution is captured in the finite element mesh on the meso-scale. The oscillatory part of the solution on the meso-scale is again damped out by a smoothing procedure. The lower frequency response on the meso-scale is resolved on the macro-mesh (shell level). The resulting solution on the meso-scale is obtained by prolongating the solution from the macro-mesh back to the finite element mesh on the meso-scale and by adding the oscillatory part of the solution previously captured on the meso-scale. Likewise, the solution on the micro-scale is obtained by prolongating the smooth part of the solution from the meso-scale and by adding the oscillatory part that has been obtained by smoothing. This process is repeated until satisfactory accuracy is obtained.

The derivation of the inter-scale transfer operators is based on the asymptotic solution expansion. For unit cells of a finite size the regularization function was introduced in [3] to obtain a well-posed inter-scale transfer operators, termed as homogenization based operators. For nonlinear systems the inter-scale transfer operators vary both in time and space.

The rate of convergence of the multigrid process has been studied in [3]. It has been found that if the stiffness of a fiber is significantly higher than that of a matrix, then the multigrid method converges in a single iteration. This behavior of the multigrid method for heterogeneous media together with its *linear* dependence on the number of degrees-of-freedom, makes it possible to solve large scale coupled global-local problems with the same amount of computational effort, or faster, than would be required to solve the corresponding uncoupled problem using direct solvers.

A different iterative approach dealing with highly nonperiodic heterogeneous media has been recently developed in [11].

### **The inverse problem - indirect calibration of constitutive equations for the interface**

An essential characteristics of the holistic approach is the need for calibration of constitutive equations of the phases to the observed macro-measurements.

The set of nonlinear functions representing the evolution of damage laws can be parametrized in the space of inelastic deformation, such as effective plastic strain/work or the inelastic portion of the crack opening/sliding displacements. These parameters are viewed as control variables within the identification problem.

The inverse problem is solved incrementally. At each new load increment, a new set of control variables is introduced corresponding to the increased value of inelastic deformation. The previously determined control variables are not updated. Thus, each new load increment (or time step) contains only a limited number of control variables.

The inverse problem for estimating the control variables within a single load increment is formulated on the basis of the regularized least squares principle. In general, the inverse problem is ill posed due to the lack of balance between the amount of observed information and the unknown data. A Tikhonov regularization procedure can be employed by which a stabilization term is added to obtain a well-posed mathematical formulation.

For parameter identification in homogeneous viscoplastic materials see [9].

### **Future research directions**

The *holistic approach* for problems in heterogeneous media is still at its embryonic stage of development, limited to idealized scenarios, such as microstructure periodicity, perfect interfaces, and quasi-static loading conditions. Further research is essential to promote this methodology from the status of “interesting and having potential” to a practical analysis and design tool.

Other issues that have not been addressed in this article, and which undoubtedly have a tremendous impact in the area of modeling and simulation of heterogeneous materials and structures, are sum-

marized below:

i. Stochastic nature of data

So far only deterministic aspect of the holistic approach has been considered. The deterministic approach utilizes mean values associated with microstructural characteristics, fabrication and environmental effects. The uncertainties in input data pose a tremendous challenge not only because we have to deal with numerical methods for stochastic differential equations [12], but more importantly, because the probability fields especially the correlations are usually unknown.

ii. Atomic and electronic scale models

In the past we had a significant success in coupling phenomena at three different scales spanning the length scales in excess of six orders of magnitude. The grand challenge is to extend the present framework to account for atomic and electronic scales. Not only that there is a need for extending the range of length scales from 6 to 10-15 orders of magnitude, even more challenging is to couple models governed by continuum mechanics principles with models obeying molecular dynamics laws [10]. For example, how does the electronic scale phenomenon described only by the atomic numbers affects the motion of atoms, and how does it translates into the formation of crystallographic defects needed for continuum models. What are the regions in the problem domain where simultaneous consideration of particle and continuum models is required? See [10] and [14] for discussion on some of these issues. In [14] an uncoupled atomistic-continuum approach has been developed, where continuum mechanics based constitutive model was built directly from the atomistics. A fully coupled atomistic-continuum model, coupling the two scales via non-local transition region was discussed in [14].

iii. Multiple time scales

The difficulty of estimating the average behavior at the larger length scales from the essential physics at smaller scales is compounded in time dependent problems. For example, in turbulence, a time average or statistical approach is often employed to account for time fluctuations at very small continuum-based spatial level, whereas atomistic scale relaxation and vibration phenomena require consideration at even smaller time scales [13].

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