structural engineering

MODELING AND SIMULATION-BASED LIFE CYCLE ENGINEERING

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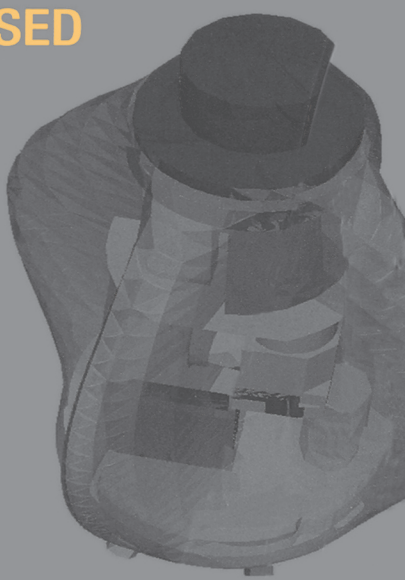

Modeling and Simulation-based Life Cycle Engineering

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Modeling and Simulation-based Life Cycle Engineering

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Contents

Preface

This book is a collection of Life Cycle Engineering [LCE] projects from the three-year collaborative research initiative between the National Science Foundation [NSF] and Sandia National Laboratories [Sandia]. Sandia has the responsibility for engineering systems that have profound impact on national security and defense, and helps to assure operability of other national systems, particularly under conditions of stress. This responsibility spans the "life cycle" of a variety of engineered systems, where "life cycle" for the system includes defining its requirements, establishing the concepts to meet the requirements, proposing designs, verifying that the design satisfies the requirements, manufacturing the system, operating and maintaining the system, and finally dismantling and disposing of the system.

With the advent of teraflop, massively parallel computers, Sandia is moving toward an engineering process in which decisions will increasingly be based on computational simulations with decreasing experimental validation. These simulations are of a magnitude unprecedented in computational size, scope of technical issues, spatial and temporal resolution, complexity in terms of coupled multiphysics phenomena, and comprehensiveness in terms of parameter-space that is being explored.

The NSF mission is to advance the fundamental science and engineering base of the United States, including a commitment to the further development of engineering processes using computer modeling and simulation. The two organizations have entered into a collaborative program to fund research projects that are focused on advancing the fundamental knowledge base needed to support advanced computer simulations.

The LCE grantees' meeting held at Albuquerque, NM in June 2001 provided an opportunity for researchers to present progress in research work and also provide a forum for the exchange of ideas. Sandia and NSF have been funding proposals that address modeling and simulation advances in several focus areas including Solid Mechanics, Thermal Transport and Engineering Design (which includes the sub-areas of Design Theory and Modeling and Simulation Uncertainty). Detailed information of the scope of each of the focus areas is given in the SCOPE AND INTRODUCTARY REMARKS. Researchers supported by NSF and Sandia, program managers from NSF and Sandia as well as contacts at Sandia attended

the meeting. This life-cycle engineering research effort is both world class and on track to meet national goals.

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Scope and Introductory Remarks

Ken P. Chong[1], Stefan Thynell[1], Harold S. Morgan[2] and George Hazelrigg[1]

INTRODUCTION

With the advent of teraflop, massively parallel computers, research is moving toward an engineering process in which decisions will increasingly be supported by computational simulations with decreasing experimental validation. Emerging, high fidelity simulations are of a magnitude unprecedented in computational size, scope of technical issues, spatial and temporal resolution, complexity in terms of coupled multiphysics phenomena, and comprehensiveness in terms of parameter-space that is being explored. However, the use of advanced simulations on teraflop computers, is impeded by an inadequate knowledge base. To expand this knowledge base, advances are required in the fundamental sciences and engineering that form the foundation of all computational analyses. Advances are needed in broad classes of technical development: the fidelity of the simulation models, experimental discovery necessary for the determination of the models and their validations, uncertainty quantification of the resulting computations, and computational techniques for the solution of the simulation models on high performance computing platforms. Sandia and NSF jointly have funded proposals that address these modeling and simulation advances in several focus areas: Solid Mechanics, Thermal Transport and Engineering Design (which includes the sub-areas of Design Theory and Modeling and Simulation Uncertainty). Detailed information of the scope of each of the focus areas is given below.

[1] National Science Foundation
[2] Sandia National Labs.

SOLID MECHANICS

This focus area seeks to improve and expand fundamental computational and material mechanics knowledge in the areas of nonlinear, large deformation, deterioration of materials, quasistatics and transient dynamics. The shift from a test-based to a simulation-based design environment requires accurate, robust and efficient computer codes which model large ranges of loadings, deformation amplitudes and rates, length- (including nano-, micro-, meso- and macro-scales) and time-scale mechanics, and damping of mechanical interfaces and joints. It seeks to develop a basic engineering understanding of numerical solution methods including finite elements, boundary elements, and gridless Lagrangian methods for challenging simulation problems such as in impact and penetration, thermomechanical aspects of material processing and manufacturing, crack initiation, propagation and arrest, design optimization and uncertainty analysis, including accurate constitutive description of materials. The solution algorithms must be robust, reliable, efficient, and scalable on parallel computing platforms. Carefully designed experimental investigations to validate and otherwise support the above technology areas are also needed.

THERMAL TRANSPORT

Thermal transport plays a central role in many engineering applications such as thermal control of engineering systems, manufacturing and materials processing, power conversion and storage, biological, and micro/quantum scale thermal/fluid processes. Because the analysis of the related thermal processes often requires excessive computing times, the thermal analysis and design of systems involving these processes are difficult. With the advent of teraflop computers, it is now possible to exploit high performance computing methodologies to address these issues, assuming that the models are accurate and correctly implemented. When analyzing existing systems, the models can be modified by comparison with data and the errors minimized, leading to an improved understanding of the process. However, when designing systems, if the conditions under which the model was validated differ from those associated with the design, errors can result. This focus area is particularly interested in proposals which emphasize the development of analytical and computational methods that represent critical thermal transport phenomena and processes with appropriate resolution, dimensionality, coupling with other physical processes, and diversity of length and time scales. Topics suitable for consideration

include, but are not limited to, convective heat transfer coupled with moving boundaries and possibly with participating media radiative heat transfer, interfacial heat transfer, phase change systems, interaction of heat transfer and material processing (such as crystallization, levitation, machining). The development and application of advanced experimental methods to better characterize critical thermal transport phenomena are also appropriate.

ENGINEERING DESIGN

There are new and emerging challenges that engineering designers face. Increasing and global competition demand that designs push limits of materials and processes, leaving less room for conservatism, and customers always want more for less. A fast-moving marketplace rapidly diminishes the value of new technologies, so that shortening the time from concept to market is increasingly important. On top of these demands, society also demands that new systems offer higher levels of safety and reliability, and lower environmental impact. These challenges have pushed conventional design approaches to their limits.

On the other hand computational capabilities are emerging that truly were inconceivable only a few years ago. Coupled with emerging models, such as finite element techniques, that represent engineered systems, these capabilities offer significant advantages. Computational design support tools enable the examination and comparison of wide ranges of design alternatives rapidly and inexpensively. The hope is that these tools will enable increased competitiveness in all the aspects noted above.

Still, despite the enormous power of computational models, they are far from perfect. All models are only abstractions of the realities that they are intended to represent. As such, the model-predicted performance of a system and the actual system performance will deviate at some level. When we use models to facilitate the understanding of nature, such deviations can be controlled and minimized. But in the case of design-support models, such control is not possible. The significant difference is that scientific models of nature are developed to fit extant data, whereas engineering design models are intended to predict future performance of systems. Studies of the inaccuracies in our ability to predict the behavior of engineered systems produce alarming results. Errors are considerable, and they cannot be controlled or minimized beyond modest limits. Thus, it is important to model the errors inherent in engineering design models and to develop a framework that will accommodate and use probabilistic results.

Recently, a framework has emerged that provides the capability to make use of probabilistic information in the context of engineering design. It is a decision

theoretic framework. Under this framework, the role of decision making in engineering design is explicitly recognized. As such, three subactivities of the design process are recognized: (1) the generation of a set of design alternatives from which the preferred design will be chosen, (2) the estimation of expectations, that is, the performance expected from each design choice, and (3) the determination of human values relevant to the design and the use of these values to effect the selection of a preferred design. Much of an axiomatic base for decision-based design has been laid in the fields of mathematics and economics. For example, the von Neumann-Morgenstern axioms define a mathematics of value valid under conditions of risk and uncertainty that appear to apply to engineering design. And probability theory appears to provide a framework for analysis of uncertainty and risk.

Research in Engineering Design has been supported in two topical areas:

Design Theory

Proposals in this focus area of Design Theory were judged in terms of their ability/potential to provide sweeping theories that would cover and regularize wide ranges of engineering design. Under this activity, research has been supported to create and/or implement an axiomatic basis for engineering design. One acceptable approach would be to build upon the concept of decision-based design and the axioms that define von Neumann-Morgenstern utility. However, other rigorous approaches have also been entertained. There is a need for a theory of value applicable to design decision-making under conditions of uncertainty and risk. There is a need for a theory for the estimation of system performance given imperfect ability to perform system modeling, imperfect estimation of model data, and imperfect knowledge of the future environment within which engineered systems must operate. And there is a need for a theory of option creation or creativity. The first such theory may already exist primarily within the fields of economics and decision theory. The second is likely find a basis in the mathematics of probability theory and forecasting. The third is more speculative, and progress in this area is likely to be difficult.

Modeling and Simulation Uncertainty

Proposals in this focus area of Modeling and Simulation Uncertainty were judged in terms of their ability/potential to provide general approaches to, and new theories for, uncertainty estimation in modeling and simulation-based design. The goal of the uncertainty estimation methodology is to understand the

impact of uncertainties on modeling and numerical simulation activities and thereby increase the confidence in decision-based design methods.

Present design methodology for engineered systems is based on incremental changes and improvements of previously successful designs. In addition, present design practice relies heavily on extensive testing of components, subsystems and prototype systems. With rapidly increasing computational capability, modeling and simulation based design is taking on increased responsibility for the success of new engineering systems. This is a fundamental paradigm shift; one whose risks and uncertainties must be assessed during the design process. This research activity addresses fundamental issues relating to the inclusion of quantitative estimation of uncertainty in mathematical modeling and computational simulation and the ascription of uncertainty to model and data elements. It complements the above mentioned research in design theory. All sources of uncertainty and error may be considered. Furthermore, techniques are sought that incorporate uncertainty quantification in the development of constitutive models for stochastic or uncertain subsystems. A variety of methods are sought to estimate the global impact of uncertainty/error sources on confidence in a design.

SCOPE

This book is a collection of Life Cycle Engineering [LCE] projects from the three-year collaborative research initiative between the National Science Foundation and Sandia National Laboratories. It addresses the LCE modeling and simulation advances in the focus areas of Solid Mechanics, Thermal Transport and Engineering Design (which includes the sub-areas of Design Theory and Modeling and Simulation Uncertainty) as described above.

Research Needs

Sunil Saigal[1], Ken P. Chong[2] and Harold S. Morgan[3]

The research needs session was chaired by the three authors listed above. The observations below are based on the contributions made by several authors in this book during the workshop as well as in written communications afterwards. The following is a summary of the discussions.

1. JOINT EFFORTS TOWARDS GRAND CHALLENGES

It was proposed that joint university/government/industry efforts are needed towards developing and validating computational models of complex mechanical phenomena, such as multi-scale problems, fracture, laminar-turbulent transition, etc.

Many of the engineering challenges that remain to be addressed are complex problems. Industry has found work-arounds to our imperfect understanding, but these work-arounds add cost and risk and limit design flexibility. Government laboratories are usually better funded to achieve a better understanding of the physics of these problems, but have still been limited to the use of empirical or semi-empirical work-arounds, which involve similar costs. Universities are well-placed to work on the fundamental mechanics of these challenges, but are rarely in a position to understand what portions of the complex problems are the most important and would allow practical design improvements. Thus, universities all too often work on scientifically interesting problems with less-than-optimal payoffs, and government and industry continue to be saddled with limited empirical work-arounds to complex problems.

The tremendous advances in computing power that have occurred over the last several decades have enabled the development of complex computational algorithms that could permit much improved solutions to these challenging problems. However, even with this greatly increased power, practical codes will still require many simplifying assumptions, especially for design. The predictions can be improved by creating codes that simulate the actual physical mechanisms. It needs to be determined which mechanisms need be simulated and to what level of accuracy? Improving these simulations will require close cooperation among computational, theoretical, and experimental researchers and engineers.

Efficient progress towards these improved simulations will require cooperation between industry, government, and universities. Industry can supply an understanding of the critical design issues and the critical limitations of existing prediction methods. Government agencies can also supply an understanding of design issues, usually with a better feel for how improved

[1] Carnegie Mellon University
[2] National Science Foundation
[3] Sandia National Labs.

simulations might change the design process. Universities can focus their research on problems whose solution is more likely to impact real systems. A continuing technical dialogue and interaction among these three groups is needed to make efficient progress, and to make the continuing case for funding research in these challenging problems.

2. MULTISCALE MODELING

The notion of multiscale material modeling has attracted much attention over the past decade. Several approaches exist: (i) the use of atomistic or discrete dislocation calculations to extract parameters used in macroscopic, phenomenological material models. (ii) quasicontinuum methods to span length scales from atoms to the continuum. (iii) Purely numerical approaches, such as meshless methods, to resolve fine scale fields. A fourth approach that is now gaining in importance is the notion of embedding fine scale theories in coarse scale ones. The fine scale theories of interest could include: (i) continuum formulations that resolve mechanics phenomena at length scales in the sub-micron to nanometer range such as the recently proposed strain gradient plasticity theories, and (ii) microforce theories. These theories are often applied to boundary value problems at length scales in the sub-micron to nanometer range. However there is a growing interest in applying them to phenomena such as microvoiding, microcracking, microscopic shear band formation, problems involving inclusions and internal surfaces, grain evolution and texture evolution in macroscopic bodies. Some of these fine scale theories analytically attain the proper response in the limit of macroscopic deformations. However, caution must be exercised in actually solving initial and boundary value problems on macroscopic dimensions (say, meters) with these theories. With any numerical method, the range of discretization will span from nanometers to centimeters or meters. This would be highly expensive, inefficient and possibly non-robust.

One alternative is to develop mathematical techniques for embedding the fine scale theories in coarser-scaled formulations. For instance strain gradient theories at the sub-micron scale might be embedded in the classical macroscopic formulation. The coarse scale formulation is thereby modified to yield a multiscale one. The variational framework is particularly well-suited to such manipulations. They can also be applied to solving boundary value problems with microforce theories while maintaining the tight coupling between the micro and macro scales.

Nanotechnology is emerging as a key area of technology innovation for the 21st century, with the hope of achieving unparalleled improvement on the standard of living of mankind. This technology hinges upon efficient and reliable nanoscale modeling and simulation methods which effectively link continuum and atomistic models to nanoscale material behaviors. It is critical to develop a novel and practical methodology combining the best features of continuum theory and atomistic simulations. As a widely used experiment for probing nanoscale mechanical properties, nanoindentation can be chosen as a focal point of study for the development and validation of the proposed methodology.

The combined continuum/atomistic methods will have high academic and industrial impact on the current pursuit of nanotechnology because of its unique methodology for predicting nanoscale mechanical properties. To continue the trend and advances indicated by the Moore's Law, the next generation of semiconductor technology will be built at the nanometer scale. The capability of predicting mechanical properties of the materials at this scale offers critical information for the designer of devices to select materials and processing techniques. The framework of continuum-atomistic linkage will have far-reaching significance in nanoscale engineering analysis.

3. FAILURE OF STRUCTURES

Failure of structures is often associated with fracture or fatigue of one or more of the elements. In the field of micro- and nano-structures, failure has numerous other manifestations. For example, micro-electro-mechanical systems (MEMS) exhibit large surface area to volume ratios. When two surfaces are brought together, the natural attraction between them, perhaps due to condensed water vapor or even van der Waal's forces, can be sufficient to overcome the relatively small restoring forces inherent in the structures. When this happens, the surfaces stick together and the MEMS has failed. A thorough understanding of this cohesion in MEMS is not available, depending upon a variety of fields, including tribology, materials science, surface chemistry and engineering.

A number of other failure modes have been observed in the mechanical elements of MEMS. Wear debris or other foreign particles entering the small gaps between components can cause the moving parts to seize. Thermally-induced or stress-induced warping of beams or plates can be quite large causing these elements to be well out of alignment with other elements of the system.

Failure of a system can also be identified as its inability to perform within the range for which it was designed. Many MEMS involve resonant structures. Uncertainties in fabrication parameters can lead to uncertain material and geometric properties, which in turn lead to uncertain response.

This variability suggests that the range of system response needs to be considered in assessing the success rate or yield of a particular process.

4. UNCERTAINTY ANALYSIS AND DESIGN CONSIDERATIONS

The research projects in the current Sandia/NSF Life Cycle Engineering program have dealt separately with advanced computational mechanics methods and uncertainty propagation methods. Most the advanced computational mechanics research has been done under deterministic assumptions, whereas the uncertainty analysis research has used simple mechanics models. The next step is to integrate the advances in these two directions. This presents new challenges in computational implementation, scale-up and efficiency. Advances in both directions have led to methods that are computationally intensive. Simple wrapping of uncertainty analysis methods around deterministic mechanics

analysis may not be efficient. The implementation will need to include parallel computing and other new computational science paradigms.

Propagation of uncertainty information through advanced computational mechanics models requires the development of new methods. Monte Carlo and response surface methods may be either too expensive or too approximate, since high-fidelity mechanics computation itself is likely to be computationally intensive. Sensitivity-based analytical approximations have been constructed through stochastic finite element and stochastic boundary element methods. Similar uncertainty propagation methods need to be developed in concert with high-fidelity mechanics methods, such as stochastic mesh-free methods, stochastic cohesive element methods, etc.

One of the challenges in model-based uncertainty simulation is the quantification of modeling error. Some work has been done to quantify the discretization error in traditional finite element analysis. Similar work is needed in the context of high-fidelity computational mechanics models, for example, mesh-free methods, methods using cohesive elements etc. Within uncertainty analysis, attempts have been made to treat computational approximations, biases, and errors as random variables; these approaches have not been entirely satisfactory and may require extensive (and expensive) calibration effort. Therefore, new efforts are needed for comprehensive characterization of model uncertainty, especially in the context of integration of advanced computational mechanics and uncertainty analysis methods. These efforts should also lead to rational approaches for the validation and acceptance/rejection of integrated models for large systems.

The use of advanced methods also presents new data requirements. Consider a simple example --- material property data for stress analysis of a beam. An isotropic strength of materials approach only requires one Young's modulus. An anisotropic linear finite element analysis requires moduli in several directions. A nonlinear analysis requires more comprehensive load-deformation data. An uncertainty analysis requires statistical data on the material properties. Thus the data requirements are different for different levels of analysis. Therefore, the integration of advanced methods will be affected by data limitations and information uncertainty. Comprehensive uncertainty quantification needs to include and develop methods to handle various types of information uncertainty.

Most of the research in the LCE effort has concentrated on developing advanced *analysis* techniques, both deterministic and non-deterministic. The next step is to develop design and life cycle management approaches that incorporate these techniques. There is a considerable gap between advances in analysis and design approaches for engineering systems. Engineering design is still mostly done using traditional deterministic analysis with simple system models calibrated with experience and design safety margins, without incorporating many of the advances in computational mechanics or uncertainty propagation. As model-based simulation gains ground for large and complex systems, the design approaches for such systems will need to incorporate these advances. Only then will the significant progress made in the LCE effort be fruitful. Therefore, new design approaches need to be developed using integrated high-fidelity computational mechanics and uncertainty analysis. Further, these approaches need to be implemented and demonstrated for *realistic systems*, in order to facilitate acceptance by the engineering community.

5. AGING AND LONG-TERM BEHAVIOR

For a large number of engineering components accumulation of damage occurs under cyclic loads far below loading conditions that would lead to instantaneous catastrophic failure. The development of modeling and simulation tools capturing the evolution of these incrementally deteriorating events is obviously essential if the entire life cycle of engineering components is to be predicted.

In the investigation of highly critical components, it is indispensable to account for the nucleation, and subsequent propagation of crack like defects. Essentially all currently available methodologies to analyze such problems are based on empirical laws, e.g. the Basquin or the Coffin-Manson Laws for crack initiation, or the Paris Law for crack propagation. While these equations are widely used, it is important to recall that they provide data correlation schemes rather than predictive capabilities. As an example, current fatigue crack growth methodologies encounter limits of applicability if small-scale yielding assumptions are not valid any longer such as at interfaces, or in layered materials, or if short cracks are of concern. No generally accepted methods exist in which crack initiation and subsequent growth - e.g. from sharp corners and intersections of interfaces with free surfaces - can be analyzed in a unified framework. To overcome these limitations, several attempts were made in the past to establish micromechanical models for fatigue failure. However, past models commonly are based on strongly simplifying assumptions, and did not take advantage either of recent advances in constitutive description of materials, or of the current state of computational tools in solid mechanics.

The main challenge in the advancement of fatigue failure is the development of the description of material separation under cyclic loading, and the determination of the associated material parameters. In an ideal world one would like to be able to predict the response of a specimen to cyclic loads from simulations on the atomistic level. For real engineering components under cyclic loading this seems to remain an elusive goal for some time to come. It seems more realistic to describe the micromechanisms of material separation processes at the crack tip by the use of appropriate constitutive models embedded in a continuum framework. Crack initiation, growth and arrest should then be computed without external interference of the analyst and depend solely on the definition of constitutive framework. To accomplish such an approach, additional and novel experimental input is needed to determine the cyclic material deterioration locally at the crack tip, and developments in computational mechanics are required to enable computations spanning the time scale of the individual damage event to the final time to failure of a component.

While the development of predictive models for aging and long-term behavior of materials and components remains, by itself, a high research priority, this development can be greatly enhanced by leveraging new technologies in information and computation, and by incorporating models into a system-level design and decision-making framework. More details are given in the following.

Synthesis of computational models with laboratory and field data

Advances in computational methods have resulted in impressive high-resolution models of materials. To make these models more useful in life-cycle engineering, however, it is necessary to provide high-resolution information on the parameters of the models. Such parameters describe spatial material properties including the distribution of initial flaws, geometrical properties, load processes arising from system operation and natural and man-made hazards, and degradation processes within the material or system. A research challenge is in developing appropriate experimental programs in the laboratory and field that would provide the type of data needed to quantify and calibrate these parameters. Since it is not possible to develop sensors to exhaustively measure the full set of high-resolution parameters inherent in the computational models, an inferential process may be needed. Such inferential processes would use a reduced set of parameters to effectively link laboratory and field experiments with high-resolution computational models.

Interface with information technology

With the rise of large-scale applications of information technology to engineering problems, such as that envisioned in the NSF-funded NEES network, there is a research opportunity in effectively using such information to develop more accurate predictive models for long-term behavior. Statistical tools would have to be supplemented with data mining, fusion and other modern information extraction and processing techniques to be effective in this research effort.

Design under uncertainty within a decision-making framework

The uncertainties inherent in the aging and long-term behavior of the materials and components of a system make it impossible to provide precise predictions of life-cycle costs. Within an axiom-based design framework, the uncertainties could, in principle, be incorporated into an optimal design that minimizes life-cycle costs, including those associated with construction, maintenance, and field-data collection and processing. There are, however, open research problems that must be addressed to bring this design framework for life-cycle engineering to fruition. These research problems are associated with developing the utility functions appropriate for life-cycle engineering, searching efficiently within a high-dimensional design space, and incorporating predictive models with uncertain parameters into the decision-making processes at the construction and maintenance life-cycle phases.

6. POLYMERS AND ELASTOMERS

In the chapter *Life–Cycle and Durability Predictions of Elastomeric Components*, it was shown that the mechanical properties of a natural vulcanized rubber are altered (degraded) due to microstructural changes, namely the scission and re-cross linking of macromolecular network junctions, that occur at sufficiently high

temperatures. In most of the existing experimental studies of the consequences of these microstructural changes, the focus has been on uniaxial extensions. These studies form a solid foundation for the development of a model that can be used in numerical life–cycle and durability predictions for elastomeric components. Research is needed in the following topics in order to continue the development of the model. First, it is necessary to determine the consequence of microstructural changes at high temperatures on the response under biaxial and shear deformations. Second, there is a paucity of experimental results on heat transfer in elastomers, and how it is affected by large deformation and microstructural changes. Third, there have been few studies that document the development of 'hot spots' in typical elastomeric components, the degradation of properties in these 'hot spots' and their influence on component performance.

Most of the existing studies on the degradation of elastomers do not consider classical viscoelastic phenomena such as stress relaxation and creep. Yet, elastomers exhibit these properties. Indeed, the conversion of mechanical energy to heat due to viscoelastic effects contributes significantly to temperature rise. Polymeric solids are also composed of cross-linked networks of macromolecules, but are stiffer than elastomers. Their viscoelastic properties need to be considered in their applications. The events leading to degradation in elastomers can also be expected to occur in polymers and to alter their viscoelastic properties. Thus, another important research need is a study of the consequences of the scission and re-cross linking process on the viscoelastic response of elastomers and polymers.

An important related subject involves the solidification or curing of a polymeric liquid to form a polymeric solid. This occurs in fabrication processes such as the casting of elastomeric components, forming of epoxy based composite materials and encapsulation of microelectronic devices. During the curing process, macromolecules cross link to form networks as the liquid evolves into a solid. This process occurs continuously in time and depends on temperature. There are volume changes as the microstructure and constituents evolve. Stresses develop in the networks that depend on their viscoelasticity and the degree of cure. The spatial and temporal variation of the changes in volume, degree of cure, heat transfer and microstructure determine the final properties of the cured product as well as its residual stresses and dimensional stability. These, in turn, determine its life-cycle and durability properties. Extensive research is needed in the development of a model that can account for these factors.

In conclusion, elastomeric and polymeric components undergo microstructural changes that influence their life-cycle and durability properties. There is need for research into the development of models that can be used in numerical simulations to predict these properties.

7. MAPPING DISCRETE MODELS TO SYSTEM RESPONSE

With the exception of idealized, canonical cases, a model for a system is nearly always in discrete form. Intrinsic to each discrete model is a set of assumptions and approximations that are used in the model parameters, constitutive relations and computational procedure. Since the formulation of this set of assumptions and approximations is dependent on the modeller's point of view and on the available

computational resources, there are, conceptually, an infinite number of discrete models corresponding to each system. Furthermore, there is no "exact" discrete model due to the intrinsic approximations; it is even difficult to determine a "best" model since more than one criterion for ranking the accuracy or suitability of the models may be of relevance.

Given that a modeller has, at his or her disposal, a large collection of models or potential approaches to modelling, the general question is: Which model or subset of models should be used? To formulate this question into a research problem, the context must be well defined. The following issues are of interest: the impact of modelling errors in the context of system failure or inefficient design, the nature, availability and cost of laboratory or field data which may be needed to calibrate the models, the definition of an appropriate utility function that could be used to develop a well-defined ranking in relation to life-cycle or other relevant costs, and the propagation of parameter and model uncertainties that lead a modeller to rely on more than a single model to assess system performance. Central to this class of research problems is the relationship, or mapping between the collection of discrete models and the characteristics of the system response.

Part I

Solid and Structural Dynamics

Computational Cohesive Zone Modeling Of Polymer Interfacial Failure

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1. INTRODUCTION

Linear elastic fracture mechanics (LEFM), based on singular stress fields and energy release rates, has proven to be quite successful in describing fracture in brittle materials (Lawn 1993). A cohesive zone description of near-tip process zones emerged early in the development of the field (Dugdale, 1960, Barenblatt, 1962), but remained relatively unused in the treatment of brittle fracture. LEFM has also been used successfully under well-defined conditions for polymers (Williams, 1984). However, it becomes limited in its treatment for polymers that exhibit significant inelasticity, large deformations, and time-dependence. Analytical challenges make the cohesive zone approach relatively difficult to use, although it is fundamentally capable of handling these complications (Dugdale, 1960, Knauss, 1973, Schapery, 1975). Implementation of the cohesive zone approach in a computational context provides a means of analyzing previously intractable problems of materials failure in a way that connects local process zones with the macroscopic deformation. For these reasons, computational cohesive zone modeling has attracted attention for brittle & elastic-plastic materials (Xu & Needleman, 1994, Camacho & Ortiz, 1996, Tvergaard & Hutchinson, 1992, Espinosa *et al.*, 1998, and Needleman and Rosakis, 1999). Failure in polymers, which is often accompanied by time-dependent and large deformation, presents unique challenges for computational analysis. In this chapter we present an implementation of cohesive zones as cohesive finite elements for tackling issues in modeling polymer interfacial fracture.

The cohesive zone approach overcomes some of the limitations of the stress intensity factor and J-integral methods that form the basis of LEFM. It can provide a description of the different stages of material failure starting from initiation to macroscopic crack propagation, while accounting for energy balance. By specifying a local cohesive law, one is able to partition the macroscopic

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fracture resistance into its component parts, providing the sort of information important for materials design and understanding adhesion.

The examples presented in this chapter demonstrate the versatility of the computational implementation to describe crack propagation in hyperelastic/viscoelastic materials, crack "pop-in", dynamic crack propagation, and 3D geometries. Specifically, we present analyses of peel testing of elastomers (Rahul-Kumar *et al.*, 1999), adhesion measurement using a compressive shear test (Jagota *et al.* 1999, Rahulkumar *et al.*, 2000), and analysis of a through-cracked tension test (S. Muraldhar *et al.* 2000).

2. COHESIVE ZONE MODEL AND NUMERICAL IMPLEMENTATION

The cohesive zone model provides local tractions that oppose separation and relative sliding of crack faces. The model can represent various crack tip phenomena (Rahul-Kumar, 1999). In comparison to LEFM where, usually, fracture is tied to a single number (*e.g.*, K_c or G_c), the cohesive zone description of the process introduces an additional parameter. The work of separating the crack faces (per unit area) corresponds to G_c; the peak stress (or characteristic opening) experienced during separation is an additional descriptor of the failure process.

Specific choices of the cohesive law and parameters have to be dictated by the particular material and failure mechanism. Here we restrict ourselves to a finite element implementation of a phenomenological, rate-independent, cohesive zone model (Xu & Needleman, 1994). Figure 1 shows two bulk finite elements that share a common face. The cohesive element defines tractions acting across this face in terms of opening and sliding displacements: $\Delta_n, \Delta_{t1}, \Delta_{t2}$. Tractions typically vanish when this displacement vector is (0,0,0). The tractions are derived from a potential, $\phi(\Delta_n, \Delta_{t1}, \Delta_{t2})$ as:

$$T_n = -\partial\phi/\partial\Delta_n, T_{t1} = -\partial\phi/\partial\Delta_{t1}, T_{t2} = -\partial\phi/\partial\Delta_{t2} \qquad (1)$$

A reduced version of the Xu-Needleman (1994) potential is given as:

$$\phi(\Delta_n, \Delta_{t1}, \Delta_{t2}) = \Gamma_0\left[1-\left(1+\frac{\Delta_n}{\delta_{cr}}\right)\exp\left(-\frac{\Delta_n}{\delta_{cr}}\right)\right]\exp\left(-\frac{\Delta_{t1}^2+\Delta_{t2}^2}{\delta_{cr}^2}\right) \qquad (2)$$

where δ_{cr} is the characteristic critical opening displacement and Γ_0 is the fracture energy of the interface. In order to penalize interpenetration of cohesive surfaces under compression the potential in equation (1) is augmented by the term $[H(\Delta_n)-1]\kappa\Delta_n^3$, where $H(\Delta_n)$ is the Heaviside step function, and κ is a penalty parameter. This modification does not affect the work of interfacial separation as it operates only under compression. When modeling interfacial separation in three

dimensions, the crack front is identified as the locus of points along the interface where the combination of openings (Δ_n, Δ_{t1}, Δ_{t2}) satisfies the relationship:

$$\left[1-\left(1+\frac{\Delta_n}{\delta_{cr}}\right)\exp\left(-\frac{\Delta_n}{\delta_{cr}}\right)\right]\exp\left(-\frac{\Delta_{t1}^2+\Delta_{t2}^2}{\delta_{cr}^2}\right)=(1-2/e) \tag{3}$$

where, e is the Euler number exp(1). This identifies a locus of openings corresponding to identical work of separation. Under pure normal separation (Δ_{t1} = Δ_{t2} = 0) the work evaluates to (1-2/e)Γ_0, for $\Delta_n = \delta_{cr}$.

The numerical implementation of a cohesive zone model for interface fracture within an implicit finite element framework is accomplished using cohesive elements. Element nodal displacements define the kinematics of deformation. Cohesive element nodes are shared with neighboring bulk finite elements that model the continuum (Figure 1). Therefore, a damage process described by a specific type of cohesive element is coupled to the deformation occurring in the bulk material.

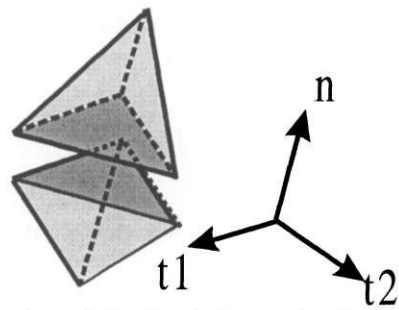

Figure 1. Schematic drawing of the local frame of reference used to define cohesive element tractions and stiffness

If cohesive tractions are given by $\{T\}=\{T_{t1}\ T_{t2}\ T_n\}^T$, finite element nodal forces can be computed as:

$$\{F\}=\int_{S_0}[Q]^T[A]^T\{T\}dS_0 \tag{4}$$

where, S_0 is the initial cohesive surface defined as the mid-plane between the two faces of the cohesive element. Matrix [Q] rotates the force vector from coordinates local to the cohesive surface to global coordinates, and [A] is a matrix of element interpolation functions that relates opening displacements $\{U\}^T=\{\Delta_n,\Delta_{t1},\Delta_{t2}\}^T$ to current nodal coordinates $\{x\}_{np}$ as

$$\{U\} = [A]\{x\}_{np} \tag{5}$$

It has been assumed in (4) that the magnitude of cohesive tractions is per unit undeformed area. This ensures that the work of separation is independent of the in-plane stretch of the element, which is appropriate for modeling fracture in solids. An approximation to the cohesive element stiffness,

$$[J]_{ij} = \left[\frac{\partial F_i}{\partial x_j}\right] \tag{6}$$

is formed by neglecting the variation in [Q] and is

$$[J] = \int_{S_0} [Q]^T [A]^T [C] [A] [Q] \, dS_0 \tag{7}$$

where [C] is the cohesive material Jacobian that relates incremental tractions to the incremental displacement jumps

$$\{T\} = [C]\{dU\}; \quad [C_{ij}] = \left[\frac{\partial T_i}{\partial u_j}\right] \tag{8a,b}$$

The nodal force vector and the cohesive element stiffness matrix are used for Newton-Raphson iterations in an implicit solution scheme. Further details can be found elsewhere (Rahulkumar *et al.*, 1999, and Rahul-Kumar *et al.*, 2000.). Implementation of this formulation has been separated into two functional units. The kernel specifies cohesive element tractions and the cohesive element Jacobian as a function of current opening displacement. The shell consists of numerical quadrature, transformations, and the like for calculating the stiffness matrix. A family of cohesive elements has been implemented for use with static and implicit-dynamic procedures in the commercial finite element package ABAQUS™, 1997.

3. APPLICATIONS

The implementation described has been used to study interfacial fracture in three experiments for adhesion of viscoelastic elastomers: the T-peel, compressive shear strength (CSS), and through crack tension (TCT) tests.

3.1 T-Peel test modeling

The peel test is employed routinely to measure the strength of elastomeric adhesives and joints (Kinloch 1987, Gent, 1996). Interpretation of peel tests is

usually based on the following two assumptions: 1) the intrinsic interface resistance is *a rate-independent* quantity, and 2) bulk dissipation in the peel arms is the major contributor to the work of separation and its rate sensitivity (Gent, 1996). T-peel experiments have been analyzed using cohesive elements to represent the intrinsic adhesion and a viscoelastic constitutive description for the bulk. The analysis allows a decoupling of bulk dissipation from the intrinsic and near-crack process zone contributions to fracture resistance.

Figure 2 shows how peel energy varies with normalized peel rate when the bulk is modeled by a standard viscoelastic linear solid, for which the viscoelastic bulk and shear relaxation modulus are given by, $K(t) = K, G(t) = G_\infty + (G_0 - G_\infty)\exp(-t/\tau_0)$, where G_∞ is the rubbery modulus and G_0 is the instantaneous modulus. The normalized velocity, v*, is defined as: $v^* = v\tau/h$, where v is the actual velocity, τ is the characteristic relaxation time and h is the thickness of the peel arm. In the limits of low and high peeling rates, $v^* \to 0, v^* \to \infty$, the entire peel arm behaves elastically (Regions I and IV). Peel energy then equals the intrinsic cohesive energy. For intermediate rates, dissipation in the bulk contributes to the overall peel energy.

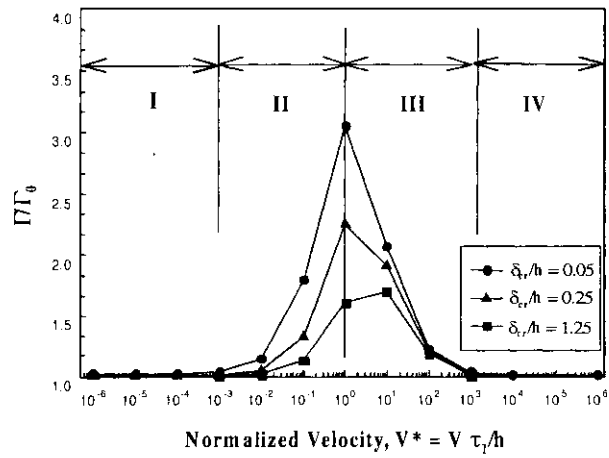

Figure 2. Predicted ratio of global fracture energy to intrinsic fracture energy and the effect of cohesive zone parameter δ_{cr} on the predicted fracture energy as a function of normalized crack velocity, V* (peeling rate).

In region II, the fracture energy at a given velocity is sensitive to the value of δ_{cr}; smaller δ_{cr} results in greater dissipation at lower velocities. The predicted fracture energies fall off rapidly in Region III and are less sensitive to δ_{cr}. The direct problem solved here, one in which cohesive zone properties are specified and total dissipation is computed, shows that total dissipation depends on *both* cohesive zone parameters. This implies that the important inverse problem, that of

partitioning measured global energy dissipation into bulk and near-tip components, cannot be resolved uniquely without the use of a cohesive zone model.

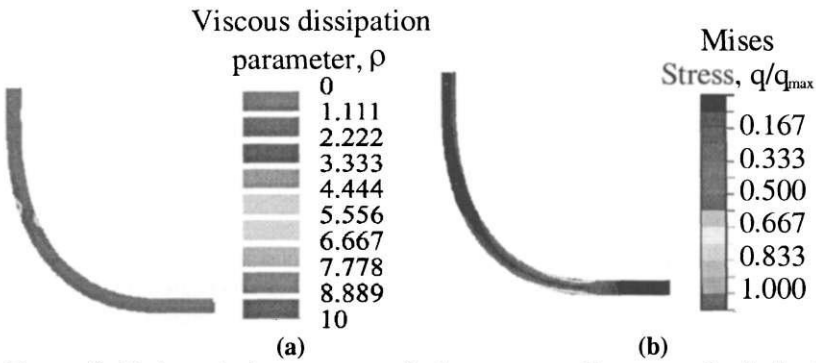

Figure 3. Deformed shapes at a velocity corresponding to peak dissipation showing (a) contours of parameter ρ, representing dissipation, and (b) von Mises stress q.

Figure 3 shows the computed peel shapes at a velocity corresponding to peak dissipation. Figure 3(a) shows contours of a parameter, ρ, which is a measure of viscous dissipation. It is defined as:, $\rho = [(\varepsilon - \varepsilon_0)/(\varepsilon_\infty - \varepsilon_0)]$, where $\varepsilon = \sqrt{2/3\mathbf{e}:\mathbf{e}}$, and **e** is the total deviatoric strain tensor. The quantities, ε_0 and ε_∞, are obtained by dividing the von Mises stress, q, at the material point by the three times the unrelaxed and relaxed shear moduli respectively of the material. The Mises stress is defined as, $q = \sqrt{3/2\mathbf{s}:\mathbf{s}}$, where **s** is the deviatoric stress tensor. At very slow and large peel rates the parameter ρ approaches 1 and 0, respectively. When loading is reversed, for a viscoelastic material, the parameter can exceed these bounds and become large. In the peel simulations, a contour plot of this parameter is a signature of the intensity and location of viscous dissipation. Figure 3(b) shows contours of the von Mises stress, q, under the same conditions.

In the low and high peel rate limits, not shown here, the peel arm deforms as an elastic material; the parameter ρ remains in the limits (0,1). Figure 3 shows that at the velocity corresponding to peak peel energy, the region of maximum dissipation is completely distinct from the region of highest stress; dissipation is localized some distance behind the crack tip. This is consistent with the prediction (Rahulkumar *et al.*, 2000), based on de Gennes' analysis of viscoelastic crack propagation (de Gennes, 1996), that dissipation is localized roughly at a distance $v\tau$ from the crack tip. These results can guide the design of adhesives. Since the relaxation time is related to the glass transition temperature of the material and the test temperature, an adhesive may be designed with an optimum glass transition temperature for specified use temperature and loading rates.

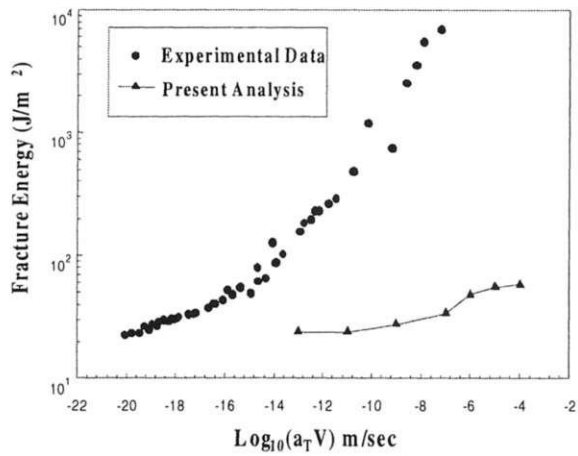

Figure 4. Experimental fracture energies on peeling of butadiene elastomeric sheets (Gent, 1996) and predictions based on fixed fracture energy and rate-dependent bulk viscoelastic loss.

The cohesive element computational was used to model experiments on peeling of polybutadiene elastomers (Chang, 1980, and Gent, 1996). The peel energy measured in these experiments qualitatively appears to be a combination of rate-independent intrinsic work of fracture and viscoelastic bulk losses. Experimentally observed increase in peel energy with peel velocity has been attributed to bulk viscoelastic losses. Here the cohesive element technique is used to test this hypothesis. Details on the characterization of the bulk viscoelastic constitutive model for the polybutadiene elastomer along with cohesive element model details are given in Rahulkumar *et al.,* 1999. As shown in Figure 4, the predicted increase in macroscopic interfacial fracture energy (adhesion) with peel rate is several orders of magnitude lower than observed experimentally. These results suggest that the interpretation of Gent's measurements of peel energy as a combination of rate-independent losses at the crack tip cohesive zone and a rate-dependent loss due to bulk viscoelasticity cannot be supported. Some additional failure mechanism appears to be operating at the crack tip that has not yet been clearly identified.

3.2 3D analysis of crack propagation in CSS test

Adhesion between an elastomer and a rigid substrate may be probed using a compressive shear strength (CSS) test shown schematically in Figure 5(a). The CSS test consists of loading a 3-ply laminate, substrate/polymer/substrate, in combined compression and shear and monitoring the force-displacement characteristics. The laminate used in the current study comprised of glass and plasticized-polyvinyl butyral (Butacite®), which is used in the manufacture of

laminated safety glazing for automotive windshields, and architectural glazing. Figure 5(b) is an *in-situ* micrograph showing polymer deformation and associated interfacial debonding during loading. Observations made during a loading a sequence reveal that an interfacial crack nucleates readily and propagates stably until reaching a critical size at which unstable debonding ensues. Modeling of such crack growth behavior is difficult and requires methods such as those presented by Jagota *et al.* (2000) and in the current contribution.

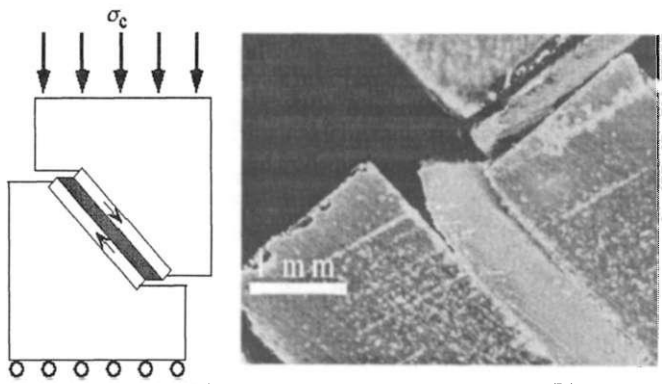

Figure 5. (a) Schematic drawing of a compressive shear test for glass/elastomer adhesion. (b). *in situ* micrograph showing polymer deformation and stable interface debonding prior to unstable failure of the interface.

A 3D analysis of the CSS test has been performed by employing 3D cohesive elements and a hyperelastic material model for the polymer. The 3D finite element discretization employed in the study is shown in Figure 6. The dimensions of the 3D CSS test specimen used in the 3D numerical study are: polymer thickness, h = 0.76 mm, length = 25 mm, and width = 4.56 mm (6h). Based on symmetry about the x-y plane, one half of width (3h) is modeled in the z direction. The polymer is modeled using 8-node hybrid brick elements, and glass is modeled using regular displacement based 8-node brick elements. A layer of 3D 8-node cohesive elements is placed along the interface between the polymer and glass. The size of cohesive elements in the fine discretized region in Figure 16 at the free edge, z=3h, are of dimension 0.047h along the length and 0.094h along the width. The 3D discretization consists of 48,900 degrees of freedom. The boundary conditions for the nodes on the bottom surface of the glass elements are specified as, $T_x = 0$, $u_y = 0$, $T_z = 0$. The nodes on the symmetry face, z=0, have, $u_z=0$. The loading consists of specifying displacements, $u_x = 0$, $u_y = \gamma h/\sqrt{2}$, and $u_z = 0$, for the nodes on the top surface of bulk polymer elements, where, γ is the equivalent shear strain in the polymer. It has been modeled as a neo-Hookean hyperelastic material with material constant, $C_{10} = (1/2)G = 1.66 \times 10^5$ Pa. Glass has been modeled as a rigid substrate. The cohesive zone parameters are: $\Gamma_0 = 4.95$ N/m, and