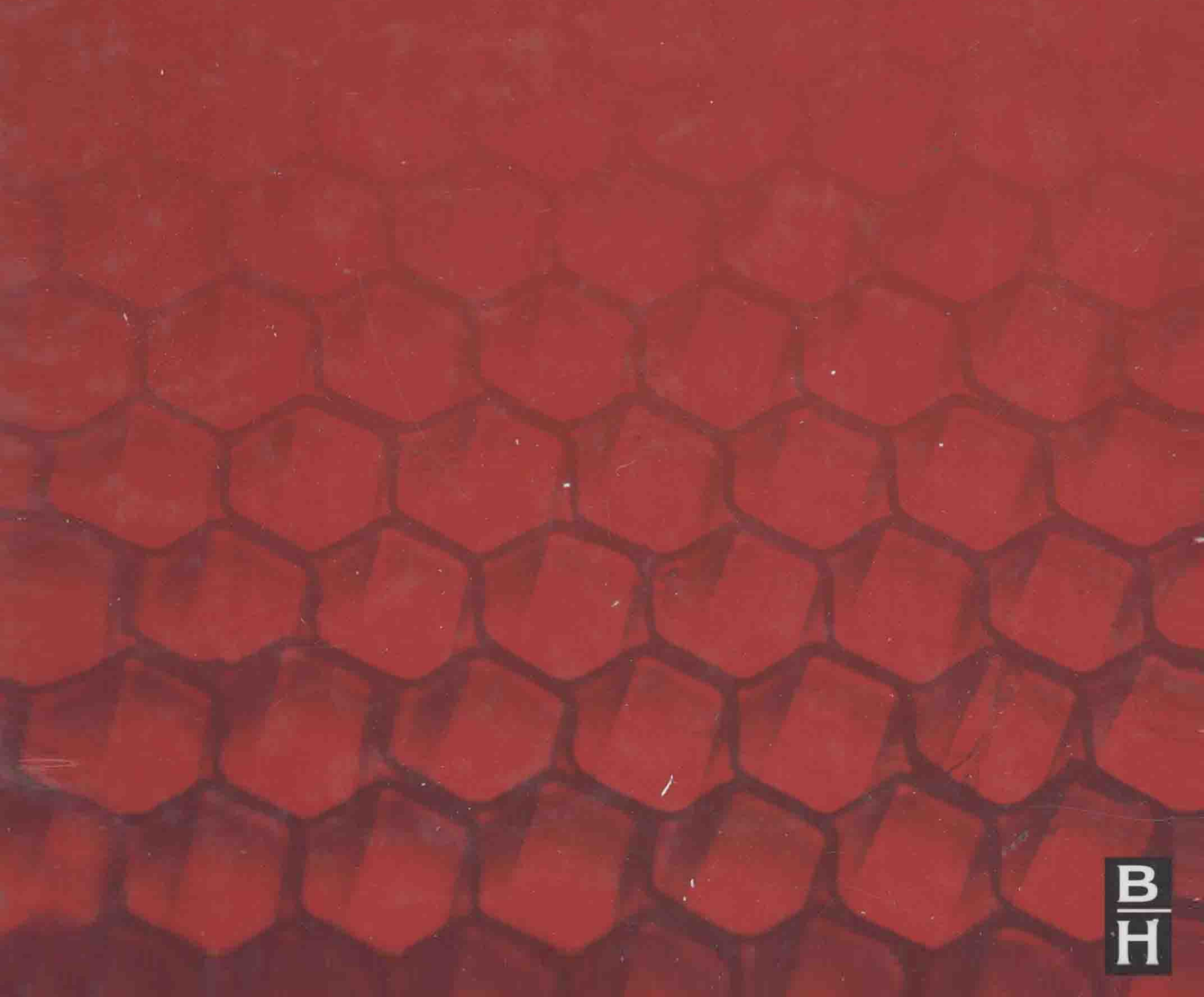
INTEGRATED DESIGN OF MULTISCALE, MULTIFUNCTIONAL MATERIALS AND PRODUCTS

DAVID L. McDOWELL
JITESH H. PANCHAL
HAE-JIN CHOI
CAROLYN CONNER SEEPERSAD
JANET K. ALLEN
FARROKH MISTREE



B
H

Integrated Design of Multiscale, Multifunctional Materials and Products

David L. McDowell
Jitesh H. Panchal
Hae-Jin Choi
Carolyn Conner Seepersad
Janet K. Allen
Farrokh Mistree

ELSEVIER

AMSTERDAM • BOSTON • HEIDELBERG • LONDON
NEW YORK • OXFORD • PARIS • SAN DIEGO
SAN FRANCISCO • SINGAPORE • SYDNEY • TOKYO

Butterworth-Heinemann is an imprint of Elsevier

B H

Butterworth-Heinemann is an imprint of Elsevier
30 Corporate Drive, Suite 400, Burlington, MA 01803, USA
Linacre House, Jordan Hill, Oxford OX2 8DP, UK

Library of Congress Cataloging-in-Publication Data
Application submitted

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library.

ISBN: 978-1-85617-662-0

For information on all Butterworth-Heinemann publications
visit our Web site at www.elsevierdirect.com

Printed in the United States of America
09 10 11 12 13   10 9 8 7 6 5 4 3 2 1

Integrated Design of Multiscale, Multifunctional Materials and Products

Preface

To some extent, design of materials has long been a preoccupation of materials scientists and engineers. However, the historical emphasis on laborious, intuitive, serendipitous materials discovery has only relatively recently been augmented by computer simulations. This speeds up discovery of new material solutions, as well as more rapidly assessing process-structure-property relations upon which modern materials science is based. Fueled by the recent emergence and rapid growth of computational methods, a materials design revolution is underway in which the classical materials selection approach is replaced by the simulation-based design of material microstructure or mesostructure to satisfy multiple performance requirements of the component or system, subject to constraints on certain material properties and other aspects of the system.

Materials typically used in applications today have complex, heterogeneous microstructures with different characteristic length scales, and these microstructures affect processing, manufacture, and in-service performance. In the past fifty years, research in theory of dislocations, phase transformations, and micromechanics of heterogeneous materials enabled explicit consideration of the role of microstructure on the properties of metallic systems and certain classes of composites. Pivotal to progress in the present materials design revolution are the works of Olson (Olson 1997) on combining elements of reductionist, bottom-up modeling with deductionist, top-down systems design of materials. The perspective of a material as a complex hierarchical system is instrumental in drawing analogy to subsystems and components considered in conventional design. Moreover, the contribution of Ashby and coworkers (Ashby 1999) regarding systematic definition and execution of the materials selection problem for various performance requirements is acknowledged as foundational to relating properties to performance.

The core of materials design is the interplay of hierarchical systems-based design of materials and multiscale/multilevel modeling methodologies, embedded within a computational framework that supports coordination of information and human decision making. We add to these developments elements of decision-based robust design of engineering systems. Why? In spite of great advances in material modeling and simulation, from atomic scales upward, these approaches have inherent uncertainty when it comes to predicting the properties of "real" materials; moreover, there are gaps of nearly intractable nature in methods for concurrent bridging of length and time scales in modeling material processing, deformation, and failure. While emerging high-performance computing and related simulation tools provide a more predictive foundation to support materials design, brute force methods based on atomistics or concurrent multiscale modeling are unlikely to have sufficient capabilities, combined with issues such as tractability and uncertainty, to support a broad range of materials design problems. A systems approach is required to address the nonlinear, hierarchical nature of real materials. Such an approach has proven to be beneficial for design of other complex systems (e.g., aircraft, automobiles, circuit boards, etc.).

Systems-based engineering design principles have developed substantially in the last few decades. An October 1998 workshop on materials design science and engineering (McDowell and Story 1998), sponsored by the National Science Foundation and cohosted by Georgia Tech and Morehouse College, was held to discuss interdisciplinary frameworks necessary to facilitate concurrent design of materials and products, and to replace "hit and miss" materials discovery with systematic methods for materials development that draw on combined elements of materials characterization and computational simulation. This is driven by an inexorable technology pull by the marketplace toward rapid development cycles for new and improved materials. Potential benefits include a virtual manufacturing environment that goes well beyond geometric modeling to include many aspects of the physical behavior of materials in simulating system-level response. Moreover, tailoring materials to enhance the performance envelope is an imperative as we consider future requirements for increasing efficiency and environmentally sustainable solutions, for example. This workshop noted that a change of culture is necessary in universities and industries to cultivate new concepts for materials design. The resulting roadmap for materials design focused on the following foundational technologies:

- Principles and approaches for more quantitative materials design.
- Enhanced modeling and simulation tools.
- Validated, reliable, and comprehensive databases.
- Methods for in situ characterization and testing.

In this book, we address the first bullet in the previous list, namely, systems strategies for concurrent robust design of materials and systems, along with elements of distributed modeling and simulation environments. Materials design falls under the general category of simulation-based design, in which computational materials science and multiscale mechanics modeling play key roles in evaluating performance metrics necessary to support materials design. Major findings of the May 2006 Report of the U.S. National Science Foundation Blue

Ribbon Panel on Simulation-Based Engineering Science (SBES) (Oden, Belytschko et al. 2006) can be summarized as follows:

- "SBES is a discipline indispensable to the nation's continued leadership in science and engineering...
- Formidable challenges stand in the way of progress in SBES research. These challenges involve resolving open problems associated with multiscale and multi-physics modeling, real-time integration of simulation methods with measurement systems, model validation and verification, handling large data, and visualization..."

The materials design approach advocated here invokes the notion of robust design, i.e., insensitivity of the desired response to any number of sources of uncertainty or variability having to do with material composition, processing, microstructure, service history, models, and model parameters, coupling of models at different length and/or time scales, chaining of design decisions or simulation outputs/inputs, etc. In many respects, it is a manifestation of SBES. To address robust design of materials, we have developed new concepts that extend existing methods and facilitate top-down design in the presence of complexity and uncertainty that is characteristic of hierarchical material systems.

Figure P.1 encompasses the goals of concurrent material and product design, showing that already established methods of design-for-manufacture of parts, subassemblies, assemblies, and overall systems can be extended to address the multiple scales that control property-performance attributes of materials. Hence, the objective of tailoring the material to specific applications (to the left of the vertical bar in Figure P.1) is patently distinct from traditional materials selection that is common in practice. The problem is that the systems-based design methods used to design parts, components, and assemblies must be extended to consider the nuances of process-structure-property relationships in materials in the presence of significant uncertainty. The hierarchy of scales from quantum to continuum on the left side of Figure P.1 may be viewed as a multiscale modeling problem, but this is a reductionist, bottom-up perspective. The materials design challenge is to develop methods that employ bottom-up modeling and simulation, calibrated and validated by characterization and measurement to the extent possible, yet permit top-down design over the hierarchy of material length scales shown in Figure P.1.

Our intention in this book is to provide a connection between several key primary disciplines or endeavors that have been traditionally distinct but naturally combine to serve as the foundation of modern materials design: (1) systems-based engineering design, (2) computational materials science and engineering, (3) robust systems design, and (4) information technology. It is targeted to serve as a useful reference in emerging methods for concurrent design of materials and products for product designers, materials scientists and

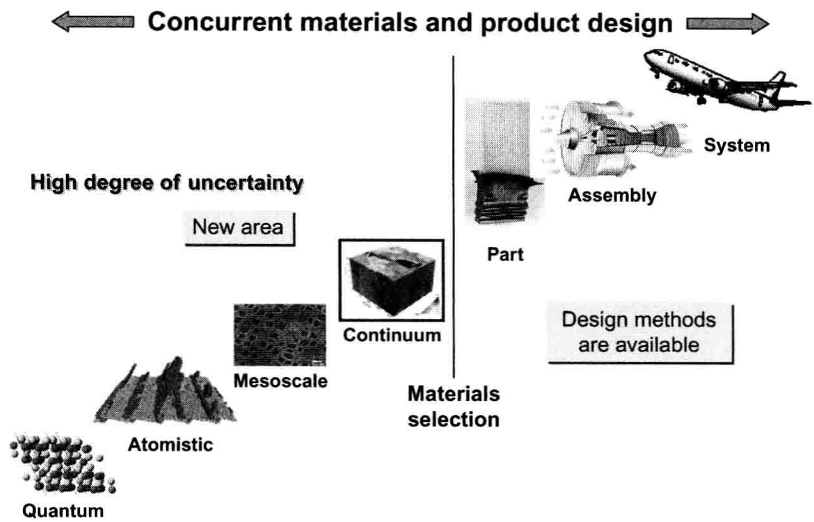


Figure P.1 Hierarchy of levels from atomic scale to system level in concurrent materials and product design. Existing systems design methods focus on levels to the right of the vertical bar, treating the materials design by selecting the material.

engineers, applied mechanics researchers, and other analysts involved in multiscale modeling of material behavior and associated process-structure-property relations.

The reader may find that the premise behind this book—that materials can be designed concurrently with products—is not the usual way of doing business in many organizations that traditionally separate the functions of materials development from systems design along organizational lines, using material properties as the mode of communication/information exchange. It also differs from the way design is taught in most engineering programs, including materials science and engineering. Indeed, the ideas presented here represent our long-term prospectus for how this might be done in the "near tomorrow" as computing power increases, engineering becomes increasingly multidisciplinary, multi-resolution, and multiscale material modeling methods blossom, and systems approaches that emerge from the engineering design, multidisciplinary optimization, and information sciences communities become a part of the engineering lexicon. To this end, we look toward the horizon beyond the current state of the curriculum, university disciplinary structures, or management of design processes in industry. We trust that the initial, embryonic ideas presented here will serve as an impetus for the students of today and technology leaders of tomorrow in various aspects of materials engineering and product development to consider the richness of opportunities that lie ahead in a digital, highly connected world.

In this book, we incorporate ideas and material from the dissertations of three former doctoral students in the Systems Realization Laboratory at Georgia Tech—Carolyn Conner Seepersad,

HaeJin Choi, and Jitesh Panchal. In addition, we have all benefited from the rich interactions among students and faculty in the Systems Realization Laboratory. At the peril of omitting some names, we acknowledge Wei Chen (Northwestern University), Tim Simpson (Penn State University), and Kemper Lewis (University of Buffalo), whose doctoral work at Georgia Tech has had a major impact on the material presented herein. In addition, several graduate students and postdoctoral fellows in mechanics of materials at Georgia Tech have contributed substantially to the formative stages of this work. These include doctoral students Ryan Austin and Jim Shepherd, who provided essential framing of computational mechanics issues and codes that contributed to several materials design scenarios presented here as examples, as well as postdocs Aijun Wang and Rajesh Kumar, who developed valuable analysis tools and methods for use in cellular materials design problems.

Pursuit of many of the concepts outlined in this book received financial support from several sources. Concepts for robust design of materials were initially developed in the context of cellular materials applications with the support of the Defense Advanced Research Projects Agency (DARPA) (N00014-99-1-1016) from 1999 to 2002, monitored by Dr. Leo Christodoulou, and by the Office of Naval Research (ONR) (N0014-99-1-0852), under Dr. Steven Fishman. Support from 2002 to 2007 by the Air Force Office of Scientific Research (AFOSR) Multi-University Research Initiative Grant on Energetic Structural Materials (1606U81, Craig Hartley, monitor) is gratefully acknowledged, as is more recent, ongoing support of the NSF (I/UCRC) Center for Computational Materials Design (CCMD), a joint venture of partner institutions Penn State and Georgia Tech.

References

Ashby, M.F. 1999. Materials Selection in Mechanical Design. Butterworth-Heinemann: Oxford, UK.

McDowell, D.L., Story, T.L., 1998. New directions in materials design science and engineering (MDS&E). Report of a NSF DMR-sponsored workshop on materials design science and engineering, Atlanta, GA, October 19–21.

Oden, J.T., Belytschko, T., Fish, J., Hughes, T.J.R., Johnson, C., Keyes, D., Laub, A., Petzold, L., Srolovitz, D., Yip, S., 2006. Simulation-based engineering science: Revolutionizing engineering science through simulation. In: A Report of the National Science Foundation Blue Ribbon Panel on Simulation-Based Engineering Science. National Science Foundation: Arlington, VA.

Olson, G.B. 1997. Computational design of hierarchically structured materials. Science, 277 (5330), 1237–1242.

Authors

DAVID L. McDOWELL *Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing*, Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332
david.mcdowell@me.gatech.edu

JITESH H. PANCHAL *Assistant Professor,* School of Mechanical and Materials Engineering, Washington State University , Pullman, WA 99163
panchal@wsu.edu

HAE-JIN CHOI *Assistant Professor*, Division of Systems and Engineering Management, School of Mechanical & Aerospace Engineering, College of Engineering, Nanyang Technological University, Singapore
hjchoi@ntu.edu.sg

CAROLYN CONNER SEEPERSAD *Assistant Professor*, Product, Process, and Materials Design Lab, Mechanical Engineering, The University of Texas at Austin, Austin, TX 78712
ccseepersad@mail.utexas.edu

JANET K. ALLEN *John and Mary Moore Chair*, School of Industrial Engineering, University of Oklahoma, Norman, OK 73019
janet.allen@ou.edu

FARROKH MISTREE *L.A. Comp Chair and Director*, School of Aerospace and Mechanical Engineering, University of Oklahoma, Norman, OK 73019
farrokh.mistree@ou.edu

About the Authors

David L. McDowell

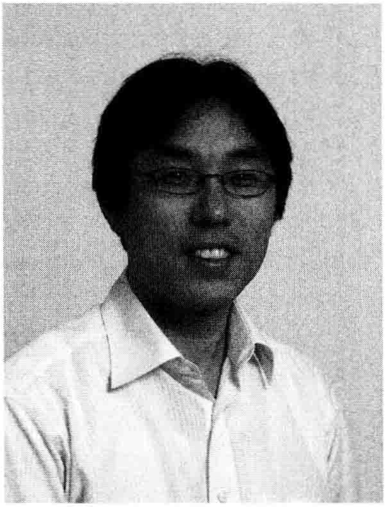
Dave McDowell joined Georgia Tech in Fall 1983 after graduating from the University of Illinois at Urbana-Champaign. Regents' Professor and Carter N. Paden, Jr. Distinguished Chair in Metals Processing, McDowell holds a dual appointment in the GWW School of Mechanical Engineering and the School of Materials Science and Engineering. He serves as Director of the Mechanical Properties Research Laboratory and as Chair of the Georgia Tech Materials Council. McDowell's research focuses on the synthesis of experiment and computation to develop physically based constitutive models for nonlinear and time-dependent behavior of materials, with emphasis on wrought and cast metals. Research topics of interest include cyclic plasticity and microstructure-sensitive fatigue modeling of metallic systems, finite strain plasticity and defect field theories, behavior of metallic foams and honeycomb materials, creep-fatigue-environment interaction, thermo-mechanical fatigue, time-dependent fracture, atomistic simulations with focus on dislocation-interface reactions, phase transformations, and multiscale modeling. McDowell currently serves on the editorial board of the International Journal of Plasticity as well as several others, and is co-Editor of the International Journal of Fatigue. For the past 15 years he has pursued definition and more systematic development of the field of multifunctional design of materials over a broad range of applications, including metal honeycombs for cooling and structural applications, lightweight transportation vehicles, components for hot sections of aircraft gas turbine engines, protective armor systems, and energetic material systems. Author of over 340 technical papers, McDowell serves as Co-Director of the NSF-sponsored Center for Computational Materials Design, a joint Penn State-Georgia Tech I/UCRC.

http://www.me.gatech.edu/faculty/mcdowell.shtml
http://mprl.me.gatech.edu/index.php
e-mail: david.mcdowell@me.gatech.edu

Jitesh H. Panchal

Jitesh Panchal is an Assistant Professor in the School of Mechanical and Materials Engineering at Washington State University. Before joining Washington State University in Fall 2008, he was a Visiting Assistant Professor in the Woodruff School of Mechanical Engineering at the Georgia Institute of Technology. He received his Bachelor of Technology (B.Tech.) degree from Indian Institute of Technology at Guwahati, and MS and PhD in Mechanical Engineering from Georgia Institute of Technology in 2003 and 2005, respectively. Panchal's research interests are in establishing design methodologies and computational tools for integrated product and materials design. His focus is on managing complexity and uncertainty in multilevel design processes. He is interested in developing open computational environments for the integrated design of products and materials. Panchal is excited about developing systematic approaches for leveraging mass-collaboration in engineering design. He is actively involved in developing new pedagogical approaches for fostering collective learning and achieving mass customization in education. He is a member of American Society of Mechanical Engineers (ASME), and American Society for Engineering Education (ASEE).

http://www.mme.wsu.edu/people/faculty/faculty.html?panchal
e-mail: panchal@wsu.edu



Hae-Jin Choi

Hae-Jin Choi is an assistant professor in the School of Mechanical and Aerospace Engineering, Nanyang Technological University (NTU), Singapore. Before joining in NTU, he served as a postdoctoral fellow in the Woodruff School of Mechanical Engineering at Georgia Tech after earning Ph.D. (2005) and M.S. (2001) degrees at Tech. He received B.S. and M.S. degrees from Yonsei University in Seoul, Korea in 1995 and 1997, respectively. His research focuses on management of uncertainty, integrated materials and products design, multiscale simulation-based design, strategic product design, and distributed collaborative product realization. Choi proposed robust design methods for managing variability and uncertainty in complex systems. Applications of the methods include design of multifunctional energetic structural materials, blast resistant panels, and multifunction linear cellular alloys. A wide range of additional design applications, such as bio mass sensors, lightweight tactical bridges, and underwater power generation systems, are currently under development. He is a member of the American Society of Mechanical Engineers and the American Institute of Aeronautics and Astronautics.

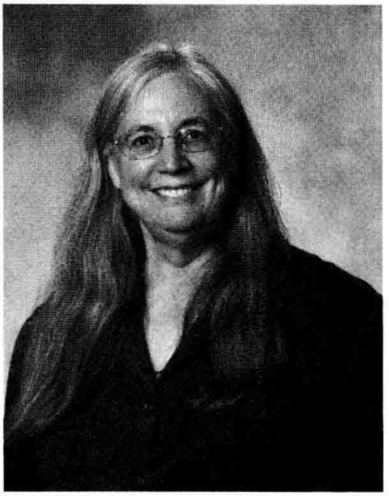
http://www3.ntu.edu.sg/home/hjchoi/
e-mail: hjchoi@ntu.edu.sg

Carolyn Conner Seepersad

Carolyn Conner Seepersad is an Assistant Professor of Mechanical Engineering at the University of Texas at Austin. She received a PhD in Mechanical Engineering from Georgia Tech in 2004, an MA/BA in Philosophy, Politics and Economics from Oxford University in 1998, and a BS in Mechanical Engineering from West Virginia University in 1996. She is a former Rhodes Scholar, Hertz Fellow, and NSF Graduate Research Fellow. Dr. Seepersad's research involves the development of methods and computational tools for engineering design, with an emphasis on multilevel design of products and materials. Topics of interest include the computational design and solid freeform (additive) fabrication of customized mesostructure, including multifunctional honeycomb structures for applications such as structural heat exchangers, acoustic energy absorbing devices, and structures with spatially tailored stiffness. Related topics include computational techniques for coordinating design exploration activities on different levels or scales, and predictive process control techniques for incorporating physics-based models into the design of manufacturing processes. Additional research interests include product customization and green design. Dr. Seepersad currently serves as a co-organizer of the annual Solid Freeform Fabrication Symposium, and she is the author of more than 60 journal papers and full-length conference publications. She teaches courses on product design, solid freeform fabrication, and design of complex engineered systems.

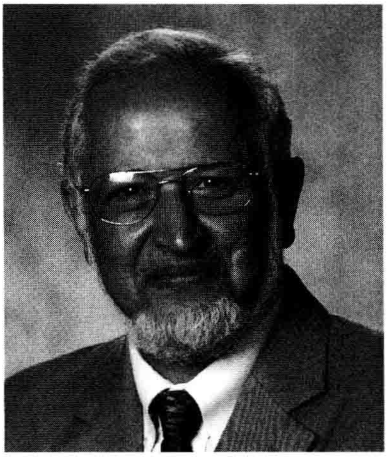
http://www.me.utexas.edu/directory/faculty/seepersad/carolyn/121/
http://www.me.utexas.edu/~ppmdlab/
e-mail: ccseepersad@mail.utexas.edu

Janet K. Allen



Janet Allen earned her doctorate from the University of California at Berkeley in 1973 and her S.B. from the Massachusetts Institute of Technology in 1967. Dr. Allen's expertise lies in the area of simulation-based design of engineering systems, especially in the management and mitigation of uncertainty in the early stages of design. There are two conceptually different approaches to accomplishing this. The first is to mitigate uncertainty by accurately modeling uncertainty and/or by reducing it. It is impossible to accomplish this completely. The second approach is to use robust design principles to improve the quality of products and processes by reducing their sensitivity to variations, thereby reducing the effects of uncertainty without removing its sources. During the course of her career, Dr. Allen has studied both aspects of the problem. Her most significant accomplishments lie in the area of robust design. However, this is by no means the only research thread embodied in Dr. Allen's research portfolio, among other things, she has studied the use of living systems theory in design, design education, modeling design processes, and design for X. Professor Allen is a Fellow of the American Society of Mechanical Engineers, a Senior Member of AIAA, a Member of ASEE and an Honorary Member of the Mechanical Engineering Honor Society, Pi Tau Sigma. She is an Associate Editor of the ASME Journal of Mechanical Design. With her students, she has authored well over 200 technical publications. A Professor Emeritus in the Woodruff School of Mechanical Engineering at the Georgia Institute of Technology, she presently holds the John and Mary Moore Chair in the School of Industrial Engineering at the University of Oklahoma.

http://www.srl.gatech.edu/Members/jallen
e-mail: janet.allen@ou.edu



Farrokh Mistree

Farrokh Mistree earned his doctorate in engineering (with minors in Operations Research and Business Administration) from the University of California, Berkeley in 1974 and earned his first degree in Naval Architecture from the Indian Institute of Technology at Kharagpur. He served at the University of New South Wales, (1974–80), The University of Houston (1981–92) and joined the Georgia Institute of Technology as Professor of Mechanical Engineering in September 1992. Professor Farrokh Mistree's *design experience* spans mechanical, aeronautical, structural, and industrial engineering. His *teaching experience* spans courses in engineering design, naval architecture, solid mechanics, operations research, and computer science. His current research focuses on learning how to manage design freedom in multiscale design (from molecular scales to reduced order models) to facilitate the integrated design of materials, product and design process chains. He is committed to developing a design pedagogy that is rooted in Decision-Based Design and adaptive action learning. It is in this context that he enjoys experimenting with ways in which design can be learned and taught. He is a Fellow of ASME, an Associate Fellow of the AIAA, a Member of ASEE and the Society of Naval Architects and Marine Engineers. Professor Mistree has co-authored two textbooks and over 350 technical publications. He was recognized for his research by receiving the ASME Design Automation Committee's 1999 Design Automation Award and was honored for outstanding teaching as recipient of the 2001 Jack M. Zeigler Woodruff School Outstanding Educator Award. He served as the National Secretary-Treasurer of Pi Tau Sigma Mechanical Engineering Honor Society (1995–2008) and as a reviewer for ABET (1996–2002). From July 1995 through December 2008, Professor Mistree served as the Associate Chair for the Woodruff School of Mechanical Engineering and the Associate Director of Georgia Tech Savannah. A Professor Emeritus in the Woodruff School of Mechanical Engineering at the Georgia Institute of Technology, he presently holds the L.A. Comp Chair and serves as Director of the School of Aerospace and Mechanical Engineering at the University of Oklahoma.

http://www.srl.gatech.edu/Members/fmistree
e-mail: farrokh.mistree@ou.edu

Photos by Gary Meek and Michelle White

Contents