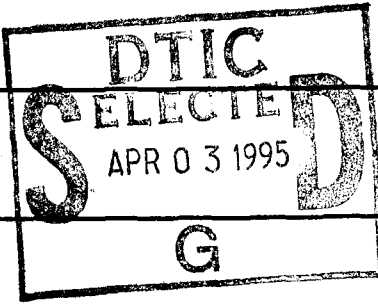


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REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0168	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0168), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE 2/15/95	3. REPORT TYPE AND DATES COVERED Final Technical Report 7/1/91-12/31/94		
4. TITLE AND SUBTITLE Transitions, Defects, and Whiskered Microstructures		5. FUNDING NUMBERS G - AFOSR 91-0301-A PR - 2304/CS T - 6912/OR		
6. AUTHOR(S) Richard James David Kinderlehrer Mitchell Luskin				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Grants and Contracts Office of Research and Technology Transfer Administration University of Minnesota Suite 201, 1100 Washington Avenue South Minneapolis, MN 55415-1226		8. PERFORMING ORGANIZATION REPORT NUMBER AFOSR-TR-95-0178		
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/NM Building 410 Bolling AFB DC 20332-6448		10. SPONSORING MONITORING AGENCY REPORT NUMBER		
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution unlimited.				
12b. DISTRIBUTION CODE				
13. ABSTRACT (Maximum 200 words)				
James and Kinderlehrer have given a new theory of magnetostriction. The theory shows excellent agreement with experiment and has motivated new experiments on the relation between domain structure and behavior by Lord and by DeGraef. The theory implies a new mechanism for magnetostriction in $Tb_x Dy_{1-x} Fe_2$ (x near 0.3). It also strongly suggests the existence of materials (termed "magnetomemory" materials by the authors) that would have magnetostrictive strain that is two orders of magnitude larger than the largest produced by current giant magnetostrictive materials. Luskin and his research group have developed an advanced computational model for the dynamics of crystals which undergo a martensitic transformation. They have used this model to compute the development of martensitic microstructure and the propagation of the interface separating the austenitic phase from the martensitic phase, and they have obtained results for the influence of the surface energy and the viscosity on the dynamics. James, Kinderlehrer, Luskin and their collaborators have studied new mechanisms for hysteresis, and have clarified the role of elastic incompatibility, shuffling, kinetics, and microstructure.				
14. SUBJECT TERMS magnetostriiction, microstructure, shape memory materials, laminates, finite element methods, martensite, weak convergence methods, relaxation, calculus of variations, continuum mechanics, local minima, kinetics, shuffling				15. NUMBER OF PAGES
				16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT	

FINAL TECHNICAL REPORT

July 1, 1991 – December 31, 1994

AFOSR-91-0301-A

Transitions, Defects, and Whiskered Microstructures

Principal Investigators: Richard James, David Kinderlehrer, Mitchell Luskin

RESEARCH REPORT

James and Kinderlehrer gave a new theory of magnetostriction and have investigated the microstructure and behavior of the highly magnetostrictive material $TbDyFe_2$ (terfenol). One of the main conclusions of this work is that the growth twins in this material do not inhibit the magnetostriction, as was thought by most workers in this field. Further improvements in the material will be limited with regard to the maximum achievable magnetostrictive strain. We propose that to achieve maximum magnetostriction, the material exchanges coarse domains for fine ones. The coarse domains exhibit an exactly coherent structure while the fine phase domain arrangement is only coherent in an average sense. We still think (as described in our proposal) that the best hope for materials with much larger magnetostriction is by combining the shape-memory and magnetostrictive effects. We are currently studying what desirable features an energy function for such a material should have, and we have come up with several possibilities.

Our theory of martensitic transformations continues to have additional applications. A wide variety of microstructures, including simple and complex twin crossings, layers within layers, laminate patches, and wedge-like microstructures observed in CuAlNi are accurately predicted by the theory.

James and Müller continued work on the passage from molecular to continuum theory for magnetism. We think that this type of calculation — the direct derivation of continuum theory from atomic theory — is very promising. These calculations are similar to our microstructure calculations in that weak convergence methods play an important role, except that it is the molecular fields that undergo rapid oscillation. We think that it should be possible to derive new continuum theories in this way.

Ball and James continued research on metastability and hysteresis. The goal is to predict the size of the hysteresis loops observed by C. Chu in his biaxial loading experiments on martensitic Cu-Al-Ni single crystals. His observations on the role of imposed disturbances suggest to us an approach based on calculating the relative minimizers of free energy; these calculations allow large disturbances of the deformation gradient but small disturbances of the deformations. The key idea is that, for reasons of geometric compatibility, a small nucleus of the energetically preferred phase necessarily must be surrounded by a transition layer. The energy penalty for this layer is more than the energy gained due to the presence of the small nucleus. This leads to metastability. The comparison with experiment is good so far.

Kinderlehrer and Ma have studied the computation of magnetostrictive configurations. They are able to produce hysteresis loops for the linear magnetostrictive material, and now have an understanding of the origins of hysteresis in these materials. The basic mechanism is local stability, as discussed above, but not related to geometric compatibility. The computed hysteresis loop does not collapse as the rate of change of the applied field goes to zero. The stability criterion which they have derived from this idea provides a good estimate of the critical field where the system enters an unstable regime analogous to the known Stoner-Wohlfarth condition. This analysis is based on replacing the entire computational system with a simple finite dimensional system intended to mimic the behavior of the closure domains observed in the computation. The major feature is an appropriate discretization of the demagnetization energy. This energy plays an important role in the behavior of large magnetic bodies, like Terfenol actuators. Also underway is the computation of a linear elastic two-dimensional model for the behavior of a twinned dendritic microstructure.

Relaxation of non-convex energy functionals remains a high priority in understanding the actual configurations attained by a material system. Often, in addition to deformation, other quantities appear in the energy. Recently, together with Fonseca and Pedregal, Kinderlehrer has attacked this issue. Beginning from the theory developed with Pedregal about weakly convergent minimizing sequences, it was shown possible to introduce minimizing sequences which both preserve (convex) constraints and integrability. In a companion paper, they treat the case of bounded variation.

Luskin and his research group have developed computational methods which now enable the theory to be used to predict the response of martensitic crystals with microstructure to a much wider class of boundary loads and temperature variations than those accessible to analytic techniques. Our computational program has motivated the development of theory which can give quantitative predictions about experiments. One successful example of this synergy was our development of the energy density for an indium-thallium alloy which we used in our three-dimensional computations of equilibria and dynamics for this crystal with general boundary loads and temperatures (Collins and Luskin [1993], Klouček and Luskin [1994a, 1994b]).

Since the computed deformation gradient approximating the deformation gradient of a solution with microstructure cannot be expected to converge pointwise under mesh refinement, we introduced a theory for the numerical analysis of microstructure which we used to rigorously analyze the convergence of the finite element approximation of several model problems. We showed that an approximate Young measure (which measures the oscillatory behavior of the computed deformation gradient) converges to the Young measure of the solution, and we also proved the convergence of the macroscopic variables defined by the integral of nonlinear functions of the approximate deformation gradients. Our theory for the analysis of numerical methods for microstructure has also allowed us to develop practical guidelines for the development of effective and efficient computational methods (Collins, Luskin, and Riordan [1993], Klouček, Li, and Luskin [1994]).

Luskin and his research group have developed methods and a code to investigate dynamical phenomena associated with martensitic transformations modeled by the balance of linear momentum

$$\rho y_{tt} = \nabla \cdot \sigma, \quad (x, t) \in \Omega \times (0, \infty), \quad (1)$$

where ρ is the density, $\sigma(\nabla y(x, t), \theta(x, t))$ is the total stress tensor, and the temperature $\theta(x, t)$ is given. Since in our theory

$$\sigma(F, \theta) = \frac{\partial W(F, \theta)}{\partial F} + \text{surface stress} + \text{viscous stress}$$

where $W(F, \theta)$ is the Helmholtz free energy density, the multi-well structure of the Helmholtz free energy density leads to an ill-posed problem (in the absence of surface stress and viscous stress) for the linearized momentum equation about some strains. We have developed stable time-discretization methods and efficient techniques for the solution of the linear equations at each time step even though the energy density is non-convex (Klouček and Luskin [1994b]).

Our computational experiments have simulated the development of martensitic microstructure and the propagation of the austenitic-martensitic phase boundary which separates the homogeneous austenitic phase from the microstructured martensitic phase (Klouček and Luskin [1994a, 1994b]). We have also done computational studies of the effects of surface stress and viscous stress on the dynamics (Klouček and Luskin [1994b]). We have recently developed methods and an extension of our code which includes thermal effects by solving (1) with the equations for the balance of energy

$$\rho e_t = \sigma \cdot \nabla y_t - \nabla \cdot q, \quad (2)$$

for the deformation and temperature where $e(\nabla y(x, t), \theta(x, t))$ is the internal energy density and $q(\nabla y(x, t), \theta(x, t), \nabla \theta(x, t))$ is the heat flux.

We used our theory of numerical analysis for microstructure to give a rigorous analysis of the convergence of a finite element approximation of the magnetization for a ferromagnetic crystal (Luskin and Ma [1992]), and we have developed an extension of the simulated annealing algorithm to solve the numerical optimization problem (Luskin and Ma [1993]). These techniques are being extended to magnetostriction problems (Kinderlehrer and Ma [1994]).

Recently, Abeyaratne, Chu and James have investigated the influence of microstructure on kinetics. The presence of microstructure introduces many little wiggles on the macroscopic energy. They consider gradient-flow kinetics of such energies, which they analyze by a change of scale calculation. The resulting macroscopic kinetic law is completely different from the microscopic one; it shows remarkably good agreement with the dynamic observations of Chu under a wide variety of imposed loading programs.

Bhattacharya, James and Swart [1994] have given a new theory of shuffling and have discussed its implications for hysteresis in shape memory materials that exhibit this phenomenon.

Our theories and computational results are being studied intensely in the mathematical community, and are gaining acceptance by materials scientists. In certain cases they have made definite predictions which have preceded the corresponding experiment; these predictions have subsequently shown excellent agreement with experiment (Chu [1993], James and Kinderlehrer [1994], Bhattacharya, James and Swart [1994]). In other cases the theories have been used to design entirely new experiments (Ball and James [1992], Chu, James and Miyazaki [1994]). These experiments have especially revealed the three dimensional behavior of transforming materials. These tests have also given a wide range of new observations, especially relating to hysteresis.

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FINAL TECHNICAL REPORT

AFOSR-91-0301-A

Transitions, Defects, and Whiskered Microstructures

Principal Investigators: Richard James, David Kinderlehrer, Mitchell Luskin

PUBLICATIONS

1. R. Abeyaratne, C. Chu and R. D. James, Kinetics and hysteresis in martensitic single crystals, Proc. Symposium on the Mechanics of Phase Transformations and Shape Memory Alloys, ASME, 1994
2. J. M. Ball C. Chu, and R. D. James, Metastability of martensite, preprint.
3. J. M. Ball and R. D. James, Proposed experimental tests of a theory of fine microstructure and the two well problem. Phil. Trans Royal Soc. Lond. A 338 (1992), 389-450.
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16. R. D. James and D. Kinderlehrer, Frustration and microstructure: an example in magnetostriction, Proc. Conference Pont a Mousson, 1991.
17. R. D. James and D. Kinderlehrer, Twinned structures in Terfenol, Proc. International Conference on Martensitic Transformations, Monterey, 1992. R. D. James and D. Kinderlehrer, Theory of magnetostriction with applications to $TbDyFe_2$, Phil. Mag. B, 68, 237-274.
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25. D. Kinderlehrer, Remarks about surface energy (with G. Vergara Caffarelli), to appear.
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41. N. Simha, Do habit planes exist for the tetragonal to monoclinic transition in zirconia?, preprint.
42. L. Truskinovsky and G. Zanzotto, Ericksen's bar revisited: finite-scale microstructures and metastability in one-dimensional elasticity, preprint.

ANNUAL TECHNICAL REPORT

AFOSR-91-0301-A

Transitions, Defects, and Whiskered Microstructures

Principal Investigators: Richard James, David Kinderlehrer, Mitchell Luskin

INVITED LECTURES OF RICHARD JAMES

Workshop on Homogenization, Mathematical Sciences Research Institute, 1991
 American Association for the Advancement of Science, Washington D. C., 1991
 Contemporary Developments in Solid Mechanics, in honor of the 60th birthday of J. K. Knowles, Caltech, 1991
 Department of Aerospace Engineering and Mechanics, University of Texas at Austin (colloquium), 1991
 Seminar on Dynamics and Flow Systems, University of Minnesota, 1991
 Theory of Martensite, a workshop organized by G. Olson, Northwestern, 1991
 Army Conference on Applied Mathematics and Computing, University of Minnesota, 1991
 The Mathematics of Nonlinear Systems, University of Bath
 International Centre for Mathematical Sciences opening meeting on Mathematics in Materials Science, 1991
 Workshop on Whiskered Microstructures, Carnegie Mellon University, 1991 (co-organized with D. Kinderlehrer and T. Einstein)
 Materials Research Society Meeting on Theory and Applications of Shape-Memory Materials, Boston, 1991
 Seminar on Mathematics in Materials Science, Heriot-Watt University, 1991
 Applied Mathematics Seminar, Courant Institute, 1991
 Department of Mathematics, Carnegie Mellon University, 1991
 Edinburgh Mathematics Society and The Royal Society of Edinburgh joint meeting, (lecture to a general audience on paper folding and the microstructure of crystals) 1992
 Thermodynamics of Materials, Oberwolfach, 1992
 Institut fur Angewandte Mathematik, Universitat Bonn, 1992
 School of Mathematics, University of Bath, 1992
 Department of Applied Mathematics, University of East Anglia (colloquium), 1992
 Department of Mathematics, Sussex University (colloquium), 1992
 Department of Applied Mathematics, University of Edinburgh (colloquium), 1992
 Transitions de Phase, University of Metz, 1992
 Edinburgh International Science Festival (general lecture on "Smart Materials"), 1992
 Mathematics in the 21st Century, a panel discussion at the Edinburgh Science Festival (panel member, together with Sir John Kingman(chair), T. B. Benjamin, Feng Kang and Jacob Palais), 1992
 The Microstructure of Crystals, conference at the ICMS co-organized with J. M. Ball, 1992
 Micromagnetics and Magnetostriction, conference at the ICMS co-organized with D. G. Lord and A. De Simone), 1992
 Science Now, BBC Radio 4 (popular talk on "Smart Materials"), 1992
 BBC World Service (popular talk on "Smart Materials"), 1992
 International Conference on Martensitic Transformations, Monterey, 1992
 Workshop on Computational Methods in Materials Science (Organizer, with R. A. Nicolaides, D. Kinderlehrer and J. Turner), Carnegie-Mellon University, 1992
 Society for Natural Philosophy, Pennsylvania State University, 1992
 Department of Mathematics, Worcester Polytechnic Institute (colloquium), 1992
 Center for the Mechanics of Composites, Texas A&M University (colloquium), 1992
 Society of Photo-Optical Instrumentation Engineers conference on Smart Structures and Materials, 1993
 Eleventh Army Conference on Applied Mathematics and Computing, Carnegie-Mellon University, 1993
 Workshop on Metastability and Hysteresis, International Centre for Mathematical Sciences, Edinburgh, 1993
 Phase Transitions, informal meeting at Talbot House, South Pomfret, Vermont, 1993
 Society of Photo-Optical Instrumentation Engineers conference on Smart Structures and Materials, 1993
 Eleventh Army Conference on Applied Mathematics and Computing, Carnegie-Mellon University, 1993
 Workshop on Metastability and Hysteresis, International Centre for Mathematical Sciences, Edinburgh, 1993
 Phase Transitions, informal meeting at Talbot House, South Pomfret, Vermont, 1993

A gathering of research workers with interests on the metastability, hysteresis, kinetics and microstructure of martensite, University of Minnesota, (host), 1993
 Department of Mechanical Engineering, M.I.T. (colloquium), 1993
 International Centre for Mechanical Sciences, Udine (8 lectures on Shape-Memory Materials), 1993
 Magnetics group, Metals Development, Ames Lab, Iowa State University, 1993
 Institute for Advanced Study, Princeton, PDE seminar, 1993
 Department of Theoretical and Applied Mechanics, University of Illinois, Champaign-Urbana (colloquium), 1993
 Workshop on Material Microstructure, Institute for Advanced Study, Princeton, 1993
 Seminar on Materials Science, Courant Institute of Mathematical Sciences, 1994
 Workshop on Micromechanics of Small Volumes, Institute for Mechanics and Materials, San Diego (lecture and co-organizer), 1994
 SPIE Conference on Smart Structures and Materials (lecture and program committee), 1994
 SIAM Conference on Emerging Issues in Mathematics and Computation from the Materials Sciences, Pittsburgh (principal lecture), 1994
 National Institute of Standards and Technology, Gaithersburg (seminar), 1994
 Department of Mechanical Engineering, Johns Hopkins University (colloquium), 1994
 12th US National Congress on Applied Mechanics, Seattle, 1994
 Meeting on Calculus of Variations and Discontinuous Structures, Como, Italy (lecture), 1994
 38th meeting of the Society for Natural Philosophy, Cornell University, Ithaca (lecture), 1994
 31st Meeting of the Society for Engineering Science, Texas A & M University, College Station (presentations), 1994
 Adaptive Quiet Structures with Active Materials, University of Maryland (Research summary), 1994
 ASME Symposium on the Mechanics of Phase Transformations and Shape Memory Alloys, Chicago (presentation), 1994
 Applied Mechanics, Division of Applied Sciences, CalTech (colloquium), 1994
 Mathematical Problems in Micromagnetics, Freiburg, Germany (lecture and colloquium), 1994
 DMV-Seminar 1994, Lecture series on "The Mathematics of Microstructure" organized by the German Mathematical Society, Heinrich-Fabri Institut, Blaubeuren (10 lectures with J. M. Ball), 1994

RECENT INVITED LECTURES OF DAVID KINDERLEHRER

First European conference on elliptic and parabolic problems, Pont a Mousson, 1991
 Mathematical Sciences Research Institute, 1991
 Three Rivers Applied Mathematics Colloquium, 1991
 American Association for the Advancement of Science Symposium, 1991
 ICIAM Conference, 1991
 Rice University, 1991
 University of Houston, 1991
 Pont a Mousson, France June 17 First European Conference on Elliptic and Parabolic Problems
 Paris, France June 20 Coll ge de France
 Washington, DC July 12 International Conference on Industrial and Applied Mathematics
 CMU, Pittsburgh, PA Sept. 27 Inaugural Conference of the Center for Nonlinear Analysis
 Leesburg, VA Oct. 18 SIAM Conference on Mathematical Methods in Material Microstructure
 Hampton University Nov. 16 Center for Nonlinear Analysis Research Workshop
 University of Indiana Dec. 5 Colloquium, Dept. of Mathematics
 Case Western Reserve Jan. 30 Joint Colloquium, Depts of Chemical Engineering and Mathematics
 Kent State University March 6 Joint Colloquium, Liquid Crystal Institute and Dept. of Mathematics
 Pennsylvania State U. March 16 Applied Mathematics Seminar
 Rome, Italy April 8 Seminar, Istituto per le Applicazioni del Calcolo
 Rome, Italy April 10 Seminar, Istituto per le Applicazioni del Calcolo
 Edinburgh, Scotland June International Centre for Mathematical Sciences programme on Mathematical Problems in Materials Science
 West Point, NY June 18 Tenth Army Conference on Applied Mathematics and

Computing

Monterey, CA July 21 ICOMAT-92
 Kent State University, 1992, ALCOM/IMA conference on Computational Problems in Liquid Crystals
 Albuquerque, NM, 1993, SPIE Smart Structures and Materials 93
 Paris, 1993, College de France
 Metz, 1993, Metz Days
 New York, 1993, Courant Institute
 Brown, Providence, 1993
 Athens, Ohio, 1993
 Trieste, Italy, 1993
 Metz Days, Univ. de Metz, 1993
 Conference on Differential Equations, Athens, OH, 1993
 Joint TMS/ASM meeting, Pittsburgh, 1993
 Mathematical Methods for Microstructure, Institute for Advanced Study, Princeton, 1993
 SISSA conference: Homogenization and related topics, Trieste, Italy, 1993
 Spring Lecture Series (Principal lecturer), University of Arkansas, 1994
 SIAM Meeting on emerging Issues in Mathematics and Computation from the Materials Sciences, conference chair, 1994
 Conference on Industrial and Applied Mathematics, Linkoping, Sweden, 1994
 Mechanical and Analytical Microstructures, Accademia dei Lincei, Rome, 1994
 SPIE Smart Structures and Materials 94, Orlando, FL
 Joint MMM/Intermag meeting, Albuquerque, NM, 1994
 Solid/Solid Phase Transitions in Inorganic Materials 94 (TMS), Nemacolin Woods, PA, 1994
 Society of Engineering Science, 1994
 Variational methods for discontinuous structures, Como, Italy, 1994
 College de France, Paris, 1993
 Courant Institute, New York, 1993
 Brown University, Providence, 1993
 University of Minnesota (Dept. of Aerospace Engineering and Mechanics), 1993
 IAC, Rome, Italy, 1993
 Colloquium, Department of Materials Science and Engineering, CMU, 1994
 Scientific Presentation, ARO Annual Review, Research Triangle Park, 1994
 Institute for Advanced Study, Princeton, 1994

RECENT INVITED LECTURES OF MITCHELL LUSKIN

Imperial College, London, July 12, 1991
 Euromech Colloquium 283, University of Strathclyde, Glasgow, July 18, 1991
 13th IMACS World Congress on Computation and Applied Mathematics, Trinity College, Dublin, July 22, 1991
 IMA, Minneapolis, Tutorial Workshop for Special Year on Applied Linear Algebra, September 4, 1991
 Xi'an Jiaotong University, China, October 21, 1991
 Peking University, Department of Mechanics, October 24, 1991
 Academia Sinica, Applied Mathematics, October 25, 1991
 Peking University, Department of Mathematics, October 26, 1991
 Tsinghua University, October 26, 1991
 Academia Sinica, Systems Science, October 27, 1991
 Ryukoku University, Otsu, Japan, October 29, 1991
 Kyoto University, Research Institute for Mathematical Sciences, October 30, 1991
 Penn State University, Math Colloquium, November 22, 1992
 Materials Research Society Annual Meeting, Boston, December 3, 1991
 Rice University, January 29, 1992
 University of Houston, January 31, 1992
 Brown University, April 9, 1992
 University of Chicago, May 1, 1992

University of Maryland, May 7, 1992
 International Centre for Mathematical Sciences, Edinburgh, June 9, 1992
 International Centre for Mathematical Sciences, Edinburgh, June 16, 1992
 International Conference on Martensitic Transformations, Monterey, July 20, 1992
 Center for Nonlinear Analysis, Carnegie Mellon University, September 16, 1992
 Society for Natural Philosophy, Penn State University, October 3, 1992
 Liquid Crystal Institute, Kent State University, November 13, 1992
 Oberwolfach Mathematics Institute, Germany, December 7, 1992
 University of Warsaw, December 11, 1992 and December 14, 1992
 Academy of Science of the Czech Republic, Institute of Computing Sciences, Prague, December 17, 1992
 Society of Photo-Optical Instrumentation Engineers Conference on Smart Structures and Materials, Albuquerque, February 3, 1993
 University of New Mexico, February 3, 1993
 American Association for the Advancement of Science Annual Meeting, Boston, February 16, 1993
 AFOSR Meeting on Computational Mathematics, Washington University, St. Louis, May 20, 1993
 Institute for Advanced Studies in Mathematics, Technion, Israel, Workshop on Defects in Nonlinear Media, June 14, 1993
 International Colloquium on Free Boundary Problems, Toledo, Spain, June 22, 1993
 Progress in the Theory and Application of the Finite Element Method II, Chalmers University of Technology, Gothenburg, Sweden, August 28, 1993
 Center for Nonlinear Partial Differential Equations, Delft Institute of Technology, Delft, Netherlands, August 31, 1993
 The Finite Element Method: Fifty Years of the Courant Element, University of Jyväskylä, Jyväskylä, Finland, September 2, 1993
 Courant Institute, New York University, New York, December 2, 1993
 Institute for Advanced Study, Princeton, New Jersey, December 6, 1993
 University of California, Los Angeles, January 3, 1994
 SIAM Conference on Emerging Issues in Mathematics and Computation from the Materials Sciences, Pittsburgh, Pennsylvania, April 18, 1994
 Massachusetts Institute of Technology, Department of Mechanical Engineering April, 28, 1994
 Brown University, Department of Applied Mathematics April 29, 1994
 European Conference on Elliptic and Parabolic Problems, Pont-à-Mousson, France, June 13, 1994
 University of Crete, Greece June 21, 1994