



Guest editorial

Wave phenomena in physics and engineering: new models, algorithms, and applications

Wave phenomena are universal phenomena that occur in nature. They are fundamental to a better understanding of physical and engineering systems. Their studies constitute an important interdisciplinary area of research with many cutting-edge scientific and technological applications.

The Workshop on *Wave Phenomena in Physics and Engineering: New Models, Algorithms, and Applications* was sponsored by the IMACS and was held as an embedded ICCSA event in Montreal, Canada, in May 2003. Selected papers presented at this conference in the area of wave propagation were expanded beyond the conference papers and the final decision about their publication in the present special issue was based on a rigorous refereeing process. This special volume of *Mathematics and Computers in Simulation* contains 15 papers and covers a substantial subset of problems in wave propagation. Collectively, the papers in this volume cover a wide range of spatial and temporal scales and provide a number of important examples of multiscale phenomena. The reader will find in this volume many inspiring applications of wave phenomena, ranging from nano- to macro-scale, as well as their analysis with tools of mathematical modeling and computational experiment. We thank all authors for their contributions and for bearing with us during the preparation of this issue. In what follows we give an overview of this special issue of *Mathematics and Computers in Simulation*.

Many of the fundamental models for wave propagation in science and engineering are based on the Helmholtz equation. The paper by R. Kechroud, A. Soulaïmani, Y. Saad, and S. Gowda discusses 2D and 3D solutions of the harmonic Helmholtz equation by finite elements. The authors survey both absorbing and transparent boundary conditions for this equation in the context of the so-called Dirichlet-to-Neumann technique. They develop and implement an efficient numerical method and apply it to the problem of acoustic wave diffraction. They compute a stabilization parameter associated with the Galerkin-least-squares technique by using a new formula and they test the developed procedure for three different preconditioners to enhance convergence.

The active control of sound is another example of an important practical problem where models based on the Helmholtz equation play a fundamental role. The contribution by J. Lončarić and S.V. Tsynkov deals with the problem of suppressing the unwanted component of a time-harmonic acoustic field on a predetermined region of interest. The authors minimize the power required for the operation of the active control system. They show that the corresponding analysis necessarily involves interactions between the sources of sound and the surrounding acoustic media which was not the case in a situation where optimal solutions were sought to minimize the L_1 or L_2 norm of the control sources.

In the paper by L.C. Lew Yan Voon and M. Willatzen two interesting examples of applicability of the Helmholtz model in quantum mechanics and acoustics are discussed. The authors focus their attention on a domain bounded by two paraboloids where they are able to solve exactly the Helmholtz equation in parabolic rotational coordinates. Based on the developed methodology, the authors analyze the energy spectrum and wave functions of an electron in a low-dimensional semiconductor structure, known as a quantum dot, as well as the acoustic eigen-frequencies and -modes of the pressure field inside an acoustic cavity.

Wave phenomena are fundamental in studying electron transport in semiconductor structures. In the paper by M. Shen, S. Saikin, M.-C. Cheng, and V. Privman a methodology for Monte-Carlo simulation of 2D spin-polarized electron transport in sub-micron semiconductor heterostructures is presented. The electron spin polarization is described by the spin density matrix, while the spatial dynamics of the electron is treated semiclassically. The authors determine the coherent dynamics of the current spin polarization and spin dephasing by the spin–orbit interaction. They also analyze the temperature dependence of the spin dephasing length.

A better understanding of many nanotechnological applications is contingent on the development of new models and numerical methods for their solution. The paper by D. Lobao and A. Povitsky is devoted to gas dynamics modeling of the plume dynamics in laser ablation, the process that has become a popular method for production of carbon nanotubes. The authors focus on the study of thermal dynamics of catalyst particles that is crucial for the carbon nanotube formation. In this process, the carbon plume interacts with the blast shock wave originated from the laser ablation. The proposed model is solved numerically with a TVD scheme and the results of numerical experiments are analyzed with a major emphasis given to furnace geometry effects.

Nanowire superlattices provide another example of physical structures, grown experimentally, with a wide range of potential applications in nanotechnology, in particular in nanoscale electronics and photonics. In the paper by M. Willatzen, R. Melnik, C. Galeriu, and L.C. Lew Yan Voon such structures are analyzed in detail, with a major emphasis given to the qualitative differences (in terms of wavefunctions and energy eigenvalues) between symmetrical and asymmetrical structures. A special attention in this paper has been given to the examination of quantum-localization effects in nanowire superlattices for radii above, at, and below the so-called critical radius.

Fluid mechanics provides a fertile ground for studying complicated wave phenomena which should be understood better in the context of novel engineering systems. In the paper by D.L. Hitt and M. McGarry the effect of flow pulsatility on the dynamics of a laminar mixing surface formed between converging microchannel flows is studied numerically. This is an important task due to the continuing developments in micro-scale fluidic systems and MEMS. The results, obtained by the authors, demonstrate the possibility of complex wave-like interfacial distortions for high-frequency pulsations.

Different types of instabilities may arise at material interfaces. For example, the shock-induced Richtmyer–Meshkov (RM) instability arises when an interface between two fluids or gases with different densities is rapidly accelerated. This type of instability has important implications in nature (e.g., supernovae explosions) as well as in many engineering applications. It is known that an accurate simulation of such instabilities is a very challenging task. In the paper by S. Dutta, J. Glimm, J.W. Grove, D.H. Sharp, and Y. Zhang a front tracking algorithm is applied to simulating RM instabilities in spherical geometry. The authors demonstrate scaling invariance with respect to the shock Mach number for fluid mixing statistics, such as growth rate and volume fraction.

The influence of magnetic fields and cavitation on the RM type instabilities has been studied numerically in the paper by R. Samulyak and Y. Prykarpatskyy. In particular, the authors have developed a two-phase equation of state for modeling the evolution of waves in mercury in the presence of cavitation bubbles. Numerical results obtained by the authors help better understand the evolution of the proposed Muon Collider target designed as a pulsed jet of mercury interacting with high intensity proton beams in a strong magnetic field.

Aeroacoustics provides many important practical wave propagation problems. One such problem is the problem of airframe noise, in particular, in the landing phase of flight where engines do not operate at full thrust. In the paper by A. Povitsky, T. Zheng, and G.N. Vatisstas propagation of acoustic waves caused by distortion of vortices in non-uniform flows is studied numerically using a high-order compact scheme. The major emphasis is given to the analysis of vortex profile effects on sound generation. In particular, the influence of strong mean flow gradients on the directivity and strength of sound waves generated by a distorted vortex is analyzed in detail for the Taylor and Vatisstas vortex models.

Direct numerical simulations form an important ingredient to physics-based predictions of laminar-to-turbulent transitions in boundary-layer flows, particularly in applications where it is desirable, or even essential, to model the various stages of transition process in an integrated manner. The paper by L. Jiang, C.-L. Chang, M. Choudhari, and C. Liu addresses two important issues in this context: instability wave propagation in boundary layers over curvilinear surfaces and robust outflow boundary conditions across the speed regime. In particular, detailed comparisons of linear and non-linear developments of instability waves in a range of boundary layer flows are used to cross-validate a high-order direct numerical simulation algorithm against the approximate but computationally more efficient technique of the so-called parabolized stability equations. The equations are approximations to the Navier–Stokes equations for instability wave propagation in mean shear flows.

Wave propagation in solids is another area of major importance in scientific and engineering applications. In the paper by P. Matus, R. Melnik, L. Wang, and I. Rybak the dynamics of a shape memory alloy rod is analyzed numerically. The authors solve a strongly coupled model of non-linear thermoelasticity describing shape memory alloy dynamics with a fully conservative numerical scheme. They show that the traditional restrictive assumptions, resulting from a standard energy inequality technique, can be removed for the proposed scheme to achieve its unconditional convergence. The proposed approximation is used to describe a complete range of behavior of the shape memory material, including hysteresis effects.

Reaction-diffusion and combustion models provide a wide range of important problems for studying wave phenomena. The paper by L. Kagan, S. Minaev, and G. Sivashinsky analyzes numerically a three-dimensional reaction-diffusion model for premixed flames with radiative heat losses. The results of numerical simulation demonstrate that cellular flames can propagate at heat-loss rates greater than the maximum that extinguishes the planar flame. Moreover, it is shown that at sufficiently high heat losses, the flame interface can break up into separate self-drifting flame balls while a significant portion of the fuel remains unconsumed.

Wave phenomena are intrinsic to many applications in life sciences, including biology and medicine. The paper by A. Bounaïm, S. Holm, W. Chen, and Å. Ødegård describes the modeling of wave propagation in human tissues accounting for frequency-dependent attenuation, as well as the wave scattering due to a tumor. The authors carry out the numerical study of the clinical amplitude–velocity reconstruction imaging (CARI) technique that has been proposed recently for better detection of breast cancer. This technique has been experimentally verified to have higher sensitivity than conventional ultrasound and,

in the present paper, the authors analyze the CARI sensitivity with 2D and 3D numerical simulation results.

In the contribution by S. Hamdi, W.H. Enright, W.E. Schiesser, and J.J. Gottlieb, new exact solitary wave solutions are derived for general types of the regularized long wave (RLW) equation and its simpler alternative, the generalized equal width wave (EW) equation, which are evolutionary partial differential equations for the simulation of one-dimensional wave propagation in non-linear media with dispersion processes. New exact solitary wave solutions are also derived for the generalized EW-Burgers equation, which models the propagation of non-linear and dispersive waves with certain dissipative effects. The analytical solutions for these model equations are obtained for any order of the non-linear terms and for any given value of the coefficients of the non-linear, dispersive and dissipative terms.

In conclusion, the editors would like to thank the referees of this special issue for their time and their contributions in making this issue a success.

We hope that this special issue will stimulate further progress in modeling and applications of wave phenomena in science and engineering. We also hope that it will help strengthen collaboration between scientists, mathematicians, and engineers in studying new fascinating and challenging problems this interdisciplinary area offers.

Roderick V.N. Melnik

Syddansk Universitet, Campusvej 55

DK-5230 Odense M., Denmark

Corresponding author

E-mail address: rmelnik@mci.sdu.dk (R.V.N. Melnik)

Alex Povitsky

University of Akron, Auburn Science and Engineering Center

Akron, OH, 44325-3903, USA

E-mail address: povitsky@uakron.edu (A. Povitsky)



Volume 65, issues 4-5, 11 May 2004 ISSN 0378-4754

MATHEMATICS AND COMPUTERS IN SIMULATION

TRANSACTIONS OF IMACS

Special Issue:
Wave Phenomena in Physics and Engineering:
New Models, Algorithms, and Applications

Guest Editors: Roderick Melnik and Alex Povitsky



INTERNATIONAL ASSOCIATION FOR
MATHEMATICS AND COMPUTERS
IN SIMULATION

Also available on

SCIENCE  DIRECT®

www.sciencedirect.com

MATHEMATICS AND COMPUTERS IN SIMULATION

Editor-in-Chief

R. Vichnevetsky

Department of Computer Science, Rutgers University, Piscataway, NJ 08855, USA

Co-Editor-in-Chief

A. Preumont

Université Libre de Bruxelles, 50 Av. F.D. Roosevelt, CP 165/42, B-1050 Brussels, Belgium

Senior Editors

E. Mosekilde
Technical University of Denmark
Physics Department
2800 Lyngby, Denmark

Syvvert P. Norsett
Norwegian University of Science & Technology
Department of Mathematical Sciences
N-7034 Trondheim, Norway

K.K. Sabelfeld
Russian Academy of Sciences
Weierstrass Institute for Applied Analysis Stochastics
Mohrenstrasse 39, 10117 Berlin, Germany

S. Steinberg
University of New Mexico
Department of Mathematics and Statistics
Albuquerque, NM 87131, USA

Editorial Board

A. Borghese
University of Milano
Department of Computer Science
Lab. of Human Motion Analysis and Virtual Reality
Via Comelico, 39, 20135 Milano, Italy

C.K. Chui
Department of Statistics
Stanford University
Sequoia Hall
390 Serra Mall, Stanford University
Stanford, CA 94305-4065, USA

J. Elsenfeld
Department of Mathematics
The University of Texas
P.O. Box 19408, Arlington, TX 76019, USA

A. Gerasoulis
Department of Computer Science
Rutgers University
New Brunswick, NJ 08903, USA

K. Gustafson
Department of Mathematics
Box 426, University of Colorado
Boulder, CO 80309, USA

A.J. Jakeman
CRES, The Australian National University
Canberra, ACT 0200, Australia

N.A. Kuznetsov
Director, Institute for Problems of
Information Transmission
Ermolovoy Street 19
GSP-4, Moscow, 101448 - Russia

L.R. Petzold
University of California
Department of Mechanical and Environmental
Engineering
Santa Barbara
CA 93106-5070, USA

J.R. Rice
Department of Computer Science
Purdue University
West Lafayette, IN 47907, USA

G. Richter
Department of Computer Science
Rutgers University
New Brunswick
NJ 08903, USA

R. Righanti
Department of Mathematics
Politecnico di Torino
Corso Duca degli Abruzzi 24
1-10129 Torino, Italy

D. Roose
KU Leuven
Department of Computer Science
Celestijnenlaan 200A
B-3001 Heverlee-Leuven
Belgium

M. Ruschitzka
Division of Computer Science
University of California
Davis, CA 95611
USA

J. Sa da Costa
Technical University of Lisbon
Department of Mechanical Engineering Co
Instituto Superior Technico
Av. Rovisco Pais 1
P-1049-001 Lisbon
Portugal

I. Troch
Technische Universität Wien
Wiedner Hauptstrasse 8-10/114
A-1040 Wien
Austria

S. Tzafestas
Intelligent Robotics and Control Unit
Computer Science Division
National Technical University of Athens
Zografou 15773
Athens
Greece

J. Vignes
Université Pierre et Marie Curie
4 Place Jussieu
F-75230 Paris Cedex 05
France

P.A. Whitlock
Computer and Information Science Dept.
2900 Bedford Avenue
Brooklyn, NY 11210
USA

Aims: The aim of the Journal is to provide an international forum for the dissemination of up-to-date information in the fields of Mathematics, Computers, in particular (but not exclusively) as they apply to the dynamics of systems, their Simulation and scientific computation in general. Published material ranges from short, concise research papers to more general tutorial articles.

MATHEMATICS AND COMPUTERS IN SIMULATION, published monthly, is the official organ of the International Association for Mathematics and Computers in Simulation (formerly AICA). This Association, founded in 1956, is a member of FIACC (the Five International Associations Coordinating Committee), together with IFIP, IFAC, IFORS and IMEKO.

Scope: Topics covered by the journal include mathematical tools (a) in the foundations of systems modelling, (b) in specific applications in engineering, and (c) in numerical analysis and the development of algorithms for simulation. They also include considerations (d) about computer hardware for simulation (digital, analog and hybrid) and (e) about special software and compilers. Finally, the journal publishes (f) with the general philosophy of systems simulation, and its impact on disciplinary and interdisciplinary research. The journal includes a Book Review section. Articles, reports and books from the international press in the disciplinary area of Mathematics and Computers in Simulation are reported.

© 2004, IMACS/Elsevier B.V. All rights reserved

The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper)

Printed in the Netherlands

doi:10.1016/S0378-4754(04)00108-9

TRANSACTIONS OF IMACS

Volume 65, Issues 4–5
11 MAY 2004

Special Issue:
Wave Phenomena in Physics and Engineering:
New Models, Algorithms, and Applications

Guest Editors:
Roderick Melnik and Alex Povitsky



ELSEVIER

Amsterdam · Boston · Jena · London · New York · Oxford ·
Paris · Philadelphia · San Diego · St. Louis



INTERNATIONAL ASSOCIATION FOR
MATHEMATICS AND COMPUTERS IN SIMULATION

MATHEMATICS AND COMPUTERS IN SIMULATION
VOLUME 65, ISSUES 4-5, 11 MAY 2004

Abstract/indexed in: ACM Computing Reviews, CAD/CAM Abstracts, Cambridge Scientific Abstracts, CompuMath Citation Index[®], Compuscience, Computer Abstracts, Current Contents[®] – Engineering, Computing & Technology Edition, Engineering Index/Compendex, INSPEC Information Services, ISI Alerting ServicesSM, Mathematical Reviews, Science Citation Index ExpandedTM, SciSearch[®], Statistical Theory and Method Abstracts, Web of ScienceSM, Zentralblatt für Mathematik

Special Issue:

**Wave Phenomena in Physics and Engineering:
New Models, Algorithms, and Applications**

Guest Editors: Roderick Melnik and Alex Povitsky

CONTENTS

Editorial	299
<i>R. Kechroud, A. Soulaïmani, Y. Saad and S. Gowda</i> Preconditioning techniques for the solution of the Helmholtz equation by the finite element method	303
<i>J. Lončarić and S.V. Tsynkov</i> Optimization of power in the problems of active control of sound	323
<i>L.C. Lew Yan Voon and M. Willatzen</i> Helmholtz equation in parabolic rotational coordinates: application to wave problems in quantum mechanics and acoustics	337
<i>M. Shen, S. Saikin, M.-C. Cheng and V. Privman</i> Monte Carlo modeling of spin FETs controlled by spin-orbit interaction	351
<i>D.C. Lobão and A. Povitsky</i> Furnace geometry effects on plume dynamics in laser ablation for nanotube synthesis	365
<i>M. Willatzen, R.V.N. Melnik, C. Galeriu and L.C. Lew Yan Voon</i> Quantum confinement phenomena in nanowire superlattice structures	385
<i>D.L. Hitt and M. McGarry</i> Numerical simulations of laminar mixing surfaces in pulsatile microchannel flows	399

CONTENTS
direct

This journal is part of **ContentsDirect**, the *free* alerting service which sends tables of contents by e-mail for Elsevier books and journals. You can register for **ContentsDirect** online at: <http://contentsdirect.elsevier.com>

<i>S. Dutta, J. Glimm, J.W. Grove, D.H. Sharp and Y. Zhang</i> Spherical Richtmyer-Meshkov instability for axisymmetric flow	417
<i>R. Samulyak and Y. Prykarpatskyy</i> Richtmyer-Meshkov instability in liquid metal flows: influence of cavitation and magnetic fields	431
<i>A. Povitsky, T. Zheng and G.H. Vatistas</i> Effect of vortex profile on sound generation in a non-uniform flow	447
<i>L. Jiang, C.-L. Chang, M. Choudhari and C. Liu</i> Instability-wave propagation in boundary-layer flows at subsonic through hypersonic Mach numbers	469
<i>P. Matus, R.V.N. Melnik, L. Wang and I. Rybak</i> Applications of fully conservative schemes in nonlinear thermoelasticity: modelling shape memory materials	489
<i>L. Kagan, S. Minaev and G. Sivashinsky</i> On self-drifting flame balls	511
<i>A. Bounaïm, S. Holm, W. Chen and Å. Ödegård</i> Quantification of the CARL breast imaging sensitivity by 2D/3D numerical time-domain ultrasound wave propagation	521
<i>S. Hamdi, W.H. Enright, W.E. Schiesser and J.J. Gottlieb</i> Exact solutions and invariants of motion for general types of regularized long wave equations	535
News of IMACS	547
IMACS Calendar of Events	549