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CRM PROCEEDINGS & LECTURE NOTES

Centre de Recherches Mathématiques
Université de Montréal

Quantum Control: Mathematical and Numerical Challenges

CRM Workshop
October 6–11, 2002
Montréal, Canada

André D. Bandrauk
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The Centre de Recherches Mathématiques (CRM) of the Université de Montréal was created in 1968 to promote research in pure and applied mathematics and related disciplines. Among its activities are special theme years, summer schools, workshops, postdoctoral programs, and publishing. The CRM is supported by the Université de Montréal, the Province of Québec (FCAR), and the Natural Sciences and Engineering Research Council of Canada. It is affiliated with the Institut des Sciences Mathématiques (ISM) of Montréal, whose constituent members are Concordia University, McGill University, the Université de Montréal, the Université du Québec à Montréal, and the Ecole Polytechnique. The CRM may be reached on the Web at www.crm.umontreal.ca.

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Preface

The workshop "Quantum Control: Mathematical and Numerical Challenges" took place at the Centre de recherches mathématiques of the Université de Montréal from October 6 to 11, 2002. It was an interdisciplinary, interuniversity and international event co-organized by André Bandrauk (Canada Research Chair, Université de Sherbrooke), Michel C. Delfour (CRM and DMS, Université de Montréal), and Claude Le Bris (École Nationale des Ponts et Chaussées, Paris, France) and co-sponsored by the three institutions through the *Natural Sciences and Engineering Research Council of Canada*[1] and the *French Ministère de la Recherche*[2]. The meeting involved more than 30 international experts and speakers in laser molecule interactions, and optimization, theory and control of molecular dynamics and emphasized participation of graduate students (18) and postdoctoral fellows (12) in applied mathematics, theoretical chemistry and physics through special grants to attend the workshop.

The workshop concentrated on advanced numerical methods and new mathematical control and optimization approaches and tools for the quantum control of matter at the molecular level using current advanced laser technology. An entirely new branch of science now known as *Laser Control of Molecular Processes* following the pioneering work of theoretical chemists such as Paul Brumer (Toronto), Herschel Rabitz (Princeton), Stuart A. Rice (Chicago), Moshe Shapiro (Weizmann Institute), and David Tannor (Weizmann Institute) is steadily making an impact on the experimental and technological world, with many outstanding contributions by internationally distinguished scientists. In parallel, mathematicians from control theory and numerical simulation, following the track opened by Jacques-Louis Lions (Collège de France), got progressively involved in this scientific endeavour and contributed to it. This conjunction of efforts motivated this workshop.

This new field of research is dedicated to *using current state of the art laser technology to control and manipulate the quantum behaviour and motion of matter at the molecular level.* The basis of this new science is the *encoding and control of quantum information* at the molecular level in order to control the time evolution of molecular processes, such as guiding the final output of a reaction to a desired target. Most of the research in this area has been numerical and theoretical, involving multidimensional time-dependent Schrödinger equations (TDSE). Coupling these molecular processes to the laser field equations (Maxwell's equations) results in a complex system of time-dependent partial differential equations. There

[1]In particular the NSERC Strategic Grant on *Molecular dynamics and photonics*, principal investigator, André Bandrauk.

[2]Une action concertée incitative jeunes chercheurs 1999, *Contrôle par laser des réactions chimiques* of the *Ministère de la Recherche* (France), principal investigator, Claude Le Bris.

are outstanding problems, both numerical and mathematical, that this workshop addressed by bringing together mathematicans, theoretical chemists and physicists working in the area of control and optimization of systems subject to quantum laws.

The co-organizers would like to thank the staff of the Centre de recherches mathématiques: Louis Pelletier, Guy Saint-Pierre and Josée Laferrière for the superb organization and the smooth administrative follow-up of the meeting and Louise Letendre who was responsible for the production and the very professional technical editorship of the present volume of proceedings. Finally we would like to thank the vice-recteur Alain Caillé for his support of the meeting through a special grant.

André Bandrauk
Michel C. Delfour
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August 2003

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An entirely new branch of science now known as *Laser Control of Molecular Processes* is steadily making an impact on the experimental and technological worlds, with internationally distinguished scientists making many outstanding contributions. In parallel, mathematicians from control theory and numerical simulation are getting progressively involved and making their contributions to this scientific endeavor.

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The volume is suitable for graduate students and research mathematicians interested in mathematical methods of control of molecular processes. It will also be useful to chemical engineers and chemists working in control and optimization of systems.

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