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PREFACE

Mathematical and computational methods with applications in chemistry and physics

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It is with pleasure that we offer the readers of the Journal of Mathematical Chemistry this Special Issue consisting of eight selected contributions to *Mathematical and computational methods with applications in chemistry and physics* presented at the 9th International Conference of Computational and Mathematical Methods in Science and Engineering, CMMSE-2009, held at Gijon, Spain, June 30–July 3, 2009. This particular Special Issue is another in a series of Special Issues dating back to CMMSE-2002 [1–6].

Since its inception in 2000, the International Conference of Computational and Mathematical Methods in Science and Engineering has been a multi-disciplinary conference, covering all numerical areas of science and engineering. In chemistry and physics the focus has been on the development of novel mathematical and computational methods and on the application of existing mathematical and computational methods to novel chemical and physical systems. The aim of CMMSE is to encourage cross-fertilization between different disciplines and to gain new insights into the emerging developments in mathematical and computational methods. New developments will be required to examine the ever more complicated science and engineering problems arising in our society.

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In this Special Issue, the first two articles are mathematical studies of highly nonlinear physical systems. The first article, by Ramos et al. develops a novel algorithm for finding the numerical solution of a class of singularly perturbed systems. The second article, by Guirao and Lampart, examines the nonlinear dynamics of a coupled lattice system which is related to the Belusov-Zhabotinskii reaction.

The next two articles are computational studies of novel chemical systems. The third article, by Yeguas et al. examines substituted N-confused porphyrins and shows that, in contrast to their non-substituted counterparts, there is no direct correlation between stability and aromaticity. The fourth article, by Laurrabaquio et al. demonstrates the extreme stability of $M@Si_{16}$ clusters and explores the possibility of using these clusters as building blocks for the construction of optoelectronic devices.

The next three articles are mathematical studies of nonlinear chemical systems. The fifth article, by Escobedo and Fernández, obtains explicit expressions of the optimal controls for a deterministic model of chemical birth and growth processes. The sixth article, by Lima and Morgado, examines a class of singular boundary value problems which model oxygen diffusion in a cell and constructs stable shooting algorithms to find solutions in the neighborhood of singularities. The seventh article, by Ray-Ronco et al. examines neutron activation analysis of fluorspar and develops a mathematical method to design the neutron activation procedure.

The eighth article, by Di Blasi et al. examines the numerical behavior of Smoothed Particle Hydrodynamics calculations and develops corrective strategies to address the particle inconsistency problem which can cause loss of accuracy in numerical solutions.

The aim of CMMSE, to encourage cross-fertilization between different disciplines and to gain new insights into the new developments in mathematical and computational methods, is well illustrated by the eight articles that have been selected for this Special Issue. We hope that the readers of JCM will find them both interesting and informative.

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