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Foreword

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Advances in experimental and computational capabilities have led to an explosion in dynamical information in chemical sciences that has energized new approaches in mathematical and computational analysis in this area. A particularly stimulating and fruitful area that is making interesting connections with the areas of geometry and analysis in classical and quantum mechanics is the development of a geometrical phase space setting for chemical dynamics.

Specific areas of mathematics that are impacting modeling, analysis, and computation in chemical systems include achieving an understanding of the phase space structure of multidimensional Hamiltonian systems and the classical-quantum correspondence, the use of Lagrangian descriptors for discovering phase space structure, exploring the dynamical significance of new invariants in symplectic dynamics (e.g., the symplectic camel), understanding the dynamical significance of higher index saddles on potential energy surfaces, exploring the role of contact geometry, non-Hamiltonian dynamics, geometric integrators, thermostats and nonholonomic mechanics in modeling and analyzing reaction dynamics, and understanding trajectory methods for quantum dynamics (e. g., Bohmian mechanics).

The papers in this two-part Special Issue on Nonlinear Dynamics in Chemical Sciences contribute to various aspects of these topics.

Several papers in the first part address the topic of geometrical aspects of chemical reaction dynamics, especially the significance of invariant phase space structures such as normally hyperbolic invariant manifolds (NHIMs). Lyu et al. investigate the role of saddle-node bifurcations in the potential for a model of a dissociation reaction, while Kuchelmeister et al. explore the nature of NHIMs in a periodically driven isomerization reaction. The role of higher index (rank 2) saddles in chemical dynamics is an important and timely topic, and Rashmi et al. condider a model for conformational isomerization in the molecule guanidine.

Non-Hamiltonian dynamics is important in the theory and application of deterministic thermostats such as the Nosé – Hoover thermostat, and fractal structure in phase space is an intriguing aspect of nonequilibrium thermostatted systems. The Hoovers provide an account of their work on the Baker Map, addressing the question of the validity of the Kaplan – Yorke conjecture.

Topological properties of the lattice of quantum states such as monodromy have been shown to be important in the spectroscopy of rotation-vibrating molecules. A detailed study of the energy-momentum map and energy band rearrangement for 2 coupled angular momenta is given by Dhont et al.

Finally, the classical mechanics of the Bohmian formulation of quantum mechanics, which can be considered to be a nonlocal hidden variable theory, is explored by Contopoulos et al., who investigate the existence of chaos in Bohmian trajectories for quantum states of simple oscillators.

We hope that the papers in this special issue will stimulate further investigations on these and other topics in this rapidly developing area of multidisciplinary research.

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