

PREFACE

Molecular modelling is undoubtedly a scientific field of growing importance, which has a high potential impact on many engineering and life sciences.

It comprises topics as various as nuclear physics, computational quantum chemistry, numerical statistical mechanics, multiscale modelling. It is closely connected to physics, chemistry, biology, materials science. The problems of molecular modelling, diverse in physical nature, are also very diverse in mathematical nature and in numerical nature. They involve high-dimensional partial differential equations, nonlinear optimization problems, stochastic analysis, and advanced linear algebra, linear and nonlinear programming, geometric integration, Monte-Carlo techniques, *etc.*

The recent years have witnessed a continuous effort of several research groups of applied mathematicians worldwide to study the models from the theoretical viewpoint and assess the quality of the numerical approaches. Both enterprises aim to, possibly, improve the efficiency of the simulations. The present special issue of M2AN collects eleven contributions all over the broad spectrum of problems of molecular modelling. Traditionally, the mission of this journal is to publish research papers of high scientific quality in the two fields of Mathematical Modelling and Numerical Analysis. The papers must present mathematical models or numerical methods that are both practically efficient and based on a rigorous theoretical foundation. The edition of a special issue on a new and lively field such as molecular modelling speaks volume. It is time for such problems to become a subject matter for applied mathematicians, as *e.g.* continuum mechanics and theoretical physics have been being for decades. Such a publishing endeavour will certainly foster interactions between practitioners of molecular modelling and applied mathematicians, for the shared benefit of the two communities.

The table of contents of this special issue reflects the diversity of problems mentioned above.

The volume opens with five contributions addressing various approaches for the calculation of electronic structures of atomic and molecular systems. The first two contributions, *Diffusion Monte-Carlo methods: numerical analysis in a simple case* by M. El Makrini, B. Jourdain and T. Lelièvre, and *Sparse grids for the Schrödinger equation* by M. Griebel and J. Hamaekers, deal with the resolution of the Schrödinger equation itself. The first one analyzes Monte-Carlo type techniques for determining the ground-state electronic wavefunction. The second one presents recent developments of techniques well-known for their success in the integration of many high-dimensional problems of the engineering sciences and their adaptation to the quantum chemistry context.

But the direct attack of the Schrödinger equation is already a challenge for systems of moderate size. The dominant approach then, is to treat approximations of the Schrödinger equation. The next three contributions of this issue indeed treat such approximations, from various standpoints. Two of these are authored by researchers in chemistry, which exemplifies the interdisciplinary character of the volume, and of the field. These contributions are: *First-order semidefinite programming for the two-electron treatment of many-electrons atoms and molecules* by D. Mazziotti, *Best N-term approximation in electronic structure calculations. II. Jastrow factors* by H.-J. Flad, W. Hackbusch and R. Schneider, *Converging self-consistent field equations in quantum chemistry: recent achievements and remaining challenges* by K. Kudin and G. Scuseria.

With the next two papers, the issue focuses on some theoretical aspects of time dependent problems. The Born-Oppenheimer approximation, time-dependent version of the clamped nuclei approximation is studied in the contribution by G. Panati, H. Spohn and S. Teufel, *The time-dependent Born-Oppenheimer approximation*. On the other hand, the theoretical well-posedness of the time dependent version of a very well known static

approximation, the Hartree model, is the topic of *Regularity of the multi-configuration time-dependent Hartree approximation in quantum Molecular Dynamics* by O. Koch and C. Lubich.

Next, problems in numerical statistical mechanics are considered. The question of the evaluation of macroscopic thermodynamics coefficients from ensemble averages is addressed by two contributions, both with a self-explanatory title: *Molecular simulation in the canonical ensemble and beyond*, by Z. Jia and B. Leimkuhler, *Theoretical and numerical comparison of some sampling methods for molecular dynamics* by E. Cancès, F. Legoll and G. Stoltz. The topics of these contributions already demonstrate the connection between molecular modelling at the microscopic scale and problems at a larger scale.

The final two contributions complement this connection, presenting two very different aspects of the intimate links between molecular modelling techniques and computational materials science. The one I co-authored with X. Blanc and C. Le Bris, *Atomistic to continuum limits for computational materials science*, summarizes some existing theoretical endeavour, while that by E. Silva, C. Först, J. Li, X. Lin, T. Zhu and S. Yip, *Multiscale materials modelling: case studies at the atomistic and electronic structure levels* concentrates on applications.

Overall, this special issue is a very appropriate place for experts to learn about the most recent and advanced developments of their field, presented in a mathematically-oriented manner. It is also an excellent opportunity for applied mathematicians not familiar with molecular modelling to discover an incredibly rich, still mostly unexplored, field. I am convinced you will enjoy reading this special issue, and I am already looking forward the next such enterprise.

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