Cambridge International
Science Publishing
Cambridge CB1 6AZ
Great Britain

Journal of Computational Methods in Sciences and Engineering
vol. 2, no. 3s-4s, 2002, p. ii
ISSN 1472–7978

Foreword

Computational Chemistry is a discipline aiming at the development and the understanding of Chemistry based on the exploitation of the potentialities of computational methods and techniques. This innovative approach takes from the experiment the ability of producing news insight into natural phenomena by means of observation of events under controlled conditions and takes from theory the principles and the methodologies for building simulated events.

The present richness of Computational Chemistry is, therefore, grounded on the continuous advance in theoretical achievements as well as on the rapid development of computational tools. Accordingly, the relevance of this approach to Science is twofold. The possibility of testing theoretical assumptions in realistic contexts and the possibility of fully mimicking complex system in an a priori fashion. This makes Computational Chemistry relevant to the progress of almost all the science and engineering disciplines.

It is now widely accepted that the various aspects of Computational Chemistry deserve an ad hoc European Conference. This European Conference on Computational Chemistry is now in its fourth edition (EUCO-CC4) and it has developed from a "mainly theory" (at its beginning) into a broader spectrum event in which not only the increasing power of the computer hardware has made the difference in the quantity and the accuracy of the results delivered but also the evolution of computing platforms towards parallel and distributed architectures has radically changed the approach to computing in Chemistry and the subjects treated.

For this reason this issue of the Journal of Computational Methods in Sciences and Engineering(JCMSE) hosts a variety of papers reflecting the broad spectrum of subjects proposed for oral presentation at EUCO-CC4. We thought that, like in other Computational Science Conferences, the process of selecting oral presentations should be more visible by making them available beforehand as papers. We hope that this effort is successful. We are aware that our inexperience and the shortage of time might have caused some problems to both the authors and the referees. We apologize for that and for the fact that this issue of the Journal on Computational Methods in Sciences and Engineering may not be at the highest level possible. We are, however, grateful to the many eminent scientists who have contributed to it by delivering their state of the art representation of Computational Chemistry. We are also grateful to the referees for their patient work performed so properly in spite of the shortage of time. We, finally, hope that our effort can contribute to the success of the Conference.

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