J Math Chem (2012) 50:379–380
DOI 10.1007/s10910-011-9964-7

GUEST EDITORIAL

Computer science and mathematics for chemistry-related applications

Jesús Vigo-Aguiar · Ian Hamilton · Stephen K. Gray

Published online: 7 January 2012

Continuing the series of conferences on computational mathematics and its applications, the "11th International Conference on Computational and Mathematical Methods in Science and Engineering" (CMMSE 2011) was held in Alicante (Spain), from 26 to 30 June 2011. A special session on "Computer science and mathematics for chemistry-related applications" was attended at this event. Rapid advances in hardware, software and mathematical tools and algorithms are making significant contributions to the development of computational models for chemistry-related applications. The objectives of the session were to enhance the communication between experimental chemistry-related research and computational work on applications.

We are pleased to offer readers of *Journal of Mathematical Chemistry* this Special Issue consisting of some of the most significant contributions in computational chemistry at CMMSE 2011. This special issue is another in a line of CMMSE Special Issues (see [1–8]).

The articles contained in this volume come from applied scientists dedicated to research progress in areas related to computational mathematics and its applications. We are pleased to present five excellent papers from invited speakers:

J. Vigo-Aguiar (✉)
Facultad Ciencias, Universidad Salamanca, Salamanca E37008, Spain
e-mail: jvigo@usal.es

I. Hamilton
Department of Chemistry, Wilfred Laurier University, Waterloo, ON N2L 3C5, Canada
e-mail: ihamilton@wlu.ca

S. K. Gray
Chemical Sciences and Engineering Division, Argonne Laboratory, 9700 South Cass Avenue, Argonne, IL 60439, USA
e-mail: gray@tcg.anl.gov

In "Dynamic optimization of a gas-liquid reactor" B. Cantó presents a mathematical model of a semi-batch GL reactor where the structural properties and the stability of the model are studied.

In "Design for an asymmetrical cyclic neutron activation process for determining fluorite grade in fluorspar concentrate" M. Castro-García discusses a new asymmetrical neutron activation process for determining fluorite grade in samples of fluorspar concentrate, showing important differences between the conventional symmetrical cyclic activation method and this new method.

In "Detecting point sources in CMB maps using an efficient parallel algorithm" P. Alonso develops an efficient algorithm for detecting point sources in cosmic microwave background maps.

In "Peptide structure prediction using distributed volunteer computing networks" Timo Strunk presents a scheme that can reliably predict peptide structure using a physical free-energy based approach for peptides of very different structure, including collapsed folds without apparent secondary structure.

In "Numerical behavior of a linear mixed kinetic-diffusion model for surfactant adsorption at the air-water interface" J. Fernández et al. use the finite element method and the backward Euler scheme to study the surfactant behaviour at the air-water interface, taking into account the mixed kinetic diffusion model evolving to the Henry isotherm.

We believe that this collection of articles will be useful and informative in presenting new perspectives and trends in computational chemistry. We hope that it provides enjoyable reading, and that it can also serve as inspiration for new outcomes in this area.

Finally, as guest editors, we would like to express our gratitude to all the authors and referees for their help in contributing excellently to these proceedings. We also greatly appreciate the help and encouragement received from Prof. P.G. Mezey (Editor-in-Chief, JOMC) in editing this Special Issue.

References

1. J. Vigo-Aguiar, J.L.G. Guirao, (eds.), *Advances in Computational and Mathematical Chemistry*. Special issue CMMSE-2010 (this volume)
2. P. Alonso, I.P. Hamilton, J. Vigo-Aguiar, (eds.), Mathematical and computational methods with applications in chemistry and physics. Special issue CMMSE-2009. J. Math. Chem. **48**(1), (2010)
3. J. Vigo-Aguiar, E.J. Brändas, (eds.), Mathematical and computational tools in theoretical chemistry. Special issue CMMSE-2008. J. Math. Chem. **48**(1), (2010)
4. J. Vigo-Aguiar, B.A. Wade, (eds.), Special issue CMMSE-2005. Dedicated to Prof. Erkki J. Brändas. J. Math. Chem. **40**(1), (2006)
5. J. Vigo-Aguiar, Special issue on computational and mathematical methods in science and engineering (CMMSE-2004). J. Comput. Appl. Math. **192**(1), (2006)
6. J. Vigo-Aguiar, B.A. Wade, Recent advances in computational and applied mathematics in science and engineering. Int. J. Comput. Math. **85**(3–4), (2008)
7. J. Vigo-Aguiar, G. VandenBerghe, Advances in computational and mathematical methods in science and engineering. J. Comput. Appl. Math. **235**(7), (2011)
8. T.E. Simos, J. Vigo-Aguiar, Special issue—selected papers from the conference on computational and mathematical methods for science and engineering (CMMSE-2002). J. Comput. Appl. Math. **158**(1), (2003)