



Journal of Computational Methods in Sciences and Engineering

Aims and Scope

The major goal of the *Journal of Computational Methods in Sciences and Engineering (JCMSE)* is the publication of new research results on computational methods in sciences and engineering. Common experience had taught us that computational methods originally developed in a given basic science, e.g. physics, can be of paramount importance to other neighbouring sciences, e.g. chemistry, as well as to engineering or technology and, in turn, to society as a whole. This undoubtedly beneficial practice of interdisciplinary interactions will be continuously and systematically encouraged by the *JCMSE*. Moreover, the *JCMSE* shall try to simultaneously stimulate similar initiatives, within the realm of computational methods, for knowledge transfer from engineering to applied as well as to basic sciences and beyond. The journal has four sections and welcomes papers on (1) Mathematics and Engineering, (2) Computer Science, (3) Biology and Medicine, and (4) Chemistry and Physics.

Editors-in-Chief

Prof. Theodore Elias Simos
Department of Computer Science and Technology
Faculty of Sciences and Technology
University of Peloponnese
GR-221 00 Tripolis Campus
Greece

Prof. George Maroulis
Department of Chemistry
University of Patras
GR-26500 Patras
Greece

Editorial Assistant

Mrs. Eleni Ralli-Simos

Mathematics and Engineering and Computer Science

Prof. Theodore Elias Simos

Senior Editors

G. Fairweather, N. Hadjisavvas, P. Mezey.

Editors

K.J. Bathe, F. Brezzi, M. Calvo, R. De Borst,

F.L. Demkovicz, M.J. Donahue, J.M. Ferrandiz,
I. Gladwell, B. Gustafsson, G.R. Johnson,
A.Q.M. Khaliq, R.W. Lewis, R. Mickens, G. Psihoyios,
B.A. Wade, J. Xu.

Biology and Medicine and Chemistry and Physics

Prof. George Maroulis

Senior Editors

D. Bonchev, S. Canuto, B. Champagne, M.L. Coote,
M. Nakano, M.G. Papadopoulos, C. Pouchan,
P. Schwerdtfeger, Z. Slanina, F. Wang, A. Zdetsis.

Editors

Y. Aoki, P.-O. Åstrand, T. Bancewicz, P. Calaminici,
V. Cherepanov, R. Fournier, P. Fuentealba, S.K. Ghosh,
F.L. Gu, K. Harigaya, U. Hohm, O. Ivanciuc, L. Jensen,
J. Kobus, Z.R. Li, M. Meuwly, M.A. Nunez, P. Piecuch,
M. Safronova, M. Swart, H. Tatewaki, A. Thakkar, H. Torii,
M. Urban, W.F. Van Gunsteren, M. Weiser, T. Wesolowski,
K. Wu, J. Yong Lee.

Submission of Papers

Authors are requested to send papers on Mathematics and Engineering and Computer Science to Prof. Theodore Elias Simos; simos@uop.gr and papers on Biology and Medicine and Chemistry and Physics to Prof. George Maroulis; maroulis@upatras.gr.

Subscription Information

Journal of Computational Methods in Sciences and Engineering (ISSN 1472-7978) will be published in 1 volume of 6 issues in 2010 (Volume 10). Institutional subscription (print and online): €657 / US\$922 (including postage and handling). Institutional subscription (online only): €600 / US\$840

Abstracted / Indexed in

Chemical Abstracts, Inspec, Mathematical Reviews,
MathSciNet, Zentralblatt MATH.

Recent Contents Volume 8, Number 4-6 (2008)

On the accuracy of Monte Carlo Potts models for grain growth / *Q. Yu, M. Nosonovsky and S.K. Esche*

High order nonlinear solver / *B. Neta and A.N. Johnson*

Investigating the prognostic accuracy of standardized data mining algorithms in intensive care unit / *L.G. Gortzis, F. Sakellaropoulos, I. Ilias, K. Stamoulis, P. Lyberopoulos and I. Dimopoulou*

The depleted hydrogen atoms in chemical graph theory / *L. Pogliani*

Inherent restrictions of the Hylleraas-Undheim-MacDonald higher roots, and minimization functionals at the excited states / *N.C. Bacalis, Z. Xiong and D. Karaoulanis*

First hyperpolarizability of donor-acceptor substituted aromatic backbone molecular systems: Effect of dihedral angle and excitation energy / *D. Makwani and R. Vijaya*

Theoretical investigation of the alkali-dimer cation K_2^+ : Potential energy, dipole moment and atomic polarizabilities / *H. Berriche, C. Ghanmi, M. Farjallah and H. Bouzouita*

Vibrational versus electronic isotropic polarizability and first hyperpolarizability of a series of cis – Ru (II) – bipyridine complexes: A non-empirical investigation / *M. Rekhis, A. Saal, C. Adamo and O. Ouamerli*

Geometric structure of the magic number clusters Li_nNa_{8-n} , Na_nK_{8-n} , and K_nLi_{8-n} / *R. Fournier*

On dispersion of nonlinear optical susceptibility for HHG in crystals / *M. Mestechkin*

✕ Order Form

Please complete this form and send it to your usual supplier or to:

IOS Press

Nieuwe Hemweg 6B
1013 BG Amsterdam
The Netherlands
Tel.: +31 20 688 3355
Fax: +31 20 687 0039
E-mail: market@iospress.nl
URL: www.iospress.nl

IOS Press c/o Accucoms US, Inc. For North America Sales and Customer Service

West Point Commons
Suite 201
Lansdale PA 19446
USA
Tel.: +1 866 855 8967
Fax: +1 215 660 5042
Email: iospress@accucoms.com

IOS
Press

Please complete this form and send it to your usual supplier or to one of the addresses on the left

Please enter my 2010 subscription to *Journal of Computational Methods in Sciences and Engineering*

- Institutional subscription (print and online): €657 / US\$922
(including postage and handling)
 Institutional subscription (online only): €600 / US\$840

Please bill me

Please charge my credit card

- Amer. Express Euro/Master Visa
Exp. Date: Security Code:
Card no.:

Name:

Address:

City/Zipcode:

Fax:

Date:

Country:

VAT no.:

Signature:

Check our website for a free electronic sample copy of *Journal of Computational Methods in Sciences and Engineering*