
Algorithmica

An International Journal in Computer Science

Volume 48 Number 4
August 2007

Special Issue

Algorithmic Methodologies for Processing
Protein Structures, Sequences, and Networks

Contents

- 301 **P. Berman, B. DasGupta, and J. Liang**
Foreword
- 303 **A. Shehu, C. Clementi, and L. E. Kavraki**
Sampling Conformation Space to Model Equilibrium Fluctuations in
Proteins
- 329 **G. Li, Z. Liu, J. Guo, and Y. Xu**
An Algorithm for Simultaneous Backbone Threading and
Side-Chain Packing
- 343 **V. Choi and N. Goyal**
An Algorithmic Approach to the Identification of Rigid Domains in
Proteins
- 363 **S. Lu, F. Zhang, J. Chen, and S.-H. Sze**
Finding Pathway Structures in Protein Interaction Networks
- 375 **N. Bouaynaya and D. Schonfeld**
Protein Communication System: Evolution and Genomic Structure
- 399 **B. Jackson and T. Jordán**
Rigid Components in Molecular Graphs
- 413 **S. Böcker and Zs. Lipták**
A Fast and Simple Algorithm for the Money Changing Problem
- 433 **L. J. Guibas and Y. Wang**
Toward Unsupervised Segmentation of Semi-Rigid Low-Resolution
Molecular Surfaces

Instructions to Authors on inside back cover

Covered in Current Contents, SCI, ISI/COMPUMATH, and
Zentralblatt für Mathematik



Springer

453 ISSN 0178-4617
48(4) 301-448

Online First
Immediately Online
www.springerlink.com

Faster publication!

Algorithmica

An International Journal in Computer Science

Subscription Information

Algorithmica is published monthly by Springer Science+Business Media, Inc. (Springer), Volumes 47–49 (4 issues each) will be published in 2007.

ISSN: 0178-4617 (print version)
ISSN: 1432-0541 (electronic version)

Subscription Rates, Orders, Inquiries:

Please contact our Customer Service department for the latest rates and pricing information:

The Americas (North, South, Central America, and the Caribbean):

MAIL: Journals Customer Service
P.O. Box 2485
Secaucus, NJ 07096, USA
TEL: 800-777-4643; 212-460-1500
(outside North America)
FAX: 201-348-4505
E-MAIL: journals-ny@springer-sbm.com

Outside the Americas:

MAIL: Journals Customer Service
Springer Distribution Center (SDC)
Haberstrasse 7
69126 Heidelberg, GERMANY
TEL: 49-6221-345-4303
FAX: 49-6221-345-4229
E-MAIL: sdc-journals@springer-sbm.com

Change of Address: Allow six weeks for all changes to become effective. All communications should include both old and new addresses (with zip codes) and should be accompanied by a mailing label from a recent issue.

Back Volumes: Prices for back volumes are available on request.

Microform Editions: Available from: University Microfilms International, 300 N. Zeeb Road, Ann Arbor, MI 48106, USA.

SpringerAlert Service: The SpringerAlert service is an innovative, free-of charge service that notifies users via e-mail whenever new SpringerLink articles and journals become available, and automatically sends the table of contents and direct links to the abstracts of a new issue of a journal in SpringerLink. Register for the SpringerAlert service at <http://www.springerlink.com/alerting>

Copyright

Submission of a manuscript implies that the work described has not been published before (except in the form of an abstract or as part of a published lecture, review, or thesis); that it is not under consideration for publication elsewhere; that its publication has been approved by all coauthors, if any, as well as—tacitly or explicitly—by the

responsible authorities at the institution where the work was carried out. Transfer of copyright to Springer becomes effective if and when the article is accepted for publication. The copyright covers the exclusive right (for U.S. government employees: to the extent transferable) to reproduce and distribute the article, including reprints, translations, photographic reproductions, microform, electronic form (offline, online), or other reproductions of similar nature.

All articles published in this journal are protected by copyright, which covers the exclusive rights to reproduce and distribute the article (e.g., as reprints), as well as all translation rights. No material published in this journal may be reproduced photographically or stored on microfilm, in electronic data bases, video disks, etc., without first obtaining written permission from Springer. The use of general descriptive names, trade names, trademarks, etc., in this publication, even if not specifically identified, does not imply that these names are not protected by the relevant laws and regulations.

An author may self-archive an author-created version of his/her article on his/her own website and his/her institution's repository, including his/her final version; however, he/she may not use the publisher's PDF version which is posted on www.springerlink.com. Furthermore, the author may only post his/her version provided acknowledgement is given to the original source of publication and a link is inserted to the published article on Springer's website. The link must be accompanied by the following text: "The original publication is available at www.springerlink.com." Please use the appropriate DOI for the article (go to Linking Options in the article, then to OpenURL and use the link with the DOI). Articles disseminated via www.springerlink.com are indexed, abstracted, and referenced by many abstracting and information services, bibliographic networks, subscription agencies, library networks, and consortia.

While the advice and information in this journal is believed to be true and accurate at the date of its publication, neither the authors, the editors, nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein. Springer publishes advertisements in this journal in reliance upon the responsibility of the advertiser to comply with all the legal requirements relating to the marketing and sale of products or services

advertised. Springer and the editors are not responsible for claims made in the advertisements published in the journal. The appearance of advertisements in Springer publications does not constitute endorsement, implied or intended, of the product advertised or the claims made for it by the advertiser.

Special regulations for photocopies in the USA. Photocopies may be made for personal or in-house use beyond the limitations stipulated under Section 107 or 108 of U.S. Copyright Law, provided a fee is paid. All fees should be paid to the *Copyright Clearance Center, Inc.*, 222 Rosewood Drive, Danvers, MA 01923, USA (WEB: <http://www.copyright.com>; FAX: 978-646-8600; TEL: 978-750-8400), stating the journal's ISSN, the volume, and the first and last page numbers of each article copied. The copyright owner's consent does not include copying for general distribution, promotion, new works, or resale. In these cases, specific written permission must first be obtained from the publisher.

The *Canada Institute for Scientific and Technical Information (CISTI)* provides a comprehensive, world-wide document delivery service for all Springer journals. For more information, or to place an order for a copyright-cleared Springer document, please contact Client Assistant, Document Delivery, CISTI, Ottawa K1A 0S2, Canada. TEL: 613-993-9251; FAX: 613-952-8243; E-MAIL: cisti.docdel@nrc.ca.

You may also contact *INFOTRIEVE* (WEB: <http://www.infotrieve.com/>; E-MAIL: orders@infotrieve.com; FAX: 310-208-5971; TEL: 800-422-4633), *UnCover*: <http://www.ingenta.com/>; *UMI*: <http://www.umi.com/>; *ISI*: <http://www.isinet.com>

Advertising

Springer, 233 Spring Street, New York, NY 10013, USA
Tel: 212-460-1572
Fax: 212-647-1898
E-mail: advertising@springer.com

Office of Publication

Springer, 233 Spring Street, New York, NY 10013, USA. Telephone: 212-460-1500;
e-mail: journals-ny@springer-sbm.com
website: springeronline.com

Production Editor: Peter Hume (Tel/Fax: 44-1493-602396; e-mail: hume@hghg98.freemove.co.uk).

Printed in the United States on acid-free paper.

© 2007 Springer Science+Business Media, Inc.

Algorithmica

An International Journal in Computer Science

Instructions to Authors

Online Manuscript Submission

Springer now offers authors, editors, and reviewers of *Algorithmica* the use of our fully web-enabled online manuscript submission and review system. To keep the review time as short as possible, we request authors submit manuscripts online to the journal's editorial office. Our online manuscript submission and review system offers authors the option to track the progress of the review process of manuscripts in real time. Manuscripts should be submitted to: <http://algo.edmgr.com>.

The online manuscript submission and review system for *Algorithmica* offers easy and straightforward log-in and submission procedures. This system supports a wide range of submission file formats: for manuscripts—Word, WordPerfect, RTF, TXT, and LaTeX; for figures—TIFF, GIF, JPEG, EPS, PPT, and Postscript. *PDF is not an acceptable file format.*

Note: In case you encounter any difficulties while submitting your manuscript online, please get in touch with the responsible Editorial Assistant by clicking on "CONTACT US" from the tool bar.

Color is published online free of charge but will only be included in the print edition when the author covers the additional expense of color printing. For an exact quote on color printing charges please contact the Production Editor.

The title page of the article should include all the authors' affiliations and the mailing address, phone, and fax numbers of the corresponding author, 5–10 key words, and a detailed abstract emphasizing the main contribution of the paper.

Footnotes other than those referring to the title or author affiliation should be avoided. If they are essential, they should be numbered consecutively.

It is suggested that the references be numbered consecutively in the order of appearance in the text. All references should be gathered together and placed after the end of the text. For journals, the following information should appear: names (including initials or first names) of all authors, year of publication, full title of paper, journal name, volume, and pages. Books cited should list author(s), year, full title, edition, publisher, and place of publication. Samples are given below:

Journals

- [1] J. Doyle and R. L. Rivest, Linear expected time of a simple union-find algorithm, *Inform. Process. Lett.*, **5** (1976), 146–148.
- [2] D. E. Knuth and A. Schönhage, The expected linearity of

a simple equivalence algorithm, *Theoret. Comput. Sci.*, **5** (1978), 281–315.

Book

- [3] A. V. Aho, J. E. Hopcroft, and J. D. Ullman, *The Design and Analysis of Computer Algorithms*, Addison-Wesley, Reading, MA, 1974, pp. 203–208.

Chapter in Book

- [4] M. J. Fischer, Efficiency of equivalence algorithms, in *Complexity of Computer Computations* (R. E. Miller and J. W. Thatcher, eds.), Plenum, New York, 1972, pp. 123–125.

Miscellaneous

Manuscripts submitted according to these instructions will reduce considerably the possibility of printer's errors in the proofs. The only corrections to be made in proofs are typographical errors. Should the author wish to correct stylistic or factual errors in proofs, he must absorb the cost. Proofs must be checked and returned to the publisher within forty-eight hours of receipt.

Twenty-five free reprints will be forwarded to the corresponding author, unless otherwise indicated. Additional reprints can be purchased by filling out the Reprint Order Form which will be sent to the corresponding author along with the proofs. Reprints are normally shipped six to eight weeks after publication of the issue in which the item appears.

Open Choice Publication

In addition to the normal publication process (whereby an article is submitted to the journal and access to that article is granted to customers who have purchased a subscription), Springer now provides an alternative publishing option: Springer Open Choice. A Springer Open Choice article receives all the benefits of a regular "subscription-based" article, but in addition is made available publicly through Springer's online platform SpringerLink. To publish via Springer Open Choice, upon acceptance please visit www.springeronline.com/openchoice to complete the relevant order form and provide the required payment information. Payment must be received in full before publication or articles will be published as regular subscription-model articles. We regret that Springer Open Choice cannot be ordered for published articles.

Algorithmica

An International Journal in Computer Science

Editor-in-Chief

Prof. Ming-Yang Kao
Department of Electrical Engineering
and Computer Science
Northwestern University
2145 Sheridan Road, Room M324
Evanston, IL 60208, USA
kao@northwestern.edu

Application Experience-Editor: **D. T. Lee**
Problems-Editor: **Bernard Chazelle**

Editorial Board

Prof. Dr. Susanne Albers
Institut für Informatik
Universität Freiburg
Georges-Köhler-Allee
79110 Freiburg, Germany

Prof. Andris Ambainis
Department of Combinatorics
and Optimization
Faculty of Mathematics
200 University Avenue West
Waterloo, Ontario
Canada N2L 3G1

Prof. Lars Arge
Department of Computer Science
University of Aarhus
IT-parken, Aabogade 34
DK-8200 Aarhus N, Denmark

Prof. James Aspnes
Department of Computer Science
Yale University
51 Prospect Street
P.O. Box 208285
New Haven, CT 06520-5285, USA

Dr. Hagit Attiya
Department of Computer Science
The Technion
Haifa 32000, Israel

Dr. Jean-Daniel Boissonnat
INRIA
Centre de Sophia Antipolis
Route des Lucioles
06565 Valbonne, France

Prof. Allan B. Borodin
Department of Computer Science
University of Toronto
Toronto, Ontario
Canada M5S 1A4

Prof. Bernard Chazelle
Department of Computer Science
Princeton University
Princeton, NJ 08544, USA

Dr. Edith Cohen
AT&T Labs – Research
Room A105
180 Park Ave., PO Box 971
Florham Park, NJ 07932-0971
USA

Prof. David P. Dobkin
Department of Computer Science
Princeton University
Princeton, NJ 08544, USA

Prof. Greg N. Frederickson
Department of Computer Science
Purdue University
West Lafayette, IN 47907, USA

Prof. Harold N. Gabow
Department of Computer Science
Campus Box 430
University of Colorado
Boulder, CO 80309, USA

Prof. Ashish Goel
Management Science and
Engineering
Stanford University
Stanford, CA 94305, USA

Prof. Leonidas J. Guibas
Department of Computer Science
Stanford University
Stanford, CA 94305, USA

Prof. John E. Hopcroft
Department of Computer Science
Room 405, Upson Hall
Cornell University
Ithaca, NY 14853, USA

Prof. Giuseppe F. Italiano
Dipartimento di Informatica,
Sistemi e Produzione
Università di Roma “Tor Vergata”
via del Politecnico 1
00 133 Roma, Italy

Prof. Tao Jiang
Department of Computer Science
and Engineering
University of California
Riverside, CA 92521, USA

Founding Editor-in-Chief (1984–2004)

C. K. Wong
IBM, Yorktown Heights, New York, USA
The Chinese University of Hong Kong, Hong Kong

Executive Committee

**John E. Hopcroft, Ming-Yang Kao, Richard M. Karp,
C. L. Liu, Franco P. Preparata**

Dr. David S. Johnson
Algorithms and Optimization
Department
AT&T Labs – Research
Room C239, 180 Park Avenue
Florham Park, NJ 07932-0971
USA

Prof. Richard M. Karp
ICSI (International Computer
Science Institute)
1947 Center St., Suite 600
Berkeley, CA 94704-1198, USA

Dr. Claire Kenyon
Department of Computer Science
Box 1910
Brown University
Providence, RI 02912, USA

Prof. Andrea S. LaPaugh
Department of Computer Science
Princeton University
Princeton, NJ 08544, USA

Prof. D. T. Lee
Institute of Information Science
Academia Sinica
Nankang, Taipei 11529
Taiwan

Prof. F. Thomson Leighton
MIT Laboratory for Computer
Science
Room NE43-328
200 Technology Square
Cambridge, MA 02139, USA

Dr. Nimrod Megiddo
Dept. K53
The IBM Almaden Research
Center
650 Harry Road
San Jose, CA 95120-6099, USA

Prof. Takao Nishizeki
Department of Information
Engineering
Faculty of Engineering
Tohoku University
Sendai 980, Japan

Prof. Rafail Ostrovsky
Department of Computer Science
University of California
Box 951596, 3732D BH
Los Angeles, CA 90095-1596
USA

Prof. Christos H. Papadimitriou
Computer Science Division
Soda Hall
University of California
Berkeley, CA 94720, USA

Prof. Ronitt Rubinfeld
Computer Science and
Artificial Intelligence Laboratory
MIT
32 Vassar Street, Bldg. 32-G698
Cambridge, MA 02139, USA

Prof. Robert Sedgwick
Department of Computer Science
Princeton University
Princeton, NJ 08544, USA

Prof. Santosh Vempala
Department of Mathematics
MIT
32 Vassar Street
Cambridge, MA 02139, USA

Prof. Jeffrey S. Vitter
School of Science
Purdue University
Mathematical Sciences Building
150 North University Street
West Lafayette, IN 47907-2067
USA

Prof. Andrew C.-C. Yao
Department of Computer Science
Princeton University
Princeton, NJ 08544, USA

Prof. Chee-Keng Yap
Courant Institute, N.Y.U.
251 Mercer Street
New York, NY 10012, USA

Aims and Scope

The development of algorithms is an integral part of computer science. The increasing complexity and scope of computer applications makes the design of efficient algorithms essential.

Algorithmica is an international journal which publishes original papers on algorithms that are either (i) theoretical papers addressing problems arising in practical areas or (ii) experimental papers that have general appeal because of their practical importance or techniques. Papers are expected to make significant contributions, judged in terms of theoretical analysis, simulations, or algorithm behavior on data from applications. The areas listed below are representative areas; papers in other areas are certainly welcome.

The fields of interest include algorithms in applied areas such as: VLSI, distributed computing, parallel processing, automated design, robotics, graphics, data base design, software tools, as well as algorithms in fundamental areas such as sorting, searching, data structures, computational geometry, and linear programming. It is expected that the areas covered by this journal will change as new technologies, methodologies, and applications develop.

In addition to these regular papers, the journal features two special sections: *Application Experience* and *Problems*.

The objective of the *Application Experience* section is to publish findings obtained from applications of theoretical results to practical situations. Included in the findings are, but not limited to, difficulties encountered in the course of the implementation or testing of algorithms, e.g., handling of degenerate cases which are often not addressed in detail but which actually occur in practice, nontrivial deviations of actual running times of the implemented algorithms from the asymptotic analytical studies, comparisons of actual performance of various algorithms proposed, and discussions of applicability of theoretical studies in practice. All submissions will be subject to the reviewing process and copies of source codes should be made available upon request by the Editor for reviewing purposes.

The *Problems* section publishes short papers presenting problems on selected topics of computer science. Special emphasis will be given to papers surveying open problems in a specific area of interest. Contributions will begin with a title and an introductory statement identifying a theme of research, followed by a list of related problems which, to the author's knowledge, are unsolved as of yet. Authors are encouraged to annotate the text with comments, background material, and appropriate references. All submissions will be subject to the reviewing process.

Special issues devoted to a single topic are also planned.