

## COMPUTER PHYSICS COMMUNICATIONS

Computer Physics Communications (CPC) publishes research papers and computer program descriptions in computational physics and physical chemistry.

### Guide for Authors

#### Useful Links

The journal's home page is located at <http://elsevier.com/locate/cpc>.

The CPC Program Library is located at <http://cpc.cs.qub.ac.uk>.

The Elsevier Editorial System (EES) is located at <http://ees.elsevier.com/cpc>.

#### Scope

Articles cover: computational models and programs in physics and physical chemistry; computational models and programs associated with the design, control and analysis of experiments; numerical methods and algorithms; algebraic computation; the impact of advanced computer architecture and special purpose computers on computing in the physical sciences; and software topics related to the physical sciences.

#### Types of contribution

Computer Physics Communications publishes the following types of papers. Special issues and conference proceedings are published on an occasional basis; enquiries should be directed to a member of the Editorial Board.

*Computational Physics Papers (CP)*. These are research papers in any area of computational physics or computational physical chemistry.

*Computer Programs in Physics Papers (CPiP)*. These are full papers describing new or revised programs to be placed in the CPC Program Library. A description of the CPC Program Library is available at <http://cpc.cs.qub.ac.uk>.

*Features articles*. These articles, which are normally arranged by invitation from an editor, are used to highlight a topical subject or to provide a review of an important body of research work that is of interest to the readership.

*New Version Announcements (NVA)*. These are short descriptions of revisions to programs in the CPC Program Library. They are intended to facilitate the rapid publication of program revisions that do not merit a full paper description.

#### Computer Programs in Physics Papers

*General*. A submitted program is expected to satisfy the following criteria: it must be of benefit to other physicists or physical chemists, or be an exemplar of good programming practice, or illustrate new or novel programming techniques which are of importance to some branch of computational physics or physical chemistry; it should be implemented in a language and executable on hardware that is widely available and well documented; it should be reliable, well engineered, and meet accepted standards for scientific programming; it should be adequately documented with comment lines and where appropriate, a separate User Manual, which together with the manuscript should make clear the structure, functionality, installation, and operation of the program. **All CPiP manuscripts must contain a Program**

**Summary section**. Further details, including a LaTeX template and Program Summary templates are available from the FAQ link at <http://cpc.cs.qub.ac.uk>.

*Program submission*. Manuscripts that describe computer programs and NVAs must be accompanied by: the program source code; job control scripts, where applicable; a README file giving the names and a brief description of all the files that make up the package and clear instructions on the installation and execution of the program; sample input and output data for at least one comprehensive test run; and, where appropriate, a user manual. At present it is not possible to submit these online

through EES so they must be sent, via email as a compressed archive file, to the CPC Program Librarian at [cpc@qub.ac.uk](mailto:cpc@qub.ac.uk). Editors and reviewers can obtain a copy of the code on request from the CPC Library. The Librarian will check the quality of the code and documentation and test the program using the data provided. Should any problems be encountered the librarian will contact the author directly and work with the author to resolve the problem.

*Standard conforming Fortran programs.* In collaboration with NAG the CPC Program Library is pleased to provide free access to the NAGWare f95 compiler's syntax checker available at <http://cpc.cs.qub.ac.uk/>. Before submission of a Fortran program, the author is encouraged to use the syntax checker to ensure that the program is error free and conforms to the appropriate Fortran standard. This will help speed up the review process and ensure that the program will port successfully to any Fortran installation.

### Manuscript preparation

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CP papers - Title, Author(s), Affiliation(s), Abstract, one to four PACS codes and up to six Keywords, Main text, Acknowledgements (if any), Appendices (if any), References, Table(s) (if any), Figure captions and figures (if any).

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NVAs - Title, Author(s), Affiliation(s), Abstract, one to four PACS codes and up to six Keywords, **Program Summary**.

*References.* References to other work should be consecutively numbered in the text using square brackets. The full reference should be given in a numerical list at the end of the paper. References should be presented in the following form:

- [1] J. Stamper, D. Tidman, *Phy. Fluids* 16 (1973) 2024
- [2] F. Scheid, *Theory and Problems of Numerical Analysis* (McGraw-Hill, New York, 1968) p. 193
- [3] G. Dolling, J.L.T. Waugh, in: *Lattice Dynamics*, ed. R.F. Wallis (Pergamon, London, 1965) p. 19
- [4] W.L. Hase, D.L. Bunker, RRKM: Program 234 in *Quantum Chemistry Program Exchange Catalog* 16, Indiana Univ., Bloomington (1984), Section IX, p. 4.
- [5] K.G. Dyall, *Comput. Phys. Commun.* 39 (1996) 141.

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