

A L^AT_EX template for CPC Computer Physics Descriptions

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Abstract

A submitted program is expected to 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.

Acceptable program descriptions can take different forms. The following Long Write-Up structure is a suggested structure but it is not obligatory. Actual structure will depend on the length of the program, the extent to which the algorithms or software have already been described in literature, and the detail provided in the user manual.

Your manuscript and figure sources should be submitted through the Elsevier Editorial System (EES) by using the online submission tool at <http://www.ees.elsevier.com/cpc>.

In addition to the manuscript you must supply: 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. These should be sent, via email as a compressed archive file, to the CPC Program Librarian at cpc@qub.ac.uk.

Keywords: keyword1; keyword2; keyword3; etc.

PROGRAM SUMMARY/NEW VERSION PROGRAM SUMMARY

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Manuscript Title:
Authors:
Program Title:
Journal Reference:
Catalogue identifier:
Licensing provisions:
Programming language:
Computer:
Operating system:
RAM: bytes
Number of processors used:
Supplementary material:
Keywords: Keyword one, Keyword two, Keyword three, etc.
Classification:
External routines/libraries:
Subprograms used:
*Catalogue identifier of previous version:**
*Journal reference of previous version:**
*Does the new version supersede the previous version?:**
Nature of problem:

Solution method:

*Reasons for the new version:**

*Summary of revisions:**

Restrictions:

Unusual features:

Additional comments:

Running time:

References

[1] Reference 1

[2] Reference 2

[3] Reference 3

* Items marked with an asterisk are only required for new versions of programs previously published in the CPC Program Library.

1.

References

- [1] P. Jönsson, X. He, C. F. Fischer, I. P. Grant, The grasp2k relativistic atomic structure package, *Comput. Phys. Commun.* 177 (2007) 597–622. doi:10.1016/j.cpc.2007.06.002.