

Guidelines for Authors

Martina Kamps and Alexander Trautmann

Jülich Supercomputing Centre (JSC), Institute for Advanced Simulation (IAS),
Forschungszentrum Jülich, 52425 Jülich, Germany
E-mail: coordination-office@fz-juelich.de

This is where the abstract should be placed. It should consist of one paragraph and give a concise summary of the material in the article below. Replace the title, authors, and addresses within the curly brackets with your own title, authors, and institutes. Preferably, do not use footnotes in the abstract or the title; the acknowledgements for funding bodies etc. are placed in a separate section at the end of the text.

1 Packages

The use of L^AT_EX macro packages can change the layout of a document substantially. The following macro packages are included in the documentclass *nic-series.cls*:

times, amssymb, amstext, amsmath, ifthen, graphicx, expdlist, alltt, overcite.

If you need other macro packages, use them with care and make sure they do not affect the given layout. Please keep in mind that your and dozens of other contributions must be uniformly inserted in the NIC proceedings.

The layout specified by *nic-series.cls* must not be changed. Characters and symbols that are already defined in T_EX or by additionally loaded packages must not be redefined.

2 Formatting the Paper

The paper may be formatted using the instructions given in the following files:

<i>nic-series.cls</i>	Class file that provides the higher level latex commands for the proceedings. Don't change the parameters.
<i>guidelines.tex</i>	Guidelines for producing a manuscript, this T _E X file.
<i>article-example.tex</i>	Sample T _E X document. Note that there are two figures (<i>pd1.pdf</i> , <i>systems.pdf</i>) embedded which you need for formatting this T _E X file.
<i>nic.bst</i>	Bibliography style for BibT _E X.

Please use *article-example.tex* as a template for your own contribution. Use `pdflatex` to compile your LaTeX source and to generate immediately a PDF file.

3 Header of the Paper

The title of a contribution should be coded as follows:

`\title{<Your contribution title>}`.

All words in headings should be capitalised except for conjunctions, prepositions (e.g. on, of, by, and, or, but, from, with, without, under) and definite and indefinite articles (the, a, an) unless they appear at the beginning.

Then the name(s) of the author(s) must be given:

```
\author{<forename1 surename1>\inst{1} \and
        <forename2 surename2>\inst{2} \and ...}.
```

If there is more than one author, separate them with the `\and` command. Numbers referring to different addresses are to be attached to each author with `\inst{<no>}`. Authors have to be specified with publicised first name.

For the author list appearing in the table of contents use abbreviations for the forenames:

```
\authorshortoc{<forename1_abbr surename1>,
               <forename2_abbr surename2>, ...}.
```

Next the address(es) of the organisation(s) is (are) required. If there is more than one address, the entries are numbered automatically with `\and` in the order in which you type them:

```
\institute{<address of institutel> \and
            <address of institute2> \and ...}.
```

In addition, you may use `\email{<email>}` to append your email address to your postal address.

The command `\maketitle` then formats the complete heading of your article. For example, see the \TeX file *article-example.tex*.

4 Headings, Equations and WWW Addresses

Please preserve the style of the headings, text fonts and line spacing to provide a uniform style for the proceedings volume.

Equations are automatically numbered sequentially throughout your contribution, as in Eq. (2). The method for long sets of equations where only one referencing equation number is wanted is given in Eq. (1).

$$\begin{aligned} F(\lambda_0 | s_0, \dots, s_m) &= \int_0^{\lambda_0} f(\lambda_0 | s_0, \dots, s_m) d\lambda_0 \\ &= \frac{F(\lambda_0, s_0, \dots, s_m)}{f(s_0, \dots, s_m)} \end{aligned} \tag{1}$$

with

$$F(\lambda_0, s_0, \dots, s_m) = \int_0^{\lambda_0} f(\lambda_0, s_0, \dots, s_m) d\lambda_0 \tag{2}$$

In \LaTeX , it is simplest to give the equation a label, as in Eq. (1) where we have used `\label{author_eq:eq1}` to identify the equation. You can then use the reference `\ref{author_eq:eq1}` when citing the equation in the text which will avoid the need to manually renumber equations due to later changes.

The same method can be used for referring to sections, subsections, tables, and figures, i.e. `\ref{author_sec:prod}` for referencing Sec. 2. Please use the following abbreviations for sections, equations, figures, and tables: Sec., Eq(s)., Fig(s)., Tab(s). Append the `\ref{...}` command with `\sim` to avoid a line break.

In order to ensure the clearness of references of all contributions the name of the author should be attached to the label. Blanks in labels are not allowed.

WWW addresses should appear in true type font. Therefore use the `\url` command, i.e. `\url{http://www.fz-juelich.de/ias/jsc}`. See also Ref. 4. The symbol “~” in the `\url` command should be realised with `\homedir`.

5 Tables

We’ve chosen a more complicated example purely as an illustration of what is possible. Tables should appear centred and the caption should be below them.

Model	$\lambda_{0.05}$	$\lambda_{0.5}$	$\lambda_{0.95}$
$\alpha = 1/16, \beta = 1/16, \text{Obs. 1}$			
α, β known	11.06	13.01	15.17
$u = 3/2$	11.08	13.03	15.20
$u = 1/2, 1 < B < 10^{400}$	11.07	13.02	15.19
$u = 1/2, B > 10^{500}$	1.83	1.99	2.17
$p(\lambda) = \lambda^{-1}$	11.14	13.10	15.28
$p(\lambda) = \lambda^{-1/2}$	11.20	13.16	15.34
$\alpha = 1, \beta = 1, \text{Obs. 6}$			
α, β known	0.23	0.46	0.81
$u = 3/2$	0.23	0.46	0.82
$u = 1/2, 10 < B < 10^{20}$	0.23	0.47	0.83
$u = 1/2, B > 10^{60}$	0.98	1.09	1.22
$p(\lambda) = \lambda^{-1}$	0.19	0.42	0.77
$p(\lambda) = \lambda^{-1/2}$	0.22	0.46	0.82

Table 1. Posterior quantiles of special observations for different Bayes models.

6 Figures

If you wish to embed a figure in PDF, PNG or JPG format in a \TeX file, use the `\includegraphics` command within the figure description and change the file-name to an appropriate one. The width of the figure can be defined by the option `[width=x-size]`. \LaTeX will automatically enlarge or reduce the figure based on the `x-size` value. The figure should appear centred and the caption should be positioned underneath.

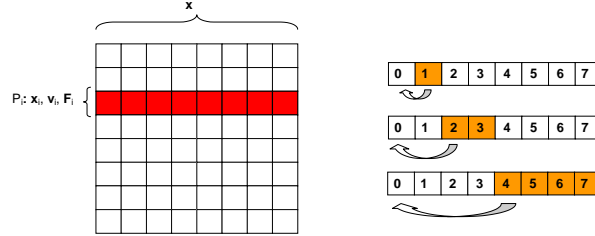


Figure 1. Integration of PDF or PNG graphics

7 Footnotes and the Bibliography

Footnotes are denoted by a letter superscript in the text^a and references are denoted by a number superscript or in special cases by a number without superscript. Using the macro package `\citesort` is not allowed.

We have used `\bibitem` to produce the bibliography. Citations in the text use the labels defined in the `\bibitem` declaration, for example, the first two papers^{1,2} are cited using the command `\cite{author_bib1,author_bib2}`. Please also attach the name of the author to the labels to ensure the clearness of references of all contributions. In special cases, e.g. see Ref. 3, the command `\citen{author_bib3}` can be used.

Please keep the sequence of the relevant information as given in this sample manuscript: author(s), title, journal, volume number, page number(s), year.

If you use a reference database and Bib_TE_X to include your bibliography into your document, you should use the bibliography style `nic.bst`.

Please use the following two commands to insert your bibliography:

```
\bibliographystyle{nic}
\bibliography{<database1>,<database2>,...}
```

Note that there is no section number for references. Furthermore, L^AT_EX will automatically generate the heading for the reference section.

Acknowledgements

This is where one places acknowledgements for funding bodies etc. Please do not forget to acknowledge the granted computing time project and the corresponding supercomputer. The acknowledgements may be placed in a separate section at the end of the text, before the Appendices. This should not be numbered, therefore use `\section*{Acknowledgements}`.

Appendix

It's preferable to have no appendices in a brief article, but if more than one is necessary then simply copy the `\section*{Appendix}` heading and type in Appendix A, Appendix B etc. between the brackets. Note that there is no section number for the appendix.

^aJust like this one.

References

1. N. Attig, M. Lewerenz, G. Sutmann, and R. Vogelsang, *Molecular Dynamics Algorithms for Massively Parallel Computers*, Proceedings of the Workshop on Molecular Dynamics On Parallel Computers, Research Centre Jülich, 8 - 10, February 1999, pp. 46-69, World Scientific, 2000.
2. D. Marx and J. Hutter, *Ab initio Molecular Dynamics: Theory and Implementation* in Modern Methods and Algorithms of Quantum Chemistry, J. Grotendorst (Ed.), John von Neumann Institute for Computing, NIC Series Vol. **3**, 329-477, 2000.
3. M. E. Tuckerman and D. Marx, *Heavy-Atom Skeleton Quantization and Proton Tunneling in "Intermediate-Barrier" Hydrogen Bonds*, Phys. Rev. Lett. **86**(21), 4946-4949, 2001.
4. <http://www.fz-juelich.de/ias/jsc>