

Guidelines for Authors

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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 acknowledgments for funding bodies etc. are placed in a separate section at the end of the text.

1 Packages

The use of \LaTeX 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

If you need other macro packages use them with caution.

2 Formatting the Paper

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

<i>nic-series.cls</i>	the 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 \TeX file.
<i>article-example.tex</i>	a sample \TeX document. Note that there are two figures (<i>pd1.pdf</i> , <i>systems.pdf</i>) you need for formatting this \TeX file.
<i>poster-example1.tex</i>	example for a poster abstract.
<i>poster-example2.tex</i>	further example for a poster abstract.
<i>nic.bst</i>	bibliography style for Bib \TeX .

You should modify the sample files with your own contribution.

Use the command `pdflatex` to compile your LaTeX source and to generate immediately a PDF file.

3 Class Option [poster]

Use the poster option for abstracts of poster presentations:

```
\documentclass[poster]{nic-series}.
```

4 Header of the Paper

The title of a contribution should be coded as follows:

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

All words in headings should be capitalized 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{author_name1\inst{1} \and  
author_name2\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>}`.

Next the address(es) of the organization(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 institute> \and  
<next institute> \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*.

5 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{eq:eq1}` to identify the equation. You can then use the reference `\ref{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 and subsections, i.e. `\ref{sec:prod}` for referencing section 2.

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 reference 4. The symbol “~” in the `\url` command should be realized with `\homedir`.

6 Tables

We’ve chosen a more complicated example purely as an illustration of what is possible.

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

7 Figures

If you wish to ‘embed’ a figure in PDF or PNG format in a \TeX file, then uncomment (% mark) the `\includegraphics` command within the figure description and change the filename to an appropriate one. Also remove the comment mark from the `[width=x-size]` option and specify the required width of the figure. \LaTeX will automatically enlarge or reduce the figure based on the `x-size` provided with the `[width= ...]` option.

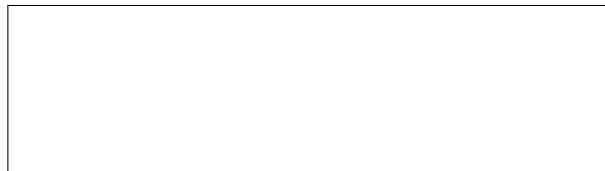


Figure 1. Integration of PDF or PNG graphics

8 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{bib1,bib2}`. In special cases, e.g. see Ref. 3, the command `\citen{bib}` can be used. Please try to 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 BibTeX 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.

Acknowledgments

This is where one places acknowledgments for funding bodies etc. The acknowledgments may be placed in a separate section at the end of the text, before the Appendices. This should not be numbered, therefore use `\section*{Acknowledgments}`.

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.

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>

^aJust like this one.