MolStat2016 Group Members

Writting Python-code in latex

Molecular Statistics

2016

For your final exam you will need to write a report as well as the code associated with your study. Some of you will probably want to write the report in LATEX. We have made this little document to show how this can be done so that your report comes out looking nice and clean.

When you have written up some Python code that you want to include in your report you can do this in the \lstlisting environment.

\begin{lstlisting}

```
# you can use comments under way to remind yourself later what the code should do.
print "I want to print this statement" # you can also comment after a line
\end{lstlisting}
```

The output of the above LATEX command is as follows:

```
# you can use comments underway to remind yourself later what the code should do
.
print "I want to print this statement" # you can also comment after a line
```

This means that you can directly copy-paste the code from you Python program into you final-report.

In order to help you set up the proper environment for the Python coding we provide the file preamble.tex, where the relevant usepackages have been imported.

The project report should include

The report is done individually, should be written in either Danish or English and be ca. 10 and no more than 20 pages long. The code associated with the study should be uploaded on the course website or emailed to the instructor. The report should be written with enough theoretical and technical background so any of your colleagues can understand what you have done, and be able to reproduce your results.

Abstract

An abstract is a brief **summary** of a research article, thesis, review, conference proceeding or any in-depth analysis of a particular subject or discipline, and is often used to help the reader quickly ascertain the paper's purpose.

1 Introduction and theory

A theoretical introduction to the subject along with motivation for the work. This includes a description of the theory and algorithms, as well as figures that could help with the understanding of the subject.

2 Implementation

Comment on what the code does and how you implemented the code. You are welcome to use code examples.

MolStat2016 Group Members

3 Results and discussion

Presentation of your results (use figures, pictures and tables). Discussion of the results. Do the results behave as expect, are there outliers and do you trust your results?

4 Conclusion

Summary of the most important findings. Perspective of your results.

- Did you achieve the goal described in the introduction?
- What would be the next step?
- Could one improve on your calculations?

You can use BibTEX for creating the references. You should cite all books Downey (2008) and web pages Heinz et al. (2015) that you've used in order to complete the report and code. Example of how to write the .bib file will be on the web page.

References

Downey, A. (2008), Think Python - ho to think like a computer scientist, Green Tea Press.

Heinz, C., Moses, B. & Hoffmann, J. (2015), 'The listings package'.

URL: http://texdoc.net/texmf-dist/doc/latex/fancyvrb/fancyvrb.pdf