PROJECT REPORT

A molecular dynamics simulation report

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ABSTRACT
This template is for authors who are preparing a report for the course "Molecular Mechanics and Multiscale Modelling of Materials" using LaTeX document preparation system and the `interact` class file.

KEYWORDS
simulation; atoms; NVE; potentials;

1. Introduction & Motivation

Here you can explain what is the motivation behind the project ...

2. Methods & Materials

Here you explain how was the model created, what are the requirements etc.

2.1. *Lists*

Numbered lists are produced using the `enumerate` environment, which will number each list item with arabic numerals by default. For example,

(1) first item
(2) second item
(3) third item

was produced by

```
\begin{enumerate}
  \item first item
  \item second item
  \item third item
\end{enumerate}
```

Alternative numbering styles can be achieved by inserting an optional argument in square brackets to each `item`, e.g. `\item[(i)] first item` to create a list numbered with roman numerals at level one.

Bulleted lists are produced using the `itemize` environment. For example,

- First bulleted item

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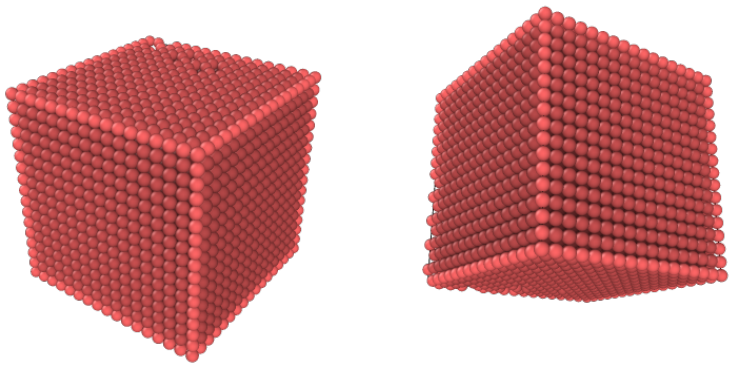

(a) An example of an individual figure sub-caption.

(b) A slightly shorter sub-caption.

Figure 1. Example of a two-part figure with individual sub-captions showing that captions are flush left and justified if greater than one line of text.

- Second bulleted item
- Third bulleted item

was produced by

```
\begin{itemize}
  \item First bulleted item
  \item Second bulleted item
  \item Third bulleted item
\end{itemize}
```

2.2. *Figures*

The `interact` class file will deal with positioning your figures in the same way as standard LaTeX. It should not normally be necessary to use the optional `[htb]` location specifiers of the `figure` environment in your manuscript; you may, however, find the `[p]` placement option or the `endfloat` package useful if a journal insists on the need to separate figures from the text.

Figure captions appear below the figures themselves, therefore the `\caption` command should appear after the body of the figure. For example, Figure 1 with caption and sub-captions is produced using the following commands:

```
\begin{figure}
\centering
\subfigure[An example of an individual figure sub-caption.]{%
\resizebox*{5cm}{!}{\includegraphics{example1.png}}}\hspace{5pt}
\subfigure[A slightly shorter sub-caption.]{%
\resizebox*{5cm}{!}{\includegraphics{example2.png}}}
\caption{Example of a two-part figure with individual sub-captions
 showing that captions are flush left and justified if greater
 than one line of text.} \label{sample-figure}
\end{figure}
```

To ensure that figures are correctly numbered automatically, the `\label` command should be included just after the `\caption` command, or in its argument.

Table 1. Example of a table showing that its caption is as wide as the table itself and justified.

	Type					
Class	One	Two	Three	Four	Five	Six
Alpha[a]	A1	A2	A3	A4	A5	A6
Beta	B2	B2	B3	B4	B5	B6
Gamma	C2	C2	C3	C4	C5	C6

[a]This footnote shows how to include footnotes to a table if required.

2.3. *Tables*

The `interact` class file will deal with positioning your tables in the same way as standard LaTeX. It should not normally be necessary to use the optional `[htb]` location specifiers of the `table` environment in your report.

The `tabular` environment can be used as shown to create tables with single horizontal rules at the head, foot and elsewhere as appropriate. The captions appear above the tables in the Interact style, therefore the `\tbl` command should be used before the body of the table. For example, Table 1 is produced using the following commands:

```
\begin{table}
\tbl{Example of a table showing that its caption is as wide as
 the table itself and justified.}
{\begin{tabular}{lcccccc} \toprule
 & \multicolumn{2}{l}{Type} \\ \cmidrule{2-7}
 Class & One & Two & Three & Four & Five & Six \\ \midrule
 Alpha\textsuperscript{a} & A1 & A2 & A3 & A4 & A5 & A6 \\
 Beta & B2 & B2 & B3 & B4 & B5 & B6 \\
 Gamma & C2 & C2 & C3 & C4 & C5 & C6 \\ \bottomrule
\end{tabular}}
\tabnote{\textsuperscript{a}This footnote shows how to include
 footnotes to a table if required.}
\label{sample-table}
\end{table}
```

To ensure that tables are correctly numbered automatically, the `\label` command should be included just before `\end{table}`.

The `\toprule`, `\midrule`, `\bottomrule` and `\cmidrule` commands are those used by `booktabs.sty`, which is called by the `interact` class file and included in the Interact LaTeX bundle for convenience. Tables produced using the standard commands of the `tabular` environment are also compatible with the `interact` class file.

2.4. *Mathematics*

2.4.1. Displayed mathematics

The `interact` class file will set displayed mathematical formulas centred on the page without equation numbers if you use the `displaymath` environment or the equivalent `\[...\]` construction. For example, the equation

$$\hat{\theta}_{w_i} = \hat{\theta}(s(t, \mathcal{U}_{w_i}))$$

was typeset using the commands

```
\[
 \hat{\theta}_{w_i} = \hat{\theta}(s(t,\mathcal{U}_{w_i}))
\]
```

For those of your equations that you wish to be automatically numbered sequentially throughout the text for future reference, use the `equation` environment, e.g.

$$\hat{\theta}_{w_i} = \hat{\theta}(s(t,\mathcal{U}_{w_i})) \tag{1}$$

was typeset using the commands

```
\begin{equation}
 \hat{\theta}_{w_i} = \hat{\theta}(s(t,\mathcal{U}_{w_i}))
\end{equation}
```

Part numbers for sets of equations may be generated using the `subequations` environment, e.g.

$$\varepsilon\rho w_{tt}(s,t) = N[w_s(s,t), w_{st}(s,t)]_s, \tag{2a}$$

$$w_{tt}(1,t) + N[w_s(1,t), w_{st}(1,t)] = 0, \tag{2b}$$

which was typeset using the commands

```
\begin{subequations} \label{subeqnexample}
\begin{equation}
     \varepsilon \rho w_{tt}(s,t) = N[w_{s}(s,t),w_{st}(s,t)]_{s},
     \label{subeqnparta}
\end{equation}
\begin{equation}
     w_{tt}(1,t)+N[w_{s}(1,t),w_{st}(1,t)] = 0,   \label{subeqnpartb}
\end{equation}
\end{subequations}
```

This is made possible by the `amsmath` package, which is called by the class file. If you put a `\label` just after the `\begin{subequations}` command, references can be made to the collection of equations, i.e. '(2)' in the example above. Or, as the example also shows, you can label and refer to each equation individually – i.e. '(2a)' and '(2b)'.

Displayed mathematics should be given end-of-line punctuation appropriate to the running text sentence of which it forms a part, if required.

3. Results

4. Discussion

5. References

The following list shows some sample references:

References

Rapaport, Dennis C., and Dennis C. Rapaport Rapaport. 2004. The art of molecular dynamics simulation. Cambridge university press.

Humphrey, William, Andrew Dalke, and Klaus Schulten. 1996. "VMD: visual molecular dynamics." Journal of molecular graphics 14, no. 1 (1996): 33-38.

This was produced by typing:

```
\begin{thebibliography}{}
\bibitem[Rapport and Dennis C.(2004)]{RD04}
Rapaport, Dennis C., and Dennis C. Rapaport Rapaport. 2004.
The art of molecular dynamics simulation.
Cambridge university press.

\bibitem[Humphrey, William, Andrew Dalke, and Klaus Schulten.(1996)]{HWA96}
Humphrey, William, Andrew Dalke, and Klaus Schulten. 1996.
"VMD: visual molecular dynamics."
Journal of molecular graphics 14, no. 1 (1996): 33-38.

\end{thebibliography}
```

Each entry takes the form:

```
\bibitem[authors' names(date of publication)]{key}
 Bibliography entry
```

where '`authors' names`' is the list of names to appear where the `bibitem` is cited in the text, and '`key`' is the tag that is to be used as an argument for the `\cite{}` commands in the text of the article. '`Bibliography entry`' is the material that is to appear in the list of references, suitably formatted. The commands

```
\usepackage{natbib}
\bibpunct[, ]{(}{)}{;}{a}{}{,}
\renewcommand\bibfont{\fontsize{10}{12}\selectfont}
```

need to be included in the preamble of your .tex file in order to generate the citations and bibliography as described above.