

Simulating Rare Events Among Thousands of Atoms with On-the-Fly Machine Learning

Jonathan Vandermause,^{1,2} Steven B. Torrisi,² Simon Batzner,³ and Boris Kozinsky¹

¹*Harvard University, School of Engineering and Applied Sciences, Cambridge, MA 02138*

²*Harvard University, Department of Physics, Cambridge, MA 02138*

³*Massachusetts Institute of Technology, Center for Computational Engineering, Cambridge, MA, 02139*

(Dated: September 9, 2018)

An article usually includes an abstract, a concise summary of the work covered at length in the main body of the article.

I. INTRODUCTION

This sample document demonstrates proper use of REVTeX 4.1 (and L^AT_EX 2_ε) in manuscripts prepared for submission to APS journals. Further information can be found in the REVTeX 4.1 documentation included in the distribution or available at <http://authors.aps.org/revtex4/>.

When commands are referred to in this example file, they are always shown with their required arguments, using normal T_EX format. In this format, #1, #2, etc. stand for required author-supplied arguments to commands. For example, in \section{#1} the #1 stands for the title text of the author's section heading, and in \title{#1} the #1 stands for the title text of the paper.

Line breaks in section headings at all levels can be introduced using \\. A blank input line tells T_EX that the paragraph has ended. Note that top-level section headings are automatically uppercased. If a specific letter or word should appear in lowercase instead, you must escape it using \lowercase{#1} as in the word “via” above.

A. Second-level heading: Formatting

This file may be formatted in either the **preprint** or **reprint** style. **reprint** format mimics final journal output. Either format may be used for submission purposes. **letter** sized paper should be used when submitting to APS journals.

1. Wide text (A level-3 head)

The `widetext` environment will make the text the width of the full page, as on page ?? (Note the use the \pageref{#1} command to refer to the page number.)

a. Note (Fourth-level head is run in) The width-changing commands only take effect in two-column formatting. There is no effect if text is in a single column.

B. Citations and References

A citation in text uses the command \cite{#1} or \onlinecite{#1} and refers to an entry in the bibliog-

raphy. An entry in the bibliography is a reference to another document.

1. Citations

Because REVTeX uses the `natbib` package of Patrick Daly, the entire repertoire of commands in that package are available for your document; see the `natbib` documentation for further details. Please note that REVTeX requires version 8.31a or later of `natbib`.

a. Syntax The argument of \cite may be a single *key*, or may consist of a comma-separated list of keys. The citation *key* may contain letters, numbers, the dash (-) character, or the period (.) character. New with `natbib` 8.3 is an extension to the syntax that allows for a star (*) form and two optional arguments on the citation key itself. The syntax of the \cite command is thus (informally stated)

\cite { *key* }, or
\cite { *optarg+key* }, or
\cite { *optarg+key* , *optarg+key...* },
where *optarg+key* signifies

key, or
**key*, or
[*pre*] *key*, or
[*pre*] [*post*] *key*, or even
*[*pre*] [*post*] *key*.

where *pre* and *post* is whatever text you wish to place at the beginning and end, respectively, of the bibliographic reference (see Ref. [?] and the two under Ref. [?]). (Keep in mind that no automatic space or punctuation is applied.) It is highly recommended that you put the entire *pre* or *post* portion within its own set of braces, for example: \cite { [{*text*}] *key* }. The extra set of braces will keep L^AT_EX out of trouble if your *text* contains the comma (,) character.

The star (*) modifier to the *key* signifies that the reference is to be merged with the previous reference into a single bibliographic entry, a common idiom in APS and AIP articles (see below, Ref. [?]). When references are merged in this way, they are separated by a semicolon instead of the period (full stop) that would otherwise appear.

b. Eliding repeated information When a reference is merged, some of its fields may be elided: for example, when the author matches that of the previous reference, it is omitted. If both author and journal match, both are omitted. If the journal matches, but the author does not, the journal is replaced by *ibid.*, as exemplified by Ref. [?]. These rules embody common editorial practice in APS

and AIP journals and will only be in effect if the markup features of the APS and AIP BibTeX styles is employed.

c. The options of the cite command itself Please note that optional arguments to the *key* change the reference in the bibliography, not the citation in the body of the document. For the latter, use the optional arguments of the `\cite` command itself: `\cite *[pre-cite] [post-cite] {key-list}`.