

This is the title [Article v1.3]

Firstname Middlename Surname^{1*}, Firstname Middlename Familyname^{1,2†§},
Firstname Initials Surname^{2†¶}, Firstname Surname^{2*}

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This version dated August 12, 2021

Abstract Please provide an abstract of no more than 250 words. Your abstract should explain the main contributions of your article, and should not contain any material that is not included in the main text. Please note that your abstract, plus the authorship material following it, must not extend beyond the title page or modifications to the LaTeX class will likely be needed.

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[‡]These authors also contributed equally to this work

Present address: [§]Department, Institute, Country; [¶]Department, Institute, Country

1 Introduction (Level 1 heading)

Your introduction goes here! Some examples of commonly used commands and features are listed below, to help you get started.

Here's a second paragraph to test paragraph indents. Lorem ipsum dolor sit amet, consectetur adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetur id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

2 Results (Level 1 heading)

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FIRST LIST

You can easily make full width checklists that take a whole page

- ☐ First thing let's do an item which breaks across lines to see how that looks
- ☐ Also remember
- ☐ And finally

SECOND LIST

This is some further description.

- ☐ First thing
- ☐ Also remember
- ☐ And finally

THIRD LIST

This is some further description.

- ☐ First thing
- ☐ Also remember
- ☐ And finally

FOURTH LIST

This is some further description.

- ☐ First thing
- ☐ Also remember
- ☐ And finally

FIFTH LIST

Full-width checklists on less than a single page are also possible

- ☐ First thing let's do an item which breaks across lines to see how that looks
- ☐ Also remember
- ☐ And finally

SIXTH LIST

This is some further description.

- ☐ First thing
- ☐ Also remember
- ☐ And finally

SEVENTH LIST

Single-column checklists are also straightforward by removing the asterisk

- ☐ First thing let's do an item which breaks across lines to see how that looks
- ☐ Also remember
- ☐ And finally

EIGHTH LIST

This is some further description.

- ☐ First thing
- ☐ Also remember
- ☐ And finally

Donec et mi. Nam vulputate metus eu enim. Vestibulum pellentesque felis eu massa.

2.1 Level 2 Heading

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2.1.1 Level 3 Heading

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Level 4 Heading

Sed commodo posuere pede. Mauris ut est. Ut quis purus. Sed ac odio. Sed vehicula hendrerit sem. Duis non odio. Morbi ut dui. Sed accumsan risus eget odio. In hac habitasse platea dictumst. Pellentesque non elit. Fusce sed justo eu urna porta tincidunt. Mauris felis odio, sollicitudin sed, volutpat a, ornare ac, erat. Morbi quis dolor. Donec pellentesque, erat ac sagittis semper, nunc dui lobortis purus, quis congue purus metus ultricies tellus. Proin et quam. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos hymenaeos. Praesent sapien turpis, fermentum vel, eleifend faucibus, vehicula eu, lacus.

3 Discussion

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Table 1. Automobile Land Speed Records (GR 5-10).

Speed (mph)	Driver	Car	Engine	Date
407.447	Craig Breedlove	Spirit of America	GE J47	8/5/63
413.199	Tom Green	Wingfoot Express	WE J46	10/2/64
434.22	Art Arfons	Green Monster	GE J79	10/5/64
468.719	Craig Breedlove	Spirit of America	GE J79	10/13/64
526.277	Craig Breedlove	Spirit of America	GE J79	10/15/65
536.712	Art Arfons	Green Monster	GE J79	10/27/65
555.127	Craig Breedlove	Spirit of America, Sonic 1	GE J79	11/2/65
576.553	Art Arfons	Green Monster	GE J79	11/7/65
600.601	Craig Breedlove	Spirit of America, Sonic 1	GE J79	11/15/65
622.407	Gary Gabelich	Blue Flame	Rocket	10/23/70
633.468	Richard Noble	Thrust 2	RR RG 146	10/4/83
763.035	Andy Green	Thrust SSC	RR Spey	10/15/97

Source: https://www.sedl.org/afterschool/toolkits/science/pdf/ast_sci_data_tables_sample.pdf

Table 1–source data 1. This is a description of a data source.

et ultrices posuere cubilia Curae; Pellentesque sit amet pede ac sem eleifend consetetur. Nullam elementum, urna vel imperdiet sodales, elit ipsum pharetra ligula, ac pretium ante justo a nulla. Curabitur tristique arcu eu metus. Vestibulum lectus. Proin mauris. Proin eu nunc eu urna hendrerit faucibus. Aliquam auctor, pede consequat laoreet varius, eros tellus scelerisque quam, pellentesque hendrerit ipsum dolor sed augue. Nulla nec lacus.

4 Methods and Materials

Guidelines can be included for standard research article sections, such as this one.

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5 Some L^AT_EX Examples

Use section and subsection commands to organize your document. L^AT_EX handles all the formatting and numbering automatically. Use ref and label commands for cross-references.

5.1 Figures and Tables

Use the table and tabular commands for basic tables — see **Table 1**, for example.

To include an image (JPEG, PNG or PDF) in your document, use the `\includegraphics` command as in the code for **Figure 2**.

If you use the following prefixes for your `\label`:

Figures `fig:`, e.g. `\label{fig:view}`

Tables `tab:`, e.g. `\label{tab:example}`

Equations `eq:`, e.g. `\label{eq:CLT}`

Boxes `box:`, e.g. `\label{box:simple}`

you can then use the convenience commands `\FIG{view}`, `\TABLE{example}`, `\EQ{CLT}` and `\BOX{simple}` *without* the label prefixes, to generate cross-references **Figure 2**, **Table 1**, **Equation 1** and **Box 1**. Alternatively, use `\autoref` with the full label, e.g. **Appendix A** (although this may not work correctly for figures and tables in the appendices or boxes nor supplements at present).

Really wide figures or tables, that take up the entire text width: use `\begin{figure*}... \end{figure*}` as in **Figure 1**. And sometimes you may want to use feature boxes like **Box 1**.

5.2 Algorithms and Pseudocode

The `algpseudocode` and `algorithms` packages is loaded by the document class. **Algorithm 1** was taken directly from the package documentation. (Please do not load `algorithm2e`; it's not compatible with `algpseudocode` nor `algorithms`!)

5.3 Citations

LaTeX formats citations and references automatically using the bibliography records in your .bib file, which you can edit

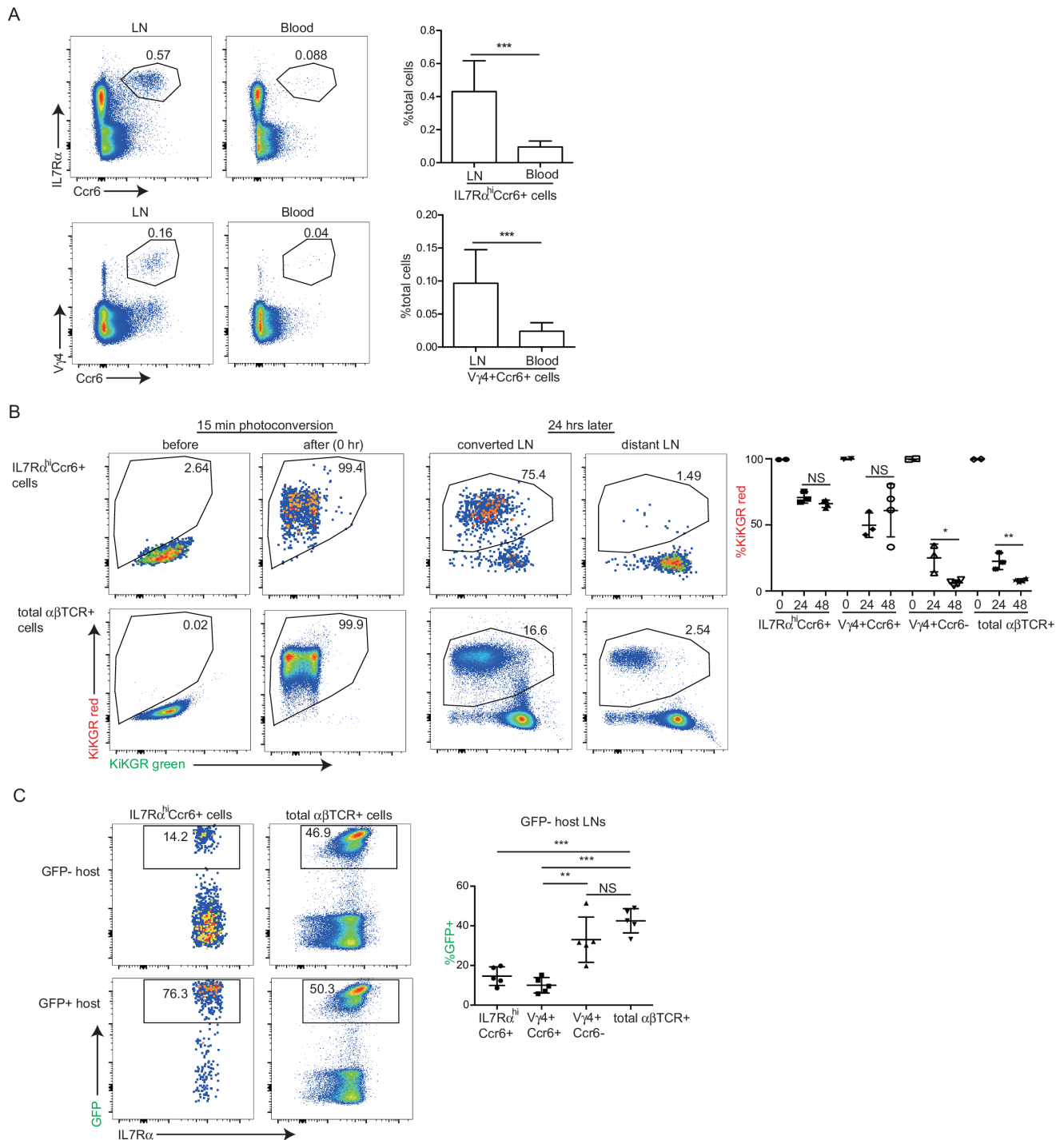


Figure 1. A very wide figure that takes up the entire page, including the gutter space.

Figure 1-Figure supplement 1. There is no limit on the number of Figure Supplements for any one primary figure. Each figure supplement should be clearly labeled, Figure 1-Figure Supplement 1, Figure 1-Figure Supplement 2, Figure 2-Figure Supplement 1 and so on, and have a short title (and optional legend). Figure Supplements should be referred to in the legend of the associated primary figure, and should also be listed at the end of the article text file.

Algorithm 1. Euclid's algorithm

```

procedure Euclid( $a, b$ )           ▷ The g.c.d. of  $a$  and  $b$ 
   $r \leftarrow a \bmod b$ 
  while  $r \neq 0$  do             ▷ We have the answer if  $r$  is 0
     $a \leftarrow b$ 
     $b \leftarrow r$ 
     $r \leftarrow a \bmod b$ 
  end while
  return  $b$                      ▷ The gcd is  $b$ 
end procedure

```

via the project menu. Use the `\cite` command for an inline citation, like [1], and the `\citep` command for a citation in parentheses Aivazian917. The LaTeX template uses a slightly-modified Vancouver bibliography style.

5.4 Mathematics

LaTeX is great at typesetting mathematics. Let X_1, X_2, \dots, X_n be a sequence of independent and identically distributed random variables with $E[X_i] = \mu$ and $\text{Var}[X_i] = \sigma^2 < \infty$, and let

$$S_n = \frac{X_1 + X_2 + \dots + X_n}{n} = \frac{1}{n} \sum_i^n X_i \quad (1)$$

denote their mean. Then as n approaches infinity, the random variables $\sqrt{n}(S_n - \mu)$ converge in distribution to a normal $\mathcal{N}(0, \sigma^2)$.

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5.5 Other Chemistry Niceties

You can use commands from the `mhchem` and `siunitx` packages. For example: $\text{C}_{32}\text{H}_{64}\text{NO}_7\text{S}$; $5\text{ }\mu\text{m}$; $30\text{ }^\circ\text{C}$; $5 \times 10^{-17}\text{ M}$

5.6 Lists

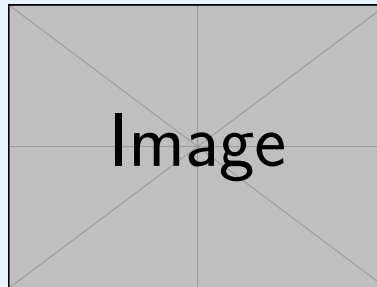
You can make lists with automatic numbering ...

1. Like this,
2. and like this.

...or bullet points ...

Box 1. This is an example feature box

This is a feature box. It floats!



Box 1 Figure 1. 'Figure' and 'table' captions in feature boxes should be entered with `\figurefig` and `\featuretable`. They're not really floats.

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- Like this,
- and like this.

...or with words and descriptions ...

Word Definition

Concept Explanation

Idea Text

Some filler text, because empty templates look really poor. Lorem ipsum dolor sit amet, consectetur adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetur id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem

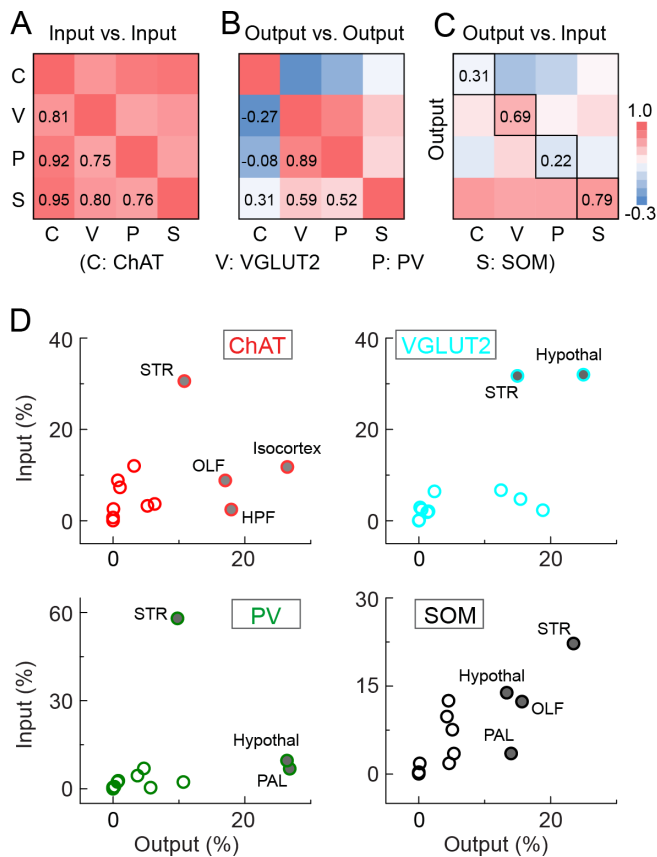


Figure 2. A column-width example.

Figure 2-Figure supplement 1. Shorter caption for main text.

Figure 2-Figure supplement 2. This is another supplementary figure.

Figure 2-source data 1. This is a description of a data source.

Figure 2-source data 2. This is another description of a data source.

vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

6 Author Contributions

FMS wrote sections X and Z. RMS contributed to the writing of sections Y and W. TMP contributed to the writing of sections Y and W. ITP contributed to all sections. ADP wrote sections W and Y, performed and analyzed the experiments in Z, made figures 4-6, and edited the whole manuscript as well as standardizing table formatting. For a more detailed description of contributions, see the GitHub issue tracking and changelog at <https://github.com/myaccount/homegithubrepository>.

7 Other Contributions

EGP provided important insights on the challenges faced by nonequilibrium simulations. FTP provided several key citations on energy conservation. For a more detailed description of contributions, see the GitHub issue tracking and changelog at <https://github.com/myaccount/homegithubrepository>.

8 Potentially Conflicting Interests

EGP has a 40% equity stake in the ReallyGoodSimulations company, which sells molecular dynamics code. DMD is a developer of the package EvenBetterMD, which is recommended in this article.

9 Funding Information

FMS acknowledges the support of NSF grant CHE-1111111.

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Author 2 name: [EEEE-FFFF-GGGG-HHHH](#)

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Appendix A Figure 1. This is a figure in the appendix

Appendix A Firstly

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Appendix B Secondly

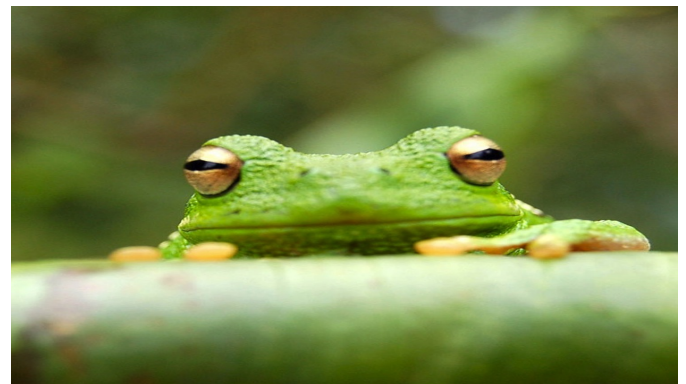
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Appendix B Figure 1. This is a figure in the appendix



Appendix B Figure 2. This is a figure in the appendix



Figure 1-Figure supplement 1. There is no limit on the number of Figure Supplements for any one primary figure. Each figure supplement should be clearly labeled, Figure 1-Figure Supplement 1, Figure 1-Figure Supplement 2, Figure 2-Figure Supplement 1 and so on, and have a short title (and optional legend). Figure Supplements should be referred to in the legend of the associated primary figure, and should also be listed at the end of the article text file.



Figure 2-Figure supplement 2. This is another supplementary figure.



Figure 2-Figure supplement 1. This is a supplementary figure's full caption, which will be used at the end of the manuscript.