# This is the title: v1.3

Firstname Middlename Surname<sup>1\*</sup>, Firstname Middlename Familyname<sup>1,2†§</sup>, Firstname Initials Surname<sup>2†¶</sup>, Firstname Surname<sup>2\*</sup>

<sup>1</sup>Institution 1; <sup>2</sup>Institution 2

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**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.

#### \*For correspondence:

email1@example.com (FMS); email2@example.com (FS)

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.

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# 2 Results (Level 1 heading)

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<sup>&</sup>lt;sup>†</sup>These authors contributed equally to this work

<sup>&</sup>lt;sup>‡</sup>These authors also contributed equally to this work

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.

#### 2.1 Level 2 Heading

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### 2.1.1 Level 3 Heading

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#### Level 4 Heading

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#### 3 Discussion

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#### 4 Methods and Materials

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

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# 5 Some LATEX Examples

Use section and subsection commands to organize your document. 上下X 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 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 algorithm2e)

#### 5.3 Citations

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

Algorithm 1. Euclid's algorithm

```
procedure EUCLID(a, b)\triangleright The g.c.d. of a and br \leftarrow a \mod b\triangleright We have the answer if r is 0a \leftarrow bb \leftarrow rr \leftarrow a \mod bend whilereturn b\triangleright The gcd is bend procedure
```

via the project menu. Use the \cite command for an inline citation, like, <sup>1</sup> and the \citep command for a citation in parentheses <sup>1</sup>. The LaTeX template uses a slightly-modified Vancouver bibliography style.

#### 5.4 Mathematics

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$$S_n = \frac{X_1 + X_2 + \dots + X_n}{n} = \frac{1}{n} \sum_{i=1}^{n} X_i$$
 (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

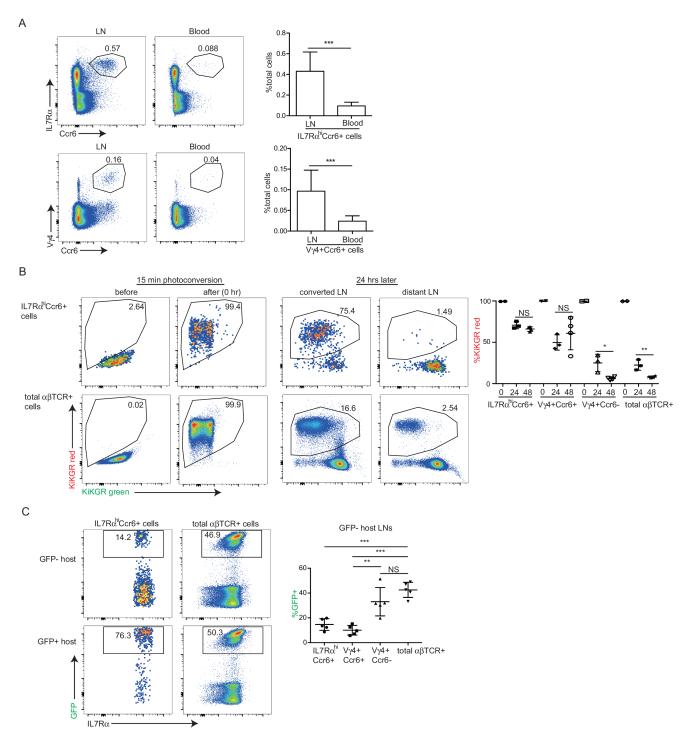
You can use commands from the mhchem and siunitx packages. For example:  $C_{32}H_{64}NO_7S$ ; 5 µm; 30 °C; 5 × 10<sup>-17</sup> M

#### 5.6 Lists

You can make lists with automatic numbering ...

- 1. Like this,
- 2. and like this.

... or bullet points ...



**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.

# 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 \featurefig and \featuretable. They're not really floats.

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Word Definition
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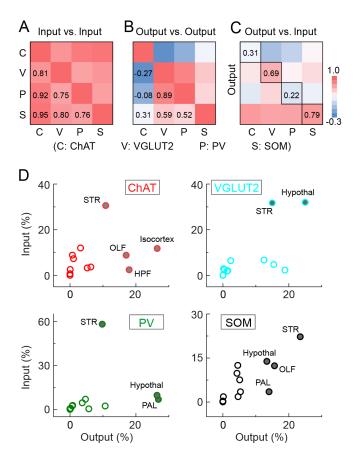


Figure 2. A column-width example.

**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.

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### **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 inportant insights on the challenges faced by nonequilibrium simulations. FTP provided several key cita-

tions on energy conservation. For a more detailed description of contributions, see the GitHub issue tracking and changelog at https://github.com/myaccount/homegithubrepository.

## 8 Competing Financial Interests

EGP has a 40% equity stake in the ReallyGoodSimulations company, which sells molecular dynamics code.

## 9 Funding Information

FMS acknowledges the support of NSF grant CHE-1111111.

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# **Appendix A** Firstly

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

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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

#### A LiveCoMS Best Practices Guide



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



**Figure 2–Figure supplement 2.** This is another supplementary figure.