

# This is the title : v1.3

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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.

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## 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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### 2.1 Level 2 Heading

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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](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.

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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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## 4 Methods and Materials

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

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## 5 Some $\text{\LaTeX}$ Examples

Use section and subsection commands to organize your document.  $\text{\LaTeX}$  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.

You can upload a figure (JPEG, PNG or PDF) using the project menu. To include it in your document, use the `\includegraphics` command as in the code for [Figure 3](#).

For a half-width figure or table with text wrapping around it, use

```
\begin{wrapfigure}{l}{.46\textwidth}
  \includegraphics[width=\hsize]{...}
  \caption{...}\label{...}
\end{wrapfigure}
```

as in [Figure 1](#). For tables:

```
\begin{wraptable}{l}{.46\textwidth}{
  \begin{tabular}{...}
  ...
  \end{tabular}}
  \caption{...}\label{...}
\end{wraptable}
```

Be careful with these, though, as they may behave strangely near page boundaries, sectional headings, or in the neighbourhood of lists or too many floats.

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 3](#), [Table 1](#), [Equation 1](#) and [Box 1](#). Alternatively, use `\autoref` with the full label, e.g. [Appendix 1](#) (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 page, including the gutter space: use `\begin{fullwidth}... \end{fullwidth}` as in [Figure 2](#). And sometimes you may want to use feature boxes like [Box 1](#).



**Figure 1.** A half-columnwidth image using `wrapfigure`, to be used sparingly. Note that using a `wrapfigure` before a sectional heading, near other floats or page boundaries is not recommended, as it may cause interesting layout issues. Use the optional argument to `wrapfigure` to control how many lines of text should be set half-width alongside it.

Some filler text to sit alongside the half-width figure. 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.

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## 5.2 Citations

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

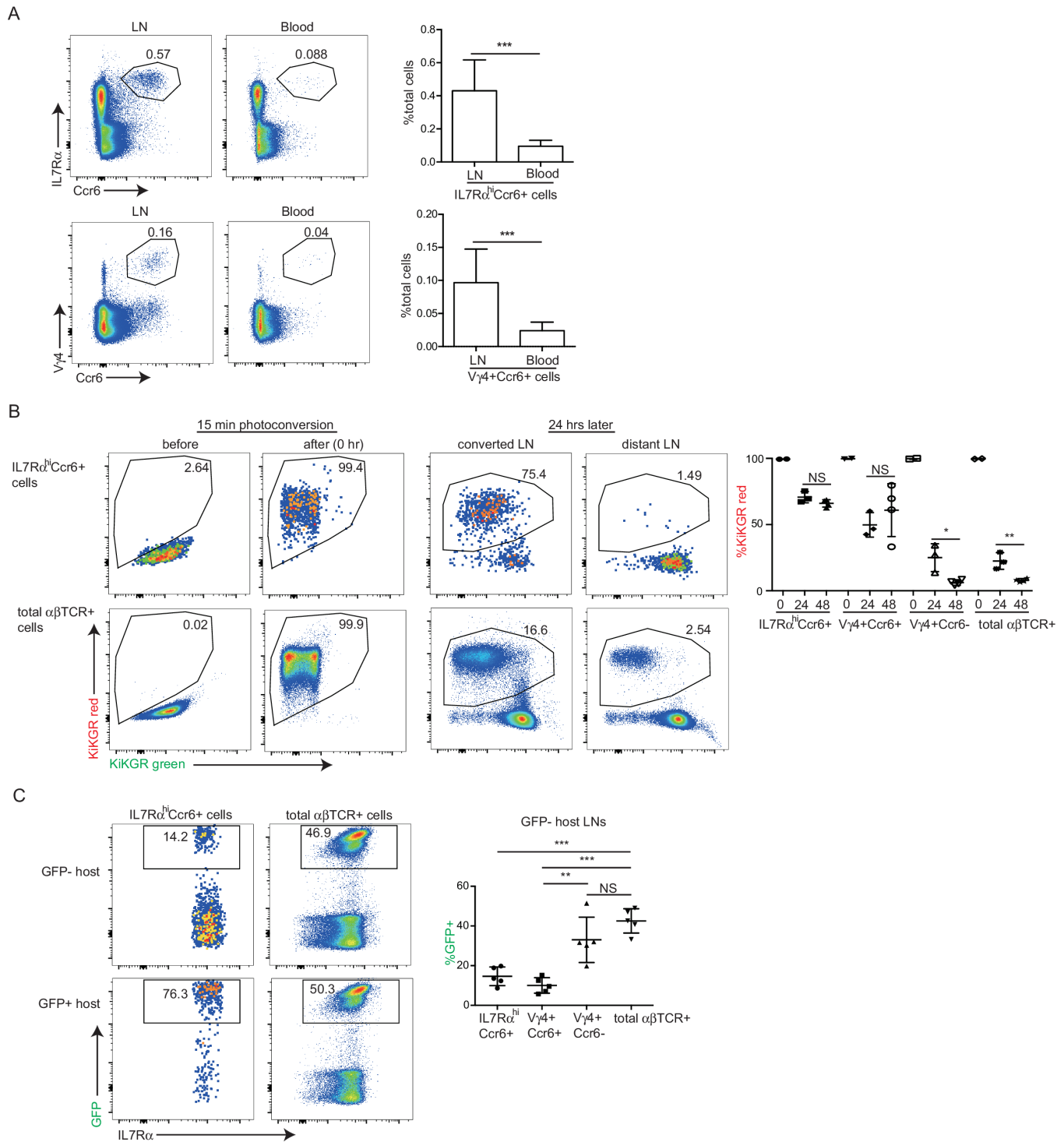
## 5.3 Mathematics

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

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

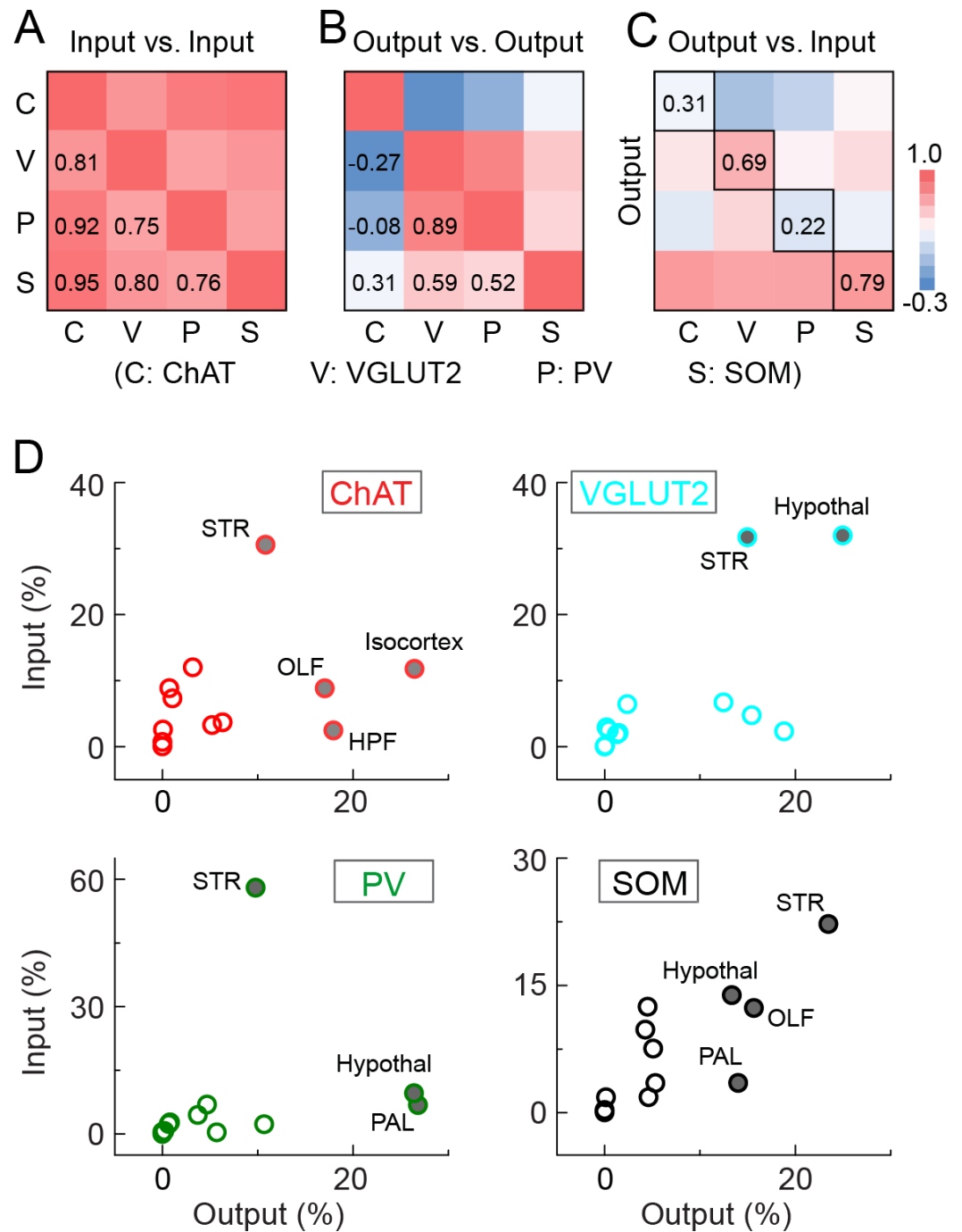
denote their mean. Then as  $n$  approaches infinity, the random variables  $\sqrt{n}(S_n - \mu)$  converge in distribution to a normal  $\mathcal{N}(0, \sigma^2)$ .

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**Figure 2.** A very wide figure that takes up the entire page, including the gutter space.

**Figure 2-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 3.** A text-width example.

**Figure 3-Figure supplement 1.** Shorter caption for main text.

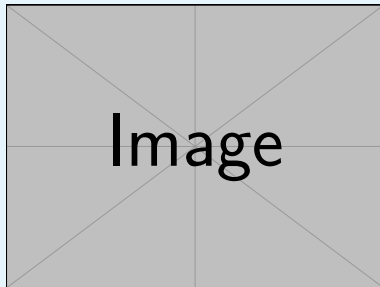
**Figure 3-Figure supplement 2.** This is another supplementary figure.

**Figure 3-source data 1.** This is a description of a data source.

**Figure 3-source data 2.** This is another description of a data source.

**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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## 5.4 Other Chemistry Niceties

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

## 5.5 Lists

You can make lists with automatic numbering ...

1. Like this,
2. and like this.

... or bullet points ...

- 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 vel leo ultrices bibendum. Aenean

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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 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 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.

## References

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## Appendix 1

### A Firstly

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

### B Secondly

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**Appendix 1 Figure 2.** This is a figure in the appendix

## Appendix 2



**Appendix 2 Figure 1.** This is a figure in the appendix



**Figure 2–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 3–Figure supplement 1.** This is a supplementary figure’s full caption, which will be used at the end of the manuscript.



**Figure 3–Figure supplement 2.** This is another supplementary figure.