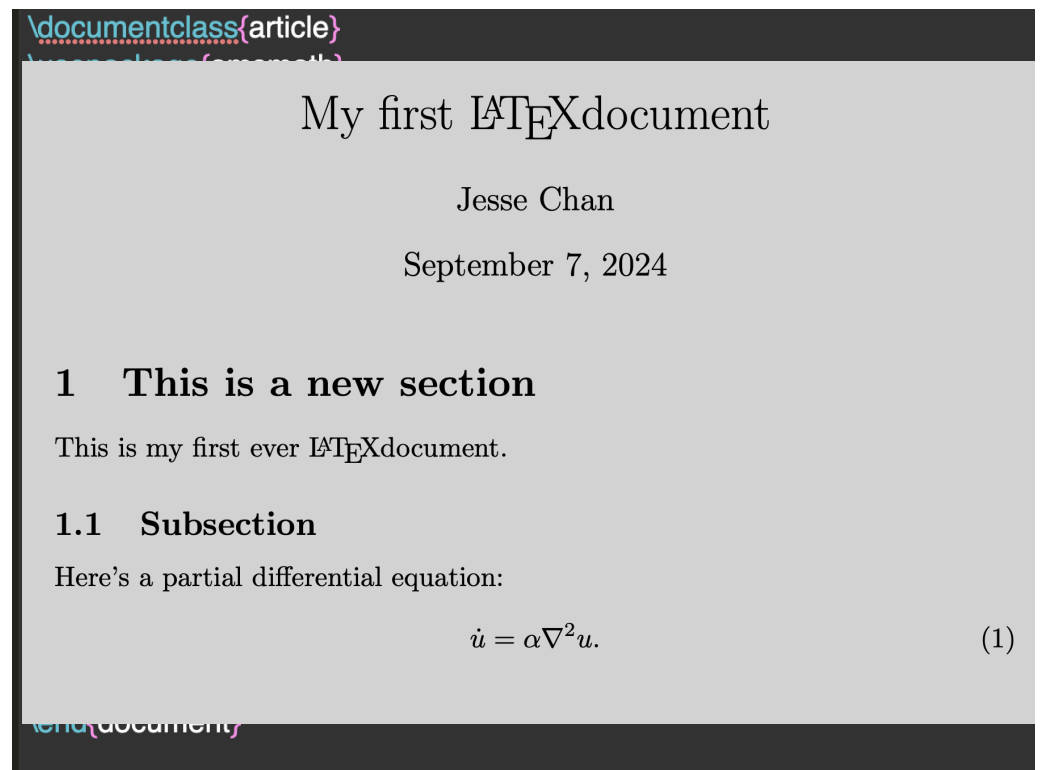


CMOR 420/520
Computational Science
LaTeX and numerical computing

Structure of a LaTeX document

- Preamble: load packages, define commands, ...
- Document: sections, mathematics, figures, ...
 - backslash “\” denotes a LaTeX command
- Compilation with “pdflatex”
 - “pdflatex simple.tex” creates both a pdf and some auxiliary files.



Preamble packages

- Using mathematical symbols and notations, tables, and images needs the correct packages
- Keep a template document that has all packages you may need in the preamble

```
1 \documentclass[10pt,letterpaper]{article}
2 \usepackage[letterpaper, margin=.75in]{geometry}
3 \usepackage[latin1]{inputenc}
4 \usepackage{float}
5 \usepackage{xy-pic}
6 \usepackage{graphicx, amsthm, amsmath, amssymb}
7 \graphicspath{{images/}{../images/}}
8 \usepackage{mathrsfs}
9 \usepackage{marginnote}
10 \usepackage{multicol}
11 \usepackage{subfiles}
12
13
14 \usepackage{tikz, pgf, calc}
15 \usetikzlibrary{arrows, matrix, positioning, fit, calc}
16 \usepackage[linewidth=1pt]{mdframed}
17 \usepackage{parskip}
18 \usepackage{cancel}
19
```

Preamble environments

- You can define environments to give a definition, Theorem, Lemma, etc.
- Keep a template document that has all environments you may need in the preamble

```
%% Theorems %%  
\newtheorem{theorem}{Theorem}[section]  
\theoremstyle{definition}  
\newtheorem{definition}{Definition}[section]  
\theoremstyle{definition}  
\newtheorem{exmp}{Example}[section]  
\newtheorem{prop}{Proposition}[section]  
\newtheorem{cor}{Corollary}[section]  
\newtheorem{lem}{Lemma}[section]  
\newtheorem*{rem}{Remark}
```

LaTeX for mathematics

- Inline math (e.g., “We’ll set $x = 10$ here...”)
- Math “environments” (e.g., “`\begin{equation}`”, “`\begin{align}`”, “`\begin{gather}`”, etc)
 - `\begin{align*}` does not create equation labels.
- Can reference sections, equations, etc.

We can write math “inline” like `$\alpha \in \mathbb{R}$`, or using environments like

```
\begin{align}
    \beta \in \mathbb{C}^2. \quad \label{eq:beta}
\end{align}
```

and reference equations later like `(\ref{eq:beta})`.

We can write math “inline” like $\alpha \in \mathbb{R}$, or using environments like

$$\beta \in \mathbb{C}^2. \tag{1}$$

and reference equations later with (1).

LaTeX special symbols

- Easy to find references for special symbols, fonts, etc.
 - [https://www.overleaf.com/learn/latex/
List of Greek letters and math symbols](https://www.overleaf.com/learn/latex/List_of_Greek_letters_and_math_symbols)
 - [https://www.cmor-faculty.rice.edu/~heinken/latex/
symbols.pdf](https://www.cmor-faculty.rice.edu/~heinken/latex/symbols.pdf)

Preamble commands

- You can define 'commands' to simplify typing equations

```
1 \newcommand{\R}{\mathbb{R}}
2 \newcommand{\C}{\mathbb{C}}
3 \newcommand{\N}{\mathbb{N}}
4 \newcommand{\Q}{\mathbb{Q}}
5 \newcommand{\sumin}{\sum_{i=1}^n}
6
7
8 \newcommand{\dt}{\Delta t}
9 \newcommand{\ukone}{u^{k+1}}
10 \newcommand{\uk}{u^k}
11 \newcommand{\utkone}{\tilde{u}^{k+1}}
12 \newcommand{\utk}{\tilde{u}^k}
13 \newcommand{\uhkone}{\hat{u}^{k+1}}
14 \newcommand{\ekone}{e^{k+1}}
15 \newcommand{\ek}{e^k}
16 \newcommand{\etkone}{\tilde{e}^{k+1}}
17 \newcommand{\etk}{\tilde{e}^k}
18 \newcommand{\ehkone}{\hat{e}^{k+1}}
```

LaTeX “floating” environments

- Figures and tables are considered “floats” in LaTeX: they can be moved (floated) around by LaTeX freely
 - “`\begin{figure}[h]`” requests that the figure be placed **here** (**t**op, **b**ottom, **t**op of next **p**age). `[!h]` strongly requests.
 - Works on all “float” environments
 - “`\includegraphics`” can edit images (crop, change aspect ratio, rotate, ...)
 - “`\includegraphics`” works without the “figure” environment too.
- * Include multiple images in one figure by inserting “`\includegraphics`” more than once in the environment

```
\begin{figure}[h]
\centering
\includegraphics[width=.25\textwidth]{chan_headshot.jpg}
\caption{This is a photo of Jesse Chan.}
\label{fig:ic}
\end{figure}
```

I can reference Figure~\ref{fig:ic} this way.



Figure 1: This is a photo of Jesse Chan.

I can reference Figure 1 this way.

LaTeX tables and alignment

- Tables and environments like “`\begin{align}`” use the alignment character “&”
- Here, “`\begin{tabular}`” defines the actual table; “`\begin{table}`” just creates the float container for the “`tabular`” instance.
- Double backslash “`\\`” adds a new line in LaTeX

* Include multiple tables in one figure/table by calling “`\tabular`” more than once in the environment

```
\begin{table}[htbp]
  \begin{tabular}{r|l|cc}
    1 & 2 & 3 & 4 \\ \hline
    5 & 6 & 7 & 8 \\
    9 & 10 & 11 & 12 \\
  \end{tabular}
\end{table}
```

1	2	3	4
5	6	7	8
9	10	11	12

Bibliographies and Bibtex

- Easy to grab citations from Google Scholar or any journal article
- Ref via `\cite{wu2024entropy}`

```
@article{wu2024entropy,
  title={Entropy stable discontinuous
  Galerkin methods for ...},
  author={Wu, Xinhui and Trask,
  Nathaniel and Chan, Jesse},
  journal={Numerical Methods for PDEs},
  pages={e23129},
  publisher={Wiley Online Library}
}
```

Google Scholar



Jesse Chan

Rice University

Verified email at rice.edu - [Homepage](#)

[finite element methods](#) [discontinuous Galerkin](#) [high order methods](#) [high performance computing](#)

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subcell positivity preservation
X Wu, N Trask, J Chan
Numerical Methods for Partial Differential Equations,
- ☐ High order entropy stable schemes for the...
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CG Taylor, L Wilcox, J Chan
arXiv preprint arXiv:2404.06630
- ☐ High order entropy stable discontinuous G...
subcell limiting
Y Lin, J Chan
Journal of Computational Physics 498, 112677

Cite

- MLA Wu, Xinhui, Nathaniel Trask, and Jesse Chan. "Entropy stable discontinuous Galerkin methods for the shallow water equations with subcell positivity preservation." *Numerical Methods for Partial Differential Equations* (2024): e23129.
- APA Wu, X., Trask, N., & Chan, J. (2024). Entropy stable discontinuous Galerkin methods for the shallow water equations with subcell positivity preservation. *Numerical Methods for Partial Differential Equations*, e23129.
- Chicago Wu, Xinhui, Nathaniel Trask, and Jesse Chan. "Entropy stable discontinuous Galerkin methods for the shallow water equations with subcell positivity preservation." *Numerical Methods for Partial Differential Equations* (2024): e23129.
- Harvard Wu, X., Trask, N. and Chan, J., 2024. Entropy stable discontinuous Galerkin methods for the shallow water equations with subcell positivity preservation. *Numerical Methods for Partial Differential Equations*, p.e23129.
- Vancouver Wu X, Trask N, Chan J. Entropy stable discontinuous Galerkin methods for the shallow water equations with subcell positivity preservation. *Numerical Methods for Partial Differential Equations*. 2024 Jul:e23129.

[BibTeX](#) [EndNote](#) [RefMan](#) [RefWorks](#)

Bibliographies and Bibtex

- Include references in a .bib file in the same directory.
- Add `\bibliography{reference file name}` and cite away
- Can customize the style of bibliography entries (MLA, Chicago, APA, etc)
- Process: compile LaTeX, then compile BibTex, then recompile LaTeX again.

```
I can reference a paper via \cite{wu2024entropy}.  
|  
\bibliographystyle{plain}  
\bibliography{references.bib}  
  
\end{document}
```

I can reference a paper via [1].

References

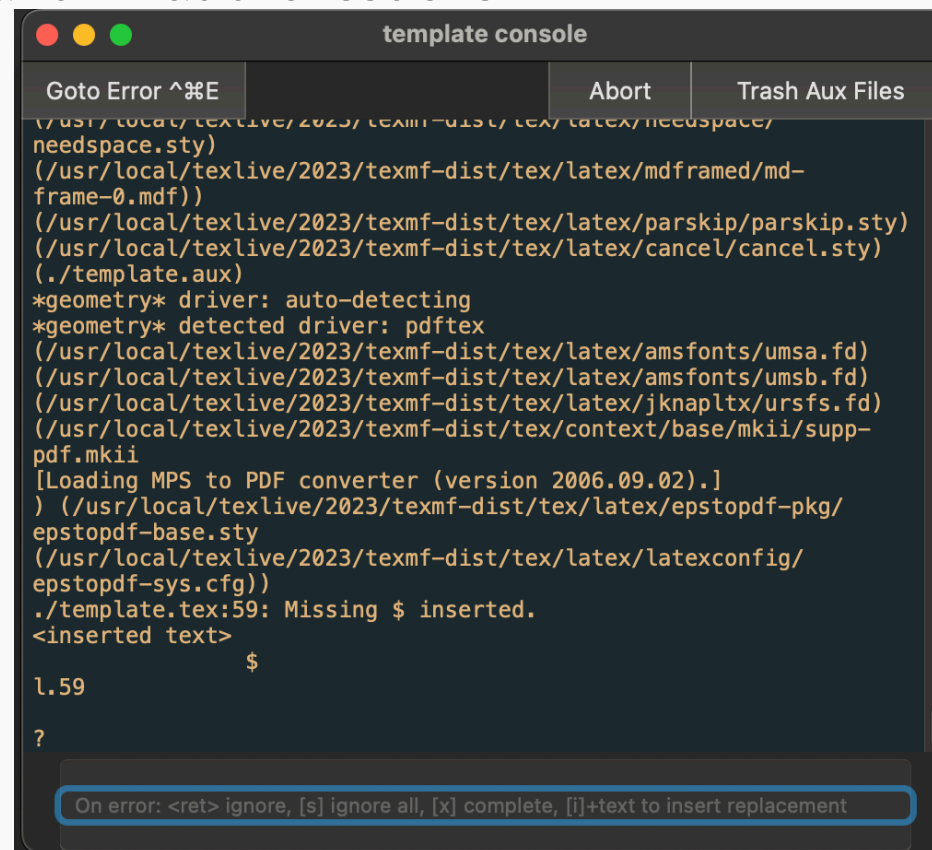
- [1] Xinhui Wu, Nathaniel Trask, and Jesse Chan. Entropy stable discontinuous galerkin methods for the shallow water equations with subcell positivity preservation. *Numerical Methods for Partial Differential Equations*, page e23129.

More about Bibtex

- Bibtex will create bibliography entries for only what is cited in the paper
- You can have a .bib file with hundreds of entries but a bibliography with just those you want/need!
- Bibtex will create a .bbl file that is essentially the bibliography
 - This file can be edited directly if desired

Error tracing

- Latex produces a console at compilation that reads through the document
- If there is error, the console stops and tells you (around) where the error is and what the issue is



The screenshot shows a terminal window titled "template console" with a dark background and light-colored text. At the top, there are three colored window control buttons (red, yellow, green) and three buttons: "Goto Error ^%E", "Abort", and "Trash Aux Files". The main area contains the output of a LaTeX compilation process. It lists various system files being loaded, such as `needspace.sty`, `mdframed/md-frame-0.mdf`, `parskip/parskip.sty`, `cancel/cancel.sty`, and `template.aux`. It also shows the detection of the `pdf` driver for geometry. The process then loads the `epstopdf` package and its configuration files. The final line of the visible output is an error message: `./template.tex:59: Missing $ inserted.` followed by `<inserted text>` and a dollar sign `$` on the next line. Below the error message, the numbers `1.59` and `?` are visible. At the bottom of the window, there is a text input field with the placeholder text: "On error: <ret> ignore, [s] ignore all, [x] complete, [i]+text to insert replacement".

```
template console
Goto Error ^%E  Abort  Trash Aux Files
(/usr/local/texlive/2023/texmf-dist/tex/latex/needspace/
needspace.sty)
(/usr/local/texlive/2023/texmf-dist/tex/latex/mdframed/md-
frame-0.mdf)
(/usr/local/texlive/2023/texmf-dist/tex/latex/parskip/parskip.sty)
(/usr/local/texlive/2023/texmf-dist/tex/latex/cancel/cancel.sty)
./template.aux)
*geometry* driver: auto-detecting
*geometry* detected driver: pdf
(/usr/local/texlive/2023/texmf-dist/tex/latex/amsfonts/umsa.fd)
(/usr/local/texlive/2023/texmf-dist/tex/latex/amsfonts/umsb.fd)
(/usr/local/texlive/2023/texmf-dist/tex/latex/jknapltx/ursfs.fd)
(/usr/local/texlive/2023/texmf-dist/tex/context/base/mkii/supp-
pdf.mkii
[Loading MPS to PDF converter (version 2006.09.02).]
) (/usr/local/texlive/2023/texmf-dist/tex/latex/epstopdf-pkg/
epstopdf-base.sty
(/usr/local/texlive/2023/texmf-dist/tex/latex/latexconfig/
epstopdf-sys.cfg))
./template.tex:59: Missing $ inserted.
<inserted text>
$
1.59
?
On error: <ret> ignore, [s] ignore all, [x] complete, [i]+text to insert replacement
```

Exercise

- Download the latex template document from Canvas
- Give it a title, author, and write the following

This is my first latex document. For $x \in \mathbb{R}$ and $y \in \mathbb{R}$ we have that

$$x + y \in \mathbb{R}.$$

I can make a table of values

1	2	3
4	5	6
7	8	9

Overleaf

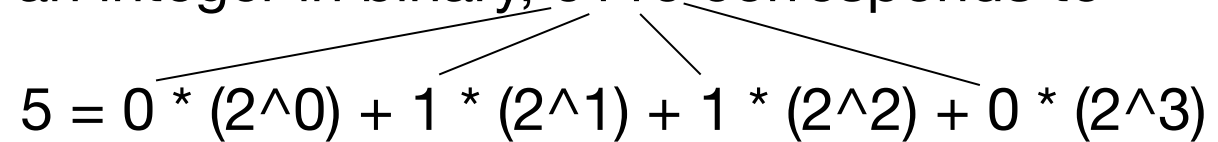
- Nowadays, most people use LaTeX via Overleaf.
- Overleaf has great resources for learning LaTeX.
- Note that Rice provides Overleaf professional! See <https://www.overleaf.com/edu/rice>
- I still prefer using LaTeX locally; it's faster, more responsive, and works offline.

Numerical computing concepts

- IEEE 754: standardized behavior (1985, 2008) to address portability issues across computer architectures.
- Several concepts are shared between C, C++, and Julia (and any programming language suitable for numerical computing)

Data types in scientific computing

- For numerical computing, it can help to know the difference between different data types (e.g., integer, float, double, long int, etc) and what distinguishes them from each other
 - Integers and decimal (float, double) behave very differently!
- To start, numbers are represented in binary in a computer.
 - If we represent an integer in binary, 0110 corresponds to



The diagram shows the binary number 0110. Four lines originate from the digits: the first line from the '0' points to the first term of the equation, the second line from the first '1' points to the second term, the third line from the second '1' points to the third term, and the fourth line from the final '0' points to the fourth term.

$$5 = 0 * (2^0) + 1 * (2^1) + 1 * (2^2) + 0 * (2^3)$$

Binary representations of integers

- $5 = 0110 = 0 * (2^0) + 1 * (2^1) + 1 * (2^2) + 0 * (2^3)$
 - Binary 0/1 digits are coefficients in a binary expansion
 - We use 4 “bits” here; 64-bit integers are most common, but 8-bit, 16-bit, and 32-bit integers are all used.
 - What does this expansion imply about the numbers that can be represented in binary?
- * They are finite! Only a finite amount of numbers can be expressed as 64 bits
- * IEEE 64 bit representation has 8-bits for an exponent to allow for representation of more numbers

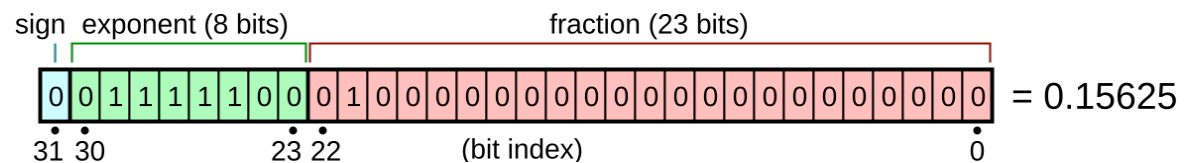
Unsigned vs signed integers

- You can have both “unsigned integer” or “signed integer” types (e.g., “unsigned int” vs “int”)
 - Both have the same bit representation, but can yield different results because they are *interpreted* differently
 - For signed integers: one bit determines the sign.
- Advantages of unsigned integers: represent larger values, provides additional information about what the variable is for.

What about decimal numbers?

- Easy to represent integers as binary; what about decimal?
- Fixed point representation: represent digits before and after a decimal point (fixed number of representable digits)
- Floating point representation: represent a number as a coefficient and exponent. Higher *relative* accuracy.

$$12.345 = \underbrace{12345}_{\text{significand}} \times \underbrace{10^{-3}}_{\text{base}^{\text{exponent}}}$$



Consequences of floating point representations

- Rounding: the sum of two floating point numbers may not be representable as another floating point number, so the result is *rounded* to the nearest representable number.
- Checking equality of floating point numbers is unreliable!

```
julia> sin(1.0 * pi) == 0.0  
false
```

- Catastrophic cancellation: subtracting large numbers from each other can result in large relative errors due to rounding.
- Overflow: results in either NaNs/Infs.

Arrays

- Arrays include vectors, matrices, tensors, ...
- Typically represents a list of numbers of one type (e.g., an array typically doesn't have both 32-bit and 64-bit numbers)
- What's the difference between arrays and other containers like Dictionaries in Python? **Speed.**
 - Arrays are very *low-overhead* containers, which make them important for efficient programs.