

**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.

The screenshot shows a LaTeX editor interface with the following content:

```
\documentclass{article}
\begin{document}
My first \LaTeX{}document

Jesse Chan
September 7, 2024

\section{This is a new section}
This is my first ever \LaTeX{}document.

\subsection{Subsection}
Here's a partial differential equation:

$$\dot{u} = \alpha \nabla^2 u. \tag{1}$$

\end{document}
```

The code is color-coded: red for backslashes, purple for curly braces, and pink for the class and document environment names. The output text is displayed below the code, showing the title "My first \LaTeX{}document", author "Jesse Chan", date "September 7, 2024", and a section header "1 This is a new section". Below it is a paragraph "This is my first ever \LaTeX{}document.", a subsection "1.1 Subsection", and a partial differential equation  $\dot{u} = \alpha \nabla^2 u.$  with the label "(1)".

# 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{xypic}
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.`    `\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}}
0 \newcommand{\uk}{u^k}
1 \newcommand{\utkone}{\tilde{u}^{k+1}}
2 \newcommand{\utk}{\tilde{u}^k}
3 \newcommand{\uhkone}{\hat{u}^{k+1}}
4 \newcommand{\ekone}{e^{k+1}}
5 \newcommand{\ek}{e^k}
6 \newcommand{\etkone}{\tilde{e}^{k+1}}
7 \newcommand{\etk}{\tilde{e}^k}
8 \newcommand{\ehkone}{\hat{e}^{k+1}}
9
```

# 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** (top, **bottom**, top of next **page**). [!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:jc}
\end{figure}
```

I can reference Figure~\ref{fig:jc} 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 \\
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}  
}
```

The screenshot shows a Google Scholar profile for Jesse Chan. At the top, there's a photo of a man with glasses and dark hair, identified as Jesse Chan from Rice University. Below the photo, his name is listed with a pencil icon for editing. It also shows a verified email at rice.edu and a homepage link. A 'FOLLOWING' button is present. Below this, a banner displays 'Save', 'Cite', 'Cited by 7', and 'Related articles'. A 'TITLE' filter dropdown is visible. The main content area lists several publications with checkboxes next to them:

- Pseudodifferential Models for Ultrasound V (S Acosta, J Chan, R Johnson, B Palacios, SIAM Journal on Applied Mathematics 84 (4), 1609-)
- Entropy stable discontinuous Galerkin methods for shallow water equations with subcell positivity preservation (X Wu, N Trask, J Chan, Numerical Methods for Partial Differential Equations, 2024)
- High order entropy stable schemes for the compressible Euler equations (J Chan, K Shukla, X Wu, R Liu, P Nalluri, Journal of Computational Physics 504, 112876)
- An Energy Stable High-Order Cut Cell Discretization for Wave Propagation (CG Taylor, L Wilcox, J Chan, arXiv preprint arXiv:2404.06630)
- High order entropy stable discontinuous Galerkin methods for shallow water equations with subcell positivity preservation (Y Lin, J Chan, Journal of Computational Physics 498, 112677)

Below the publications, citation styles are listed: MLA, APA, Chicago, Harvard, and Vancouver. Each style has a corresponding citation entry. At the bottom right, there are buttons for BibTeX, EndNote, RefMan, and 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

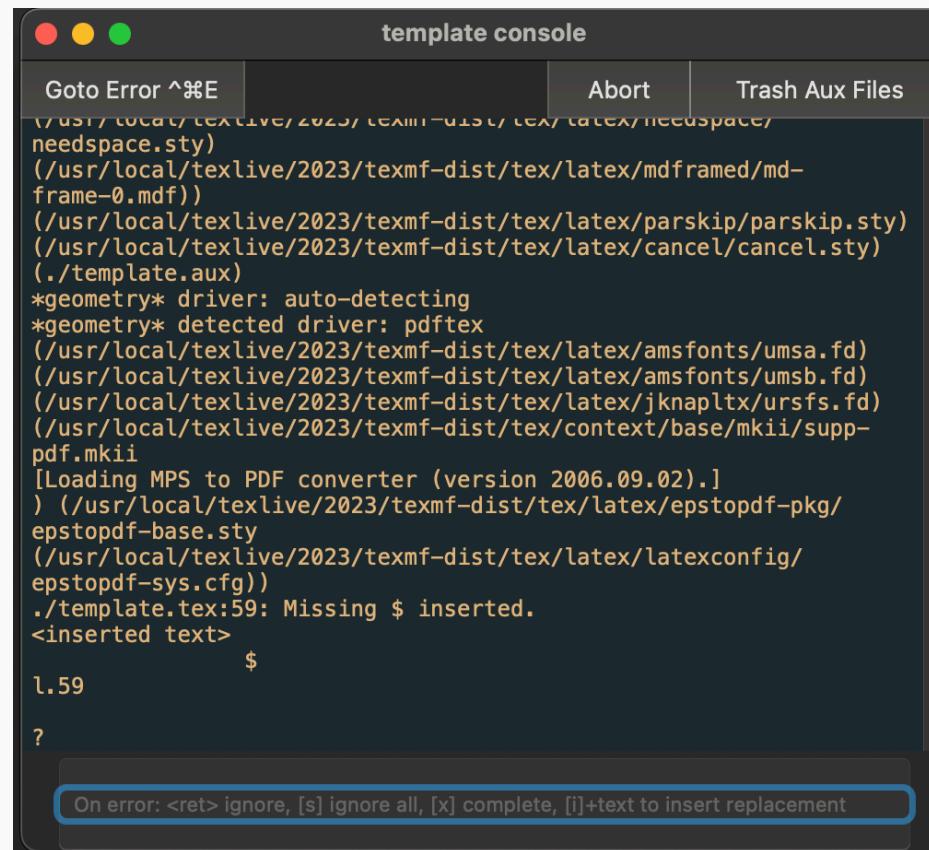
- [1] Xinhui Wu, Nathaniel Trask, and Jesse Chan. Entropy stable discontinuous galerkin methods for the shallow water equations with subcell positivity preservation. *Numerical Methods for Partial Differential Equations*, page e23129.

# 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". The window has three buttons in the top-left corner (red, yellow, green). The title bar also contains "Abort" and "Trash Aux Files" buttons. The main area of the terminal displays the following LaTeX compilation log:

```
(/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: pdftex
(/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>
$
```

l.59

?

In the bottom right corner of the terminal window, there is a small text input field with a blue border containing the message: "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

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

# Binary representations of integers

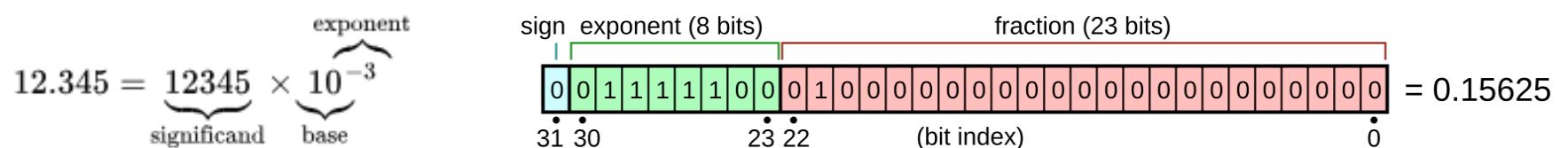
- $5 = 0110 = 0 * (2^0) + 1 * (2^1) + 1 * (2^2) + 0 * (2^3)$
- Binary 0/1 digits are coefficients in a binary expansion
- We use 4 “bits” here; 64-bit integers are most common, but 8-bit, 16-bit, and 32-bit integers are all used.
- What does this expansion imply about the numbers that can be represented 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.



[https://en.wikipedia.org/wiki/Floating-point\\_arithmetic](https://en.wikipedia.org/wiki/Floating-point_arithmetic)

# 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.