Enzo - P / Cello Scaling and other things

scaling, chemistry

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ABSTRACT

Nam dui ligula, fringilla a, euismod sodales, sollicitudin vel, wisi. Morbi auctor lorem non justo. Nam lacus libero, pretium at, lobortis vitae, ultricies et, tellus. Donec aliquet, tortor sed accumsan bibendum, erat ligula aliquet magna, vitae ornare odio metus a mi. Morbi ac orci et nisl hendrerit mollis. Suspendisse ut massa. Cras nec ante. Pellentesque a nulla. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Aliquam tincidunt urna. Nulla ullamcorper vestibulum turpis. Pellentesque cursus luctus mauris.

CCS CONCEPTS

Computing methodologies → Massively parallel algorithms; Simulation evaluation;
Software and its engineering → Designing software;

KEYWORDS

awesomeness

ACM Reference format:

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1 INTRODUCTION

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2 THE BODY OF THE PAPER

Typically, the body of a paper is organized into a hierarchical structure, with numbered or unnumbered headings for sections, subsections, sub-subsections, and even smaller sections. The command \section that precedes this paragraph is part of such a hierarchy. LaTeX handles the numbering and placement of these headings for you, when you use the appropriate heading commands around the titles of the headings. If you want a sub-subsection or smaller part to be unnumbered in your output, simply append an asterisk to the command name. Examples of both numbered and unnumbered headings will appear throughout the balance of this sample document.

Because the entire article is contained in the **document** environment, you can indicate the start of a new paragraph with a blank line in your input file; that is why this sentence forms a separate paragraph.

2.1 Type Changes and Special Characters

We have already seen several typeface changes in this sample. You can indicate italicized words or phrases in your text with the command \textit; emboldening with the command \textbf and typewriter-style (for instance, for computer code) with \texttt. But remember, you do not have to indicate typestyle changes when such changes are part of the *structural* elements of your article; for instance, the heading of this subsection will be in a sans serif³ typeface, but that is handled by the document class file. Take care with the use of⁴ the curly braces in typeface changes; they mark the beginning and end of the text that is to be in the different typeface.

You can use whatever symbols, accented characters, or non-English characters you need anywhere in your document; you can find a complete list of what is available in the \(\mathbb{E}T_EX\) \(User's Guide \) [?].

2.2 Math Equations

You may want to display math equations in three distinct styles: inline, numbered or non-numbered display. Each of the three are discussed in the next sections.

2.2.1 Inline (In-text) Equations. A formula that appears in the running text is called an inline or in-text formula. It is produced by the **math** environment, which can be invoked

 $^{^{1}\}mathrm{This}$ is an abstract footnote

²This is a footnote.

 $^{^3}$ Another footnote here. Let's make this a rather long one to see how it looks.

⁴Another footnote.

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with the usual \begin ...\end construction or with the short form \$...\$. You can use any of the symbols and structures, from α to ω , available in LATEX [?]; this section will simply show a few examples of in-text equations in context. Notice how this equation: $\lim_{n\to\infty} x = 0$, set here in in-line math style, looks slightly different when set in display style. (See next section).

2.2.2 Display Equations. A numbered display equation—one set off by vertical space from the text and centered horizontally—is produced by the **equation** environment. An unnumbered display equation is produced by the **displaymath** environment.

Again, in either environment, you can use any of the symbols and structures available in LaTeX; this section will just give a couple of examples of display equations in context. First, consider the equation, shown as an inline equation above:

$$\lim_{n \to \infty} x = 0 \tag{1}$$

Notice how it is formatted somewhat differently in the **dis-playmath** environment. Now, we'll enter an unnumbered equation:

$$\sum_{i=0}^{\infty} x + 1$$

and follow it with another numbered equation:

$$\sum_{i=0}^{\infty} x_i = \int_0^{\pi+2} f \tag{2}$$

just to demonstrate LATEX's able handling of numbering.

2.3 Citations

Citations to articles [????], conference proceedings [?] or maybe books [??] listed in the Bibliography section of your article will occur throughout the text of your article. You should use BibTeX to automatically produce this bibliography; you simply need to insert one of several citation commands with a key of the item cited in the proper location in the .tex file [?]. The key is a short reference you invent to uniquely identify each work; in this sample document, the key is the first author's surname and a word from the title. This identifying key is included with each item in the .bib file for your article.

The details of the construction of the .bib file are beyond the scope of this sample document, but more information can be found in the *Author's Guide*, and exhaustive details in the *Later's Guide* by Lamport [?].

This article shows only the plainest form of the citation command, using \cite.

2.4 Tables

Because tables cannot be split across pages, the best placement for them is typically the top of the page nearest their initial cite. To ensure this proper "floating" placement of tables, use the environment **table** to enclose the table's contents and the table caption. The contents of the table itself must go in the **tabular** environment, to be aligned properly

Table 1: Frequency of Special Characters

Non-English or Math	Frequency	Comments
Ø	1 in 1,000	For Swedish names
π	1 in 5	Common in math
\$	4 in 5	Used in business
Ψ_1^2	1 in 40,000	Unexplained usage

in rows and columns, with the desired horizontal and vertical rules. Again, detailed instructions on **tabular** material are found in the PTFX User's Guide.

Immediately following this sentence is the point at which Table 1 is included in the input file; compare the placement of the table here with the table in the printed output of this document.

To set a wider table, which takes up the whole width of the page's live area, use the environment **table*** to enclose the table's contents and the table caption. As with a singlecolumn table, this wide table will "float" to a location deemed more desirable. Immediately following this sentence is the point at which Table 2 is included in the input file; again, it is instructive to compare the placement of the table here with the table in the printed output of this document.

It is strongly recommended to use the package booktabs [?] and follow its main principles of typography with respect to tables:

- Never, ever use vertical rules.
- (2) Never use double rules.

It is also a good idea not to overuse horizontal rules.

2.5 Figures

Like tables, figures cannot be split across pages; the best placement for them is typically the top or the bottom of the page nearest their initial cite. To ensure this proper "floating" placement of figures, use the environment **figure** to enclose the figure and its caption.

This sample document contains examples of .eps files to be displayable with IATEX. If you work with pdfIATEX, use files in the .pdf format. Note that most modern TEX systems will convert .eps to .pdf for you on the fly. More details on each of these are found in the *Author's Guide*.

As was the case with tables, you may want a figure that spans two columns. To do this, and still to ensure proper "floating" placement of tables, use the environment figure* to enclose the figure and its caption. And don't forget to end the environment with figure*, not figure!

2.6 Theorem-like Constructs

Other common constructs that may occur in your article are the forms for logical constructs like theorems, axioms, corollaries and proofs. ACM uses two types of these constructs: theorem-like and definition-like.

Here is a theorem:

Table 2: Some Typical Commands

Command	A Number	Comments
\author	100	Author
\table	300	For tables
\table*	400	For wider tables

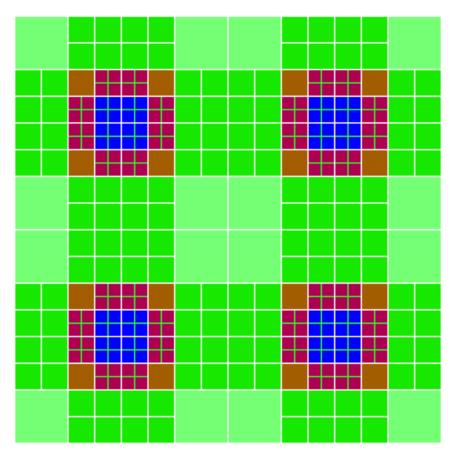


Figure 3: A sample black and white graphic that needs to span two columns of text.

Theorem 2.1. Let f be continuous on [a,b]. If G is an antiderivative for f on [a,b], then

$$\int_{a}^{b} f(t) dt = G(b) - G(a).$$

Here is a definition:

Definition 2.2. If z is irrational, then by e^z we mean the unique number that has logarithm z:

$$\log e^z = z.$$

The pre-defined theorem-like constructs are **theorem**, **conjecture**, **proposition**, **lemma** and **corollary**. The pre-defined definition-like constructs are **example** and **definition**. You can add your own constructs using the *amsthm* interface [?]. The styles used in the **\theoremstyle** command are **acmplain** and **acmdefinition**.

Another construct is **proof**, for example,

PROOF. Suppose on the contrary there exists a real number L such that

$$\lim_{x \to \infty} \frac{f(x)}{g(x)} = L.$$

Then

$$\begin{split} l &= \lim_{x \to c} f(x) = \lim_{x \to c} \left[gx \cdot \frac{f(x)}{g(x)} \right] = \lim_{x \to c} g(x) \cdot \lim_{x \to c} \frac{f(x)}{g(x)} = 0 \cdot L = 0, \\ \text{which contradicts our assumption that } l \neq 0. \end{split}$$

3 CONCLUSIONS

This paragraph will end the body of this sample document. Remember that you might still have Acknowledgments or Appendices; brief samples of these follow. There is still the Bibliography to deal with; and we will make a disclaimer , Thomas Bolden

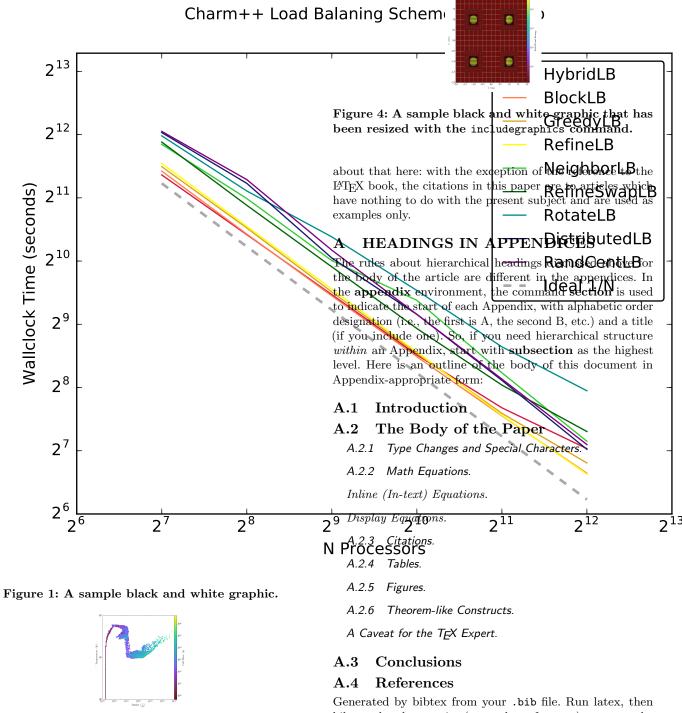


Figure 2: A sample black and white graphic that has been resized with the includegraphics command.

Generated by bibtex from your .bib file. Run latex, then bibtex, then latex twice (to resolve references) to create the .bbl file. Insert that .bbl file into the .tex source file and comment out the command \thebibliography.

B MORE HELP FOR THE HARDY

Of course, reading the source code is always useful. The file acmart.pdf contains both the user guide and the commented code.

ACKNOWLEDGMENTS

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