# Introduction to Programming and Computing for Scientists

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**Lund University** 

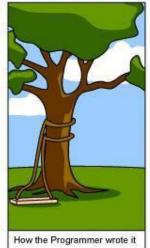
Lecture 2

# Software development is not simply programming



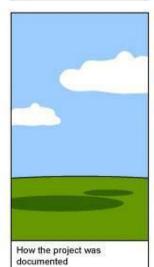


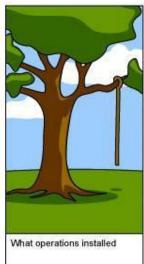


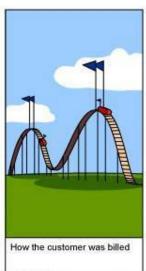


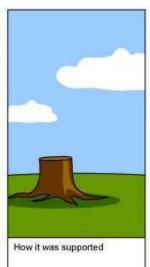


described it











**Author unknown** 

Most software/IT projects fail, even with excellent programmers

# Software development is many things



# Software development as a process: a simplified picture

#### **Requirement collection**

understanding of the problem

#### **Testing and bug-fixing**

there is no code without bugs





#### **Documenting**

undocumented software dies early

#### **Design and planning**

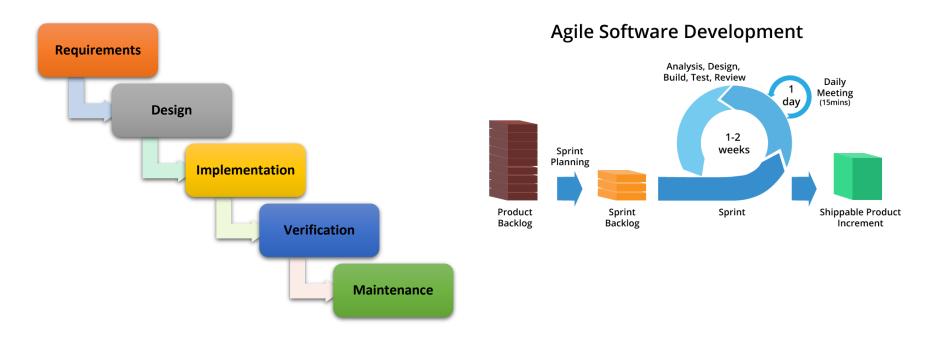
mix of engineering and art



### **Programming**

### Different software development methodologies

- Waterfall model: a straightforward sequential approach
- Agile development: too many bugs to do long-term planning

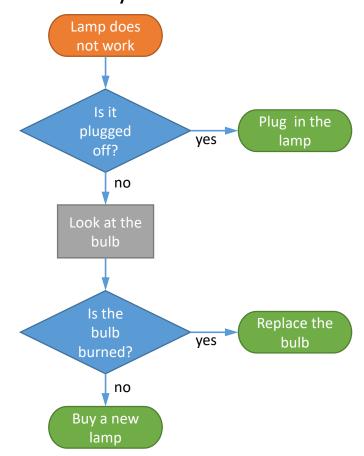


 There are also rapid prototyping, incremental development, various combinations of methodologies, and even cowboy coding (every student does it)

### Most programs implement an algorithm

- Algorithm is a well-defined sequence of actions to be performed
  - Starts from initial state
    - May need initial input
  - Proceeds through a sequence of instructions in a strict order
    - May include conditional statements
  - Terminates with a final state
- Algorithms can be expressed through:
  - Human language (ambiguous)
  - Pseudocode (no standard)
  - Flowcharts
  - Other charts, tables, programming languages

- Flowchart is a graphical representation of an algorithm
  - Warning: complex flowcharts may lead to "spaghetti code" with many redirections



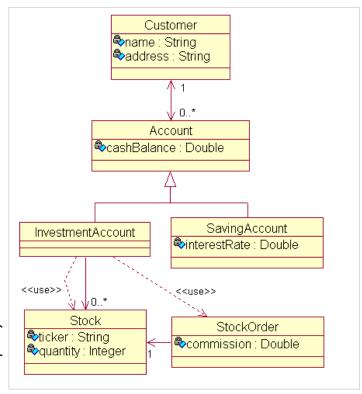
# Flowchart symbols overview

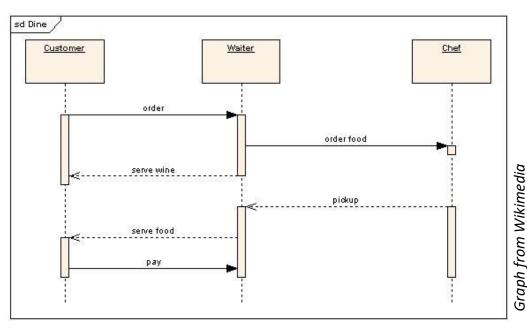
- Can be found in any presentation-making software
- Often used to describe not only algorithms, but also workflows

Start and end	
Flow arrows	
Process	
Conditional	
Data	
Document	
Disk	
Tape	

# Unified Modelling Language (UML)

- A standard way to visualize complex processes or systems
  - You may never need to use it, unless you'll become a professional developer
- Designed for object-oriented methods
- Uses diagrams to describe systems:
  - Structure diagrams show objects and their relations
  - Behaviour diagrams show activities and state changes
- There are many different "styles" of diagrams, but each has well-defined "language"





### A bit of legalism

- Even if you are not a professional programmer, the code that you write is an Intellectual Property
  - Much like scientific publications, music, photos etc
  - Computer programs and even their design are protected by copyright
    - Different laws exist in different countries
- In Swedish universities, it is your Intellectual Property
  - In other countries and companies, your employer may own the code check the contract
  - You should remember to mention code written by you in your CV
- What does ownership give you:
  - Right to authorise <u>copying</u> (including copying for usage)
  - Right to authorise modifications
  - Right to authorise <u>distribution</u>

### Software licenses

- Software license is a legal instrument that defines rules of software usage, modification and distribution
- Different licenses allow different freedoms
  - Proprietary (end-user license agreements, EULA): least permissive
  - Open Source: some limitations, several combinations exist
  - Public domain: basically, no license, everything is permitted
- Scientific software has no common approach regarding licenses
  - Large pieces of code are in a "grey zone", having no explicit license and used without clear rules
- We like Open Source licenses because they allow <u>free code usage</u>, <u>modification</u> and <u>sharing</u>
  - A number of different Open Source licenses exist (see next slide)
  - Open Source software can still be sold (if anyone wants to pay)
  - Software developed using public funding (as in universities) should normally have an Open Source license
- Note: documents and data also have licenses! We like Open Access ones.

# Some Open Source licenses

- GPL, Apache and BSD are the most commonly used ones
  - Some, like GPL, are "contagious"
  - It is up to the code owner to decide what license to use

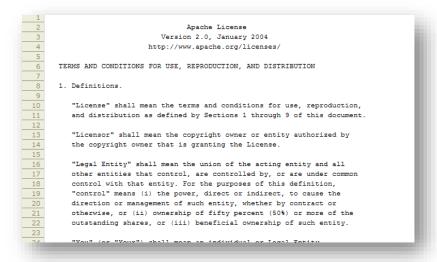


Comparison of the Open Source Licences  The bullets mark if the the licence explicitly states the item in question. Implicit items are not marked by this chart	Must distribute license with binray or source	Cannot use contributors name to endorse	There has to be a notification for changed files	Any change must distributed in source form	Lets you provide warrenty if you want to, normally no	Lets you explicitly charge for providing warrenty or gurantee or transfer of code	All derivative work must be under the same license ▲	Must show License when Run from command line	Non derivative works can have different license	May exclude countries where there is a contradiction with patent in that ocuntry	Must describe any deviation due to regulation
Apache License 2.0	•	•	•	•							
Common Development and Distribution License	•		•				•				
GNU General Public License (GPL)	•		•	•		•	•			•	
GNU Library General Public License (LGPL)	•		•			•				•	
Microsoft Public License (Ms-PL)	•	•									
Microsoft Reciprocal License (Ms-RL)	•	•							•		
Mozilla Public License 1.1 (MPL)	•	1705	•								
New BSD License	•	•									
The MIT License	•										

Graph from stackoverflow.com , original spelling

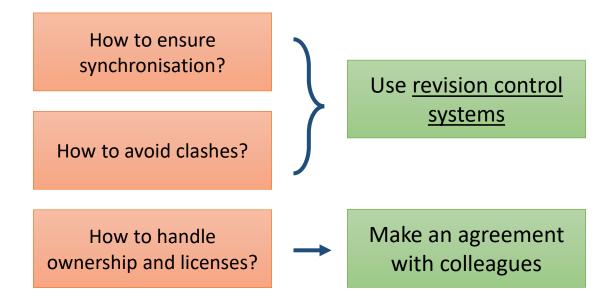
### Practical use of licenses

- Licenses protect (or not) both the developers and the software
  - If everybody is allowed to change the code, the original author can not guarantee its <u>quality</u> or features
  - If nobody is allowed to change it, the author will be held <u>responsible</u> for all wrongdoings
  - In practice, a good balance is needed: changes should be allowed under certain conditions
- License is implemented as a <u>piece of text</u>, distributed together with the software
  - Some add it to every file
  - If a software package has many files, license can be a separate file

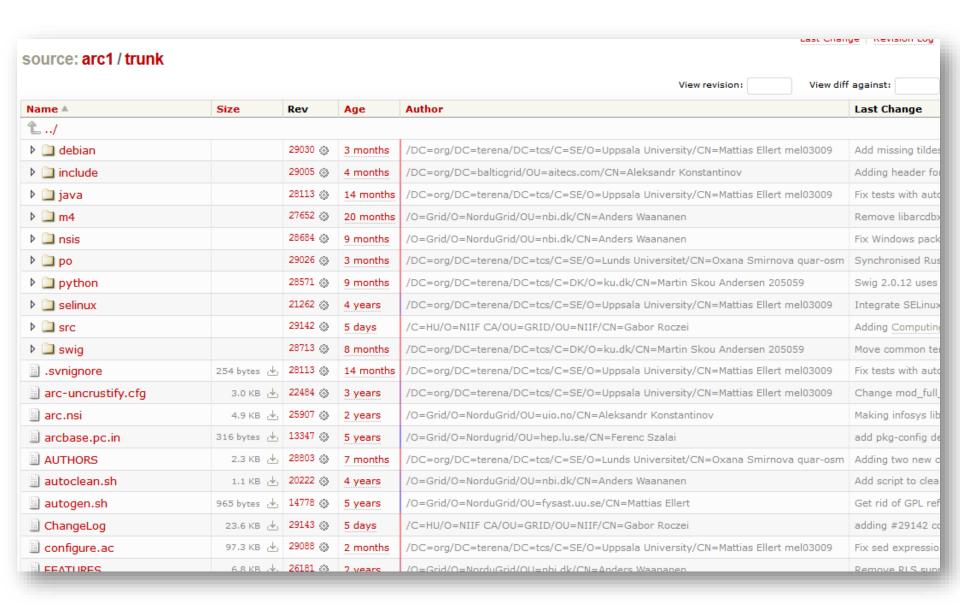


### When you're not the lone developer

- When your code grows big, it is always good to split it into separate files
  - A program is one algorithm (rarely a few)
  - Software is a collection of various algorithms that work together
- Large softwares consist of many files and are usually developed by several people



# Example of a complex software with many authors



### Revision control systems

- **Revision** in our context stands for an updated piece of code (or several pieces)
- Since several developers may update different pieces of code simultaneously, a system is needed to keep everything synchronised and to avoid clashes
- Sometimes bad updates need to be reverted, too previous revisions need to be kept
- When a software is ready to be used, it has to be <u>tagged</u>, for reference
  - A tag is basically a snapshot of all the code, labelled by a number or a special string
  - Tags are a good reference point for testing
  - When tested and proven to work as expected, a tag is released as a new software version
- Therefore, the main functionalities of such common development systems are:
  - Reference software repository ("master copy")
  - Accepting changes (<u>commits</u>) from different developers
  - Revision history ("backup" of files)
  - Versioning

### Few words on software versions

- Software changes very often, so it is important to know what exact code was used
  - Primarily, to make results <u>reproducible</u>
  - But also to simplify maintenance, debugging, user support etc.
- Most code developed by students has no versions very bad practice!
- Some examples of versions:
  - Operating systems: Windows 10, iOS 9.3.5, Ubuntu 16.04 "Yakkety Yak", Android 7.0 "Nougat", Fedora 20 "Heisenbug"
  - Software: ROOT v6.06/06, gcc 4.9.2, Photoshop CS5.5, Office 2013, Linux kernel 4.7
- In the Linux world, most common versioning scheme is MM.mm.bb
  - MM major version with massive changes; usually backwards incompatible with MM-1
  - mm minor version with some new functionality; versions MM.mm and MM.mm-1 are usually compatible
  - bb <u>bugfix</u> version, always compatible with MM.mm.bb-1

### General principles of work with revision control systems

- There is a code repository, from which software releases are made
  - Repository can be centralised or distributed
- Each developer makes clone or checkout an own working copy of the repository
  - Many systems allow to clone/checkout only a part of the entire repository
- After doing local code changes, the developer synchronises commit or push the change to the repository
  - In most systems, only the differences are communicated to the repository
  - It is a good practice to commit often, avoid mega-commits
- If the system notices that the code has changed meanwhile, it will try to merge the changes, if they were committed to different parts of the code
  - Beware! The changes may still turn out to be incompatible, no system is clever enough to figure it
  - If automatic merging is impossible, you will have to do it manually
- Changes can be reverted to any previous revision if it turns out they caused troubles
- Release manager can decide which changes should be accepted for the software release

### Traditional approach: central code repository

A straightforward approach is to have one central repository

• A **trunk** would contain the main reference code, and **branches** would contain

specialised/private developments

Name A	Size	Rev	Age	Author
<b>L</b> /				
▼		29096 💮	7 weeks	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala Univ
Darc_trunk_bdii5		17248 💮	5 years	/O=Grid/O=NorduGrid/OU=nsc.liu.se/CN=Daniel Jol
		29096 💮	7 weeks	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala Uni
Dianitor		12565 💮	6 years	/O=GermanGrid/OU=UniLuebeck/CN=Hajo Nils Krab
▶ 🛄 jss		4648 ⊗	9 years	anonymous
▶ 🛄 v_0_2		316 💮	12 years	aleks
▷ 🛄 v_0_4		4659 💮	9 years	aleks
▶ 🗀 v_0_6		12819 💮	6 years	/O=Grid/O=NorduGrid/OU=fys.uio.no/CN=Adrian Ta
Þ 🗀 v_0_8		17741 📎	5 years	/O=Grid/O=NorduGrid/OU=fys.uio.no/CN=Adrian Ta
▶ 🛄 v_0_8_1_1		16791 💮	5 years	/O=Grid/O=NorduGrid/OU=nsc.liu.se/CN=Daniel Jo
▶ 🛄 v_0_8_2		18196 💮	4 years	/O=Grid/O=NorduGrid/OU=nsc.liu.se/CN=Daniel Jo
▶ 🛄 v_0_8_3		20021 💮	4 years	/C=HU/O=NIIF CA/OU=GRID/OU=NIIF/CN=Ivan Ma
▶ 🗎 tags		24575 💮	3 years	/O=Grid/O=NorduGrid/OU=nbi.dk/CN=Anders Waar
trunk		20022 💮	4 years	/C=HU/O=NIIF CA/OU=GRID/OU=NIIF/CN=Ivan Ma

#### Plus

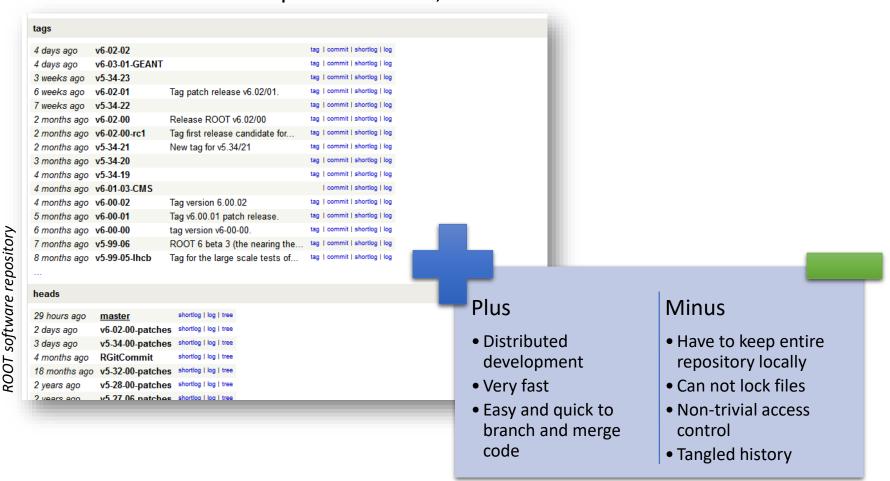
- Easy to control and manage
- Easy to prevent conflicts
- Each developer makes a checkout of only the code they need

#### Minus

- No general agreement how to deal with branches
- Single point of failure if the server goes down (or is slow)

# Modern approach: distributed repository

- Every developer has a local copy of the entire repository
  - Can commit off-line and synchronise later
    - Allows for frequent commits, hence better revision control



### Most popular revision control systems

- Git: a distributed system
  - Developed by Linus Torvalds in 2005
  - Open Source (GPL/LGPL)
  - Each local copy is a complete repository, with all the revision history and such
  - Light-weight easy to merge branches
  - No own access control, but many add-ons
  - Basis for popular platforms: Github, Gitlab
  - Very well documented: http://git-scm.com/book



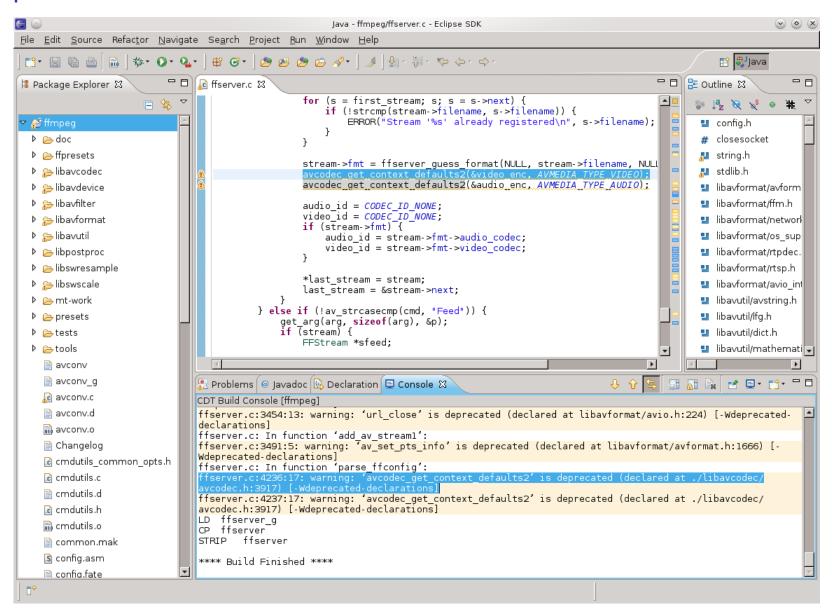
- Subversion (SVN): a centralised system
  - Release 1.0.0 in 2004
  - Open Source (Apache)
  - Branches retain no knowledge of the trunk
  - Strict history and revision control
  - Allows authorisation per directory
  - Well documented, e.g.: <u>http://svnbook.red-bean.com/</u>



# Integrated Development Environment (IDE)

- For non-professional developers, a good editor and command-line build tools is enough to write and build software
  - Warning: avoid building in your SVN/Git working copy! This may create many files that you don't want to commit!
- For professionals, special IDEs exist, that include:
  - Context-aware software <u>editor</u>
  - <u>Build</u> automation tools
    - Some include compilers and interpreters
  - Debugging tools
  - Some integrate with revision control systems
- Very many IDEs exist for C++
  - There are no good IDEs for Linux (they are not really needed there)
  - Geany is actually a light-weight IDE
    - Some even use Emacs editor as an IDE
  - Eclipse is one of the most powerful and complicated
  - On Windows, Microsoft Visual Studio is the best

### Eclipse screenshot



### There is no code without bugs

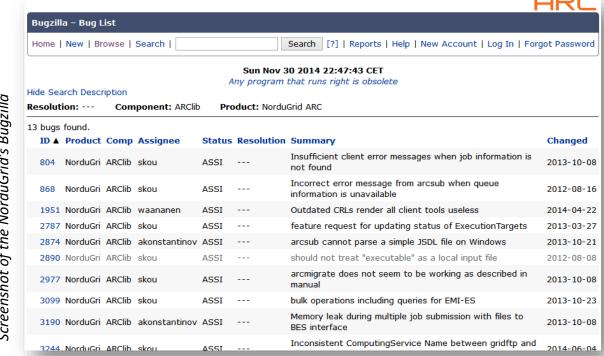
- With an Open Source code, everybody can find a bug... or many...
- So we need a system where bugs can be reported and followed-up: a bug tracking system
- Such system is essentially a database where every authorised person can register a discovered defect
- Typical information to be entered:
  - Summary of the problem and ways to <u>reproduce</u> it
  - Software version that has the problem
  - Operating system version where the problem occurs
  - Severity of the problem
- Bugs have life cycle: from being new, to assigned, to fixed
  - Different systems have different such states
  - States are changed by administrators in charge of bug tracking
    - E-mail notifications are sent to all the involved parties (reporters, developers etc) on each state change
- When you find a bug, please always report it!

### Bug tracking systems

- Many bug tracking systems exist
  - Some are stand-alone
  - Some are integrated with revision control systems
    - Some are even distributed
  - Some are integrated with IDEs
  - Some are a part of larger issue-tracking systems

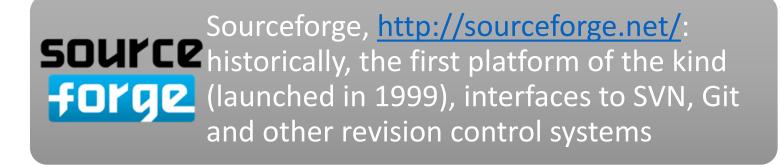
#### Some commonly used bug trackers:

- Bugzilla (standalone), http://www.bugzilla.org/
- JIRA (project management tool), https://www.atlassian.com/software/iira
- Savannah (development service), http://savannah.gnu.org/
- Trac (integrated with Wiki), http://trac.edgewall.org/
- Redmine (project management), http://www.redmine.org/



### Software development hosting platforms

• If you start a new software project and don't want to set up an own code repository, Wiki, bug tracker etc, several free Open Source hosting services exist



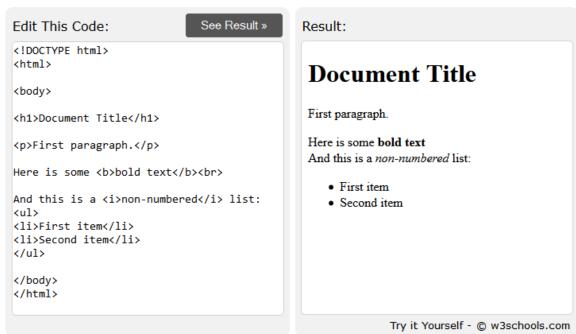


GitHub, <a href="https://github.com/">https://github.com/</a>: the most popular and largest IT-project hosting service (started in 2008), based on Git (obviously); free for Open Source projects

 Some other hosting services: BitBucket, several Google platforms, GitLab, Launchpad, Savannah, Assembla etc

### Simplest languages: markup languages

- Markup languages add special tags to <u>plain text</u>
  - These tags will be processed and interpreted by software
  - Tags must be distinguishable from normal text
- An example of a markup language at work you see every day in Web pages
  - Did you ever try to click "show source code" on a Web page?
  - If yes, you probably noted <!DOCTYPE html in the very beginning</li>
  - HTML stands for HyperText Markup Language
    - Was developed at CERN, inspired by an earlier SGML (Standard Generalized Markup Language)



# Usage of markup languages for text processing; LaTeX

- Once your results are ready, it is time to publish!
  - Or to write a project report
- Softwares that make your papers looking good are called word processors
  - All good word processors cost money (like Microsoft Office)
  - All free word processors are desperately bad (like LibreOffice)
- What do word processors do under the hood?
  - They make use of different markup languages to add special tags to your text and figures, and convert them to a visually pleasant layout (hopefully)
- LaTeX is a markup language for word processing, with which you add the tags yourself, and LaTeX system converts it to a publishable material



- It is free
- It supports most complex mathematics
- It is extensible
- It is accepted by all publishers

#### Minus

- You don't see the result "live"
- Tables and figures are very difficult to pin into place
- No way to track changes (unless you use a revision control system)

### So what is LaTeX?

- Actually, the language itself is called TeX
  - TeX was released in 1978, designed by Donald Knuth in Stanford
  - The goal was to create a complete typesetting system that would produce identical results on any computer
    - Hence the markup language: plain text can be transferred everywhere
  - Stable since 1989, when support for non-English languages was added to TeX 3.0
    - Software version is currently 3.14159265 (guess the next version....)
    - Public domain software
- Some basic TeX rules:
  - TeX tags (commands) start with a backslash \ and use curly brackets \ } to group command input
  - Simple mathematics is included in \$\$
    - $\sqrt{2}$  results in  $\sqrt{2}$
  - Paragraphs are separated by blank lines
  - Comments start with %

### From TeX to LaTeX

- Plain TeX uses elementary instructions and is rather difficult to learn and use for complex documents
- Leslie Lamport developed LaTeX in 1984 using TeX, to provide a higher-level language
  - Added pre-defined commands for sections, cross-references, bibliography etc
  - Easy to use with non-Latin scripts
  - Current version: LaTeX2ε (since 1994)
  - Several online platforms exist

```
\documentclass[a4paper]{article}
\begin{document}
\section*{Document Title}
First paragraph.

Here is some \textbf{bold} text\\
And this is a \textit{non-numbered} list:
\begin{itemize}
\item First item
\item Second item
\end{document}
\end{document}
```

#### Document Title

First paragraph.

Here is some **bold** text

And this is a non-numbered list:

- First item
- Second item

Exercise: go to <a href="https://v2.overleaf.com">https://v2.overleaf.com</a> and try to reproduce this document

### More LaTeX features

- Can do almost all imaginable formatting, section numbering, headers and footers, lists etc
  - Note: (La)TeX uses own fonts, not system ones
    - This ensures identical results everywhere

Is very good with equations	\begin{equation}
Can include figures	<pre>\begin{figure} \includegraphics{cat.jpg}</pre>
Can create tables	<pre>\begin{table} \begin{tabular}</pre>
Handles cross references	<pre>\label{sec:intro} \ref{sec:intro}</pre>
Handles bibliography	<pre>\begin{thebibliography} \bibitem{mybook} \cite{mybook}</pre>
Can include other files	<pre>\input{section2.tex} \include{appendix.tex}</pre>
Can auto-generate table of contents etc	\tableofcontents
Can even do nice slides	\documentclass{beamer}

### Steps to create a LaTeX document

Writing a LaTeX document is similar to real software development:

Edit the text files and the bibliography

Pre-process the files

Create the final publishable document

• You can use Linux command line, any of Windows IDEs (*TeXnicCenter* is good), or one of the many online LaTeX systems (Overleaf is perhaps the most popular)

# A more advanced document: part 1

```
\documentclass[a4paper,12pt,twoside]{article}
                                                          Use additional features:
                                                          utf8: non-latin fonts
\usepackage[utf8]{inputenc}
                                                          graphicx: pictures
\usepackage[pdftex] {graphicx}
                                                          hyperref: web links
\usepackage[pdftex]{hyperref}
\author{Oxana Smirnova}
\title{LaTeX exercise paper}
\date{\today}
                                                               Create title here
\begin{document}
                                                         Empty line starts a new
 \maketitle
                                                         paragraph
 \begin{center}
  \texttt{oxana.smirnova@hep.lu.se}
 \end{center}
\section{Introduction}
                                                    Use labels for cross-referencing from text
\label{sec:intro}
This is introduction. Summary will be given in Section \ref{sec:sum}.
\section{About Linux}
\label{sec:linux}
\begin{figure}[h]
  \begin{center}
                                                                     Use <u>Upload</u> button to upload a picture to Overleaf
    \includegraphics[width=2cm] {penguin.png}
    \caption{Penguin symbolises Linux}
    \label{fig:penguin}
                                                                     Use labels to cross-reference figures as well
  \end{center}
\end{figure}
```

# A more advanced document: part 2

```
Figure \ref{fig:penguin} shows a \textit{penguin}. For more details, check
the Linux Web page~\cite{linux}.
                                                                      Cited papers are defined in the end of the document
\subsection{Linux flavours}
\label{sec:flavours}
Table~\ref{tab:flavours} lists some Linux flavours~\footnote{Only one is shown
for simplicity }.
                                                                         Tables are difficult: & divides cells and
\begin{table}[h]
                                                                          \\ divides rows
  \begin{center}
    \beta = \frac{1}{2}
      \textbf{Distribution}&RedHat&Debian&SuSE\\ \hline \hline
      Fedora 23
                                             \\ \hline
                           & X
                                &
    \end{tabular}
    \caption{Different flavours of Linux}
    \label{tab:flavours}
  \end{center}
\end{table}
\section{About mathematics}
\label{sec:math}
In-line math in \LaTeX \ is enclosed in \$ symbols. Backslash \textbackslash \
is used to denote special symbols.
                                                                                    Remember {} to group characters
Subscripts and superscripts are always math: $A x$, $A {xy}$,
e^x and e^{x^2}. Using underscore \ outside math without \textbackslash \
causes big\ troubles.
All special symbols are also math: $\alpha$, $\beta$, $\gamma$, $\delta$, $\sin
x$, $\hbar$, $\lambda$, $\ldots$ More information can be
found in Ref.~\cite{latex}.
```

# A more advanced document: part 3

```
Equation~\ref{eq:chi2} shows $\chi^2$.
                                                                      Auto-numbered equations is why we love LaTeX
                                                                       Use labels to cross-reference equations, too
\begin{equation}
\label{eq:chi2}
 \c^2 = \sum_i \left(\frac{F i-D i}{\sum_i \right)^2}
\end{equation}
\section{Summary}
\label{sec:sum}
We learned the following:
\begin{itemize}
 \item Linux is good
 \item \LaTeX \ is good for:
    \begin{enumerate}
     \item Structuring documents
     \item Writing mathematial equations
    \end{enumerate}
\end{itemize}
We can also write unformatted text using \texttt{verbatim} environment, but
sometimes we have to specify this in the preamble:
\begin{verbatim}
 \usepackage{verbatim}
                                                                            99 indicates maximum number of papers in the
\end{verbatim}
                                                                            bibliography list
\begin{thebibliography}{99}
 \bibitem{linux} Linux web site: \url{www.linux.com}
 \bibitem{latex} Leslie Lamport, \textsl{LaTeX: A Document Preparation
System}, second edition, Addison-Wesley (1994).
\end{thebibliography}
                                                                            Papers are referenced not by labels
                                                                            but by <u>bibitem</u> tags
\end{document}
```

### Summary

- Software development is a profession and requires professional tools
- Open Source code drives the technological and scientific progress
- "Language" can mean many things: a programming language, a visual modelling language, a markup language...
  - ...and actually many other languages