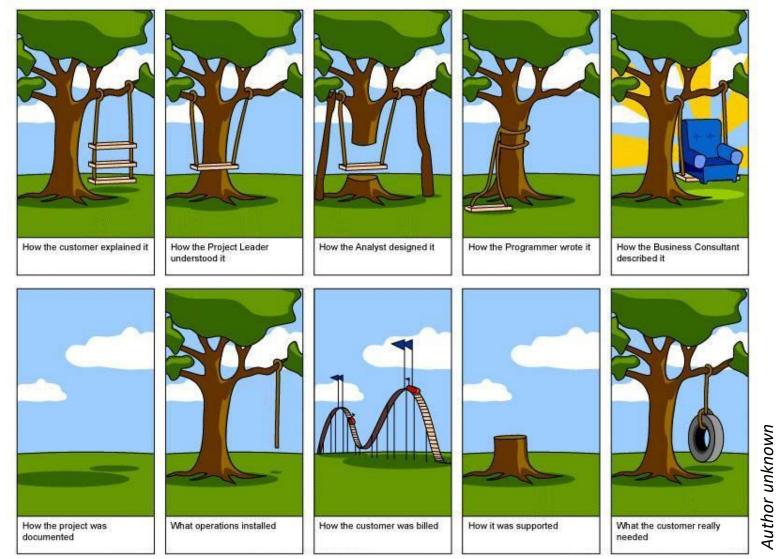
# Introduction to Programming and Computing for Scientists

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Lund University

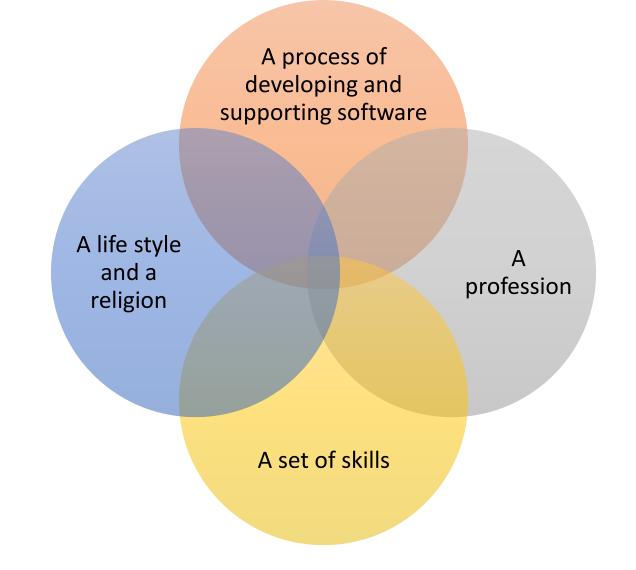
Lecture 2: Essentials of code development in a collaborative environment

#### Software development is not simply programming

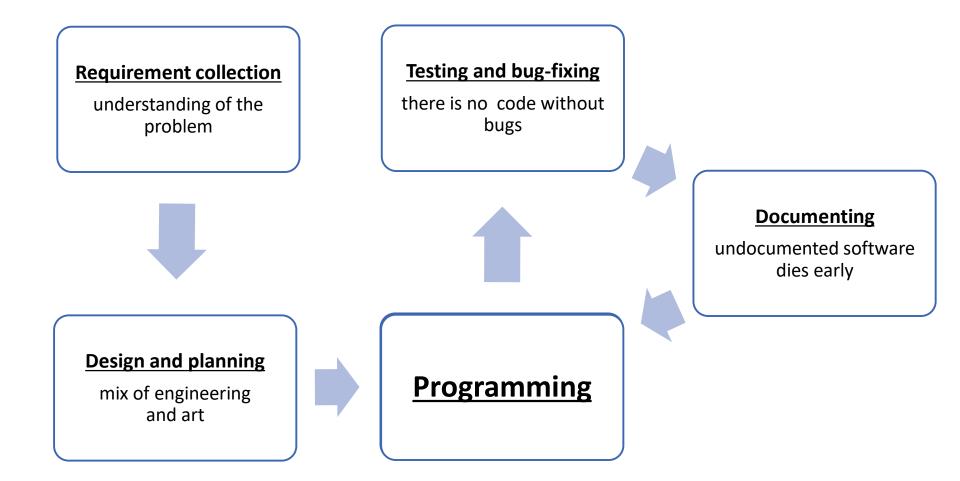


• Most software/IT projects fail, even with excellent programmers

#### Software development is many things

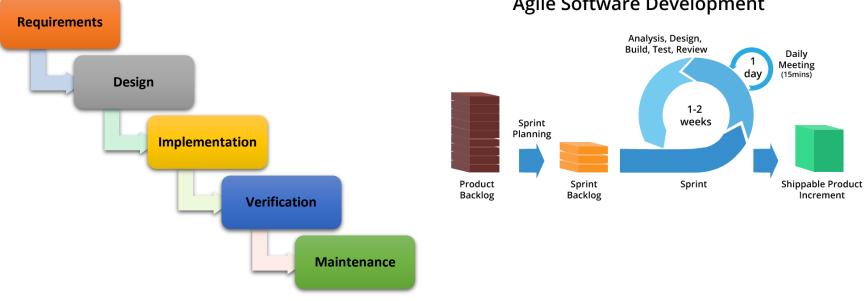


#### Software development as a process: a simplified picture



### Different software development methodologies

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



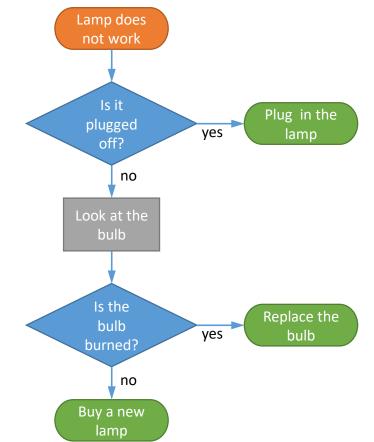
Agile Software Development

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

#### Most programs implement an algorithm

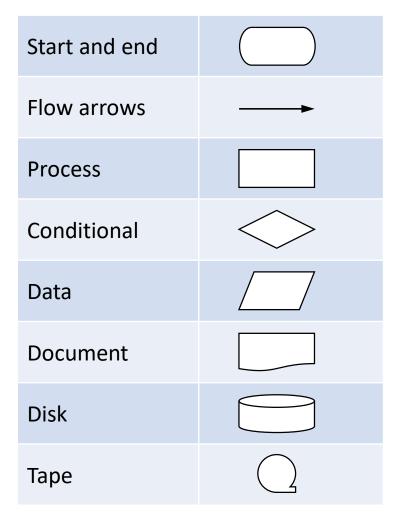
- Algorithm is a well-defined sequence of actions to be performed
  - Starts from initial state
    - May need initial input
  - Proceeds through a sequence of instructions in a strict order
    - May include conditional statements
  - Terminates with a final state
- Algorithms can be expressed through:
  - 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



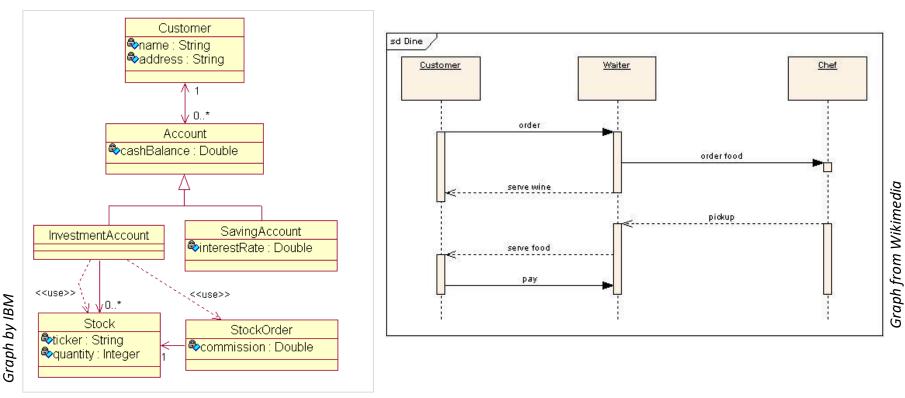
#### Flowchart symbols overview

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



## 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"



Oxana Smirnova (Lund University)

## 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 free code usage, modification and sharing
  - 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
- <u>Note</u>: 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

ache	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 $\blacktriangle$	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	com original spelling
SD	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) New BSD License The MIT License	•••••	• •• •	••••	• •• •	•	•	••	•	••••	•	•	Granh from stackoverflow com original spelling

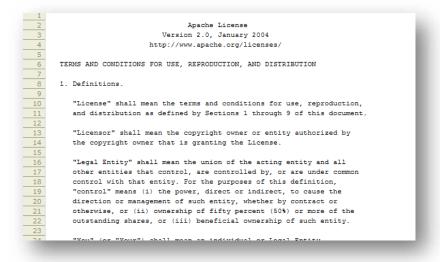
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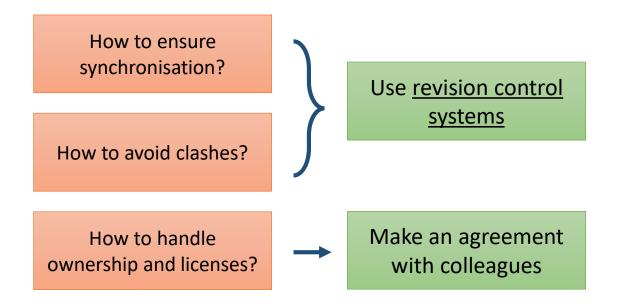
#### Practical use of licenses

- 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

#### source: arc1 / trunk

case onlarige internation cog

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#### 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 (commits) 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 **reproducible**
  - 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 11, iOS 15.6.1, Ubuntu 22.10 "Kinetic Kudu", Android 9.0 "Pie", Fedora 20 "Heisenbug"
  - Software: ROOT v6.26/06, gcc 12.2, Photoshop CS5.5, Office 2019, Linux kernel 5.19.5
- In the Linux world, most common versioning scheme is MM.mm.bb
  - MM <u>major</u> version with massive changes; usually <u>backwards incompatible</u> 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 <u>code repository</u>, 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

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	🕨 🛄 arc_trunk_bdii5		17248 🛞	5 years	/O=Grid/O=NorduGrid/OU=nsc.liu.se/CN=Daniel Johan
	🕨 🛄 compat		29096 🛞	7 weeks	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala Univer
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	🕨 🛄 trunk		20022 🛞	4 years	/C=HU/O=NIIF CA/OU=GRID/OU=NIIF/CN=Ivan Marto

#### Plus

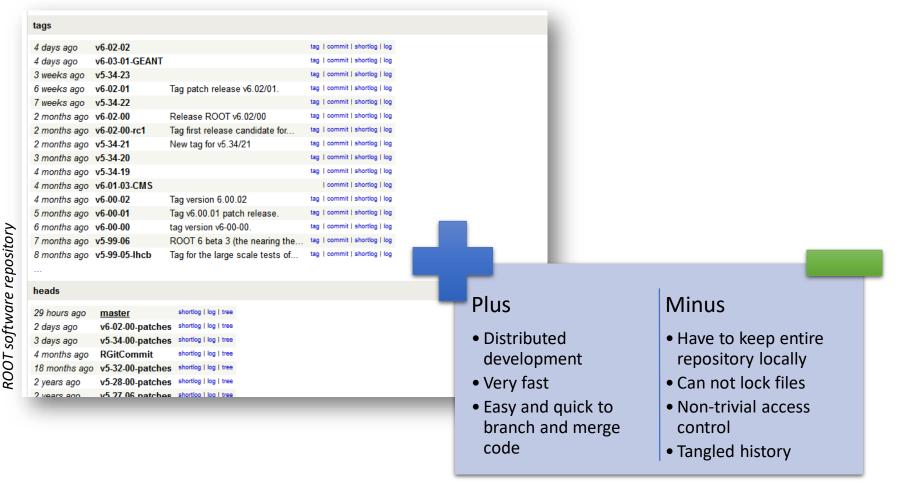
- Easy to control and manage
- Easy to prevent conflicts
- Each developer makes a checkout of only the code they need

#### 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: <u>http://git-scm.com/book</u>



- 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 Git/SVN 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
  - <u>Debugging</u> tools
  - Some integrate with revision control systems
- Very many IDEs exist for C++
  - There are <u>no good IDEs for Linux (they are not really needed there</u>)
  - **Code::Blocks** is a good IDE, available at LUNARC
    - 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

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#### 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

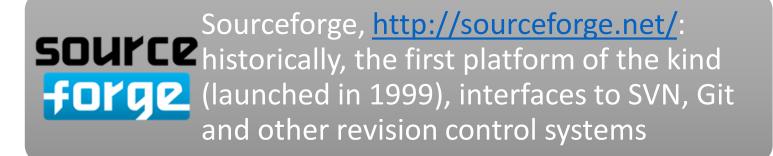
Some commonly used bug trackers:

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

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Hide S	Sun Nov 30 2014 22:47:43 CET Any program that runs right is obsolete Hide Search Description						
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	js found. ▲ <b>Produc</b> t	Comp	Assignee	Status	Resolution	Summary	Changed
804	NorduGr	ARClib	skou	ASSI		Insufficient client error messages when job information is not found	2013-10-0
868	8 NorduGr	ARClib	skou	ASSI		Incorrect error message from arcsub when queue information is unavailable	2012-08-1
195	51 NorduGr	ARClib	waananen	ASSI		Outdated CRLs render all client tools useless	2014-04-2
278	87 NorduGr	ARClib	skou	ASSI		feature request for updating status of ExecutionTargets	2013-03-2
287	74 NorduGr	ARClib	akonstantinov	ASSI		arcsub cannot parse a simple JSDL file on Windows	2013-10-2
289	0 NorduGri	ARClib	skou	ASSI		should not treat "executable" as a local input file	2012-08-0
297	77 NorduGri	ARClib	skou	ASSI		arcmigrate does not seem to be working as described in manual	2013-10-0
309	9 NorduGr	ARClib	skou	ASSI		bulk operations including queries for EMI-ES	2013-10-2
319	0 NorduGr	ARClib	akonstantinov	ASSI		Memory leak during multiple job submission with files to BES interface	2013-10-0
	4 NorduGr	ADCIL	-	ASSI		Inconsistent ComputingService Name between gridftp and	2014-06-0

### 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, <u>https://github.com/</u>: 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 plain text
  - 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)

Edit This Code:	See Result »	Result:
html <html></html>		Document Title
<body></body>		
<h1>Document Title</h1>		First paragraph.
First paragraph.		Here is some <b>bold text</b>
Here is some <b>bold text&lt;</b>	/b>	And this is a <i>non-numbered</i> list:
And this is a <i>non-numbe <ul></ul></i>	ered list:	<ul><li>First item</li><li>Second item</li></ul>
<li>First item</li>		
<li>Second item</li>		
		Try it Yourself - © w3schools.com

Oxana Smirnova (Lund University)

Programming for Scientists

#### 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

_			
-	Plus	Minus	
	• It is free	<ul> <li>You don't see the result "live"</li> </ul>	
	<ul> <li>It supports most complex mathematics</li> </ul>	<ul> <li>Tables and figures are very difficult to pin into</li> </ul>	
	• It is extensible	place	
	<ul> <li>It is accepted by all publishers</li> </ul>	<ul> <li>No way to track changes (unless you use a</li> </ul>	
		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 \$\$
    - $\$  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{itemize}
\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 <u>https://v2.overleaf.com</u> 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

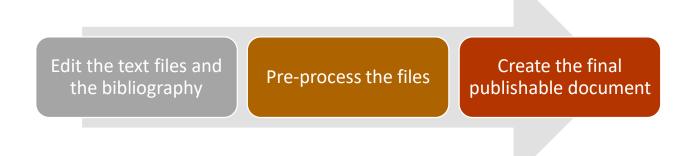
Is very good with equations	\begin{equation}
Can include figures	<pre>\begin{figure} \includegraphics{cat.jpg}</pre>
Can create tables	<pre>\begin{table} \begin{tabular}</pre>
Handles cross references	<pre>\label{sec:intro} \ref{sec:intro}</pre>
Handles bibliography	<pre>\begin{thebibliography} \bibitem{mybook} \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	<pre>\documentclass{beamer}</pre>

Oxana Smirnova (Lund University)

Programming for Scientists

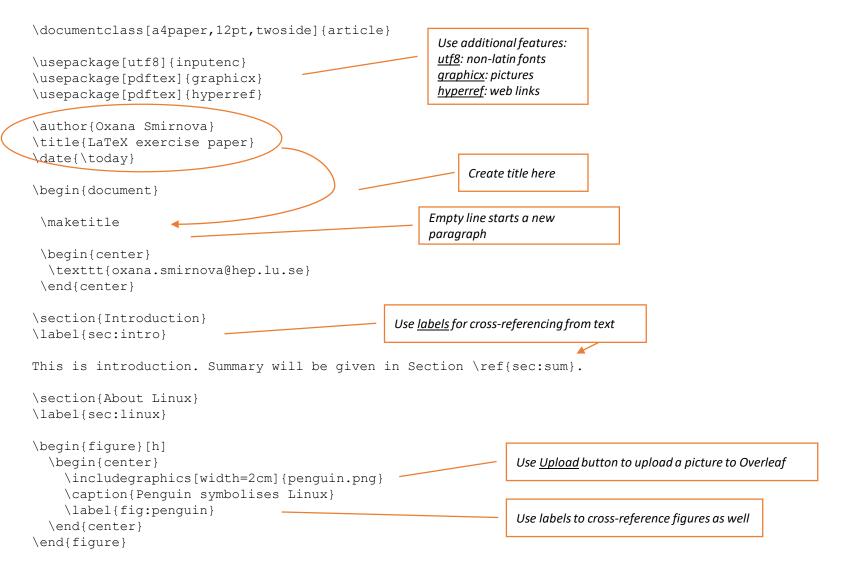
#### Steps to create a LaTeX document

• Writing a LaTeX document is similar to real software development:



• 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)

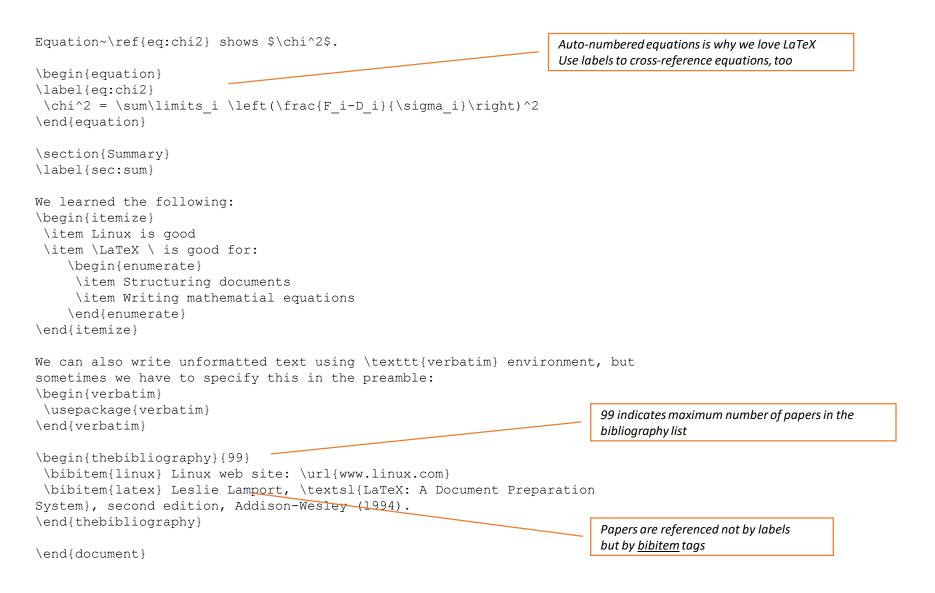
#### A more advanced document: part 1



#### 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}
    \left( \left| c \right| \right)  | is for border, c is for centering
      \textbf{Distribution}&RedHat&Debian&SuSE\\ \hline \hline
      Fedora 23
                                               \\ \hline
                            γ3
                                   æ
                                           æ
    \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



#### 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