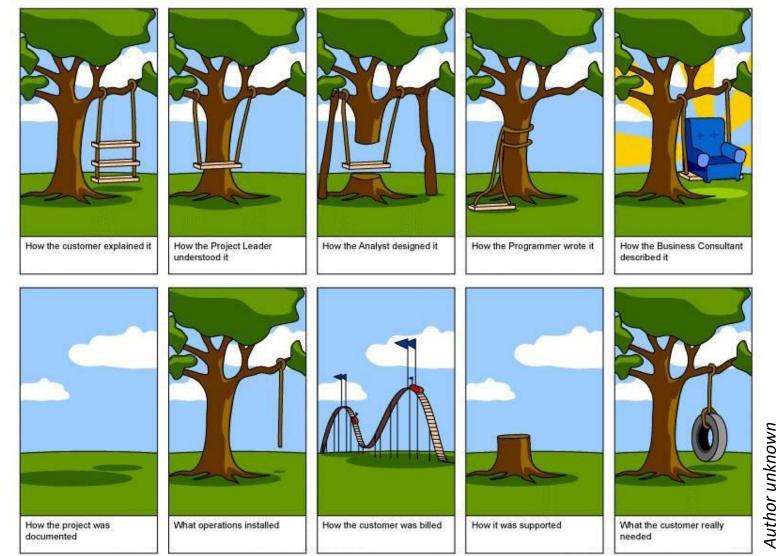
Introduction to Programming and Computing for Scientists

Oxana Smirnova

Lund University

Lecture 6

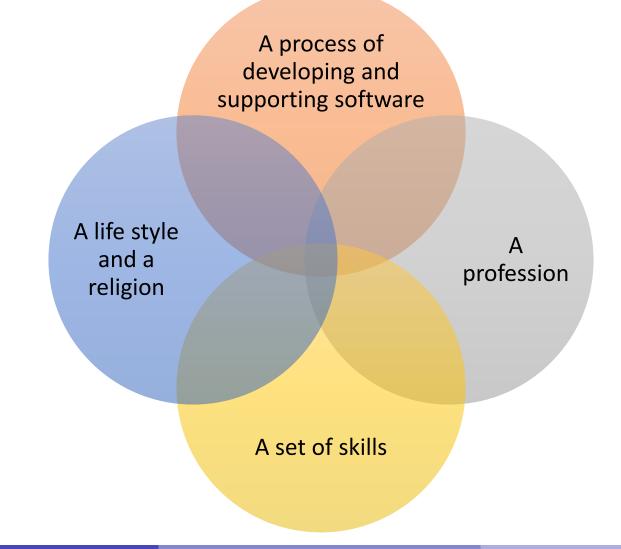
Knowing programming languages is not enough



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

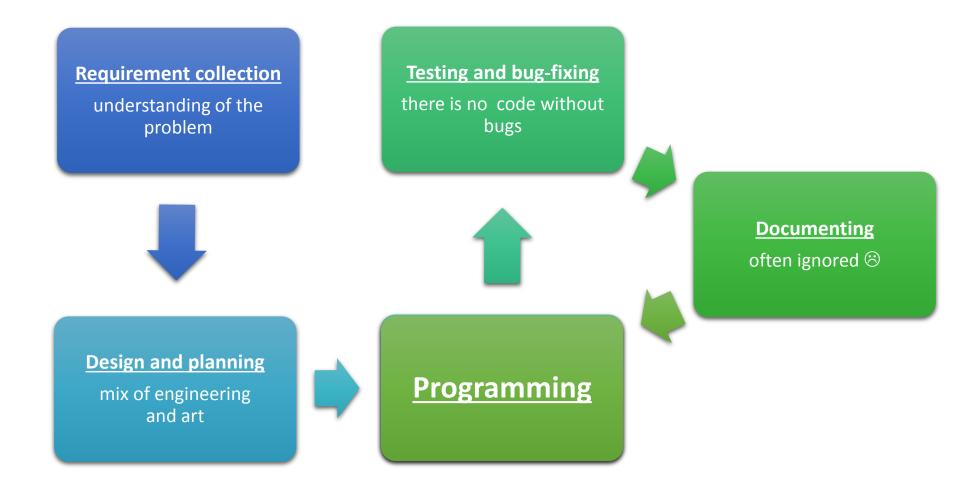
From programming to software development

• Software development is many things:



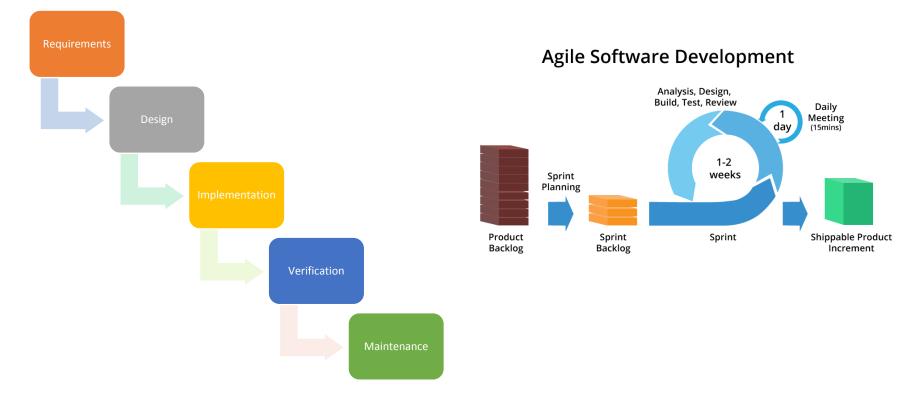
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Software development as a process: simplified picture



Different software development methodologies

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

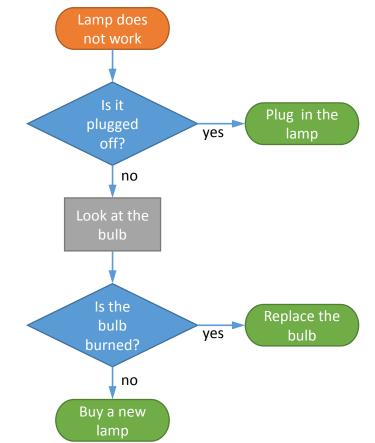


 There are also rapid prototyping, incremental development, various combinations of methodologies, and even cowboy coding (every student does it)

Most programs implement an algorithm

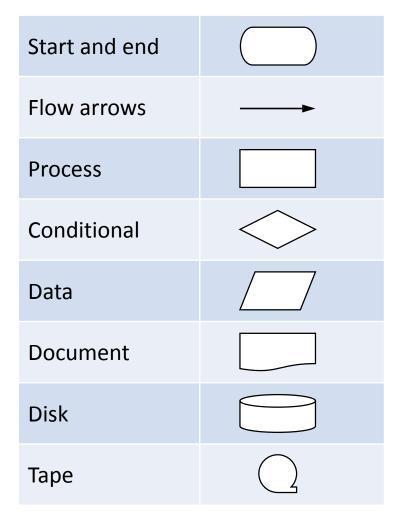
- Algorithm is a well-defined sequence of actions to be performed
 - Starts from initial state
 - May need initial input
 - Proceeds through a sequence of **instructions** in a strict order
 - May include conditional statements
 - Terminates with a final state
- Algorithms can be expressed through:
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

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



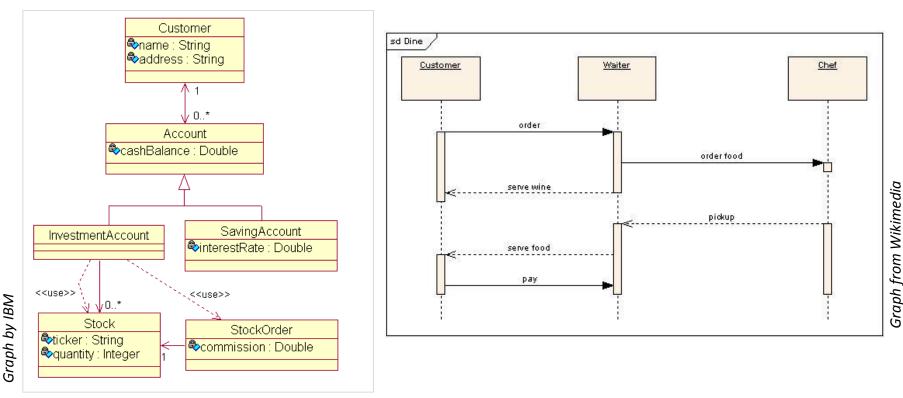
Flowchart symbols overview

- 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"



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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 •
 - GPL is "contagious"

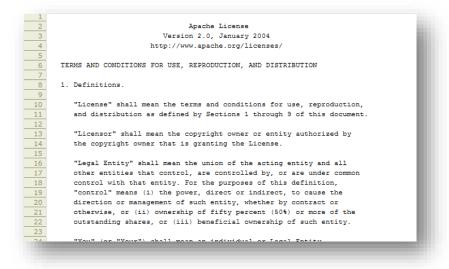
It is up to the code owner to decide what license to use •

Apache GNU	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	.com . oriainal spellina
BSD	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	•••••••	• •• •	••••	•	•	••	••	•	••••	•	•	Graph from stackoverflow.com ,



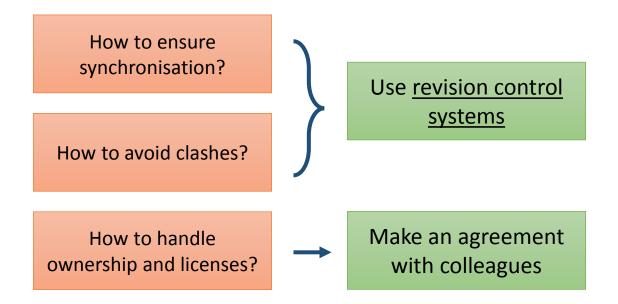
Practical use of licenses

- 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 quality or features
 - If nobody is allowed to change it, the author will be held responsible for all wrongdoings
 - In practice, a good balance is needed: changes should be allowed under certain conditions
- License is implemented as a piece of text, 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				Lest Cherry	ye ivevision Loy
				View revision: View diff	against:
Name 🔺	Size	Rev	Age	Author	Last Change
t /					
🕨 🛄 debian		29030 🛞	3 months	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala University/CN=Mattias Ellert mel03009	Add missing tilde
🕨 🛄 include		29005 🛞	4 months	/DC=org/DC=balticgrid/OU=aitecs.com/CN=Aleksandr Konstantinov	Adding header f
🕨 🛄 java		28113 🛞	14 months	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala University/CN=Mattias Ellert mel03009	Fix tests with au
Þ 🛄 m4		27652 🛞	20 months	/O=Grid/O=NorduGrid/OU=nbi.dk/CN=Anders Waananen	Remove libarcd
🕨 🛄 nsis		28684 🛞	9 months	/O=Grid/O=NorduGrid/OU=nbi.dk/CN=Anders Waananen	Fix Windows pac
🕨 🛄 ро		29026 🛞	3 months	/DC=org/DC=terena/DC=tcs/C=SE/O=Lunds Universitet/CN=Oxana Smirnova quar-osm	Synchronised Ru
🕨 🛄 python		28571 🛞	9 months	/DC=org/DC=terena/DC=tcs/C=DK/O=ku.dk/CN=Martin Skou Andersen 205059	Swig 2.0.12 use
🕨 🛄 selinux		21262 🛞	4 years	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala University/CN=Mattias Ellert mel03009	Integrate SELinu
🕨 🛄 src		29142 🛞	5 days	/C=HU/O=NIIF CA/OU=GRID/OU=NIIF/CN=Gabor Roczei	Adding Computi
🕨 🛄 swig		28713 🛞	8 months	/DC=org/DC=terena/DC=tcs/C=DK/O=ku.dk/CN=Martin Skou Andersen 205059	Move common t
🗄 .svnignore	254 bytes 🕁	28113 🛞	14 months	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala University/CN=Mattias Ellert mel03009	Fix tests with au
📓 arc-uncrustify.cfg	3.0 КВ 🕁	22484 📎	3 years	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala University/CN=Mattias Ellert mel03009	Change mod_ful
📓 arc.nsi	4.9 КВ 🕁	25907 🛞	2 years	/O=Grid/O=NorduGrid/OU=uio.no/CN=Aleksandr Konstantinov	Making infosys l
📓 arcbase.pc.in	316 bytes 🕁	13347 🛞	5 years	/O=Grid/O=Nordugrid/OU=hep.lu.se/CN=Ferenc Szalai	add pkg-config o
AUTHORS	2.3 KB 🕁	28803 🛞	7 months	/DC=org/DC=terena/DC=tcs/C=SE/O=Lunds Universitet/CN=Oxana Smirnova quar-osm	Adding two new
📓 autoclean.sh	1.1 KB 🕁	20222 🛞	4 years	/O=Grid/O=NorduGrid/OU=nbi.dk/CN=Anders Waananen	Add script to cle
📄 autogen.sh	965 bytes 🕁	14778 💮	5 years	/O=Grid/O=NorduGrid/OU=fysast.uu.se/CN=Mattias Ellert	Get rid of GPL re
📄 ChangeLog	23.6 КВ 🕁	29143 💮	5 days	/C=HU/O=NIIF CA/OU=GRID/OU=NIIF/CN=Gabor Roczei	adding #29142 (
🗒 configure.ac	97.3 КВ 🕁	29088 🛞	2 months	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala University/CN=Mattias Ellert mel03009	Fix sed expressi
	6.8 KB	26181 🚳	2 years	/O=Grid/O=NorduGrid/OU=pbi_dk/CN=Apders_Waapapen	Remove RLS sur

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 **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 8.1, iOS 8.0, Ubuntu 14.10 "Utopic Unicorn", Android 4.4 "KitKat", Fedora 20 "Heisenbug"
 - Software: ROOT v6.02/02, gcc 4.9.2, Photoshop CS5.5, Office 2013, Linux kernel 3.16
- 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 **checkout** an own **working copy** of the repository
 - Many systems allow to check out only a part of the entire repository
- After doing local code changes, the developer uploads commit 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, a conflict will be reported, and commit will fail
- Commits can be reverted to any previous revision if it turns out they caused troubles
- Release manager can decide which commits 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 🔺	Size	Rev	Age	Author
1L/				
🗢 🛄 branches		29096 🛞	7 weeks	/DC=org/DC=terena/DC=tcs/C=SE/O=Uppsala Univer
🕨 🛄 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
🕨 🛄 janitor		12565 🚷	6 years	/O=GermanGrid/OU=UniLuebeck/CN=Hajo Nils Krabbe
Þ 🛄 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 Taga
Þ 🛄 v_0_8		17741 🛞	5 years	/O=Grid/O=NorduGrid/OU=fys.uio.no/CN=Adrian Taga
▶ 🛄 v_0_8_1_1		16791 💮	5 years	/O=Grid/O=NorduGrid/OU=nsc.liu.se/CN=Daniel Johan
▶ 🛄 v_0_8_2		18196 💮	4 years	/O=Grid/O=NorduGrid/OU=nsc.liu.se/CN=Daniel Johan
▶ 🛄 v_0_8_3		20021 🛞	4 years	/C=HU/O=NIIF CA/OU=GRID/OU=NIIF/CN=Ivan Marte
🕨 🛄 tags		24575 🛞	3 years	/O=Grid/O=NorduGrid/OU=nbi.dk/CN=Anders Waanar
👂 🛄 trunk		20022 🛞	4 years	/C=HU/O=NIIF CA/OU=GRID/OU=NIIF/CN=Ivan Marte

Plus

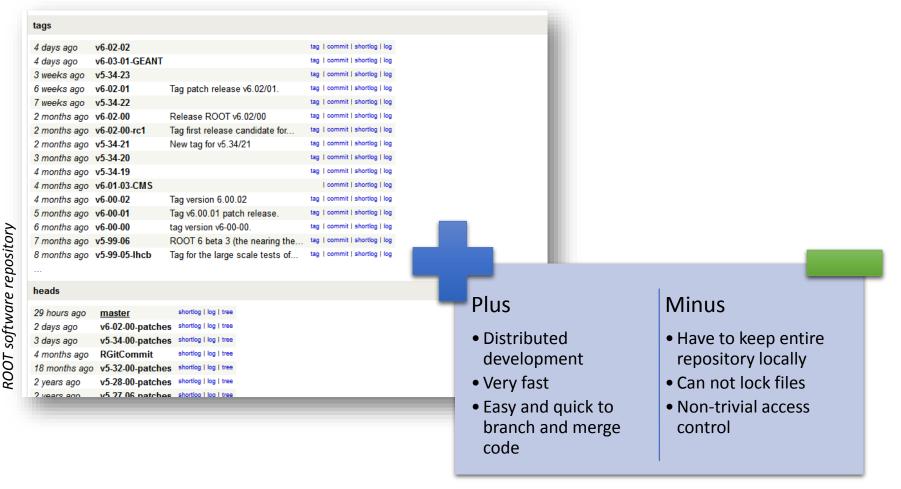
- Easy to control and manage
- Easy to prevent conflicts
- Each developer makes a checkout of only the code they need

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

- Subversion (SVN): a centralised system
 - One of the most commonly used systems
 - Release 1.0.0 in 2004
 - Open Source (Apache)
 - Branches retain no knowledge of the trunk
 - Allows authorisation per directory
 - Well documented, O'Reilly book is online for free: <u>http://svnbook.red-bean.com/</u>



- Git: a distributed system
 - Developed by Linus Torvalds in 2005 when the other system he was using fell victim to copyright battles
 - 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
 - Git book also exists: <u>http://git-scm.com/book</u>



Integrated Development Environment (IDE)

- For non-professional developers, a good editor and configure; make is enough to write and build software
 - Warning: avoid doing **configure**; **make** in your working copy! They 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>)
 - **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

	Java - ffmpeg/ffserver.c - Eclipse SDK	0 0
<u>F</u> ile <u>E</u> dit <u>S</u> ource Refac <u>t</u> or <u>N</u> avigate	Se <u>a</u> rch <u>P</u> roject <u>R</u> un <u>W</u> indow <u>H</u> elp	
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 Fimpeg Godoc Fifpresets Fibavcodec Fibavfilter Fibavfilter Fibavtil Fibavutil Fibavscale Fibswscale Fibswscale Fibswscale Fibswscale Fibswscale Fibswscale Fibavtork Fibswscale Fibavtork Fibswscale Fibavtork Fibswscale Fibavtork Fibswscale Fibavtork Fibavtork	<pre>for (s = first_stream; s; s = s->next) { if (!strcmp(stream->filename, s->filename)) { ERROR("Stream '%s' already registered\n", s->filename); } stream->fmt = ffserver_guess_format(NULL, stream->filename, NULL avcodec_get_context_defaults2(&video_enc, AVMEDIA_TYPE_VIDEO); avcodec_get_context_defaults2(&audio_enc, AVMEDIA_TYPE_AUDIO); audio_id = CODEC_ID_NONE; video_id = cODEC_ID_NONE; if (stream->fmt) { audio_id = stream->fmt->audio_codec; video_id = stream->fmt->video_codec; video_id = stream->fmt->video_codec; video_id = stream->next; } else if (!av_strcasecmp(cmd, "Feed")) { get_arg(arg, sizeof(arg), &p); if (stream *sfeed; // // //</pre>	 I² × × • • * config.h closesocket string.h stdlib.h libavformat/avform libavformat/ffm.h libavformat/rtpdec. libavformat/rtpdec. libavformat/rtpdec. libavformat/rtpdec. libavformat/avio_int libavutil/dict.h libavutil/dict.h libavutil/mathemati
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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), 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/

Home New Browse Search Search [?] Reports Help New Account Log In Forgot Password							
Sun Nov 30 2014 22:47:43 CET Any program that runs right is obsolete Hide Search Description							
13 bugs	ion:	Com	ponent: ARClib	Рго	duct: Nordu		
		Comp	Assignee	Status	Resolution	Summary	Changed
804	NorduGri	ARClib	skou	ASSI		Insufficient client error messages when job information is not found	2013-10-08
868	NorduGri	ARClib	skou	ASSI		Incorrect error message from arcsub when queue information is unavailable	2012-08-16
1951	NorduGri	ARClib	waananen	ASSI		Outdated CRLs render all client tools useless	2014-04-22
2787	NorduGri	ARClib	skou	ASSI		feature request for updating status of ExecutionTargets	2013-03-22
2874	NorduGri	ARClib	akonstantinov	ASSI		arcsub cannot parse a simple JSDL file on Windows	2013-10-21
2890	NorduGri	ARClib	skou	ASSI		should not treat "executable" as a local input file	2012-08-08
2977	NorduGri	ARClib	skou	ASSI		arcmigrate does not seem to be working as described in manual	2013-10-08
3099	NorduGri	ARClib	skou	ASSI		bulk operations including queries for EMI-ES	2013-10-23
3190	NorduGri	ARClib	akonstantinov	ASSI		Memory leak during multiple job submission with files to BES interface	2013-10-08
		ARClib		ASSI		Inconsistent ComputingService Name between gridftp and	2014-06-04

Software development hosting services

• 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 newest and largest IT-project hosting service (started in 2008), based on Git (obviously); free for Open Source projects



Google Code, <u>http://code.google.com/</u>: started in 2005, offers Git, SVN and Mercurial revision control systems

• Some other hosting services: RubyForge, Tigris.org, BountySource, Launchpad, BerliOS, JavaForge, GNU Savannah, Gitorious

Yet another kind of language: 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
 - HTML stands for Hypertext Markup Language
 - Was developed at CERN, inspired by an earlier SGML

Edit This Code:	See Result »	Result:
<pre><!DOCTYPE html> <html> <body> <h1>Document Title</h1> First paragraph. Here is some bold text<!-- And this is a <i-->non-number First item Second item </body> </html></pre>		Document Title First paragraph. Here is some bold text And this is a <i>non-numbered</i> list: • First item • Second item
		Try it Yourself - © w3schools.com

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	 You don't see the result "live" 	
	 It supports most complex mathematics 	 Tables and figures are very difficult to pin into 	
	 It is extensible 	place	
	 It is accepted by all publishers 	 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 \$\$
 - $\$ 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: LaTeX2ɛ (since 1994)

```
\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

LaTeX example produced with the help of <u>https://www.writelatex.com</u>

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

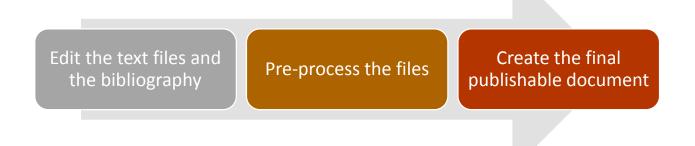
Is very good with equations	\begin{equation}
Can include figures	<pre>\begin{figure} \includegraphics{cat.jpg}</pre>
Can create tables	<pre>\begin{table} \begin{tabular}</pre>
Handles cross references	<pre>\label{sec:intro} \ref{sec:intro}</pre>
Handles bibliography	<pre>\begin{thebibliography} \bibitem{mybook}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

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Programming for Scientists

Steps to create a LaTeX document

• Writing a LaTeX document resembles software development:



- You can use Linux command line, any of Windows IDEs (*TeXnicCenter* is good), or one of the many online LaTeX systems
- There is also software called LyX, which is based on LaTeX and produces "live" visual result
 - Beware that LyX files are a heavy extension of LaTeX, and can not be used without LyX (not portable!)

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