C.E.C.I

Consortium des Equipements
de Calcul Intensif
en Fédération Wallonie-Bruxelles

Introduction to Scientific Software Deployment and Development

damien.francois@uclouvain.be

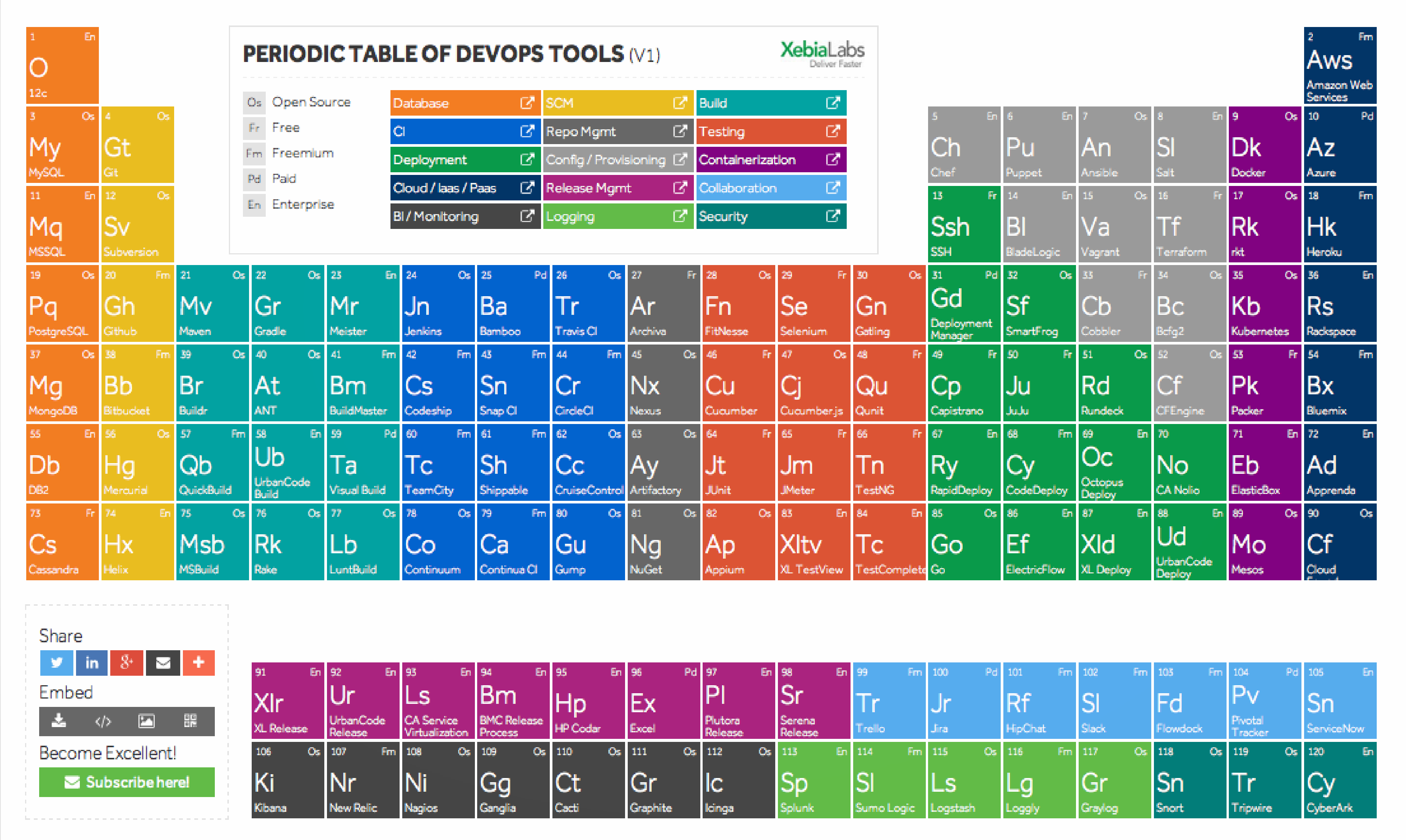
October 2020

http://www.ceci-hpc.be/training.html

UCL Université catholique de Louvain

INSTITUT DE CALCUL INTENSIF ET DE STOCKAGE DE MASSE

What is this?



PERIODIC TABLE OF DEVOPS TOOLS (V1)

XebiaLabs
Deliver Faster

Os	Open Source
Fr	Free
Fm	Freemium
Pd	Paid
En	Enterprise

Database	SCM	Build
CI	Repo Mgmt	Testing
Deployment	Config / Provisioning	Containerization
Cloud / Iaas / Paas	Release Mgmt	Collaboration
BI / Monitoring	Logging	Security

1 En O 12c																	2 Fm Aws Amazon Web Services
3 Os My MySQL	4 Os Gt Git											5 En Ch Chef	6 En Pu Puppet	7 Os An Ansible	8 En Sl Salt	9 Os Dk Docker	10 Pd Az Azure
11 En Mq MSSQL	12 Os Sv Subversion											13 Fr Ssh SSH	14 En Bl BladeLogic	15 Os Va Vagrant	16 Fr Tf Terraform	17 Os Rk rkt	18 Fm Hk Heroku
19 Os Pq PostgreSQL	20 Fm Gh Github	21 Os Mv Maven	22 Os Gr Gradle	23 En Mr Meister	24 Os Jn Jenkins	25 Pd Ba Bamboo	26 Os Tr Travis CI	27 Fr Ar Archiva	28 Os Fn FitNesse	29 Fr Se Selenium	30 Os Gn Gatling	31 Pd Gd Deployment Manager	32 Os Sf SmartFrog	33 Fr Cb Cobbler	34 Os Bc Bcfg2	35 Os Kb Kubernetes	36 En Rs Rackspace
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55 En Db DB2	56 Os Hg Mercurial	57 Fm Qb QuickBuild	58 En Ub UrbanCode Build	59 Pd Ta Visual Build	60 Fm Tc TeamCity	61 Fm Sh Shippable	62 Os Cc CruiseControl	63 Os Ay Artifactory	64 Fr Jt JUnit	65 Fr Jm JMeter	66 Fr Tn TestNG	67 En Ry RapidDeploy	68 Fm Cy CodeDeploy	69 En Oc Octopus Deploy	70 No CA Nolio	71 En Eb ElasticBox	72 En Ad Apprenda
73 Fr Cs Cassandra	74 En Hx Helix	75 Os Msb MSBuild	76 Os Rk Rake	77 Os Lb LuntBuild	78 Os Co Continuum	79 Fm Ca Continua CI	80 Os Gu Gump	81 Os Ng NuGet	82 Os Ap Appium	83 En Xltv XL TestView	84 En Tc TestComplete	85 Os Go Go	86 En Ef ElectricFlow	87 En Xld XL Deploy	88 En Ud UrbanCode Deploy	89 Os Mo Mesos	90 Os Cf Cloud

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91 En Xlr XL Release	92 En Ur UrbanCode Release	93 En Ls CA Service Virtualization	94 En Bm BMC Release Process	95 En Hp HP Codar	96 Pd Ex Excel	97 En Pl Plutora Release	98 En Sr Serena Release	99 Fm Tr Trello	100 Pd Jr Jira	101 Fm Rf HipChat	102 Fm Sl Slack	103 Fm Fd Flowdock	104 Pd Pv Pivotal Tracker	105 En Sn ServiceNow
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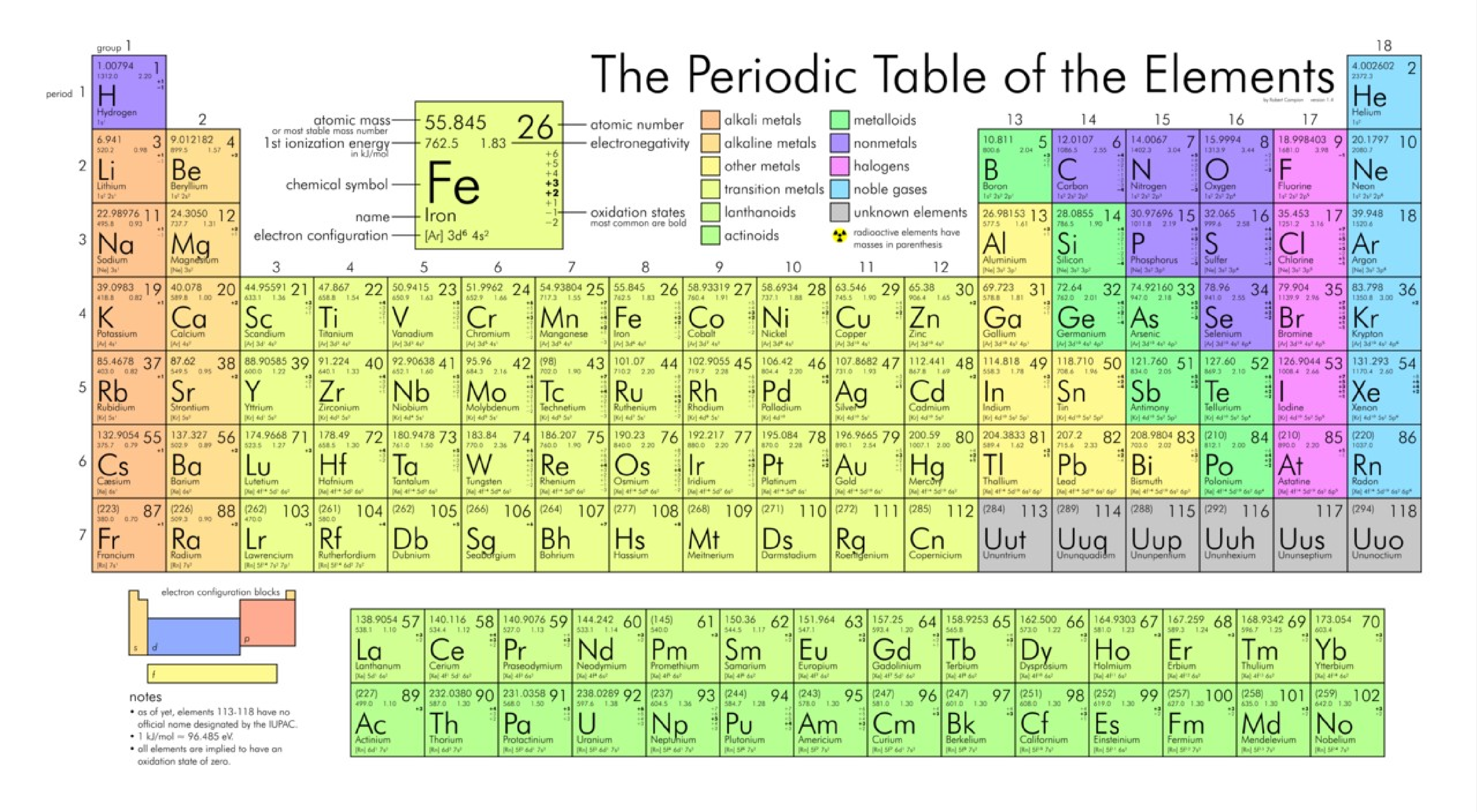
https://xebialabs.com/periodic-table-of-devops-tools/

Not this...



The Periodic Table of the Elements

period \ group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H Hydrogen 1.00794																	2 He Helium 4.002602
2	3 Li Lithium 6.941	4 Be Beryllium 9.012182											5 B Boron 10.811	6 C Carbon 12.0107	7 N Nitrogen 14.0067	8 O Oxygen 15.9994	9 F Fluorine 18.998403	10 Ne Neon 20.1797
3	11 Na Sodium 22.98976	12 Mg Magnesium 24.3050											13 Al Aluminium 26.98153	14 Si Silicon 28.0855	15 P Phosphorus 30.97696	16 S Sulfer 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948
4	19 K Potassium 39.0983	20 Ca Calcium 40.078	21 Sc Scandium 44.95591	22 Ti Titanium 47.867	23 V Vanadium 50.9415	24 Cr Chromium 51.9962	25 Mn Manganese 54.93804	26 Fe Iron 55.845	27 Co Cobalt 58.93319	28 Ni Nickel 58.6934	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.64	33 As Arsenic 74.92160	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798
5	37 Rb Rubidium 85.4678	38 Sr Strontium 87.62	39 Y Yttrium 88.90585	40 Zr Zirconium 91.224	41 Nb Niobium 92.90638	42 Mo Molybdenum 95.96	43 Tc Technetium (98)	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.9055	46 Pd Palladium 106.42	47 Ag Silver 107.8682	48 Cd Cadmium 112.441	49 In Indium 114.818	50 Sn Tin 118.710	51 Sb Antimony 121.760	52 Te Tellurium 127.60	53 I Iodine 126.9044	54 Xe Xenon 131.293
6	55 Cs Cæsium 132.9054	56 Ba Barium 137.327	71 Lu Lutetium 174.9668	72 Hf Hafnium 178.49	73 Ta Tantalum 180.9478	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.217	78 Pt Platinum 195.084	79 Au Gold 196.9665	80 Hg Mercury 200.59	81 Tl Thallium 204.3833	82 Pb Lead 207.2	83 Bi Bismuth 208.9804	84 Po Polonium (210)	85 At Astatine (210)	86 Rn Radon (220)
7	87 Fr Francium (223)	88 Ra Radium (226)	103 Lr Lawrencium (262)	104 Rf Rutherfordium (261)	105 Db Dubnium (262)	106 Sg Seaborgium (266)	107 Bh Bohrium (264)	108 Hs Hassium (277)	109 Mt Meitnerium (268)	110 Ds Darmstadium (271)	111 Rg Roentgenium (272)	112 Cn Copernicium (285)	113 Uut Ununtrium (284)	114 Uuq Ununquadium (289)	115 Uup Ununpentium (288)	116 Uuh Ununhexium (292)	117 Uus Ununseptium	118 Uuo Ununoctium (294)

57 La Lanthanum 138.9054	58 Ce Cerium 140.116	59 Pr Praseodymium 140.9076	60 Nd Neodymium 144.242	61 Pm Promethium (145)	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.9253	66 Dy Dysprosium 162.500	67 Ho Holmium 164.9303	68 Er Erbium 167.259	69 Tm Thulium 168.9342	70 Yb Ytterbium 173.054
89 Ac Actinium (227)	90 Th Thorium 232.0380	91 Pa Protactinium 231.0358	92 U Uranium 238.0289	93 Np Neptunium (237)	94 Pu Plutonium (244)	95 Am Americium (243)	96 Cm Curium (247)	97 Bk Berkelium (247)	98 Cf Californium (251)	99 Es Einsteinium (252)	100 Fm Fermium (257)	101 Md Mendelevium (258)	102 No Nobelium (259)

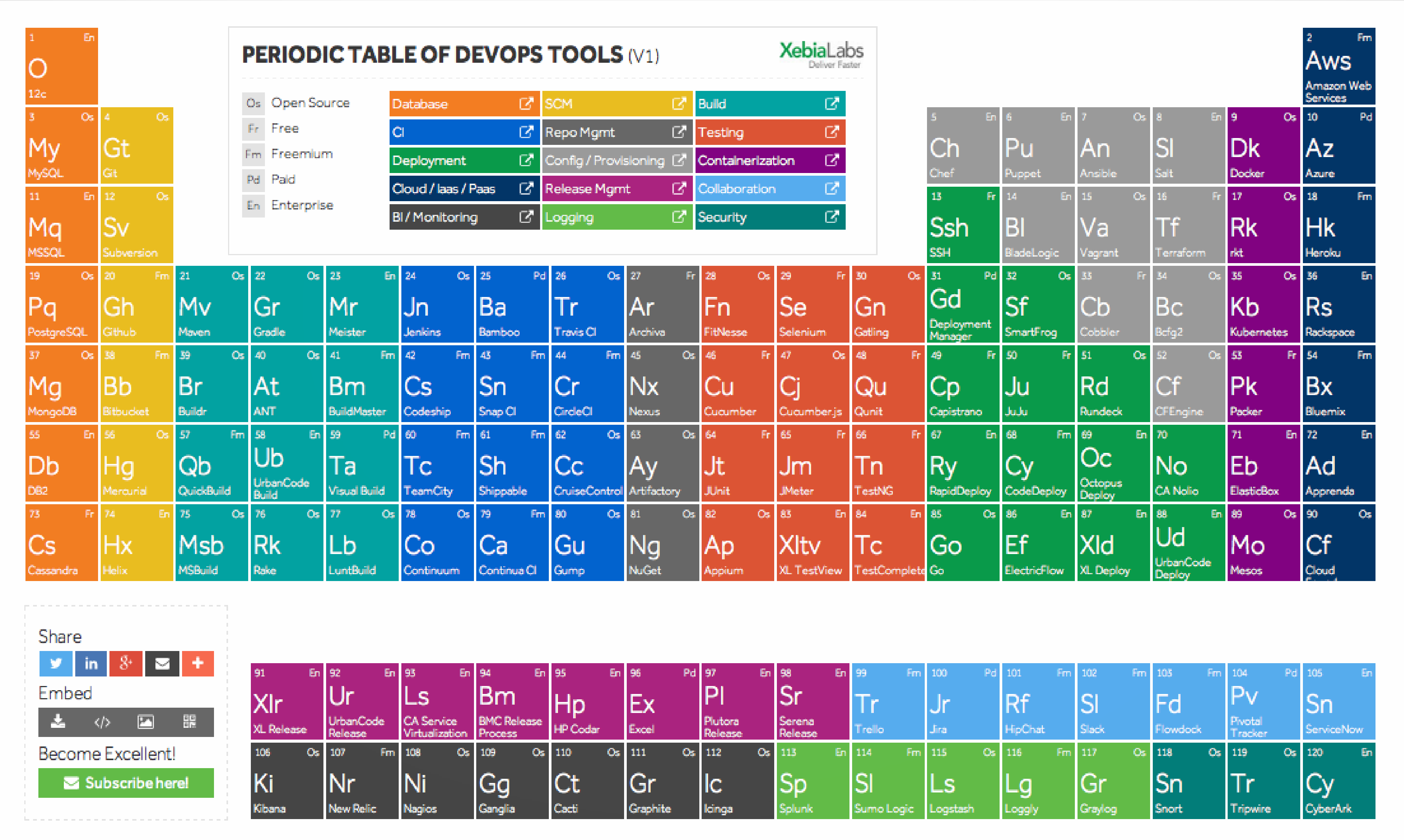
atomic mass or most stable mass number — 55.845; atomic number — 26
1st ionization energy in kJ/mol — 762.5; electronegativity — 1.83
chemical symbol — Fe
oxidation states most common are bold — +6 +5 +4 +3 +2 +1 −1 −2
name — Iron
electron configuration — [Ar] $3d^6$ $4s^2$

alkali metals	metalloids
alkaline metals	nonmetals
other metals	halogens
transition metals	noble gases
lanthanoids	unknown elements
actinoids	radioactive elements have masses in parenthesis

notes
- as of yet, elements 113-118 have no official name designated by the IUPAC.
- 1 kJ/mol ≈ 96.485 eV.
- all elements are implied to have an oxidation state of zero.

Source: Wikipedia

… but this:



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https://xebialabs.com/periodic-table-of-devops-tools/

Goal of this session:

“Give you access to the same tools
the professionals are using
for **developing** and **deploying** programs.”

Dev's toolkit :

1. Programming languages
2. Good practices/principles/style
3. Text editor
4. Source control management
5. Debuggers / Profilers
6. Databases
7. Packaging / Distributing tools
8. Comments and documentation
9. Tests
10. Licensing

1. Programming language

Be aware of the 'other' paradigm...

Imperative – “Do this”
BASIC, Assembly

Structured – Subroutines, scopes
C, FORTRAN77
algorithms + data : good for explicit computing

Object-Oriented – Encapsulation, Inheritance, ...
C++, Python
objects + messages : good for modeling

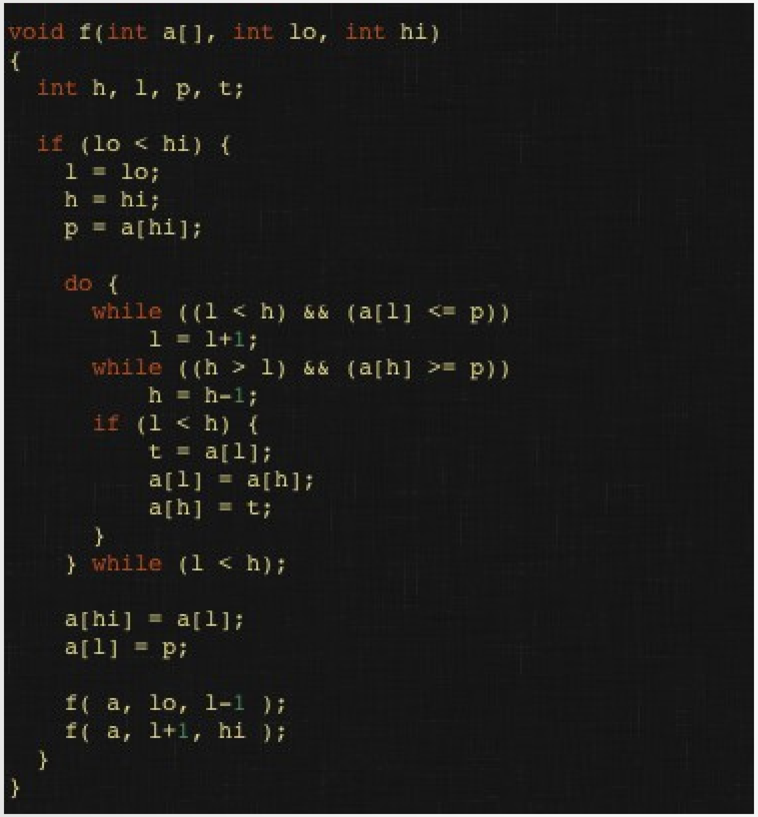
Declarative – “I need this”
SQL

Functional – Pure functions, lazy evaluation
Haskell, Scala
functions o functions : good for reasoning

Logic – Predicates and rules
Prolog, Datalog
facts + rules : good for searching

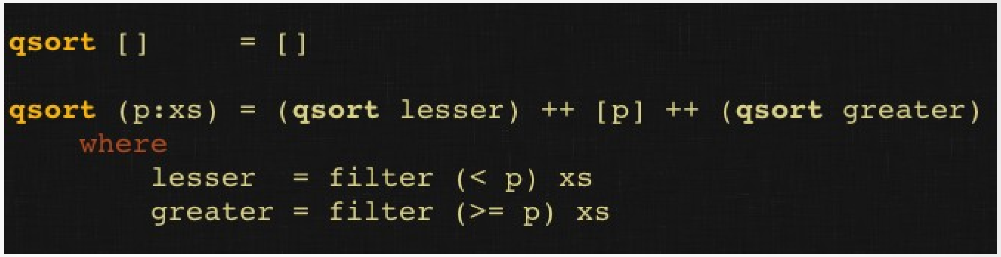
1. Programming language

C



```c
void f(int a[], int lo, int hi)
{
  int h, l, p, t;

  if (lo < hi) {
    l = lo;
    h = hi;
    p = a[hi];

    do {
      while ((l < h) && (a[l] <= p))
          l = l+1;
      while ((h > l) && (a[h] >= p))
          h = h-1;
      if (l < h) {
          t = a[l];
          a[l] = a[h];
          a[h] = t;
      }
    } while (l < h);

    a[hi] = a[l];
    a[l] = p;

    f( a, lo, l-1 );
    f( a, l+1, hi );
  }
}
```

Haskell



```haskell
qsort []     = []

qsort (p:xs) = (qsort lesser) ++ [p] ++ (qsort greater)
    where
        lesser  = filter (< p) xs
        greater = filter (>= p) xs
```

Purely functional
Static strong typing
Lazy evaluation

Completely different mindset, often very concise and (mostly) bugfree

1. Programming language

- Good reasons for choosing language X:
  - it offers useful paradigms for your problem
  - it offers high-level constructs/tools - e.g. for parsing arguments
  - it offers (directly or indirectly) useful libraries - e.g. for linear algebra
- Ok reasons for choosing language X:
  - standard in your community – easier to get accepted
- Bad reasons for choosing language X:
  - it runs fast – probably needs high skills to be fast
  - it is the language you already know

2. Good practices

- Write for humans, not for computers
- Use the appropriate language(s)
- Organize for change, and make incremental changes
- Plan for mistakes, automate testing
- Automate repetitive tasks
- Use modern source-code management system
- Document the design and purpose, not the implementation
- Optimize only when it works already
- Follow good coding principles

https://github.com/Droogans/unmaintainable-code/blob/master/README.md

2. Good practices

Paul F. Dubois. 1999. Ten Good Practices in Scientific Programming. *Computing in Science and Eng.* 1, 1 (January 1999), 7-11. DOI=10.1109/MCISE.1999.743610 http://dx.doi.org/10.1109/MCISE.1999.743610

Wilson G, Aruliah DA, Brown CT, Chue Hong NP, Davis M, Guy RT, et al. (2014) Best Practices for Scientific Computing. *PLoS Biol* 12(1): e1001745. doi:10.1371/journal.pbio.1001745

Dubois PF, Epperly T, Kumfert G (2003) Why Johnny can't build (portable scientific software). *Comput Sci Eng* 5: 83–88. doi: 10.1109/mcise.2003.1225867

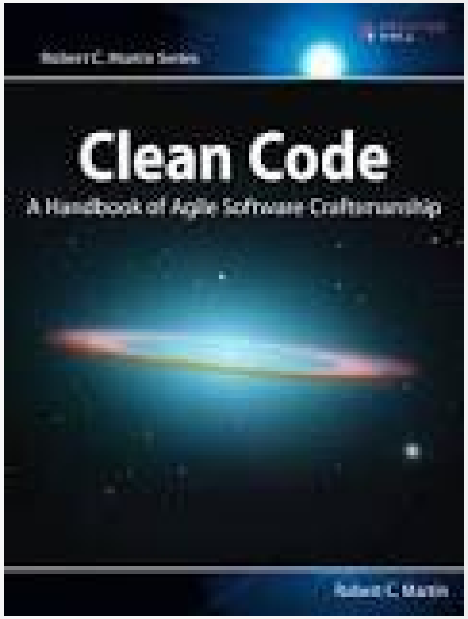
Prlić A, Procter JB (2012) Ten Simple Rules for the Open Development of Scientific Software. *PLoS Comput Biol* 8(12): e1002802. doi:10.1371/journal.pcbi.1002802

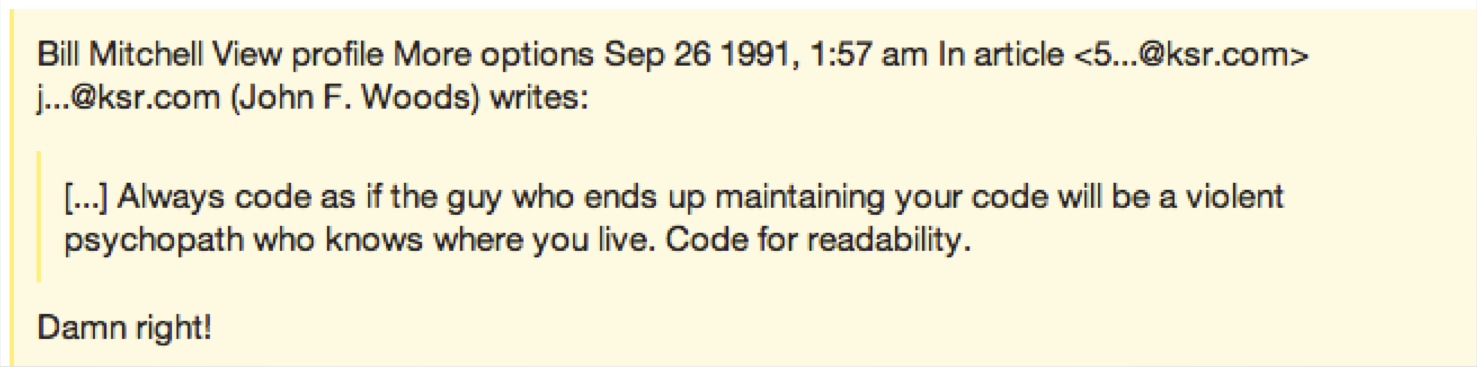
Victor R. Basili, Jeffrey C. Carver, Daniela Cruzes, Lorin M. Hochstein, Jeffrey K. Hollingsworth, Forrest Shull, Marvin V. Zelkowitz, "*Understanding the High-Performance-Computing Community: A Software Engineer's Perspective,*" *IEEE Software*, vol. 25, no. 4, pp. 29-36, July/August, 2008

Wilson G, Bryan J, Cranston K, Kitzes J, Nederbragt L, Teal TK (2017) Good enough practices in scientific computing. *PLoS Comput Biol* 13(6): e1005510. https://doi.org/10.1371/journal.pcbi.1005510

2. Good coding principles

- Don't repeat yourself (DRY)
- Keep it simple, Stupid (KISS)
- One level of abstraction
- Single responsibility principle
- Separation of concern
- Avoid premature optimization
- Many others...





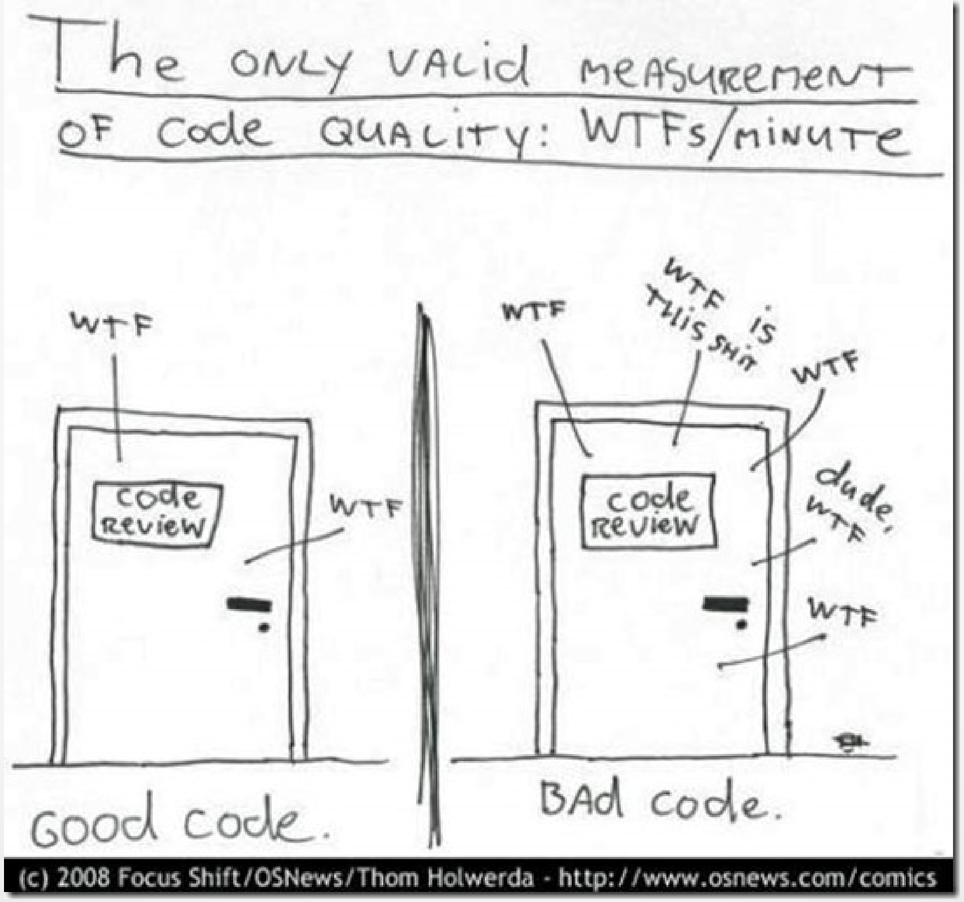
Bill Mitchell View profile More options Sep 26 1991, 1:57 am In article <5...@ksr.com> j...@ksr.com (John F. Woods) writes:

> [...] Always code as if the guy who ends up maintaining your code will be a violent psychopath who knows where you live. Code for readability.

Damn right!

Clean Code: A Handbook of Agile Software Craftsmanship, R. C. Martin, Prentice Hall, 2008

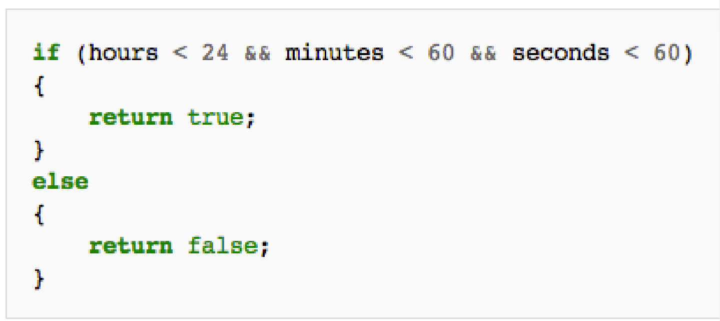
Good principle for good quality



(c) 2008 Focus Shift/OSNews/Thom Holwerda - http://www.osnews.com/comics

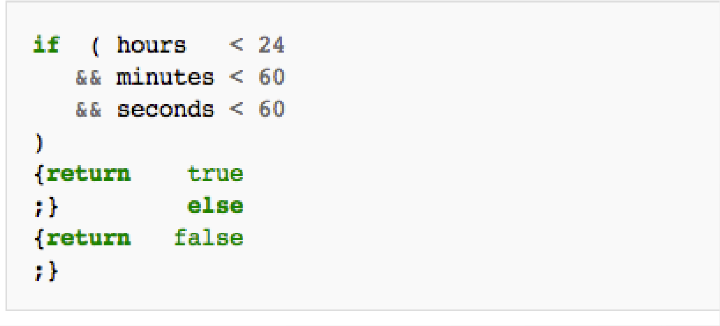
2. Good style

- Makes sure the code is readable by all
  - easily
  - quickly



```
if (hours < 24 && minutes < 60 && seconds < 60)
{
    return true;
}
else
{
    return false;
}
```

vs



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if  ( hours   < 24
   && minutes < 60
   && seconds < 60
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{return    true
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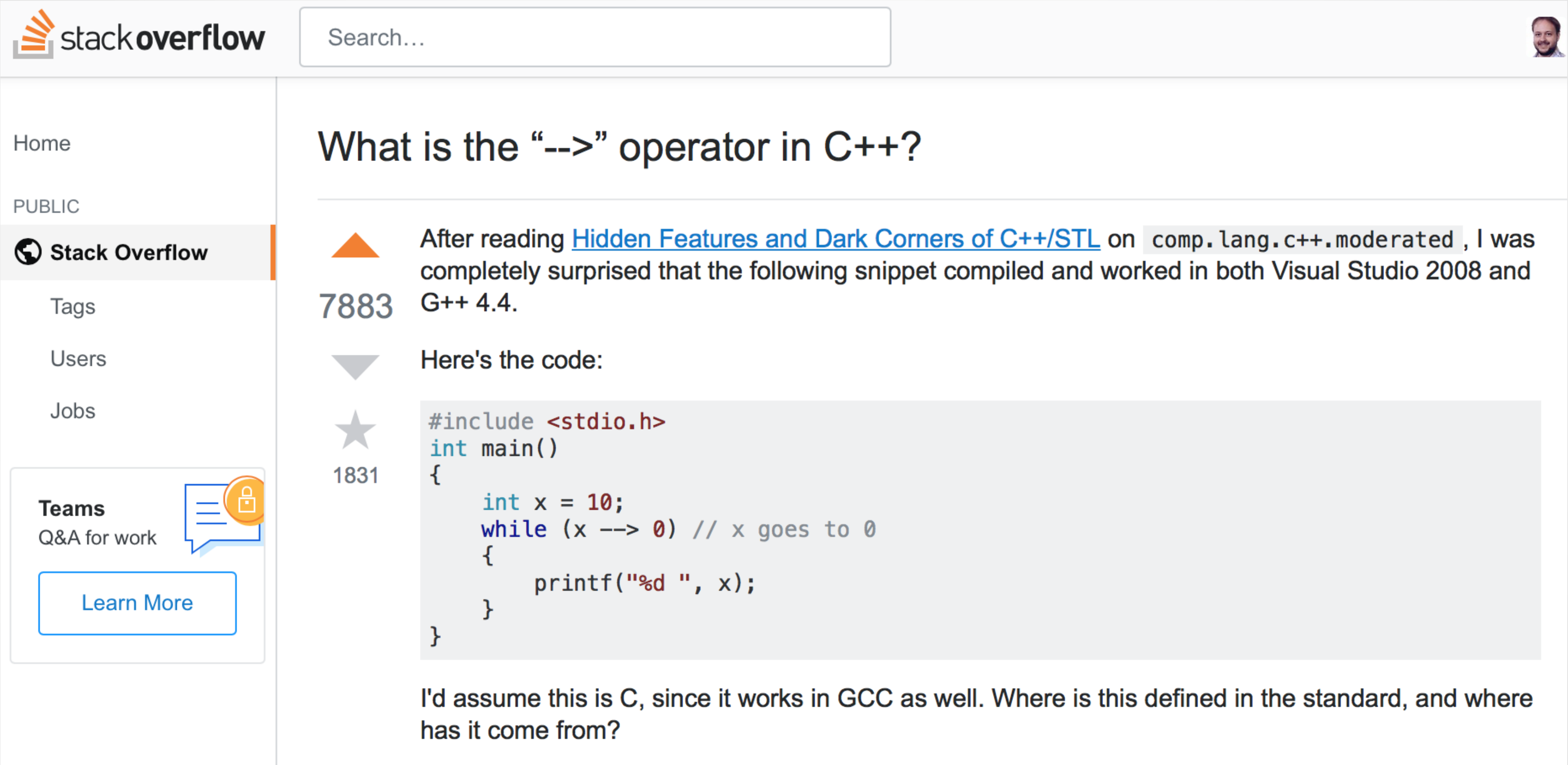
2. Good style



What is the “-->” operator in C++?

After reading Hidden Features and Dark Corners of C++/STL on `comp.lang.c++.moderated`, I was completely surprised that the following snippet compiled and worked in both Visual Studio 2008 and G++ 4.4.

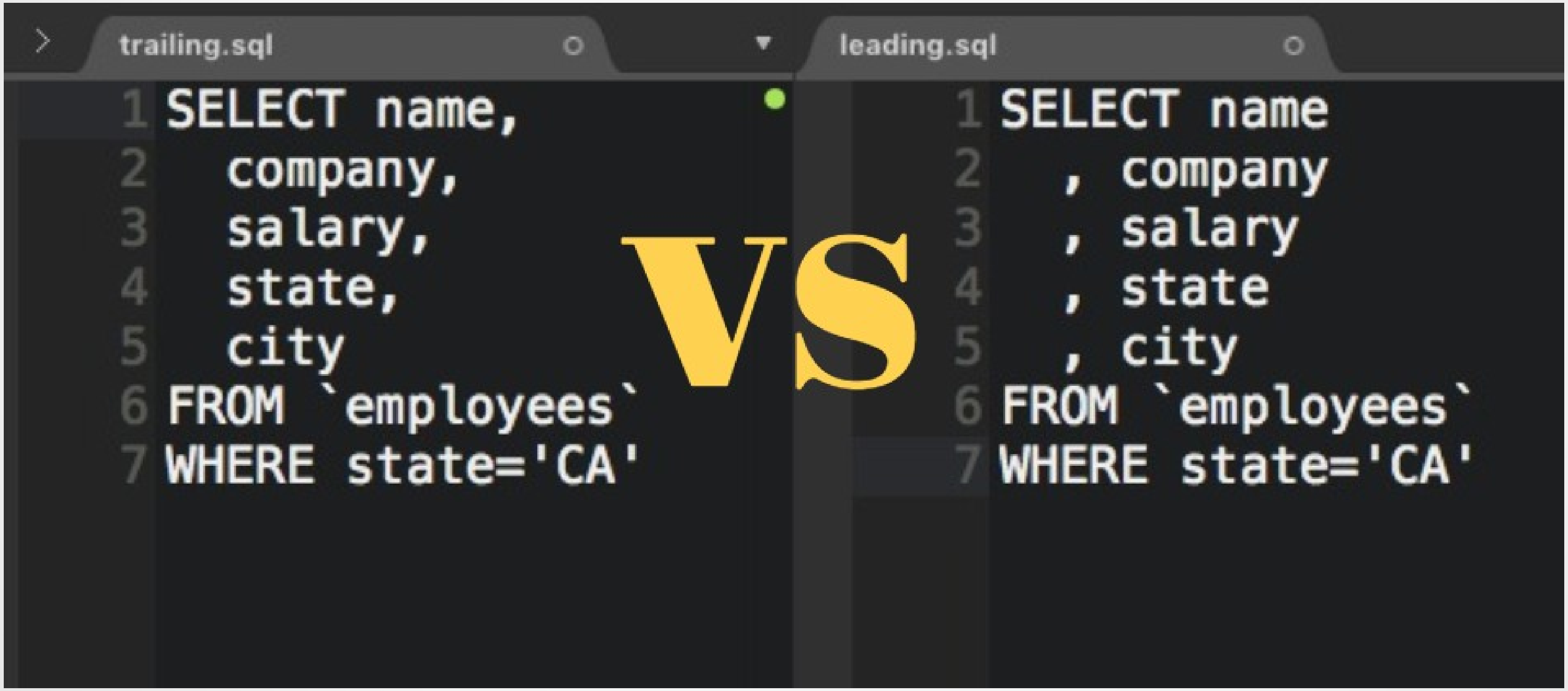
Here's the code:

```
#include <stdio.h>
int main()
{
    int x = 10;
    while (x --> 0) // x goes to 0
    {
        printf("%d ", x);
    }
}
```

I'd assume this is C, since it works in GCC as well. Where is this defined in the standard, and where has it come from?

https://stackoverflow.com/questions/1642028/what-is-the-operator-in-c

2. Good style



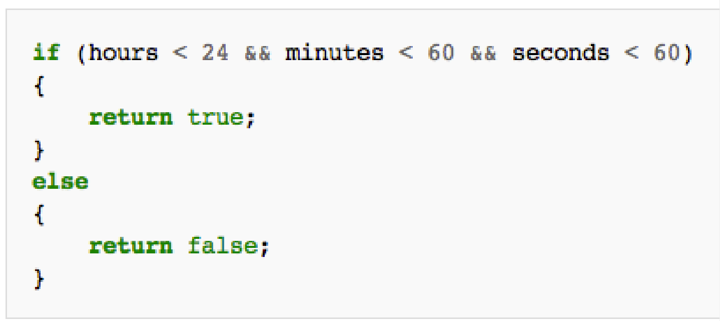
```sql
SELECT name,
  company,
  salary,
  state,
  city
FROM `employees`
WHERE state='CA'
```

```sql
SELECT name
  , company
  , salary
  , state
  , city
FROM `employees`
WHERE state='CA'
```

https://towardsdatascience.com/winning-arguments-with-data-leading-with-commas-in-sql-672b3b81eac9

2. Good style

- Makes sure the code is readable by all
  - easily
  - quickly
- Depends on
  - the language
  - the project



```
if (hours < 24 && minutes < 60 && seconds < 60)
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```

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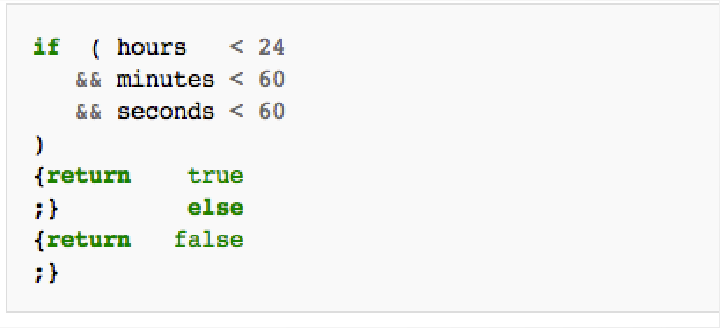
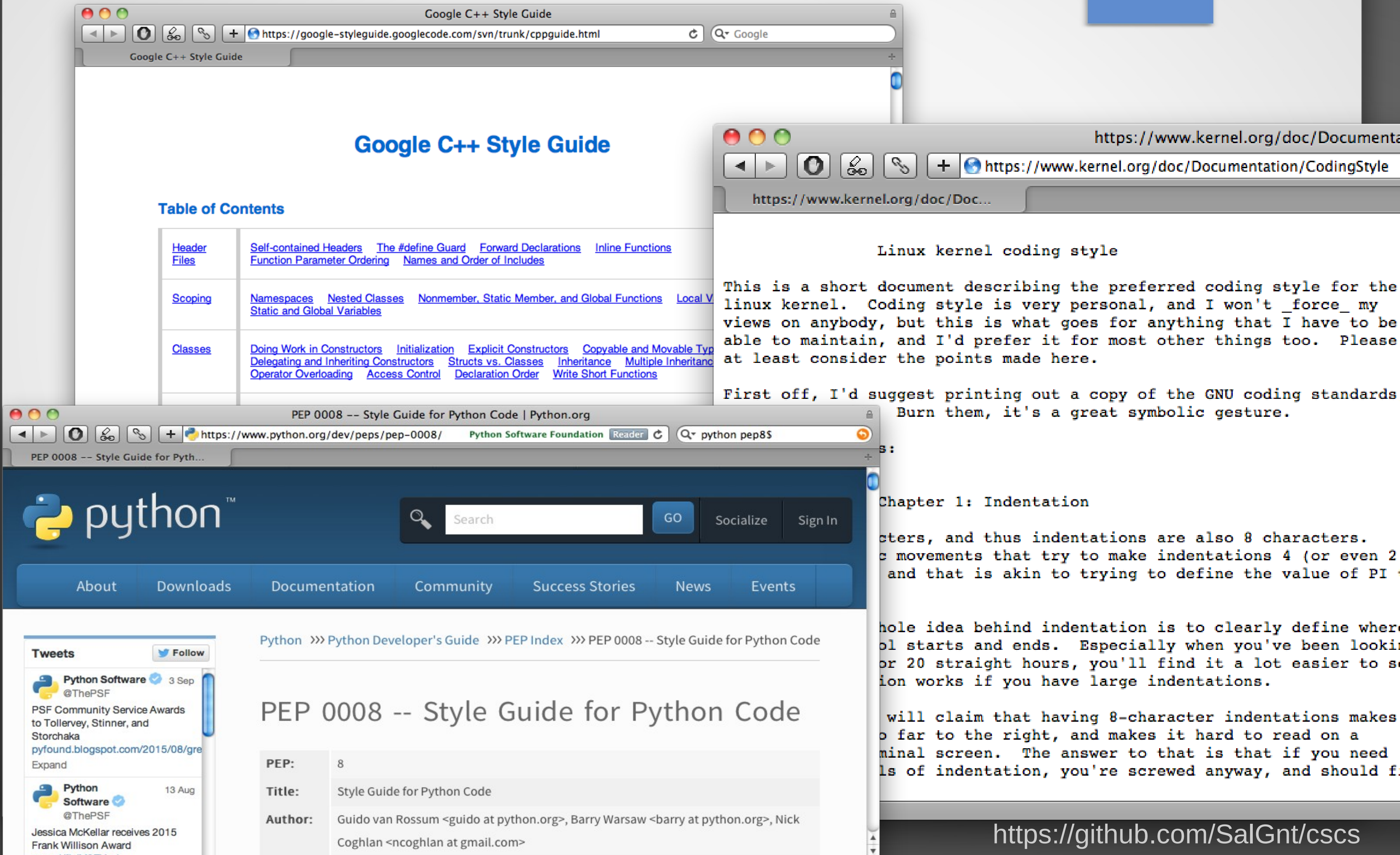


```
if  ( hours   < 24
   && minutes < 60
   && seconds < 60
)
{return     true
;}          else
{return    false
;}
```

2. Good style



Google C++ Style Guide

https://google-styleguide.googlecode.com/svn/trunk/cppguide.html

Google C++ Style Guide

Google C++ Style Guide

Table of Contents

Header Files	Self-contained Headers The #define Guard Forward Declarations Inline Functions Function Parameter Ordering Names and Order of Includes
Scoping	Namespaces Nested Classes Nonmember, Static Member, and Global Functions Local V Static and Global Variables
Classes	Doing Work in Constructors Initialization Explicit Constructors Copyable and Movable Typ Delegating and Inheriting Constructors Structs vs. Classes Inheritance Multiple Inheritanc Operator Overloading Access Control Declaration Order Write Short Functions

https://www.kernel.org/doc/Documenta

https://www.kernel.org/doc/Documentation/CodingStyle

https://www.kernel.org/doc/Doc...

```
                    Linux kernel coding style

This is a short document describing the preferred coding style for the
linux kernel.  Coding style is very personal, and I won't _force_ my
views on anybody, but this is what goes for anything that I have to be
able to maintain, and I'd prefer it for most other things too.  Please
at least consider the points made here.

First off, I'd suggest printing out a copy of the GNU coding standards
           Burn them, it's a great symbolic gesture.

s:

Chapter 1: Indentation

cters, and thus indentations are also 8 characters.
c movements that try to make indentations 4 (or even 2
 and that is akin to trying to define the value of PI

hole idea behind indentation is to clearly define where
ol starts and ends.  Especially when you've been looki
or 20 straight hours, you'll find it a lot easier to se
ion works if you have large indentations.

 will claim that having 8-character indentations makes
o far to the right, and makes it hard to read on a
minal screen.  The answer to that is that if you need
ls of indentation, you're screwed anyway, and should f
```

PEP 0008 -- Style Guide for Python Code | Python.org

https://www.python.org/dev/peps/pep-0008/

PEP 0008 -- Style Guide for Pyth...

python™

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PSF Community Service Awards to Tollervey, Stinner, and Storchaka pyfound.blogspot.com/2015/08/gre

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Python Software @ThePSF 13 Aug

Jessica McKellar receives 2015 Frank Willison Award

Python >>> Python Developer's Guide >>> PEP Index >>> PEP 0008 -- Style Guide for Python Code

PEP 0008 -- Style Guide for Python Code

PEP:	8
Title:	Style Guide for Python Code
Author:	Guido van Rossum <guido at python.org>, Barry Warsaw <barry at python.org>, Nick Coghlan <ncoghlan at gmail.com>

3. Text editor

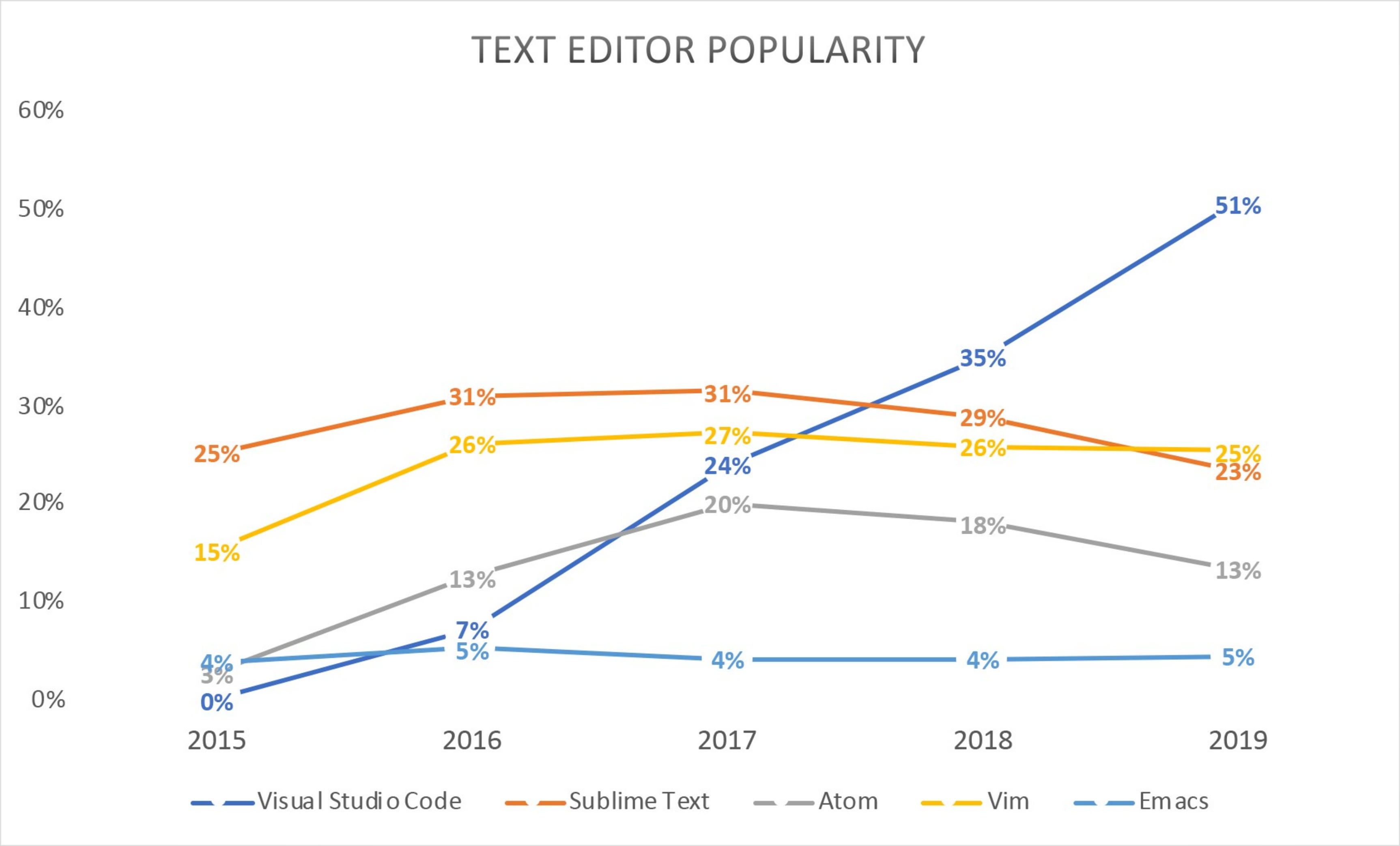
- Some files are better edited directly on the clusters;

- If you prefer a graphical user interface, some good candidates are:
  - Sublime text: http://www.sublimetext.com/
  - Atom: https://atom.io/
  - VSCode https://code.visualstudio.com/download

- Choose one and learn it from inside out

https://jaxbot.me/articles/why-i-use-vim

3. Text editor



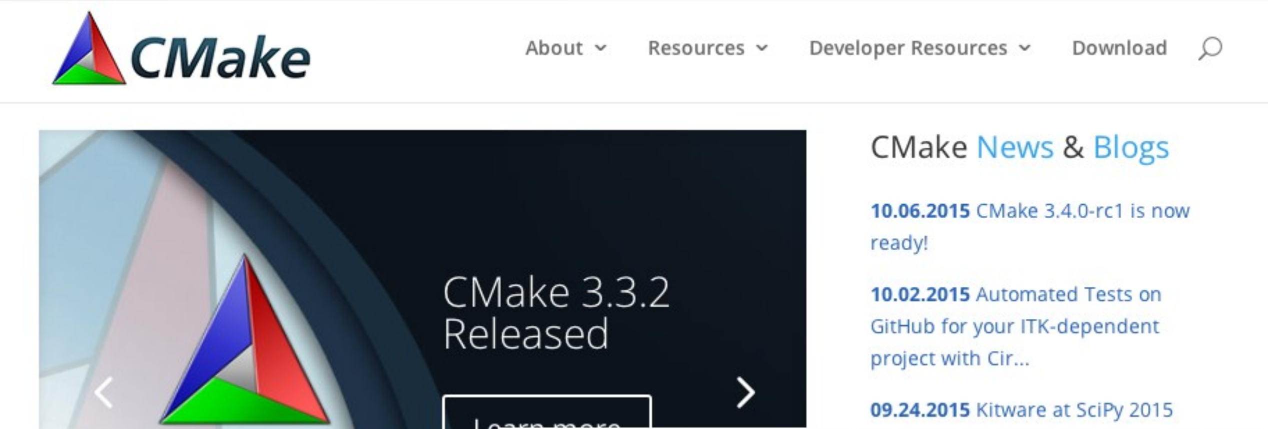
https://blog.robenkleene.com/2020/09/21/the-era-of-visual-studio-code/

Dev's toolkit :

1. Programming language
2. Good practices / Code Style Guides
3. Text editor / IDE
4. **Source control management**
5. **Debuggers / Profilers**
6. **Databases**
7. Packaging / Distributing tools
8. Comments and documentation
9. Tests
10. Licensing

Own dedicated sessions

7. Packaging Fortran/C/C++ code



CMake 3.3.2 Released

Learn more

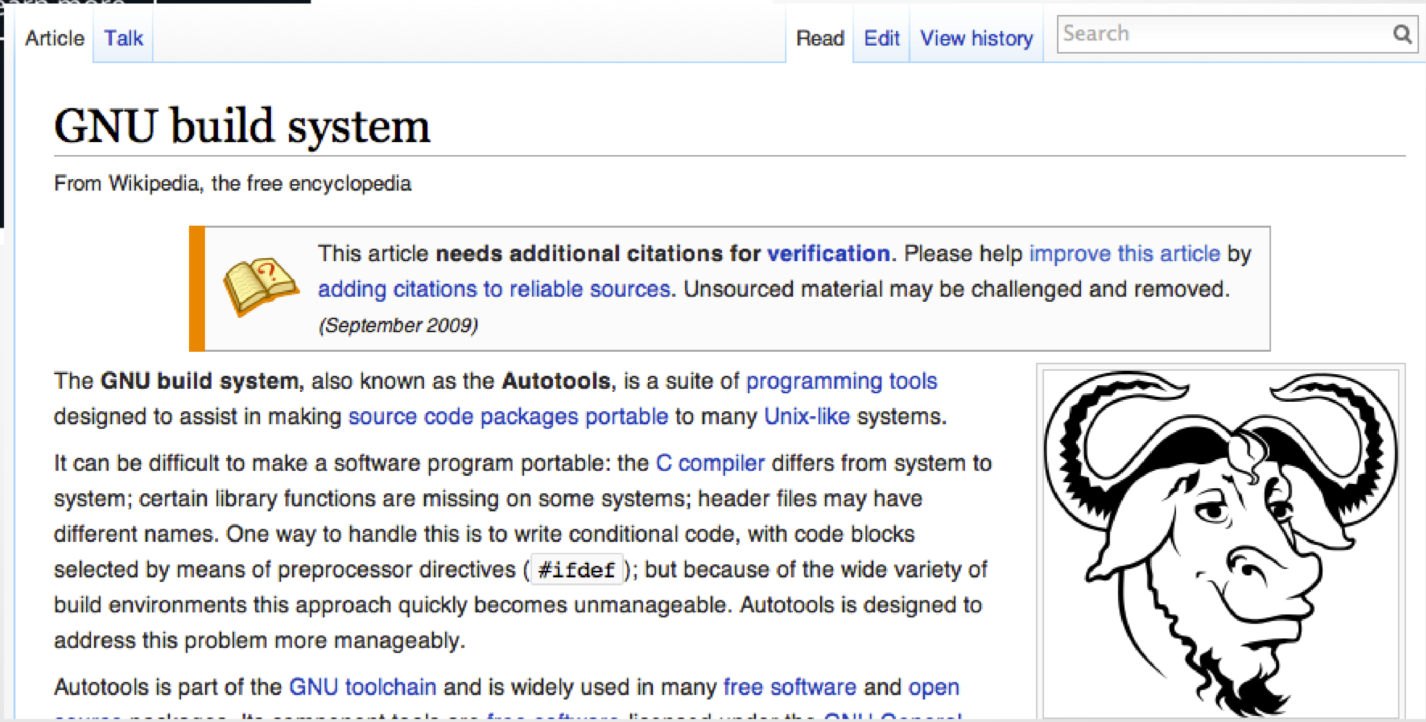
CMake News & Blogs

10.06.2015 CMake 3.4.0-rc1 is now ready!

10.02.2015 Automated Tests on GitHub for your ITK-dependent project with Cir...

09.24.2015 Kitware at SciPy 2015

Making sure it compiles on your laptop is not enough



GNU build system

From Wikipedia, the free encyclopedia

This article **needs additional citations for verification**. Please help improve this article by adding citations to reliable sources. Unsourced material may be challenged and removed. *(September 2009)*

The **GNU build system**, also known as the **Autotools**, is a suite of programming tools designed to assist in making source code packages portable to many Unix-like systems.

It can be difficult to make a software program portable: the C compiler differs from system to system; certain library functions are missing on some systems; header files may have different names. One way to handle this is to write conditional code, with code blocks selected by means of preprocessor directives (`#ifdef`); but because of the wide variety of build environments this approach quickly becomes unmanageable. Autotools is designed to address this problem more manageably.

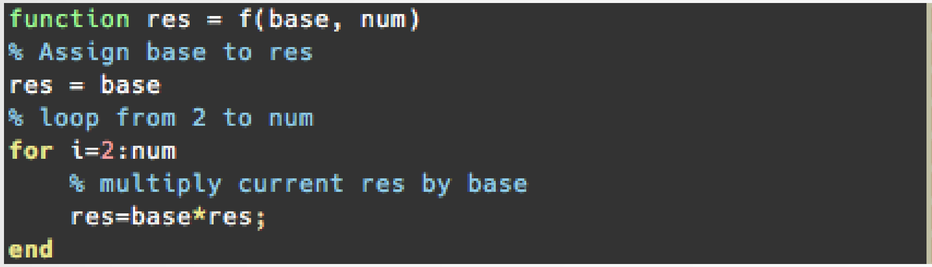
Autotools is part of the GNU toolchain and is widely used in many free software and open source packages. Its component tools are free software licensed under the GNU General

It has to compile on all the clusters...

https://cmake.org/ , https://en.wikipedia.org/wiki/GNU_build_system

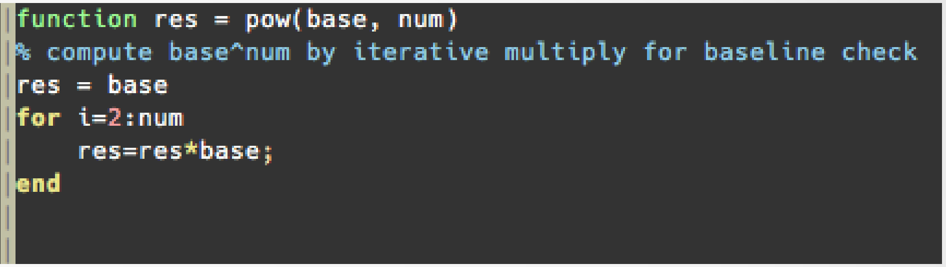
8. Comments / Documentation

Lots of useless comments



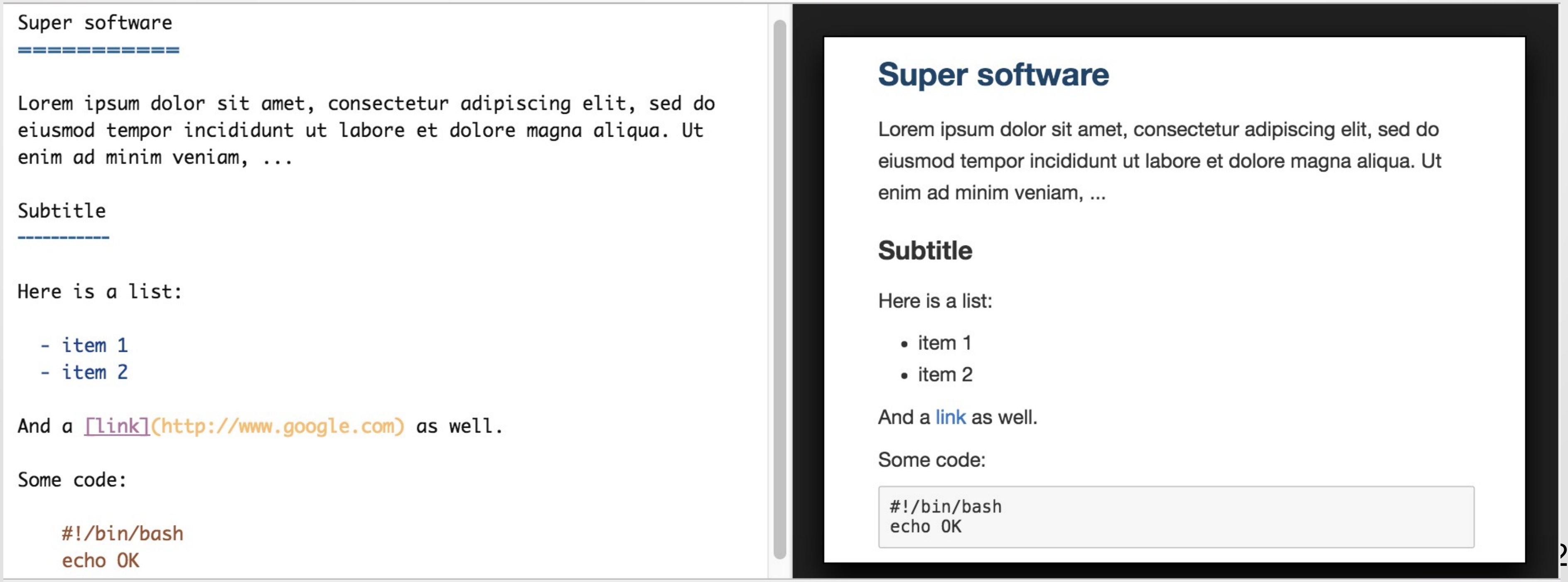
```
function res = f(base, num)
% Assign base to res
res = base
% loop from 2 to num
for i=2:num
    % multiply current res by base
    res=base*res;
end
```

Less comments but useful comments



```
function res = pow(base, num)
% compute base^num by iterative multiply for baseline check
res = base
for i=2:num
    res=res*base;
end
```

Write doc in a lightweight markup language (Markdown, rst, etc.)



```
Super software
==============

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do
eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut
enim ad minim veniam, ...

Subtitle
--------

Here is a list:

  - item 1
  - item 2

And a [link](http://www.google.com) as well.

Some code:

    #!/bin/bash
    echo OK
```

Super software

Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, ...

Subtitle

Here is a list:

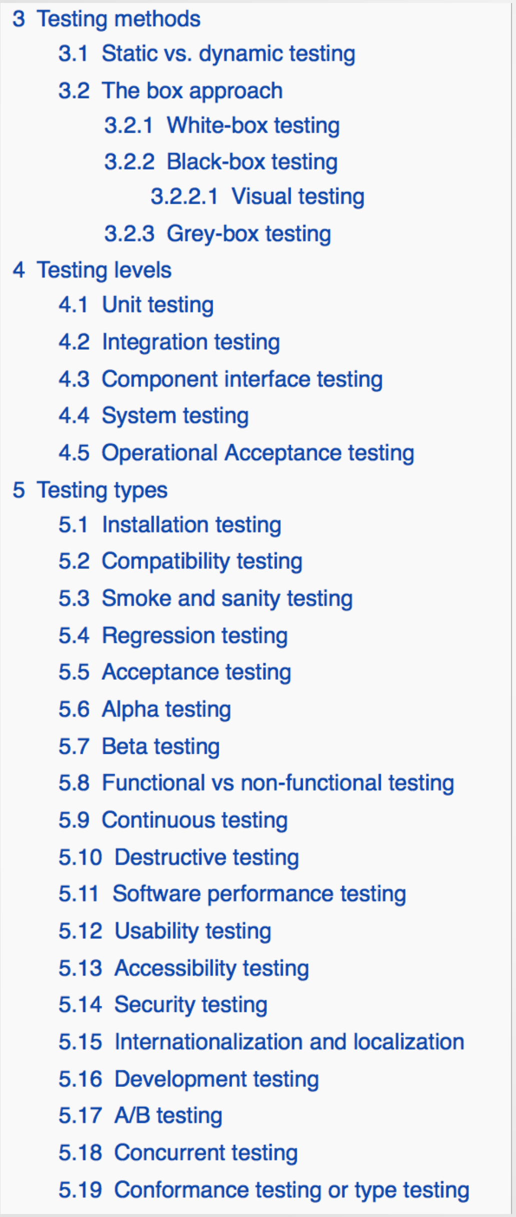
- item 1
- item 2

And a link as well.

Some code:

```
#!/bin/bash
echo OK
```

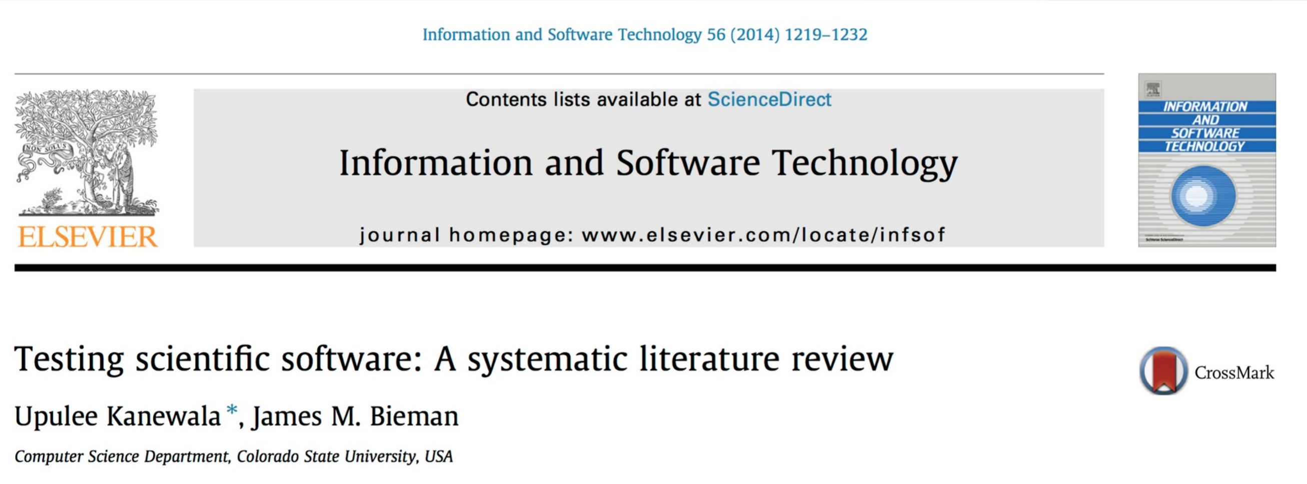
9. Tests - TDD



3 Testing methods
- 3.1 Static vs. dynamic testing
- 3.2 The box approach
  - 3.2.1 White-box testing
  - 3.2.2 Black-box testing
    - 3.2.2.1 Visual testing
  - 3.2.3 Grey-box testing

4 Testing levels
- 4.1 Unit testing
- 4.2 Integration testing
- 4.3 Component interface testing
- 4.4 System testing
- 4.5 Operational Acceptance testing

5 Testing types
- 5.1 Installation testing
- 5.2 Compatibility testing
- 5.3 Smoke and sanity testing
- 5.4 Regression testing
- 5.5 Acceptance testing
- 5.6 Alpha testing
- 5.7 Beta testing
- 5.8 Functional vs non-functional testing
- 5.9 Continuous testing
- 5.10 Destructive testing
- 5.11 Software performance testing
- 5.12 Usability testing
- 5.13 Accessibility testing
- 5.14 Security testing
- 5.15 Internationalization and localization
- 5.16 Development testing
- 5.17 A/B testing
- 5.18 Concurrent testing
- 5.19 Conformance testing or type testing



Information and Software Technology 56 (2014) 1219–1232

Contents lists available at ScienceDirect

Information and Software Technology

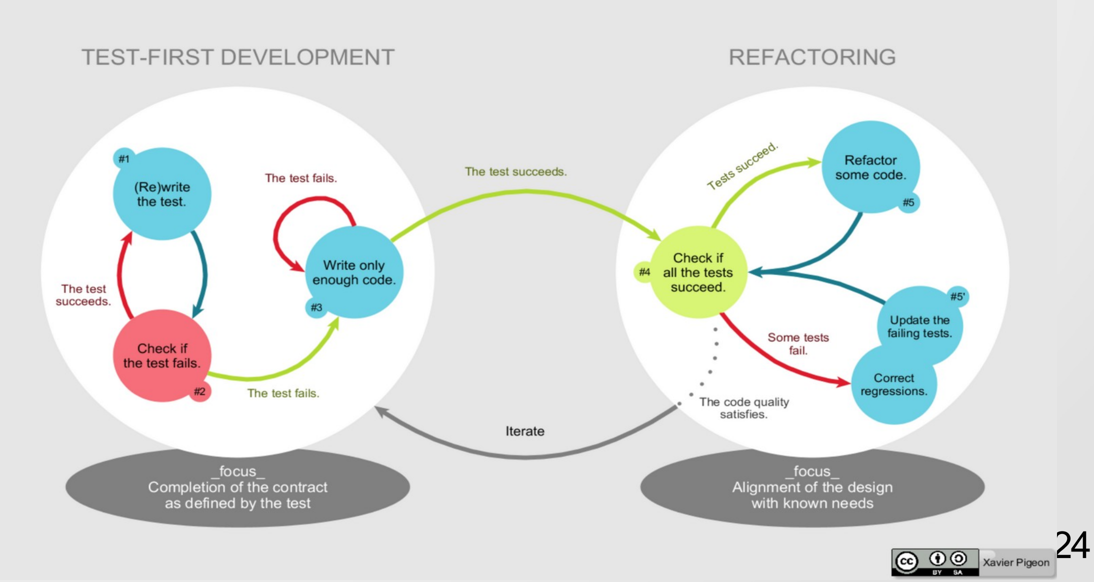
journal homepage: www.elsevier.com/locate/infsof

ELSEVIER

Testing scientific software: A systematic literature review

Upulee Kanewala *, James M. Bieman

Computer Science Department, Colorado State University, USA



http://dx.doi.org/10.1016/j.infsof.2014.05.006

10. Licensing your code: Why?

- **Commercial reason** :
  - you want to make money out of it – forbid distribution
    – forbid reverse engineering

- **Scientific reason** :
  - you want to it to be used and get citations
    – you need to allow usage, and/or modification, etc.
    – you require others to cite your work
  - you want to protect yourself from liability claims

10. Licensing your code: How?

- Choose a license type, e.g.
  - Apache License 2.0
  - BSD 3-Clause "New" or "Revised" license
  - BSD 2-Clause "Simplified" or "FreeBSD" license
  - GNU General Public License (GPL)
  - GNU Library or "Lesser" General Public License (LGPL)
  - MIT license
  - Mozilla Public License 2.0
  - Common Development and Distribution License
  - Eclipse Public License
- Copy/adapt the text
- Distribute a LICENSE file with your code

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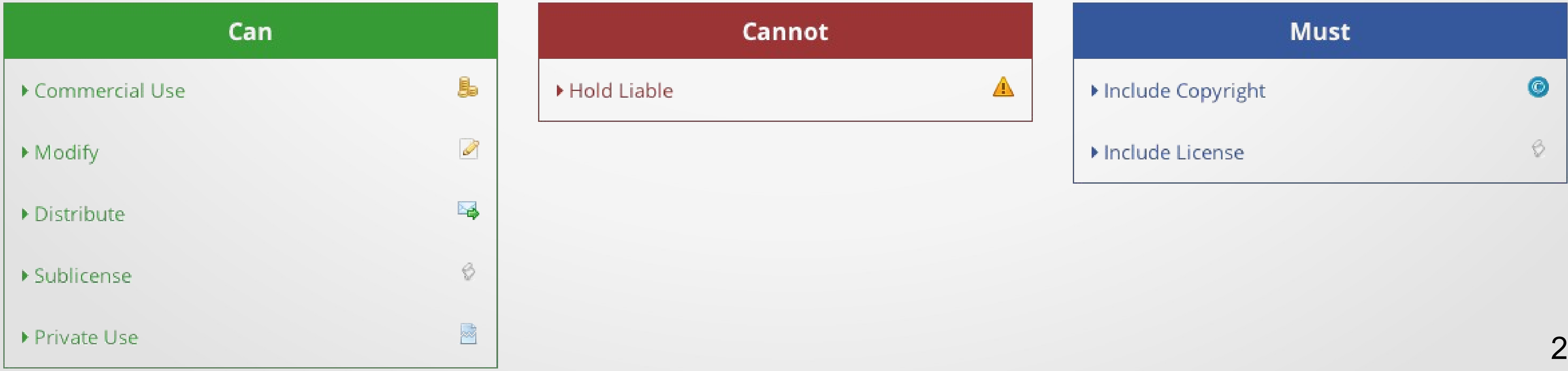
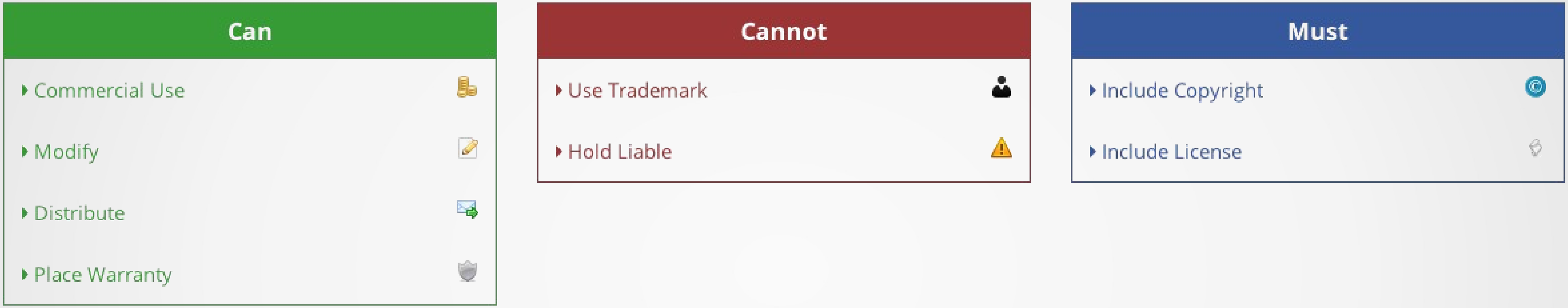


Can	Cannot	Must
Commercial Use	Hold Liable	Include Copyright
Modify		Include License
Distribute		
Sublicense		
Private Use		

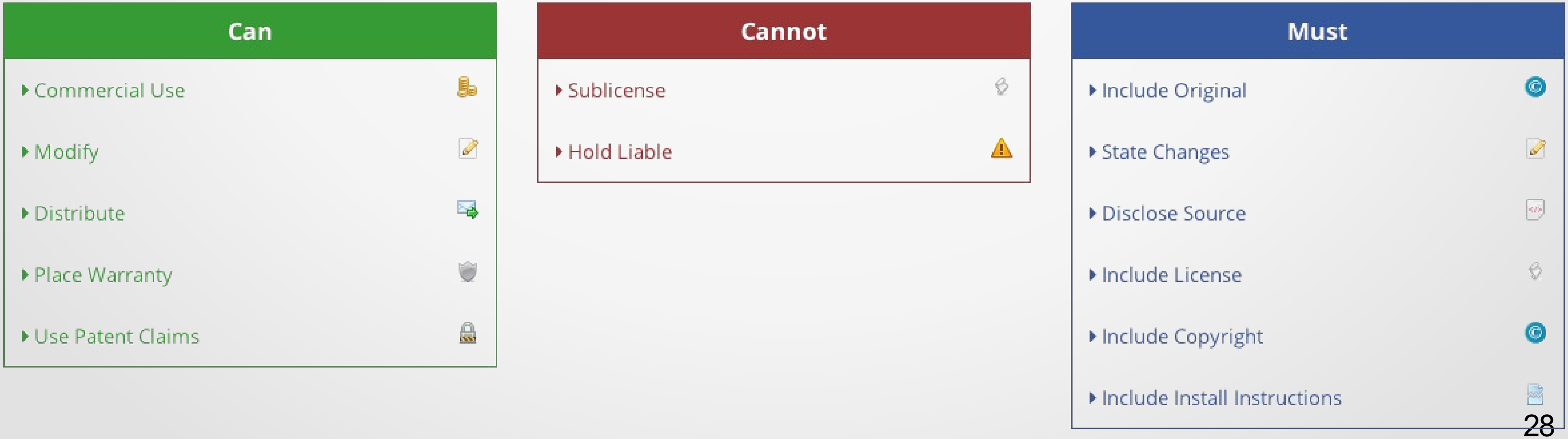
10. Licensing your code: BSD,GPL

BSD



Can	Cannot	Must
Commercial Use	Use Trademark	Include Copyright
Modify	Hold Liable	Include License
Distribute		
Place Warranty		

GPL



Can	Cannot	Must
Commercial Use	Sublicense	Include Original
Modify	Hold Liable	State Changes
Distribute		Disclose Source
Place Warranty		Include License
Use Patent Claims		Include Copyright
		Include Install Instructions

Reproduced from https://tldrlegal.com

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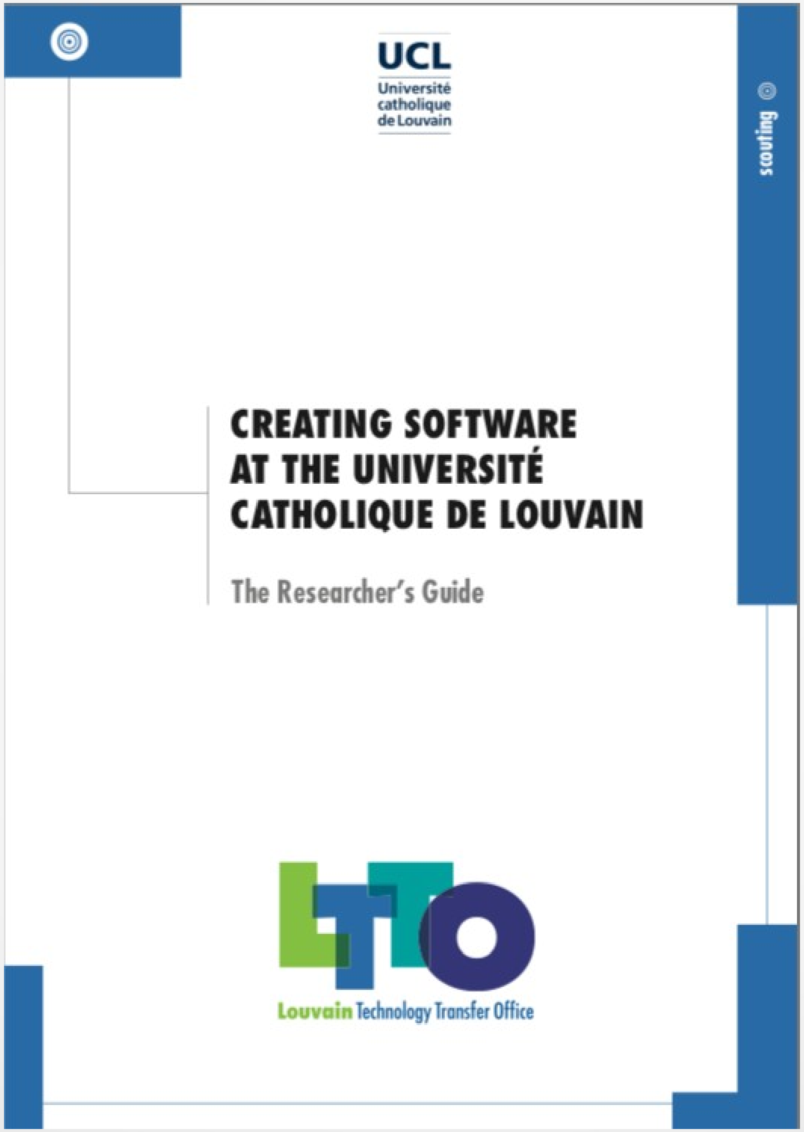

UCL
Université catholique de Louvain

scouting

CREATING SOFTWARE AT THE UNIVERSITÉ CATHOLIQUE DE LOUVAIN

The Researcher's Guide

LTTO
Louvain Technology Transfer Office

http://www.ltto.com/upload/documents/02-guide-software-PDF-LIEU.pdf

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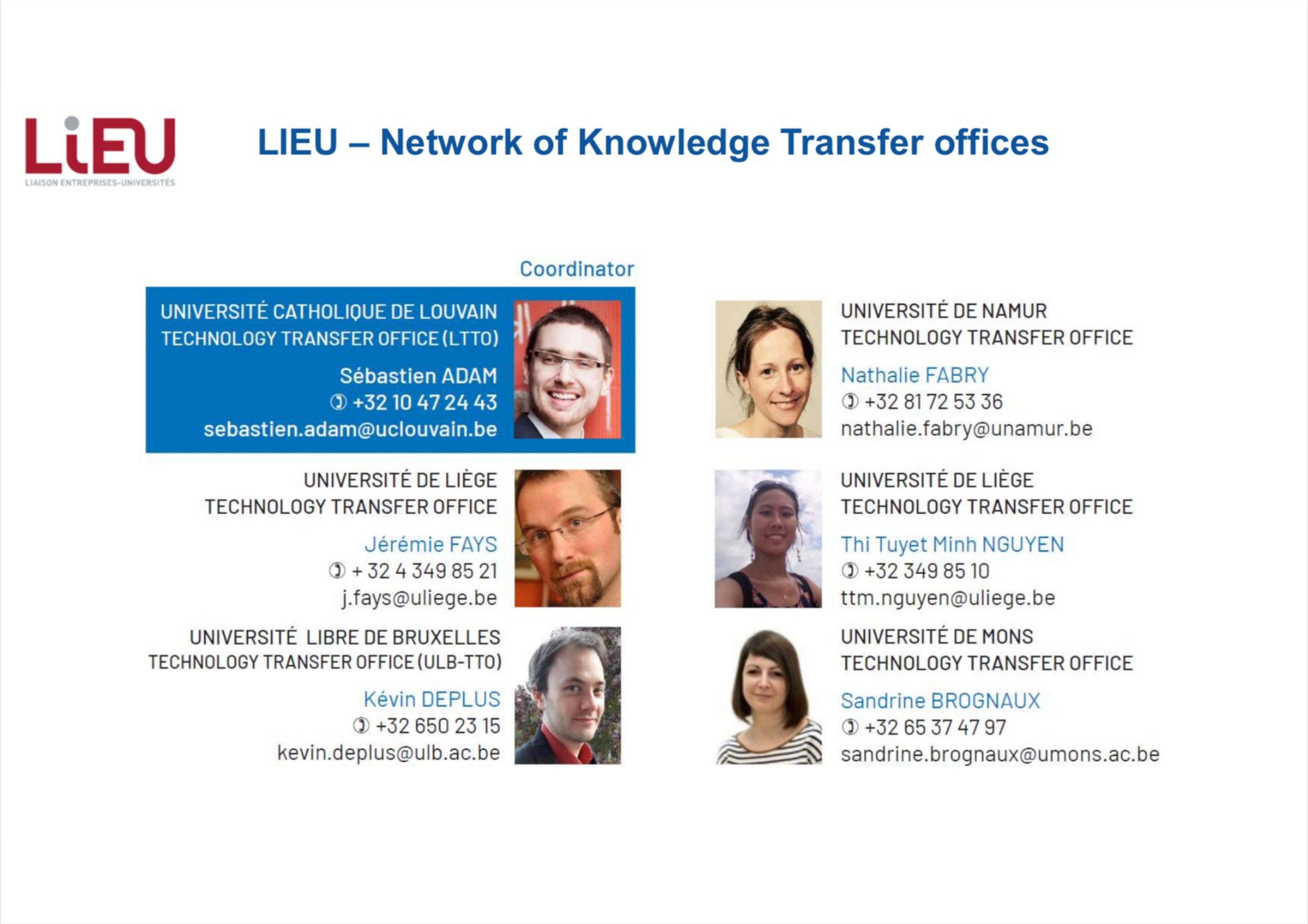

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Slide credit Sébastien ADAM

Ops' toolkit :

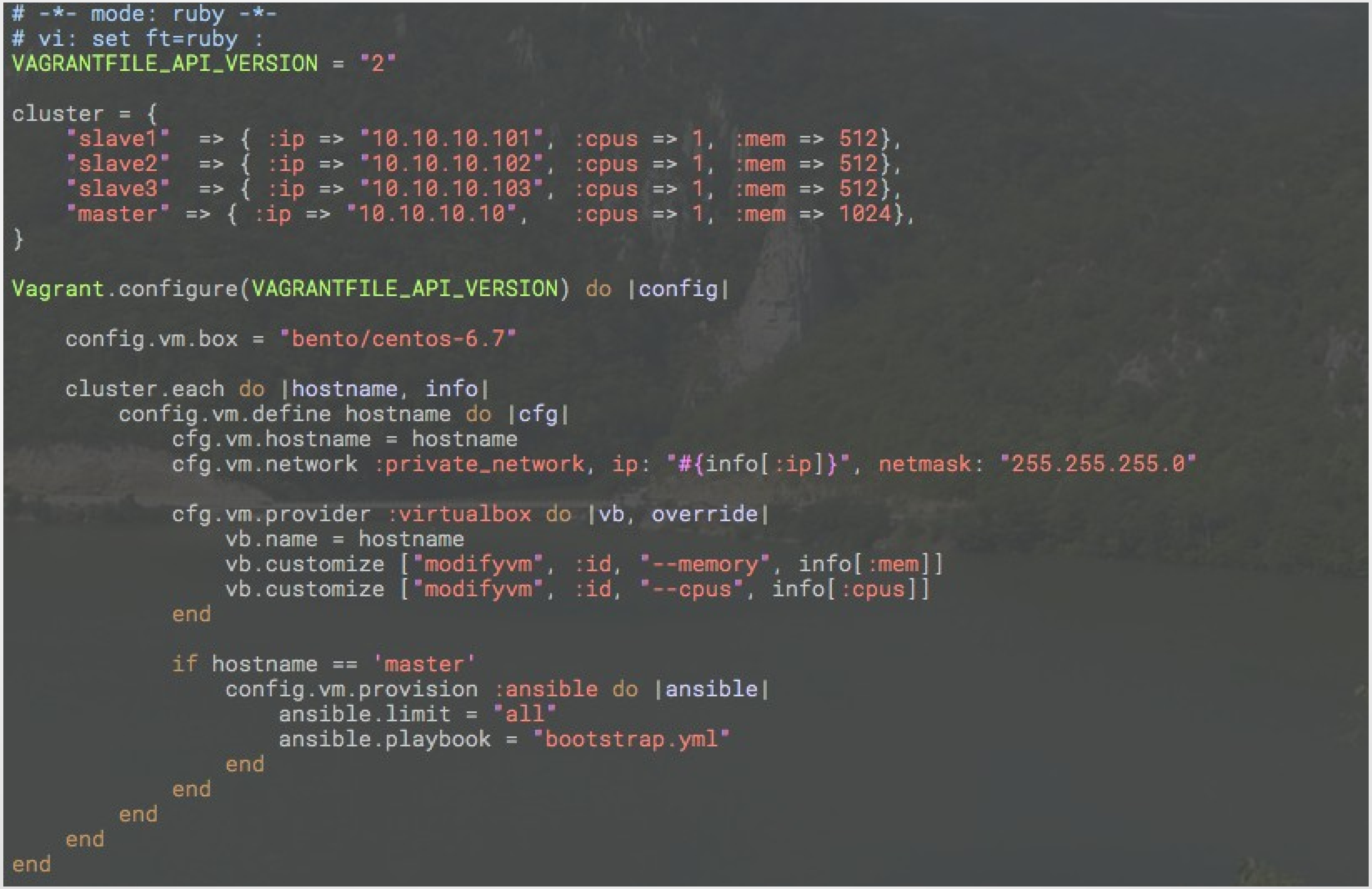
1. Virtualization platforms
2. Multi-host connexions
3. Configuration management
4. Installing
5. Automatic build tests
6. Monitoring

1. Virtualization

- Install on your laptop an environment similar to that of the cluster to test your workflow
- With
  - VirtualBox: https://www.virtualbox.org/
  - Vagrant: https://www.vagrantup.com/
- you can build a virtual cluster in one command:

“vagrant up”

1. Virtualization



```
# -*- mode: ruby -*-
# vi: set ft=ruby :
VAGRANTFILE_API_VERSION = "2"

cluster = {
    "slave1"  => { :ip => "10.10.10.101", :cpus => 1, :mem => 512},
    "slave2"  => { :ip => "10.10.10.102", :cpus => 1, :mem => 512},
    "slave3"  => { :ip => "10.10.10.103", :cpus => 1, :mem => 512},
    "master" => { :ip => "10.10.10.10",    :cpus => 1, :mem => 1024},
}

Vagrant.configure(VAGRANTFILE_API_VERSION) do |config|

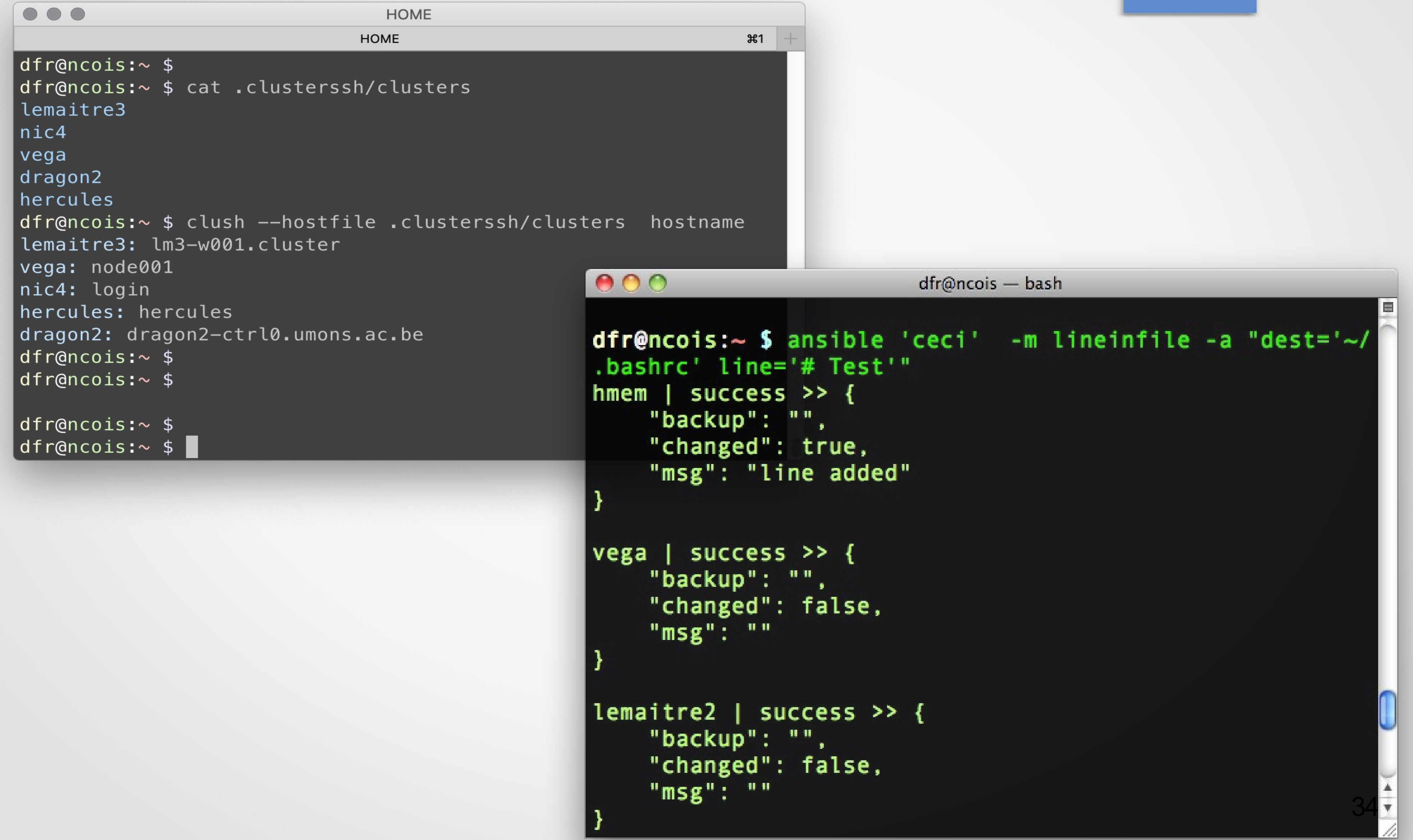
    config.vm.box = "bento/centos-6.7"

    cluster.each do |hostname, info|
        config.vm.define hostname do |cfg|
            cfg.vm.hostname = hostname
            cfg.vm.network :private_network, ip: "#{info[:ip]}", netmask: "255.255.255.0"

            cfg.vm.provider :virtualbox do |vb, override|
                vb.name = hostname
                vb.customize ["modifyvm", :id, "--memory", info[:mem]]
                vb.customize ["modifyvm", :id, "--cpus", info[:cpus]]
            end

            if hostname == 'master'
                config.vm.provision :ansible do |ansible|
                    ansible.limit = "all"
                    ansible.playbook = "bootstrap.yml"
                end
            end
        end
    end
end
```

2. Multi-host SSH



```
dfr@ncois:~ $
dfr@ncois:~ $ cat .clusterssh/clusters
lemaitre3
nic4
vega
dragon2
hercules
dfr@ncois:~ $ clush --hostfile .clusterssh/clusters  hostname
lemaitre3: lm3-w001.cluster
vega: node001
nic4: login
hercules: hercules
dragon2: dragon2-ctrl0.umons.ac.be
dfr@ncois:~ $
dfr@ncois:~ $

dfr@ncois:~ $
dfr@ncois:~ $
```

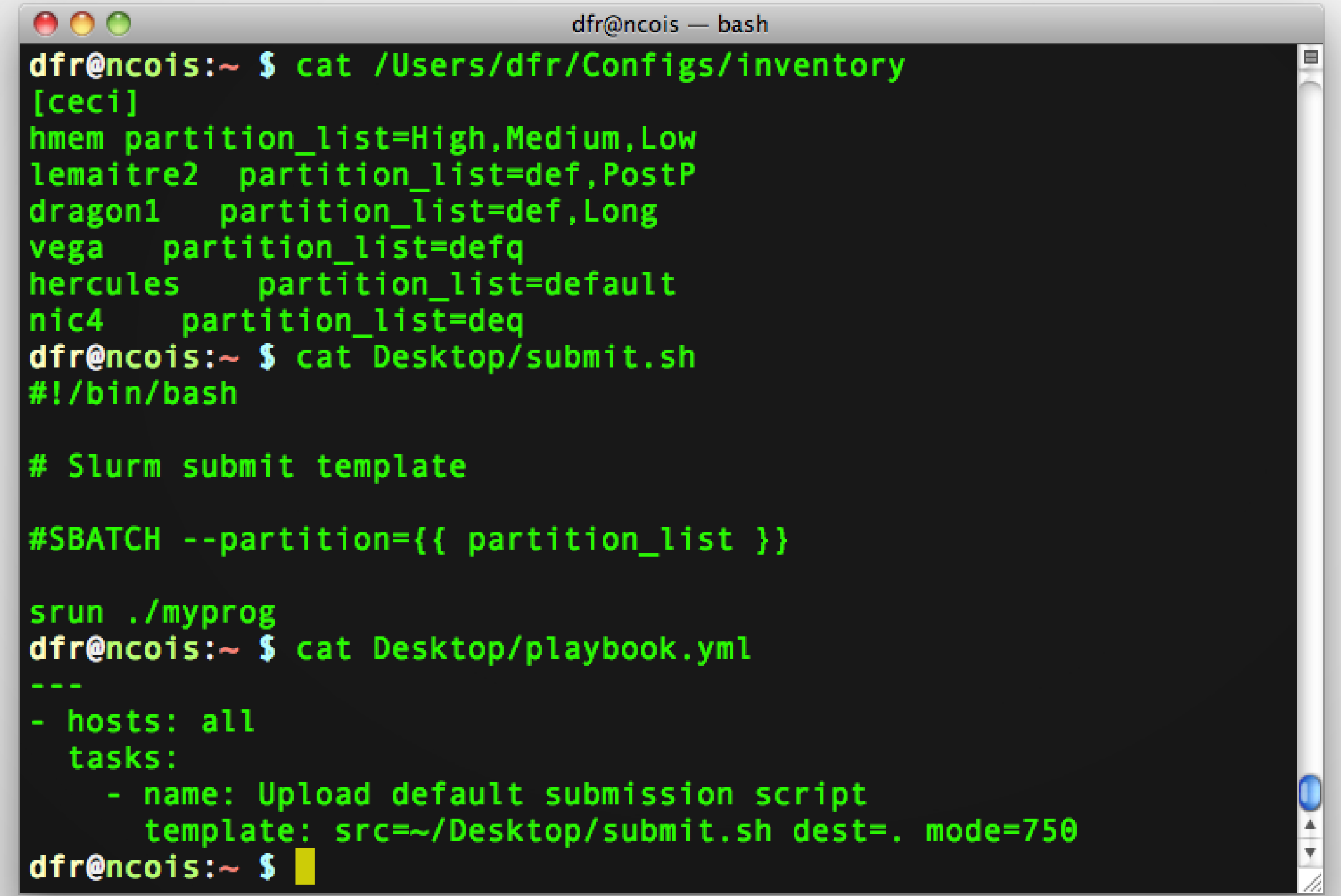
```
dfr@ncois:~ $ ansible 'ceci'  -m lineinfile -a "dest='~/
.bashrc' line='# Test'"
hmem | success >> {
    "backup": "",
    "changed": true,
    "msg": "line added"
}

vega | success >> {
    "backup": "",
    "changed": false,
    "msg": ""
}

lemaitre2 | success >> {
    "backup": "",
    "changed": false,
    "msg": ""
}
```

https://clustershell.readthedocs.io http://www.ansible.com/

3. Configuration Management



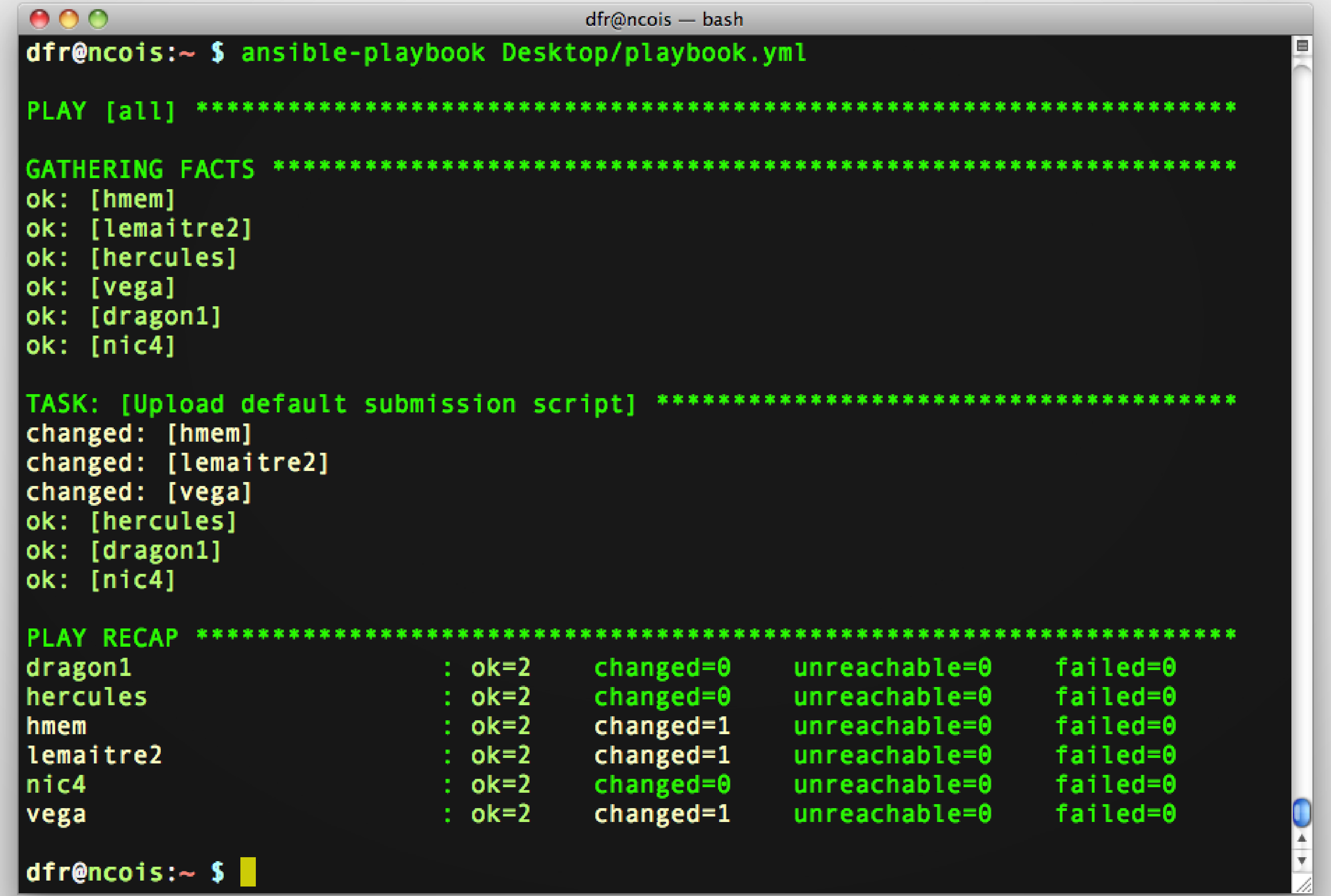
```
dfr@ncois:~ $ cat /Users/dfr/Configs/inventory
[ceci]
hmem partition_list=High,Medium,Low
lemaitre2  partition_list=def,PostP
dragon1   partition_list=def,Long
vega   partition_list=defq
hercules    partition_list=default
nic4    partition_list=deq
dfr@ncois:~ $ cat Desktop/submit.sh
#!/bin/bash

# Slurm submit template

#SBATCH --partition={{ partition_list }}

srun ./myprog
dfr@ncois:~ $ cat Desktop/playbook.yml
---
- hosts: all
  tasks:
    - name: Upload default submission script
      template: src=~/Desktop/submit.sh dest=. mode=750
dfr@ncois:~ $
```

3. Configuration Management



```
dfr@ncois:~ $ ansible-playbook Desktop/playbook.yml

PLAY [all] ********************************************************************

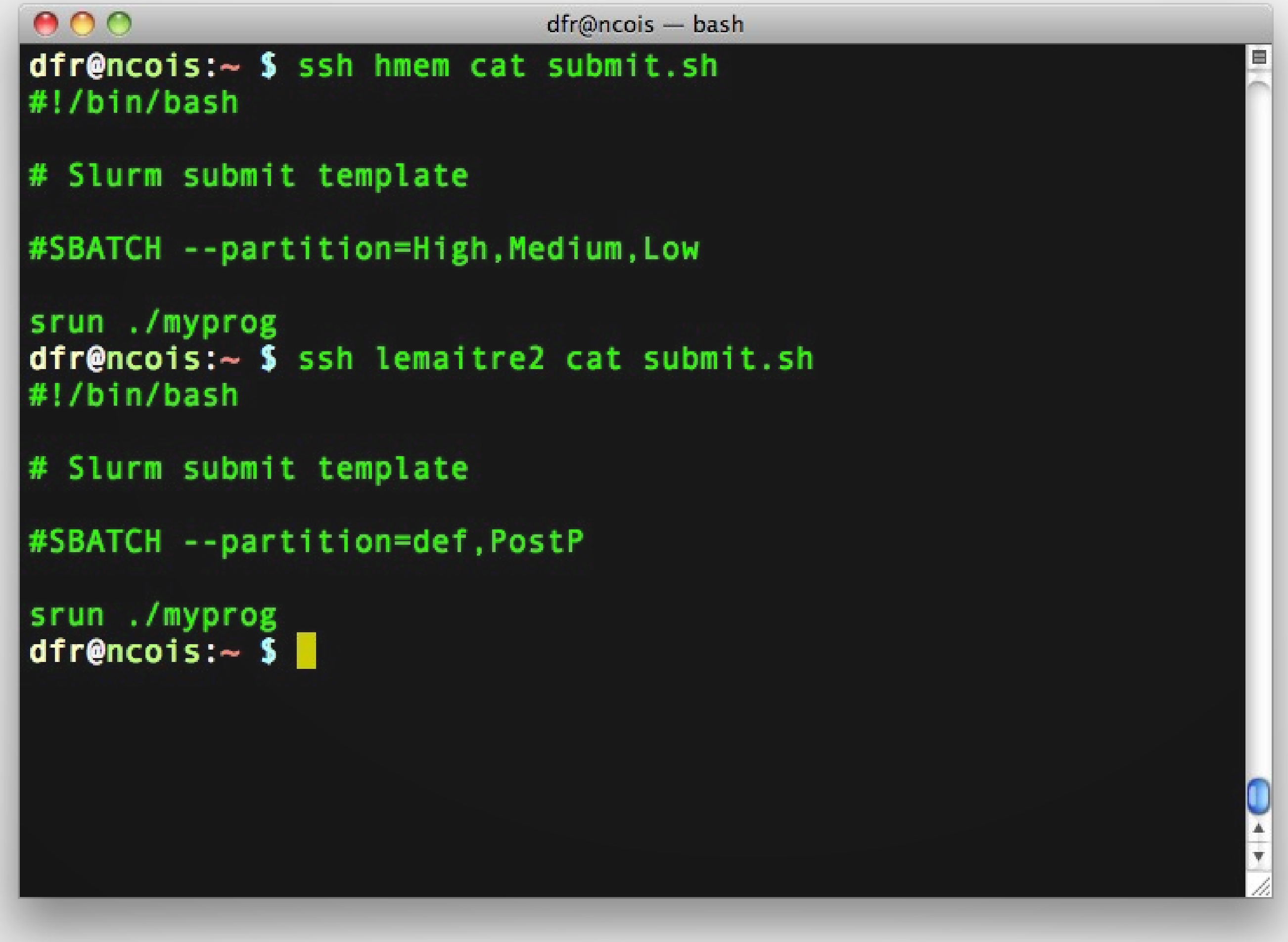
GATHERING FACTS ***************************************************************
ok: [hmem]
ok: [lemaitre2]
ok: [hercules]
ok: [vega]
ok: [dragon1]
ok: [nic4]

TASK: [Upload default submission script] **************************************
changed: [hmem]
changed: [lemaitre2]
changed: [vega]
ok: [hercules]
ok: [dragon1]
ok: [nic4]

PLAY RECAP ********************************************************************
dragon1                    : ok=2    changed=0    unreachable=0    failed=0
hercules                   : ok=2    changed=0    unreachable=0    failed=0
hmem                       : ok=2    changed=1    unreachable=0    failed=0
lemaitre2                  : ok=2    changed=1    unreachable=0    failed=0
nic4                       : ok=2    changed=0    unreachable=0    failed=0
vega                       : ok=2    changed=1    unreachable=0    failed=0

dfr@ncois:~ $
```

3. Configuration Management



dfr@ncois — bash

```
dfr@ncois:~ $ ssh hmem cat submit.sh
#!/bin/bash

# Slurm submit template

#SBATCH --partition=High,Medium,Low

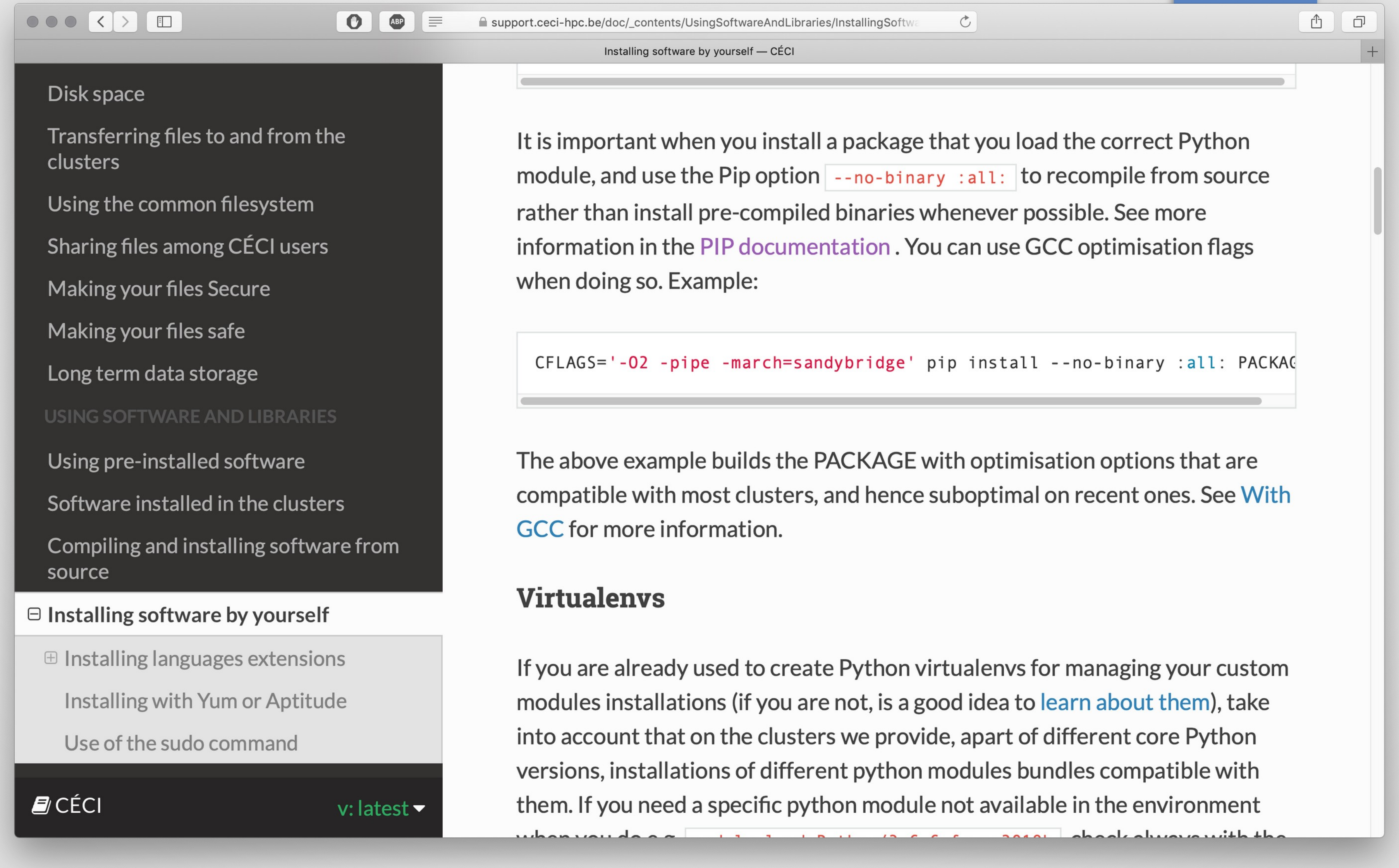
srun ./myprog
dfr@ncois:~ $ ssh lemaitre2 cat submit.sh
#!/bin/bash

# Slurm submit template

#SBATCH --partition=def,PostP

srun ./myprog
dfr@ncois:~ $
```

4. Easy installing


support.ceci-hpc.be/doc/_contents/UsingSoftwareAndLibraries/InstallingSoftw
Installing software by yourself — CÉCI

- Disk space
- Transferring files to and from the clusters
- Using the common filesystem
- Sharing files among CÉCI users
- Making your files Secure
- Making your files safe
- Long term data storage

USING SOFTWARE AND LIBRARIES

- Using pre-installed software
- Software installed in the clusters
- Compiling and installing software from source
- ⊟ Installing software by yourself
  - ⊞ Installing languages extensions
  - Installing with Yum or Aptitude
  - Use of the sudo command

CÉCI v: latest

It is important when you install a package that you load the correct Python module, and use the Pip option `--no-binary :all:` to recompile from source rather than install pre-compiled binaries whenever possible. See more information in the PIP documentation . You can use GCC optimisation flags when doing so. Example:

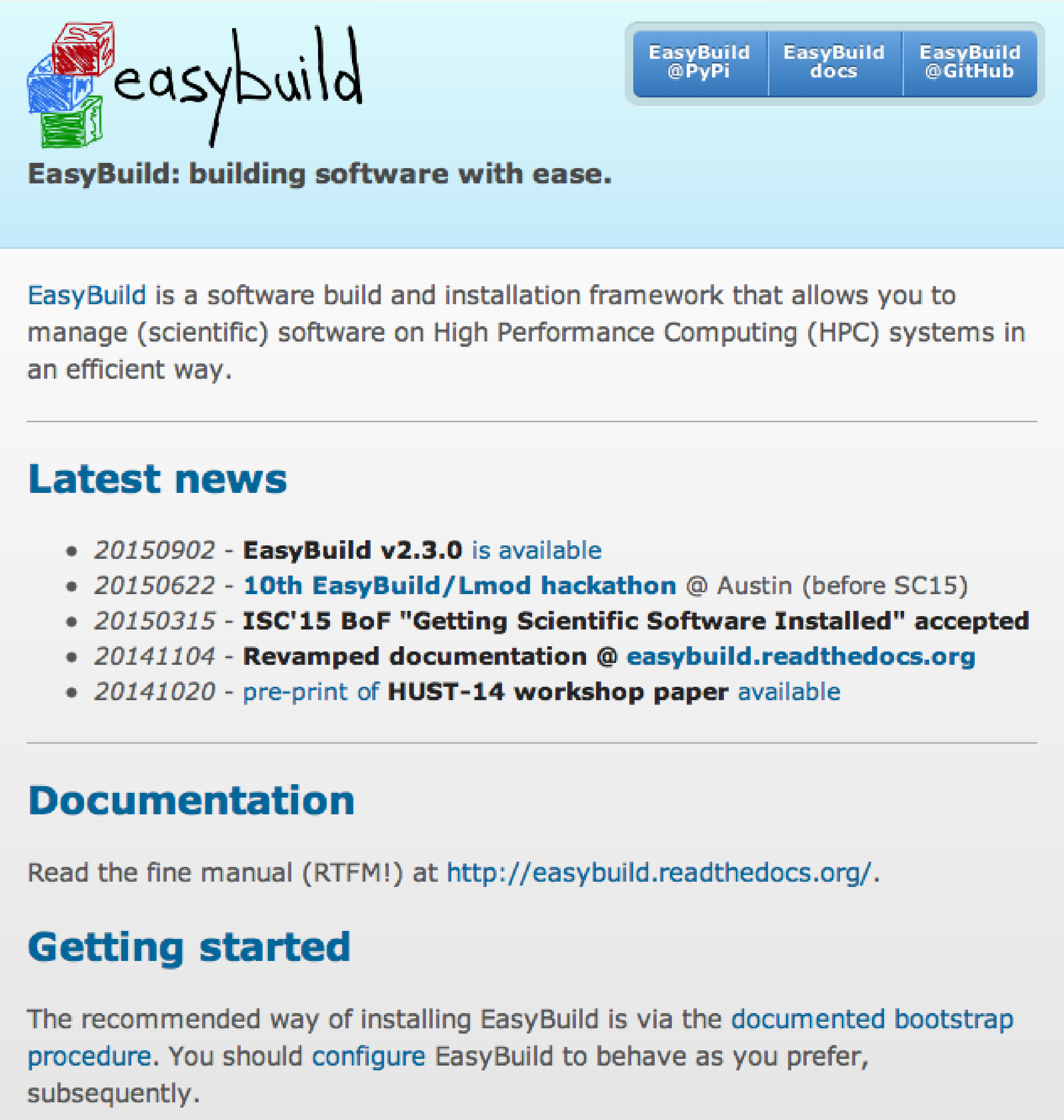
```
CFLAGS='-O2 -pipe -march=sandybridge' pip install --no-binary :all: PACKAG
```

The above example builds the PACKAGE with optimisation options that are compatible with most clusters, and hence suboptimal on recent ones. See With GCC for more information.

Virtualenvs

If you are already used to create Python virtualenvs for managing your custom modules installations (if you are not, is a good idea to learn about them), take into account that on the clusters we provide, apart of different core Python versions, installations of different python modules bundles compatible with them. If you need a specific python module not available in the environment when you do e.g. `module load Python/3.6.6-foss-2018b` check always with the

4. Easy installing



EasyBuild: building software with ease.

EasyBuild is a software build and installation framework that allows you to manage (scientific) software on High Performance Computing (HPC) systems in an efficient way.

Latest news

- *20150902* - **EasyBuild v2.3.0** is available
- *20150622* - **10th EasyBuild/Lmod hackathon** @ Austin (before SC15)
- *20150315* - **ISC'15 BoF "Getting Scientific Software Installed" accepted**
- *20141104* - **Revamped documentation @ easybuild.readthedocs.org**
- *20141020* - pre-print of **HUST-14 workshop paper** available

Documentation

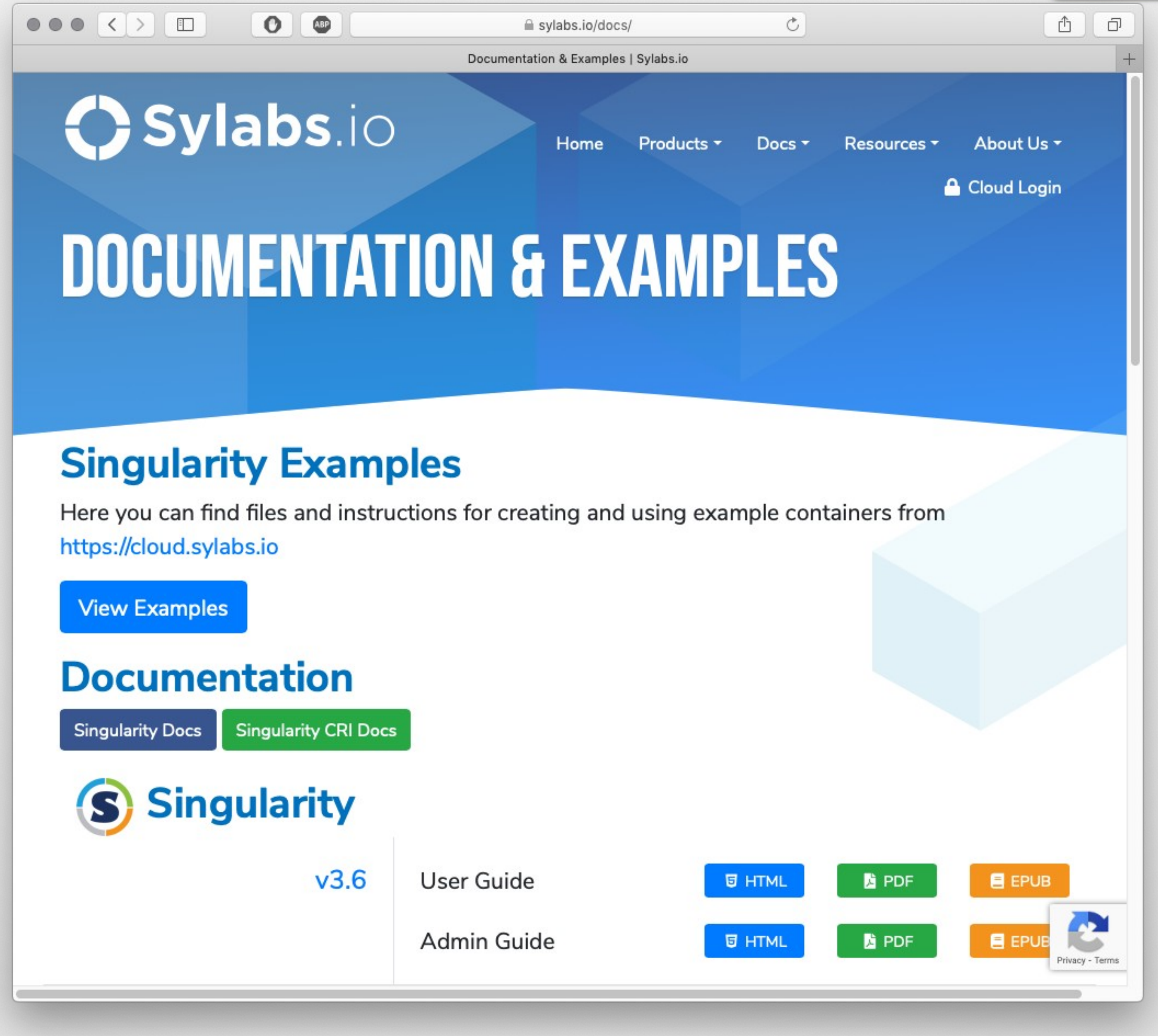
Read the fine manual (RTFM!) at http://easybuild.readthedocs.org/.

Getting started

The recommended way of installing EasyBuild is via the documented bootstrap procedure. You should configure EasyBuild to behave as you prefer, subsequently.

https://easybuild.readthedocs.io/en/latest/

4. Easy installing



sylabs.io/docs/

Documentation & Examples | Sylabs.io

DOCUMENTATION & EXAMPLES

Singularity Examples

Here you can find files and instructions for creating and using example containers from https://cloud.sylabs.io

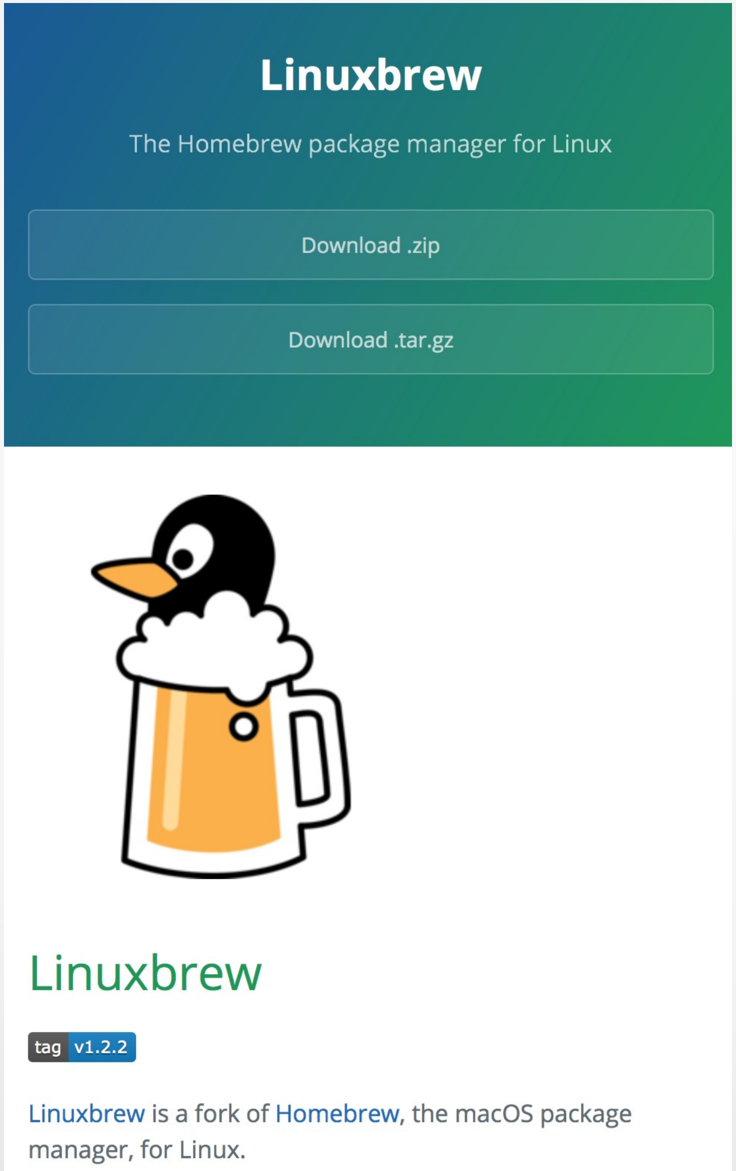
Documentation

Singularity

v3.6				
	User Guide	HTML	PDF	EPUB
	Admin Guide	HTML	PDF	EPUB

https://sylabs.io/docs/

4. Easy installing



Linuxbrew

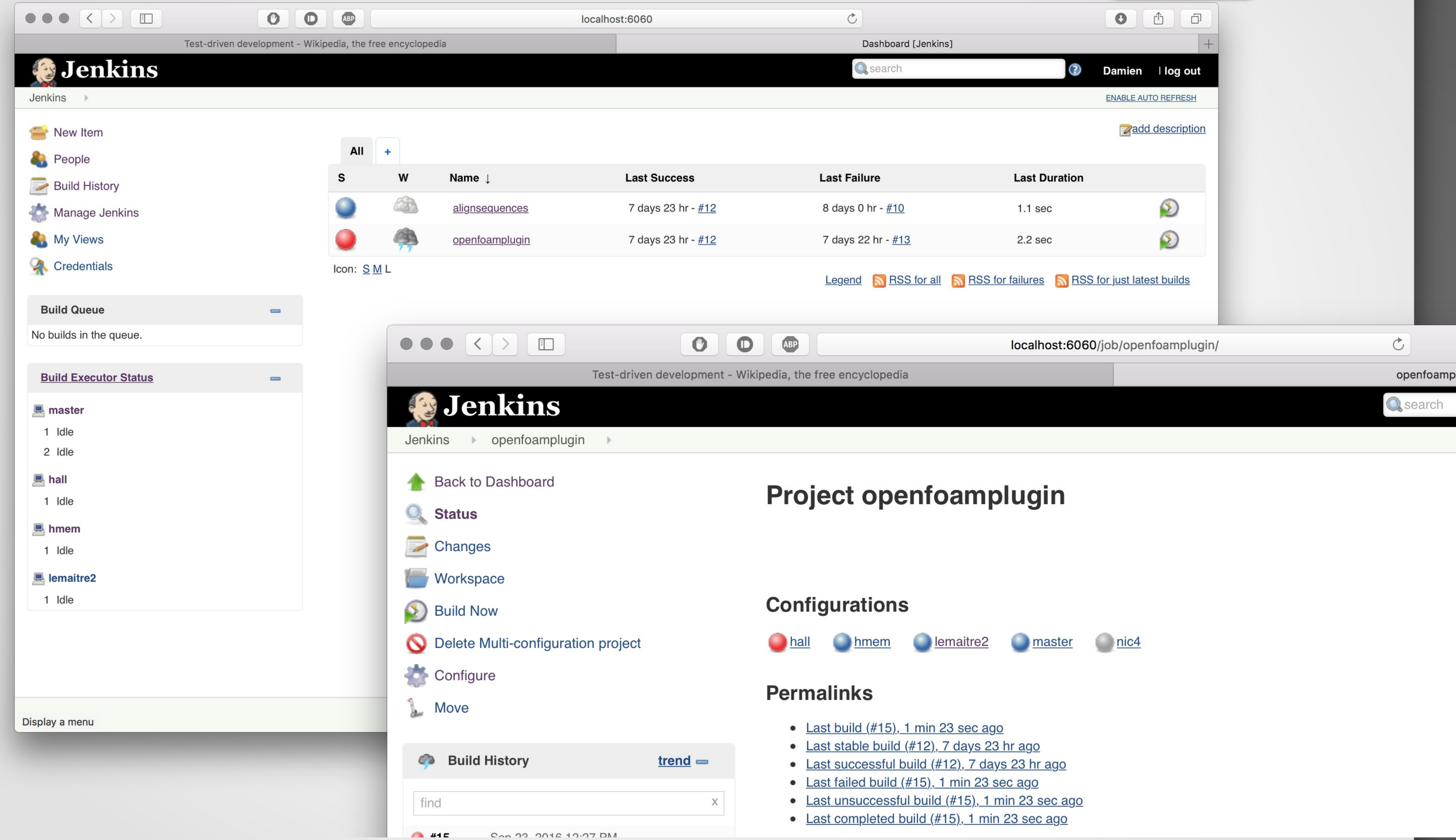
The Homebrew package manager for Linux

Linuxbrew

Linuxbrew is a fork of Homebrew, the macOS package manager, for Linux.

http://linuxbrew.sh

5. Automatic build tests



localhost:6060

Test-driven development - Wikipedia, the free encyclopedia | Dashboard [Jenkins]

Jenkins | search | Damien | log out

Jenkins › | ENABLE AUTO REFRESH

- New Item
- People
- Build History
- Manage Jenkins
- My Views
- Credentials

add description

All | +

S	W	Name ↓	Last Success	Last Failure	Last Duration	
●	☁	alignsequences	7 days 23 hr - #12	8 days 0 hr - #10	1.1 sec	
🔴	⛈	openfoamplugin	7 days 23 hr - #12	7 days 22 hr - #13	2.2 sec	

Icon: S M L

Legend | RSS for all | RSS for failures | RSS for just latest builds

Build Queue

No builds in the queue.

Build Executor Status

master
1 Idle
2 Idle
hall
1 Idle
hmem
1 Idle
lemaitre2
1 Idle

Display a menu

localhost:6060/job/openfoamplugin/

Test-driven development - Wikipedia, the free encyclopedia | openfoamp

Jenkins | search

Jenkins › openfoamplugin ›

- Back to Dashboard
- Status
- Changes
- Workspace
- Build Now
- Delete Multi-configuration project
- Configure
- Move

Build History trend

find

#15 Sep 23, 2016 12:27 PM

Project openfoamplugin

Configurations

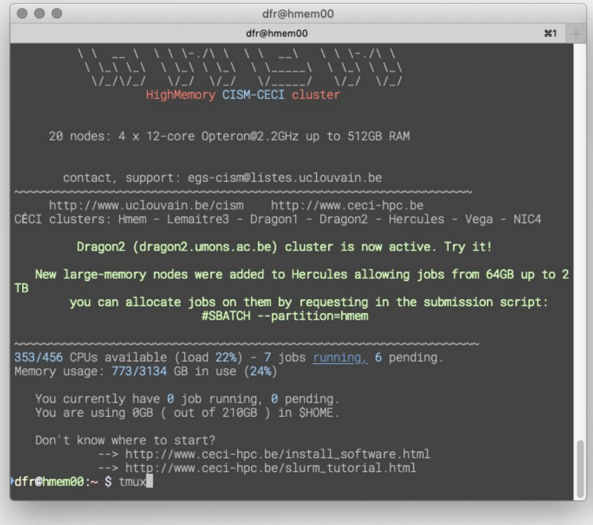
🔴 hall ● hmem ● lemaitre2 ● master ○ nic4

Permalinks

- Last build (#15), 1 min 23 sec ago
- Last stable build (#12), 7 days 23 hr ago
- Last successful build (#12), 7 days 23 hr ago
- Last failed build (#15), 1 min 23 sec ago
- Last unsuccessful build (#15), 1 min 23 sec ago
- Last completed build (#15), 1 min 23 sec ago

https://www.jenkins.io

6. Terminal multiplexing



```
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           \/_/\/_/   \/_/  \/_/   \/_____/   \/_/  \/_/
                  HighMemory CISM-CECI cluster


     20 nodes: 4 x 12-core Opteron@2.2GHz up to 512GB RAM


       contact, support: egs-cism@listes.uclouvain.be
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
     http://www.uclouvain.be/cism    http://www.ceci-hpc.be
CÉCI clusters: Hmem - Lemaitre3 - Dragon1 - Dragon2 - Hercules - Vega - NIC4

        Dragon2 (dragon2.umons.ac.be) cluster is now active. Try it!

   New large-memory nodes were added to Hercules allowing jobs from 64GB up to 2
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        you can allocate jobs on them by requesting in the submission script:
                          #SBATCH --partition=hmem

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353/456 CPUs available (load 22%) - 7 jobs running, 6 pending.
Memory usage: 773/3134 GB in use (24%)

   You currently have 0 job running, 0 pending.
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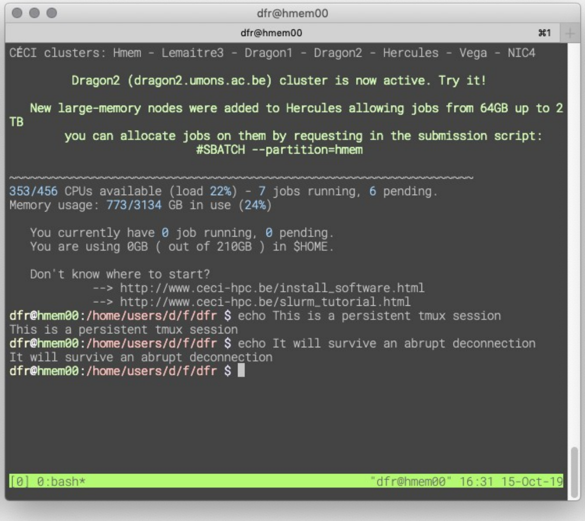
dfr@hmem00:~ $ tmux
```



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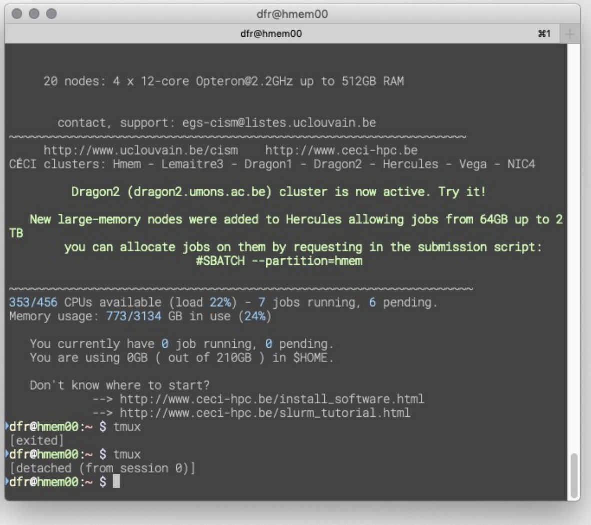
dfr@hmem00:/home/users/d/f/dfr $ echo This is a persistent tmux session
This is a persistent tmux session
dfr@hmem00:/home/users/d/f/dfr $ echo It will survive an abrupt deconnection
It will survive an abrupt deconnection
dfr@hmem00:/home/users/d/f/dfr $







[0] 0:bash*                                            "dfr@hmem00" 16:31 15-Oct-19
```



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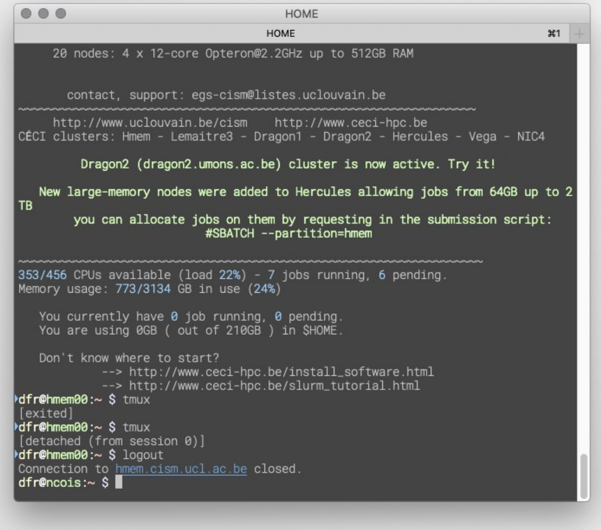
dfr@hmem00:~ $ tmux
[exited]
dfr@hmem00:~ $ tmux
[detached (from session 0)]
dfr@hmem00:~ $
```



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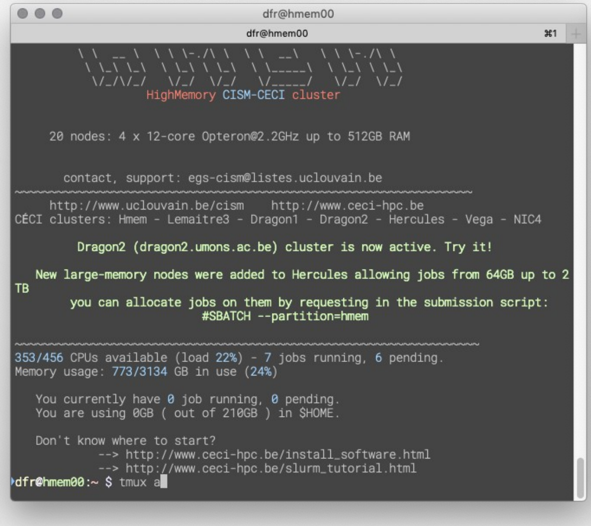
dfr@hmem00:~ $ tmux
[exited]
dfr@hmem00:~ $ tmux
[detached (from session 0)]
dfr@hmem00:~ $ logout
Connection to hmem.cism.ucl.ac.be closed.
dfr@ncois:~ $
```



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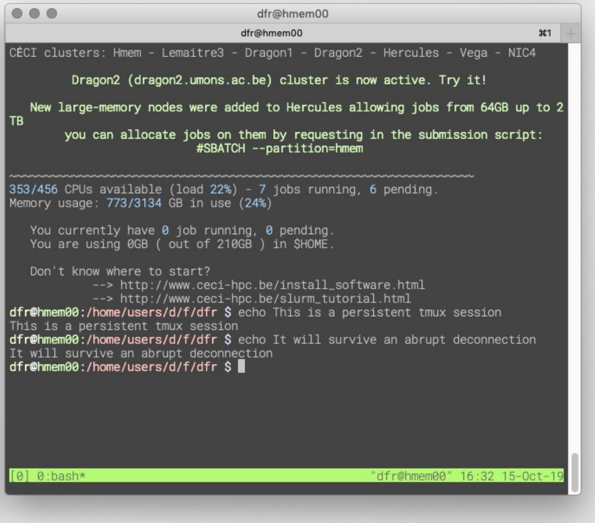
dfr@hmem00:~ $ tmux a
```



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It will survive an abrupt deconnection
dfr@hmem00:/home/users/d/f/dfr $







[0] 0:bash*                                            "dfr@hmem00" 16:32 15-Oct-19
```

Commands: tmux or screen

Dev's toolkit :

1. Programming language
2. Good practices / Code Style Guides
3. Text editor / IDE
4. Source control management
5. Debuggers / Profilers
6. Databases
7. Packaging / Distributing tools
8. Comments and documentation
9. Tests
10. Licensing

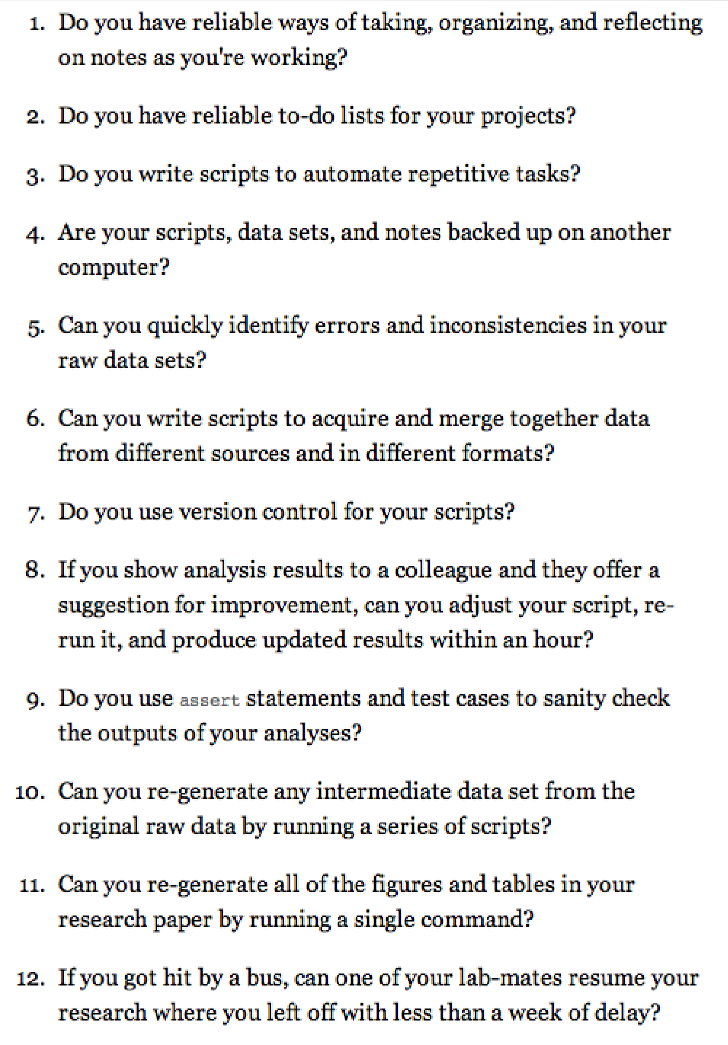
Ops' toolkit :

1. Virtualization platforms (Virtual box, Vagrant)
2. Multi-host connexions (clustershell)
3. Configuration management/ (ansible)
4. Installing (easybuild)
5. Automatic build tests (jenkins)
6. Terminal multiplexing (tmux, screen)

The 'Phillip' test

- 12 simple questions
- ordered by 'difficulty'
- measures quality of organization
- for research programming

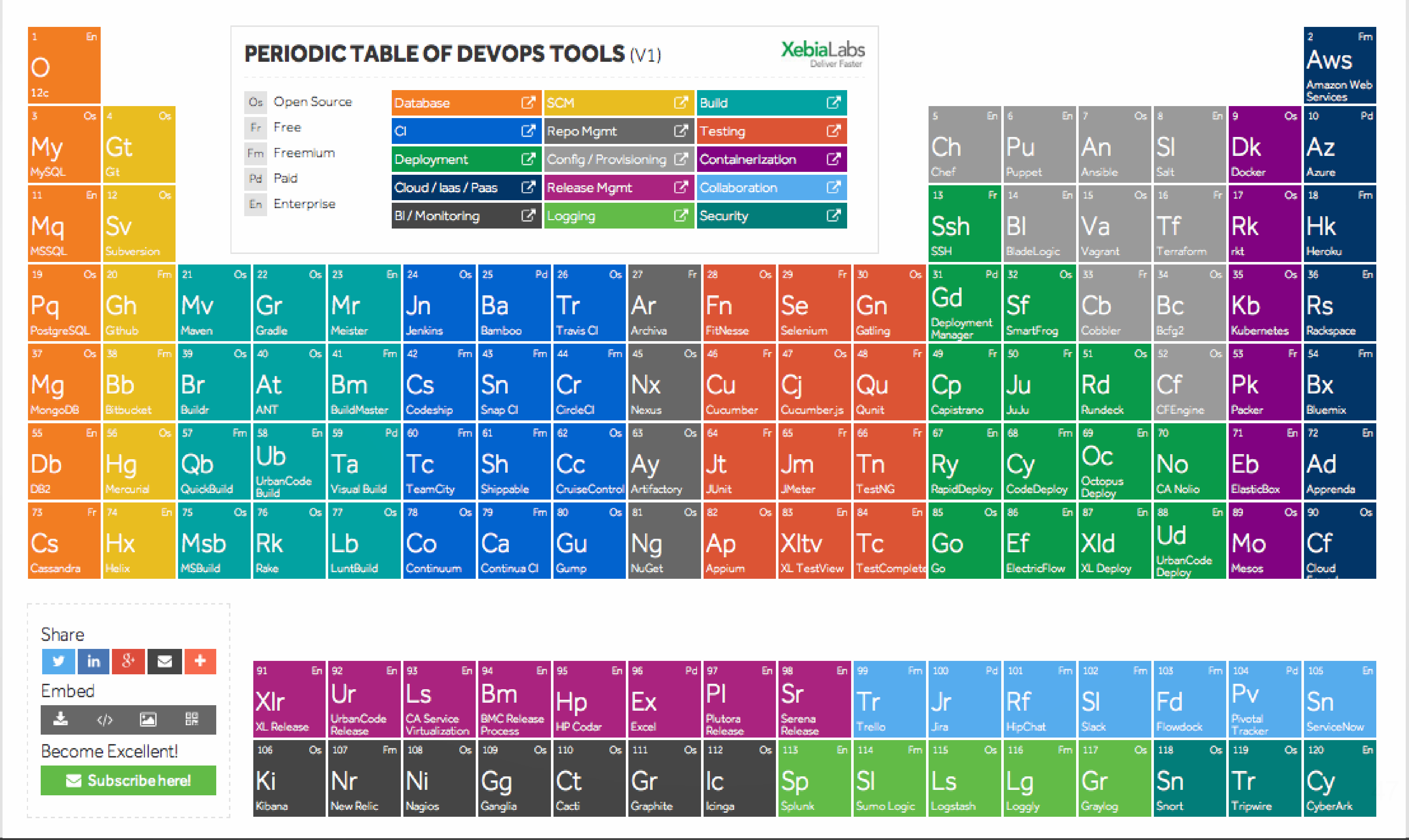
If you do not score at least a 7 there is room for improvement using the tools presented here



1. Do you have reliable ways of taking, organizing, and reflecting on notes as you're working?
2. Do you have reliable to-do lists for your projects?
3. Do you write scripts to automate repetitive tasks?
4. Are your scripts, data sets, and notes backed up on another computer?
5. Can you quickly identify errors and inconsistencies in your raw data sets?
6. Can you write scripts to acquire and merge together data from different sources and in different formats?
7. Do you use version control for your scripts?
8. If you show analysis results to a colleague and they offer a suggestion for improvement, can you adjust your script, re-run it, and produce updated results within an hour?
9. Do you use `assert` statements and test cases to sanity check the outputs of your analyses?
10. Can you re-generate any intermediate data set from the original raw data by running a series of scripts?
11. Can you re-generate all of the figures and tables in your research paper by running a single command?
12. If you got hit by a bus, can one of your lab-mates resume your research where you left off with less than a week of delay?

http://pgbovine.net/research-programming-workflow.htm

Work quicker & more reliably



PERIODIC TABLE OF DEVOPS TOOLS (V1)

XebiaLabs
Deliver Faster

Os	Open Source
Fr	Free
Fm	Freemium
Pd	Paid
En	Enterprise

Database	SCM	Build
CI	Repo Mgmt	Testing
Deployment	Config / Provisioning	Containerization
Cloud / Iaas / Paas	Release Mgmt	Collaboration
BI / Monitoring	Logging	Security

1 En O 12c																	2 Fm Aws Amazon Web Services
3 Os My MySQL	4 Os Gt Git											5 En Ch Chef	6 En Pu Puppet	7 Os An Ansible	8 En Sl Salt	9 Os Dk Docker	10 Pd Az Azure
11 En Mq MSSQL	12 Os Sv Subversion											13 Fr Ssh SSH	14 En Bl BladeLogic	15 Os Va Vagrant	16 Fr Tf Terraform	17 Os Rk rkt	18 Fm Hk Heroku
19 Os Pq PostgreSQL	20 Fm Gh Github	21 Os Mv Maven	22 Os Gr Gradle	23 En Mr Meister	24 Os Jn Jenkins	25 Pd Ba Bamboo	26 Os Tr Travis CI	27 Fr Ar Archiva	28 Os Fn FitNesse	29 Fr Se Selenium	30 Os Gn Gatling	31 Pd Gd Deployment Manager	32 Os Sf SmartFrog	33 Fr Cb Cobbler	34 Os Bc Bcfg2	35 Os Kb Kubernetes	36 En Rs Rackspace
37 Os Mg MongoDB	38 Fm Bb Bitbucket	39 Os Br Buildr	40 Os At ANT	41 Fm Bm BuildMaster	42 Fm Cs Codeship	43 Fm Sn Snap CI	44 Fm Cr CircleCI	45 Os Nx Nexus	46 Fr Cu Cucumber	47 Os Cj Cucumber.js	48 Fr Qu Qunit	49 Fr Cp Capistrano	50 Fr Ju JuJu	51 Os Rd Rundeck	52 Os Cf CFEngine	53 Fr Pk Packer	54 Fm Bx Bluemix
55 En Db DB2	56 Os Hg Mercurial	57 Fm Qb QuickBuild	58 En Ub UrbanCode Build	59 Pd Ta Visual Build	60 Fm Tc TeamCity	61 Fm Sh Shippable	62 Os Cc CruiseControl	63 Os Ay Artifactory	64 Fr Jt JUnit	65 Fr Jm JMeter	66 Fr Tn TestNG	67 En Ry RapidDeploy	68 Fm Cy CodeDeploy	69 En Oc Octopus Deploy	70 No CA Nolio	71 En Eb ElasticBox	72 En Ad Apprenda
73 Fr Cs Cassandra	74 En Hx Helix	75 Os Msb MSBuild	76 Os Rk Rake	77 Os Lb LuntBuild	78 Os Co Continuum	79 Fm Ca Continua CI	80 Os Gu Gump	81 Os Ng NuGet	82 Os Ap Appium	83 En Xltv XL TestView	84 En Tc TestComplete	85 Os Go Go	86 En Ef ElectricFlow	87 En Xld XL Deploy	88 En Ud UrbanCode Deploy	89 Os Mo Mesos	90 Os Cf Cloud
			91 En Xlr XL Release	92 En Ur UrbanCode Release	93 En Ls CA Service Virtualization	94 En Bm BMC Release Process	95 En Hp HP Codar	96 Pd Ex Excel	97 En Pl Plutora Release	98 En Sr Serena Release	99 Fm Tr Trello	100 Pd Jr Jira	101 Fm Rf HipChat	102 Fm Sl Slack	103 Fm Fd Flowdock	104 Pd Pv Pivotal Tracker	105 En Sn ServiceNow
			106 Os Ki Kibana	107 Fm Nr New Relic	108 Os Ni Nagios	109 Os Gg Ganglia	110 Os Ct Cacti	111 Os Gr Graphite	112 Os Ic Icinga	113 En Sp Splunk	114 Fm Sl Sumo Logic	115 Os Ls Logstash	116 Fm Lg Loggly	117 Os Gr Graylog	118 Os Sn Snort	119 Os Tr Tripwire	120 En Cy CyberArk

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