

# Introduction to Scientific Software Deployment and Development

damien.francois@uclouvain.be  
November 2023

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

PERIODIC TABLE OF DEVOPS TOOLS (V1)															XebiaLabs Deliver Faster					
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 Bcf2	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 Juku	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 Os 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 LunrBuild	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			

Os	Open Source	Database	SCM	Build
Fr	Free	CI	Repo Mgmt	Testing
Fm	Freemium	Deployment	Config / Provisioning	Containerization
Pd	Paid	Cloud / IaaS / PaaS	Release Mgmt	Collaboration
En	Enterprise	BI / Monitoring	Logging	Security

Share

Embed

Become Excellent!

Subscribe here!

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

# Goal of this session:

“Promote the tools  
the professionals are using for  
**developing** and **deploying** programs,  
to make them **correct**, **maintainable**, **shareable**, and **fast**,  
*efficiently.*”

“...to make them **correct and maintainable**, ..., *efficiently*”

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>

Koehler Leman J *et al* "**Better together: Elements of successful scientific software development in a distributed collaborative community**. *PLoS Comput Biol*. 2020 doi: 10.1371/journal.pcbi.1007507.

“...to make them **correct** and **maintainable**, ..., *efficiently*”

Follow programming good practices:

1. Write for humans, not for computers
2. Use the appropriate language
3. Organize for change and make incremental changes
4. Follow good coding principles
5. Plan for mistakes, automate testing
6. Use modern source-code management system
7. Document the design and purpose, not the implementation
8. Optimize only when it works already
9. Debug cleverly

# 1. Write for humans, not for computers

---

“Indeed, the ratio of time spent reading versus writing is well over 10 to 1. We are constantly reading old code as part of the effort to write new code. ...[Therefore,] making it easy to read makes it easier to write.”



# 1. Write for humans, not for computers

---

Structure clear but goal not obvious

```
1 for i in range(n):
2     for j in range(m):
3         for k in range(l):
4             temp_value = X[i][j][k] * 12.5
5             new_array[i][j][k] = temp_value + 150
```

**VS**

Sweet spot in-between...

Goal clear but structure less obvious

```
1 PIXEL_NORMALIZATION_FACTOR = 12.5
2 PIXEL_OFFSET_FACTOR = 150
3
4 for row_index in range(row_count):
5     for column_index in range(column_count):
6         for color_channel_index in range(color_channel_count):
7             normalized_pixel_value = (
8                 original_pixel_array[row_index][column_index][color_channel_index]
9                 * PIXEL_NORMALIZATION_FACTOR
10            )
11            transformed_pixel_array[row_index][column_index][color_channel_index] = (
12                normalized_pixel_value + PIXEL_OFFSET_FACTOR
13            )
```

# 1. Write for humans, not for computers

## Avoid naming anti-patterns:

A.1	<i>“Get” - more than an accessor</i>	A getter that performs actions other than returning the corresponding attribute without documenting it. Example: method <code>getImageData</code> which, no matter the attribute value, every time returns a new object (see Fig. 1).	B.6	<i>Expecting but not getting a collection</i>	The name of a method suggests that a collection should be returned but a single object or nothing is returned. Example: method <code>getStats</code> with return type <code>Boolean</code> (see Fig. 15).
A.2	<i>“Is” returns more than a Boolean</i>	The name of a method is a predicate suggesting a true/false value in return. However the return type is not <code>Boolean</code> but rather a more complex type thus allowing a wider range of values without documenting them. Example: <code>isValid</code> with return type <code>int</code> (see Fig. 6).	C.1	<i>Method name and return type are opposite</i>	The intent of the method suggested by its name is in contradiction with what it returns. Example: method <code>disable</code> with return type <code>ControlEnableState</code> . The inconsistency comes from “disable” and “enable” having opposite meanings (see Fig. 16).
A.3	<i>“Set” method returns</i>	A set method having a return type different than <code>void</code> and not documenting the return type/values with an appropriate comment (see Fig. 7).	C.2	<i>Method signature and comment are opposite</i>	The documentation of a method is in contradiction with its declaration. Example: method <code>isNavigateForwardEnabled</code> is in contradiction with its comment documenting “a back navigation”, as “forward” and “back” are antonyms (see Fig. 17).
A.4	<i>Expecting but not getting a single instance</i>	The name of a method indicates that a single object is returned but the return type is a collection. Example: method <code>getExpansion</code> returning <code>List</code> (see Fig. 9).	D.1	<i>Says one but contains many</i>	The name of an attribute suggests a single instance, while its type suggests that the attribute stores a collection of objects. Example: attribute <code>target</code> of type <code>Vector</code> . It is unclear whether a change affects one or multiple instances in the collection (see Fig. 18).
B.1	<i>Not implemented condition</i>	The comments of a method suggest a conditional behavior that is not implemented in the code. When the implementation is default this should be documented (see Fig. 10).	D.2	<i>Name suggests Boolean but type does not</i>	The name of an attribute suggests that its value is true or false, but its declaring type is not <code>Boolean</code> . Example: attribute <code>isReached</code> of type <code>int[]</code> where the declared type and values are not documented (see Fig. 19).
B.2	<i>Validation method does not confirm</i>	A validation method (e.g., name starting with “validate”, “check”, “ensure”) does not confirm the validation, i.e., the method neither provides a return value informing whether the validation was successful, nor documents how to proceed to understand (see Fig. 11).	E.1	<i>Says many but contains one</i>	The name of an attribute suggests multiple instances, but its type suggests a single one. Example: attribute <code>stats</code> of type <code>Boolean</code> . Documenting such inconsistencies avoids additional comprehension effort to understand the purpose of the attribute (see Fig. 20).
B.3	<i>“Get” method does not return</i>	The name suggests that the method returns something (e.g., name starts with “get” or “return”) but the return type is <code>void</code> . The documentation should explain where the resulting data is stored and how to obtain it (see Fig. 12).	F.1	<i>Attribute name and type are opposite</i>	The name of an attribute is in contradiction with its type as they contain antonyms. Example: attribute <code>start</code> of type <code>MAssociationEnd</code> . The use of antonyms can induce wrong assumptions (see Fig. 21).
B.4	<i>Not answered question</i>	The name of a method is in the form of predicate whereas the return type is not <code>Boolean</code> . Example: method <code>isValid</code> with return type <code>void</code> (see Fig. 13).	F.2	<i>Attribute signature and comment are opposite</i>	The declaration of an attribute is in contradiction with its documentation. Example: attribute <code>INCLUDE_NAME_DEFAULT</code> whose comment documents an “exclude pattern”. Whether the pattern is included or excluded is thus unclear (see Fig. 22).
B.5	<i>Transform method does not return</i>	The name of a method suggests the transformation of an object but there is no return value and it is not clear from the documentation where the result is stored. Example: method <code>javaToNative</code> with return type <code>void</code> (see Fig. 14).			



# 1. Write for humans, not for computers

The screenshot shows a Stack Overflow question page. The header includes the Stack Overflow logo, a search bar, and the word 'Products'. The left sidebar contains navigation links for Home, PUBLIC, Questions (highlighted), Tags, Users, Companies, COLLECTIVES, Explore Collectives, TEAMS, and Create free Team. The main content area features the question title 'What does the ????! operator do in C?' with metadata: 'Asked 11 years ago', 'Modified 1 year, 2 months ago', and 'Viewed 379k times'. A blue notification box states: 'Highly active question. You have enough reputation to answer or unprotect this question.' Below this, the question body text reads: 'I saw a line of C that looked like this:'. A code block contains the snippet: `!ErrorHasOccured() ????! HandleError();`. The question text continues: 'It compiled correctly and seems to run ok. It seems like it's checking if an error has occurred, and if it has, it handles it. But I'm not really sure what it's actually doing or how it's doing it. It does look like the programmer is trying express their feelings about errors.' The final paragraph asks: 'I have never seen the ????! before in any programming language, and I can't find documentation for it anywhere. (Google doesn't help with search terms like ????!). What does it do and how does the code sample work?'

# 1. Write for humans, not for computers

stackoverflow Products Search...

Home

PUBLIC

Questions

Tags

Users

Companies

COLLECTIVES

Explore Collectives

TEAMS

Create free Team

## What does the ?!?! operator do in C?

Asked 11 years ago Modified 1 year, 2 months ago Viewed 379k times

**Highly active question.** You have enough reputation to answer or unprotect this question.

```
2471 if (ErrorHasOccured())  
HandleError();
```

I saw a line of C that looked like this:  
!ErrorHasOccured() ?!?! HandleError();

It compiled correctly and seems to run ok. It seems like it's checking if an error has occurred, and if it has, it handles it. But I'm not really sure what it's actually doing or how it's doing it. It does look like the programmer is trying express their feelings about errors.

I have never seen the ?!?! before in any programming language, and I can't find documentation for it anywhere. (Google doesn't help with search terms like ?!?!). What does it do and how does the code sample work?

<https://stackoverflow.com/questions/7825055/what-does-the-operator-do-in-c>

## 2. Use the appropriate language

---



are all valid choices in a scientific context.

## 2. Use the appropriate language

---

What they have in common:

- Computation-efficiency concern
- Optimized libraries available for linear algebra, signal processing, learning, etc.
- Support for parallel computing
- Extensions/libraries for using accelerators (GPUs)

## 2. Use the appropriate language

---



### **“Functional programming”**

Very close to mathematical formulation

Imposes constraints that make code less prone to bugs and easier to make parallel

Not very popular in HPC (yet)

### 3. Organize for change and make incremental changes

---

Scientific software specifications are always changing:

- ◆ Work from working state to another working state
- ◆ Document the changes and why they were made
- ◆ Refactor upon “code smell”

Keyword: **modularity**: small independent interchangeable building blocks (e.g. functions)

# 3 1/2 . Avoid “code smells” / anti-patterns

**{ PRAGMATIC WAYS }**  
TIPS FOR CLEANER CODE

## DUPLICATE CODE

DUPLICATE CODE CAN OCCUR AS A RESULT OF A SHORT DEADLINE, LACK OF COMMUNICATION, OR JUST OUT OF PURE LAZINESS BY THE DEVELOPER.

LEARN ABOUT THE DIFFERENT **REFACTORING** METHODS TO CLEAN UP DUPLICATE CODE.

**THE D.R.Y. PRINCIPLE STANDS FOR DON'T REPEAT YOURSELF**

LEARN MORE CLEAN CODE TIPS AT [PRAGMATICWAYS.COM](https://pragmaticways.com)

**{ PRAGMATIC WAYS }**  
TIPS FOR CLEANER CODE

## SPECULATIVE GENERALITY

CODE THAT'S CREATED FOR **FUTURE USE** IS **SPECULATIVE GENERALITY**. THIS CODE IS NOT CURRENTLY TIED TO ANY REQUIREMENTS BUT THE INTENTIONS ON **FUTURE REQUIREMENTS**.

THIS CODE CROWDS THE PROJECT AND WILL PROBABLY **NEVER** END UP GETTING USED. **DELETE ANY CODE THAT ISN'T BEING UTILIZED TODAY, EVEN IF YOU "MIGHT USE IT LATER."**

**CREATE CLASSES FOR CURRENT REQUIREMENTS ONLY**

LEARN MORE CLEAN CODE TIPS AT [PRAGMATICWAYS.COM](https://pragmaticways.com)

**{ PRAGMATIC WAYS }**  
TIPS FOR CLEANER CODE

## CONDITIONAL COMPLEXITY

WE'VE ALL SEEN IT, THE **LARGE CONDITIONAL BLOCKS** OF **10+ IF-ELSE STATEMENTS**.

THESE COMPLEX CONDITIONALS ARE USUALLY A RESULT OF POOR (OR JUST LACK OF) **DESIGN PLANNING**, OR JUST NATURALLY GREW WITH THE LIFE OF THE PROJECT (NEW REQUIREMENTS, FEATURES, ETC.)

**CONSIDER REFACTORING WITH A DESIGN PATTERN**

LEARN MORE CLEAN CODE TIPS AT [PRAGMATICWAYS.COM](https://pragmaticways.com)

**{ PRAGMATIC WAYS }**  
TIPS FOR CLEANER CODE

## SOLUTION SPRAWL

"YOU BECOME AWARE OF THIS SMELL WHEN ADDING OR UPDATING A SYSTEM FEATURE CAUSES YOU TO **MAKE CHANGES** TO MANY DIFFERENT PIECES OF CODE."

IF THE PROBLEM IS OF **SPRAWLING OBJECT CREATION** RESPONSIBILITY, THEN REFACTOR USING THE **FACTORY DESIGN PATTERN**.

**REFACTOR CODE TO LIMIT A FEATURE'S EXPOSURE**

LEARN MORE CLEAN CODE TIPS AT [PRAGMATICWAYS.COM](https://pragmaticways.com)

**{ PRAGMATIC WAYS }**  
TIPS FOR CLEANER CODE

## LONG PARAMETER LIST

METHODS WITH LONG PARAMETER LISTS (OVER 4 PARAMETERS LONG) ARE **HARDER TO READ** AND UNDERSTAND.

THE FUNCTION IS PROBABLY DOING **MORE THAN ONE THING**, IN WHICH CASE YOU COULD SPLIT THE METHOD UP INTO **MULTIPLE TARGETED FUNCTIONS**. OTHERWISE CONSIDER GROUPING THE PARAMETERS TOGETHER IN A **DATA OBJECT**.

**USE LESS THAN 4 PARAMETERS PER FUNCTION**

LEARN MORE CLEAN CODE TIPS AT [PRAGMATICWAYS.COM](https://pragmaticways.com)

**{ PRAGMATIC WAYS }**  
TIPS FOR CLEANER CODE

## DEAD CODE

AS JEFF ATWOOD PUTS IT, "RUTHLESSLY DELETE CODE THAT ISN'T BEING USED. THAT'S WHY WE HAVE SOURCE CONTROL SYSTEMS!"

DEAD CODE IN A PROJECT JUST ADDS MORE CONFUSION TO THE CODE BASE, MORE NONSENSE TO MAINTAIN. CLEAN UP OLD CODE AND DELETE DEAD CODE - YOU'LL KNOW YOU BROKE SOMETHING IF YOUR TEST CASES FAIL!

**DELETE DEAD CODE, INCLUDING OLD COMMENTED OUT CODE**

LEARN MORE CLEAN CODE TIPS AT [PRAGMATICWAYS.COM](https://pragmaticways.com)

**{ PRAGMATIC WAYS }**  
TIPS FOR CLEANER CODE

## ODDBALL SOLUTION

WHEN YOU HAVE MULTIPLE SOLUTIONS TO THE SAME PROBLEM, YOU HAVE AN **ODDBALL SOLUTION**.

THERE SHOULD ONLY BE **ONE WAY TO SOLVE THE SAME PROBLEM**. ASSESS IF THE OTHER SOLUTION(S) ARE ACTUALLY NEEDED. IF NOT, **REMOVE THEM**. IF SO, CONSIDER IMPLEMENTING THE **ADAPTER DESIGN PATTERN** TO UNIFY THE INTERFACES.

**CREATE ONE AND ONLY ONE WAY TO SOLVE A PROBLEM**

LEARN MORE CLEAN CODE TIPS AT [PRAGMATICWAYS.COM](https://pragmaticways.com)

**{ PRAGMATIC WAYS }**  
TIPS FOR CLEANER CODE

## PRIMITIVE OBSESSION

ADDING PRIMITIVE VARIABLES IS LIKE SNEAKING CHOCOLATE ON A DIET, "**JUST ONE LITTLE PIECE WON'T HURT**." ONE AFTER THE OTHER, BEFORE YOU KNOW IT, YOU'VE BLOATED THE PROGRAM WITH A MESS OF **PRIMITIVE OBSESSION**.

INTRODUCE A **PARAMETER OBJECT** OR CREATE A **WHOLE OBJECT** TO CLEAN UP THE PRIMITIVE OBSESSION IN YOUR PROJECT.

**CREATE OBJECTS TO REPRESENT DATA**

LEARN MORE CLEAN CODE TIPS AT [PRAGMATICWAYS.COM](https://pragmaticways.com)

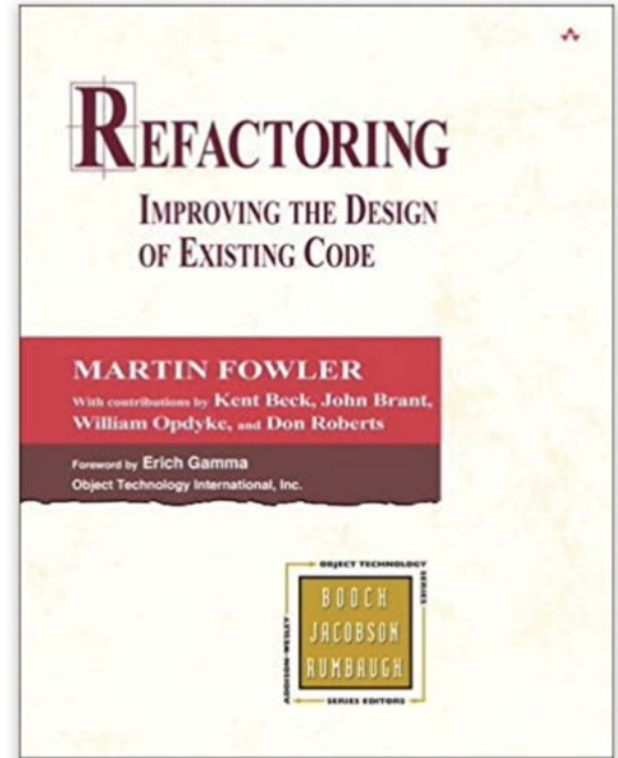
## 3 1/2 . Avoid “code smells” e.g. nested if’s

### don’t

```
function getSign(x) {
  result = NULL;
  if (x == 0)
    result = “zero”;
  else {
    if (x > 0)
      result = “positive”;
    else {
      if (x < 0)
        result = “negative”
      else
        result = “NaN”;
    }
  }
  return result;
}
```

### do

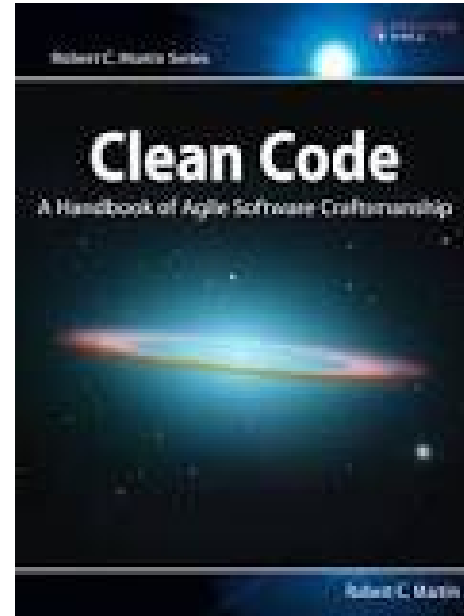
```
function getSign(x) {
  if (x == 0)
    return “zero”;
  if (x > 0)
    return “positive”;
  if (x == 0)
    return “negative”;
  return “Nan”;
}
```





## 4. Follow good coding principles

- Don't repeat yourself (DRY)
- Keep it simple (KISS)
- One level of abstraction
- Single responsibility principle
- Separation of concern
- Avoid premature optimization
- Follow style guidelines
- 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!

# 4. Follow good coding principles and style



Home

PUBLIC

Stack Overflow

Tags

Users

Jobs

Teams

Q&A for work



Learn More

## What is the "-->" operator in C++?

7883

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:

1831

```
#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>

# 4. Follow good coding principles and style



Home

PUBLIC

Stack Overflow

Tags

Users

Jobs

Teams

Q&A for work

Learn More

## What is the "-->" operator in C++?

7883 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:

**while (x-- > 0)**

1831

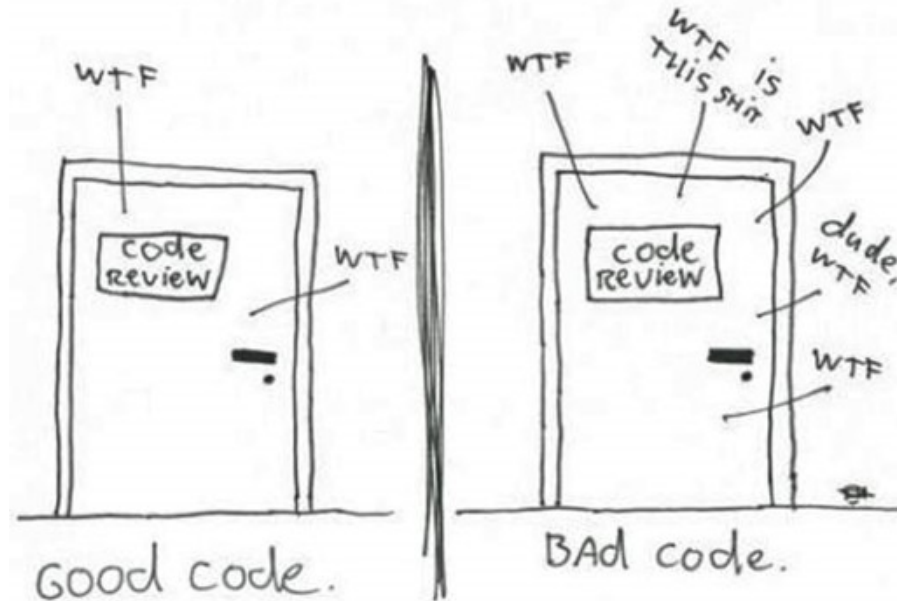
```
#include <stdio.h>
int main()
{
    int x = 10;
    while (x --> 0) // x goes to 0
    {
        printf("%d ", x);
    }
}
```

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>

## 4. Follow good coding principles and style

The ONLY VALID MEASUREMENT  
OF CODE QUALITY: WTFs/MINUTE



# 4. Follow good coding principles and style

The image displays three overlapping browser windows, each showing a different coding style guide:

- Top Window: Google C++ Style Guide**  
URL: <https://google-styleguide.googlecode.com/svn/trunk/cppguide.html>  
Title: 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 Variables](#), [Static and Global Variables](#)
  - Classes: [Doing Work in Constructors](#), [Initialization](#), [Explicit Constructors](#), [Copyable and Movable Type](#), [Delegating and Inheriting Constructors](#), [Structs vs. Classes](#), [Inheritance](#), [Multiple Inheritance](#), [Operator Overloading](#), [Access Control](#), [Declaration Order](#), [Write Short Functions](#)
- Middle Window: Linux kernel coding style**  
URL: <https://www.kernel.org/doc/Documentation/>  
Title: Linux kernel coding style  
Text:

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 been able to maintain, and I'd prefer it for most other things too. At least consider the points made here.

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

... goes:

Chapter 1: Indentation

... characters, and thus indentations are also 8 characters. ... sthetic movements that try to make indentations 4 ( ... ep, and that is akin to trying to define the val

... whole idea behind indentation is to clearly de ... control starts and ends. Especially when you've b ... h for 20 straight hours, you'll find it a lot ea ... cation works if you have large indentations.
- Bottom Window: PEP 0008 -- Style Guide for Python Code | Python.org**  
URL: <https://www.python.org/dev/peps/pep-0008/>  
Title: PEP 0008 -- Style Guide for Python Code  
Navigation: About, Downloads, Documentation, Community, Success Stories, News, Events  
Tweets: Python Software Foundation (@ThePSF) 3 Sep

## 4. Follow good coding principles : gracefully handle user errors

---

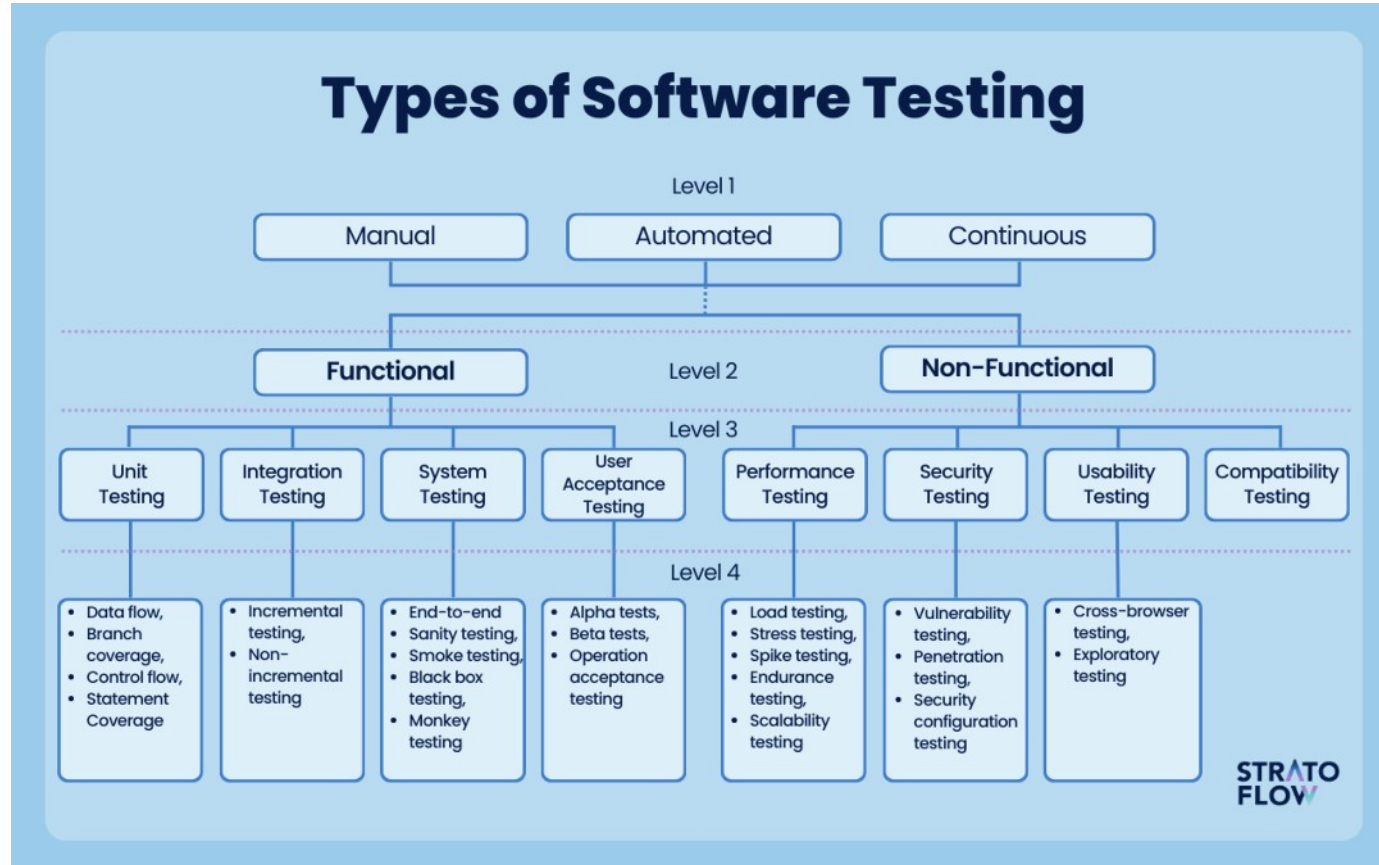
Use error handling techniques:

- ◆ Return codes
- ◆ Exceptions
- ◆ Callbacks
- ◆ “Result” structs

Be informative in the error messages.

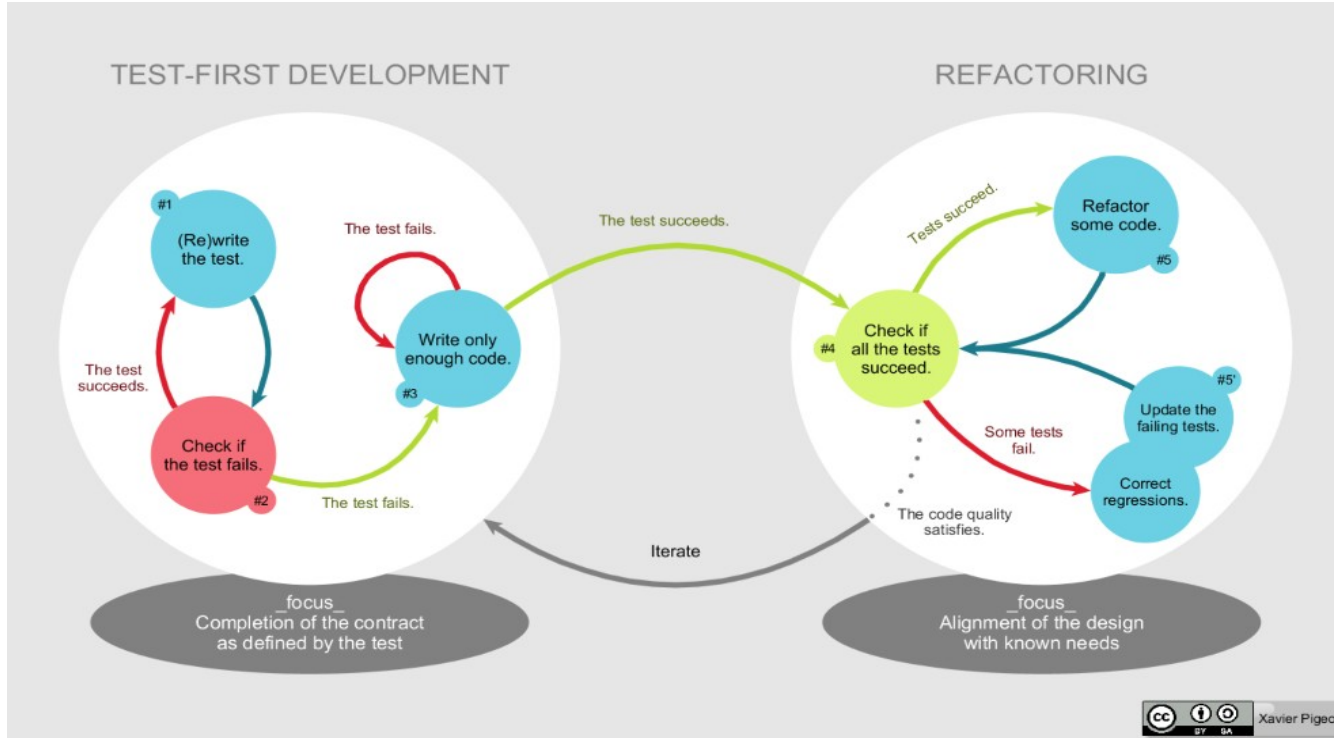
- ◆ “r no good” **vs** “Error: Input argument Rate (r) must be positive”
- ◆ Grade errors: “Warning”, “Error”, “Fatal”

# 5. Plan for mistakes, automate testing; Test-driven development



# 5. Plan for mistakes, automate testing; Test-driven development

Write the tests before you even write the code





# 6. Use modern source-code management system



# git

for your code, papers, thesis, etc.

2021

## Introduction to code versioning

by Dr Olivier Mattelaer (UCLouvain/CISM)

📅 Wednesday 27 Oct 2021, 09:00 → 12:00 Europe/Brussels

📍 comodal (louvain-la-neuve or remote)

### Description

Code versioning is very important to master, even for non programmers. It allows tracking the changes made to a submission script, a piece of code, a configuration file, or even a dataset and propagate the changes in a consistent and systematic way to all clusters.

### Contents:

- Notions of code versioning
- Working as a team with code versioning
- Using git to access code from others
- Publishing code

### Prerequisite:

- Being able to use SSH with private keys
- Being familiar with a text editor
- Mastering the Linux command line and the GNU utilities (mkdir, cp, scp, etc.)

**Type:** Hands-on

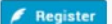
**Target audience:** Rookie programmer

**Must:** This session is a must-have for anyone not familiar with code versioning or git.

**Organized by** UCLouvain/CISM

**Registration**  Participants

 11 / 60

 Register

**Contact**  [egs-cism@listes.uclouvain.be](mailto:egs-cism@listes.uclouvain.be)  
 0494424767

## 7. Document the purpose and design, not the implementation

---



```
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
```

VS

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

## 7. Document the purpose and design, not the implementation



```
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
```

VS

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

# 7. Document the purpose and design, not the implementation

## Learn Markdown

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

Some code:

```
#!/bin/bash
```

**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
```

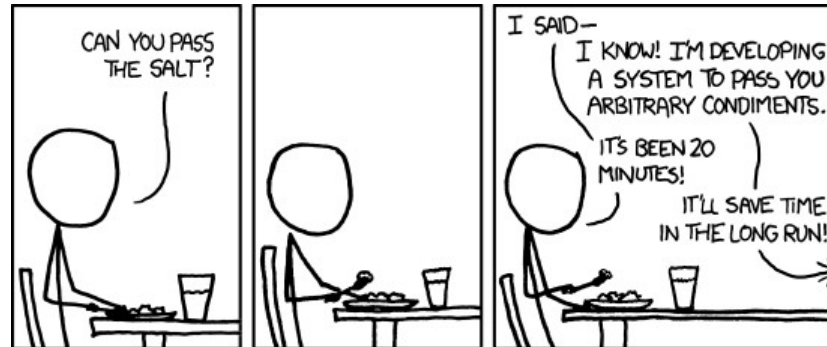
## 8. Optimize only when it works already

---

- ◆ Do not try to make it fast when it is not working yet

(focus on data structures, organization, etc. rather than on micro-optimizations)

- ◆ Do not try to make it universal for all possible future needs at the beginning “YAGNI” (do not close doors either)



# 8. Optimize only when it works already

Use a profiler

2021  
Debugging/profiling scientific code and scientific libraries

by Bernard Van Renterghem (UCL CISM)  
Wednesday 27 Oct 2021, 13:00 → 16:00 Europe/Brussels  
somodal (bouvain-la-baronne or remote)

Description  
When a piece of software does not work the way it is expected to, it needs debugging. Then, when it works, it needs profiling to remove the bottlenecks. This session will also present the standard optimized libraries that will allow you to code faster and more efficiently.

Contents

- Debugging principles
- The GDB debugger (gdb)
- The Intel debugger
- Advanced features of Intel Cluster studio
  - the support of MIC architecture (Devic Phi)
  - the Guided Auto Parallelism
  - the OpenMP support
- Intel MKL

Prerequisite

- Being able to use SSH with private keys
- Being familiar with a text editor
- Mastering the Linux command line and the GNU utilities (ls, cp, mv, etc.)
- Previous knowledge of either C, Fortran, Octave, Python or R
- Working knowledge of C or Fortran
- Familiarity with OpenMP and MPI

Type: Hands-on  
Target audience: Programmers  
Note: This session is important for programmers who want to optimize their code for usage on a cluster.

Organized by: UCLouvain/CISM  
Registration: Participants 1 / 100 Register

Contact: [cpu\\_comp@info.uclouvain.be](mailto:cpu_comp@info.uclouvain.be)  
[bern.vanrenterghem@uclouvain.be](mailto:bern.vanrenterghem@uclouvain.be)

Incorporate benchmarks in your tests

Intel VTune Amplifier 2019  
Hotspots by CPU Utilization

Analysis Configuration | Collection Log | Summary | Bottom-up | Caller/Callee | Top-down Tree | Platform | jacobi.c x | jacobi.c x

Source | Assembly

Source	Effective Time by Utilization			
	Idle	Poor	Ok	Excellent
82 while (k <= maxit && error > tol) {				
83				
84 error = 0.0;				
85 #pragma omp parallel	0.0%	39.9%	0.0%	0.0%
86 {				
87				
88 /* copy new solution into old */				
89 #pragma omp for private(i) // or collapse(2)				
90 for (j=0; j<m; j++){				
91 for (i=0; i<n; i++){	0.0%	2.1%	0.0%	0.0%
92 UOLD(j,i) = U(j,i);	0.0%	7.7%	0.0%	0.0%
93 }				
94				
95 /* compute stencil, residual and update */				
96 #pragma omp for private(i, resid) reduction(+:error) // or co				
97 for (j=1; j<m-1; j++){				
98 for (i=1; i<n-1; i++){	0.0%	0.8%	0.0%	0.0%
99 resid =(	0.0%	10.2%	0.0%	0.0%
100 ax * (UOLD(j,i-1) + UOLD(j,i+1))	0.0%	3.1%	0.0%	0.0%
101 + ay * (UOLD(j-1,i) + UOLD(j+1,i))	0.0%	3.8%	0.0%	0.0%
102 + b * UOLD(j,i) - F(j,i)	0.0%	2.3%	0.0%	0.0%
103 ) / b;	0.0%	0.0%	0.0%	0.0%
104				

# 9. Debug cleverly

## Use a debugger

2021

### Debugging/profiling scientific code and scientific libraries

by Bernard Van Renterghem (UCL CISM)

Wednesday 27 Oct 2021, 13:00 → 16:00 Europe/Brussels

isomodal (bouvain-la-neuve or remote)

**Description**

When a piece of software does not work the way it is expected to, it needs debugging. Then, when it works, it needs profiling to remove the bottlenecks. This session will also present the standard optimized libraries that will allow you to code faster and more efficiently.

**Contents**

- Debugging principles
- The GDB debugger (gdb)
- The Intel debugger
- Advanced features of Intel Cluster studio
  - the support of MIC architecture (Data PaaS)
  - the Guided Auto Parallelism
  - the OpenMP support
- Intel NPL

**Prerequisite**

- Being able to use SSH with private keys
- Being familiar with a text editor
- Mastering the Linux command line and the GNU utilities (ls, cp, mv, etc.)
- Possessing knowledge of either C, Fortran, Octave, Python or R
- Working knowledge of C or Fortran
- Familiarity with OpenMP and MPI

**Type: Hands-on**

**Target audience: Programmers**

**Note:** This session is important for programmers who want to optimize their code for usage on a cluster.

Organized by UCLouvain/CISM

Registration [Participants](#)

Contact [bernard.van.renterghem@uclouvain.be](mailto:bernard.van.renterghem@uclouvain.be)

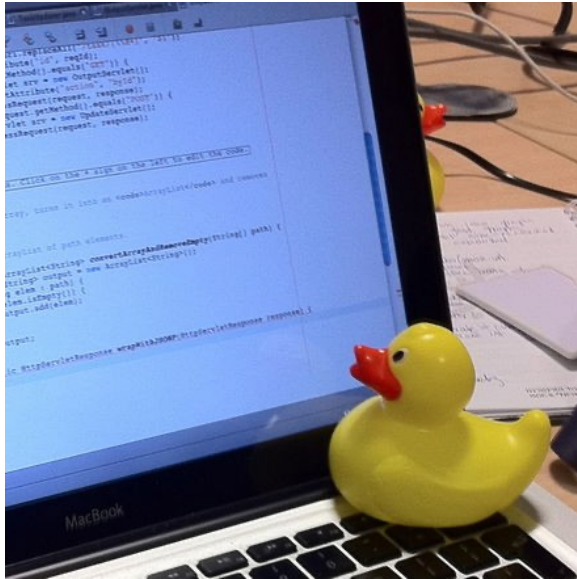
The screenshot shows the Remote Python Debugger (RPDB) interface. The top menu includes File, Breakpoints, Control, Window, and Help. The toolbar contains various icons for running, stepping, and debugging. The main window is divided into several panes:

- Namespace:** A tree view showing the current namespace. The 'main' function is expanded, showing attributes like \_\_class\_\_, \_\_doc\_\_, \_\_name\_\_, func\_closures, func\_code, func\_defaults, func\_dict, func\_globals, and func\_name.
- Source:** The source code of the file `/data/sys/bin/winpdb-1.3.6/winpdb.py`. The code includes a `main()` function that calls `rpdb2.get_version()` and `rpdb2._print`. A breakpoint is set at line 4637, which is highlighted in blue. The code also includes a `get_version()` function and a `if __name__ == '__main__':` block.
- Threads:** A table showing the current threads. The main thread is in a 'waiting at break point' state.
- Stack:** A table showing the current stack frames. The top frame is `winpdb.py` at line 4637, and the bottom frame is `rpdb2.py` at line 14044.
- Console:** The console output shows the RPDB version (RPDB-1.3.6) and copyright information. It also displays the startup sequence, including password generation and successful attachment to the debuggee.

At the bottom, the state is 'State: WAITING AT BREAK POINT'.

# 9. Debug cleverly

## Use a method



Describe out loud to an imaginary rubber duck (or a willing colleague) each line in your code in simple terms and why it is obviously correct.

At some point, if you get hesitant, that is probably where the bug is!

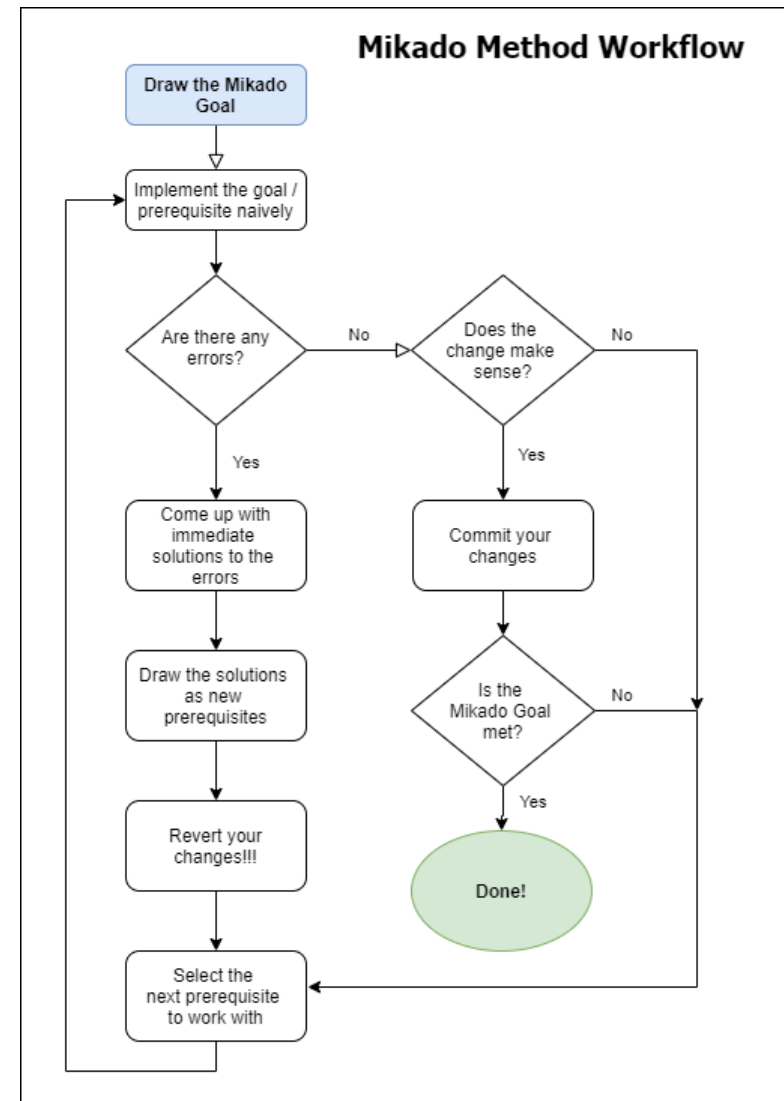
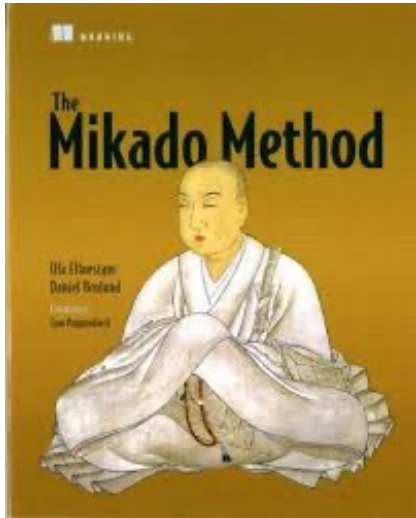
Dig that part of the code until you are confident again that it works.

Or discover that it does actually not work as expected ...



# 9. Debug cleverly

Use a method



“... to make them ... **shareable** ..., *efficiently*”

1. Automate the compiling process
2. Learn about containers
3. License your code

# 1. Automate the compiling process



About Resources Developer Resources Download



## 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

Article Talk

Read Edit View history

Search

## 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.

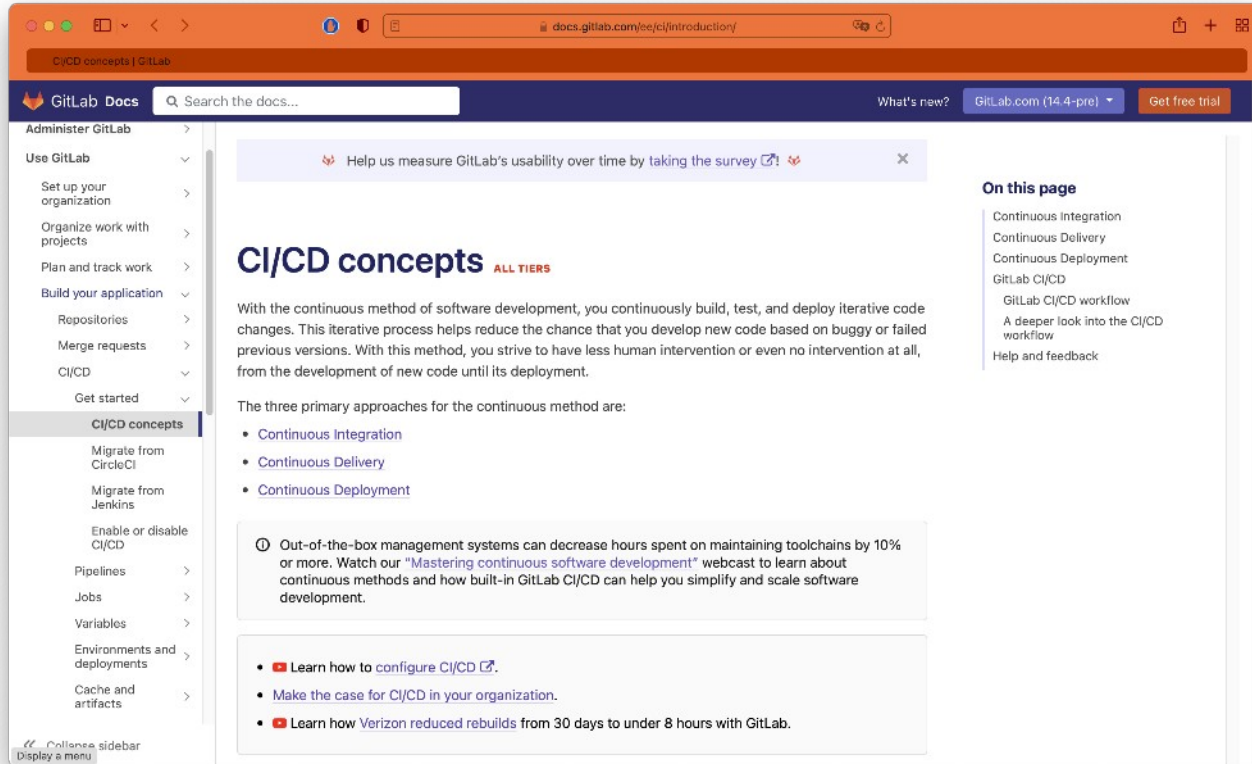
Autotools is part of the [GNU toolchain](#) and is widely used in many [free software](#) and [open source packages](#). Its component tools are [free software](#), licensed under the [GNU General](#)



Making sure it compiles on your laptop is not enough

It has to compile on all the clusters...

# 1. Automate the compiling process



The screenshot shows a web browser window displaying the GitLab Docs page for CI/CD concepts. The browser's address bar shows the URL `docs.gitlab.com/ee/ci/introduction/`. The page header includes the GitLab Docs logo, a search bar, and navigation links for "What's new?", "GitLab.com (14.4-pre)", and "Get free trial".

The left sidebar contains a navigation menu with the following items:

- Administer GitLab
- Use GitLab
  - Set up your organization
  - Organize work with projects
  - Plan and track work
  - Build your application
    - Repositories
    - Merge requests
    - CI/CD
    - Get started
- CI/CD concepts** (highlighted)
- Migrate from CircleCI
- Migrate from Jenkins
- Enable or disable CI/CD
- Pipelines
- Jobs
- Variables
- Environments and deployments
- Cache and artifacts

The main content area features a survey notification: "Help us measure GitLab's usability over time by taking the survey". Below this is the main heading "CI/CD concepts ALL TIERS".

The text explains: "With the continuous method of software development, you continuously build, test, and deploy iterative code changes. This iterative process helps reduce the chance that you develop new code based on buggy or failed previous versions. With this method, you strive to have less human intervention or even no intervention at all, from the development of new code until its deployment."

The text continues: "The three primary approaches for the continuous method are:"

- [Continuous Integration](#)
- [Continuous Delivery](#)
- [Continuous Deployment](#)

A callout box contains the text: "Out-of-the-box management systems can decrease hours spent on maintaining toolchains by 10% or more. Watch our 'Mastering continuous software development' webcast to learn about continuous methods and how built-in GitLab CI/CD can help you simplify and scale software development."

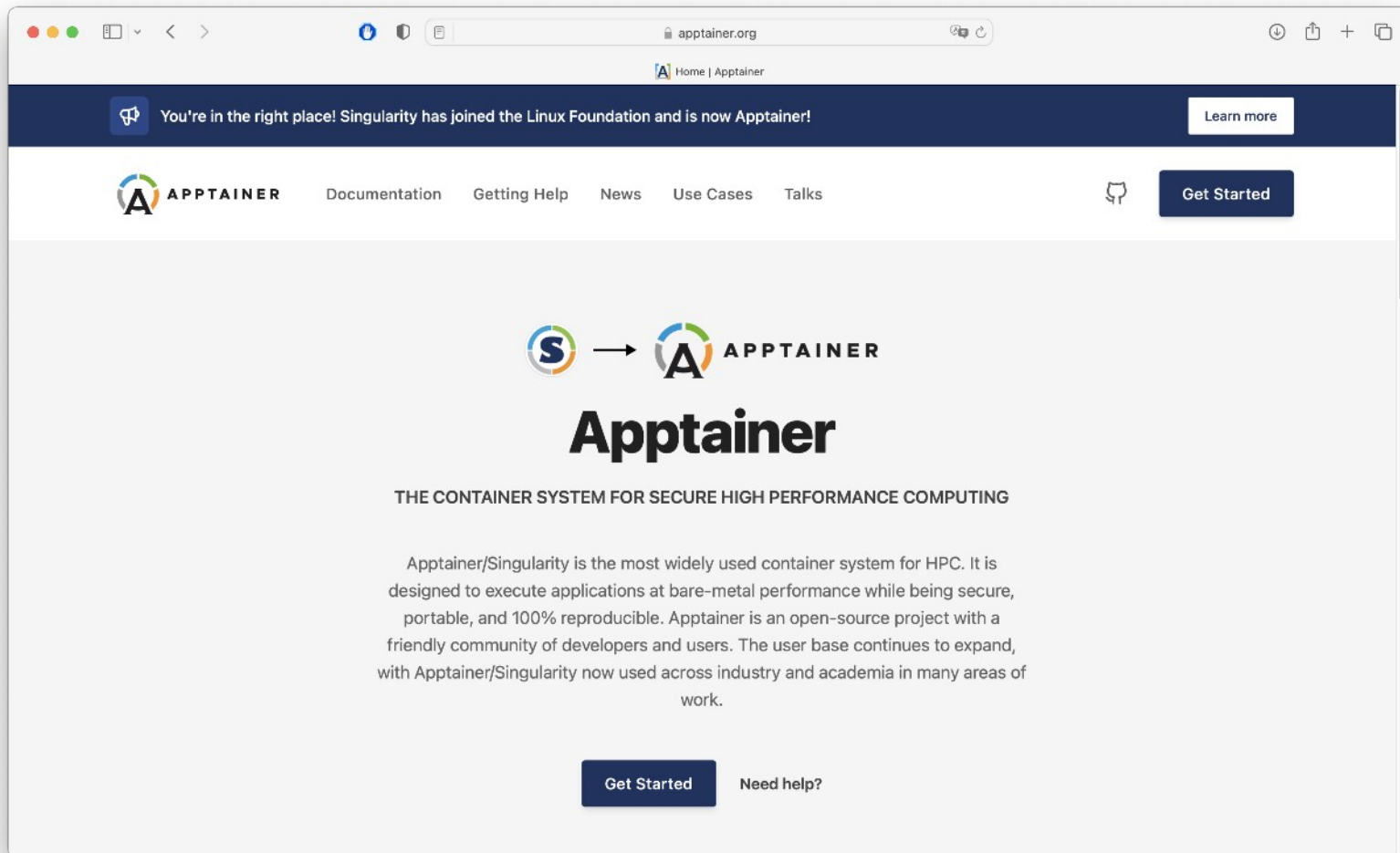
Below this, a list of links is provided:

- [Learn how to configure CI/CD](#)
- [Make the case for CI/CD in your organization](#)
- [Learn how Verizon reduced rebuilds from 30 days to under 8 hours with GitLab](#)

The right sidebar, titled "On this page", lists the following sections:

- Continuous Integration
- Continuous Delivery
- Continuous Deployment
- GitLab CI/CD
  - GitLab CI/CD workflow
  - A deeper look into the CI/CD workflow
  - Help and feedback

## 2. Learn about containers






The image shows a browser window displaying the Apptainer website. The browser's address bar shows 'apptainer.org'. The website has a dark blue header with a navigation menu and a 'Learn more' button. The main content area features the Apptainer logo, a transition from the Singularity logo, and the text 'Apptainer THE CONTAINER SYSTEM FOR SECURE HIGH PERFORMANCE COMPUTING'. Below this is a paragraph describing Apptainer/Singularity as a widely used container system for HPC. At the bottom, there are 'Get Started' and 'Need help?' buttons.

apptainer.org

Home | Apptainer

You're in the right place! Singularity has joined the Linux Foundation and is now Apptainer! [Learn more](#)

**APPTAINER** Documentation Getting Help News Use Cases Talks  [Get Started](#)

 →  **APPTAINER**

# Apptainer

THE CONTAINER SYSTEM FOR SECURE HIGH PERFORMANCE COMPUTING

Apptainer/Singularity is the most widely used container system for HPC. It is designed to execute applications at bare-metal performance while being secure, portable, and 100% reproducible. Apptainer is an open-source project with a friendly community of developers and users. The user base continues to expand, with Apptainer/Singularity now used across industry and academia in many areas of work.

[Get Started](#) [Need help?](#)

### 3. License your code: Why?

---

- ♦ **Commercial reason :**
  - you want to make money out of it – control 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






# 3. License your code: e.g. MIT

Copyright (c) <year> <copyright holders>

Permission is hereby granted, free of charge, to any person obtaining a copy of this software and associated documentation files (the "Software"), to deal in the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the Software, and to permit persons to whom the Software is furnished to do so, subject to the following conditions:

The above copyright notice and this permission notice shall be included in all copies or substantial portions of the Software.

THE SOFTWARE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE AND NONINFRINGEMENT. IN NO EVENT SHALL THE AUTHORS OR COPYRIGHT HOLDERS BE LIABLE FOR ANY CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.





Can	
▶ Commercial Use	
▶ Modify	
▶ Distribute	
▶ Sublicense	
▶ Private Use	

Cannot	
▶ Hold Liable	



Must	
▶ Include Copyright	
▶ Include License	

# 3. License your code: e.g. BSD, GPL

## BSD Can

- ▶ Commercial Use 
- ▶ Modify 
- ▶ Distribute 
- ▶ Place Warranty 






## Cannot

- ▶ Use Trademark 
- ▶ Hold Liable 

## Must

- ▶ Include Copyright 
- ▶ Include License 

## GPL Can

- ▶ Commercial Use 
- ▶ Modify 
- ▶ Distribute 
- ▶ Place Warranty 
- ▶ Use Patent Claims 

## Cannot

- ▶ Sublicense 
- ▶ Hold Liable 

## Must

- ▶ Include Original 
- ▶ State Changes 
- ▶ Disclose Source 
- ▶ Include License 
- ▶ Include Copyright 
- ▶ Include Install Instructions 



# 3. License your code: finding help



## LIEU – Network of Knowledge Transfer offices

Coordinator

UNIVERSITÉ CATHOLIQUE DE LOUVAIN  
TECHNOLOGY TRANSFER OFFICE (LTTO)

Sébastien ADAM

☎ +32 10 47 24 43

sebastien.adam@uclouvain.be



UNIVERSITÉ DE LIÈGE  
TECHNOLOGY TRANSFER OFFICE

Jérémie FAYS

☎ + 32 4 349 85 21

j.fays@uliege.be



UNIVERSITÉ LIBRE DE BRUXELLES  
TECHNOLOGY TRANSFER OFFICE (ULB-TTO)

Kévin DEPLUS

☎ +32 650 23 15

kevin.deplus@ulb.ac.be



UNIVERSITÉ DE NAMUR  
TECHNOLOGY TRANSFER OFFICE

Nathalie FABRY

☎ +32 81 72 53 36

nathalie.fabry@unamur.be



UNIVERSITÉ DE LIÈGE  
TECHNOLOGY TRANSFER OFFICE

Thi Tuyet Minh NGUYEN

☎ +32 349 85 10

ttn.nguyen@uliege.be



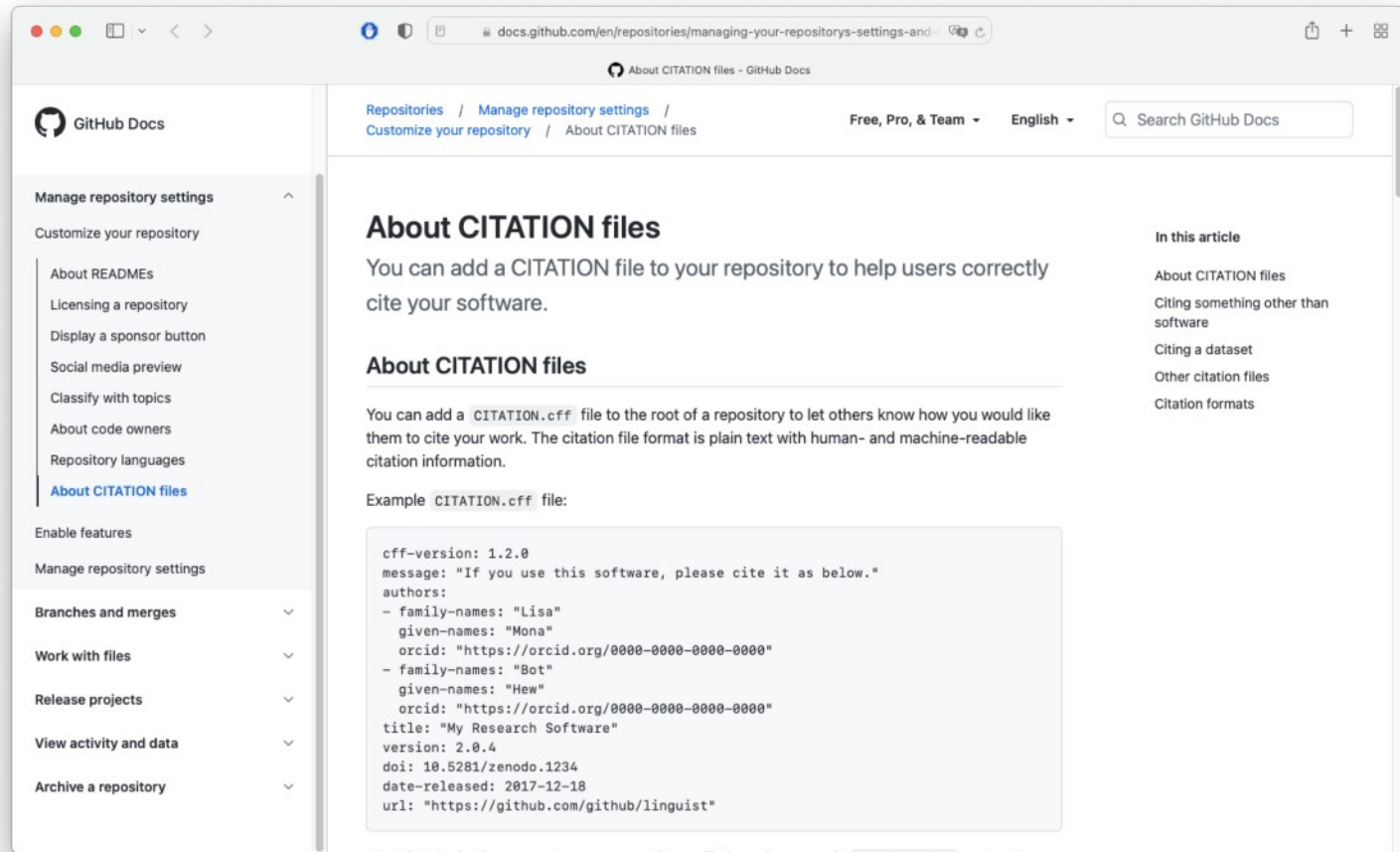
UNIVERSITÉ DE MONS  
TECHNOLOGY TRANSFER OFFICE

Sandrine BROGNAUX

☎ +32 65 37 47 97

sandrine.brognaux@umons.ac.be

# 3 1/2. GitHub CITATION files



The screenshot shows the GitHub Docs website. The browser address bar displays `docs.github.com/en/repositories/managing-your-repositorys-settings-and-features/customizing-your-repository/about-citation-files`. The page title is "About CITATION files - GitHub Docs". The breadcrumb navigation shows "Repositories / Manage repository settings / Customize your repository / About CITATION files". The left sidebar contains a navigation menu with "About CITATION files" selected. The main content area has a heading "About CITATION files" and a sub-heading "You can add a CITATION file to your repository to help users correctly cite your software." Below this, there is a section titled "About CITATION files" with a sub-heading "You can add a CITATION.cff file to the root of a repository to let others know how you would like them to cite your work. The citation file format is plain text with human- and machine-readable citation information." An example CITATION.cff file is provided in a code block:

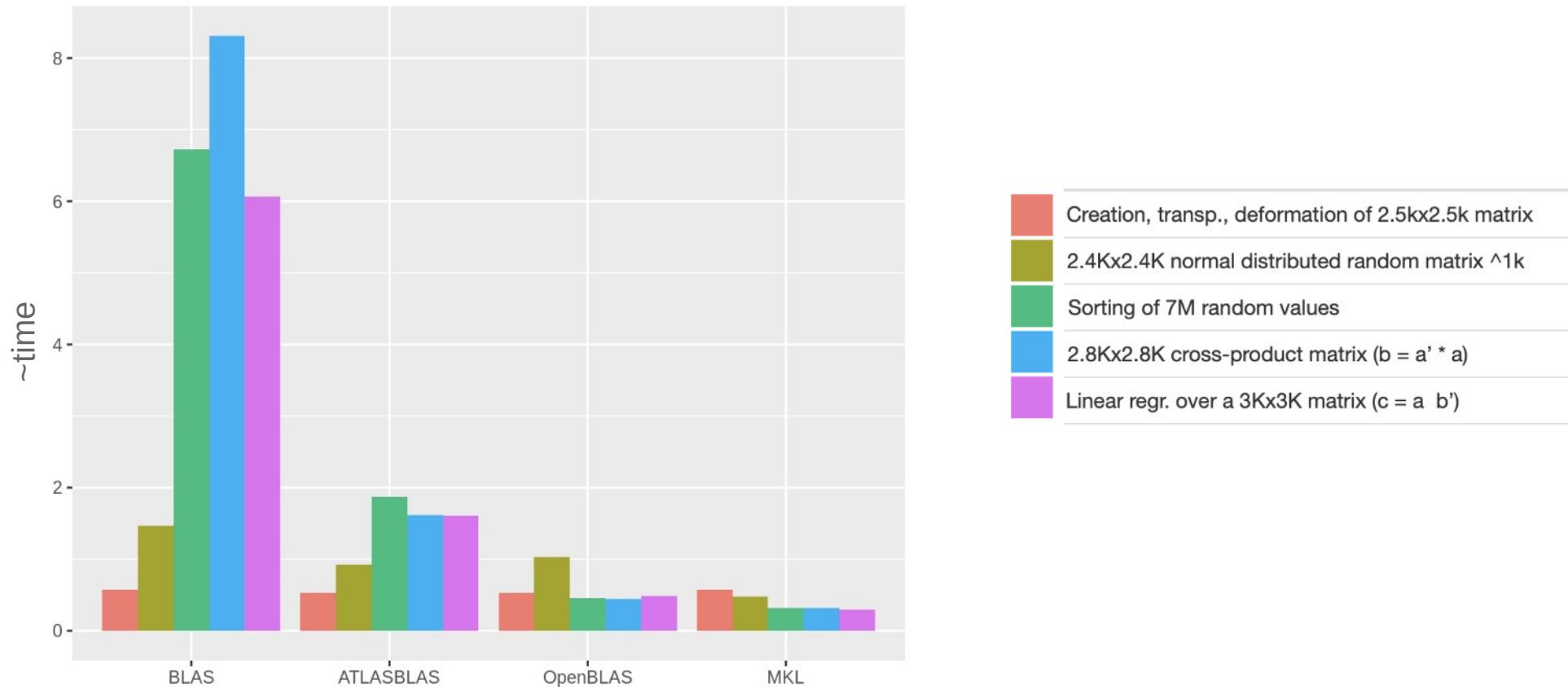
```
cff-version: 1.2.0
message: "If you use this software, please cite it as below."
authors:
  - family-names: "Lisa"
    given-names: "Mona"
    orcid: "https://orcid.org/0000-0000-0000-0000"
  - family-names: "Bot"
    given-names: "Hew"
    orcid: "https://orcid.org/0000-0000-0000-0000"
title: "My Research Software"
version: 2.0.4
doi: 10.5281/zenodo.1234
date-released: 2017-12-18
url: "https://github.com/github/linguist"
```

On the right side, there is a section titled "In this article" with a list of links: "About CITATION files", "Citing something other than software", "Citing a dataset", "Other citation files", and "Citation formats".

“... to make them ... **fast** ..., *efficiently*”

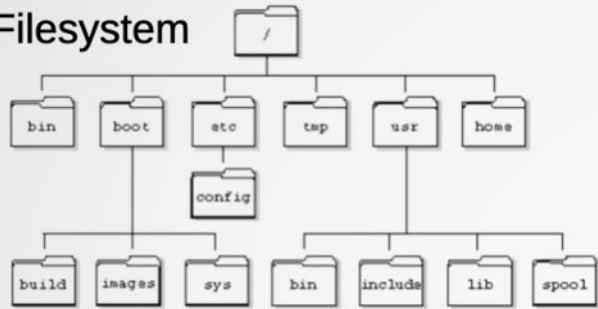
1. Use optimized libraries
2. Choose the right storage system
3. Think parallel from the start
4. Integrate checkpoint/restart from the start

# 1. Use optimized libraries

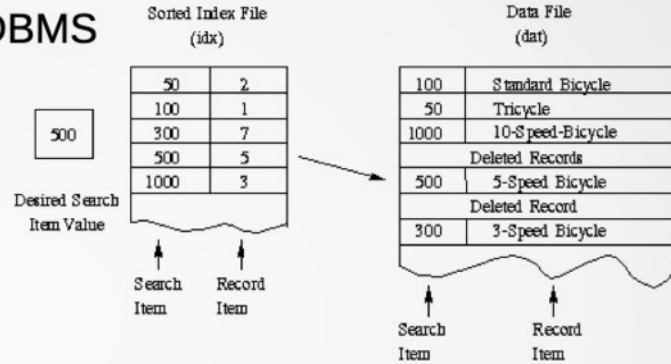


## 2. Choose the right storage system

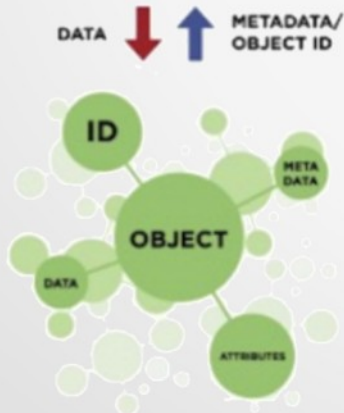
### Filesystem



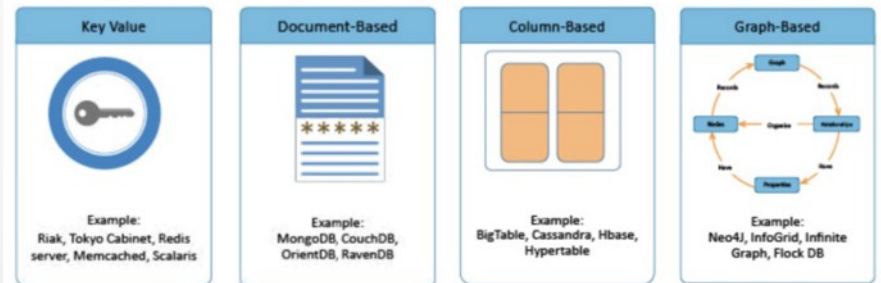
### RDBMS



### Objects store



### NoSQL



### 3. Think parallel from the start

---

1. Identify data flows and independent tasks
2. Make data decomposition easy
3. Make work decomposition easy

```
data = [(x1,y1), (x2,y2), .., (x10,y10)]
for i = 1 .. 10
  s[i] = ( data[xi] + data[yi] )
  ss[i] = ( data[xi]^2 + data[yi]^2 )
end
```






```
begin=0, end=10
data = [(x1,y1), (x2,y2), .., (x10,y10)]
for i = begin .. end
  s[i] = ( data[xi] + data[yi] )
end
for i = begin .. end
  ss[i] = ( data[xi]^2 + data[yi]^2 )
end
```

## 4. Integrate checkpoint/restart from the start

---

1. Allow starting from a non-initial state
2. Save variables to disk frequently

```
data = [(x1,y1), (x2,y2), .., (x10,y10)]
for i = 1 .. 10
    res[i] = ( data[xi]^2 + data[yi]^2 )
end
```



```
if exists(i) and exists(res)
    begin=load(i)
    res=load(res)
else
    begin = 1
end=10
data = [(x1,y1), (x2,y2), .., (x10,y10)]
for i = begin .. end
    res[i] = ( data[xi]^2 + data[yi]^2 )
    save(res, i)
end
```

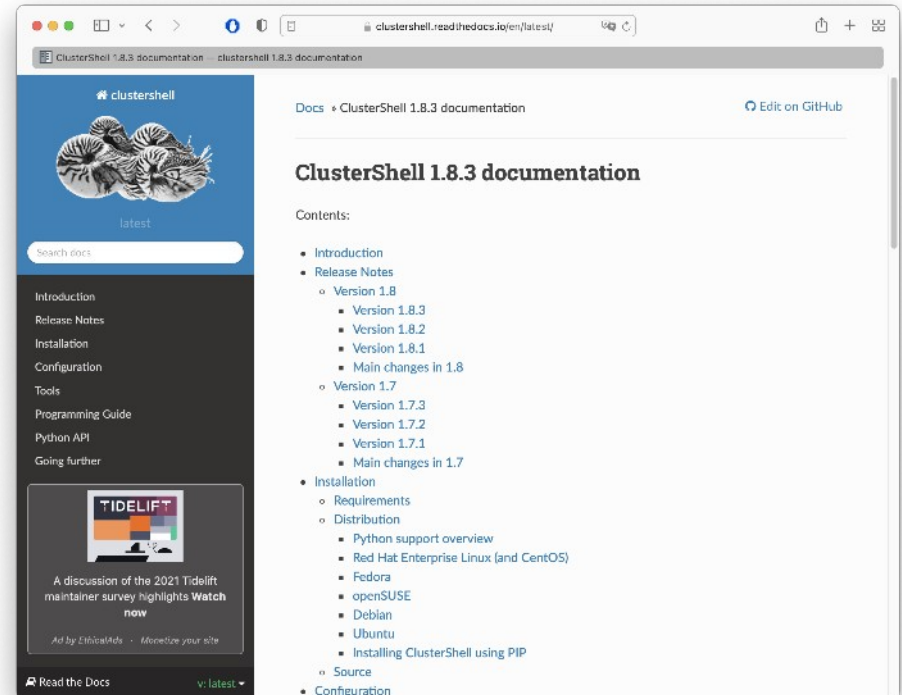
“ ..., *efficiently*”

1. Perform “multi-host” SSH
2. Master configuration management
3. Use terminal multiplexing
4. Install software like a boss
5. Avoid the boilerplate
6. BACKUPS!



# 1. Perform “multi-host” SSH

```
> clush -Bw lemaitre3,hercules,nic5,dragon2 "emacs --version"
-----
dragon2,hercules,lemaitre3 (3)
-----
GNU Emacs 24.3.1
Copyright (C) 2013 Free Software Foundation, Inc.
GNU Emacs comes with ABSOLUTELY NO WARRANTY.
You may redistribute copies of Emacs
under the terms of the GNU General Public License.
For more information about these matters, see the file named COPYING.
-----
nic5
-----
GNU Emacs 26.1
Copyright (C) 2018 Free Software Foundation, Inc.
GNU Emacs comes with ABSOLUTELY NO WARRANTY.
You may redistribute copies of GNU Emacs
under the terms of the GNU General Public License.
For more information about these matters, see the file named COPYING.
-----
> clush -Bw lemaitre3,hercules,nic5,dragon2 "scontrol version"
-----
dragon2,lemaitre3 (2)
-----
slurm 20.02.7
-----
hercules
-----
slurm 20.02.6
-----
nic5
-----
slurm 20.02.3
> clush -w lemaitre3,hercules,nic5,dragon2 "squeue -tPD | wc -l"
nic5: 1420
lemaitre3: 288
dragon2: 145
hercules: 102
>
```



The screenshot shows a web browser displaying the ClusterShell 1.8.3 documentation page. The page has a blue header with the ClusterShell logo and a search bar. The main content area is white with a dark sidebar on the left containing navigation links: Introduction, Release Notes, Installation, Configuration, Tools, Programming Guide, Python API, and Going further. The main content area displays the title "ClusterShell 1.8.3 documentation" and a "Contents:" section with a list of links: Introduction, Release Notes, Version 1.8 (with sub-links for 1.8.3, 1.8.2, 1.8.1, and Main changes in 1.8), Version 1.7 (with sub-links for 1.7.3, 1.7.2, 1.7.1, and Main changes in 1.7), Installation (with sub-links for Requirements, Distribution, Python support overview, Red Hat Enterprise Linux (and CentOS), Fedora, openSUSE, Debian, Ubuntu, and Installing ClusterShell using PIP), Source, and Configuration. At the bottom of the page, there is a "Read the Docs" logo and a "v: latest" dropdown menu.

## 2. Master configuration management

---



ANSIBLE

```
> ansible -i lemaitre3,nic5 'all' -m lineinfile -a "dest=myfile line='Contents' create=true"
nic5 | CHANGED => {
  "ansible_facts": {
    "discovered_interpreter_python": "/usr/libexec/platform-python"
  },
  "backup": "",
  "changed": true,
  "msg": "line added"
}
lemaitre3 | SUCCESS => {
  "ansible_facts": {
    "discovered_interpreter_python": "/usr/bin/python"
  },
  "backup": "",
  "changed": false,
  "msg": ""
}
```

## 2. Master configuration management



```
>> cat inventory playbook.yml myfile
```

	File: <b>inventory</b>
1	[all]
2	
3	lemaitre3 short_name="lm3"
4	nic5 short_name="nic5"

	File: <b>playbook.yml</b>
1	---
2	- hosts:
3	- lemaitre3
4	- nic5
5	tasks:
6	- name: Upload templated file
7	template: src=myfile dest=. mode=700

	File: <b>myfile</b>
1	This cluster's short name is {{ short_name }}

## 2. Master configuration management



```
> ansible-playbook -i inventory playbook.yml --diff

PLAY [lemaitre3,nic5] *****

TASK [Gathering Facts] *****
ok: [nic5]
ok: [lemaitre3]

TASK [Upload templated file] *****
--- before: ./myfile
+++ after: /Users/dfrancois/.ansible/tmp/ansible-local-40594k4ng0q9q/tmpd689k7ap/myfile
@@ -1 +1 @@
-Contents
+This cluster's short name is nic5

changed: [nic5]
--- before: ./myfile
+++ after: /Users/dfrancois/.ansible/tmp/ansible-local-40594k4ng0q9q/tmpa5narr9m/myfile
@@ -1 +1 @@
-Contents
+This cluster's short name is lm3

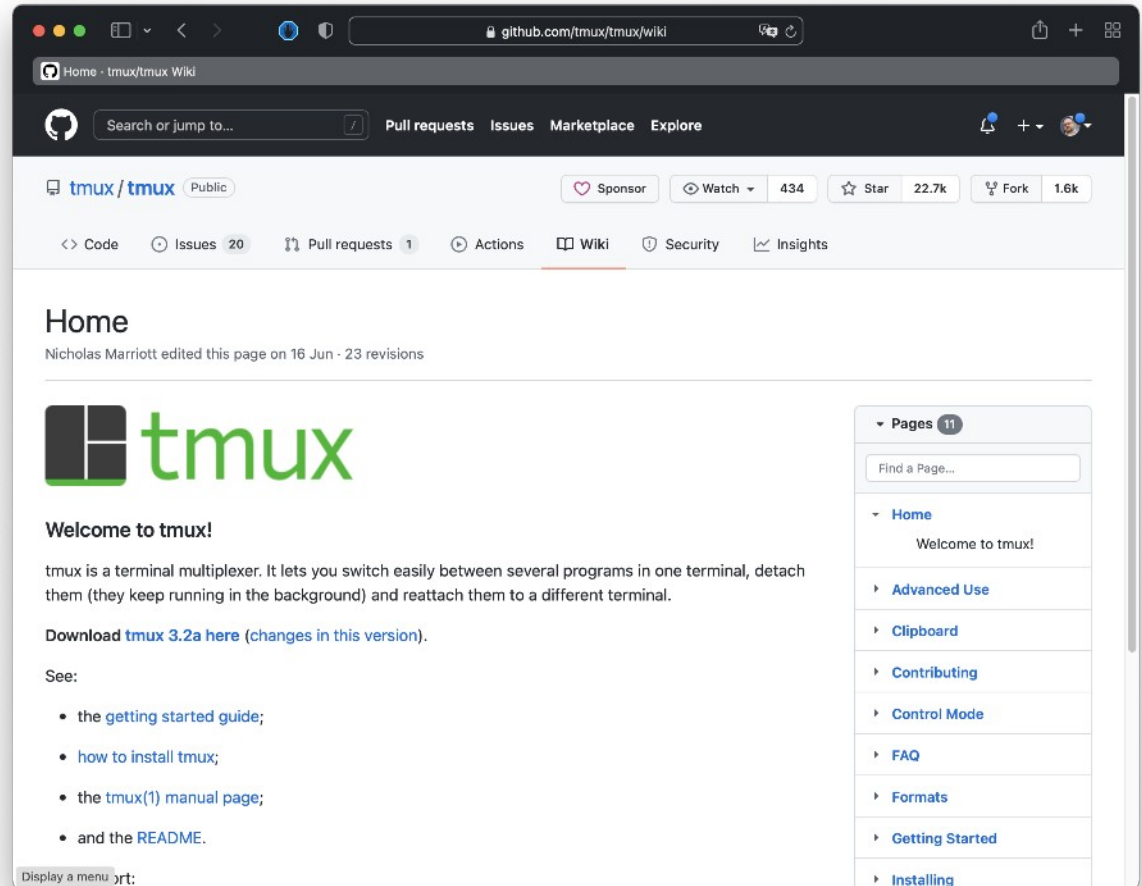
changed: [lemaitre3]

PLAY RECAP *****
lemaitre3      : ok=2    changed=1    unreachable=0    failed=0    skipped=0    rescued=0    ignored=0
nic5          : ok=2    changed=1    unreachable=0    failed=0    skipped=0    rescued=0    ignored=0

> clush -w lemaitre3,nic5 "cat myfile"
nic5: This cluster's short name is nic5
lemaitre3: This cluster's short name is lm3
```

# 3. Use terminal multiplexing

Do not let SSH disconnections harm your workflow (and much more)



# 4. Install software like a boss

```
[dfr@lemaitre3 ~]$ eb --search emacs
== found valid index for /usr/easybuild/easyconfigs, so using it...
== found valid index for /usr/easybuild/easyconfigs, so using it...
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-24.3-GCC-4.8.3-bare.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-24.3-GCC-4.8.3.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-24.4-GCC-4.9.2.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-24.5-GCC-4.9.3-2.25.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-25.1-foss-2016a.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-25.3-GCCcore-6.3.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-25.3-GCCcore-6.4.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-25.3-GCCcore-7.3.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-26.3-GCCcore-8.3.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-27.1-GCCcore-9.3.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-27.1-GCCcore-10.2.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-24.3-GCC-4.8.3-bare.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-24.3-GCC-4.8.3.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-24.4-GCC-4.9.2.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-24.5-GCC-4.9.3-2.25.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-25.1-foss-2016a.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-25.3-GCCcore-6.3.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-25.3-GCCcore-6.4.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-25.3-GCCcore-7.3.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-26.3-GCCcore-8.3.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-27.1-GCCcore-9.3.0.eb
* /usr/easybuild/easyconfigs/e/Emacs/Emacs-27.1-GCCcore-10.2.0.eb
```



EasyBuild @PyPi    EasyBuild docs    EasyBuild @GitHub

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](http://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.

# 4. Install software like a boss (module tips)

Setup your \$PS1 as [\u@h W] (\${LOADEDMODULES##\*:}) \\$ to see latest loaded module

Use direnv to automatically load modules based on the current working directory

Create module collections with module save

Write and use your own modules with module use PATH

```
help([[Setup env so that Slurm commands  
operate on Debug partition]])
```

```
local partition='debug'
```

```
setenv("SQUEUE_PARTITION", partition)  
setenv("SINFO_PARTITION", partition)  
setenv("SBATCH_PARTITION", partition)  
setenv("SRUN_PARTITION", partition)
```

A terminal window showing the execution of several commands related to module management and environment setup. The commands include: `echo $PS1`, `find project_1/`, `cd project_1`, `module save`, `module use PATH`, and `ml`. The output shows the current loaded modules and the environment variables set by the `ml` command.

```
[dfr@lemaitre3 ~] (releases/2021b) echo $PS1
[\u@lemaitre3 W] (${LOADEDMODULES##*:}) \$
[dfr@lemaitre3 ~] (releases/2021b) find project_1/
project_1/
project_1/program.py
project_1/.envrc
[dfr@lemaitre3 ~] (releases/2021b) cd project_1
direnv: loading /home/users/dfr/dfr/project_1/.envrc
direnv: export +CMAKE_LIBRARY_PATH +CMAKE_PREFIX_PATH +CPATH +EBDEVELBINUTILS +EBDEVELBZIP2 +EBDEVELGCCCORE +EBDEVELGMP +EBDEVELLIBFFI +EBDEV
VELLIBREADLINE +EBDEVELNCURSES +EBDEVLOPENSSL +EBDEVLPYTHON +EBDEVELSQLITE +EBDEVETCL +EBDEVEXLZ +EBDEVELZLIB +EBEXTSLISTPYTHON +EBROOTBI
NUTILS +EBROOTBZIP2 +EBROOTGCCCORE +EBROOTGMP +EBROOTLIBFFI +EBROOTLIBREADLINE +EBROOTNCURSES +EBROOTOPENSSL +EBROOTPYTHON +EBROOTSQLITE +EB
ROOTTCL +EBROOTXZ +EBROOTZLIB +EBVERSIONBINUTILS +EBVERSIONBZIP2 +EBVERSIONGCCCORE +EBVERSIONGMP +EBVERSIONLIBFFI +EBVERSIONLIBREADLINE +EBV
ERSIONNCURSES +EBVERSIONOPENSSL +EBVERSIONPYTHON +EBVERSIONSQLITE +EBVERSIONTCL +EBVERSIONXZ +EBVERSIONZLIB +LD_LIBRARY_PATH +LIBRARY_PATH +
PKG_CONFIG_PATH +PYTHONPATH +XDG_DATA_DIRS +_ModuleTable006 +_ModuleTable007 +_ModuleTable008 +_ModuleTable009 +_ModuleTable010 +_Modul
eTable011 +_ModuleTable012 +_ModuleTable013 +_ModuleTable014 +_ModuleTable015 +_LMOD_REF_COUNT_CMAKE_LIBRARY_PATH +_LMOD_REF_COUNT_CM
AKE_PREFIX_PATH +_LMOD_REF_COUNT_CPATH +_LMOD_REF_COUNT_LD_LIBRARY_PATH +_LMOD_REF_COUNT_LIBRARY_PATH +_LMOD_REF_COUNT_MANPATH +_LMOD_R
EF_COUNT_PATH +_LMOD_REF_COUNT_PKG_CONFIG_PATH +_LMOD_REF_COUNT_PYTHONPATH +_LMOD_REF_COUNT_XDG_DATA_DIRS +LOADEDMODULES +MANPATH +PATH +
_LMFILES +_ModuleTable001 +_ModuleTable002 +_ModuleTable003 +_ModuleTable004 +_ModuleTable005 +_ModuleTableSz_
[dfr@lemaitre3 project_1] (Python/3.9.6-GCCcore-11.2.0) $ ml

Currently Loaded Modules:
 1) tis/2018.01 (S) 5) zlib/1.2.11-GCCcore-11.2.0 9) libreadline/8.1-GCCcore-11.2.0 13) GMP/6.2.1-GCCcore-11.2.0
 2) StdEnv (H) 6) binutils/2.37-GCCcore-11.2.0 10) Tcl/8.6.11-GCCcore-11.2.0 14) libffi/3.4.2-GCCcore-11.2.0
 3) releases/2021b (S) 7) bzip2/1.0.8-GCCcore-11.2.0 11) SQLite/3.36-GCCcore-11.2.0 15) openssl/1.1
 4) GCCcore/11.2.0 8) ncurses/6.2-GCCcore-11.2.0 12) XZ/5.2.5-GCCcore-11.2.0 16) Python/3.9.6-GCCcore-11.2.0

Where:
S: Module is Sticky, requires --force to unload or purge
H: Hidden Module
[dfr@lemaitre3 project_1] (Python/3.9.6-GCCcore-11.2.0) $ cd ..
direnv: unloading
[dfr@lemaitre3 ~] (releases/2021b) $ ml

Currently Loaded Modules:
 1) tis/2018.01 (S) 2) StdEnv (H) 3) releases/2021b (S)

Where:
S: Module is Sticky, requires --force to unload or purge
H: Hidden Module
[dfr@lemaitre3 ~] (releases/2021b) $
```

# 5. Avoid the boilerplate



```
1 {
2   "project_name": "project_name",
3   "repo_name": "{ cookiecutter.project_name.lower().replace(' ', '_') }",
4   "author_name": "Your name (or your organization/company/team)",
5   "description": "A short description of the project.",
6   "open_source_license": ["MIT", "BSD-3-Clause", "No license file"],
7   "s3_bucket": "[OPTIONAL] your-bucket-for-syncing-data (do not include 's3://')",
8   "aws_profile": "default",
9   "python_interpreter": ["python3", "python"]
10 }
```



```
— LICENSE
— Makefile
— README.md
— data
  — external
  — interim
  — processed
  — raw
— docs
— models
— notebooks
— references
— reports
  — figures
— requirements.txt
— setup.py
— src
  — __init__.py
  — data
    — make_dataset.py
  — features
    — build_features.py
  — models
    — predict_model.py
    — train_model.py
  — visualization
    — visualize.py
— tox.ini
```

<- Makefile with commands like `make data` or `make train`  
<- The top-level README for developers using this project.  
<- Data from third party sources.  
<- Intermediate data that has been transformed.  
<- The final, canonical data sets for modeling.  
<- The original, immutable data dump.  
<- A default Sphinx project; see sphinx-doc.org for details  
<- Trained and serialized models, model predictions, or model summaries  
<- Jupyter notebooks. Naming convention is a number (for ordering), the creator's initials, and a short '-' delimited description, e.g. `1.0-jqp-initial-data-exploration`.  
<- Data dictionaries, manuals, and all other explanatory materials.  
<- Generated analysis as HTML, PDF, LaTeX, etc.  
<- Generated graphics and figures to be used in reporting  
<- The requirements file for reproducing the analysis environment, e.g. generated with `pip freeze > requirements.txt`  
<- makes project pip installable (pip install -e .) so src can be imported  
<- Source code for use in this project.  
<- Makes src a Python module  
<- Scripts to download or generate data  
<- Scripts to turn raw data into features for modeling  
<- Scripts to train models and then use trained models to make predictions  
<- Scripts to create exploratory and results oriented visualizations  
<- tox file with settings for running tox; see tox.readthedocs.io

<https://cookiecutter.readthedocs.io/en/stable/>

<https://github.com/search?q=cookiecutter&type=Repositories>



## 6. BACKUPS!!!

---

# 3-2-1 Backup Rule



X3

Maintain at least 3  
copies of your data



X2

Keep 2 copies stored  
at separate locations



X1

Store at least 1 copy  
at an off-site location

## 6. BACKUPS!!!

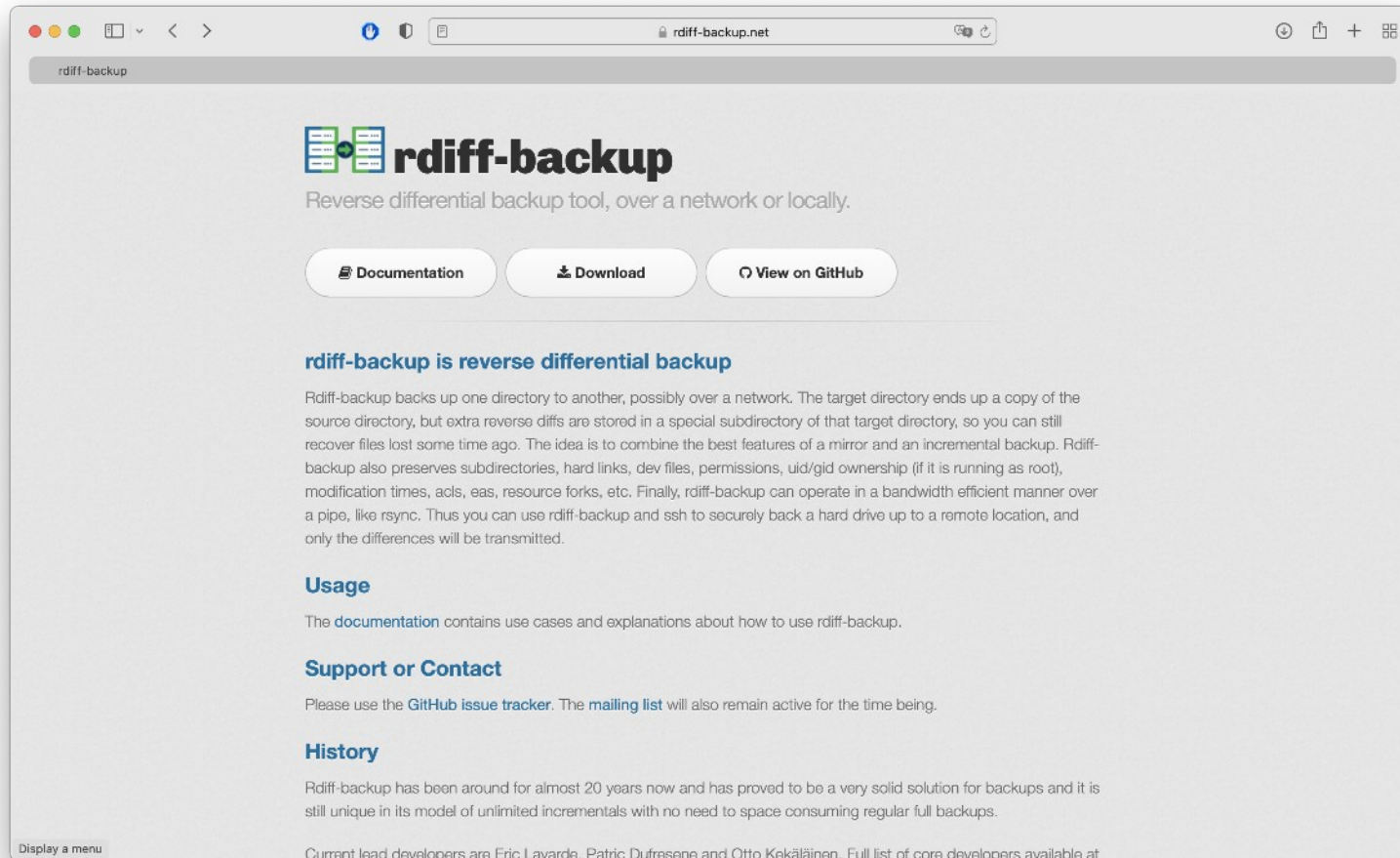
---

### **Schrodinger's Backup**

“The condition of any backup is unknown until a restore is attempted.”

@nixcraft

# 6. BACKUPS!!!



The screenshot shows the homepage of the rdiff-backup project. At the top, there is a navigation bar with the project name 'rdiff-backup'. Below this, the project logo is displayed, followed by the tagline 'Reverse differential backup tool, over a network or locally.' Three buttons are visible: 'Documentation', 'Download', and 'View on GitHub'. The main content area features a section titled 'rdiff-backup is reverse differential backup' with a detailed paragraph explaining the tool's capabilities. Below this, there are sections for 'Usage', 'Support or Contact', and 'History', each with a brief introductory sentence.

rdiff-backup

## rdiff-backup

Reverse differential backup tool, over a network or locally.

[Documentation](#) [Download](#) [View on GitHub](#)

### rdiff-backup is reverse differential backup

Rdiff-backup backs up one directory to another, possibly over a network. The target directory ends up a copy of the source directory, but extra reverse diffs are stored in a special subdirectory of that target directory, so you can still recover files lost some time ago. The idea is to combine the best features of a mirror and an incremental backup. Rdiff-backup also preserves subdirectories, hard links, dev files, permissions, uid/gid ownership (if it is running as root), modification times, acls, eas, resource forks, etc. Finally, rdiff-backup can operate in a bandwidth efficient manner over a pipe, like rsync. Thus you can use rdiff-backup and ssh to securely back a hard drive up to a remote location, and only the differences will be transmitted.

### Usage

The [documentation](#) contains use cases and explanations about how to use rdiff-backup.

### Support or Contact

Please use the [GitHub issue tracker](#). The [mailing list](#) will also remain active for the time being.

### History

Rdiff-backup has been around for almost 20 years now and has proved to be a very solid solution for backups and it is still unique in its model of unlimited incrementals with no need to space consuming regular full backups.

Current lead developers are Eric Lavarde, Patric Dufresene and Otto Kekäläinen. Full list of core developers available at

# This was:

“A short catalog of *tools*  
the professionals are using for  
**developing** and **deploying** programs,  
to make them **correct**, **maintainable**, **shareable**, and **fast**,  
*efficiently.*”

# We discussed:

- ◆ good practices
- ◆ important choices
- ◆ useful tools
- ◆ practical references

# The “Phillip test” (by Philip Guo)

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?

# Work faster & more reliably

**PERIODIC TABLE OF DEVOPS TOOLS (V1)** Xebialabs  
Deliver Faster

Os: Open Source	Database	SCM	Build
Fr: Free	CI	Repo Mgmt	Testing
Fm: Freemium	Deployment	Config / Provisioning	Containerization
Pd: Paid	Cloud / IaaS / PaaS	Release Mgmt	Collaboration
En: Enterprise	BI / Monitoring	Logging	Security

1 En															2 Fm				
O 12c															Aws Amazon Web Services				
3 Os	4 Os													5 En	6 En	7 Os	8 En	9 Os	10 Pd
My MySQL	Gt Git													Ch Chef	Pu Puppet	An Ansible	Sl Salt	Dk Docker	Az Azure
11 En	12 Os													13 Fr	14 En	15 Os	16 Fr	17 Os	18 Fm
Mq MySQL	Sv Subversion													Ssh SSH	Bl BladeLogic	Va Vagrant	Tf Terraform	Rk rkt	Hk Heroku
19 Os	20 Fm	21 Os	22 Os	23 En	24 Os	25 Pd	26 Os	27 Fr	28 Os	29 Fr	30 Os	31 Pd	32 Os	33 Fr	34 Os	35 Os	36 En		
Pq PostgreSQL	Gh Github	Mv Maven	Gr Gradle	Mr Meister	Jn Jenkins	Ba Bamboo	Tr Travis CI	Ar Archiva	Fn FitNesse	Se Selenium	Gn Gatling	Gd Deployment Manager	Sf SmartFrog	Cb Cobbler	Bc Bcf2	Kb Kubernetes	Rs Rackspace		
37 Os	38 Fm	39 Os	40 Os	41 Fm	42 Fm	43 Fm	44 Fm	45 Os	46 Fr	47 Os	48 Fr	49 Fr	50 Fr	51 Os	52 Os	53 Fr	54 Fm		
Mg MongoDB	Bb Bitbucket	Br Buildr	At ANT	Bm BuildMaster	Cs Codeship	Sn Snap CI	Cr CircleCI	Nx Nexus	Cu Cucumber	Cj Cucumber.js	Qu Qunit	Cp Capistrano	Ju Juju	Rd Rundeck	Cf CFEngine	Pk Packer	Bx Bluemix		
55 En	56 Os	57 Fm	58 En	59 Pd	60 Fm	61 Fm	62 Os	63 Os	64 Fr	65 Fr	66 Fr	67 En	68 Fm	69 En	70 Os	71 En	72 En		
Db DB2	Hg Mercurial	Qb QuickBuild	Ub UrbanCode Build	Ta Visual Build	Tc TeamCity	Sh Shippable	Cc CruiseControl	Ay Artifactory	Jt JUnit	Jm JMeter	Tn TestNG	Ry RapidDeploy	Cy CodeDeploy	Oc Octopus Deploy	No CA Nolio	Eb ElasticBox	Ad Apprenda		
73 Fr	74 En	75 Os	76 Os	77 Os	78 Os	79 Fm	80 Os	81 Os	82 Os	83 En	84 En	85 Os	86 En	87 En	88 En	89 Os	90 Os		
Cs Cassandra	Hx Helix	Msb MSBuild	Rk Rake	Lb LunrBuild	Co Continuum	Ca Continus CI	Gu Gump	Ng NuGet	Ap Appium	Xltv XL TestView	Tc TestComplete	Go Go	Ef ElectricFlow	Xld XL Deploy	Ud UrbanCode Deploy	Mo Mesos	Cf Cloud Foundry		

Share

Embed

Become Excellent!

Subscribe here!

91 En	92 En	93 En	94 En	95 En	96 Pd	97 En	98 En	99 Fm	100 Pd	101 Fm	102 Fm	103 Fm	104 Pd	105 En
Xlr XL Release	Ur UrbanCode Release	Ls CA Service Virtualization	Bm BMC Release Process	Hp HP Codar	Ex Excel	Pl Plutora Release	Sr Serena Release	Tr Trello	Jr Jira	Rf HipChat	Sl Slack	Fd Flowdock	Pv Pivotal Tracker	Sn ServiceNow
106 Os	107 Fm	108 Os	109 Os	110 Os	111 Os	112 Os	113 En	114 Fm	115 Os	116 Fm	117 Os	118 Os	119 Os	120 En
Ki Kibana	Nr New Relic	Ni Nagios	Gg Ganglia	Ct Cacti	Gr Graphite	lc Icinga	Sp Splunk	Sl Sumo Logic	Ls Logstash	Lg Loggly	Gr Graylog	Sn Snort	Tr Tripwire	Cy CyberArk