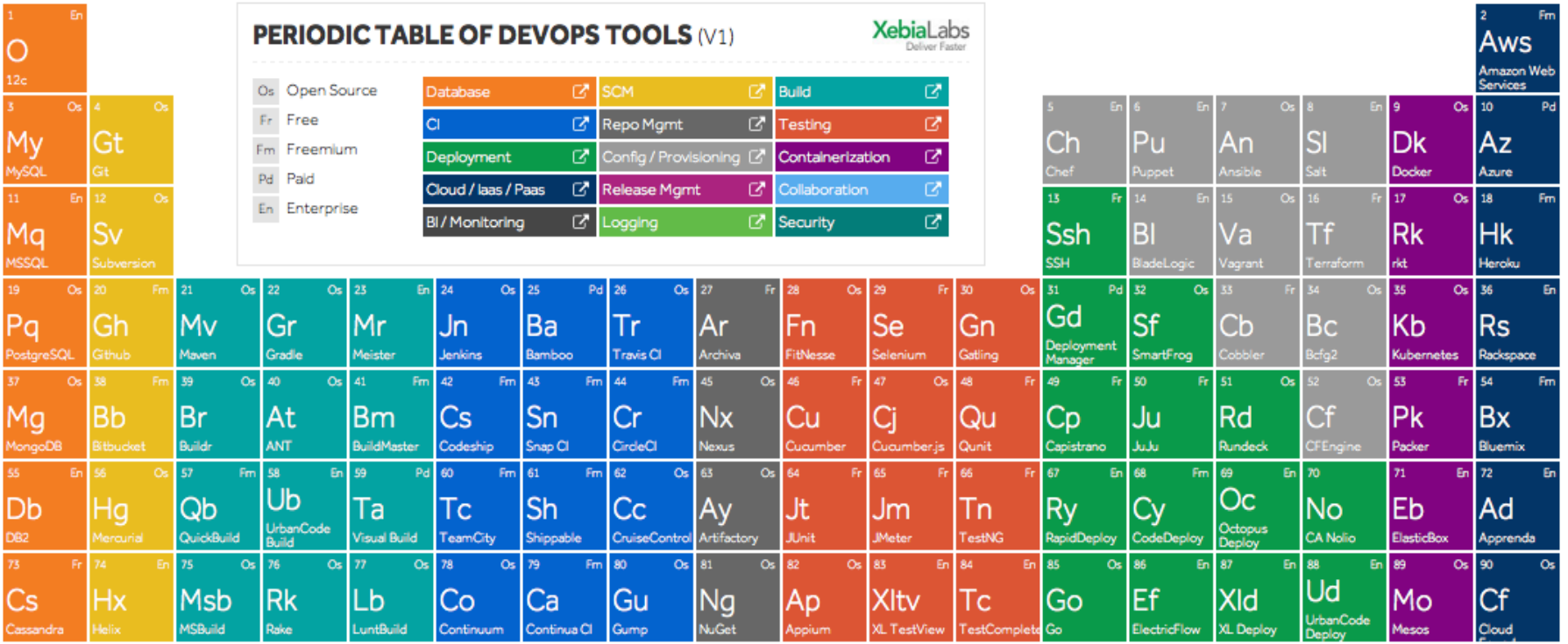
Introduction to Scientific Software Deployment and Development

damien.francois@uclouvain.be
November 2023

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



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

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."

Robert C. Martin *Clean code A Handbook of Agile Software Craftsmanship,* 2009

1. Write for humans, not for computers

Structure clear but goal not obvious

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

vs

Sweet spot in-between...

Goal clear but structure less obvious

```
PIXEL_NORMALIZATION_FACTOR = 12.5
PIXEL_OFFSET_FACTOR = 150

for row_index in range(row_count):
    for column_index in range(column_count):
        for color_channel_index in range(color_channel_count):
            normalized_pixel_value = (
                original_pixel_array[row_index][column_index][color_channel_index]
                * PIXEL_NORMALIZATION_FACTOR
            )
            transformed_pixel_array[row_index][column_index][color_channel_index] = (
                normalized_pixel_value + PIXEL_OFFSET_FACTOR
            )
```

https://towardsdatascience.com/data-scientists-your-variable-names-are-awful-heres-how-to-fix-them-89053d2855be

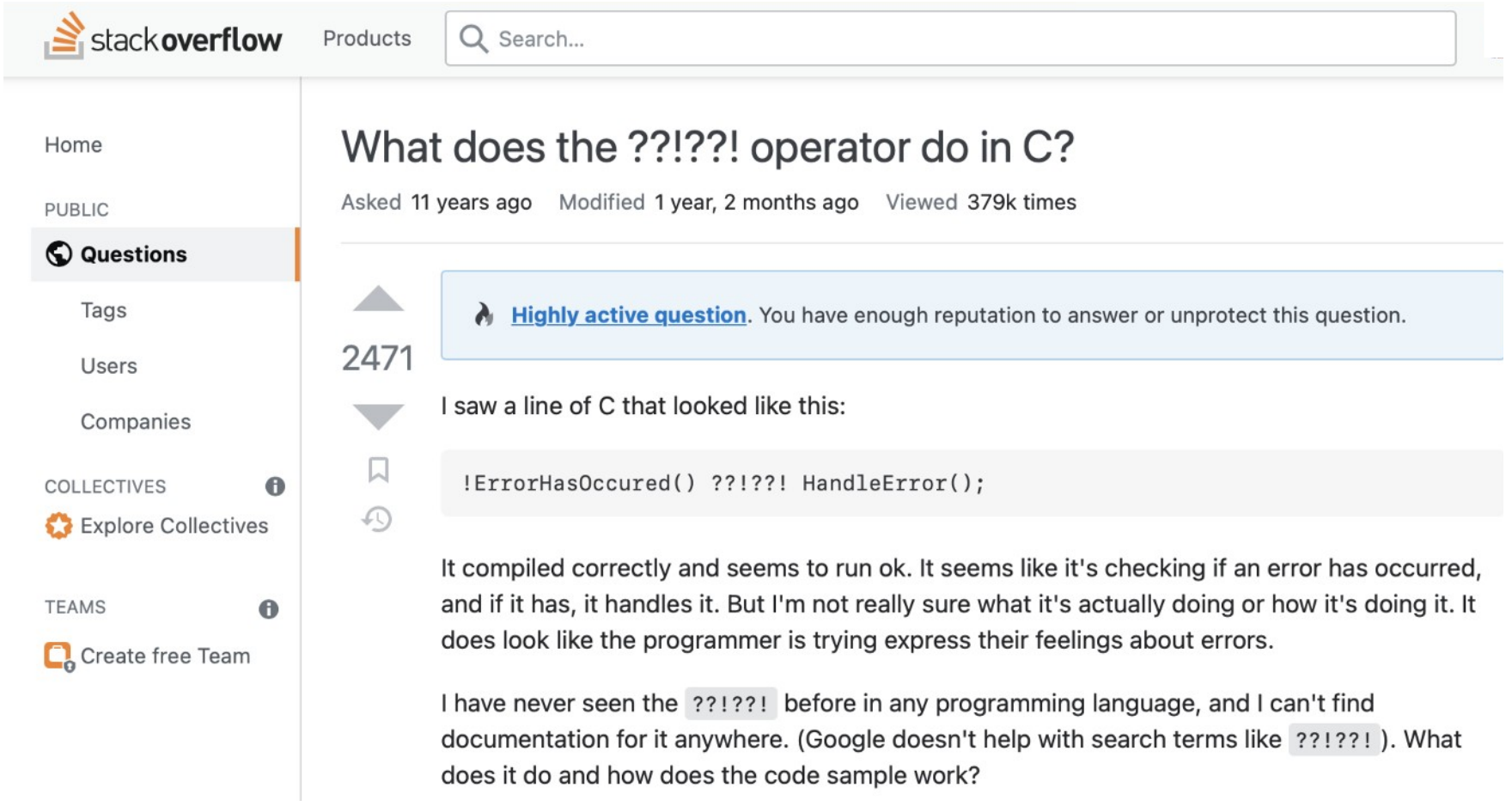
1. Write for humans, not for computers

Avoid naming anti-patterns:

A.1	*"Get" - more than an accessor*	A getter that performs actions other than returning the corresponding attribute without documenting it. Example: method `getImageData` which, no matter the attribute value, every time returns a new object (see Fig. 1).
A.2	*"Is" returns more than a Boolean*	The name of a method is a predicate suggesting a true/false value in return. However the return type is not Boolean but rather a more complex type thus allowing a wider range of values without documenting them. Example: `isValid` with return type `int` (see Fig. 6).
A.3	*"Set" method returns*	A set method having a return type different than `void` and not documenting the return type/values with an appropriate comment (see Fig. 7).
A.4	*Expecting but not getting a single instance*	The name of a method indicates that a single object is returned but the return type is a collection. Example: method `getExpansion` returning `List` (see Fig. 9).
B.1	*Not implemented condition*	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).
B.2	*Validation method does not confirm*	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).
B.3	*"Get" method does not return*	The name suggests that the method returns something (e.g., name starts with "get" or "return") but the return type is `void`. The documentation should explain where the resulting data is stored and how to obtain it (see Fig. 12).
B.4	*Not answered question*	The name of a method is in the form of predicate whereas the return type is not Boolean. Example: method `isValid` with return type `void` (see Fig. 13).
B.5	*Transform method does not return*	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 `javaToNative` with return type `void` (see Fig. 14).
B.6	*Expecting but not getting a collection*	The name of a method suggests that a collection should be returned but a single object or nothing is returned. Example: method `getStats` with return type Boolean (see Fig. 15).
C.1	*Method name and return type are opposite*	The intent of the method suggested by its name is in contradiction with what it returns. Example: method `disable` with return type `ControlEnableState`. The inconsistency comes from "disable" and "enable" having opposite meanings (see Fig. 16).
C.2	*Method signature and comment are opposite*	The documentation of a method is in contradiction with its declaration. Example: method `isNavigateForwardEnabled` is in contradiction with its comment documenting "a back navigation", as "forward" and "back" are antonyms (see Fig. 17).
D.1	*Says one but contains many*	The name of an attribute suggests a single instance, while its type suggests that the attribute stores a collection of objects. Example: attribute `target` of type `Vector`. It is unclear whether a change affects one or multiple instances in the collection (see Fig. 18).
D.2	*Name suggests Boolean but type does not*	The name of an attribute suggests that its value is true or false, but its declaring type is not Boolean. Example: attribute `isReached` of type `int[]` where the declared type and values are not documented (see Fig. 19).
E.1	*Says many but contains one*	The name of an attribute suggests multiple instances, but its type suggests a single one. Example: attribute `stats` of type Boolean. Documenting such inconsistencies avoids additional comprehension effort to understand the purpose of the attribute (see Fig. 20).
F.1	*Attribute name and type are opposite*	The name of an attribute is in contradiction with its type as they contain antonyms. Example: attribute `start` of type `MAssociationEnd`. The use of antonyms can induce wrong assumptions (see Fig. 21).
F.2	*Attribute signature and comment are opposite*	The declaration of an attribute is in contradiction with its documentation. Example: attribute `INCLUDE_NAME_DEFAULT` whose comment documents an "exclude pattern". Whether the pattern is included or excluded is thus unclear (see Fig. 22).

Arnaoudova, *et al*. Linguistic antipatterns: what they are and how developers perceive them. Empir Software Eng 21, 104–158 (2016).

1. Write for humans, not for computers



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

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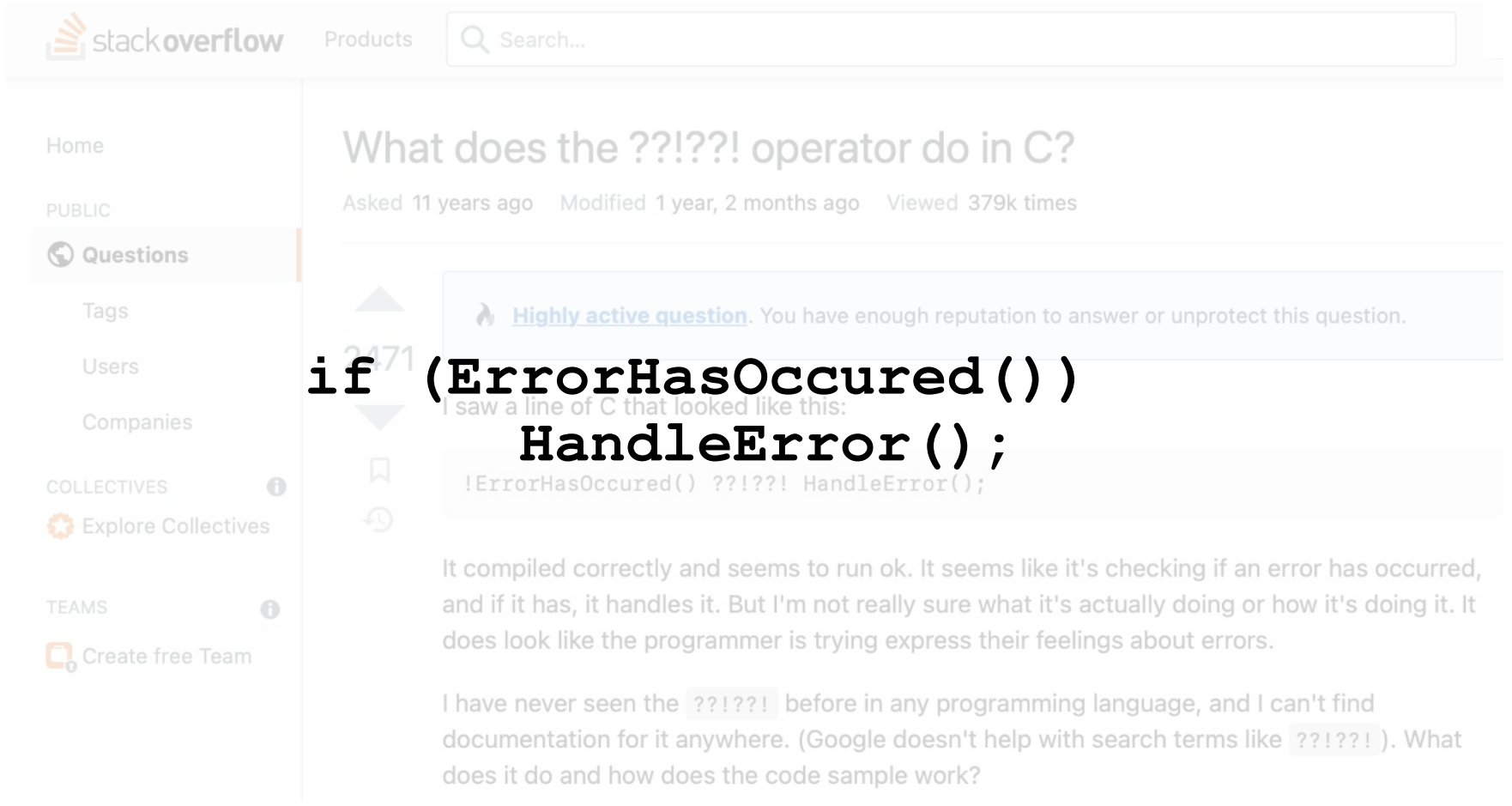



```
if (ErrorHasOccured())
    HandleError();
```

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)

https://madhadron.com/programming/seven_ur_languages.html

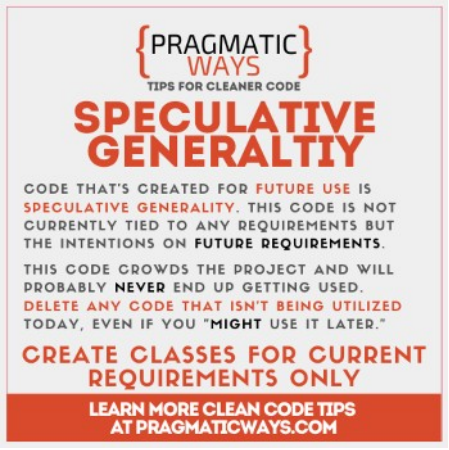
3. Organize for change and make incremental changes

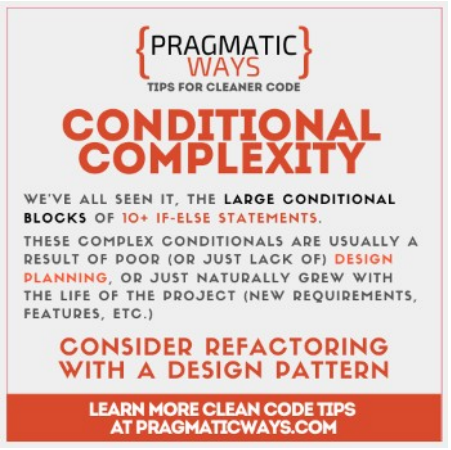
Scientific software specifications are always changing:

- 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 ½ . Avoid “code smells” / anti-patterns





https://pragmaticways.com/31-code-smells-you-must-know/

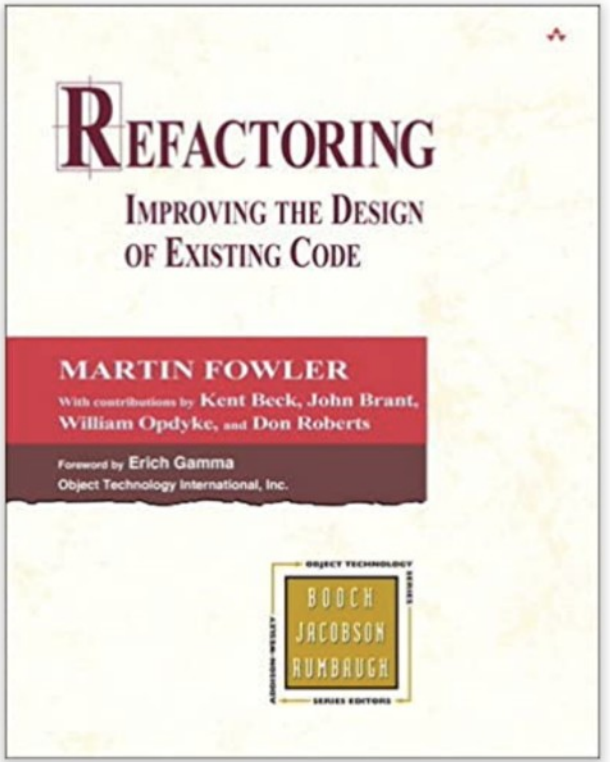
3 ½ . Avoid “code smells” e.g. nested `if`’s

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

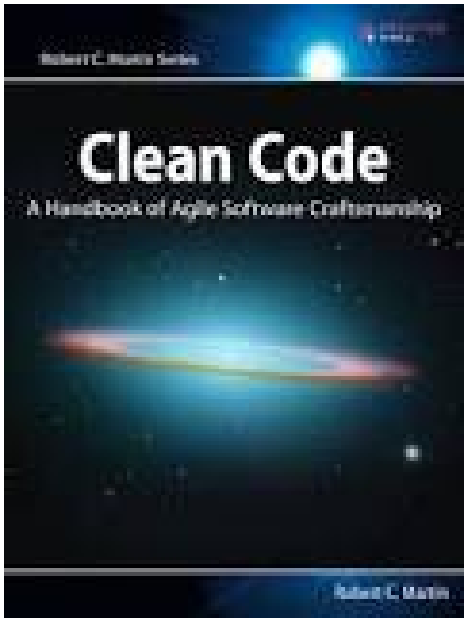
```
function getSign(x) {
    if (x == 0)
        return “zero”;
    if (x > 0)
        return “positive”;
    if (x == 0)
        return “negative”;
    return “Nan”;
}
```



https://refactoring.com/catalog/replaceNestedConditionalWithGuardClauses.html

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!

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

4. Follow good coding principles and style

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

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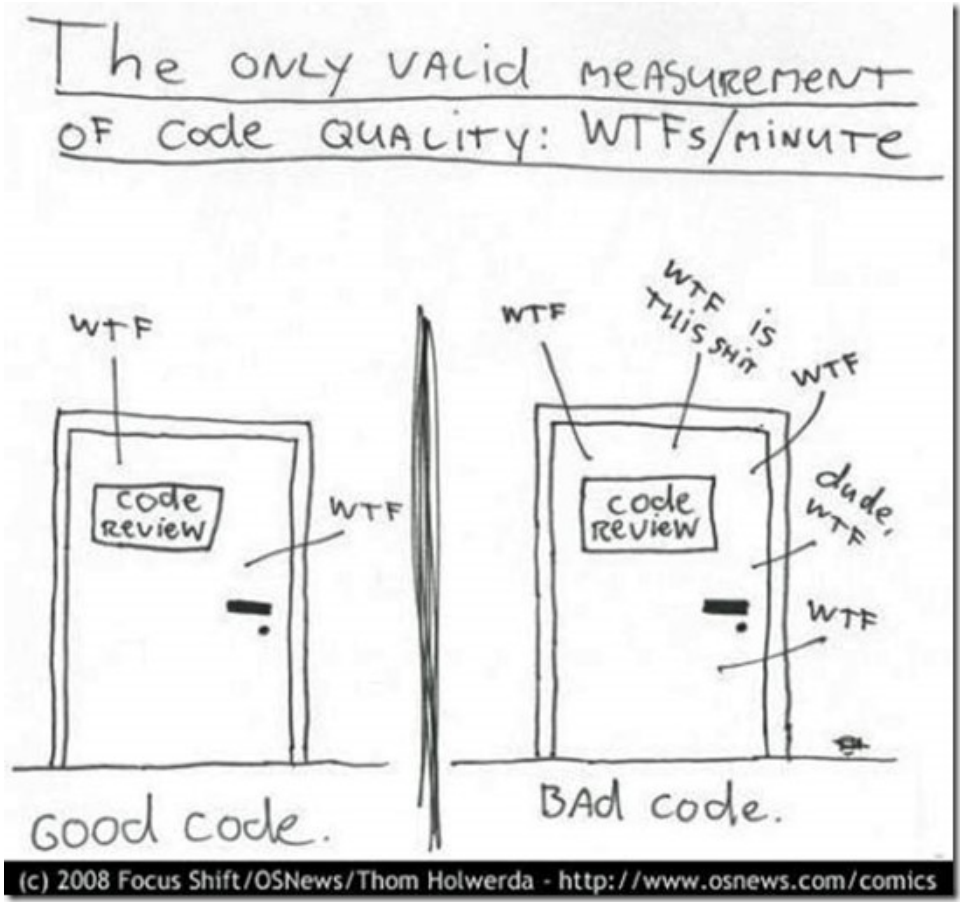

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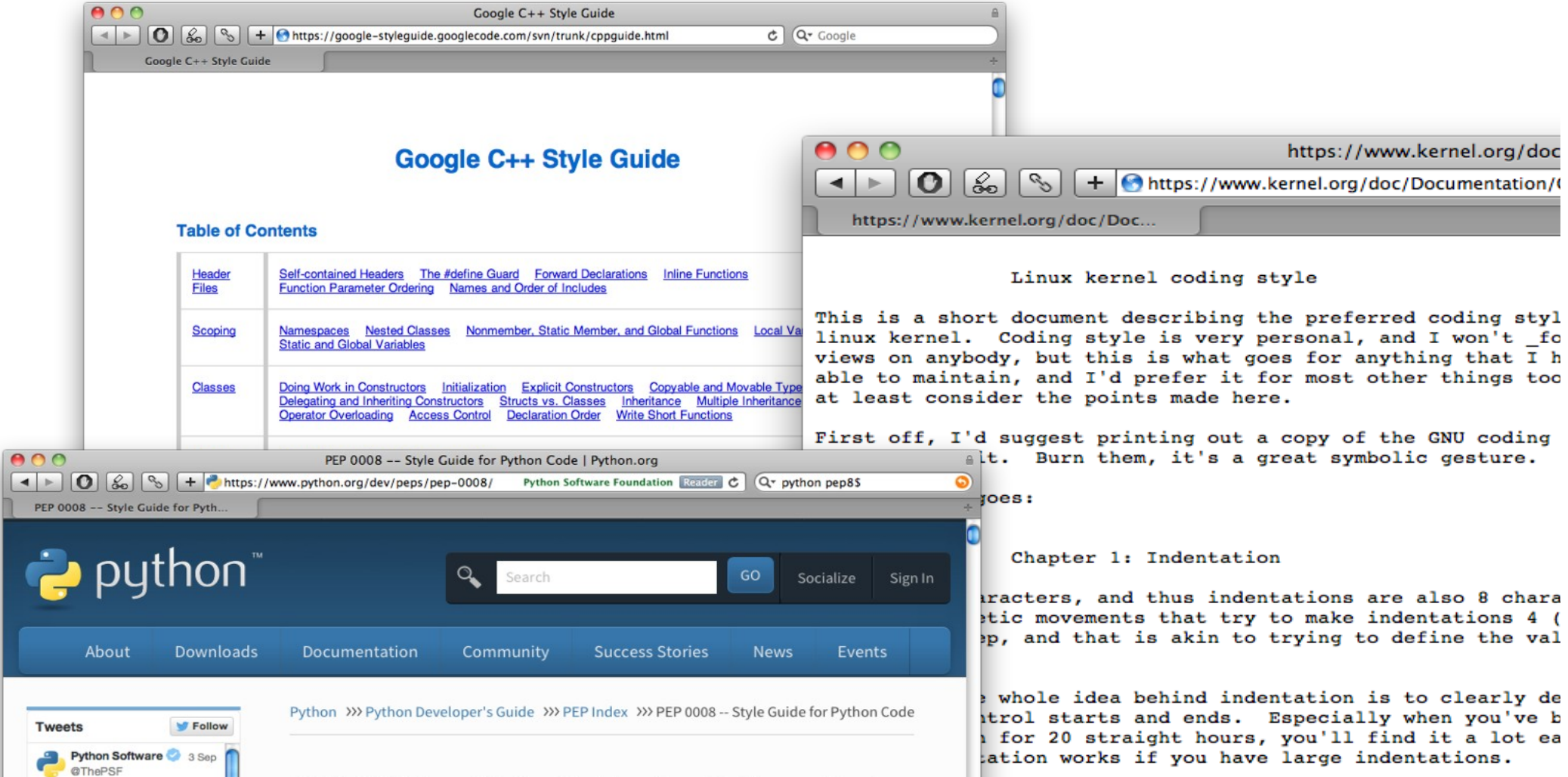


4. Follow good coding principles : gracefully handle user errors

Use error handling techniques:

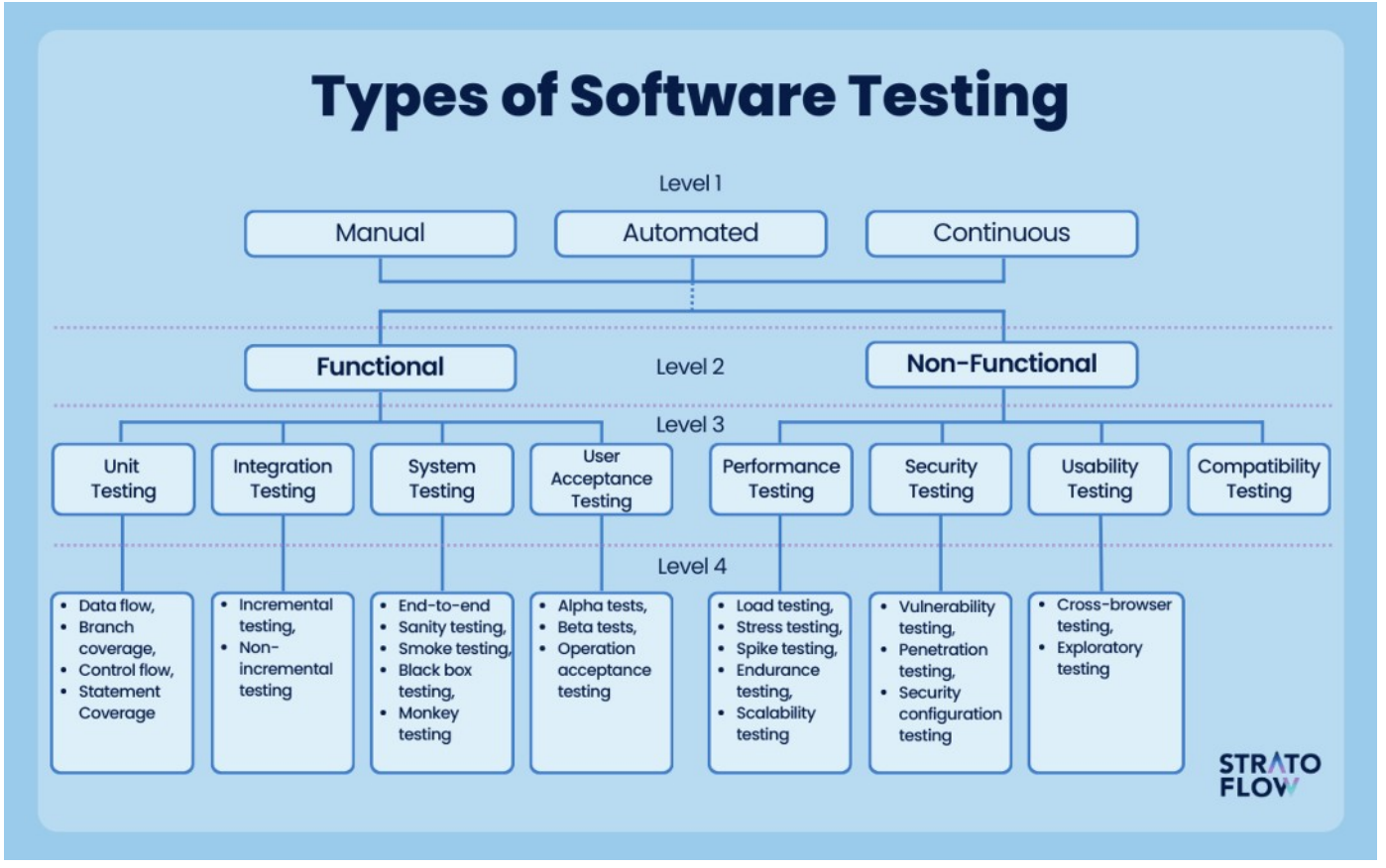
- Return codes
- Exceptions
- Callbacks
- “Result” structs

Be informative in the error messages.

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

https://andreabergia.com/blog/2023/05/error-handling-patterns/

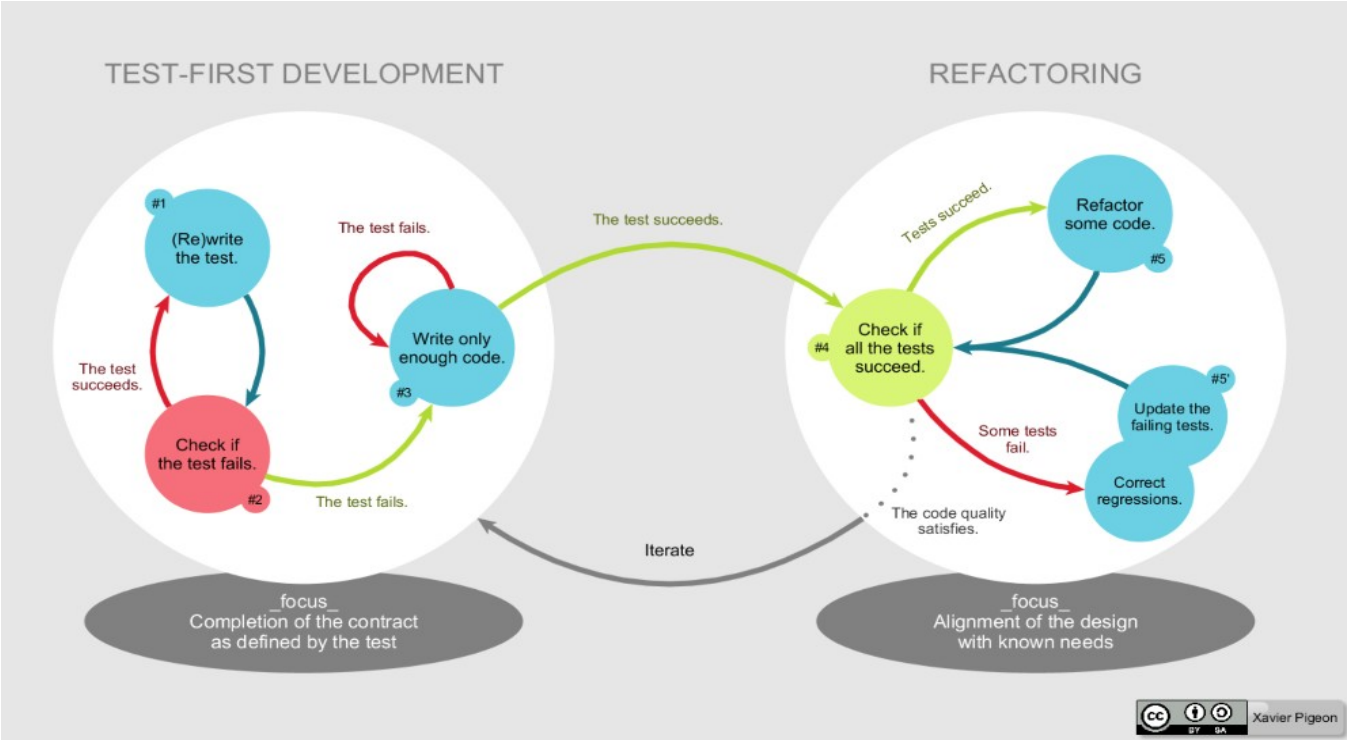
5. Plan for mistakes, automate testing; Test-driven development



https://stratoflow.com/types-of-software-testing/

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

Write the tests before you even write the code



https://en.wikipedia.org/wiki/Test-driven_development

6. Use modern source-code management system

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 event 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
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
```

https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1006561

7. Document the purpose and design, not the implementation

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end
```

https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1006561

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
---------

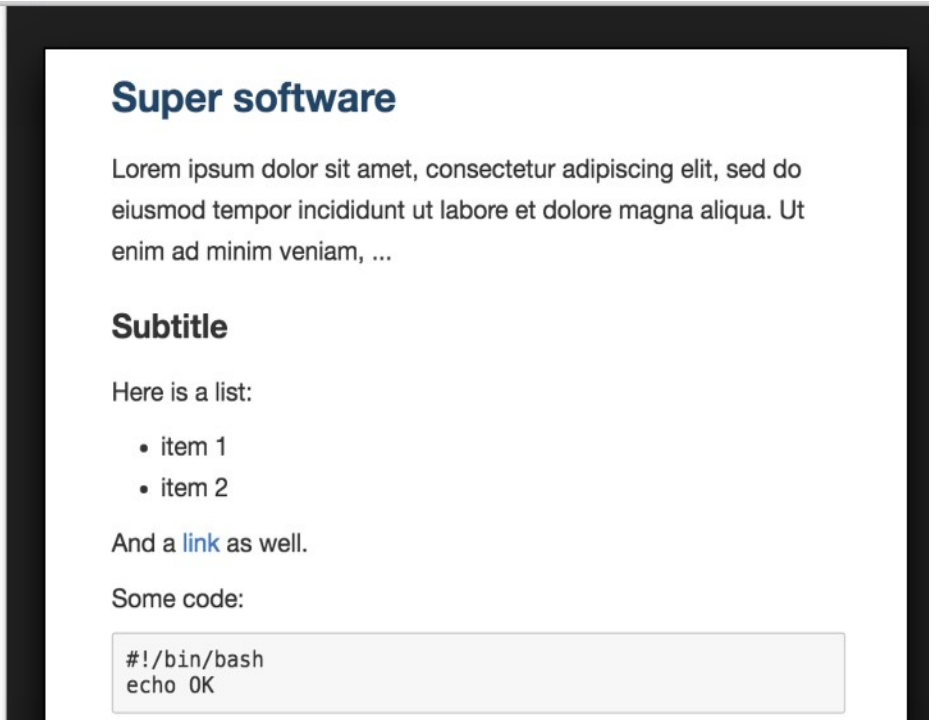
Here is a list:

  - item 1
  - item 2

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

Some code:

    #!/bin/bash
```



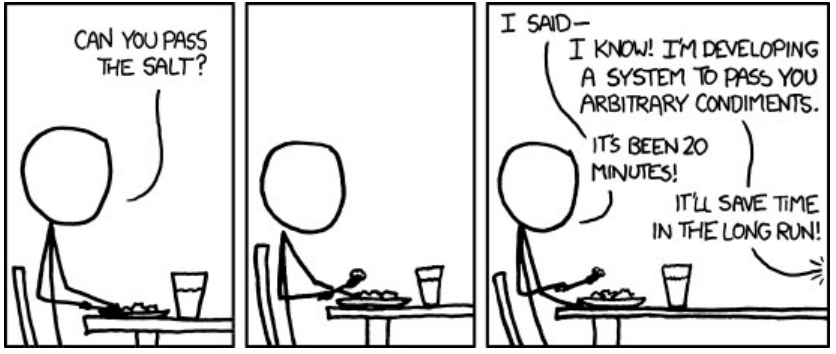
https://daringfireball.net/projects/markdown/

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)

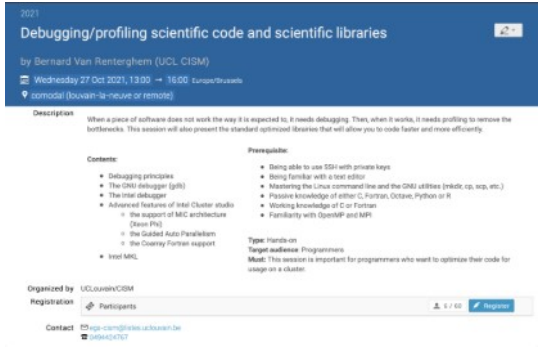
- Do not try to make it universal for all possible future needs at the beginning “YAGNI” (do not close doors either)



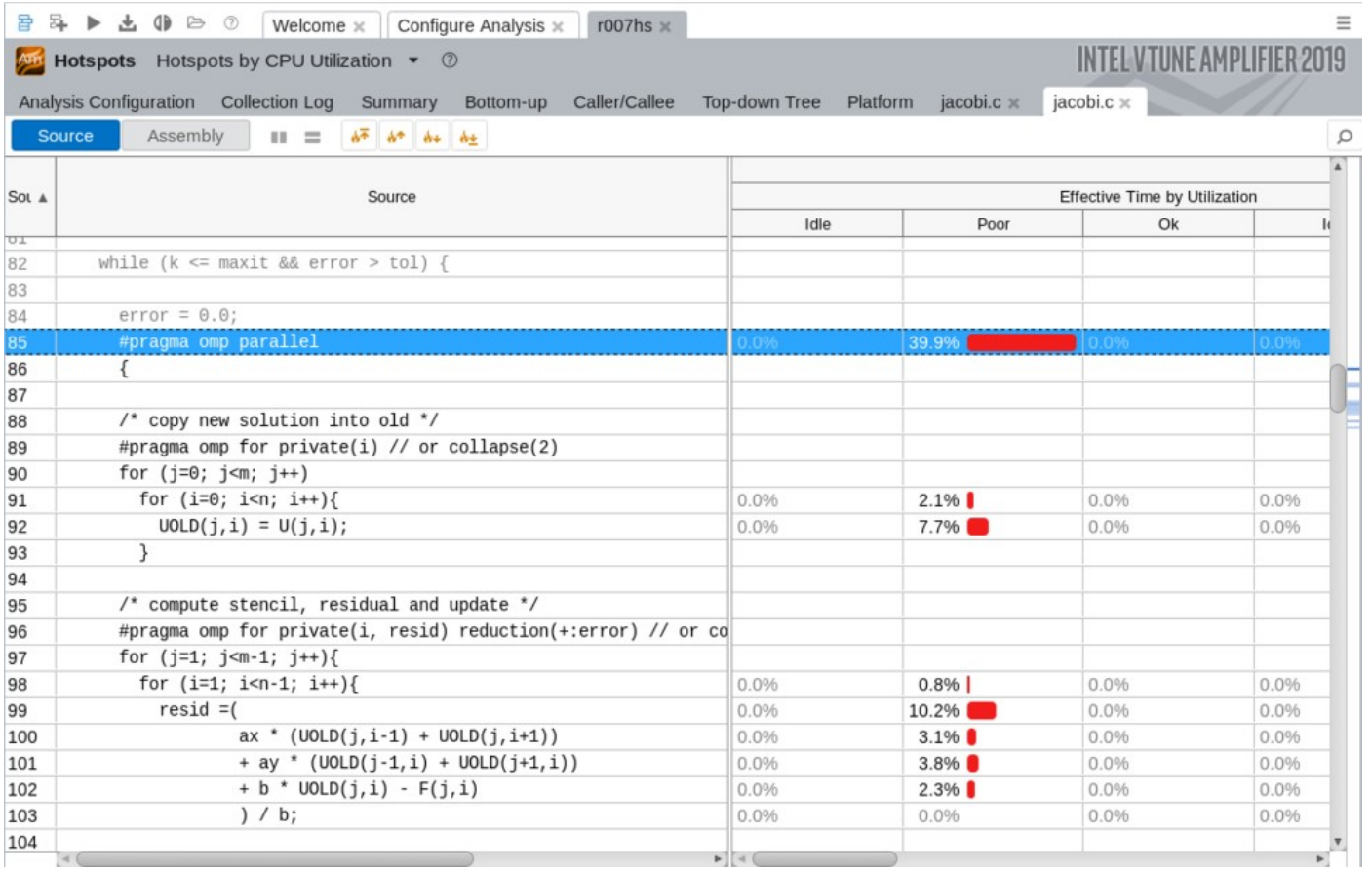
https://xkcd.com/974/

8. Optimize only when it works already

Use a profiler

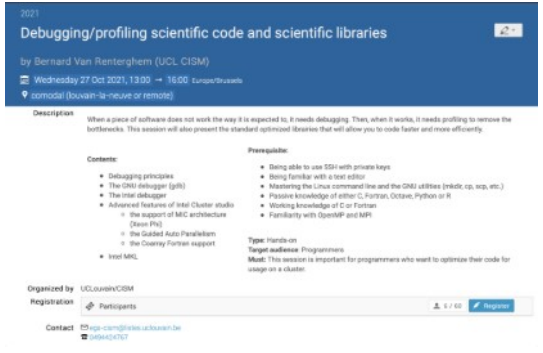


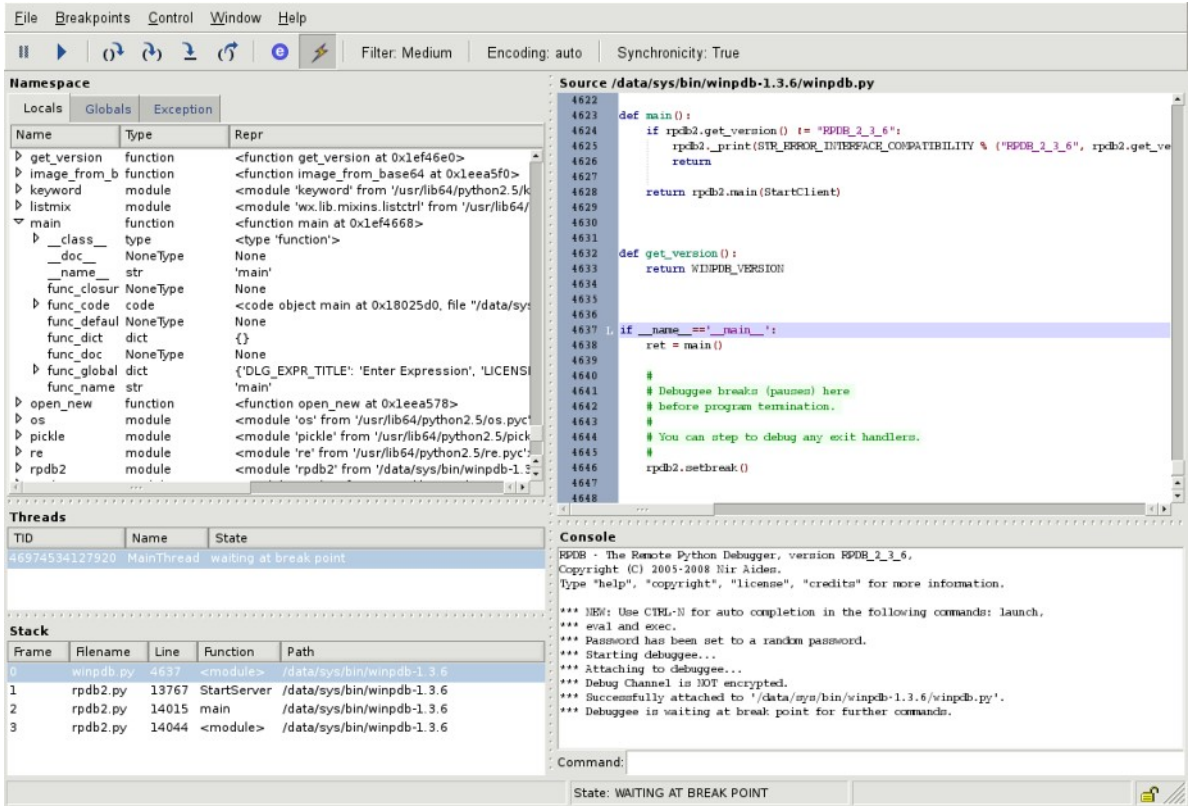
Incorporate benchmarks in your tests



9. Debug cleverly

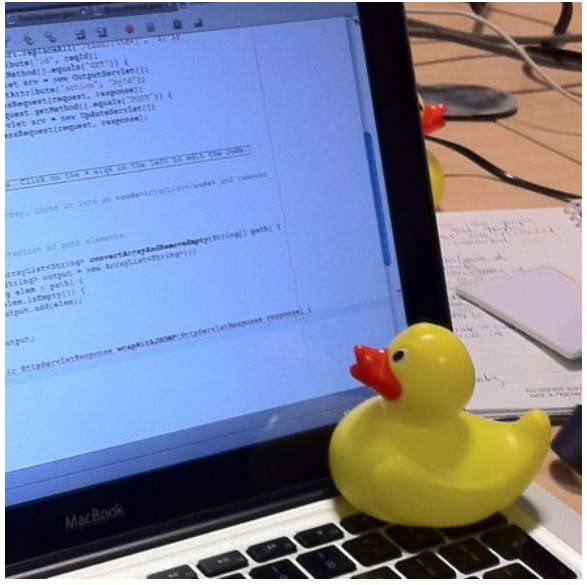
Use a debugger





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!

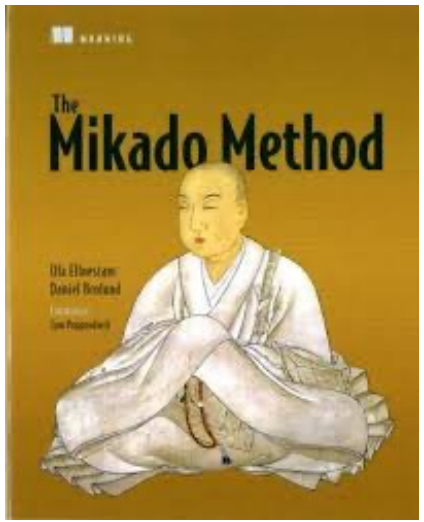
Dig that part of the code until you are confident again that it works.

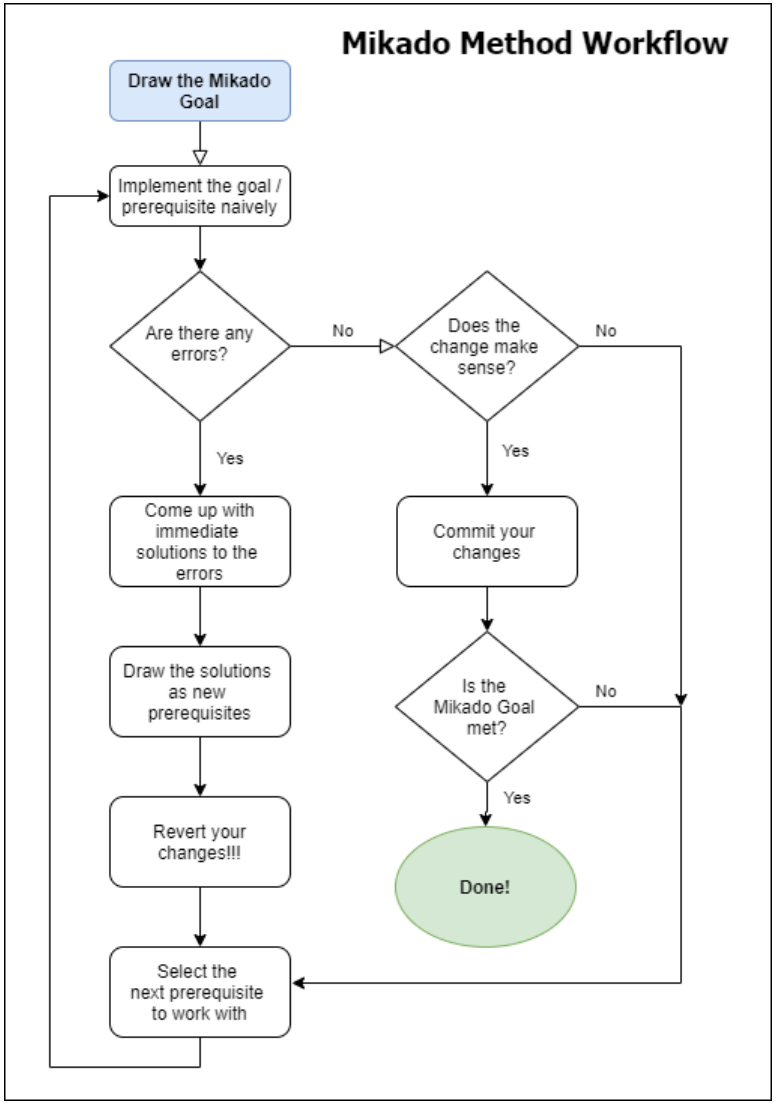
Or discover that it does actually not work as expected ...

https://en.wikipedia.org/wiki/Rubber_duck_debugging

9. Debug cleverly

Use a method



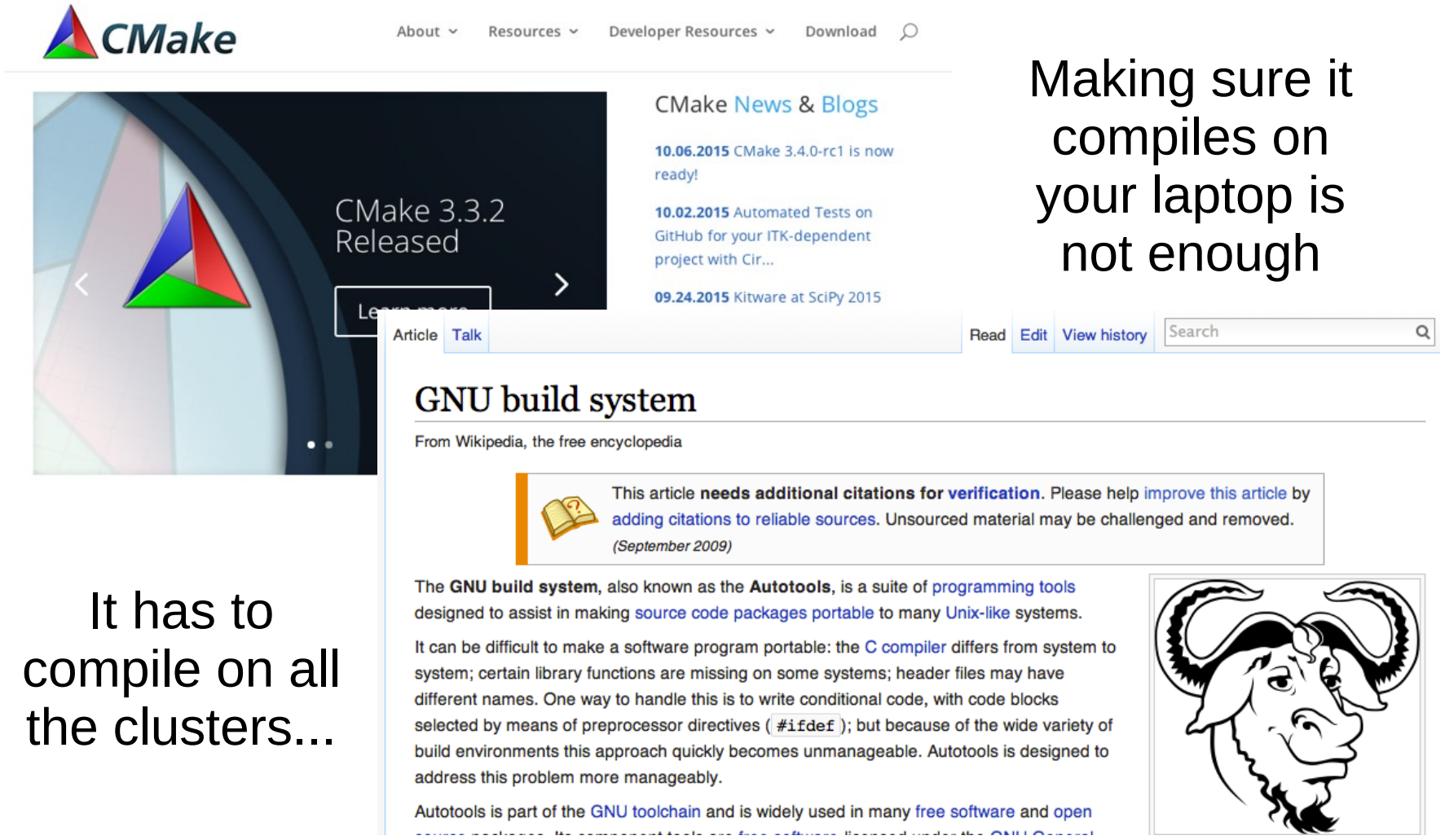


The Mikado Method, O. Ellnestam & D. Brolund, Manning, 2014

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

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

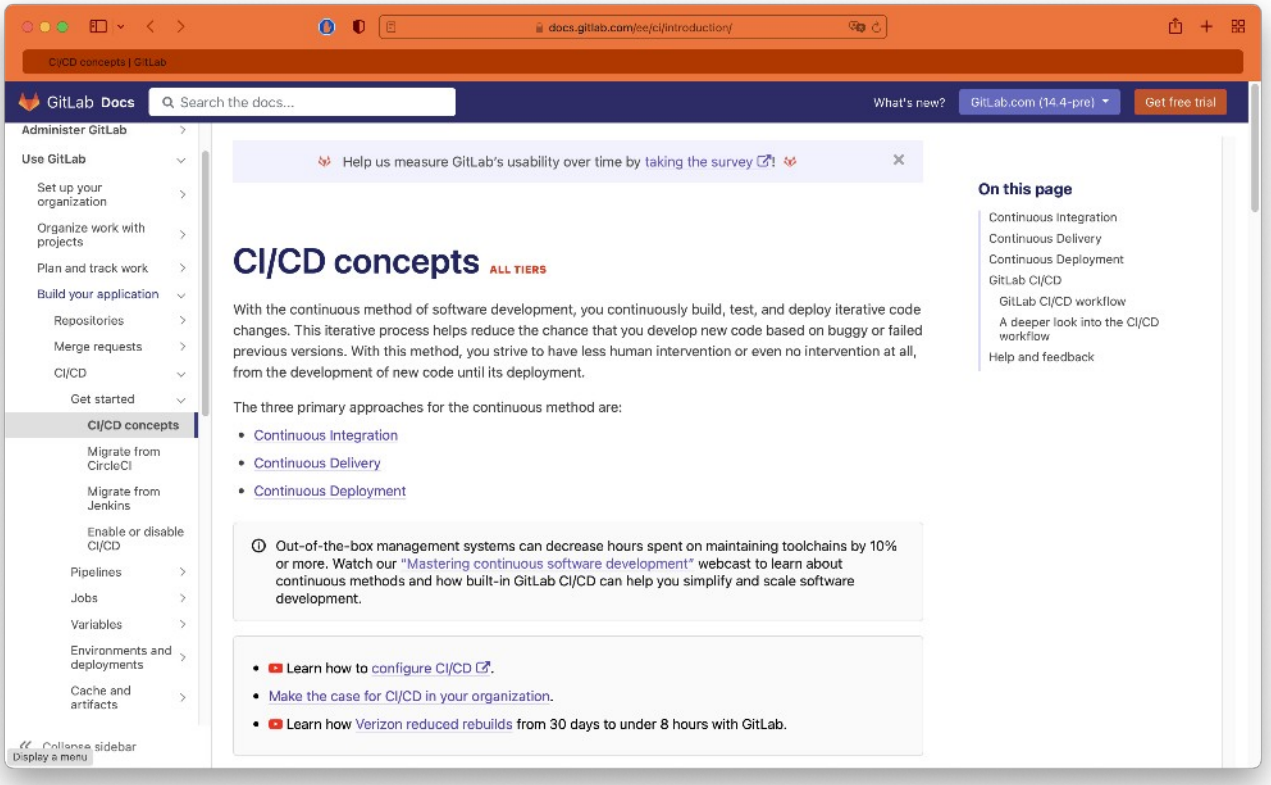
1. Automate the compiling process



Making sure it compiles on your laptop is not enough

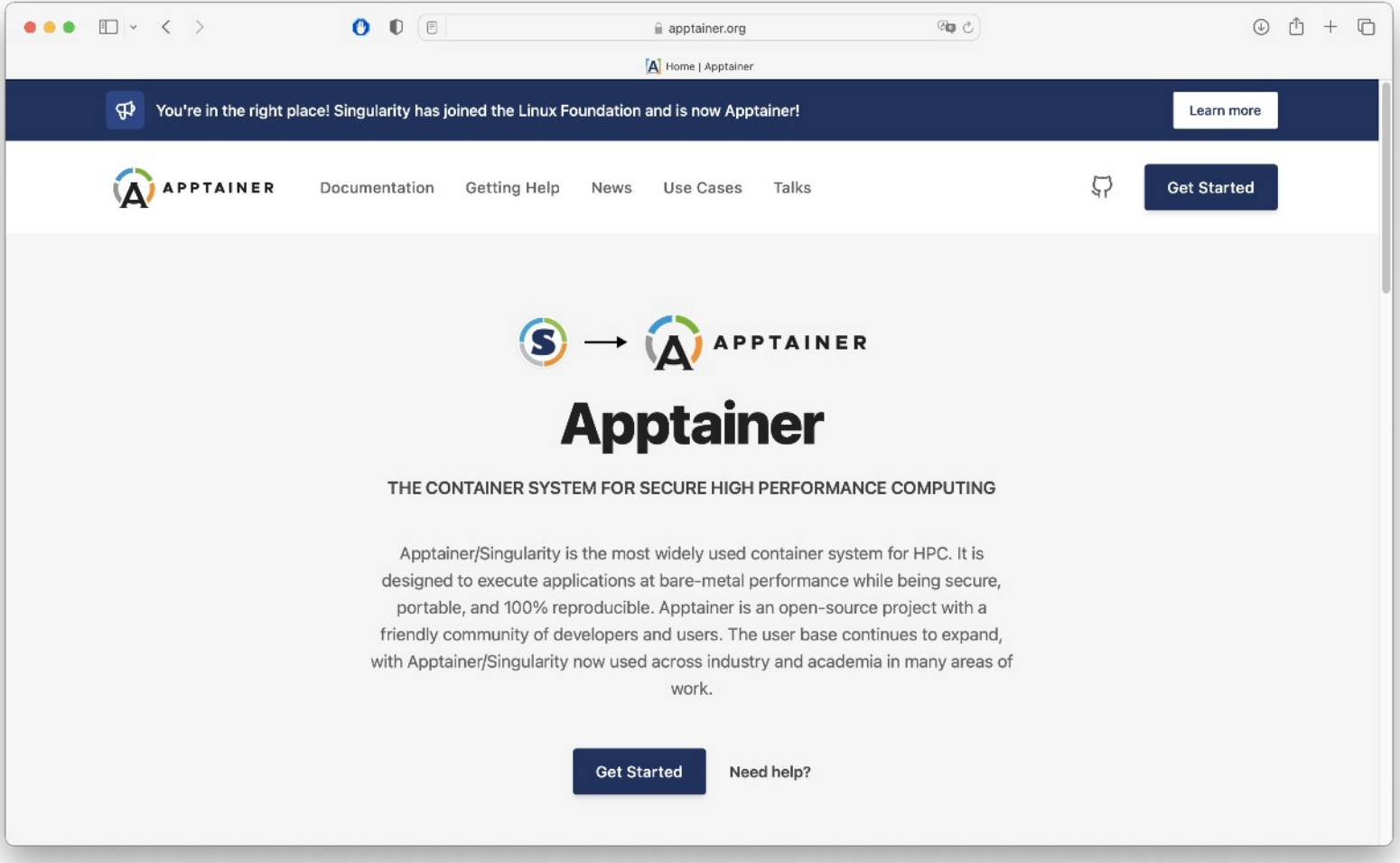
It has to compile on all the clusters...

1. Automate the compiling process



https://docs.gitlab.com/ee/ci/introduction/

2. Learn about containers



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>

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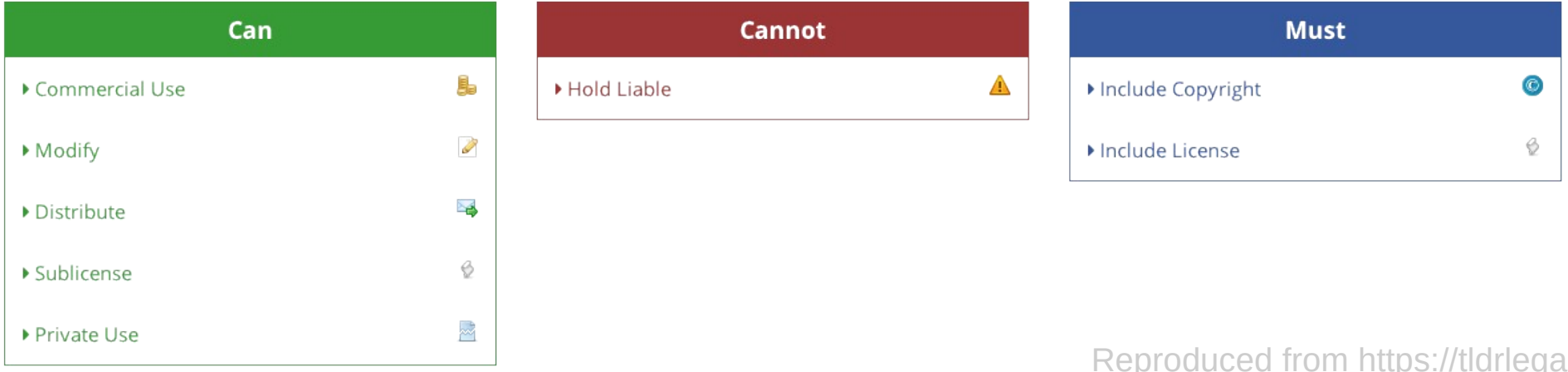

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BSD

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

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3. License your code: finding help

LIEU – Network of Knowledge Transfer offices

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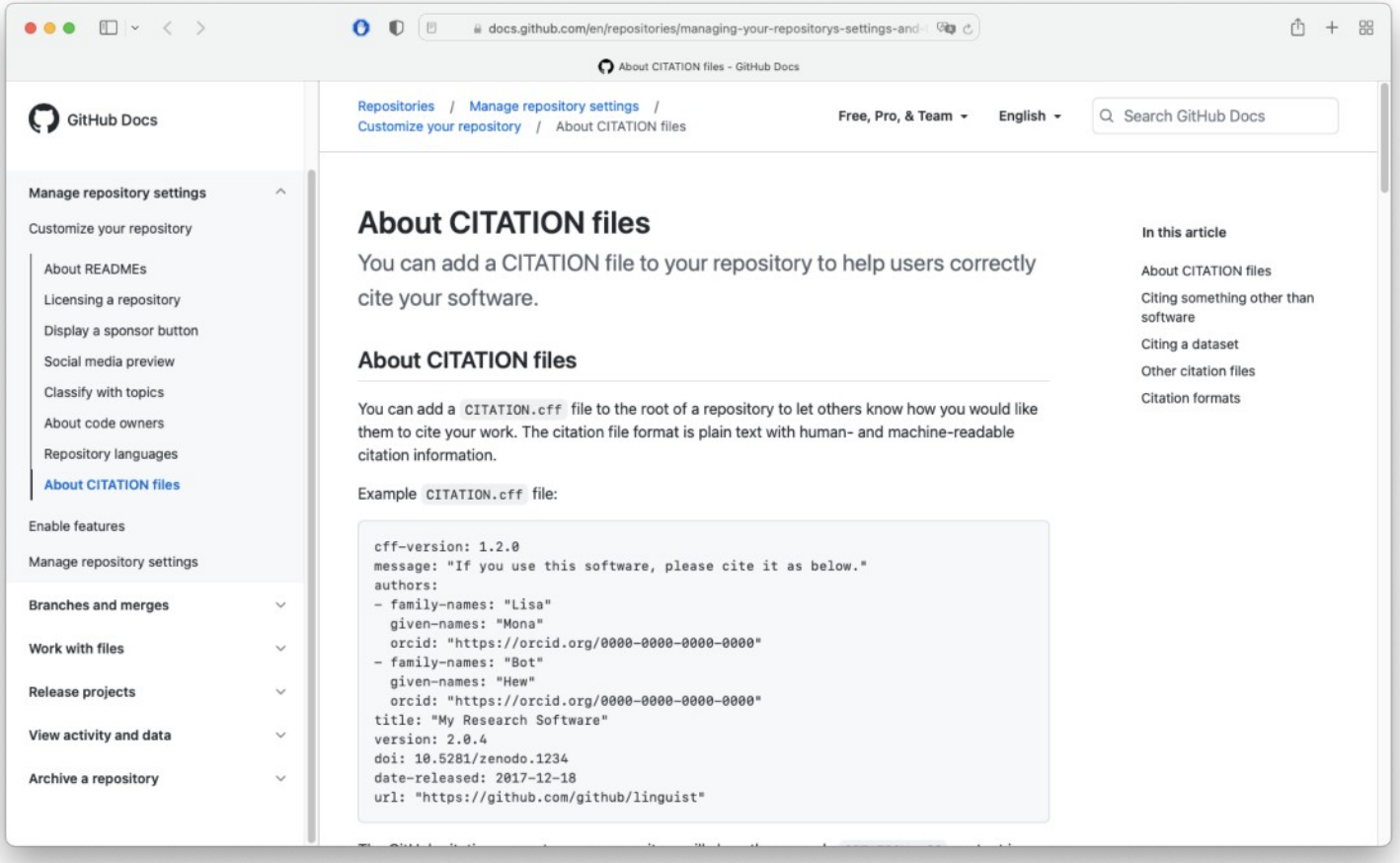
Slide credit: Sébastien ADAM

3 ½. GitHub CITATION files

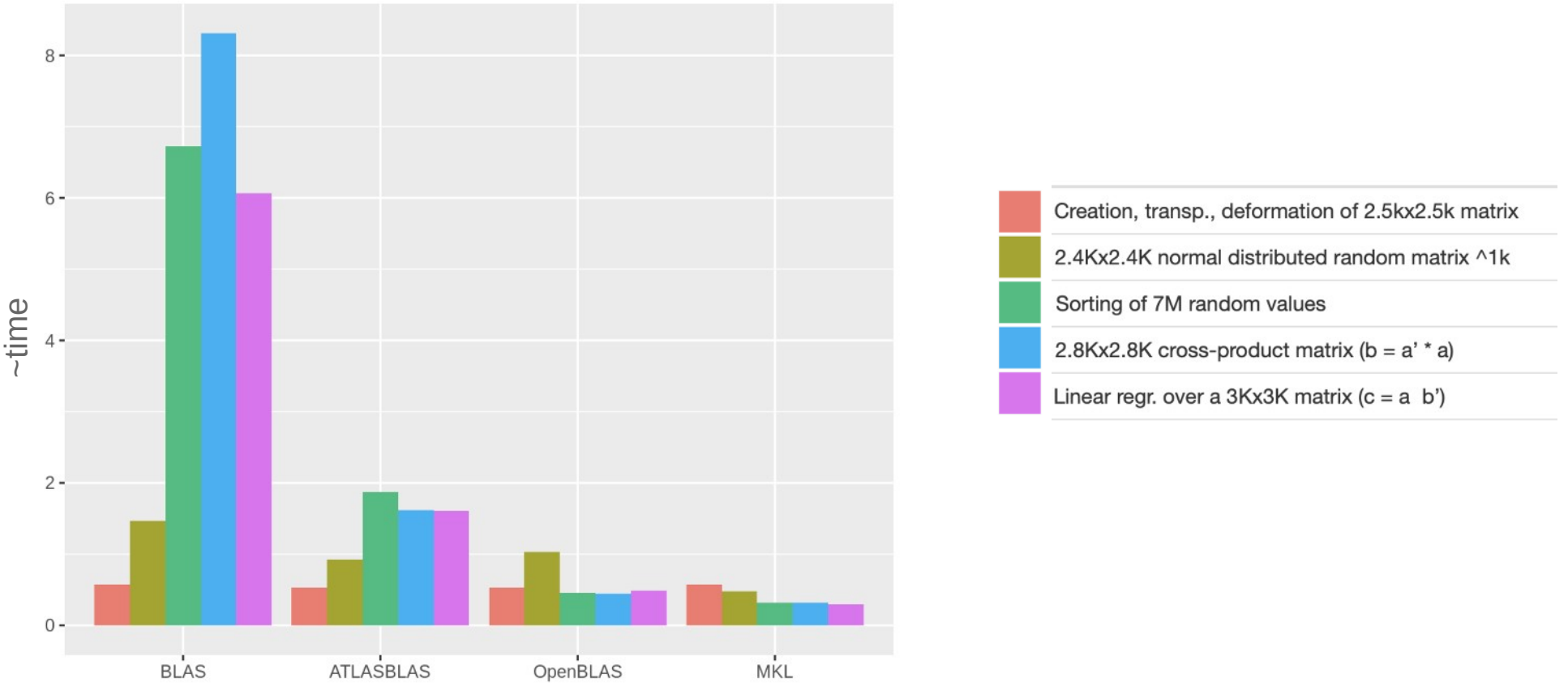


https://docs.github.com/en/repositories/managing-your-repositorys-settings-and-features/customizing-your-repository/about-citation-files

“… 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

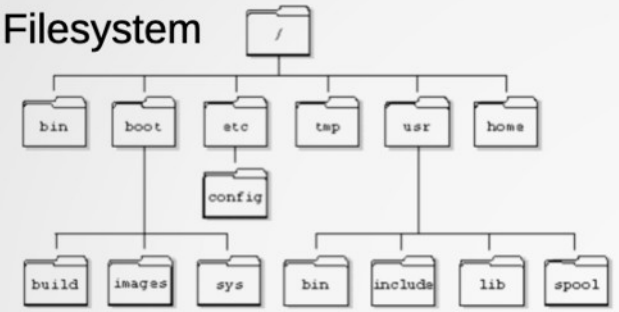
1. Use optimized libraries



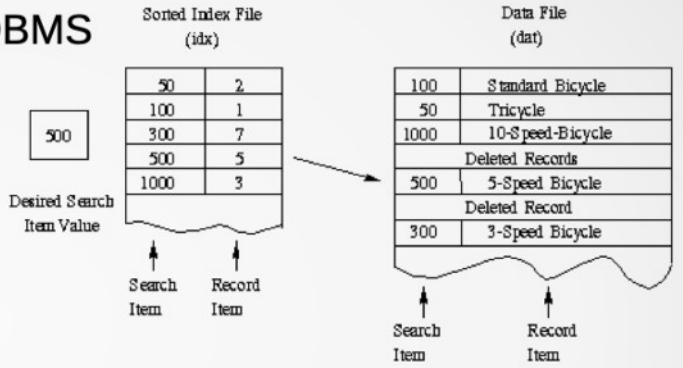
https://csantill.github.io/RPerformanceWBLAS/

2. Choose the right storage system

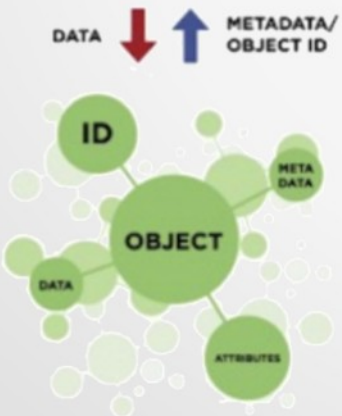
Filesystem



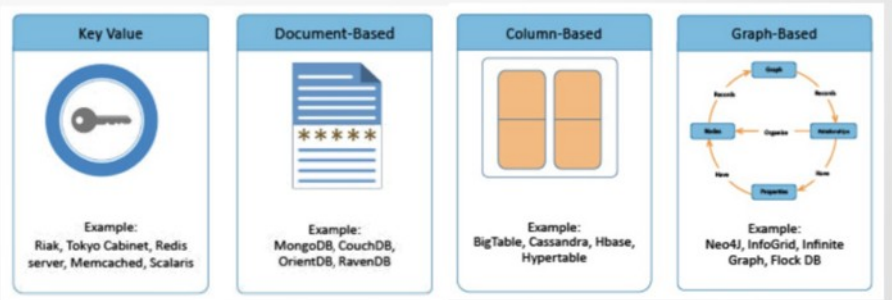
RDBMS



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
```

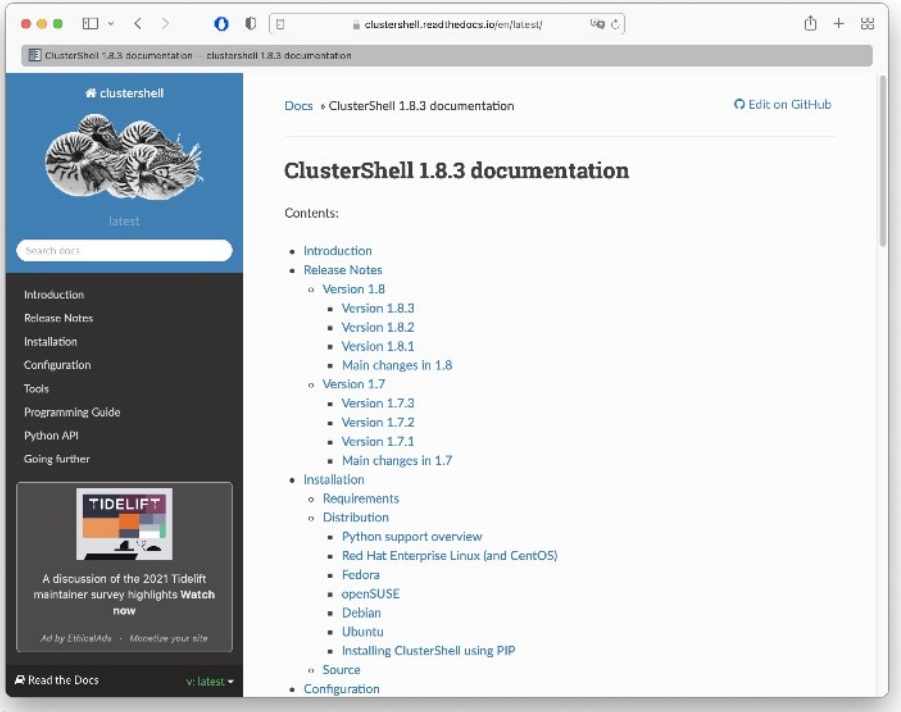
```
if exists(i) and exists(res)
    begin=load(i)
    res=load(res)
else
    begin = 1
end=10
data = [(x1,y1), (x2,y2), .., (x10,y10)]
for i = begin .. end
  res[i] = ( data[xi]^2  + data[yi]^2 )
  save(res, i)
end
```

“ …, *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
❯
```



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

2. Master configuration management

```
❯ 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: **inventory**

```
1  [all]
2
3  lemaitre3 short_name="lm3"
4  nic5      short_name="nic5"
```

File: **playbook.yml**

```
1  ---
2  - hosts:
3      - lemaitre3
4      - nic5
5    tasks:
6      - name: Upload templated file
7        template: src=myfile dest=. mode=700
```

File: **myfile**

```
1  This cluster's short name is {{ short_name }}
```

https://www.ansible.com

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

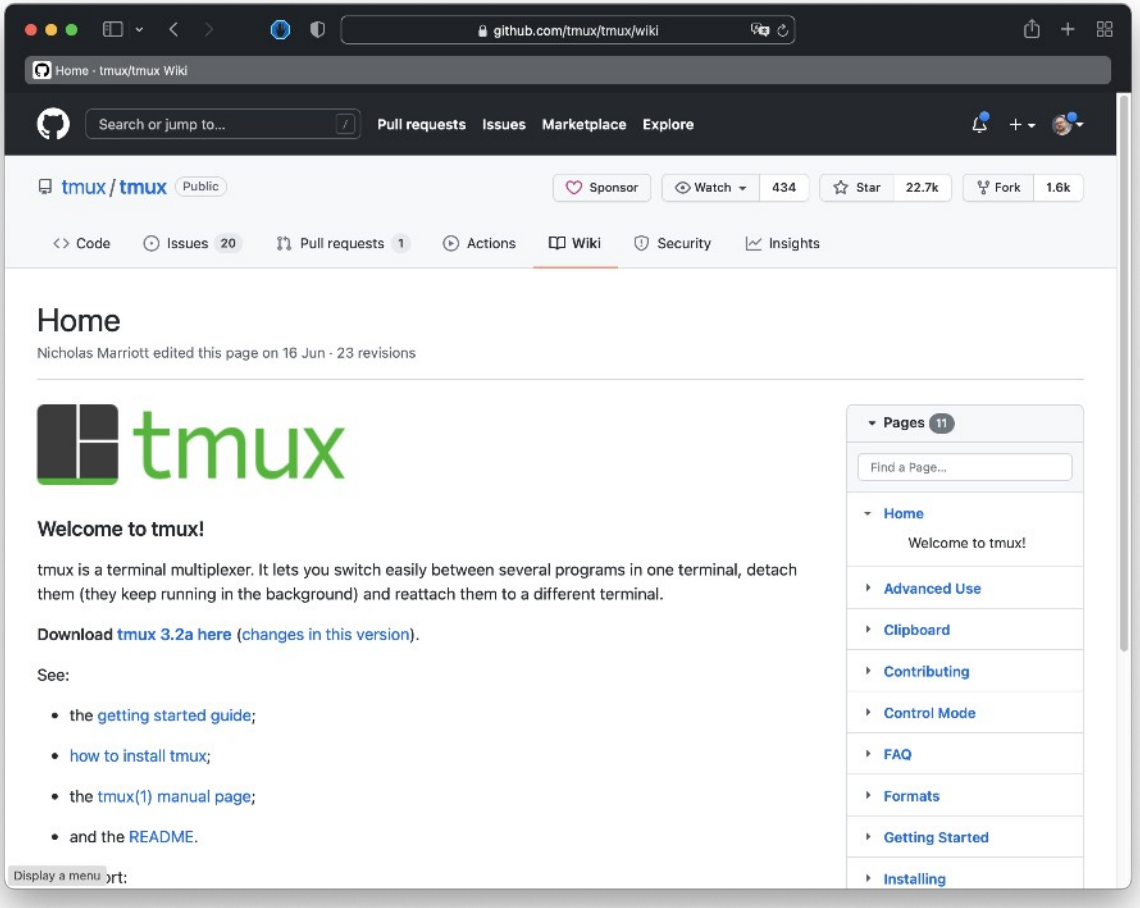
changed: [lemaitre3]

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

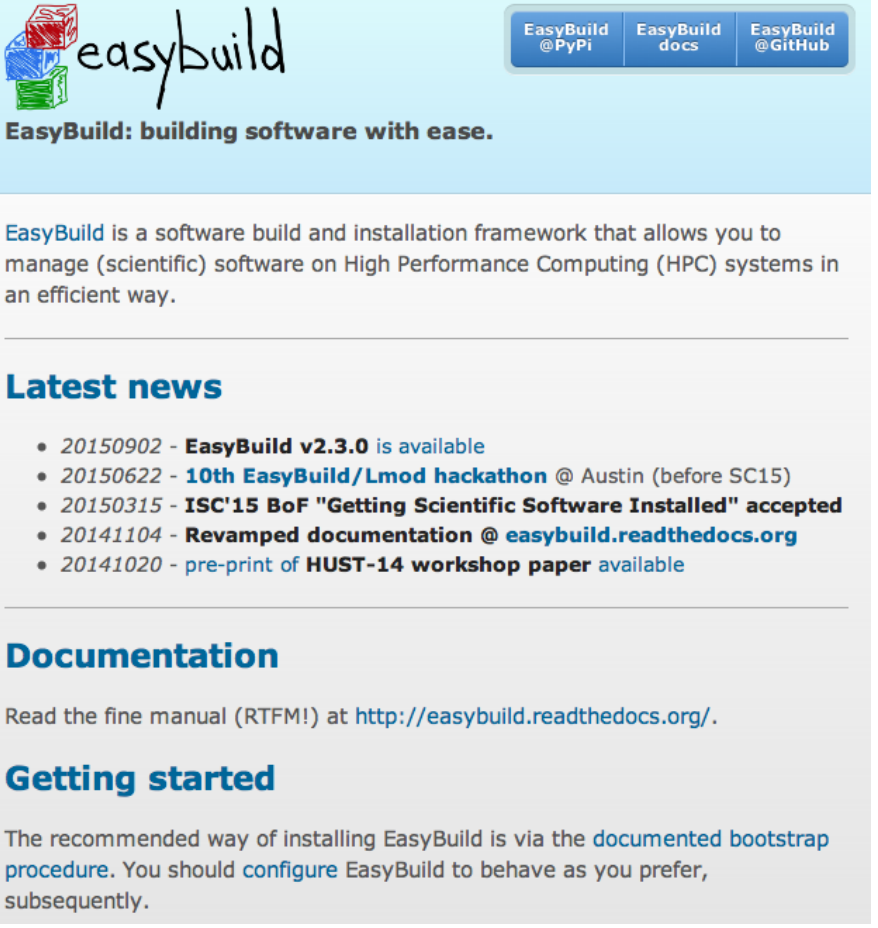
Do not let SSH disconnections harm your workflow
(and much more)



https://github.com/tmux/tmux/wiki

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
```



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

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

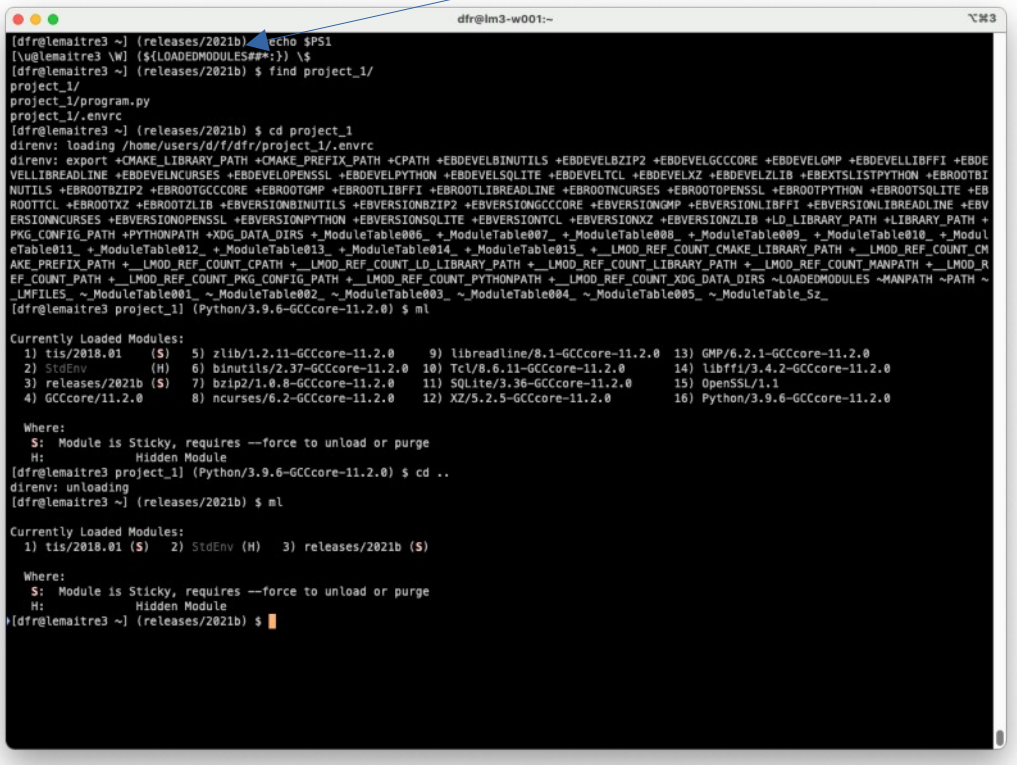
Create module collections with `module save`

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)
```



https://github.com/direnv/direnv/

5. Avoid the boilerplate

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

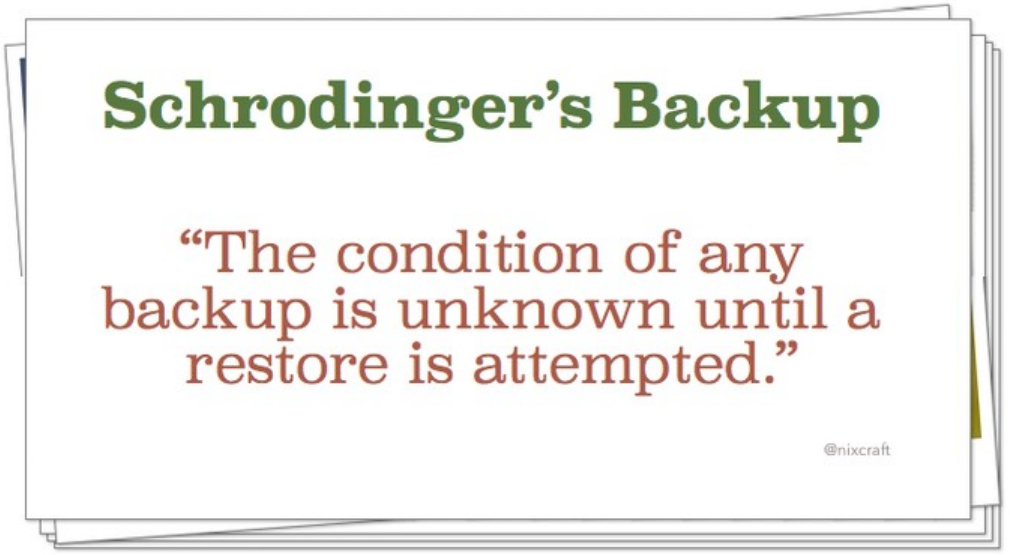
```
├── LICENSE
├── Makefile           <- Makefile with commands like `make data` or `make train`
├── README.md          <- The top-level README for developers using this project.
├── data
│   ├── external       <- Data from third party sources.
│   ├── interim        <- Intermediate data that has been transformed.
│   ├── processed      <- The final, canonical data sets for modeling.
│   └── raw            <- The original, immutable data dump.
│
├── docs               <- A default Sphinx project; see sphinx-doc.org for details
│
├── models             <- Trained and serialized models, model predictions, or model summaries
│
├── notebooks          <- 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`.
│
├── references         <- Data dictionaries, manuals, and all other explanatory materials.
│
├── reports            <- Generated analysis as HTML, PDF, LaTeX, etc.
│   └── figures        <- Generated graphics and figures to be used in reporting
│
├── requirements.txt   <- The requirements file for reproducing the analysis environment, e.g.
│                         generated with `pip freeze > requirements.txt`
│
├── setup.py           <- makes project pip installable (pip install -e .) so src can be imported
├── src                <- Source code for use in this project.
│   ├── __init__.py    <- Makes src a Python module
│   │
│   ├── data           <- Scripts to download or generate data
│   │   └── make_dataset.py
│   │
│   ├── features       <- Scripts to turn raw data into features for modeling
│   │   └── build_features.py
│   │
│   ├── models         <- Scripts to train models and then use trained models to make
│   │   │                 predictions
│   │   ├── predict_model.py
│   │   └── train_model.py
│   │
│   └── visualization  <- Scripts to create exploratory and results oriented visualizations
│       └── visualize.py
│
└── tox.ini            <- 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

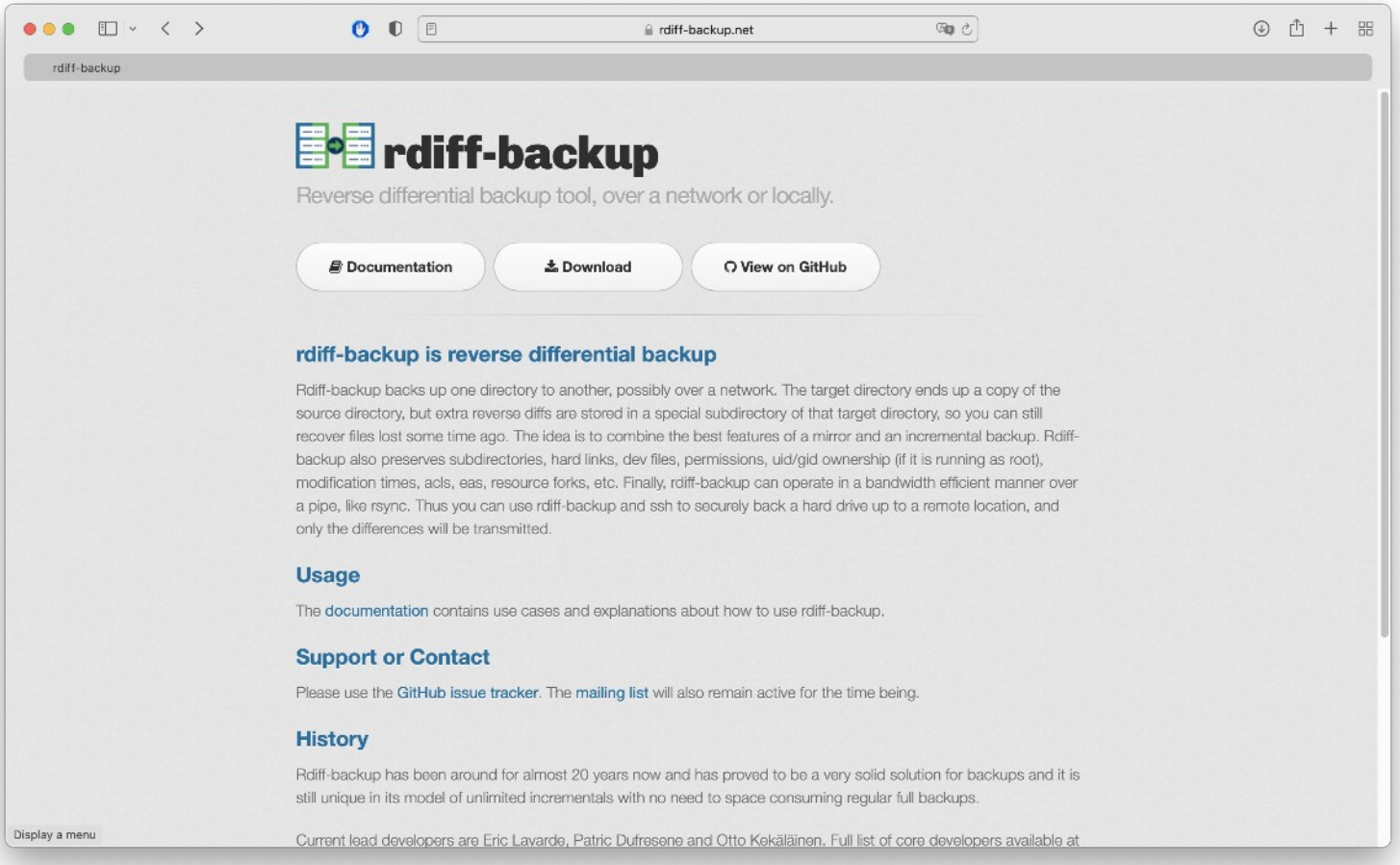
6. BACKUPS!!!

https://securityboulevard.com/2020/05/3-2-1-backup-rule-the-rule-of-thumb-to-solve-your-data-loss-problems/

6. BACKUPS!!!


Schrodinger's Backup
"The condition of any backup is unknown until a restore is attempted."
@nixcraft

6. BACKUPS!!!



https://rdiff-backup.net

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.”

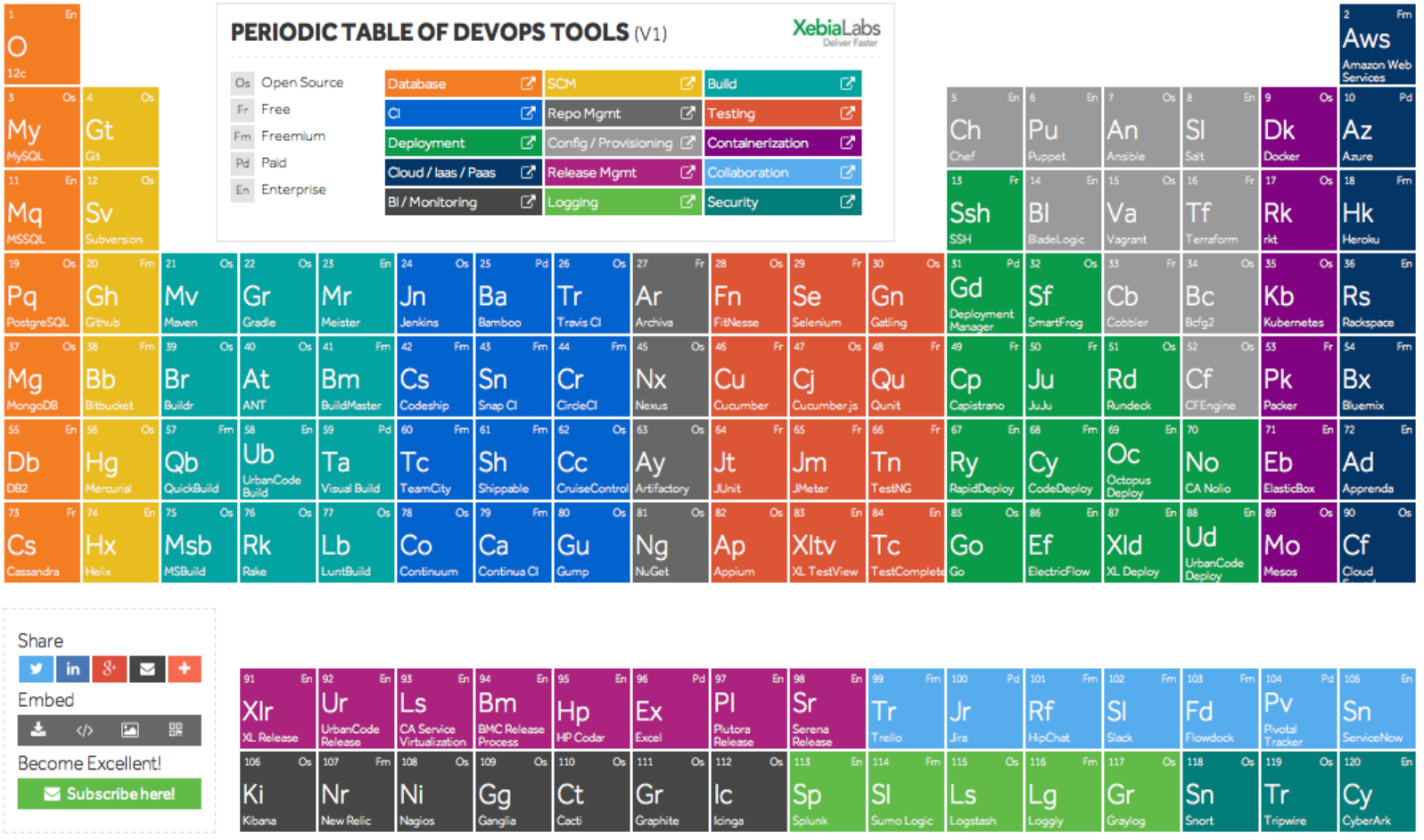
We discussed:

- 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