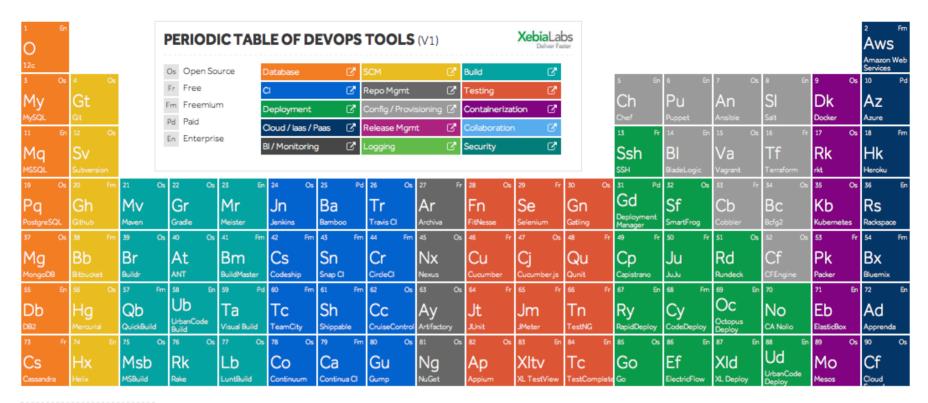
Introduction to Scientific Software Deployment and Development

damien.francois@uclouvain.be November 2022

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



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Xlr	Ur	Ls	Bm	Нр	Ex		Sr	Tr	Jr	Rf	SI	Fd	Pv	Sn
XL Release	UrbanCode Release	CA Service Virtualization	BMC Release Process	HP Codar	Excel		Serena Release	Trello	Jira	HipChat	Slack	Flowdock	Pivotal Tracker	ServiceNow
106 O:	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	Nr	Ni	Gg	Ct	Gr	lc	Sp	SI	Ls	Lg	Gr	Sn	Tr	Cy
Kibana	New Relic	Nagios	Ganglia	Cacti	Graphite	lcinga	Splunk	Sumo Logic	Logstash		Graylog	Snort	Tripwire	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*"

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

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

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
- Organize for change and make incremental changes
 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

"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."



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

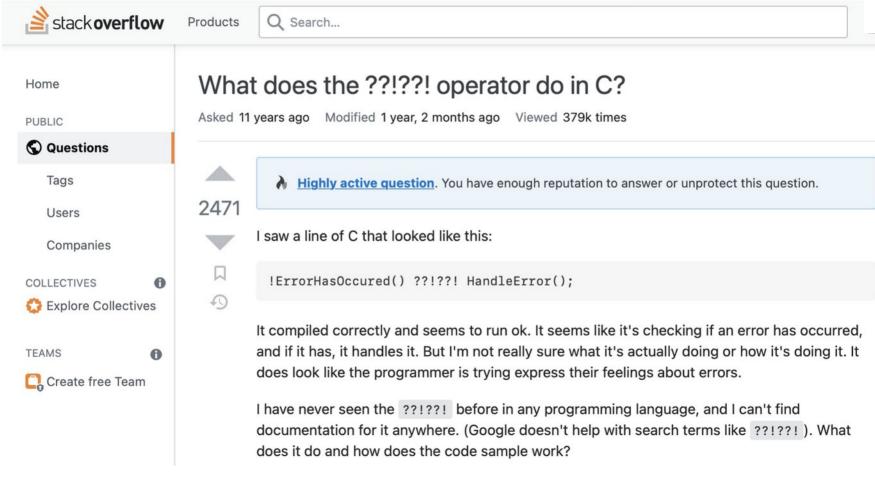
Sweet spot in-between...

Goal clear but structure less obvious

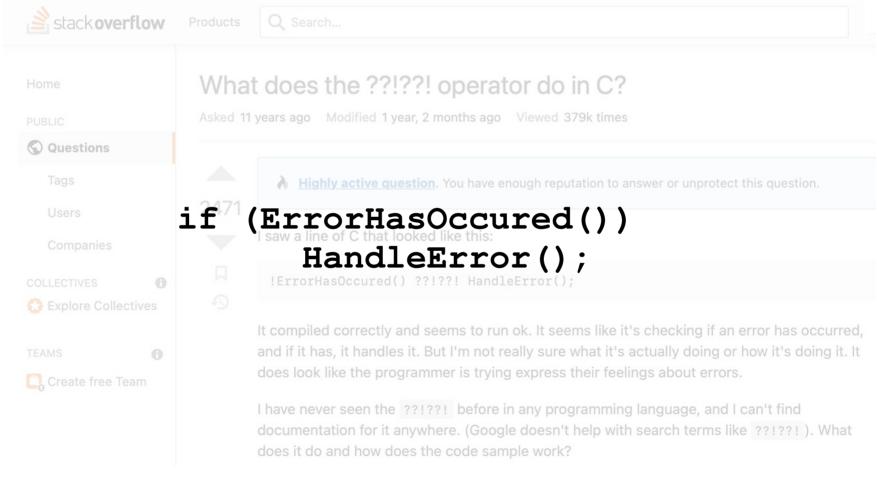
Avoid naming anti-patterns:

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).		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).		
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		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).		
A.3	"Set" method returns	type int (see Fig. 6). A set method having a return type different than void and not documenting the return type/values with an appropriate comment (see Fig. 7).		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).		
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).	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		
B.1	Not implemented condition	The comments of a method suggest a conditional behavior that is not implemented in the code. When the implementa-			whether a change affects one or multiple instances in the collection (see Fig. 18).		
		tion is default this should be documented (see Fig. 10).		Name suggests Boolean but	The name of an attribute suggests that its value is true or false, but its declaring type is not Boolean. Example: attribute		
Ry	Validation method does not	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). 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		type does not	isReached of type int[] where the declared type and values are not documented (see Fig. 19).		
	confirm				The name of an attribute suggests multiple instances, but its type suggests a single one. Example: attribute stats of		
B.3	"Get" method does not return			Says many but contains one	type Boolean. Documenting such inconsistencies avoids additional comprehension effort to understand the purpose of the attribute (see Fig. 20).		
		data is stored and how to obtain it (see Fig. 12).	-	A44-21-1	The name of an attribute is in contradiction with its type		
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]).		Attribute name and type are opposite	as they contain antonyms. Example: attribute start of type MAssociationEnd. The use of antonyms can induce wrong assumptions (see Fig. 21).		
B.5	Transform method does not re- turn	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).		Attribute signature and com- ment 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).

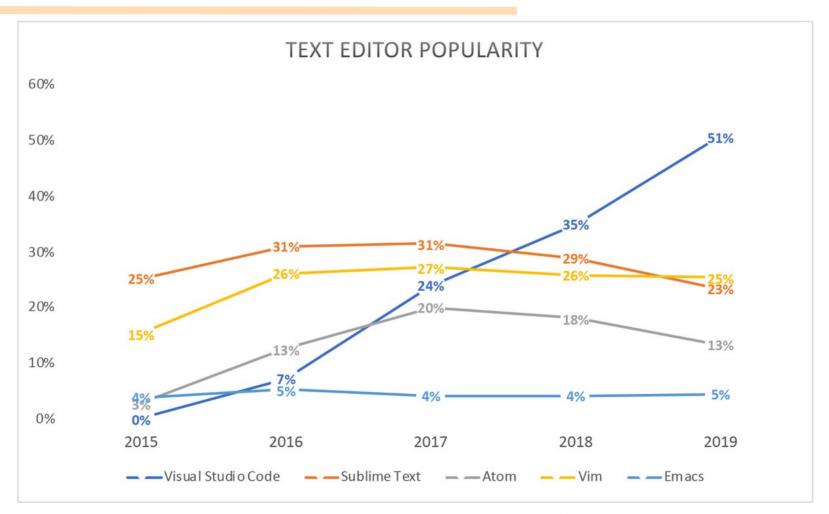


https://stackoverflow.com/questions/7825055/what-does-the-operator-do-in-c



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

1. Write for humans, not for computers (and learn your editor)



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

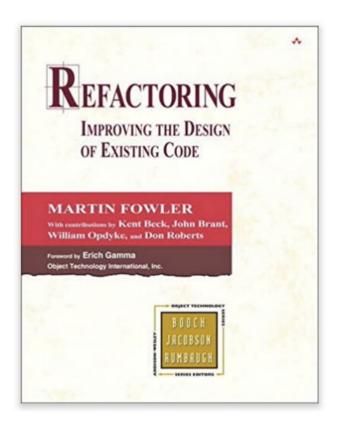
Scientific software specifications are always changing:

- 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)

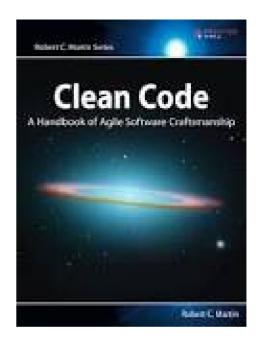
3 ½ . Avoid "code smells"

```
static MappedField validateQuerv(final Class clazz, final Mapper mapper, final StringBuilder origProp, final FilterOperator op, final
                MappedField mf = null;
final String prop origProp.toString();
boolean hasTranslations = false;
42
                                                                             What's a prop?
43
44
                if (!origProp.substring(0) 1).equals("$")) {
    final String[] parts | prop.split(regex: "\\.");
                                                                            -Whal's a part?
46
                    if (clazz == null) return null: }
47
                    MappedClass mc = mapper.getMappedClass(clazz);
48
                     //CHECKSTYLE:OFF
49
                    for (int i = 0; ; ) {
50
                         VCHECKSTYLE: ON
                        final String part = parts[i];
                        boolean fieldIsArrayOperator = part.equals("$");
                        mf = mc.getMappedField(part);
                        //translate from java field name to stored field name
                        if (mf == nul) && !fieldIsArrayOperator) {
                            mf = mc.getMappedFieldByJavaField(part);
                            if (validateNames && mf == null) {
                                throw new ValidationException (format("The field '%s' could not be found in '%s' while validating - %s; if you wis
61
                            hasTranslations = true:
                            if (mf != null)
                                parts[i] = mf.getNameToStore();
66
67
                            mf != null 66 mf.isMap()) {
                              skip the map key validation.
                                                                        Control the loop
                        if (i >= parts.length)
                            break;
                        if (!fieldIsArrayOperator)
                             //catch people trying to search/update into @Reference/@Serialized fields
                            if (validateNames 66 ! canQueryPast(mf)) {
                                throw new ValidationException(format("Cannot use dot-notation past '%s' in '%s'; found while validating - %s", pa
79
                            if (mf == null && mc.isInterface()) {
80
                                break;
                             else if (mf == null)
                                throw new ValidationException(format("The field '%s' could not be found in '%s'", prop, mc.getClazz().getName())
82
83
84
                          //get the next MappedClass for the next field validation
                            mc = mapper.getMappedClass((mf.isSingleValue()) ? mf.getType() : mf.getSubClass());
85
86
                                    Comments, because cade is unclear
87
88
                    //record new property string if there has been a translation to any part
89
                    if (hasTranslations) {
90
                       origorop.setlength(e); // clear existing content Parameter Mutation
91
92
                        origProp.append(parts[0]);
                        for (int i = 1; i < parts.length; i++) {
```



4. Follow good coding principles

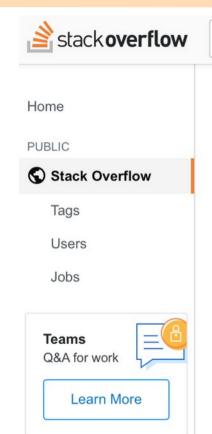
- Don't repeat yourself (DRY)
- Keep it simple (KISS)
- One level of abstraction
- Single responsibility principle
- Separation of concern
- Avoid premature optimization
- Follow style guidelines
- Many others...



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!



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



7883

Search

After reading <u>Hidden Features and Dark Corners of C++/STL</u> 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.

 $\overline{}$

Here's the code:



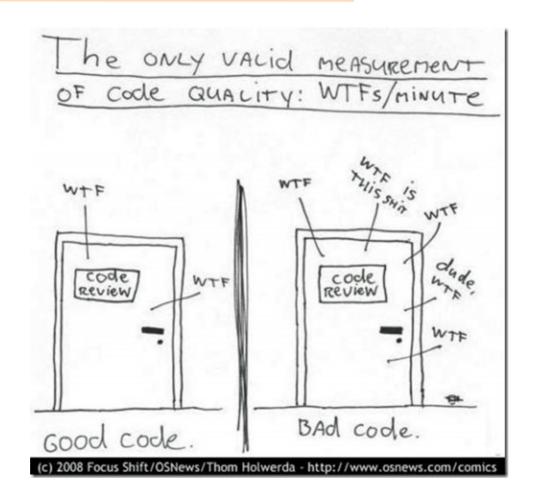
1831

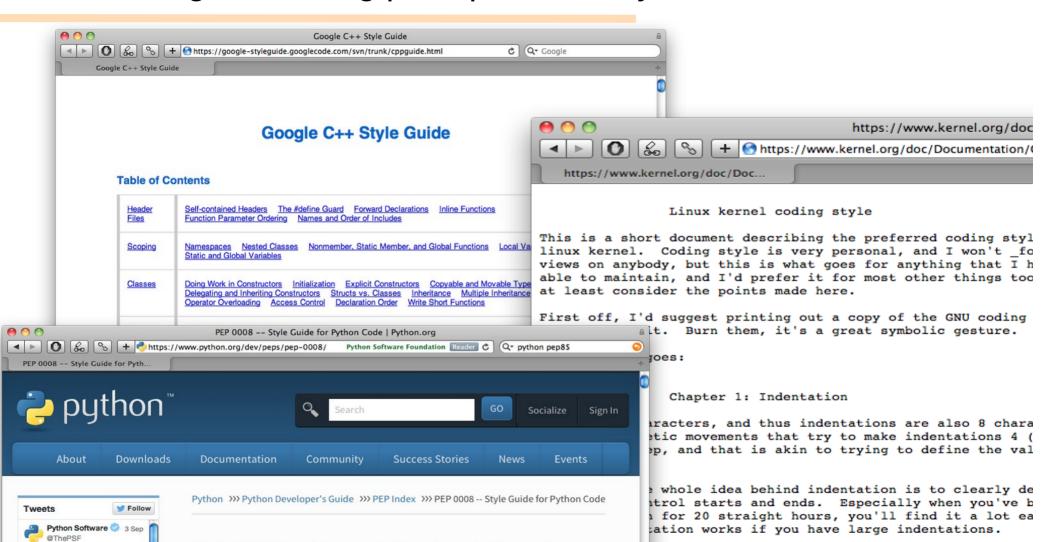
#include <stdio.h>
int main()
{
 int x = 10;
 while (x --> 0) // x goes to 0
 {
 printf("%d ", x);
 }
}

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

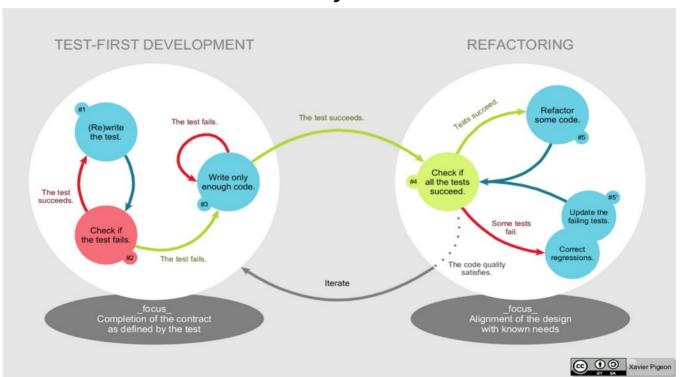






5. Plan for mistakes, automate testing; Test-driven development

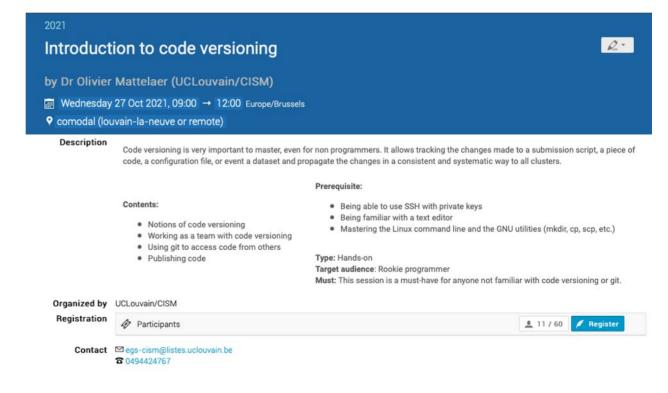
Write the tests before you even write the code



6. Use modern source-code management system



for your code, papers, thesis, etc.



7. Document the purpose and design, not the implementation

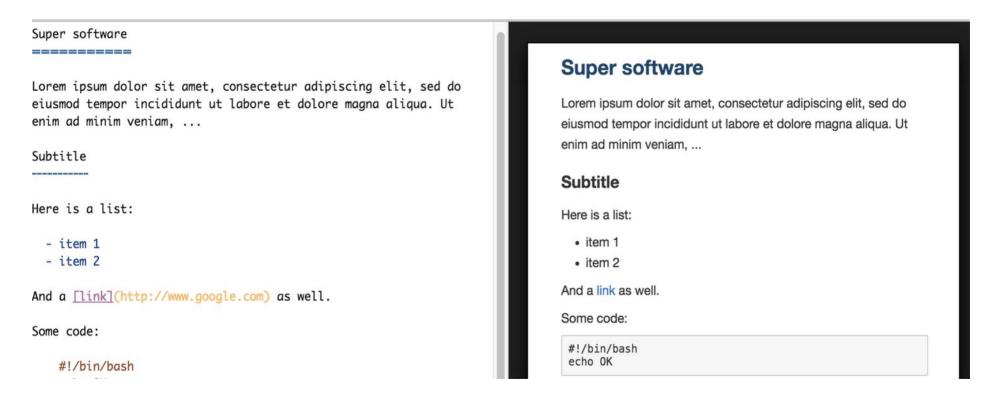
```
function res = f(base, num)
% Assign base to res
res = base
% loop from 2 to num
for i=2:num
% multiply current res by base
  res=base*res;
end
```

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 or RestructuredText

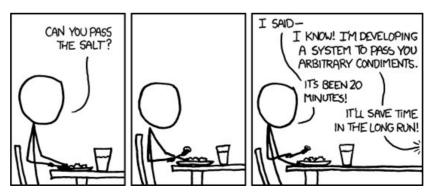


8. Optimize only when it works already

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 (do not close doors either)



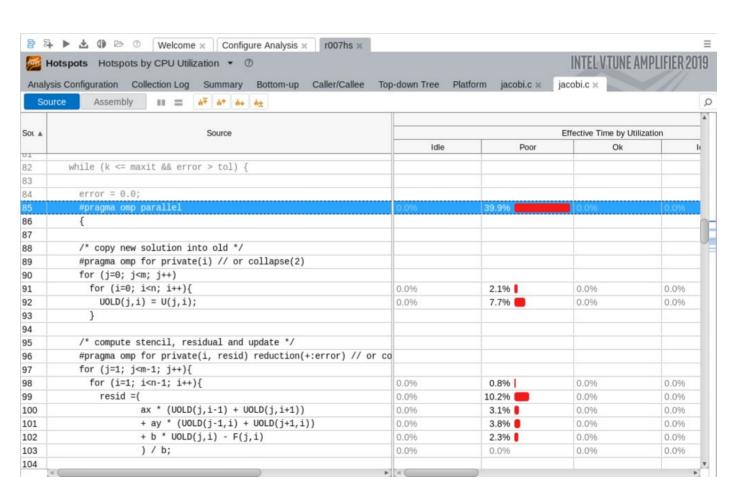
https://xkcd.com/974/

8. Optimize only when it works already

Use a profiler



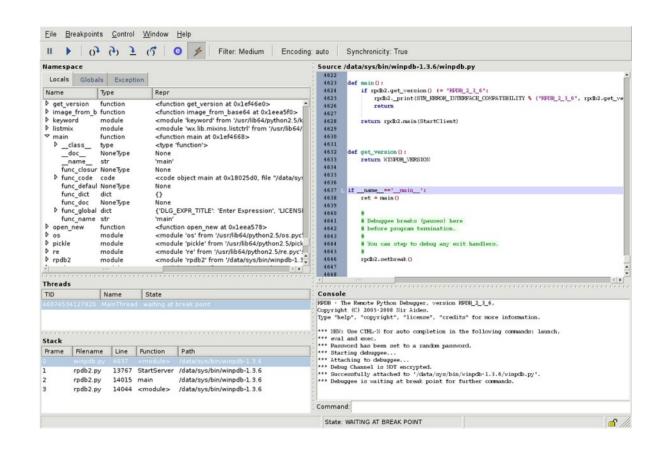
Incorporate benchmarks in your tests



9. Debug cleverly

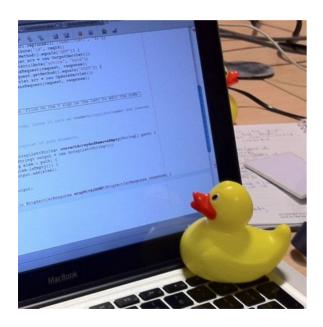
Use a debugger





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.

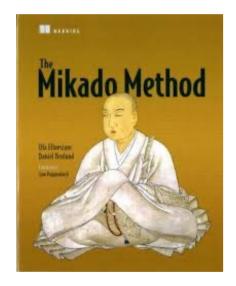
At some point, if you get hesitant, that is probably where the bug is!

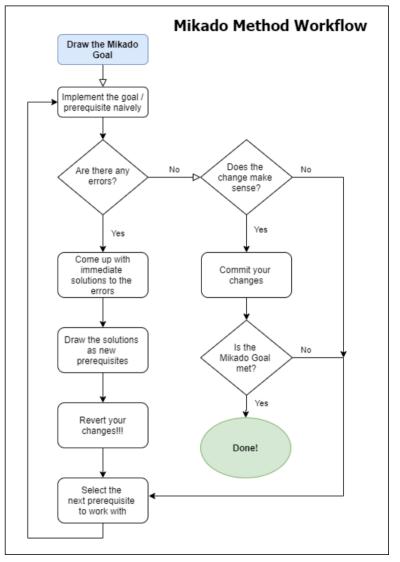
Dig that part of the code until you are confident again that it works.

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

9. Debug cleverly

Use a method



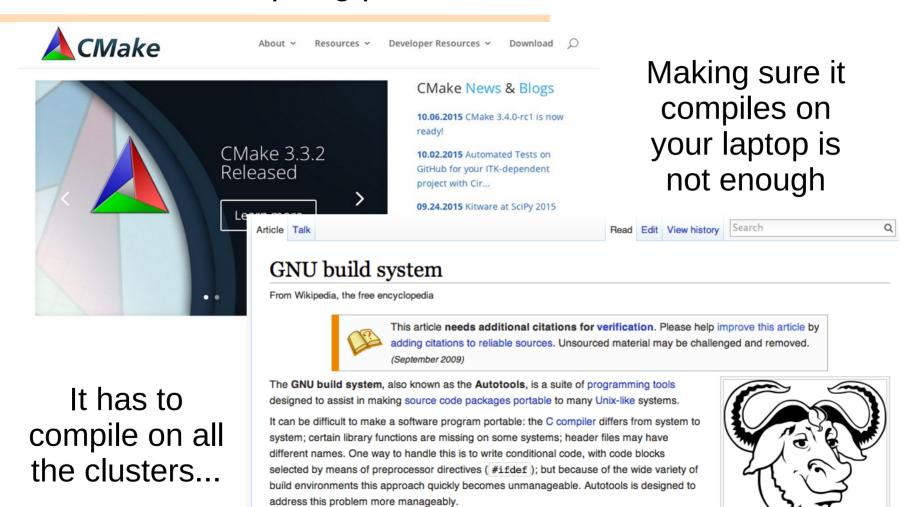


The Mikado Method, O. Ellnestam & D. Brolund, Manning, 2014

"... to make them ... **shareable** ..., *efficiently*"

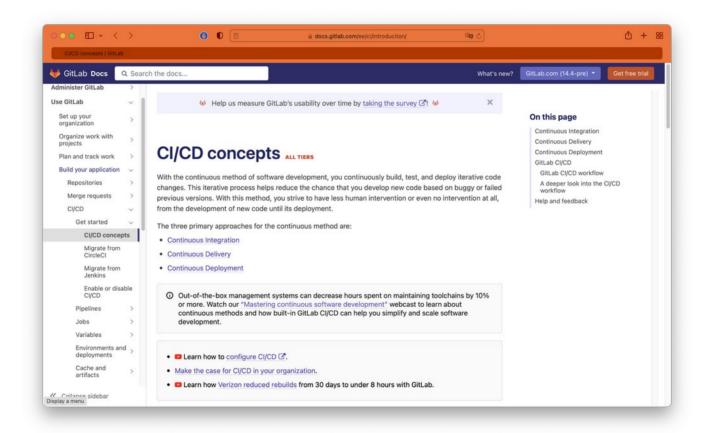
- 1. Automate the compiling process
- 2. Learn about containers
- 3. License your code

1. Automate the compiling process

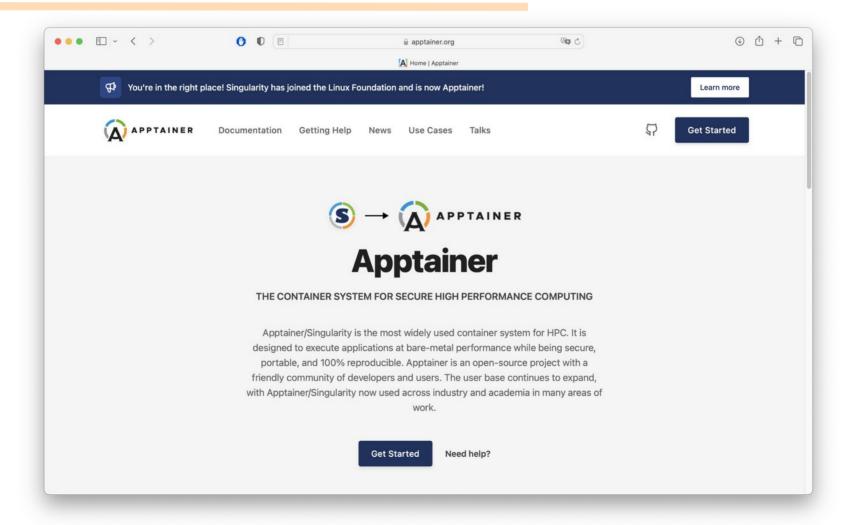


Autotools is part of the GNU toolchain and is widely used in many free software and open

1. Automate the compiling process



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

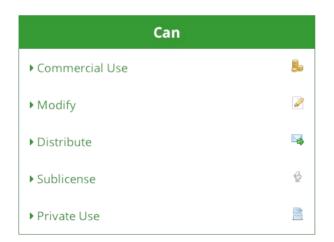
3. License your code: e.g. MIT

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

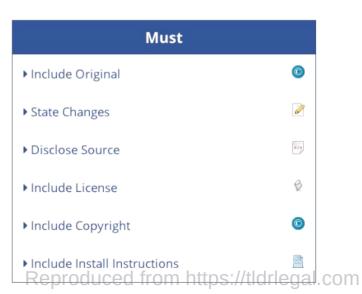












3. License your code: finding help



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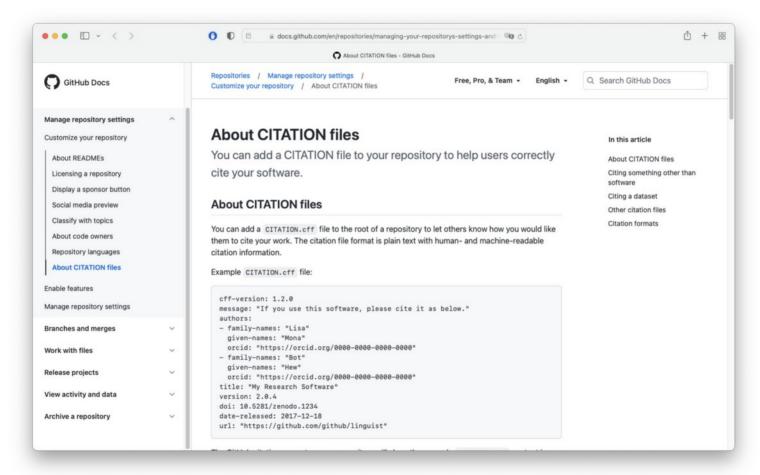
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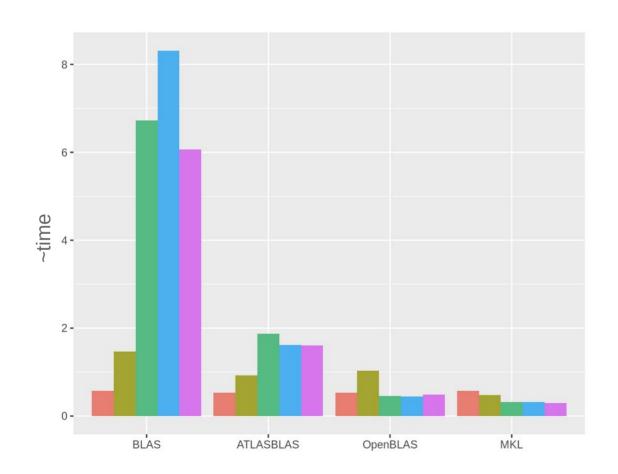
3 ½. GitHub CITATION files

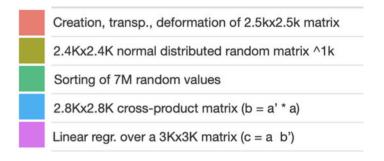


"... to make them ... **fast** ..., *efficiently*"

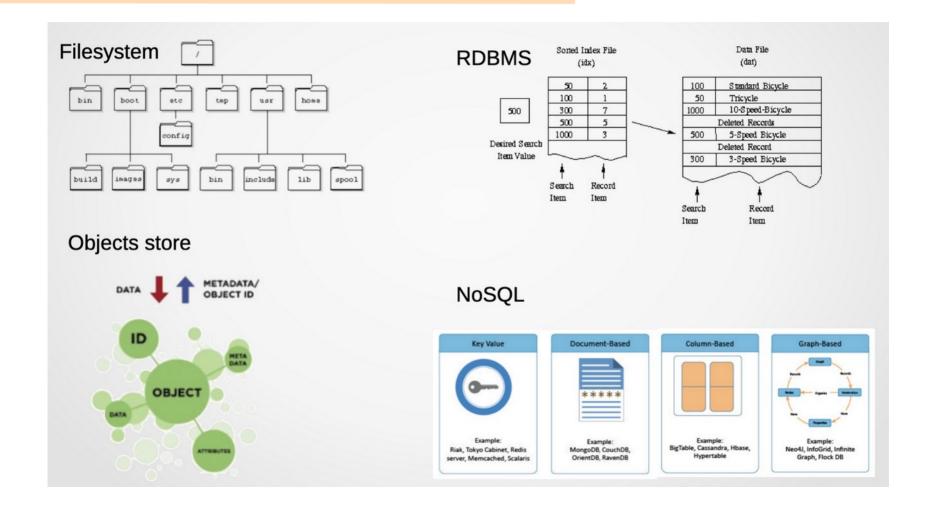
- 1. Use optimized libraries
- 2. Choose the right storage system
- 3. Think parallel from the start
- 4. Integrate checkpoint/restart from the start

1. Use optimized libraries





2. Choose the right storage system



3. Think parallel from the start

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

```
begin=0, end=10
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
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

```
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 = 1 .. 10
    res[i] = ( data[xi]^2 + data[yi]^2 )
end

end

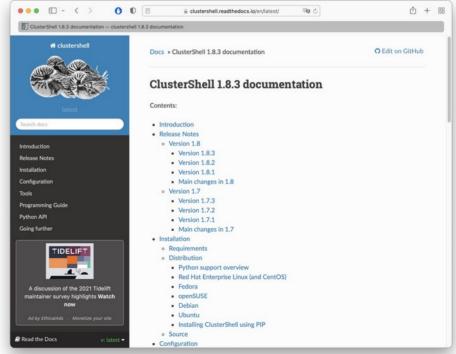
res[i] = ( data[xi]^2 + data[yi]^2 )
    save(res, i)
end
```

" ..., 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.
GNU Emacs 26.1
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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
       [all]
       lemaitre3 short_name="lm3"
       nic5
                short name="nic5"
       File: playbook.yml
      - hosts:
          lemaitre3
          - nic5
        tasks:
          - name: Upload templated file
            template: src=myfile dest=. mode=700
      File: myfile
       This cluster's short name is {{ short_name }}
```



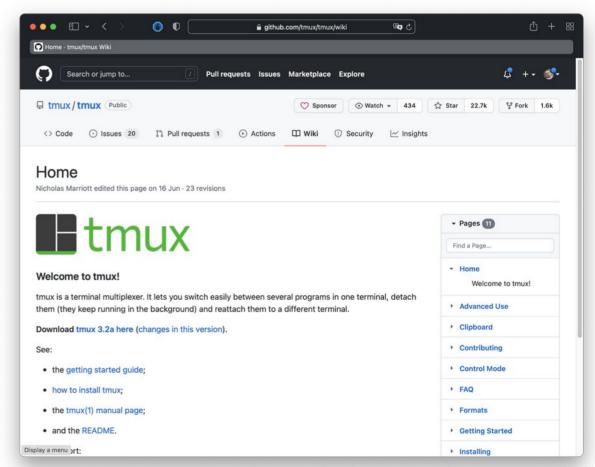
2. Master configuration management

```
ansible-playbook -i inventory playbook.yml --diff
ok: [lemaitre3]
-- before: ./mvfile
+++ after: /Users/dfrancois/.ansible/tmp/ansible-local-40594k4ng0g9g/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]
lemaitre3
                     : ok=2
                                      unreachable=0
                                                    failed=0
                                                             skipped=0
                                                                       rescued=0
                                                                                 ianored=0
nic5
                     : ok=2
                            changed=1
                                                   failed=0
                                                            skipped=0
                                      unreachable=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
```



EasyBuild EasyBuild @PyPi docs @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
- 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.

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
                    <- Makefile with commands like 'make data' or 'make train'
                    <- The top-level README for developers using this project.
 README.md
 data
  - external
                    <- Data from third party sources.
   - interim
                    <- Intermediate data that has been transformed.
  - processed
                    <- The final, canonical data sets for modeling.
                    <- The original, immutable data dump.
 - docs
                    <- A default Sphinx project: see sphinx-doc.org for details
                    <- Trained and serialized models, model predictions, or model summaries
 models
                    <- Jupyter notebooks. Naming convention is a number (for ordering).

    notebooks

                       the creator's initials, and a short '-' delimited description, e.g.
                        `1.0-igp-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'
                    <- makes project pip installable (pip install -e .) so src can be imported
- setup.pv
                    <- Source code for use in this project.
   -- __init__.py
                    <- Makes src a Python module
   - data
                    <- Scripts to download or generate data
      __ make_dataset.pv
                    <- Scripts to turn raw data into features for modeling

    features

      build_features.py
   - models
                    <- Scripts to train models and then use trained models to make
      — predict model.pv
      train_model.py
  visualization <- Scripts to create exploratory and results oriented visualizations</p>
      - 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!!!

3-2-1 Backup Rule

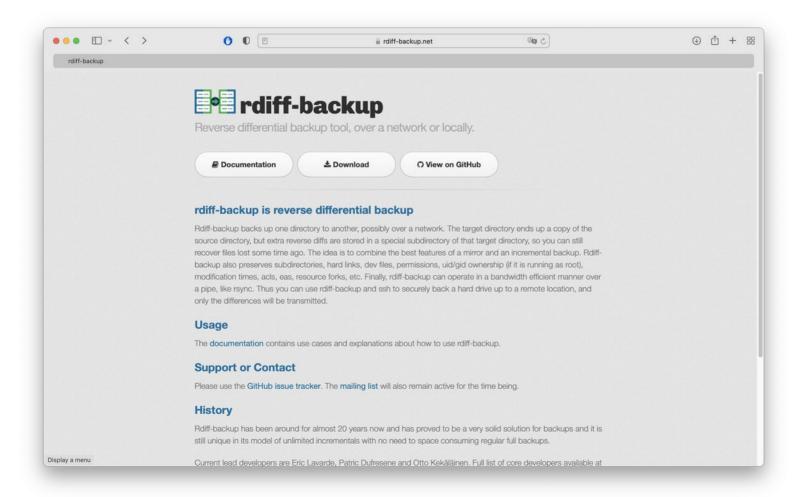


Maintain at least 3 copies of your data

Keep 2 copies stored at separate locations

Store at least 1 copy at an off-site location

6. BACKUPS!!!



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

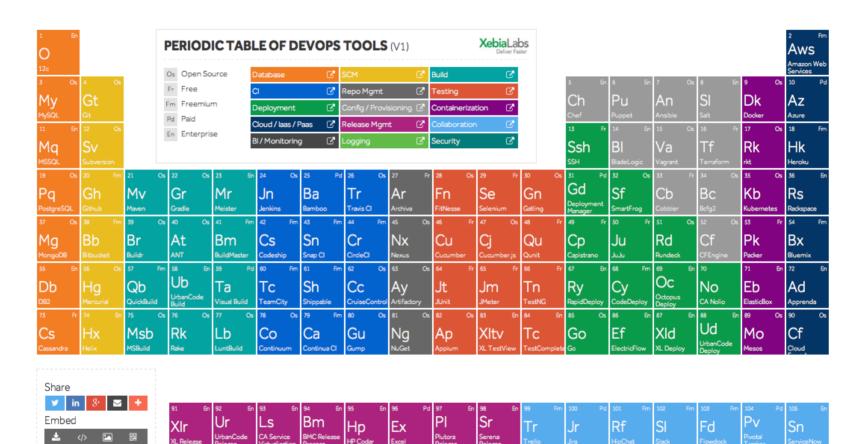
The "Phillip test" (by Philip Guo)

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, rerun 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



111

Gr

Sn

Gr

Lg

Су

Gg

ICt

Become Excellent!

✓ Subscribe here!

Ki