



Consortium des Équipements
de Calcul Intensif
en Fédération Wallonie-Bruxelles

Introduction to Scientific Software Deployment and Development

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



What is this?



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 O 12c	2 Fm Aws Amazon Web Services																
3 Os My MySQL	4 Os Gt GT																
11 En Mq MSSQL	12 Os Sv Subversion																
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 Juju	51 Os Rd Rundeck	52 Os Cf CFEngine	53 Fr Pk Packer	54 Fm Bx Bluemix
55 En Db DB2	56 Os Hg Mercurial	57 Fm Qb QuickBuild	58 En Ub UrbanCode Build	59 Pd Ta Visual Build	60 Fm Tc TeamCity	61 Fm Sh Shippable	62 Os Cc CruiseControl	63 Os Ay Artifactory	64 Fr Jt JUnit	65 Fr Jm JMeter	66 Fr Tn TestNG	67 En Ry RapidDeploy	68 Fm Cy CodeDeploy	69 En Oc Octopus Deploy	70 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 Continuum 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 Foundry

Share



Embed



Become Excellent!



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 Pivotal 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:



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

Dev's toolkit :



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

1. Programming language



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

1. Programming language



Be aware of the 'other' paradigm...

Imperative – “Do this”
BASIC, Assembly

Structured – Subroutines, scopes
C, FORTRAN77

algorithms + data : good for explicit computing

Object-Oriented – Encapsulation, Inheritance, ...
C++, Python

objects + messages : good for modeling

Declarative – “I need this”
SQL

Functional – Pure functions, lazy evaluation
Haskell, Scala

functions o functions : good for reasoning

Logic – Predicates and rules
Prolog, Datalog

facts + rules : good for searching

1. Programming language

C

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

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

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

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

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

Haskell

```
qsort [] = []

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

Purely functional
Static strong typing
Lazy evaluation

2. Good practices



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

2. Good practices



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

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

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

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

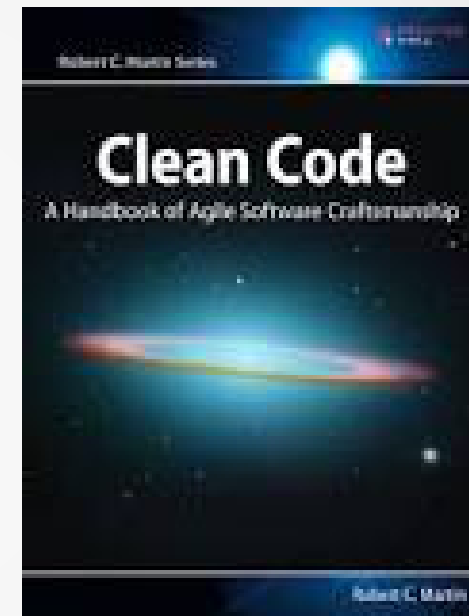
Victor R. Basili, Jeffrey C. Carver, Daniela Cruzes, Lorin M. Hochstein, Jeffrey K. Hollingsworth, Forrest Shull, Marvin V. Zelkowitz, "Understanding the High-Performance-Computing Community: A Software Engineer's Perspective," *IEEE Software*, vol. 25, no. 4, pp. 29-36, July/August, 2008

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

2. Good coding principles



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

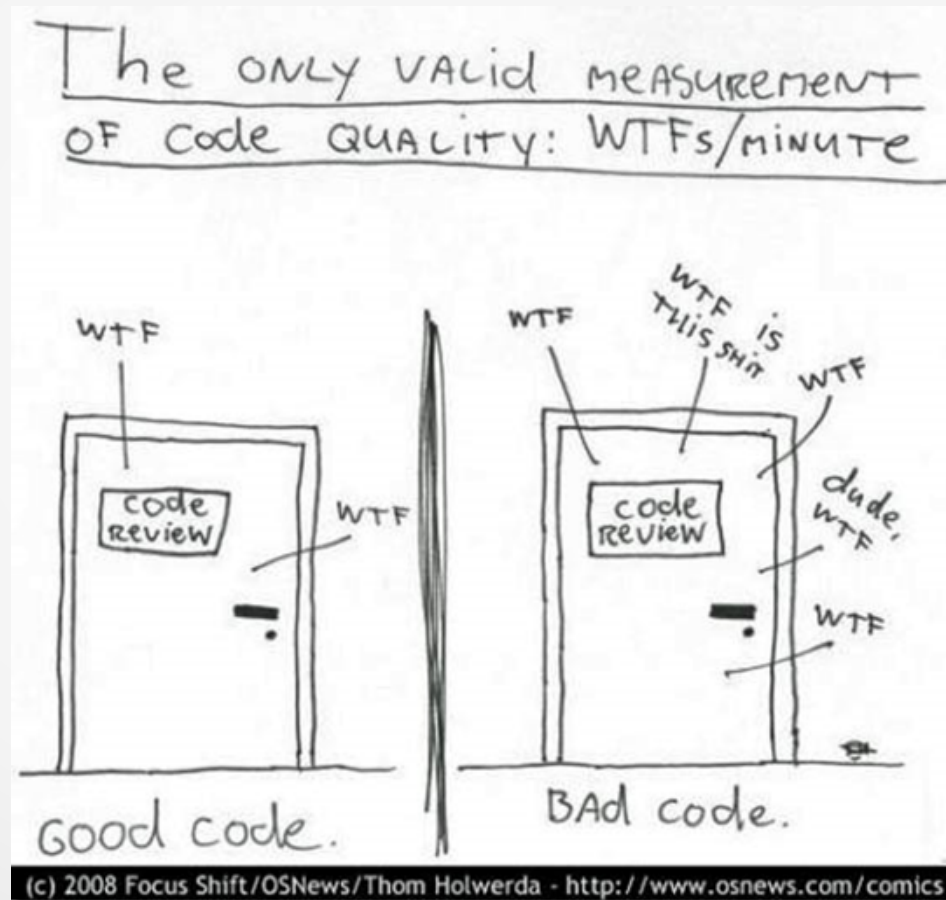


Bill Mitchell View profile More options Sep 26 1991, 1:57 am In article <5...@ksr.com>
j...@ksr.com (John F. Woods) writes:

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

Damn right!

How to measure code quality



2. Good style

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

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

VS

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

2. Good style



Search...



Home

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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?

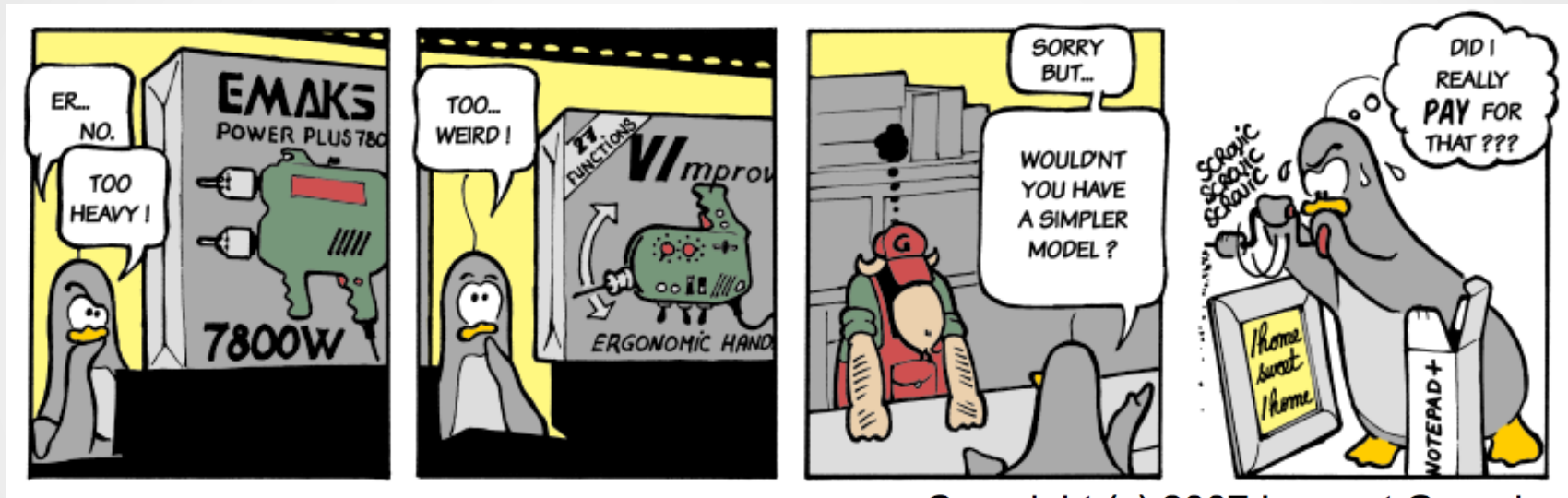
3. Text editor

- Some files are better edited directly on the clusters;



- If you prefer a graphical user interface, some good candidates are:
 - Sublime text: <http://www.sublimetext.com/>
 - Notepad++: <https://notepad-plus-plus.org/>
 - Text Wrangler: <http://www.barebones.com/>
 - Textmate: <https://macromates.com/>
 - Atom: <https://atom.io/>
- Choose one and learn it from inside out

3. Text editor



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Dev's toolkit :



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

} Own dedicated sessions

7. Packaging Fortran/C/C++ code



Making sure it
compiles on your
laptop is not
enough

A screenshot of the CMake website. The top navigation bar includes 'About', 'Resources', 'Developer Resources', and 'Download'. A large banner on the left features the CMake logo and the text 'CMake 3.3.2 Released'. To the right, there is a 'CMake News & Blogs' section with three entries: '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...', and '09.24.2015 Kitware at SciPy 2015'. Below the news section, there are tabs for 'Article' and 'Talk', and a search bar with 'Read', 'Edit', and 'View history' options.

It has to compile
on all the
clusters...

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](#)



8. Comments / Documentation



Lots of useless comments

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

Less comments but useful comments

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

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

Super software

=====

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

Subtitle

Here is a list:

- item 1
- item 2

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

Some code:

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

Super software

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

Subtitle

Here is a list:

- item 1
- item 2

And a [link](#) as well.

Some code:

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

9. Tests - TDD



3 Testing methods

3.1 Static vs. dynamic testing

3.2 The box approach

3.2.1 White-box testing

3.2.2 Black-box testing

3.2.2.1 Visual testing

3.2.3 Grey-box testing

4 Testing levels

4.1 Unit testing

4.2 Integration testing

4.3 Component interface testing

4.4 System testing

4.5 Operational Acceptance testing

5 Testing types

5.1 Installation testing

5.2 Compatibility testing

5.3 Smoke and sanity testing

5.4 Regression testing

5.5 Acceptance testing

5.6 Alpha testing

5.7 Beta testing

5.8 Functional vs non-functional testing

5.9 Continuous testing

5.10 Destructive testing

5.11 Software performance testing

5.12 Usability testing

5.13 Accessibility testing

5.14 Security testing

5.15 Internationalization and localization

5.16 Development testing

5.17 A/B testing

5.18 Concurrent testing

5.19 Conformance testing or type testing

Information and Software Technology 56 (2014) 1219–1232

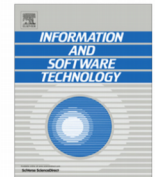
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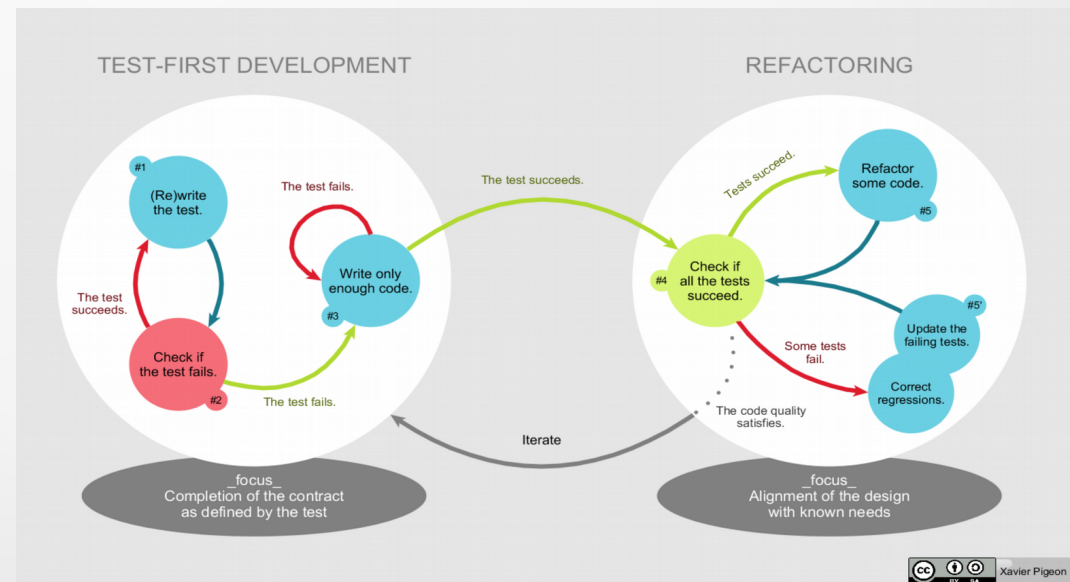


Testing scientific software: A systematic literature review



Upulee Kanewala*, James M. Bieman

Computer Science Department, Colorado State University, USA



10. Licensing your code: Why?



- **Commercial reason :**
 - you want to make money out of it – forbid distribution
 - forbid reverse engineering
- **Scientific reason :**
 - you want to it to be used and get citations
 - you need to allow usage, and/or modification, etc.
 - you require others to cite your work
 - you want to protect yourself from liability claims

10. Licensing your code: How?



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

10. Licensing your code: MIT



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

Cannot	
▶ Hold Liable	

Must	
▶ Include Copyright	
▶ Include License	

10. Licensing your code: BSD, GPL



BSD

Can	
▶ Commercial Use	
▶ Modify	
▶ Distribute	
▶ Place Warranty	

Cannot	
▶ Use Trademark	
▶ Hold Liabile	

Must	
▶ Include Copyright	
▶ Include License	

GPL

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

Cannot	
▶ Sublicense	
▶ Hold Liabile	

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

Ops' toolkit :



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

1. Virtualization

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

“vagrant up”



1. Virtualization

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

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

Vagrant.configure(VAGRANTFILE_API_VERSION) do |config|

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

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

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

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

2. Multi-host SSH



```
dfr@ncois — bash
dfr@ncois:~ $ pdsh -g ceci hostname
nic4: master2
hmem: hmem00.cism.ucl.ac.be
vega: node001
hercules: hercules
dragon1: dragon1-h1.umons.ac.be
lemaitre2: lemaitre2.cism.ucl.ac.be
dfr@ncois:~ $
```

```
dfr@ncois — bash
dfr@ncois:~ $ ansible 'ceci' -m lineinfile -a "dest='~/
.bashrc' line='# Test'"
hmem | success >> {
  "backup": "",
  "changed": true,
  "msg": "line added"
}
vega | success >> {
  "backup": "",
  "changed": false,
  "msg": ""
}
lemaitre2 | success >> {
  "backup": "",
  "changed": false,
  "msg": ""
}
```

3. Configuration Management



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

# Slurm submit template

#SBATCH --partition={{ partition_list }}

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

3. Configuration Management



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

PLAY [all] *****

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

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

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

dfr@ncois:~ $ █
```

3. Configuration Management



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

# Slurm submit template

#SBATCH --partition=High,Medium,Low

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

# Slurm submit template

#SBATCH --partition=def,PostP

srun ./myprog
dfr@ncois:~ $ █
```

4. Easy installing



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
- 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. Easy installing



```
dfr@manneback:~$ eb -S . 2>/dev/null | head -20
== temporary log file in case of crash /tmp/eb-_Y2XSC/easybuild-18L_LH.log
== Searching (case-insensitive) for '.' in /usr/lib/python2.6/site-packages/easybuild_easyconfigs-2.3.0-py2.6.egg/easybuild/easyconfigs
CFGS1=/usr/lib/python2.6/site-packages/easybuild_easyconfigs-2.3.0-py2.6.egg/easybuild/easyconfigs
* $CFGS1/TEMPLATE.eb
* $CFGS1/a/ABAQUS/ABAQUS-6.12.1-linux-x86_64.eb
* $CFGS1/a/ABAQUS/ABAQUS-6.13.5-linux-x86_64.eb
* $CFGS1/a/ABAQUS/ABAQUS-6.14.1-linux-x86_64.eb
* $CFGS1/a/ABINIT/ABINIT-7.0.3-x86_64_linux_gnu4.5.eb
* $CFGS1/a/ABINIT/ABINIT-7.0.5-x86_64_linux_gnu4.5.eb
* $CFGS1/a/ABINIT/ABINIT-7.10.4-intel-2015a-incl-deps.eb
* $CFGS1/a/ABINIT/ABINIT-7.10.4-intel-2015a.eb
* $CFGS1/a/ABINIT/ABINIT-7.11.6-intel-2015a.eb
* $CFGS1/a/ABINIT/ABINIT-7.2.1-x86_64_linux_gnu4.5.eb
* $CFGS1/a/ABINIT/ABINIT-7.4.3-goolf-1.4.10-ETSF_IO-1.0.4.eb
* $CFGS1/a/ABYSS/ABYSS-1.3.4-goalf-1.1.0-no-OFED-Python-2.7.3.eb
* $CFGS1/a/ABYSS/ABYSS-1.3.4-goolf-1.4.10-Python-2.7.3.eb
* $CFGS1/a/ABYSS/ABYSS-1.3.4-ictce-4.0.6-Python-2.7.3.eb
* $CFGS1/a/ABYSS/ABYSS-1.3.4-ictce-5.3.0-Python-2.7.3.eb
* $CFGS1/a/ABYSS/ABYSS-1.3.6-goolf-1.4.10-Python-2.7.5.eb
* $CFGS1/a/ABYSS/ABYSS-1.3.7-intel-2015a-Python-2.7.9.eb
dfr@manneback:~$ eb -S . | cut -d/ -f3 | sort -u | wc -l
742
dfr@manneback:~$
```



4. Easy installing



CDE: Automatically create portable Linux applications

CDE (formerly known as CDEpack) automatically packages up the **C**ode, **D**ata, and **E**nvironment required to deploy and run your Linux programs on other machines without any installation or configuration. CDE is the easiest way to completely eliminate [dependency hell](#).

To get started, download the CDE binary ([32-bit](#) or [64-bit](#)) and follow these steps:

1. Package



Prepend any set of Linux commands with the "cde" binary, and CDE will run them and automatically package up all files (e.g., executables, libraries, plug-ins, config/data files) accessed during execution.

2. Deliver



A package is simply a directory that can be compressed and delivered to any x86-Linux machine. It contains all the files and environment variables required to run your original commands. Packages can range from 10 to 100 MB in size.

3. Run



After receiving the package, the user can now run those same commands from within the package on **any** modern x86-Linux distro. The user does not need to first compile, install, or configure anything.

4. Easy installing

A screenshot of the AppImage website. The page has a teal background. At the top left is the 'AppImage' logo. To the right are navigation links: 'Documentation', 'Source', 'Wiki', and 'Community'. Further right is a 'Star' button with a GitHub icon and the number '1,844'. On the left side, there is a large blue square icon with a white downward arrow and a gear. To the right of this icon, the text 'Linux apps that run anywhere' is displayed in white. Below this text are two user testimonials in white text. At the bottom center, there is a small, faint warning icon (a triangle with an exclamation mark).

4. Easy installing



Shifter vs Charlie Cloud vs Docker vs Singularity

	Shifter	Charlie Cloud	Docker	Singularity
Privilege model	SUID	UserNS	Root Daemon	SUID/UserNS
Support current production Linux distros	Yes	No	No	Yes
Internal image build/bootstrap	No*	No*	No**	Yes
No privileged or trusted daemons	Yes	Yes	No	Yes
No additional network configurations	Yes	Yes	No	Yes
No additional hardware	Maybe	Yes	Maybe	Yes
Access to host filesystem	Yes	Yes	Yes***	Yes
Native support for GPU	No	No	No	Yes
Native support for InfiniBand	Yes	Yes	No	Yes
Native support for MPI	Yes	Yes	No	Yes
Works with all schedulers	No	Yes	No	Yes
Designed for general scientific use cases	Yes	No	No	Yes
Contained environment has correct perms	Yes	No	Yes	Yes
Containers are portable, unmodified by use	No	No	No	Yes
Trivial HPC install (one package, zero conf)	No	Yes	Yes	Yes
Admins can control and limit capabilities	Yes	No	No	Yes

* Relies on Docker

** Depends on upstream

*** With security implications



4. Easy installing



Linuxbrew

The Homebrew package manager for Linux

Download .zip

Download .tar.gz

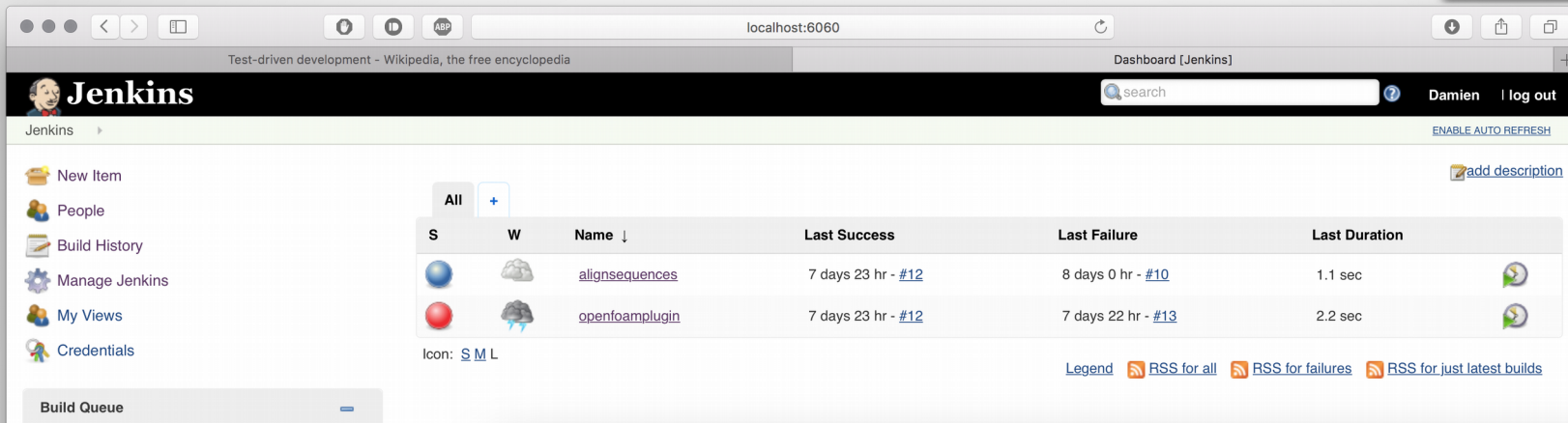


Linuxbrew

tag v1.2.2

Linuxbrew is a fork of [Homebrew](#), the macOS package manager, for Linux.

5. Automatic build tests



Test-driven development - Wikipedia, the free encyclopedia

Dashboard [Jenkins]

Jenkins

Search: Damien | log out

ENABLE AUTO REFRESH

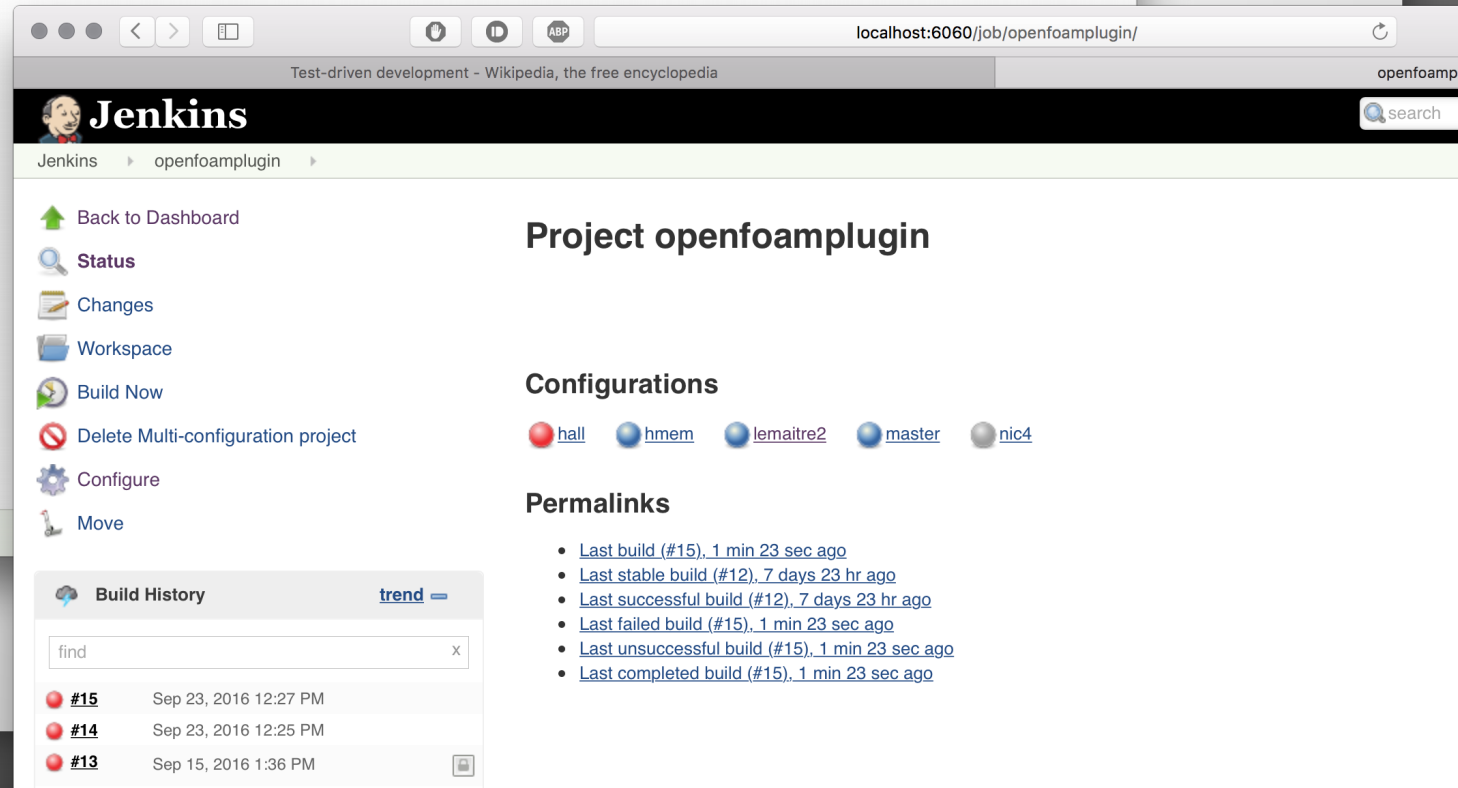
add description

All +

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

icon: [S](#) [M](#) [L](#)

[Legend](#) [RSS for all](#) [RSS for failures](#) [RSS for just latest builds](#)



Test-driven development - Wikipedia, the free encyclopedia

openfoamplugin

Jenkins

Back to Dashboard

Status

Changes

Workspace

Build Now

Delete Multi-configuration project

Configure

Move

Project openfoamplugin

Configurations

hall hmem lemaitre2 master nic4

Permalinks

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

Build History

trend

find

#15	Sep 23, 2016 12:27 PM
#14	Sep 23, 2016 12:25 PM
#13	Sep 15, 2016 1:36 PM

6. Monitoring



`multitail -q 2 "**/res"`

- [main](#)
- [features](#)
- [examples](#)
- [screenshots!](#)
- [download](#)
- [to do](#)

```
dfr@hmem00.cism.ucl.ac.be b/res (Fri Oct 16 12:57:23 2015) [0.020000] — bash
1
2
3
4 General info
5 █
What is it in short?
MultiTail allows you to monitor logfiles and
00] a/res
1
2
3
4
5
6
7
01] b/res
01] b/res
```

```
dfr@hmem00.cism.ucl.ac.be c/res (Fri Oct 16 13:07:23 2015) [0.010000] — bash
1
2
3
4
5 █
00] a/res
3
4
5
6
7
8
01] b/res
1
02] c/res
```

Useful with command 'screen'

6. Monitoring



Name: lucid (1) swatch.1p.gz
Provided by: swatch_3.2.3-1_all 🐛

Synopsis

Description

Command Line Options

The Configuration File

Special Option

For Perl Hacks Only

Configuration Example

See Also

Notes

Author

Availability

NAME
swatch - simple watcher

SYNOPSIS

```
swatch [ --awk-file FILE ] [ --extra-include-dir DIR ] [ --help | -h ] [ --input FILE ] [ --pid-file FILE ] [ --restart-time TIME ] [ --script-dir PATH ] [ --tail-args ARGUMENTS ] [ --tail-program NAME ] [ --tail-program-name FILENAME ] [ --version ] [ file_to_examine ] | [ --tail-file FILE ] [ --debug [ level ] ] [ --dump-script filename ]
```

DESCRIPTION

Swatch is designed to monitor system activity. In order for Swatch to be useful, it requires a configuration file which contains pattern(s) to look for and action(s) to perform when each pattern is found.

```
dfr@hmem00 -- bash
dfr@hmem00:~/test-mt $ cat ~/.swatchrc
watchfor /warning/ -style-config | -O
echo
mail addresses=damien.francois@uclouvain.be, subject=Alert
dfr@hmem00:~/test-mt $ swatch --tail-file **/*res
*** swatch version 3.2.3 (pid:41469) started at Fri Oct 16 12:54:48 CEST 2015
warning
```

```
From: Damien Francois (damien.francois@uclouvain.be) <dfr@hmem.cism.ucl.ac.be>
Subject: Alert
Date: 16 Oct 2015 12:54:52 GMT+02:00
To: Damien François <damien.francois@uclouvain.be>
```

warning

Dev's toolkit :



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

Ops' toolkit :



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

The 'Phillip' test



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

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

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

Work quicker & more reliably



PERIODIC TABLE OF DEVOPS TOOLS (V1)																		XebiaLabs Deliver Faster		2
1	3		4															2		
O 12c En	My MySQL Os		Gt Git Os															Aws Amazon Web Services Fm		
11	12																10			
Mq MSSQL En	Sv Subversion Os																Az Azure Pd			
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36			
Pq PostgreSQL Os	Gh Github Fm	Mv Maven Os	Gr Gradle Os	Mr Meister En	Jn Jenkins Os	Ba Bamboo Pd	Tr Travis CI Os	Ar Archiva Fr	Fn FitNesse Os	Se Selenium Fr	Gn Gatling Os	Gd Deployment Manager Pd	Sf SmartFrog Os	Cb Cobbler Fr	Bc Bcfq2 Os	Kb Kubernetes Os	Rs Rackspace En			
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54			
Mg MongoDB Os	Bb Bitbucket Fm	Br Buildr Os	At ANT Os	Bm BuildMaster Fm	Cs Codeship Fm	Sn Snap CI Fm	Cr CircleCI Fm	Nx Nexus Os	Cu Cucumber Fr	Cj Cucumber.js Os	Qu Qunit Fr	Cp Capistrano Fr	Ju Juju Fr	Rd Rundeck Os	Cf CFEngine Os	Pk Packer Fr	Bx Bluemix Fm			
55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72			
Db DB2 En	Hg Mercurial Os	Qb QuickBuild Fm	Ub UrbanCode Build En	Ta Visual Build Pd	Tc TeamCity Fm	Sh Shippable Fm	Cc CruiseControl Os	Ay Artifactory Os	Jt JUnit Fr	Jm JMeter Fr	Tn TestNG Fr	Ry RapidDeploy En	Cy CodeDeploy Fm	Oc Octopus Deploy En	No CA Nolio Os	Eb ElasticBox En	Ad Apprenda Fm			
73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90			
Cs Cassandra Fr	Hx Helix En	Msb MSBuild Os	Rk Rake Os	Lb LunrBuild Os	Co Continuum Os	Ca Continua CI Fm	Gu Gump Os	Ng NuGet Os	Ap Appium Os	Xltv XL TestView En	Tc TestComplete En	Go Go Os	Ef ElectricFlow En	Xld XL Deploy En	Ud UrbanCode Deploy En	Mo Mesos Os	Cf Cloud Os			

PERIODIC TABLE OF DEVOPS TOOLS (V1)

Legend:

- Os: Open Source
- Fr: Free
- Fm: Freemium
- Pd: Paid
- En: Enterprise

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

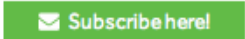
Share



Embed



Become Excellent!



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