Reproducible Research at the Cloud Era

Overview, Hands-on and Open Challenges

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http://RR-tutorials.rtfd.io

Before the tutorial starts: Visit
https://goo.gl/l9mCsM

for *preliminary setup instructions*!

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Summary

About me

https://varrette.gforge.uni.lu

- **2003 – 2007**: PhD between INP Grenoble & UL
  - ↪ *Security in Large Scale Distributed Systems: Authentication and Result Checking*
- **2007 – now**: *Research Associate* at UL
  - ↪ Part of the PCOG Team led by Prof. P. Bouvry
  - ↪ Manager of the UL High Performance Computing Facility
    - ✓ ≃ 197 **T**Flops (2017), 5.844 **P**B, 4 sysadmins

Research Interests: Distributed Computing Platforms

- Security (crash/cheating faults, obfuscation) in DGVCS
- Performance of HPC/cloud platforms
  - ↪ Energy Efficiency, Performance, Cost...

Disclaimer: Acknowledgements

- A **large** part of these slides were **courtesy** borrowed, with permission, from:
  - ↪ Lucas Nussbaum (INRIA, Univ. Lorraine)
  - ↪ Arnaud Legrand (INRIA, Univ. Grenoble)
  - ↪ Valentin Plugaru (Univ. of Luxembourg)
  - ↪ and many others...

- In particular, to know more about **Reproducible Research**:
  - ↪ Webinars on Reproducible Research `https://github.com/alegrand/RR_webinars`
  - ↪ Reproducible build `https://reproducible-builds.org/`
    - ✓ initiative of various free software projects

...

Agenda: Dec. 12th, 2016

Time	Session
09:00 – 10:00	Reproducible Research in Computer Science
10:00 – 10:30	Hands-On: Build these slides using Vagrant
10:30 – 11:00	**Coffee Break**
11:00 – 11:30	Hands-On: Reproducible Software Environment with Easybuild
	Hands-On: Docker
	Reproducible Results
12:15 –	**Lunch**

Tutorial Pre-Requisites / Setup

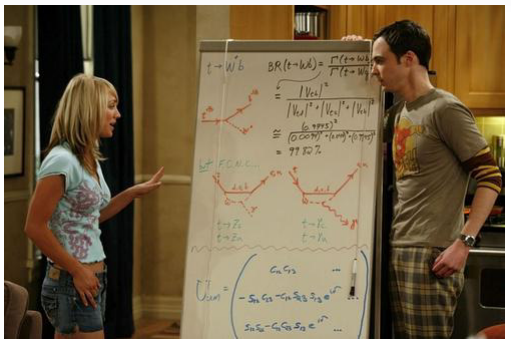
http://RR-tutorials.readthedocs.io/en/latest/setup/

- Create (if need) accounts for the **cloud services** we will use:
  - ↪ Github, Vagrant Cloud and Docker Hub
- Install **mandatory software**, *i.e.* (apart from Git):
  - ↪ Virtual Box https://www.virtualbox.org/
  - ↪ Vagrant https://www.vagrantup.com
  - ↪ Docker https://www.docker.com/
- Check installed software and download the boxes we will use:

```
$> git clone https://github.com/Falkor/RR-tutorials.git
$> cd RR-tutorials
$> make setup
$> vagrant up &&  docker pull ubuntu:14.04  # might take some time...
```

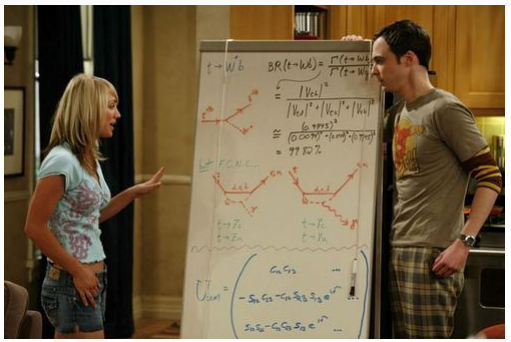
Summary

Validation in (Computer) Science



- Two classical approaches for validation:
  - ↪ **Formal**: equations, proofs, etc.
  - ↪ **Experimental**, on a scientific instrument
- Often a mix of both:
  - ↪ In Physics
  - ↪ In Computer Science
- Quite a lot of **formal** work in Computer Science
- But also quite a lot of experimental validation
  - ↪ Distributed computing, networking
    - ✓ testbeds: IoT-LAB, Grid'5000...
  - ↪ Language/image processing ⇝ evaluations using large corpuses

Validation in (Computer) Science



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How good are we at performing experiments?

(Poor) State of Experimentation in CS

- **1994**: survey of 400 papers[1]
  - ↪ among published CS articles in ACM journals
  - ↪ **40%-50%** of those **requiring** an experimental validation **had none**
- **1998**: survey of 612 papers[2]
  - ↪ too many papers have **no experimental validation at all**
  - ↪ too many papers use an informal (assertion) form of validation
  - ↪ 2009 update: situation is improving[3]

[1] Paul Lukowicz et al. "Experimental Evaluation in Computer Science: A Quantitative Study". In: **Journal of Systems and Software** 28 (1994), pages 9–18.

[2] M.V. Zelkowitz and D.R. Wallace. "Experimental models for validating technology". In: **Computer** 31.5 (May 1998), pages 23–31.

[3] Marvin V. Zelkowitz. "An update to experimental models for validating computer technology". In: **J. Syst. Softw.** 82.3 (Mar. 2009), pages 373–376.

(Poor) State of Experimentation in CS

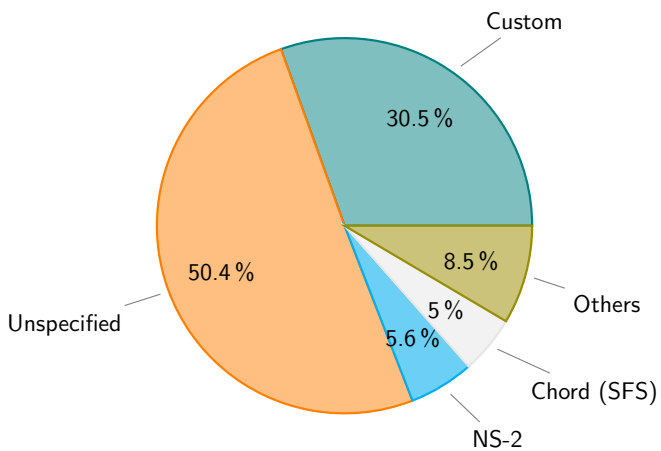
- Most papers **do not use** even basic statistical tools
  - ↪ Papers published at the Europar conference[4]

Year	#Papers	With error bars	Percentage
2007	89	5	5.6%
2008	89	3	3.4%
2009	86	2	2.4%
2010	90	6	6.7%
2011	81	7	8.6%
2007-2001	**435**	**23**	**5.3%**

[4] Study carried out by E. Jeannot.

(Poor) State of Experimentation in CS

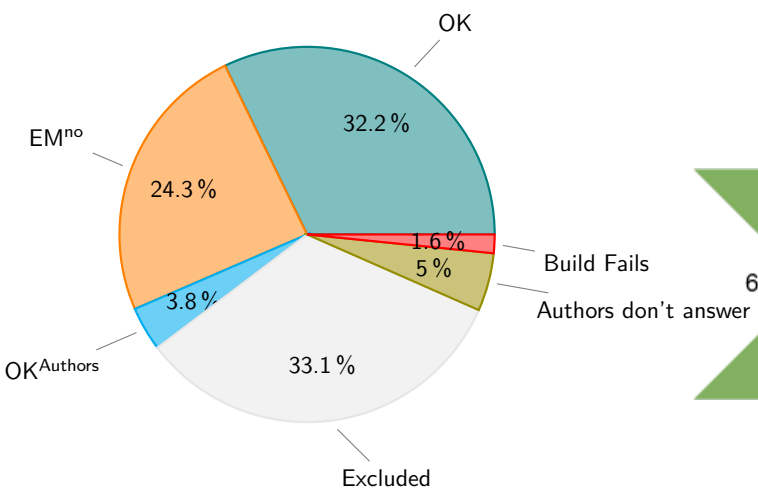
- **2007**: Survey of simulators used in P2P research[5]
  - ↪ 287 papers surveyed on P2P networking subject
  - ↪ **141** of these papers **reports the use of a simulator**
    - ✓ 30% use a custom tool
    - ✓ 50% don't report the used tool!

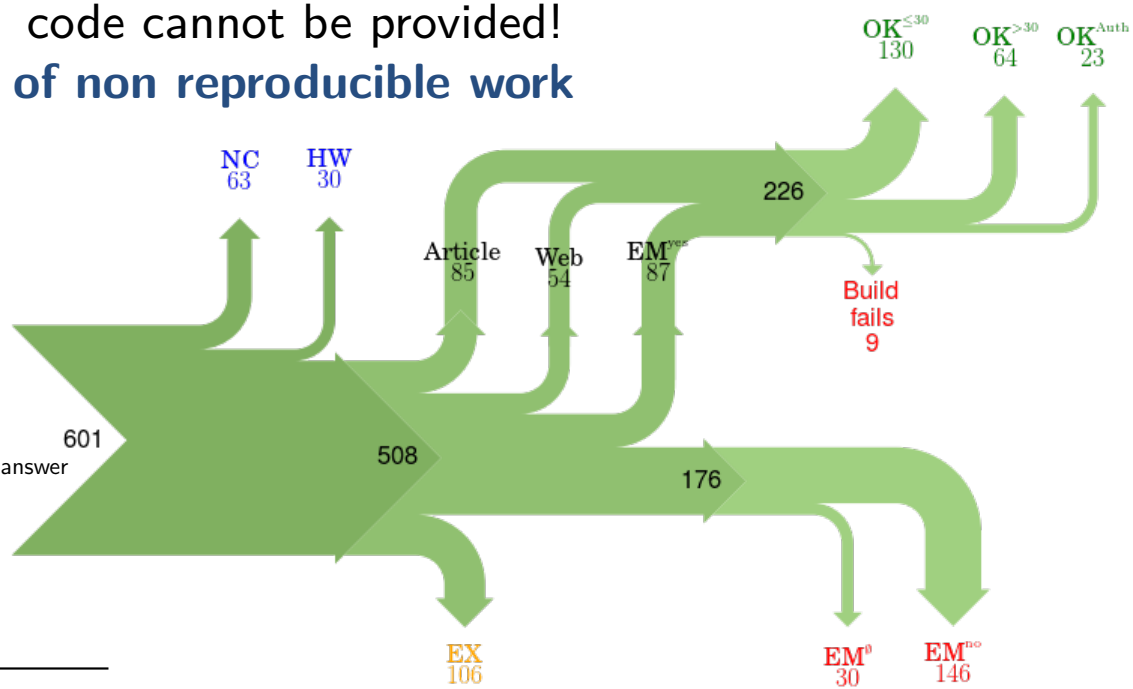


[5] S. Naicken et al. "The state of peer-to-peer simulators and simulations". In: **SIGCOMM Comput. Commun. Rev.** 37.2 (Mar. 2007), pages 95–98.

(Poor) State of Experimentation in CS

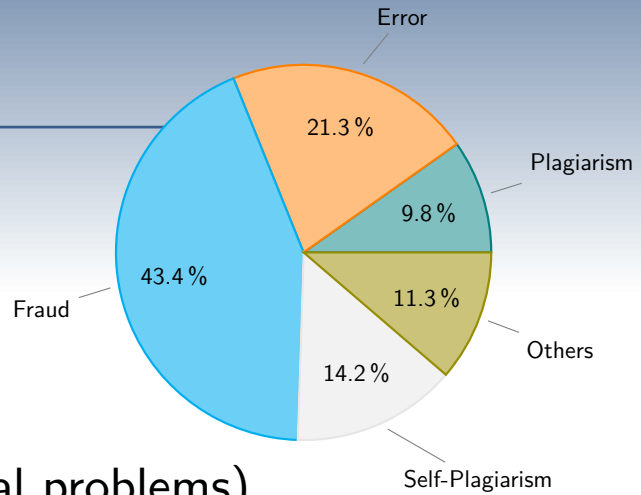
- **2015**: **601 papers** from ACM conferences and journals analysed[6]
  - ↪ **Obj.**: attempt to locate any source code that backed up the published results; **if found, try to build the code**.
  - ↪ EM^{no} (**146 papers!**): code cannot be provided!
  - ↪ Original study: **80% of non reproducible work**





[6] Christian Collberg et al. **Repeatability and Benefaction in Computer Systems Research**. Technical report. http://reproducibility.cs.arizona.edu/. Feb. 2015.

And in Other Sciences?



- **Biology**: Increase in **retracted papers**[7],
  - ↪ **Fraud** (data fabrication or falsification)
  - ↪ **Error** (plagiarism, scientific mistake, ethical problems)
    - ✓ see also Reproducibility: A tragedy of errors[8]
    - ✓ cf.Duke University scandal with scientific misconduct on lung cancer
  - ↪ High number of **failing clinical trials**
    - ✓ Do We Really Know What Makes Us Healthy?, 2007
    - ✓ Lies, Damned Lies, and Medical Science, 2010
- **Psychology**:
  - ↪ unreplicable study about extrasensory perception (ESP)
- **Machine Learning**: Trouble at the lab, The Economist, 2013

  *According to some estimates, three-quarters of published scientific papers in the field of machine learning are bunk because of this "overfitting". **Sandy Pentlan, MIT***

[7] R Grant Steen. "Retractions in the scientific literature: is the incidence of research fraud increasing?" In: **J Med Ethics** 37 (2011). http://dx.doi.org/10.1136/jme.2010.040923, pages 249–253.

[8] David B. Allison et al. **Reproducibility: A tragedy of errors**. http://www.nature.com/news/reproducibility-a-tragedy-of-errors-1.19264. Feb. 2016.

And in Other Sciences?

- **Medicine**: Study shows lower fertility for mices exposed to transgenic maize (AFSSA report[9])
  - ↪ Several calculation errors have been identified
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  - ↪ caused by timing system failure in 2012

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- ☹: Not everything is perfect
- ☺: But some errors are properly identified
  - ↪ Stronger experimental culture in other (older?) sciences?
  - ↪ Long history of costly experiments, scandals, ...

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What About You (as Rewiever) ?

> *"This may be an interesting contribution but. . . "*

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- There is no label/legend/. . . What is the **meaning of this graph**?
  - ↪ If only I could access the generation script

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- **Which code / data set** did I use to generate this figure?
- It **worked yesterday**!
- 6 months later: just **why** did I do that?

Why is it Hard to Reproduce? (any Scientific Work)

- **Human error**:
  - ↪ Experimenter **bias** *crowdsourced research?*
  - ↪ Programming **errors** or data manipulation **mistakes**
  - ↪ Poorly selected statistical test
- There is just **no real incentive in doing so**:
  - ↪ Legal barriers, **copyright** *Many ongoing discussions in US*
  - ↪ **Competition** issue *researchware, bibliometry, ...*
  - ↪ Publication **bias** *only the idea matters, not the gory details...*
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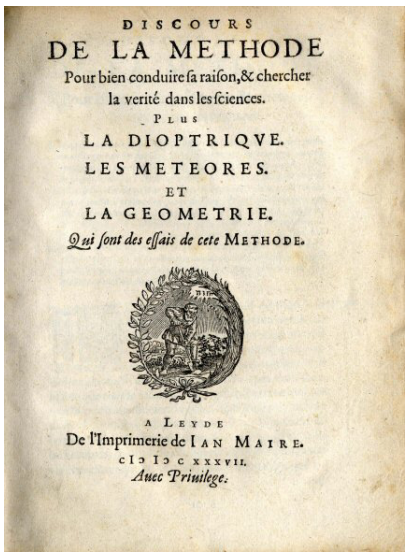
- **Technical difficulty**:
  - ↪ ~~Hardware and software evolve too quickly. It's not worth it~~
  - ↪ ~~No resources for storing so much data/information~~
  - ↪ ~~Lack of easy-to-use tools~~

Summary

Reproducible Research Movement

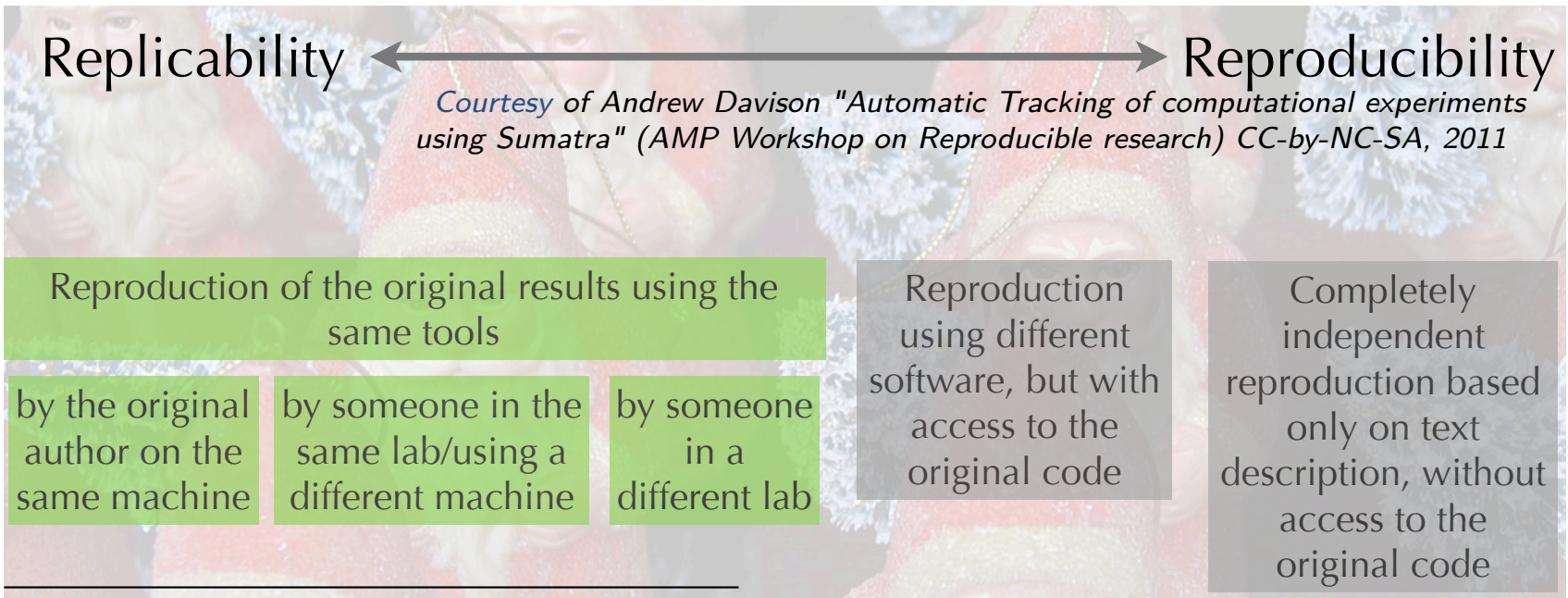
- Originated mainly in **Computational Sciences**
  - ↪ Computational biology, data-intensive physics, etc.
- Explores methods and tools to enhance experimental practices
  - ↪ Enable others to reproduce and build upon one's work

- **Nothing New**
  - ↪ Fundamental basis of the scientific method
  - ↪ K. Poppler, 1934: *non-reproducible single occurrences are of no significance to science*


DISCOURS
DE LA METHODE
Pour bien conduire sa raison,& chercher la verité dans les sciences.
PLUS
LA DIOPTRIQVE.
LES METEORES.
ET
LA GEOMETRIE.
Qui sont des essais de cette METHODE.
A LEYDE
De l'Imprimerie de IAN MAIRE.
cIↃ IↃ c XXXVII.
Avec Privilege.

Replicability vs. Reproducibility

- Terminology varies[10]
  - ↪ **Replicability** ∼ same result
  - ↪ **Reproducibity** ∼ same scientific conclusions



[10] Dror G. Feitelson. **From Repeatability to Reproducibility and Corroboration**. Technical report. http://www.cs.huji.ac.il/~feit/papers/Repeat15SIGOPS.pdf. Hebrew University of Jerusalem, 2015.

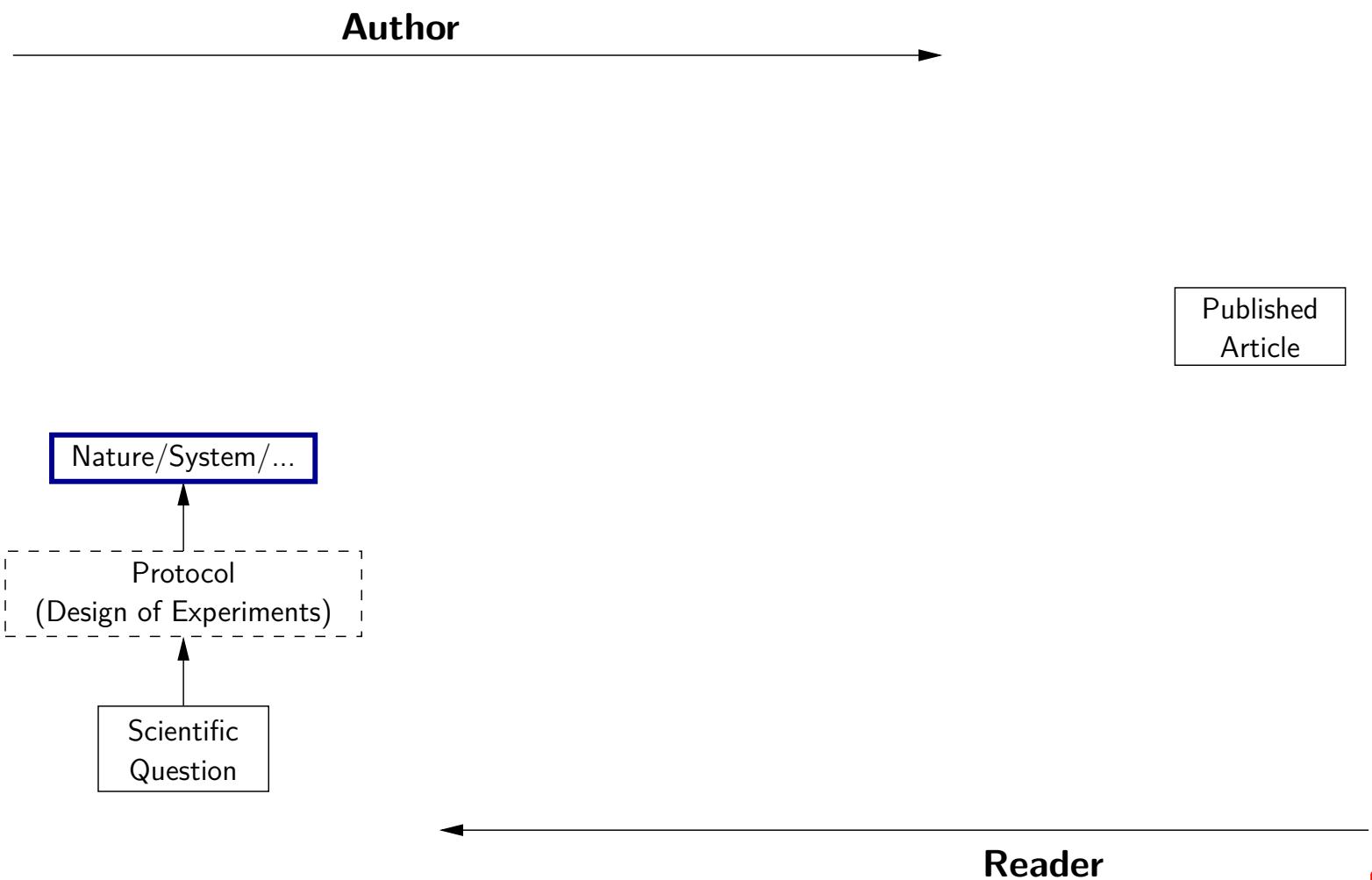
Reproducibility in Practice

Reproducibility (Wikipedia)

- the ability of an entire experiment or study to be **reproduced**,
  - ↪ either by the researcher
  - ↪ or by someone else working independently.
- One of the main principles of the scientific method.

- For an experiment involving software, reproducibility means:
  - ↪ **open access** to the scientific article describing it
  - ↪ **open data** sets used in the experiment
  - ↪ **source code** of all the components
  - ↪ **environment** of execution
  - ↪ **stable references** between all this

The Research Pipeline



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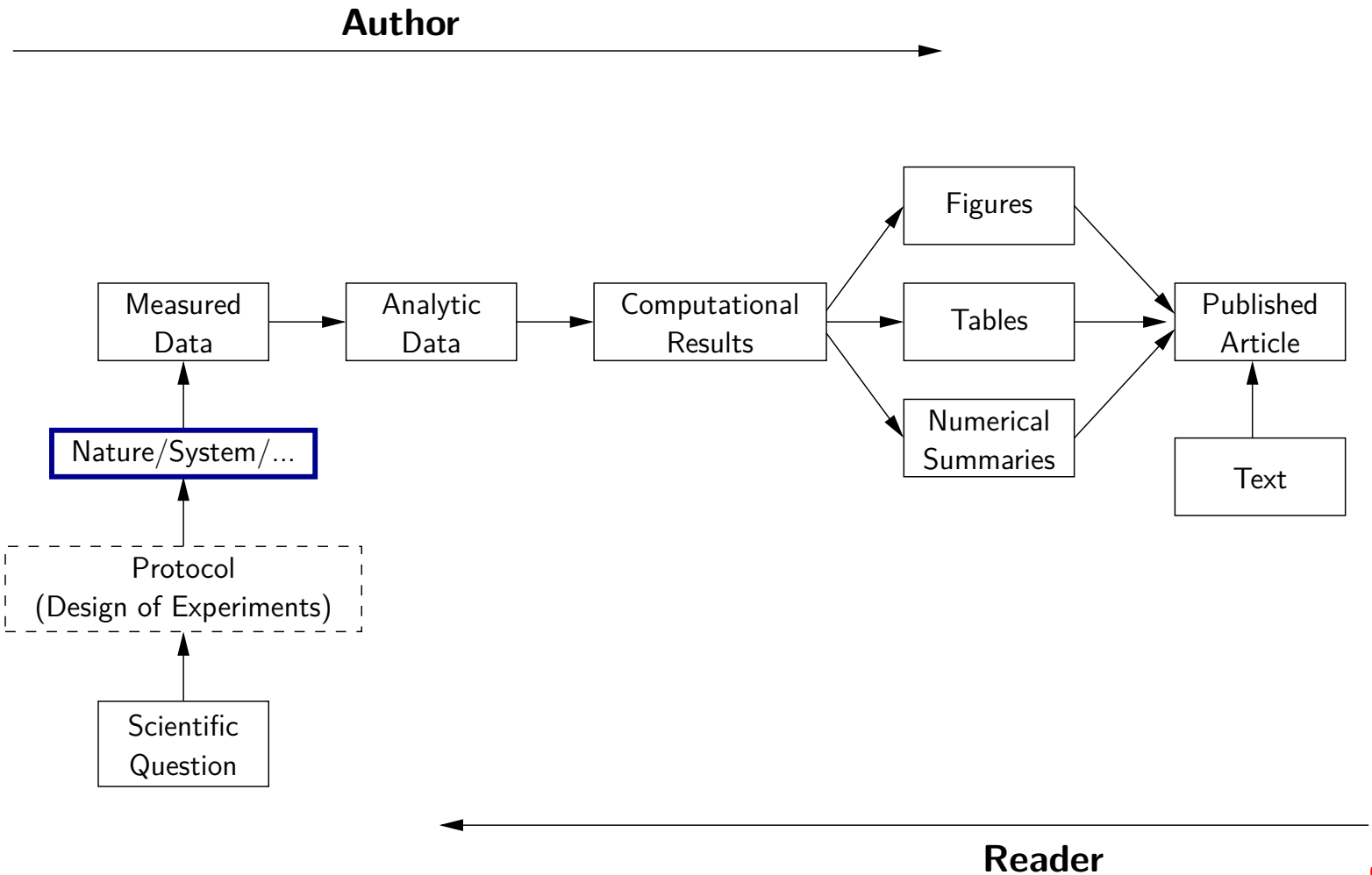

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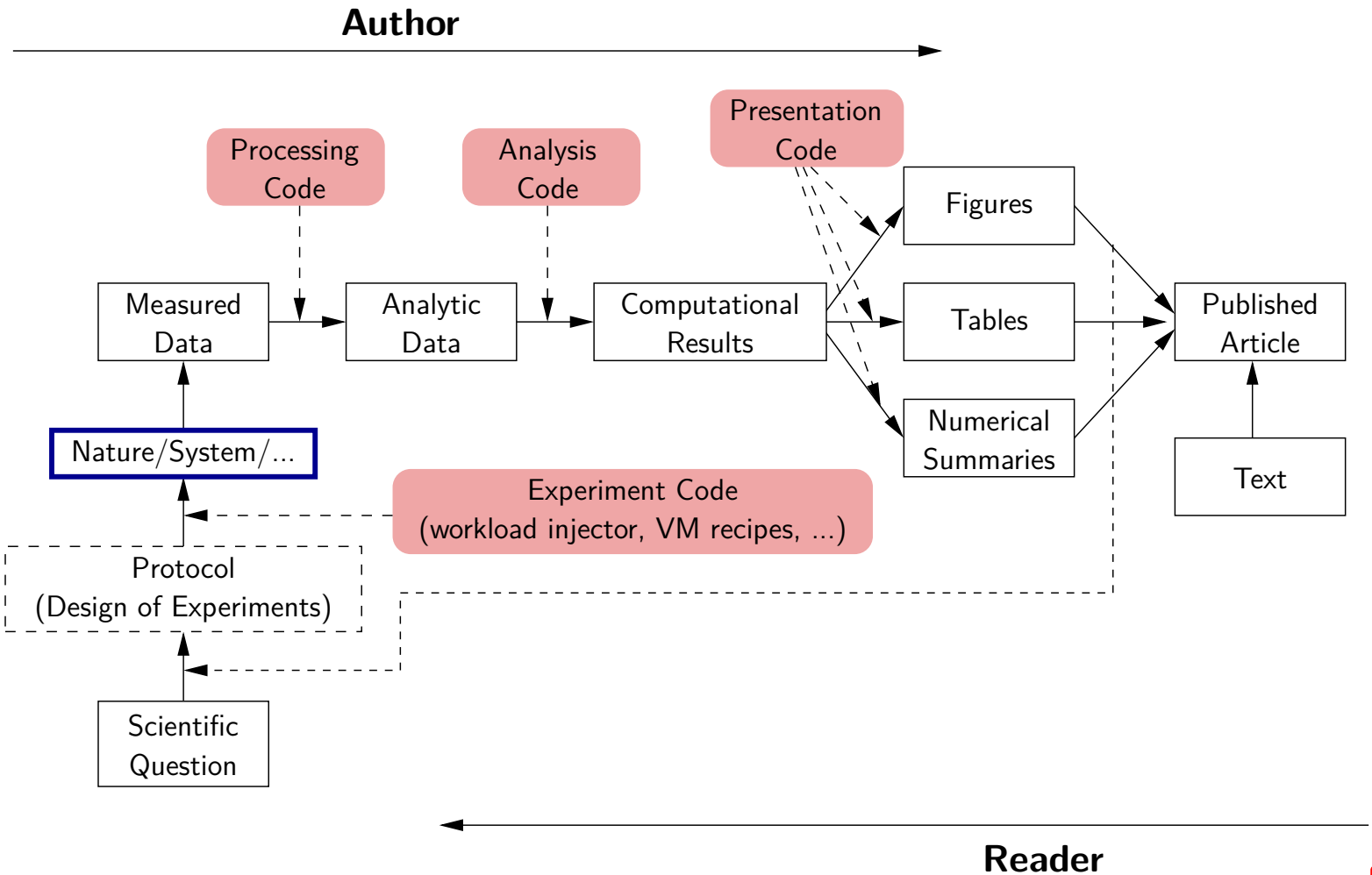

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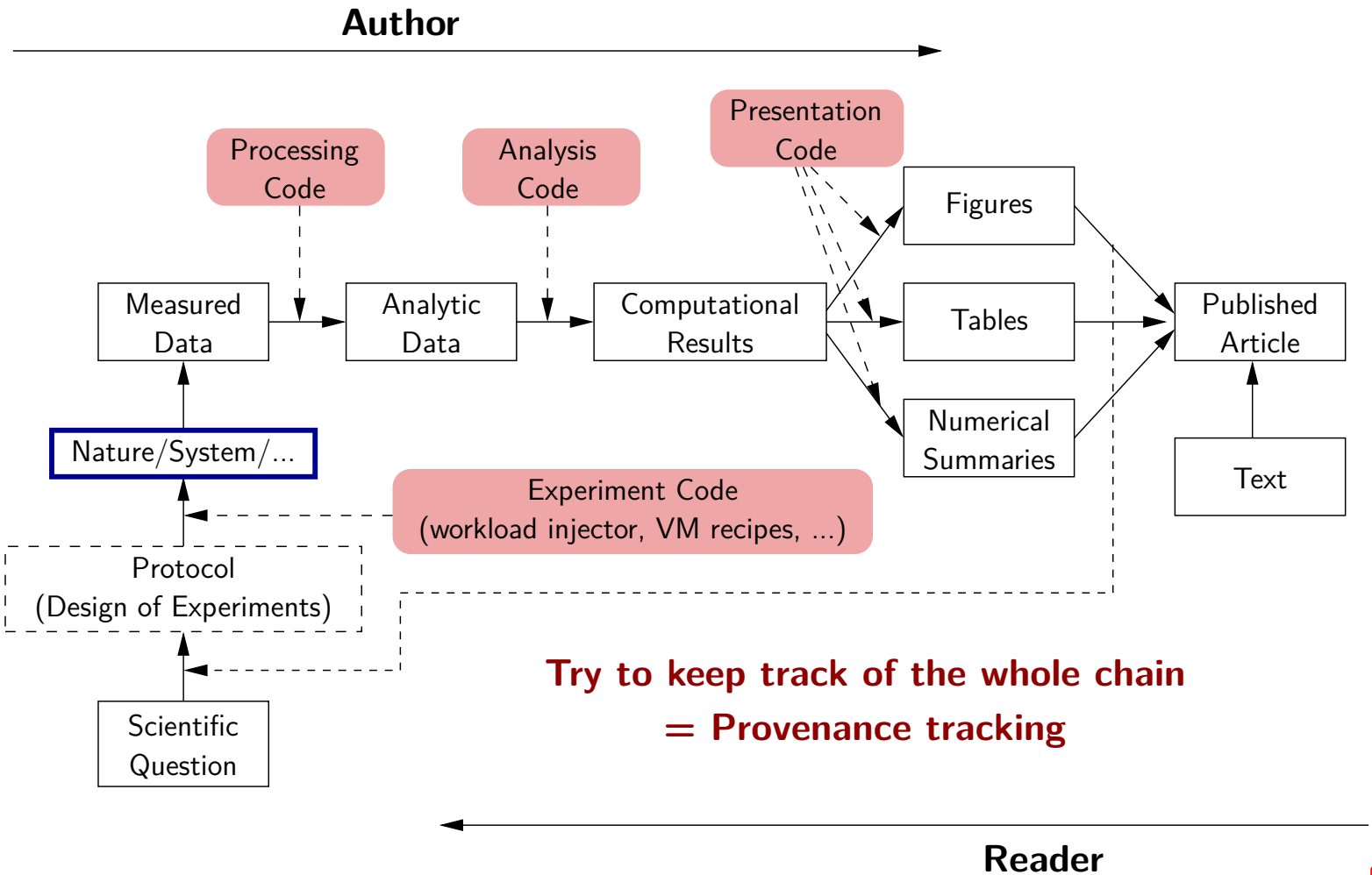

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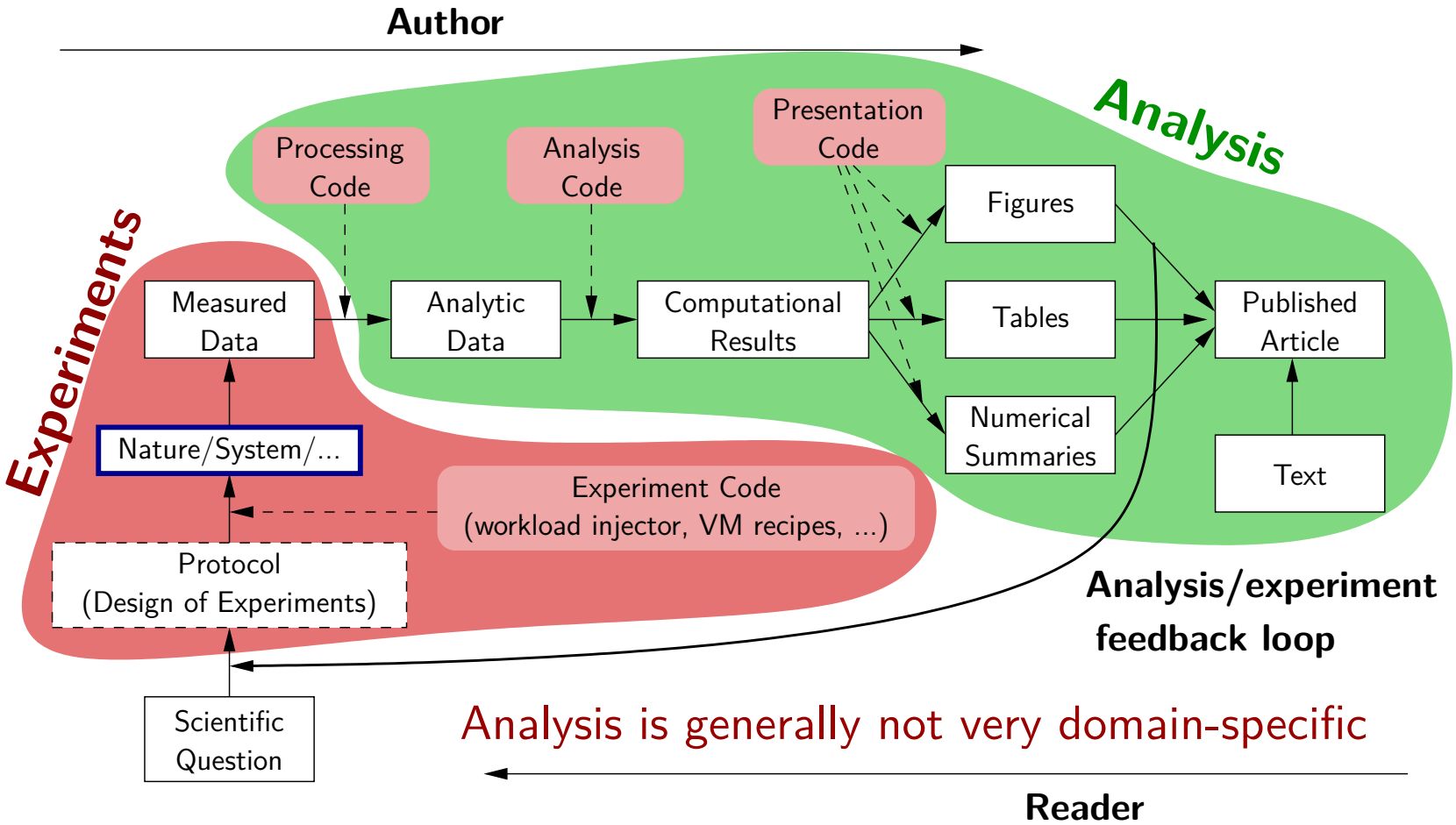

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Reproducible Research Challenges

- The **Distributed/Cloud Computing point-of-view**:
  - ↪ **Experiments** remains **the HARD part** and is very domain-specific
    - ✓ Rely on large, distributed, hybrid, prototype hardware/software
    - ✓ Measure execution times (makespans, traces, . . .)
    - ✓ Many parameters, very costly and hard to **reproduce**

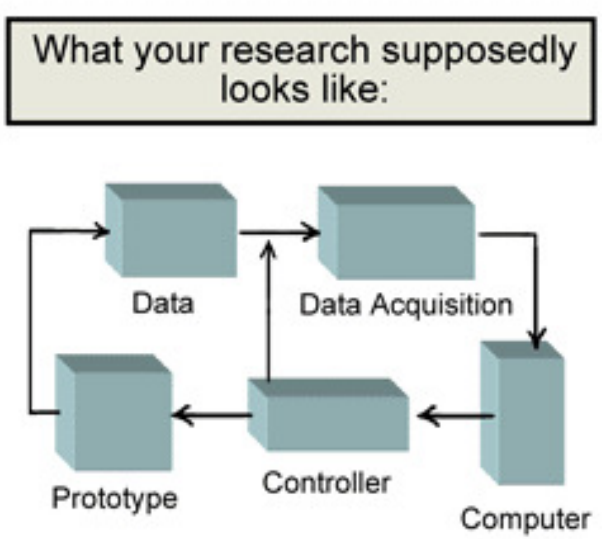

Figure 1. Experimental Diagram

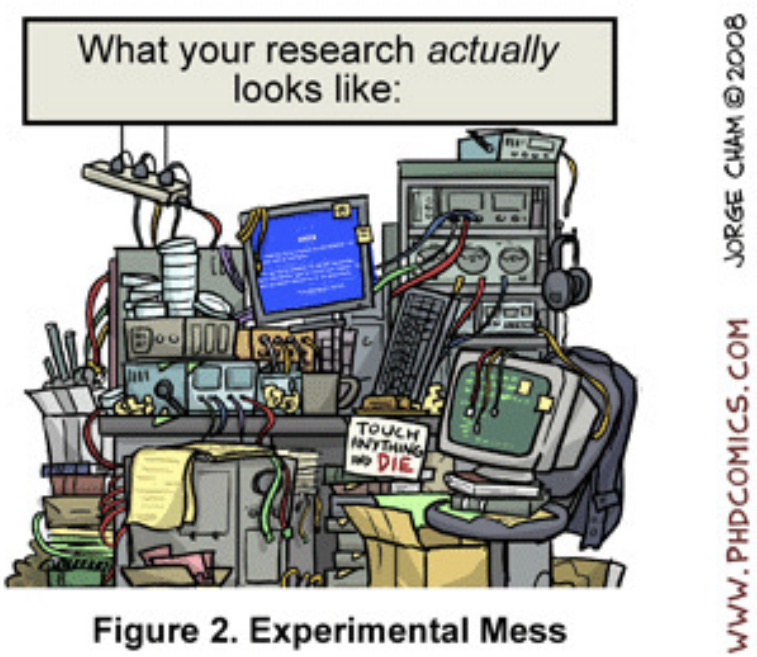

Figure 2. Experimental Mess

Environment Management

Controlling/Providing your Environment

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Q1: How to describe/provide the software environment used?

"I used OpenFOAM with OpenMPI on Debian"

- Obvious solution: **Virtual Machines**
  - ↪ Easy way to [automatically] test recipes
  - ↪ **Yet** provides **only** the final result, **not the logic behind**

RR: Trying to Bridge the Gap

- Accurate, organized and **easy-to{read|take|share} Docs**
  - ↪ Markdown, mkdocs, org-mode, Read the Docs...

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- **Sharing Code and Data**
  - ↪ `git`, Github, Bitbucket, Gitlab...
- **Mastering your environment clean and automated** by:
  - ↪ Using common building tools make, cmake etc.
  - ↪ Using a constrained environment
    - ✓ Sandboxed Ruby/Python,Vagrant, Docker
  - ↪ Automate its building through cross-platform recipes
  - ↪ Automatically test your recipes for Environment configuration

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All covered in this tutorial!

Summary

Easy-to-{Read | Take | Share} Docs

- **Reproducible** research assumes accurate and organized Docs
- You need to **document** your:
  - ↪ **Hypotheses**: keep track of your ideas/line of thoughts
  - ↪ **Experiments**: details on how and why an experiment was run
    - ✓ including failed or ambiguous attempts.
  - ↪ **Initial analysis or interpretation** of these experiments
    - ✓ was the outcome conform to the expectation or not?
    - ✓ does it (in)validate the hypothesis?
  - ↪ **Organization**: keep track of things to do/ x/test/improve
- **Stucture**:
  - ↪ General information about the document
  - ↪ **commonly used commands** and how to set up experiments
  - ↪ Experiment results
    - ✓ by **date** (`tags`)
    - ✓ by **experiment campaigns** (`date/time`)

Documentation Tools / Format

Recommandation

- Plain-text with Markdown syntax
  - ↪ Easy to **track over Git** (`text` files, **not** Word/RFT etc.)
  - ↪ Easy to **export** to any format using `pandoc` / `multimarkdown`
  - ↪ **Supports online/offline** Wikis / Blogging platforms

- **Focus on writing**, viewers for all platform
  - ↪ Mac OS: MOU, Marked 2
  - ↪ Linux: Remarkable, Retext
  - ↪ Windows: MarkdownPad, Remarkable
- Git Based Markdown Blogging
  - ↪ Octopress, Jekyll

Git-based Markdown Wiki

- **Permits to work offline**
  - ↪ Gollum, as embedded in GitLab
    - ✓ run `gollum` (from root directory) `http://localhost:4567`

Recommandation: MkDocs

`http://www.mkdocs.org/`

- Better for **Hierarchical structure** of the docs
  - ↪ fully configured by `mkdocs.yml` and files in `docs/`
  - ↪ local [interpreted] site: `mkdocs serve` (from root directory)
    `http://localhost:8000`
- compliant with Read the Docs
  - ↪ trigger **automatic doc rebuild** upon [git] push
  - ↪ cf `http://rr-tutorials.readthedocs.io/` ☺

Mkdocs Workflow

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- Tools:
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- Configuration:
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$> mkdocs serve     # Run LOCAL builtin server http://localhost:8000
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Hands-On 1: Markdown & MkDocs

Your Turn!

http://rr-tutorials.readthedocs.io/en/latest/hands-on/docs/

- **Easy-to-{Read | Take | Share} Docs with MkDocs**
  - ↪ installation of MkDocs — http://www.mkdocs.org/#installation
  - ↪ initialization — `mkdocs new .`
  - ↪ Markdown basis
  - ↪ **Local** serve — `mkdocs serve`

Summary

Sharing Code and Data

What kinds of systems are available?

- *Good*: The cloud — Dropbox, Google Drive, Figshare...
- **Better** - **Version Control systems** (VCS)
  - ↪ SVN, Git and Mercurial
- **Best** - **Version Control Systems** on the **Public/Private Cloud**
  - ↪ GitHub, Bitbucket, Gitlab

Sharing Code and Data

What kinds of systems are available?

- *Good*: The cloud — Dropbox, Google Drive, Figshare...
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- **Best** - **Version Control Systems** on the **Public/Private Cloud**
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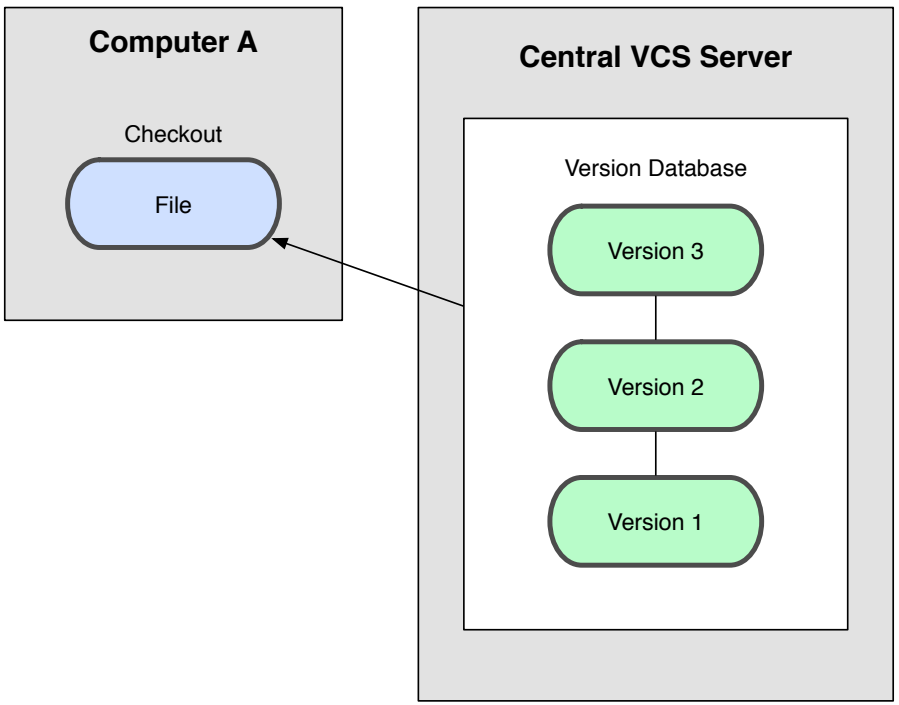
- **Which one?**
  - ↪ Depends on the level of privacy you expect
    - ✓ ... but you probably already know these tools ☺
  - ↪ **Few handle GB files...**

Centralized VCS – CVS, SVN



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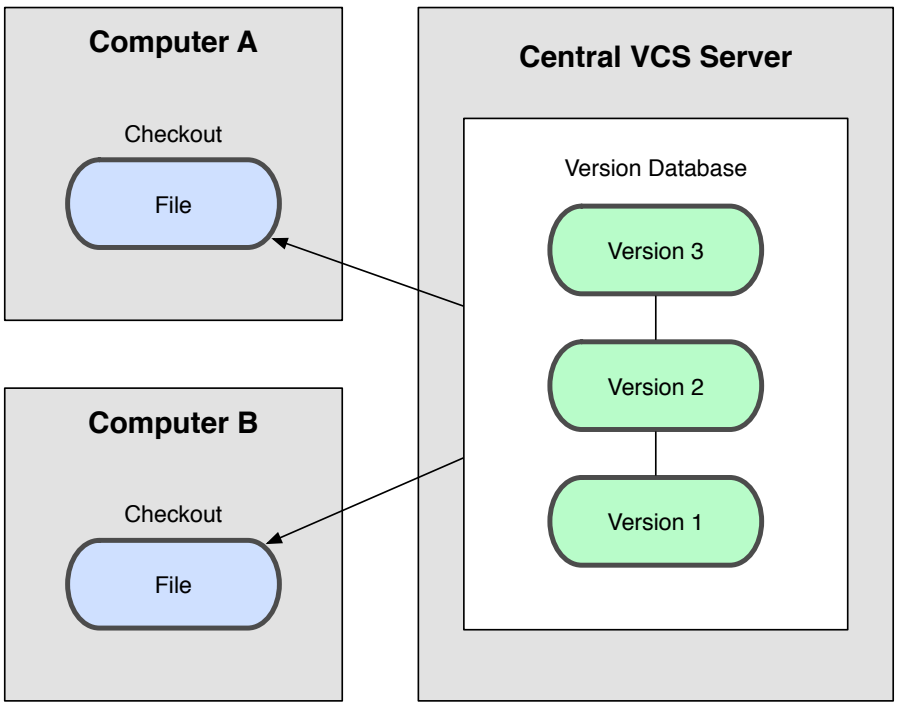
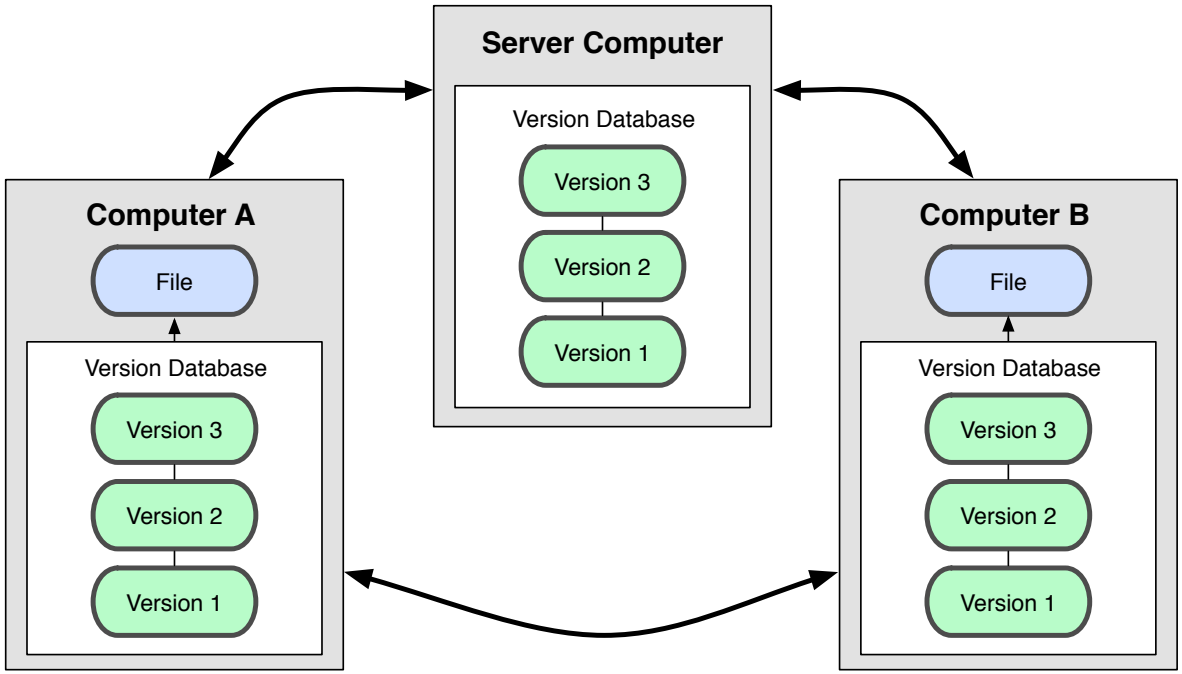
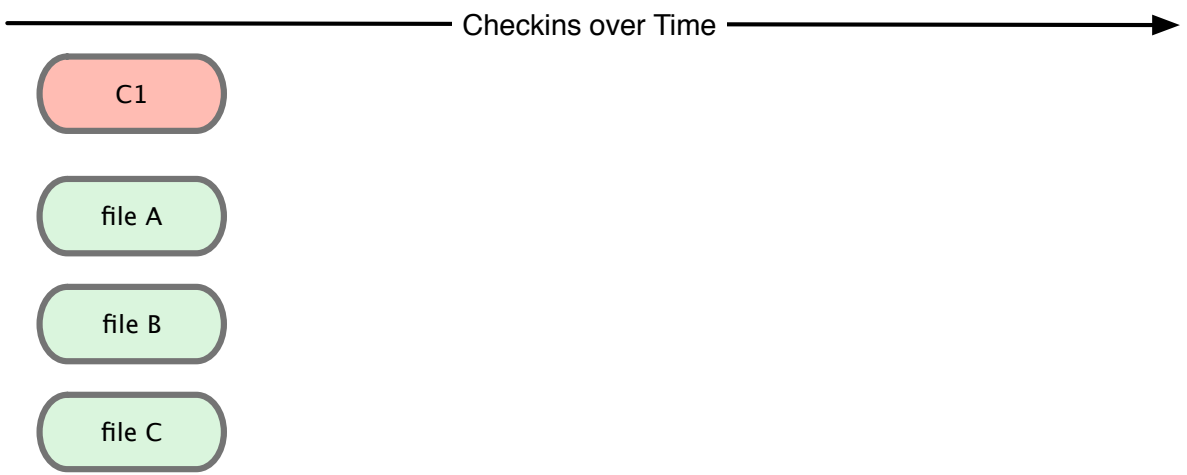


Distributed VCS – Git



Everybody has the full history of commits

Tracking changes (most VCS)



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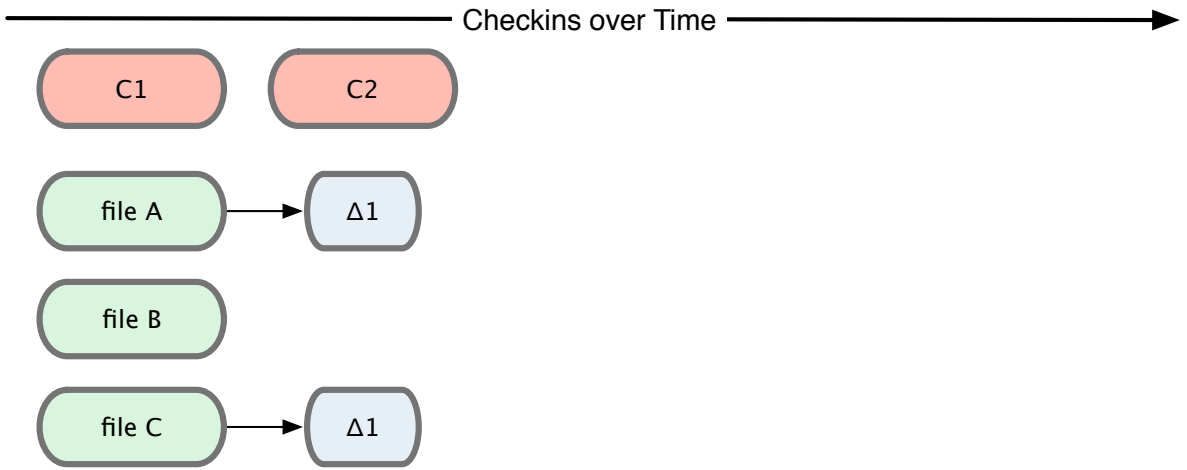

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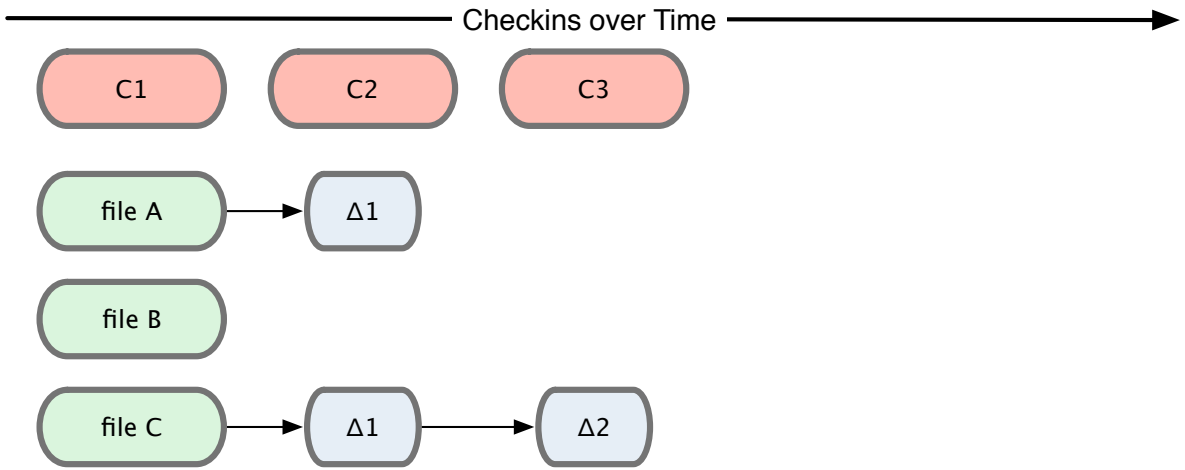

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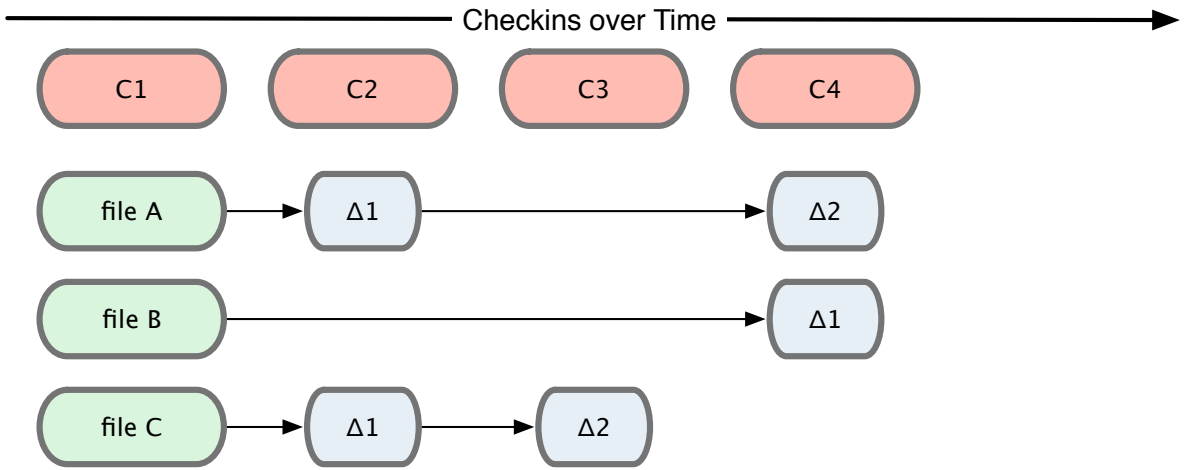

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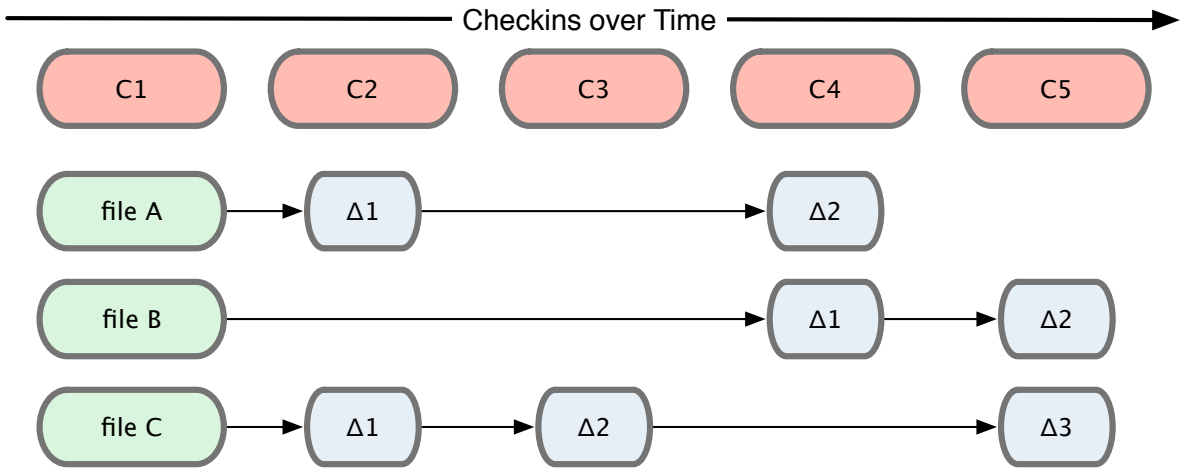

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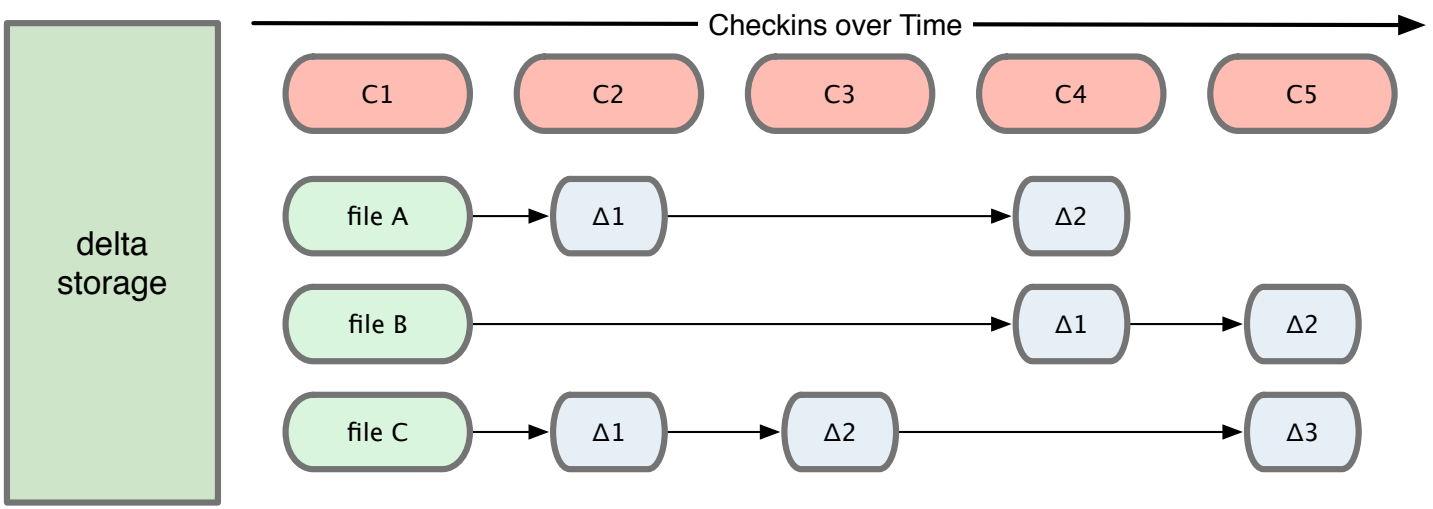

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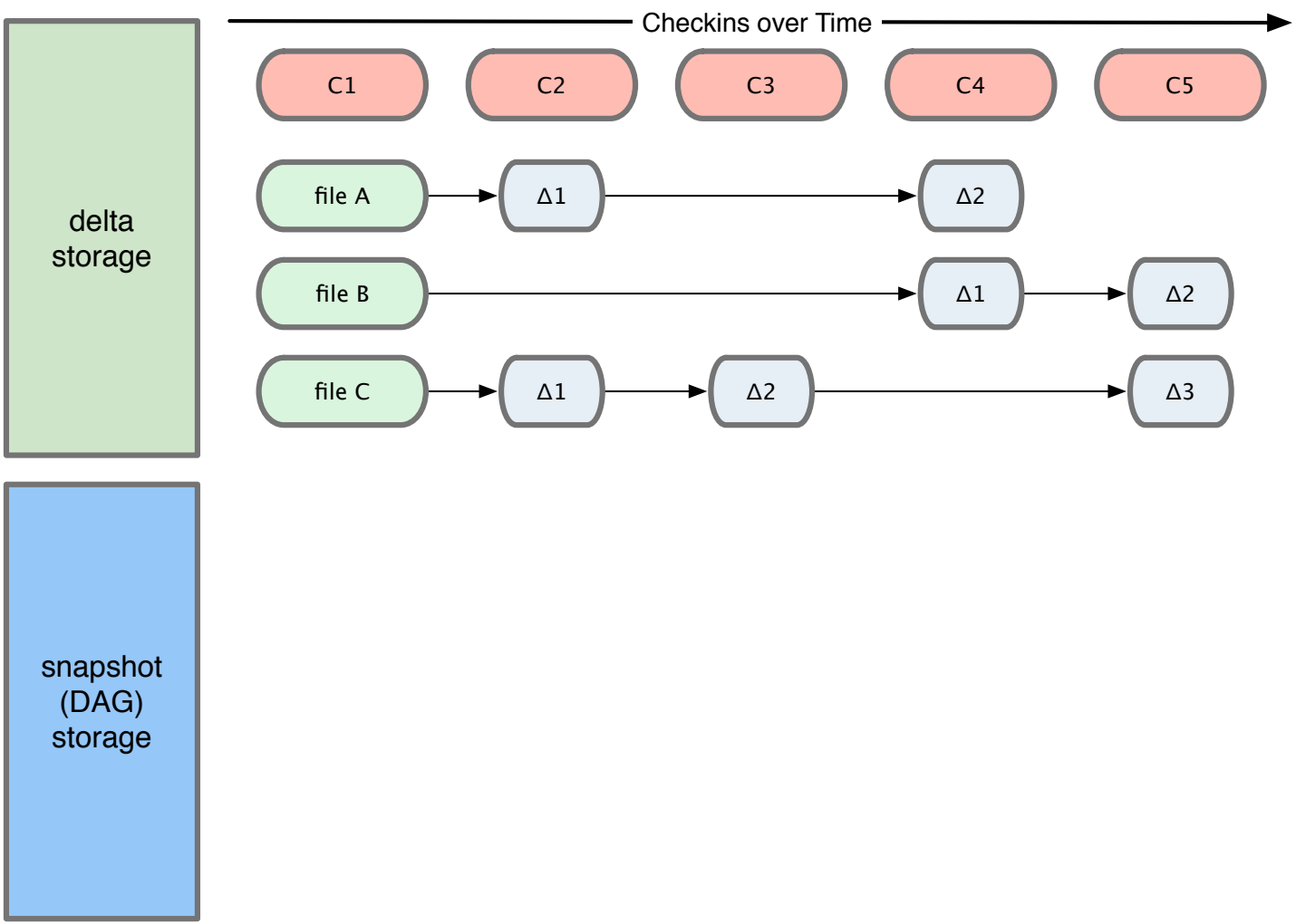

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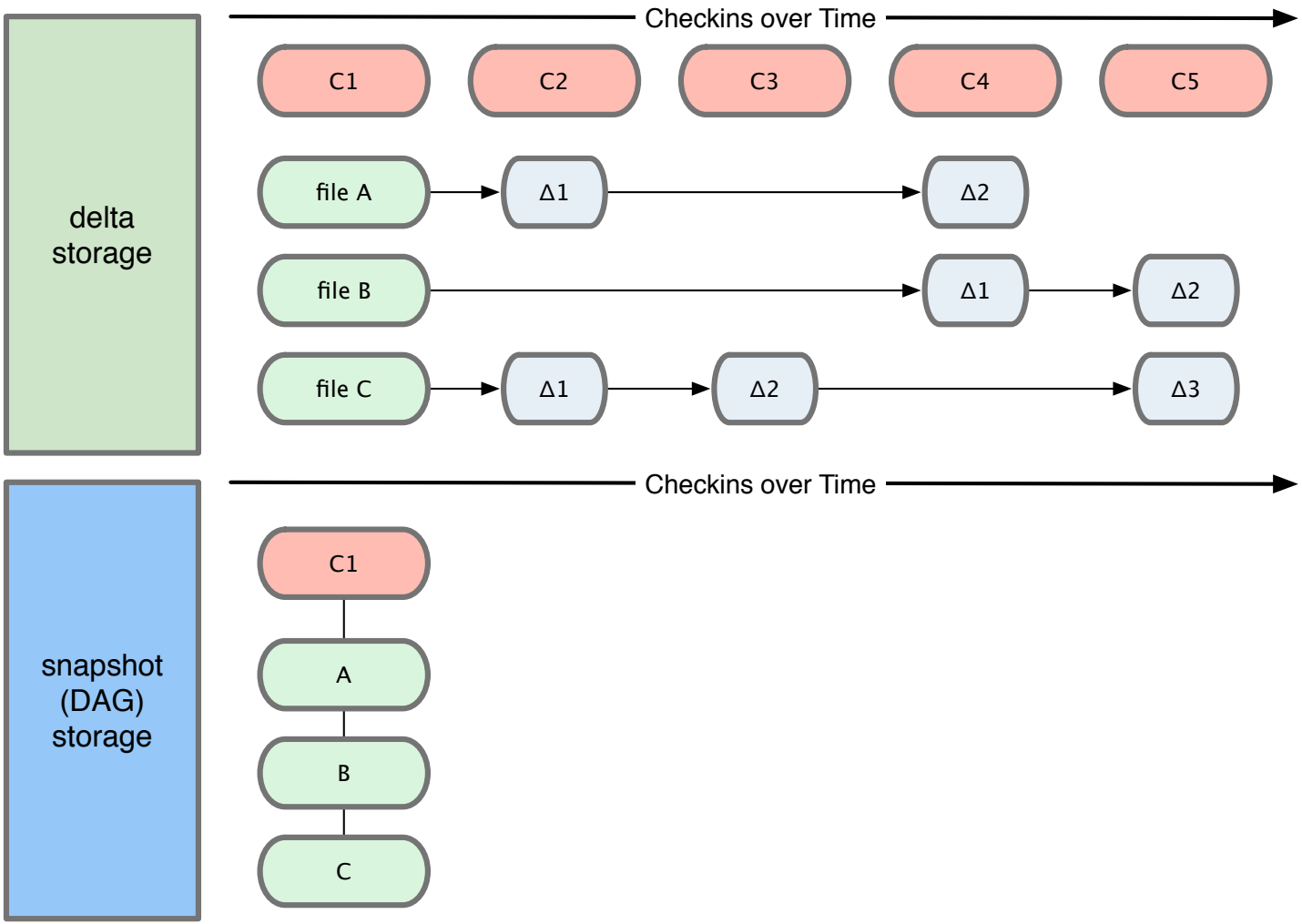

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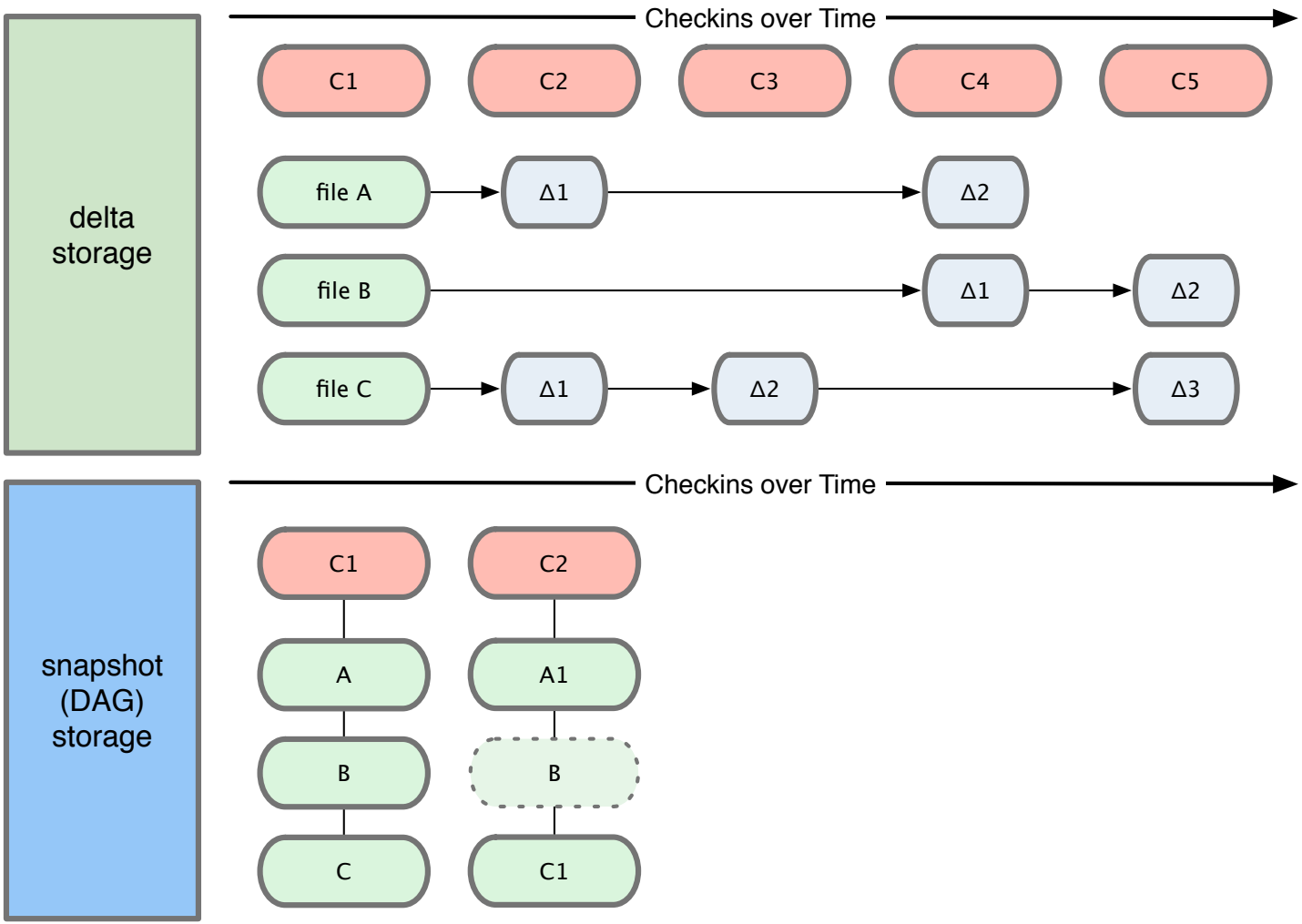

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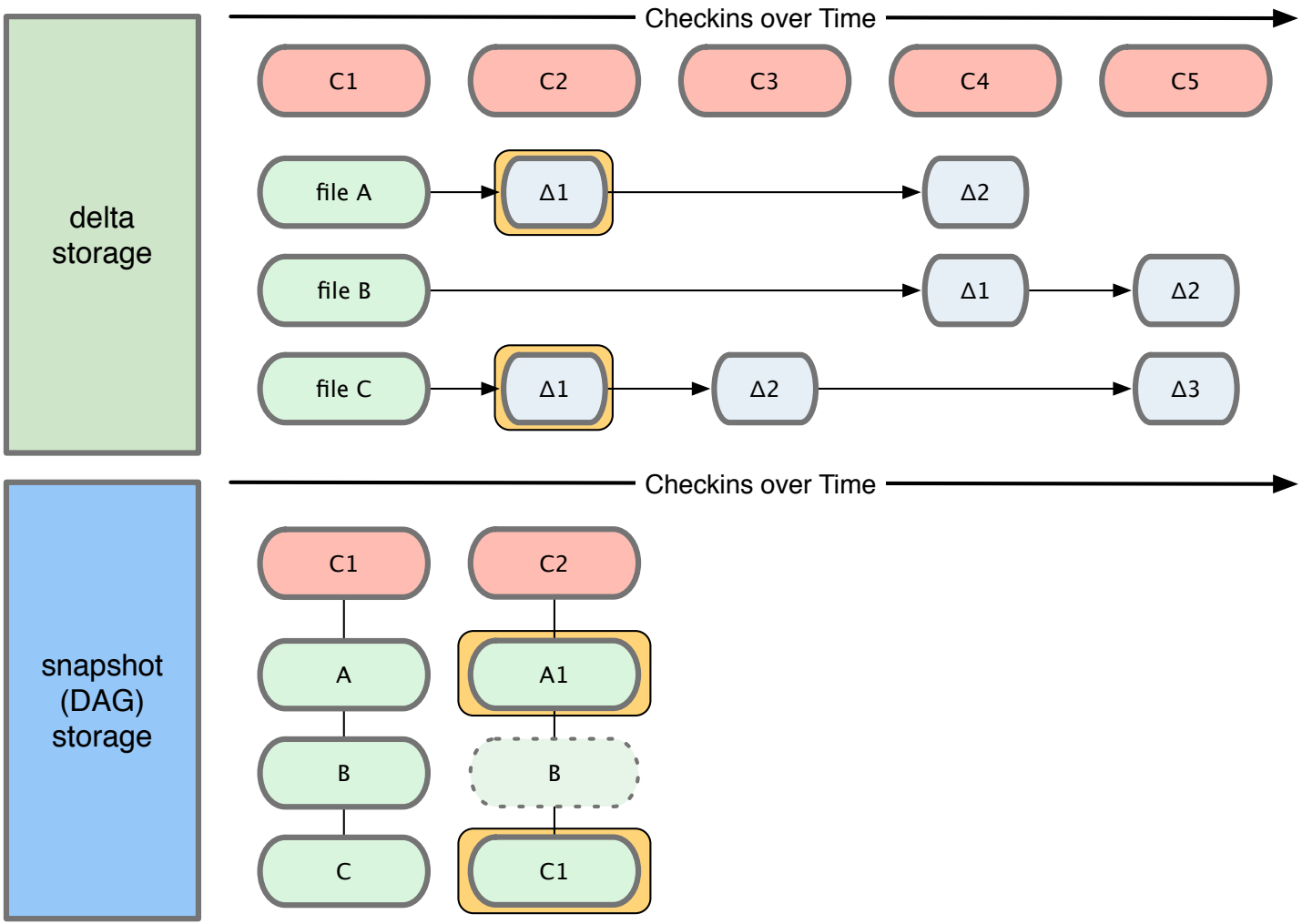

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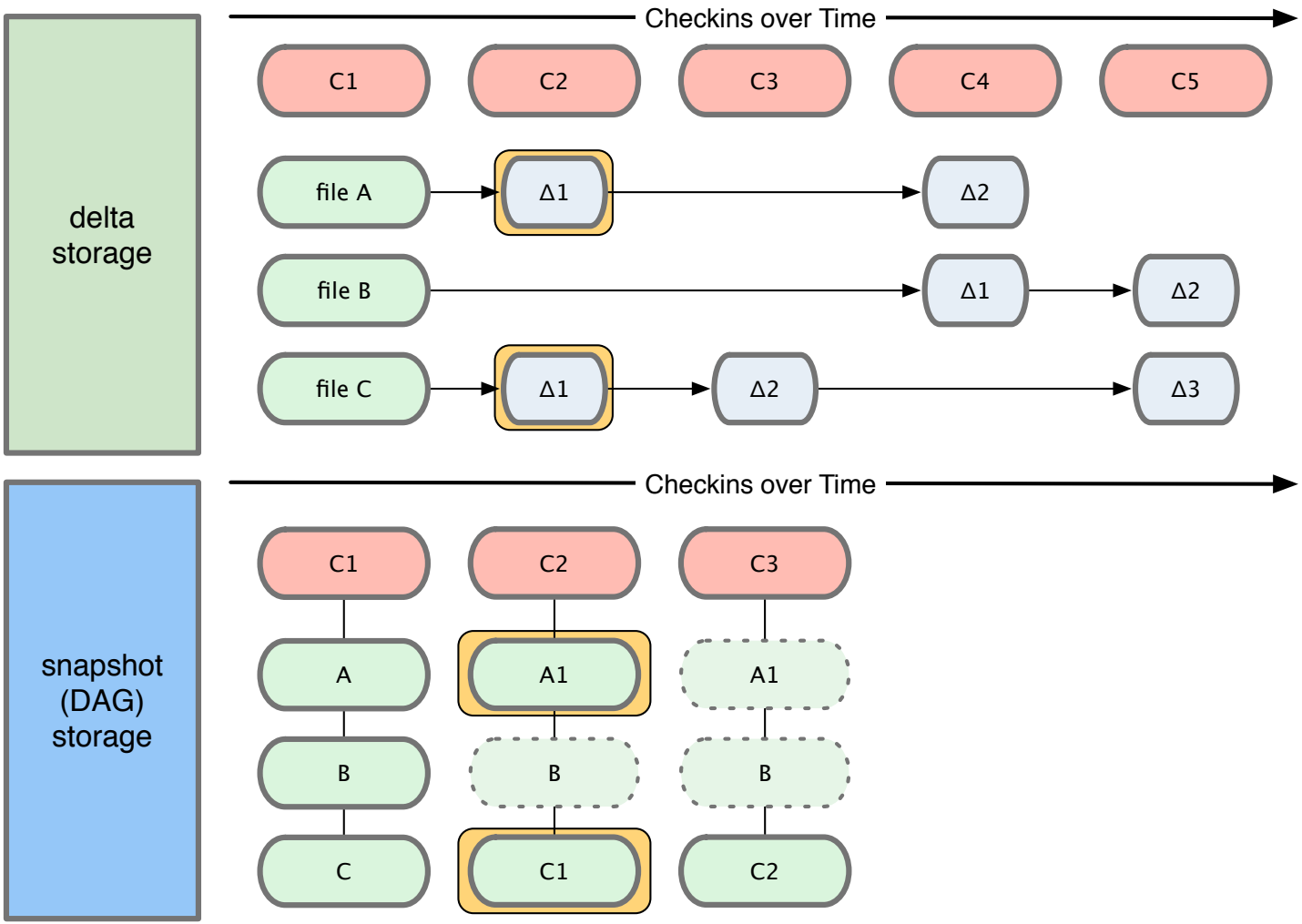

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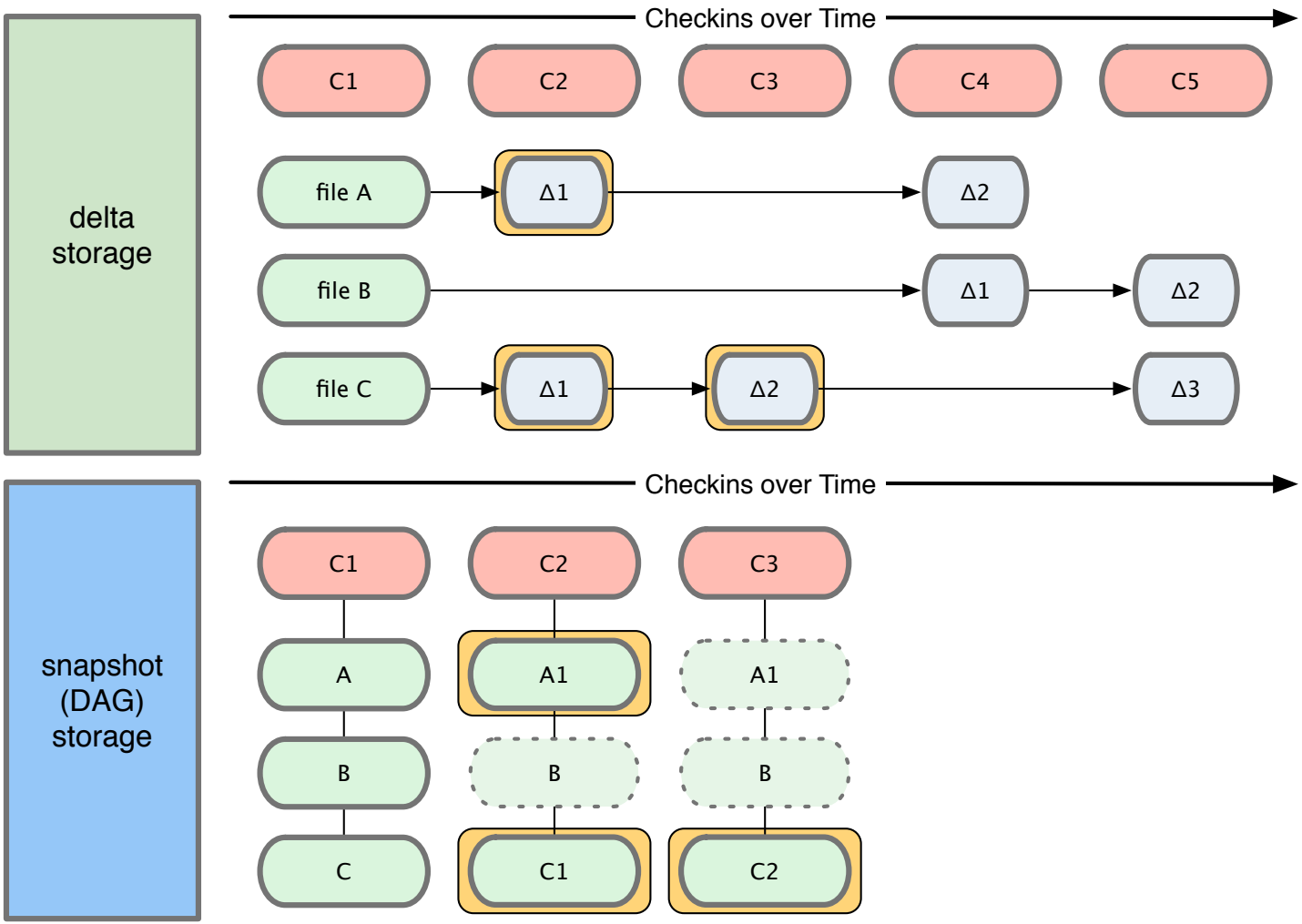

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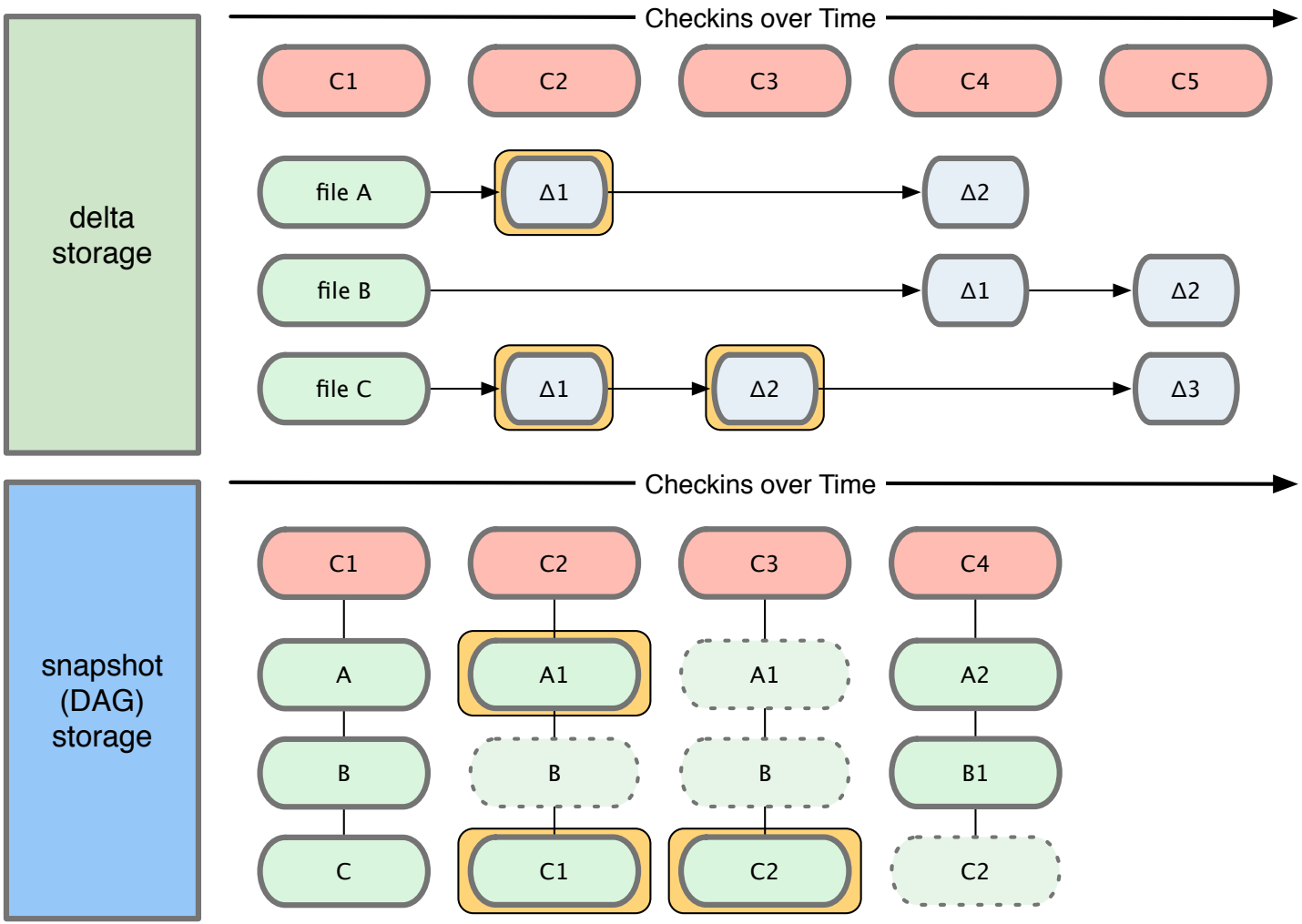

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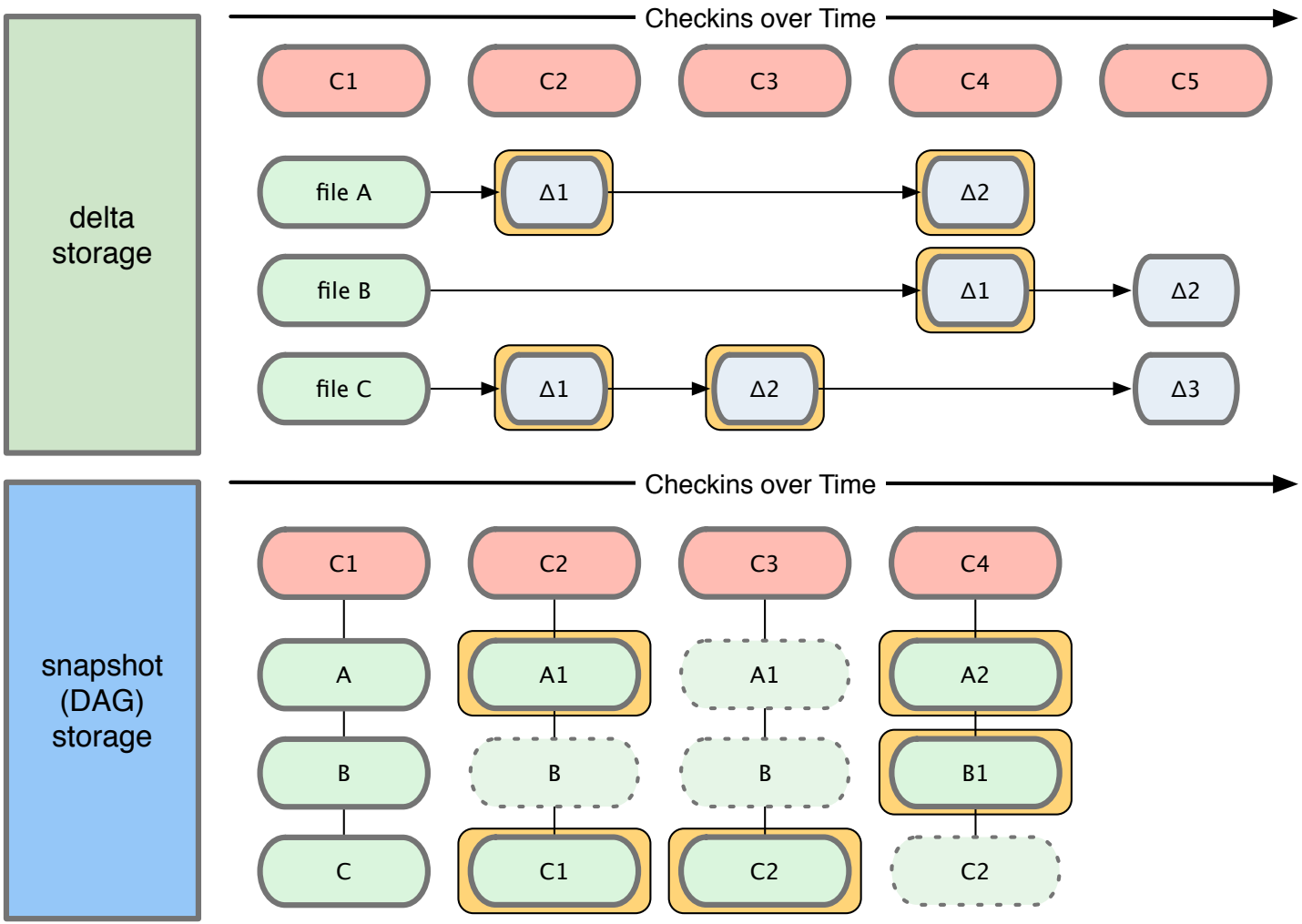

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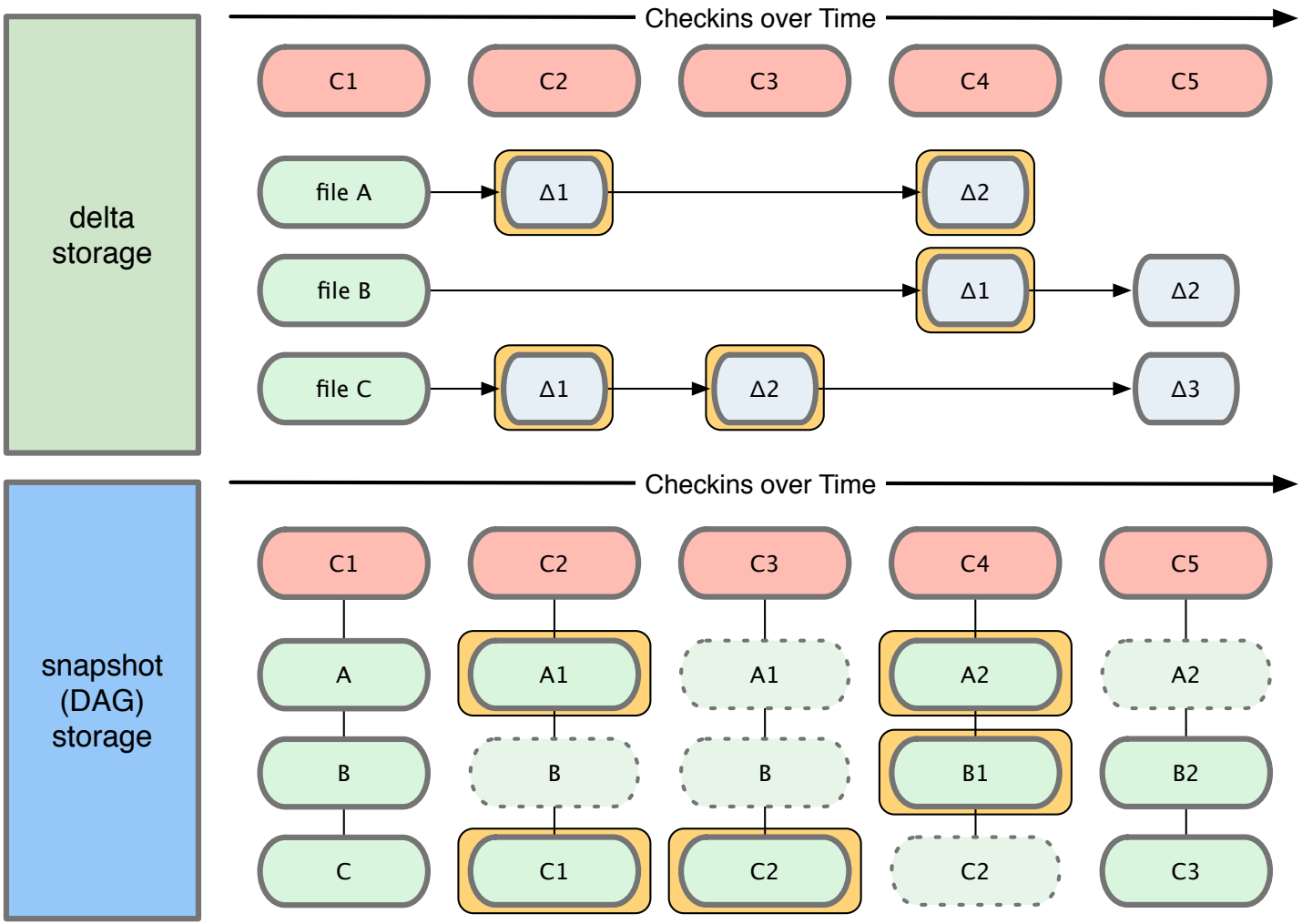

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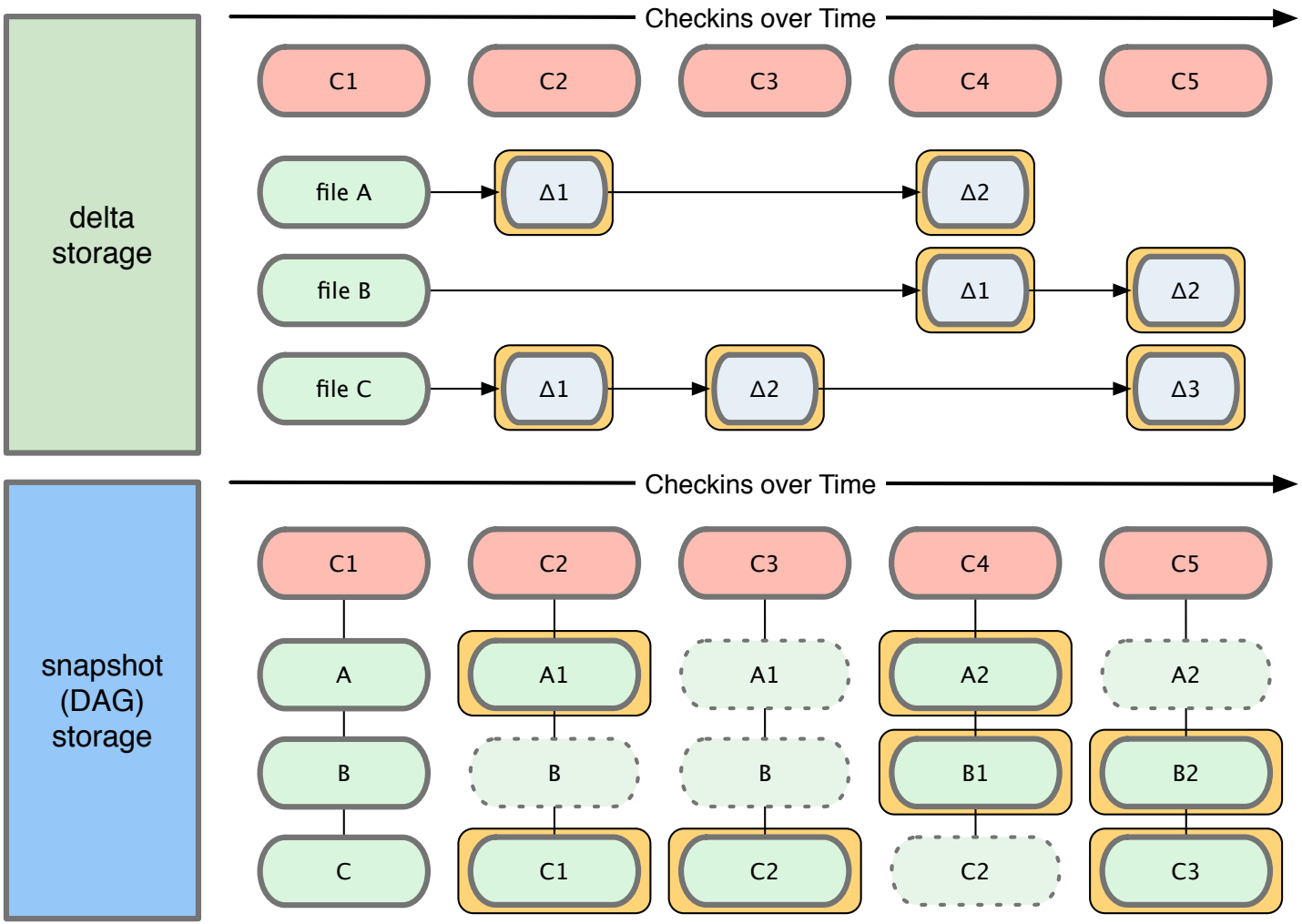
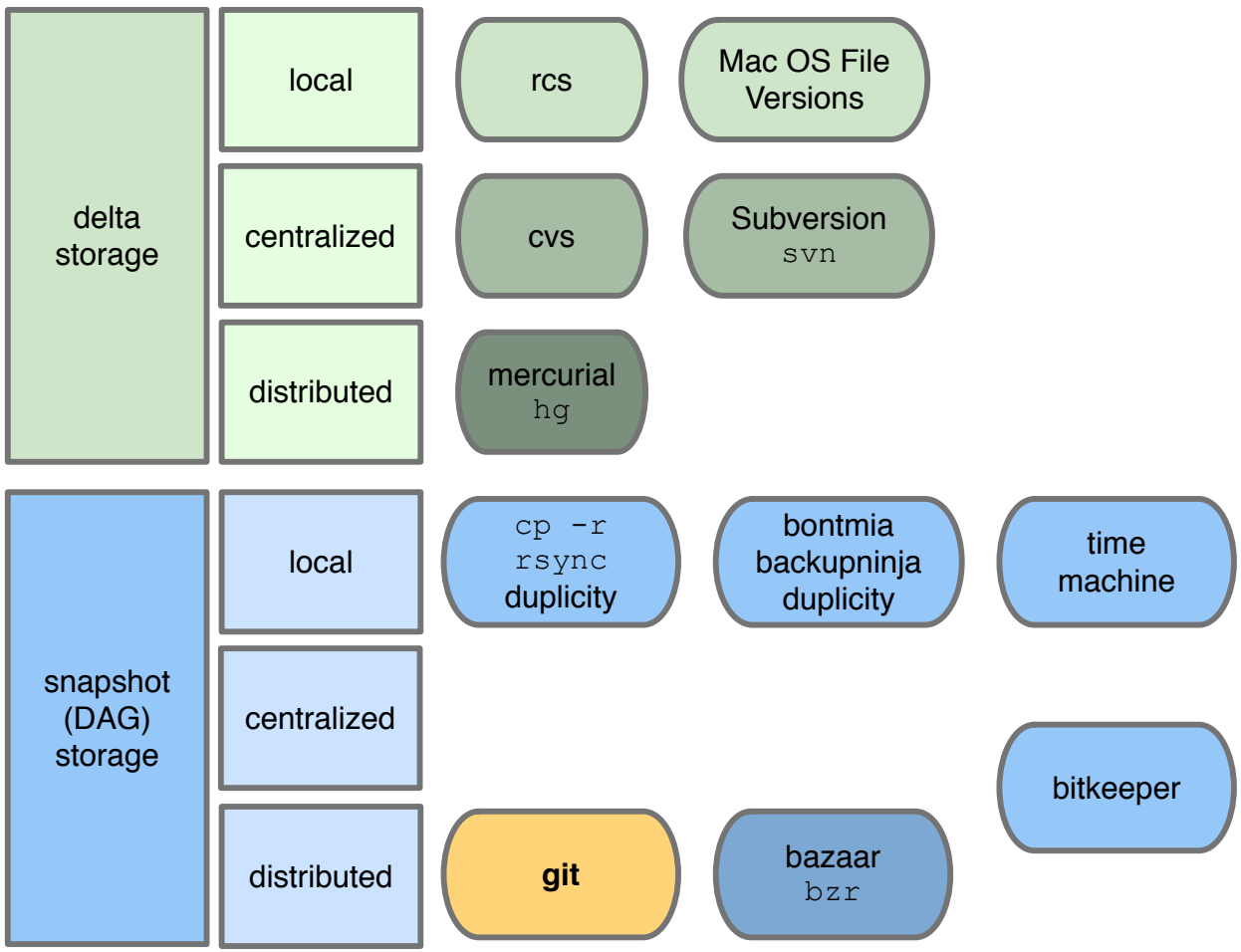


VCS Taxonomy



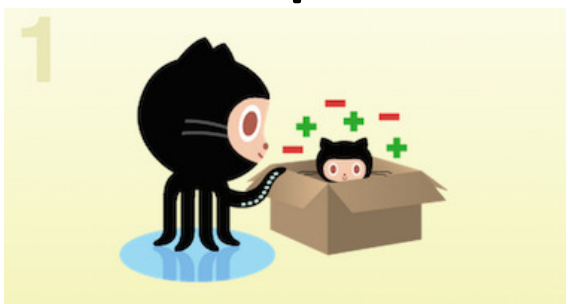
Git at the heart of RR

http://git-scm.org

Git on the Cloud: Github `github.com`

(Reference) web-based Git repository hosting service

Set up Git



Create Repository

Fork repository

Work together

So what makes Git so useful?

(almost) Everything is local

- everything is fast
- every clone is a backup
- you work **mainly offline**

Ultra Fast, Efficient & Robust

- Snapshots, not patches (deltas)
- **Cheap branching and merging**
  - ↪ Strong support for thousands of parallel branches
- Cryptographic integrity everywhere

Other Git features

- **Git doesn't delete**
  - ↪ **Immutable** objects, Git generally only adds data
  - ↪ If you mess up, you can usually recover your stuff
    - ✓ Recovery can be tricky though

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Git Tools / Extension

- cf. **Git submodules** or **subtrees**
- **Introducing git-flow**
  - ↪ workflow with a strict branching model
  - ↪ offers the `git` commands to follow the workflow

```
$> git flow init
$> git flow feature { start, publish, finish } <name>
$> git flow release { start, publish, finish } <version>
```

Hands-on 2: Practical Git http://git-scm.com/downloads

Installation on Linux / Mac OS

```
$> apt-get install git-core git-flow          # On Debian-like systems
$> yum install git gitflow                    # On CentOS-like systems
$> brew install git git-flow                  # On Mac OS, using Homebrew
```

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- Incl. Git Bash/GUI & Shell Integration
  - ↪ install **Git bash** + command prompt
  - ↪ select checkout windows / commit unix

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- Incl. Git Bash/GUI & Shell Integration
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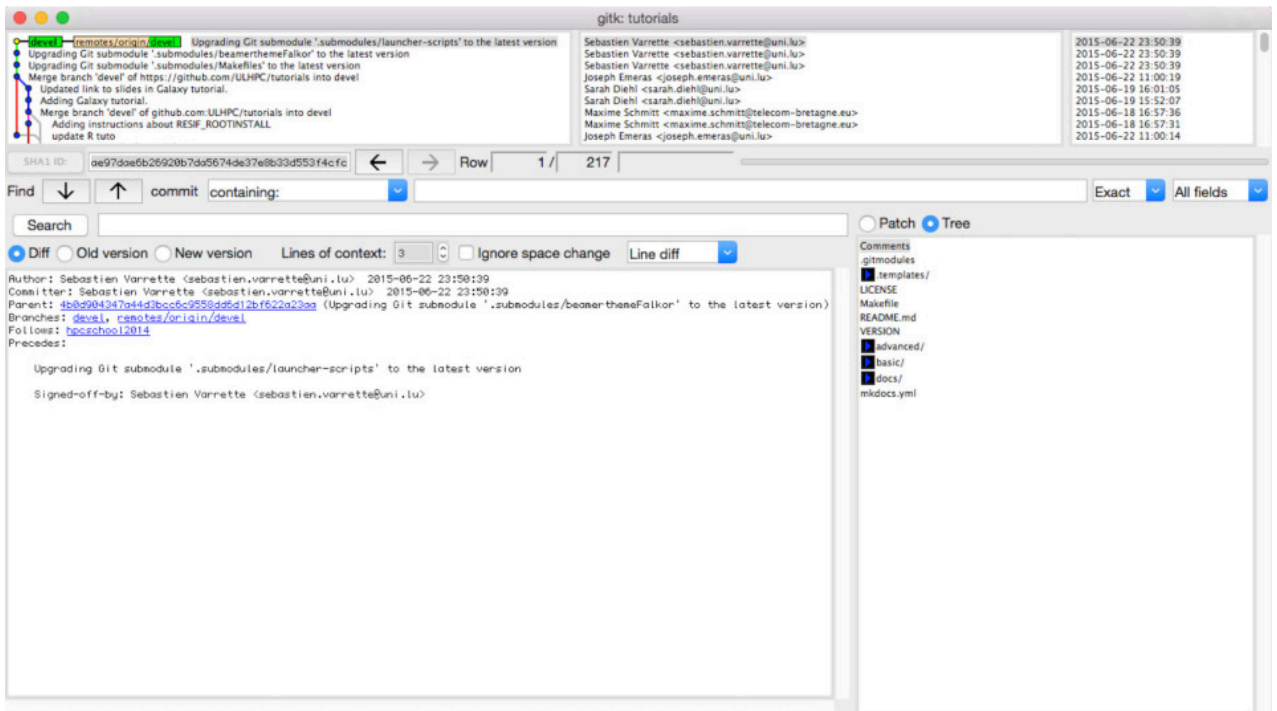
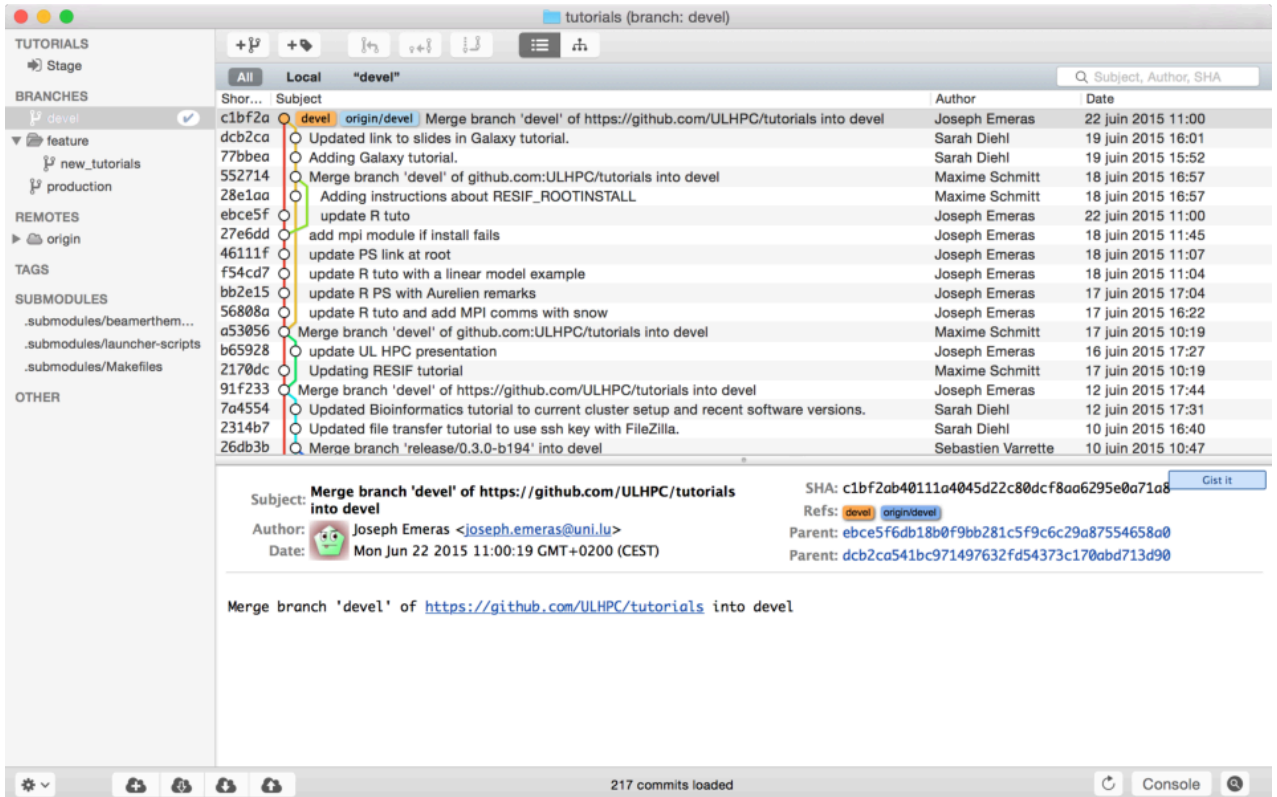
- **Your turn!** http://rr-tutorials.readthedocs.io/en/latest/setup/
  - ↪ Ensure you have git installed

Git GUI (default) Gitk

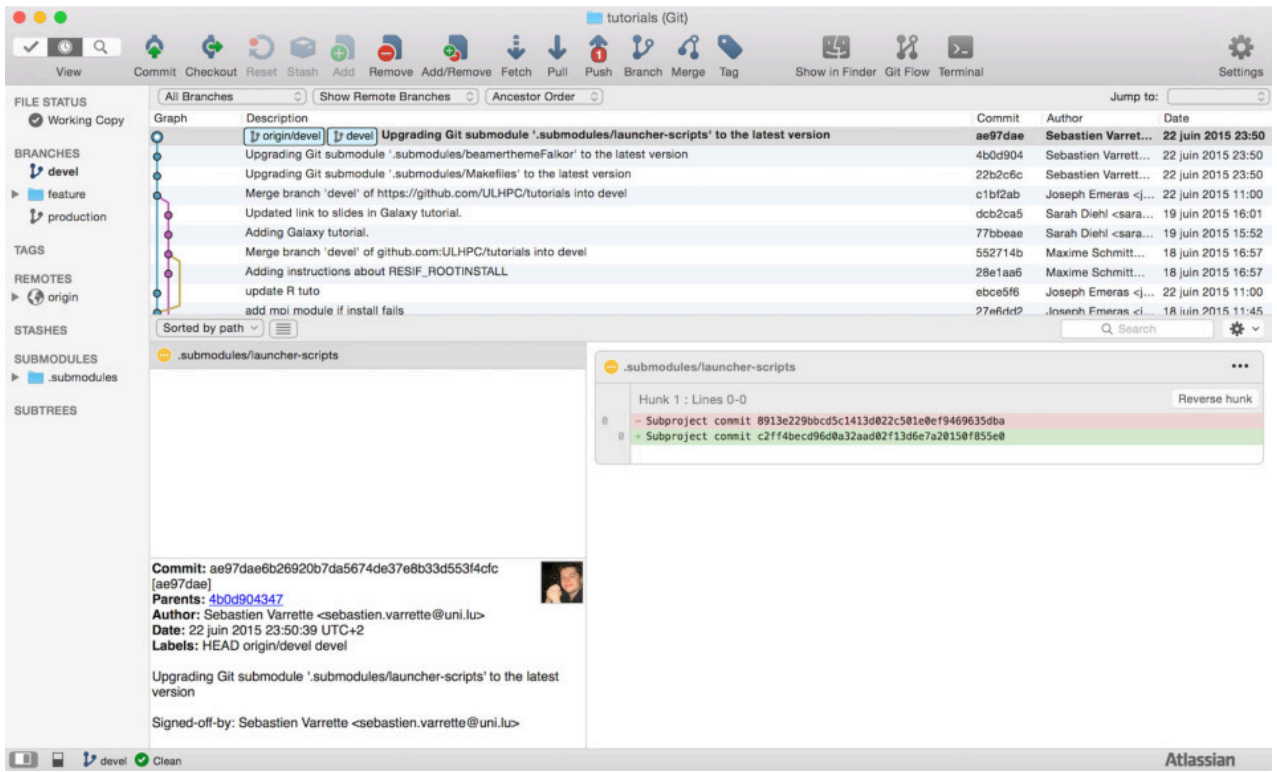


Git GUI (Mac OS) GitX-dev



http://rowanj.github.io/gitx/

Git GUI (Windows/Mac) SourceTree



http://www.sourcetreeapp.com/

1. Let it install a default git ignore file
2. make it load your SSH key created with Putty

Preliminary Configurations

- Global Git configuration are stored in `~/.gitconfig`
  - ↪ **Ex**: see my personal `.gitconfig`
- You **SHOULD** at least configure your name and email to commit
  - ↪ open a terminal (Git bash under windows) for the below commands

```
$> git config --global user.name "Firstname LastName"
$> git config --global user.email "Firstname.LastName@uni.lu"
$> git config --global color.ui true                    # Colors
$> git config --global core.editor vim                  # Editor
```

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```

Your Turn!

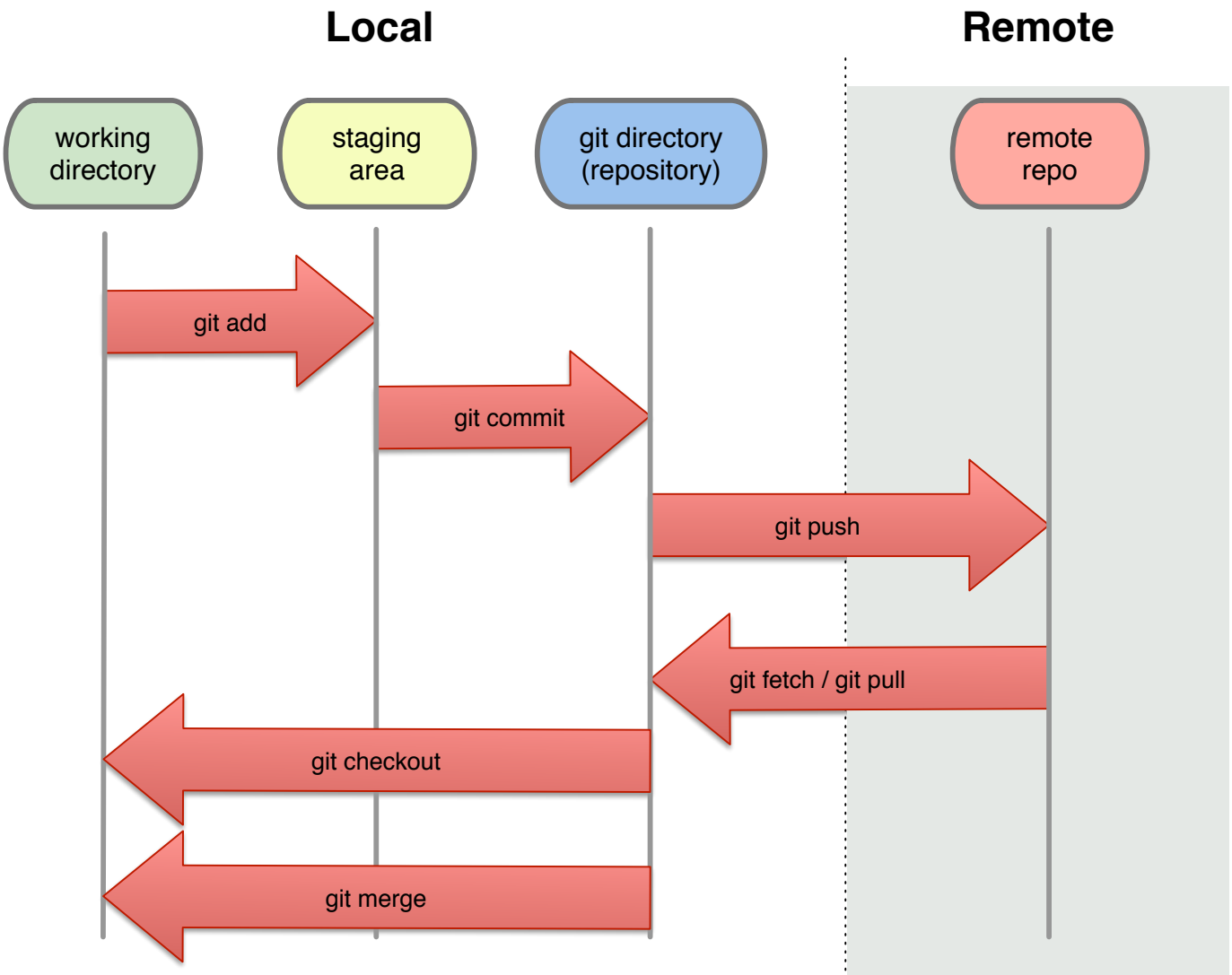
- Then check the changes by: `git config -l | grep user`

Git Commands Aliases

- You can also create git command aliases in `~/.gitconfig`.
  - ↪ **Ex** copy/paste from my personal `.gitconfig`

```
[alias]
    up = pull origin
    pu = push origin
    st = status
    df = diff
    ci = commit -s
    co = checkout
    br = branch
    w  = whatchanged --abbrev-commit
    ls = ls-files
    gr = log --graph --oneline --decorate
    amend = commit --amend
```

Git Workflow



Creating a Repository

```
$> git [flow] init
```

- Initializes a new git (flow) repository in the current directory

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Your Turn!

```
$> cd /tmp
$> mkdir firstproject
$> cd firstproject

$> git init
Initialized empty Git repository in /private/tmp/firstproject/.git/
```

Cloning a Repository

```
$> git clone [--recursive] <url> [<path>]
```

Type	URL Format / Example	Port
Local	`/path/to/project.git`	n/a
SSH	`git+ssh://user@server:port/project.git`	22
Git	`git://server/project.git`	9418
HTTPS	`https://github.com/Falkor/falkorlib.git`	443

Cloning a Repository

```
$> git clone [--recursive] <url> [<path>]
```

Your Turn!

```
$> cd /tmp
$> git clone https://github.com/Falkor/RR-tutorials.git
Cloning into 'tutorials'...
remote: Counting objects: 1247, done.
remote: Compressing objects: 100% (63/63), done.
remote: Total 1247 (delta 32), reused 0 (delta 0), pack-reused 1181
Receiving objects: 100% (1247/1247), 15.74 MiB | 3.08 MiB/s, done.
Resolving deltas: 100% (588/588), done.
Checking connectivity... done.
$> git clone --recursive \
       https://github.com/Falkor/RR-tutorials.git /tmp/tutorials2
```

Inspecting a Repository

```
$> git status [-s]                    # -s:  short / simplified output
```

Inspecting a Repository

```
$> git status [-s]                # -s:  short / simplified output
```

Your Turn!

```
$> cd /tmp/firstproject
$> git status
On branch master

Initial commit

nothing to commit

# Create an empty file
$> touch README.md
```

```
$> git status
On branch master

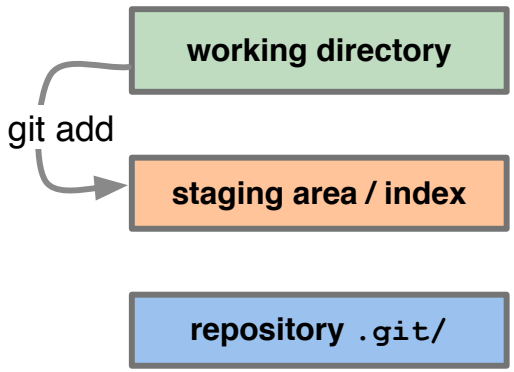
Initial commit

Untracked files:
    README

nothing added to commit but untracked
files present
$> git status -s
?? README
```

Add / Tracking [new] file(s)

```
$> git add [-f] <pattern>
```



- Adds changes to the index
  - ↪ Add a specific file: `git add README`
  - ↪ Add a set of files: `git add *.py`
- Beware that empty directory cannot be added **directly**
  - ↪ due to the internal file representation (**blobs**)
  - ↪ **Tips**: add an hidden file `.empty` (or `.gitignore`)

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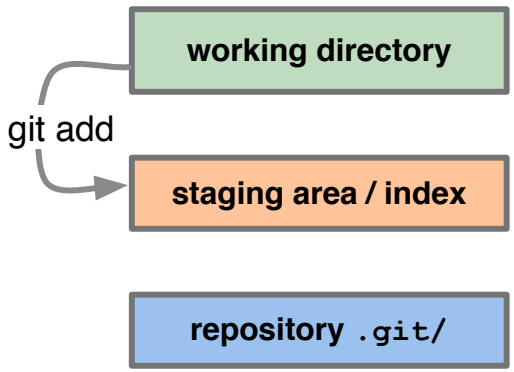

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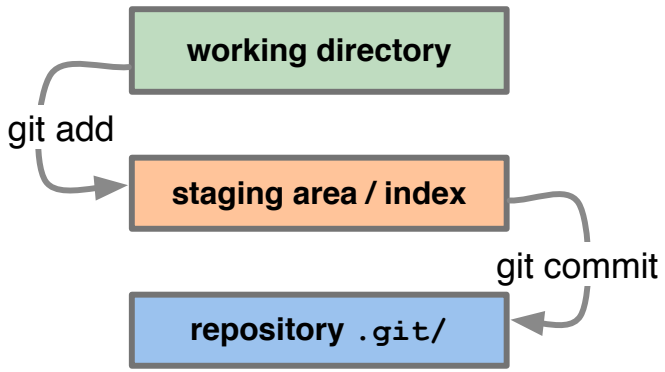
Your Turn!

```
$> cd /tmp/firstproject
$> git status -s
?? README
```

```
$> git add README
$> git status -s
A  README
```

Committing your changes

```
$> git commit [-s] [-m "msg"]
```



- Commit all changes: `git commit -a`

Committing your changes

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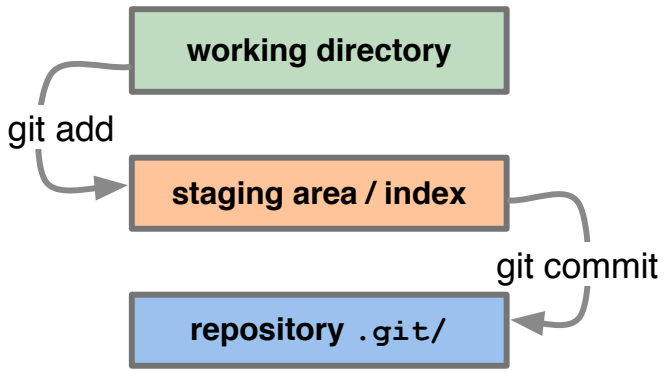

- Commit all changes: `git commit -a`

Your Turn!

```
$> cd /tmp/firstproject
$> git commit -s -m "add README"    # OR git ci -m "add README"
[master (root-commit) ee60f53] add README
 1 file changed, 0 insertions(+), 0 deletions(-)
 create mode 100644 README
$> git status               # OR git st
On branch master
nothing to commit, working directory cleant
```

Removing Files

```
$> git rm [-rf] [--cached] <file>
```

- `--cached`: remove from Staging area
  - ↪ otherwise (default): from index **and** file system

Ignoring Files

Ignoring files from staging: '.gitignore'

- you can create a `.gitignore` file listing patterns to ignore
  - ↪ Blank lines or lines starting with \# are ignored
  - ↪ End pattern with slash (/) to specify a directory
  - ↪ Negate pattern with exclamation point (!)
- Collection of useful `.gitignore` templates

```
.DS_Store
*~
```

```
*.asv
*.m~
*.mex*
tmp/*
```

- LaTeX `.gitignore`
- Python `.gitignore`
- Ruby `.gitignore`

Moving Files

```
$> git mv <source> <destination>
```

```
# Equivalent of:
mv <source> <destination>
git rm <source>
git add <destination>
```

Moving Files

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$> git mv <source> <destination>
```

```
# Equivalent of:
mv <source> <destination>
git rm <source>
git add <destination>
```

Your Turn!

```
$> cd /tmp/firstproject
$> git mv README README.md
$> git status
On branch master
Changes to be committed:
    renamed:    README -> README.md
$> git commit -m "a first move"
```

Check the Commit History

```
$> git log [-p] [--stat] [--graph --oneline --decorate]
```

- `-p` / `--stat`: show the differences introduced in each commit
- You can also perform some date filtering

  ```
  $> git log --since=2.weeks
  ```

- Ncurses-based text-mode interface: `tig`

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  ```
  $> git log --since=2.weeks
  ```

- Ncurses-based text-mode interface: `tig`

Your Turn!

```
$> cd /tmp/firstproject
$> git log --oneline --graph --decorate     # OR git gr
* f1f0c27 (HEAD -> master) a first move
* ee60f53 add README
$> git log -p -1          # only the last commit OR git show
$> tig
```

Show differences

```
$> git diff [--cached] [<ref>]
```

- Check **un-staged** changes: `git diff`
  - ↪ `--cached`: check **staged** changes
- Relative to a specific revision:

```
$> git diff 1776f5
$> git diff HEAD^
```

Undoing Things

```
$> git commit --amend                    # Change the last commit
```

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$> git commit --amend                    # Change the last commit
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```
$> git unstage <file>                    # or git reset HEAD <file>
```

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```

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$> git unstage <file>                    # or git reset HEAD <file>
```

```
$> git checkout -- <file>    # DANGER! Un-modify modified file
```

- Restore to the last committed/cloned version: **all** changes are lost!

Undoing Things

```
$> git commit --amend                    # Change the last commit
```

```
$> git unstage <file>                    # or git reset HEAD <file>
```

```
$> git checkout -- <file>    # DANGER! Un-modify modified file
```

```
$> git revert <commit>                   # revert a <commit>
```

- Make a new commit that undoes all changes made in <commit>

Undoing Things

```
$> git commit --amend                    # Change the last commit
```

```
$> git unstage <file>                    # or git reset HEAD <file>
```

```
$> git checkout -- <file>    # DANGER! Un-modify modified file
```

```
$> git revert <commit>                   # revert a <commit>
```

Your Turn!

```
$> cd /tmp/firstproject
$> git commit --amend
$> echo 'toto' >> README.md
```

```
$> cat README.md && git status
$> git checkout -- README
$> git status
```

Git Summary

Basic Workflow

Edit files	`vim` / `emacs` / `subl` ...
Stage the changes	`git add`
Review your changes	`git status`
Commit the changes	`git commit`

Git Summary

For cheaters: A Basicerer Workflow

Edit files	`vim` / `emacs` / `subl` ...
Stage & commit the changes	`git commit -a`

Git Summary

For cheaters: A Basicerer Workflow

Edit files	`vim` / `emacs` / `subl` ...
Stage & commit the changes	`git commit -a`

- **Advices**: **Commit early, commit often!**
  - ↪ commits = save points
    - ✓ use descriptive commit messages
  - ↪ Don't get out of sync with your collaborators
  - ↪ Commit the sources, not the derived files

- **Not covered here (by lack of time)**
  - ↪ Branches, tags, remotes, submodules, subtrees, etc...

Summary

Environment Management

- RR assumes that you **Master your environment**
- Keep it **clean and automated** by:
  - ↪ Using common building tools — make, cmake etc.
  - ↪ Using a constrained environment
    - ✓ Sandboxed Ruby environment — `bundler`, `Gemfile`
    - ✓ Sandboxed Python — `pip freeze`, `pyenv`, `virtualenv`
    - ✓ VMs or Containers — Vagrant, Docker
  - ↪ Automate its building through cross-platform recipes
  - ↪ Automatically test your recipes for Environment configuration

Controlled Ruby Environment

- Consider using RVM, rbenv and more importantly Bundler
  - ↪ Bring the flexibility of `Rakefile` (`Makefile` + Ruby)
  - ↪ Bundler: **reproducible** running environment **across** developpers
  - ↪ easy configuration through `Gemfile[.lock]` + `bundle` command
- RVM: sandboxed environment per project (**alternative**: rbenv)
  - ↪ easy configuration through `.ruby-{version,gemset}` files

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Typical setup of a freshly cloned project:

```
$> gem install bundler # assuming it is not yet available
$> bundle              # clone ruby deps/env as defined in Gemfile*
$> rake -T             # To list the available tasks
```

Controlled Ruby Environment

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$> bundle              # clone ruby deps/env as defined in Gemfile*
$> rake -T             # To list the available tasks
```

Recommended Gems

`rake`, `bundler`, `falkorlib`

Controlled Python Environment

- `pip`: Python package manager
  - ↪ "nice" python packages: `mkdocs`...
  - ↪ Windows: install via Chocolatey

```
$> pip install <package>                    # install <package>
```

Controlled Python Environment

- `pip`: Python package manager
  - ↪ "nice" python packages: `mkdocs`...
  - ↪ Windows: install via Chocolatey

```
$> pip install <package>                    # install <package>
```

```
$> pip install -U pip                       # upgrade on Linux/Mac OS
```

Controlled Python Environment

- `pip`: Python package manager
  - ↪ "nice" python packages: `mkdocs`...
  - ↪ Windows: install via Chocolatey

```
$> pip install <package>                    # install <package>
```

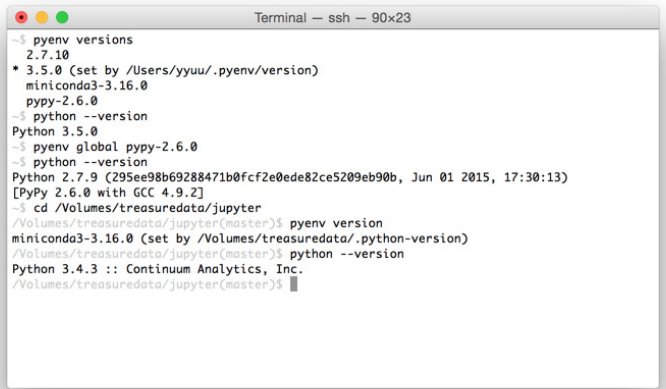
```
$> pip install -U pip                       # upgrade on Linux/Mac OS
```

- Dump python environment to a requirements file

```
$> pip freeze -l > requirements.txt         # as Ruby Gemfiles
```

Pyenv / VirtualEnv / Autoenv

- pyenv: ≃ RVM/rbenv for Python
- virtualenv ≃ RVM Gemset
- (optional) autoenv
  - ↪ Directory-based shell environments
  - ↪ easy config through .env file. **Ex**:




```
# (rootdir)/.env : autoenv configuration file
pyversion=‘head .python-version‘
pvenv=‘head .python-virtualenv‘

pyenv virtualenv --force --quiet ${pyversion} ${pvenv}-${pyversion}
# activate it
pyenv activate ${pvenv}-${pyversion}
```

Constrained VM environment

- Let's see how to reproduce a simple yet practical example in a **constrained** and **reproducible** VM environment.

Challenge 1: Reproduce the Build of these Slides

- Several **tricky** issues illustrating previous best practices
  - ↪ grab the sources — `git`
  - ↪ use of a constrained environment — Vagrant
  - ↪ installing the prerequisite software environment — `apt-get`
    - ✓ [un]common mix here: `make`, `latex-beamer`, `biber`, `pandoc`...
    - ✓ generally the **major challenge** in reproducing computations...

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`http://rr-tutorials.readthedocs.io/en/latest/hands-on/vagrant/`

IF NOT YET DONE: `http://rr-tutorials.readthedocs.io/en/latest/setup/`

Grab the [Code/Data] Source

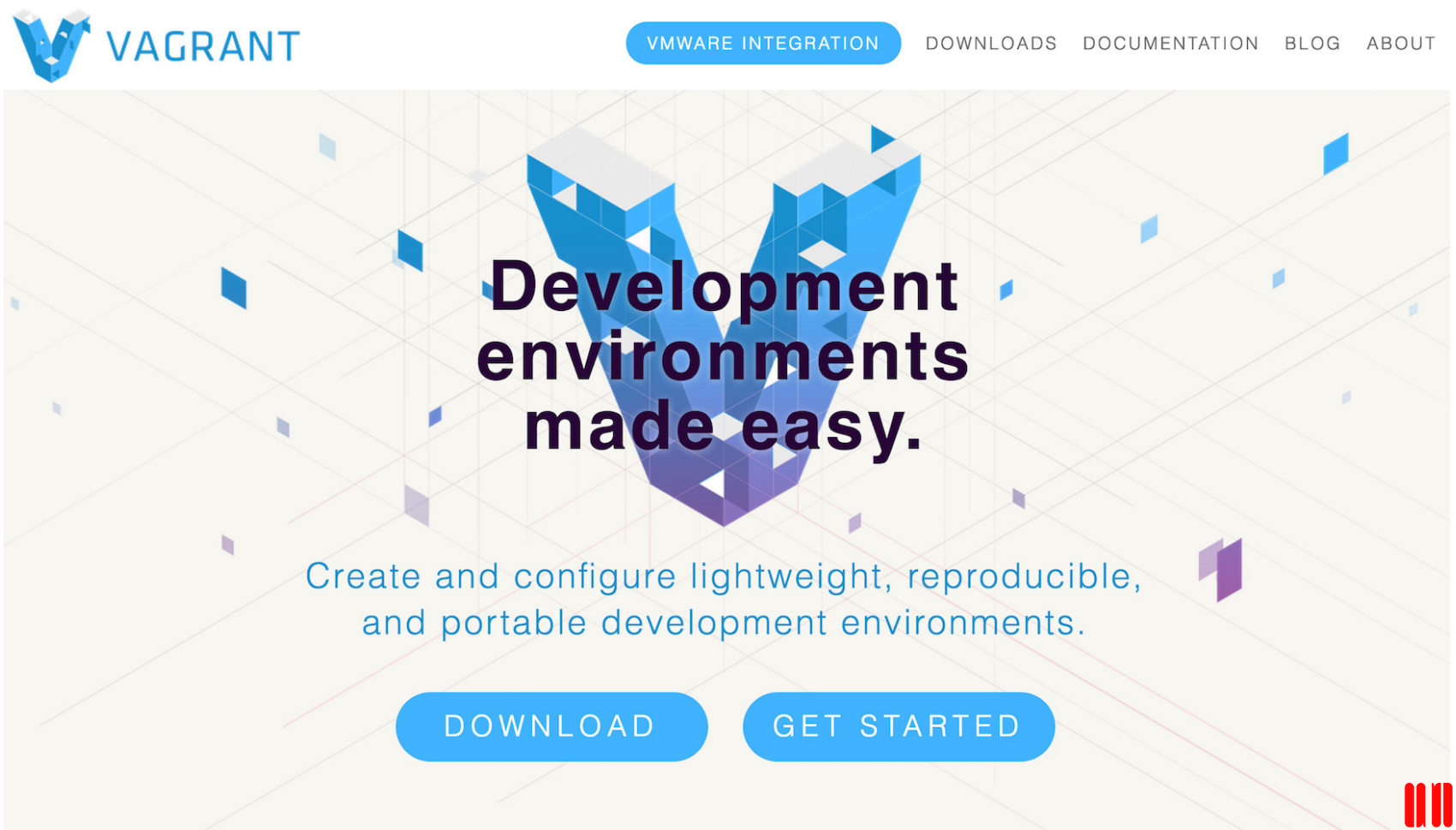
- You should have now Git installed
- Get the `RR-tutorials` repository from Github

```
$> git clone https://github.com/Falkor/RR-tutorials.git
$> cd RR-tutorials
$> make setup  # OR git submodule init && git submodule update
```

- **Notable** elements within this cloned repository:
  - ↪ the LaTeX slides sources `slides/2016/cloudcom2016/src/`
  - ↪ Documentation sources `mkdocs.yml` and `docs/`
  - ↪ Vagrant configuration for **this** project `Vagrantfile`
  - ↪ Bats unit tests `tests/`
  - ↪ Continuous Integration settings through Travis-CI `.travis.yml`

Use a Constrained Environment

http://vagrantup.com/



What is Vagrant ?

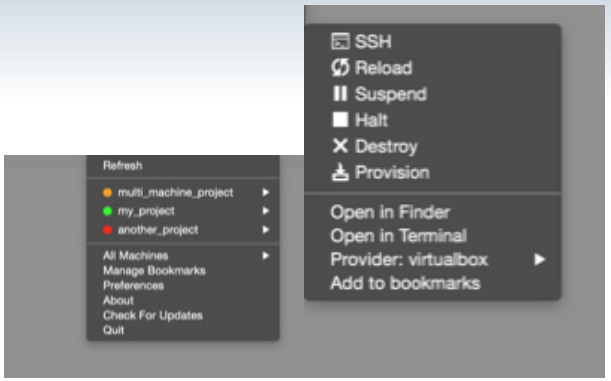
Create and configure **lightweight**, **reproducible**, and **portable** development environments

- **Command line** tool `vagrant [...]`
- Easy and Automatic per-project VM management
  - ↪ Supports many hypervisors: VirtualBox, VMWare...
  - ↪ Easy text-based configuration (Ruby syntax) `Vagrantfile`
- Supports **provisioning** through configuration management tools
  - ↪ Shell
  - ↪ Puppet `https://puppet.com/`
  - ↪ Salt... `https://saltstack.com/`

Cross-platform: runs on Linux, Windows, MacOS

Installation Notes

http://rr-tutorials.readthedocs.io/en/latest/setup/



- **Mac OS X**:
  - ↪ best done using Homebrew and Cask

```
$> brew install caskroom/cask/brew-cask
$> brew cask install virtualbox    # install virtualbox
$> brew cask install vagrant
$> brew cask install vagrant-manager # cf http://vagrantmanager.com/
```

- **Windows / Linux**:
  - ↪ install Oracle Virtualbox and the Extension Pack
  - ↪ install Vagrant

Why use Vagrant?

- Create new VMs quickly and easily: only one command!
  - ↪ `vagrant up`
- Keep the number of VMs under control
  - ↪ All configuration in `VagrantFile`
- **Reproducibility**
  - ↪ Identical environment in development and production
- **Portability**
  - ↪ **avoid** sharing 4 GB VM disks images
  - ↪ Vagrant Cloud to share your images
- **Collaboration made easy**:

```
$> git clone ...
$> vagrant up
```

Minimal default setup

```
$> vagrant init [-m] <user>/<name> # setup vagrant cloud image
```

- A `Vagrantfile` is configured for box `<user>/<name>`
  - ↪ Find existing box: Vagrant Cloud https://vagrantcloud.com/
  - ↪ You can have multiple (named) box within the **same** `Vagrantfile`
    - ✓ See `ULHPC/puppet-sysadmins/Vagrantfile`

```
Vagrant.configure(2) do |config|
   config.vm.box = '<user>/<name>'
   config.ssh.insert_key = false
end
```

Box name	Description
`ubuntu/trusty64`	Ubuntu Server 14.04 LTS
`debian/contrib-jessie64`	Vanilla Debian 8 "Jessie"
`centos/7`	CentOS Linux 7 x86_64
`svarrette/RR-tutorials`	IEEE CloudCom 2016 Tuto

Pulling and Running a Vagrant Box

```
$> vagrant up          # boot the box(es) set in the Vagrantfile
```

- Base box is downloaded and stored locally `~/.vagrant.d/boxes/`
- A new VM is created and configured with the base box as template
  - ↪ The VM is booted and (eventually) provisioned
  - ↪ Once within the box: `/vagrant` = directory hosting `Vagrantfile`

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$> vagrant status                  # State of the vagrant box(es)
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```
$> vagrant status                  # State of the vagrant box(es)
```

```
$> vagrant ssh                  # connect inside it, CTRL-D to exit
```

Stopping Vagrant Box

```
$> vagrant { destroy | halt }                    # destroy / halt
```

- Once you have finished your work within a *running* box
  - ↪ save the state for later with `vagrant halt`
  - ↪ reset changes / tests / errors with `vagrant destroy`
  - ↪ commit changes by generating a new version of the box

Back to Hands-on 1

Your Turn! http://rr-tutorials.readthedocs.io/en/latest/hands-on/vagrant/

- **Steps [1-4]** to cover the following elements:
  - ↪ **Basic Usage of Vagrant**
  - ↪ **Build these Slides**
    - ✓ find the prerequisite software environment `apt-get`
    - ✓ [un]common mix here: `make`, `latex-beamer`, `biber`, `pandoc...`

- **Hints**:
  - ↪ if a package is missing, find the appropriate one `apt-cache search`
  - ↪ Ubuntu Package Search for a missing `*.sty` http://packages.ubuntu.com/
    - ✓ `Search the contents of packages` for Distribution `Trusty`

Vagrant Box Provisioning

- Now you have *hopefully* a working **documented procedure**
  - ↪ it's time to **bundle it** for provisioning the box upon boot
  - ↪ key for sustainable reproducible environment
- Simple case: **inline** provisioning **i.e.** list commands to run

Vagrant Box Inline Provisioning

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```
config.vm.provision "shell", inline: <<-SHELL
  sudo apt-get update --fix-missing
  sudo apt-get upgrade
  # Complete the below list of missing packages
  apt-get -yq --no-install-suggests --no-install-recommends install \
        git make latex-beamer biber latex-make [...]
SHELL
```

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        git make latex-beamer biber latex-make [...]
SHELL
```

```
$> vagrant provision          # test your provisioning config
```

Vagrant Box Inline Provisioning

Your Turn! http://rr-tutorials.readthedocs.io/en/latest/hands-on/vagrant/

- **Steps 5**:
  - ↪ adapt the `Vagrantfile` to embed your commands
  - ↪ recall that relative paths are expanded relative to the location of the root `Vagrantfile`
  - ↪ inline command are run as the `vagrant` user, **not** `root`

- **IMPORTANT**:
  - ↪ all your commands should run **in a non-interactive** way

```
apt-get install -y <package>    # Debian / Ubuntu
yum     install -y <package>    # CentOS/ Redhat
```

Vagrant Box Shell Provisioning

- Embed your inline commands in a **Shell/Python/Ruby** script
  ↪ see sample script `vagrant/bootstrap.sample.sh`

```
config.vm.provision "shell", path: "<script>.{sh|py|rb}"
```

Your Turn! http://rr-tutorials.readthedocs.io/en/latest/hands-on/vagrant/

- **Steps 6**: copy and adapt `vagrant/bootstrap.sample.sh`
  ↪ adapt the `Vagrantfile` to provision the VM with your script
  ↪ test a reproducible provisioning from scratch

```
$> vagrant destroy && vagrant up && vagrant ssh
$> make -C make -C /vagrant/slides/2016/cloudcom2016/src/
```

Vagrant Box Packaging

- At some moment, you probably want to diffuse your custom box!
  - ↪ **Ex**: `svarrette/RR-tutorials` used for this tutorial
  - ↪ use Vagrant Cloud as a global storage media
  - ↪ `VBoxManage list runningvms` to get the real box name

```
$> vagrant package --base <real-box-name> --output <name>.box
```

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  - ↪ `VBoxManage list runningvms` to get the real box name

```
$> vagrant package --base <real-box-name> --output <name>.box
```

- **BEFORE packaging your box**:
  - ↪ Use official insecure SSH key `config.ssh.insert_key=false`
  - ↪ **Purge** the VM to reduce its size see `vagrant/purge.sh`
    - ✓ remove useless [big] packages `aptitude purge [...]`
    - ✓ Empty logs/history etc.
    - ✓ Zero out the free space `dd if=/dev/zero of=/EMPTY bs=1M`
  - ↪ **Up-to-date** Virtualbox **Guest additions** `vagrant vbguest`

Detailed Pre-Packaging Steps (1/2)

- Ensure you **DO NOT** reset the default (insecure) SSH key
  - ↪ default **expected** setting to SSH your box
  - ↪ **before** `vagrant up`, ensure replacement of SSH keys **is not done**

```
config.ssh.insert_key = false    # in Vagrantfile
```

- **Purge** the VM, in particular to **Zero out the free space**
  - ↪ see `vagrant/purge.sh`

```
# Remove APT cache
apt-get clean -y   && apt-get autoclean -y && apt-get autoremove -y
# Remove bash history
unset HISTFILE
rm -f /root/.bash_history && rm -f /home/vagrant/.bash_history
# Zero out free space to aid VM compression
dd if=/dev/zero of=/EMPTY bs=1M
rm -f /EMPTY
```

Detailed Pre-Packaging Steps (2/2)

- Ensure an **Up-to-date Virtualbox Guest additions**
  - ↪ ensure optimized usage of the box
  - ↪ simplified management with the vbguest plugin

```
# Install the 'vbguest' plugin
$> vagrant plugin install vagrant-vbguest
$> vagrant vbguest --status
GuestAdditions versions on your host (5.1.8) and guest (4.3.36)
do not match.
# Upgrade the GuestAdditions
$> vagrant vbguest --do install --auto-reboot [--force]
```

- If you want the **manual** way:
  - ↪ copy `/Applications/VirtualBox.app/Contents/MacOS/VBoxGuestAdditions.iso`
  - ↪ mount in **within** the VM
  - ↪ execute `VBoxLinuxAdditions.run`

Vagrant Box Packaging

```
# Locate the internal name of the running VM and repackage it
$> VBoxManage list runningvms
"RR-tutorials_default_1481463725786_57301" {...}
$> vagrant package \
    --base vagrant-vms_default_1431034026308_70455 \
    --output <os>-<version>-<arch>.box
```

Vagrant Box Packaging

```
# Locate the internal name of the running VM and repackage it
$> VBoxManage list runningvms
"RR-tutorials_default_1481463725786_57301" {...}
$> vagrant package \
    --base vagrant-vms_default_1431034026308_70455 \
    --output <os>-<version>-<arch>.box
```

- Now you can upload the generated box on Vagrant Cloud.
  - ↪ select '`New version`', enter the new version number
  - ↪ add a new box provider (`Virtualbox`)
  - ↪ upload the generated box

Vagrant Box Packaging

```
# Locate the internal name of the running VM and repackage it
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```

- Now you can upload the generated box on Vagrant Cloud.
  - ↪ select '`New version`', enter the new version number
  - ↪ add a new box provider (`Virtualbox`)
  - ↪ upload the generated box

- Upon successful upload: **release** the uploaded box
  - ↪ by default it is unreleased
  - ↪ Now people using the `<user>/<name>` box will be notified of a pending update

Vagrant Box Packaging

Your Turn! http://rr-tutorials.readthedocs.io/en/latest/hands-on/vagrant/

- **Steps 7-8**: Package your box and diffuse it on Vagrant Cloud
  - ↪ Make preliminary checks
  - ↪ Purge the VM
  - ↪ Package it and Upload to Vagrant Cloud

Vagrant Box Generation

- You might rely on Falkor/vagrant-vms
  - ↪ use it at your own risks
  - ↪ based on packer and veewee

```
$> git clone https://github.com/Falkor/vagrant-vms.git
$> cd vagrant-vms
$> gem install bundler && bundle install
$> rake setup
```

Vagrant Box Generation

- You might rely on Falkor/vagrant-vms
  - ↪ use it at your own risks
  - ↪ based on packer and veewee

```
$> git clone https://github.com/Falkor/vagrant-vms.git
$> cd vagrant-vms
$> gem install bundler && bundle install
$> rake setup
```

```
# initiate a template for a given Operating System:
$> rake packer:{Debian,CentOS,openSUSE,scientificlinux,ubuntu}:init
# Build a Vagrant box
$> rake packer:{Debian,CentOS,openSUSE,scientificlinux,ubuntu}:build
# If things goes fine:
$> vagrant box add packer/<os>-<version>-<arch>/<os>-<version>-<arch>.box
```

Advanced Provisioning: Puppet

- Shell provisioning is a reasonable good basis but **not sufficient**
  - ↪ **hard to be cross-platform** `apt-get` vs. `yum`
- You quickly something more **consistent**
  - ↪ Puppet `https://puppet.com/`
  - ↪ Salt... `https://saltstack.com/`

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  - ↪ Salt... `https://saltstack.com/`

Puppet: Reproducible/Cross-Platform IT Environment

- Advanced configuration management and **IT Automation**
  - ↪ cross-platform w. Puppet's Resource Abstraction Layer (RAL)
  - ↪ Git-based workflow
- Embed environment management in **manifests** and **modules**
  - ↪ **nodes manifests**: nodes definitions
  - ↪ **modules**: (reusable) set of recipe to configure a given service
    - ✓ Large Community Recipes / Modules `https://forge.puppet.com/`

Puppet Operational modes

- **Masterless** - apply Puppet manifests directly on the target system.
  - ↪ No need of a complete client-server infrastructure.
  - ↪ Have to distribute manifests and modules to the managed nodes.

```
$> puppet apply --modulepath /modules/ /manifests/file.pp
```

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```
$> puppet apply --modulepath /modules/ /manifests/file.pp
```

- **Master / Client** Setup
  - ↪ server (running as `puppet`) listening on 8140 on the Puppet Master
  - ↪ client (running as `root`) on each managed node.
    - ✓ Run as a service (default), via cron (with random delays), manually or via MCollective
  - ↪ Client and Server have to share SSL certificates
    - ✓ certificates must be signed by the Master CA

```
$> puppet agent --test [--noop] [--environment <environment>]
```

Puppet DSL

- A Declarative Domain Specific Language (DSL)
  - ↪ defines **STATES** (and **not** procedures)
- Puppet code is written in **manifests** `<file>.pp`
  - ↪ **declare resources** that affect elements of the system
    - ✓ each resource has a type (`package`, `service`, `file`, `user`, `exec` ...)
    - ✓ each resource has a **uniq** title
  - ↪ resources are grouped in **classes**
- Classes and configuration files are organized in **modules**
- **Example** of resources types:

```
file { '/etc/motd':
  content => "Toto"
}
```

```
package { 'openssh':
  ensure => present,
}
```

```
service { 'httpd':
  ensure => running,
  enable => true,
}
```

Puppet Classes

- **Containers** of different resources
  - ↪ Can have parameters since Puppet 2.6

```
class mysql (
  $root_password = 'default_value',
  $port          = '3306',
) {
  package { 'mysql-server':
    ensure => present,
  }
  service { 'mysql':
    ensure    => running,
  }
  [...]
}
```

Puppet Classes Declaration

- To use a class previously defined, we **declare** it
- "Old style" class declaration, without parameters:

```
include mysql
```

- "New style" (from Puppet 2.6) with explicit parameters:

```
class { 'mysql':
  root_password => 'my_value',
  port          => '3307',
}
```

- A class is **uniq** to a given node

Puppet Defines

- Similar to parametrized classes . . .
  - ↪ . . . but can be used multiple times (with different titles).

```
# Definition of a define
define apache::virtualhost (
  $ensure   = present,
  $template = 'apache/virtualhost.conf.erb' ,
  [...] ) {
  file { "ApacheVirtualHost_${name}":
    ensure  => $ensure,
    content => template("${template}"),
  }
}
# Declaration of a define:
apache::virtualhost { 'www.uni.lu':
  template => 'site/apache/www.uni.lu-erb'
}
```

Puppet Variables and Facts

- Can be defined in different places and by different actors:
  - ↪ by client nodes as facts
  - ↪ defined by users in Puppet code, on Hiera on in the ENC
  - ↪ built-in and be provided directly by Puppet
- Facts using `facter`:
  - ↪ runs on clients and collects facts that the server can use as variables

```
$> facter
architecture => x86_64
fqdn => toto.uni.lu
kernel => Linux
memorytotal => 16.00 GB
operatingsystem => Centos
operatingsystemrelease => 6.3
osfamily => RedHat
virtual => physical
[...]
```

- Can be used outside Puppet
- Good tool to **abstract** your environment
  - ↪ permits **reproducible** and cross-platform developments

Puppet User Variables

- In Puppet manifests:

```
$role = 'mail'
$package = $::operatingsystem ? {
    /(?i:Ubuntu|Debian|Mint)/ => 'apache2',
    default                   => 'httpd',
}
```

- In an External Node Classifier (ENC)
  - ↪ Common ENC: Puppet DashBoard, the Foreman, Puppet Enterprise.
- In an Hiera backend

```
$syslog_server = hiera(syslog_server)
```

Puppet Nodes

- A **node**/system is identified by its **certname**
  - ↪ defaults to the node's fqdn

```
node 'web01' {
  include apache
}
```

```
node /^www\d+$/ {
  include apache
}
```

- Nodes classification can be done by External Node Classifier (ENC)
  - ↪ Puppet DashBoard, The Foreman and Puppet Enterprise
- Nodes classification can be done also by Hiera
  - ↪ In `/etc/puppet/manifests/site.pp`

```
hiera_include('classes')
```

Vagrant Puppet Provisionning

- Operate in **masterless** mode
- Embed your manifests and modules in your repository
  - ↪ grab community modules with `librarian-puppet`, `r10K`

```
config.vm.provision :puppet  do |puppet|
    puppet.hiera_config_path = 'hieradata/hiera.yaml'
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Vagrant Puppet Provisionning

- Operate in **masterless** mode
- Embed your manifests and modules in your repository
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Your Turn! ... **Or not ☺(no time)**

Software/Modules Management

- **Software Management Challenge**
  - ↪ Not so much standardization
    - ✓ every machine/app has a different software stack / installation procedure
    - ✓ Sites share unique hardware among teams with very different requirements
    - ✓ **You** want to experiment with many exotic architectures
- Software Flavor vs. Dependency nightmare vs Performance
  - ↪ **Ex**: 3 compilers + 3 MPI + n software
  - ↪ Complex set of CLI options,
  - ↪ One of the main limits for RR
- Some Tools can help you!
  - ↪ Easybuild `http://easybuild.readthedocs.io/`
  - ↪ Spack `http://spack.readthedocs.io/`
  - ↪ CDE
  - ↪ Kameleon `http://kameleon.imag.fr/`

EasyBuild

http://easybuild.readthedocs.io/

- Easybuild: open-source framework to (automatically) build scientific software
- **Why?**: *"Could you please install this software on the cluster?"*
  - ↪ Scientific software are often **painful** to build
    - ✓ non-standard build tools / incomplete build procedure
    - ✓ hardcoded parameters and/or poor/outdated documentation
  - ↪ EasyBuild helps to facilitate this task
    - ✓ consistent software build and installation framework
    - ✓ automatically generates LMod modulefiles

EasyBuild Installation

http://easybuild.readthedocs.io/

```
# pick an installation prefix to install EasyBuild to
export EASYBUILD_PREFIX=$HOME/.local/easybuild
# download script
curl -O goo.gl/RK3Gpf    # Get bootstrap_eb.py
# bootstrap EasyBuild
python bootstrap_eb.py $EASYBUILD_PREFIX
# update $MODULEPATH, and load the EasyBuild module
module use $EASYBUILD_PREFIX/modules/all
module load EasyBuild
```

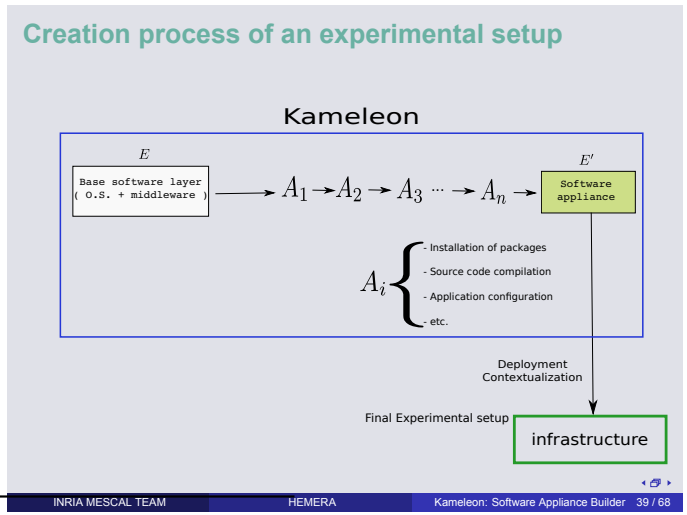
EasyBuild Usage

http://easybuild.readthedocs.io/

```
# Load EasyBuild module
module load EasyBuild
# Check version
eb --version
# Look for HPL
eb -S HPL
# Check what needs to be built to compile HPL 2.1 with Intel compiler
HPL-2.1-intel-2016b.eb
# Check what needs to be built to compile HPL 2.1 with GCC/OpenMPI/...
eb HPL-2.1-foss-2016b.eb -Dr
# Build HPL and its dependencies
eb HPL-2.1-foss-2016b.eb -r
# See available HPL now
module avail HPL
# Amending an existing easyconfig
eb HPL-2.1-foss-2016b.eb --try-software-version=2.2
```

Kameleon: Reproducible SW[11]

- Uses *recipes* (high-level description)
  - ↪ Similar to cfengine, Puppet, Chef in the sysadmin world
- Persistent cache to allow re-generation without external resources
  - ↪ Linux distribution mirror ⇝ self-contained archive
  - ↪ Supports LXC, Docker, VirtualBox, qemu, Kadeploy images, etc.



[11] Cristian Camilo Ruiz Sanabria et al. "Reproducible Software Appliances for Experimentation". In: **TRIDENTCOM'2014**.

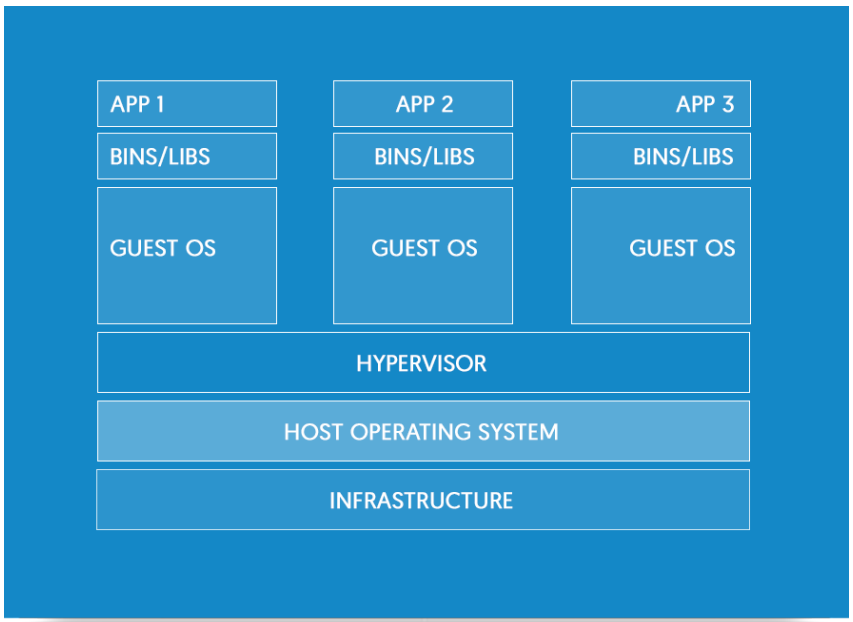
Courtesy of L. Nussbaum

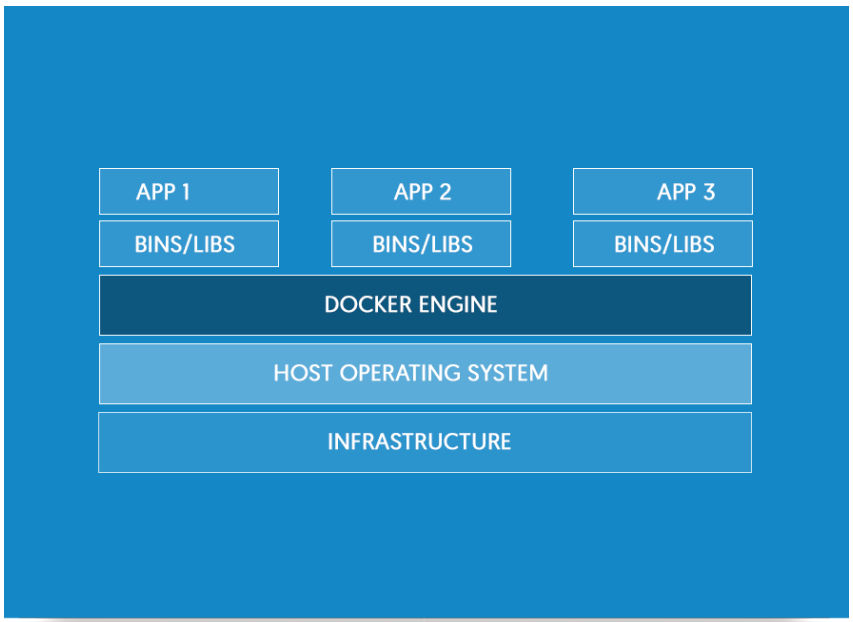
Lighweight Constrained Env.: Docker

http://www.docker.com

- Open-source engine
- Automates the deployment of any application
  - ↪ **lightweight**, **portable**, **self-sufficient** container
  - ↪ will run virtually anywhere
- Tries to achieve deterministic builds by isolating your service
  - ↪ build done from a snapshotted OS and running imperative steps on top of it
- **Dependency hell**:
  - ↪ Docker works with images that consume minimal disk space
  - ↪ all images are **versioned**, **archivable**, and **shareable** DockerHub
- `Dockerfiles`: resolving imprecise documentation

VM vs. Containers





- **Virtual machines**
  - ↪ app + binaries + libraries
  - ↪ incl. an entire guest OS
- **Container**
  - ↪ app + binaries + libraries
  - ↪ kernel shared
  - ↪ run on **any** computer

Pulling and Running Images

```
$> docker pull <name>:<tag>
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- Pull a **public** image such as ubuntu or centos
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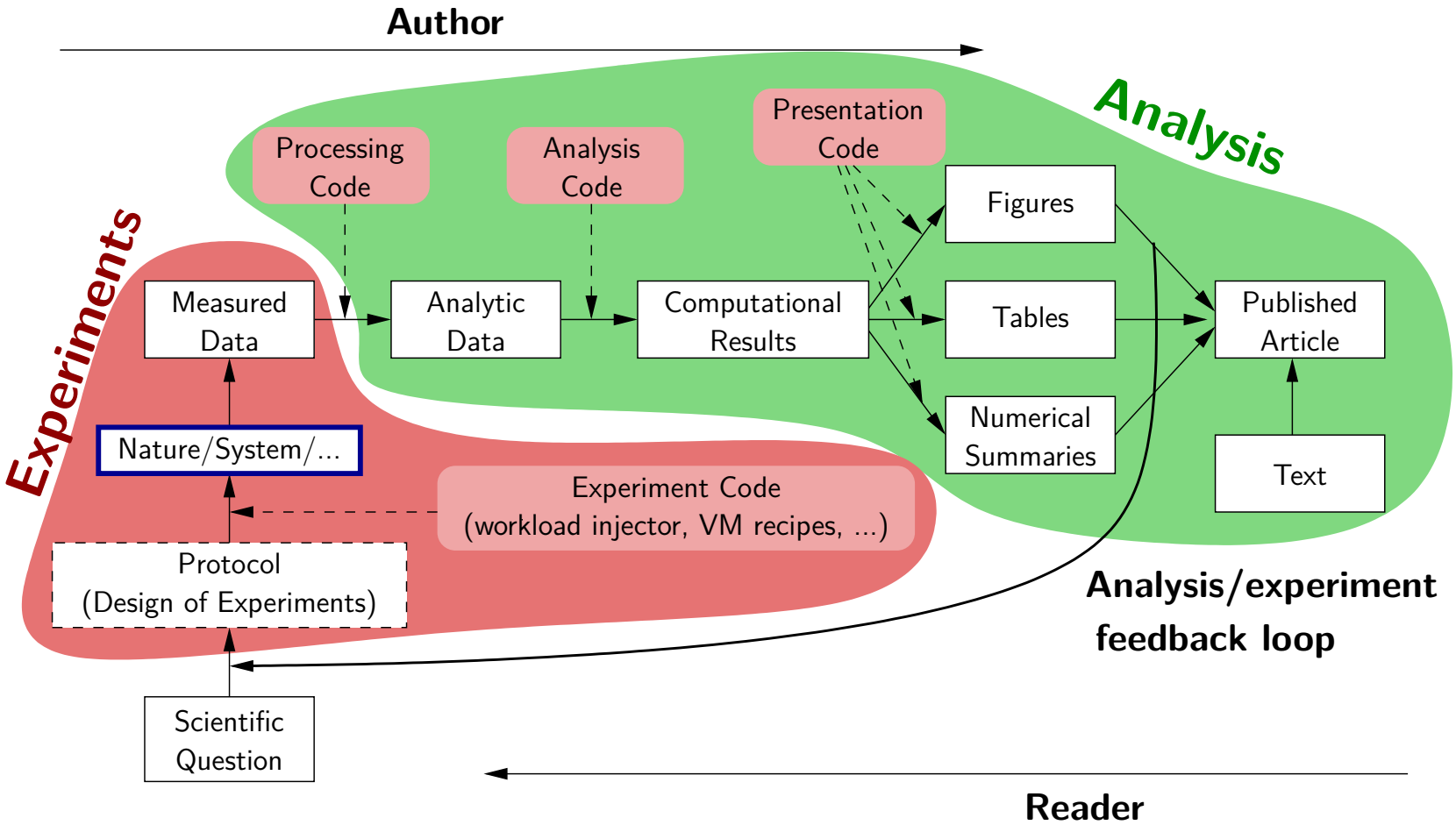
Your Turn!

http://rr-tutorials.readthedocs.io/en/latest/hands-on/docker/

Summary

The Research Pipeline



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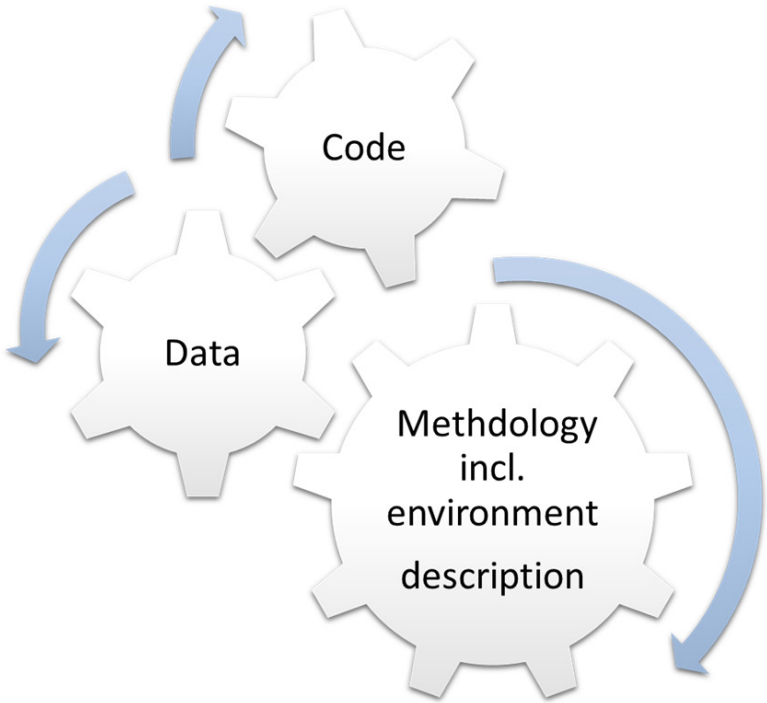
  - ↪ Markdown, mkdocs, org-mode, Read the Docs...
- **Sharing Code and Data**
  - ↪ `git`, Github, Bitbucket, Gitlab...
- **Mastering your environment clean and automated** by:
  - ↪ Using common building tools make, cmake etc.
  - ↪ Using a constrained environment
    - ✓ Sandboxed Ruby/Python,Vagrant, Docker
  - ↪ Automate its building through cross-platform recipes
  - ↪ Automatically test your recipes for Environment configuration

Sharing Code and Data

- Is this enough?
  1. Use a work ow that **documents both data and process**
  2. Use the machine readable **CSV format**
  3. Provide **raw** data and **meta** data, not just statistical outputs
  4. **Never** do data manipulation and statistical tests **by hand**
  5. Use R, Python or another free software to read and process raw data
     - ✓ ideally to produce complete reports with code, results and prose

Reproducibility axes

- Always keep track of:
  - ↪ your **methodology**
  - ↪ your **code**
  - ↪ your (input) **data**
- Can you later come back and:
  - ↪ reproduce your experiment
  - ↪ including its environment
  - ↪ . . . and obtain the same results?



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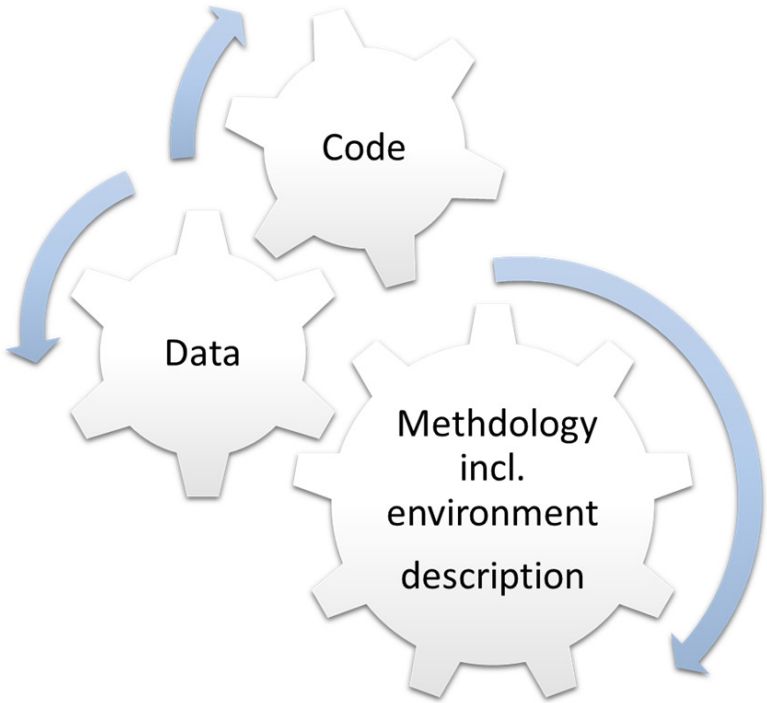
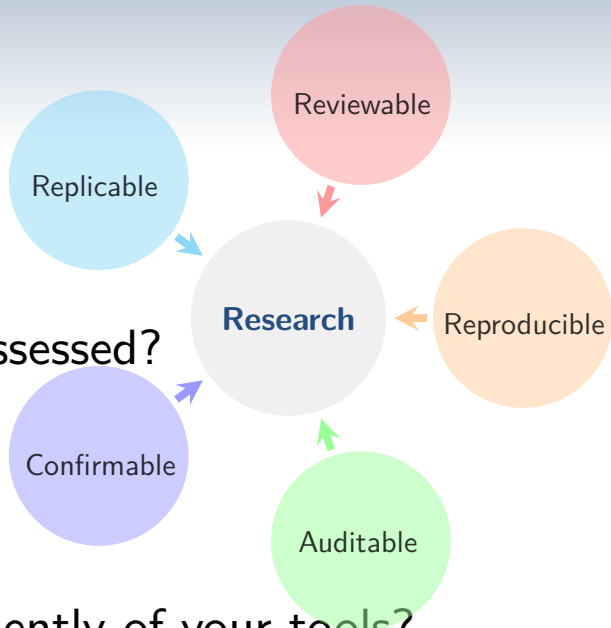


- If **not**, then **now** is the best time to start
  - ↪ documenting your processes
  - ↪ describing your environment (software **and hardware**!)
  - ↪ versioning and tagging your code and data
  - ↪ (. . . and keep backups of it all)

Reproducibility levels



Is your research[12]:

- reviewable
  - ↪ desc. of your methods can be independently assessed?
- replicable
  - ↪ are the tools available to duplicate the results?
- confirmable
  - ↪ can the main conclusions be attained independently of your tools?
- auditable
  - ↪ do you have records such that your research can be later defended?
  - ↪ . . . or differences between independent confirmations resolved?
- **open or reproducible**, such that
  - ↪ the procedures can be fully audited **and**
  - ↪ the results can be replicated or independently reproduced **and**
  - ↪ the results can be extended or the method applied to new problems

[12] ICERM Report 2013: "Reproducibility in Computational and Experimental Mathematics"

Open challenges

Sometimes you need to:

- Continue your computation **elsewhere**
  - ↪ another HPC node/cluster, supercomputer, cloud instance
- Continue your computation **in a different environment**
  - ↪ another software stack (*just* OS, *some* libraries / compiler flags)
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Keep track of your environment changes!

Questions?

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