Introduction to High Performance Scientific Computing

Autumn, 2016

Lecture 2

Imperial College
London

Announcements

- Lecture recordings at panopto.imperial.ac.uk
  - Will be available by end of day (search for ‘M3C’)

- Webpage: imperialhpsc.bitbucket.org

Assessment

4 Programming assignments
HW1: Assigned 19/10, due 26/10 (**5%**)
HW2: Assigned 27/10, due 7/11 (**20%**)
HW3: Assigned 10/11, due 21/11 (**20%**)
HW4: Assigned 24/11, due 1/12 (**15%**)

1 Programming Project (40%)
Assigned 2/12, due 15/12

Submitting HW2 **commits you to the course**

Main topics

- **Version control with git and bitbucket**
  - **Background on version control**
  - **Working locally on your computer**
  - **Moving material back and forth from the cloud**

Software version control

- Originally used for large projects with many developers
- Now a standard tool in software engineering
- Slowly becoming a standard tool in scientific computing

Software version control

- Originally used for large projects with many developers
- Now a standard tool in software engineering
- Slowly becoming a standard tool in scientific computing
- Useful for:
  - Collaboratively developing software
  - Keeping track of changes to code
  - Managing different versions of code in an organized manner
- The more complicated the problem, the more important it is to use version control!

Local version control

- SVN
  - Was standard tool 5-10 years ago, now losing popularity
  - Uses client-server model
  - Master version and history stored centrally on server
  - What happens if server is down?

- Git
  - Rapidly gaining popularity
  - Uses distributed model
  - Software history stored locally in *.git* subdirectory

Local projects

Good programming practice:

1. **Make a plan/outline**
2. **Take notes and add comments**
3. **Careful testing and validation**

Local projects

Good programming practice:

1. **Make a plan/outline**
2. **Take notes and add comments**
3. **Careful testing and validation**

Git helps with 2. and 3.

Local projects with git

Where you make changes →

Local projects with git

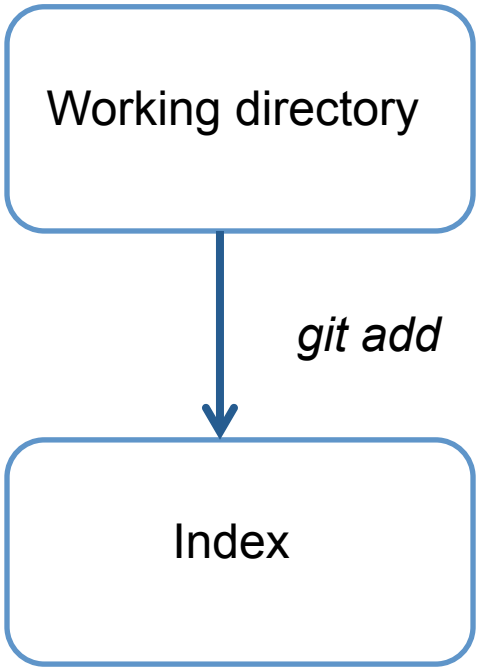
Where you make changes → Working directory

Index

'Archived' version(s) → Repository

Local projects with git

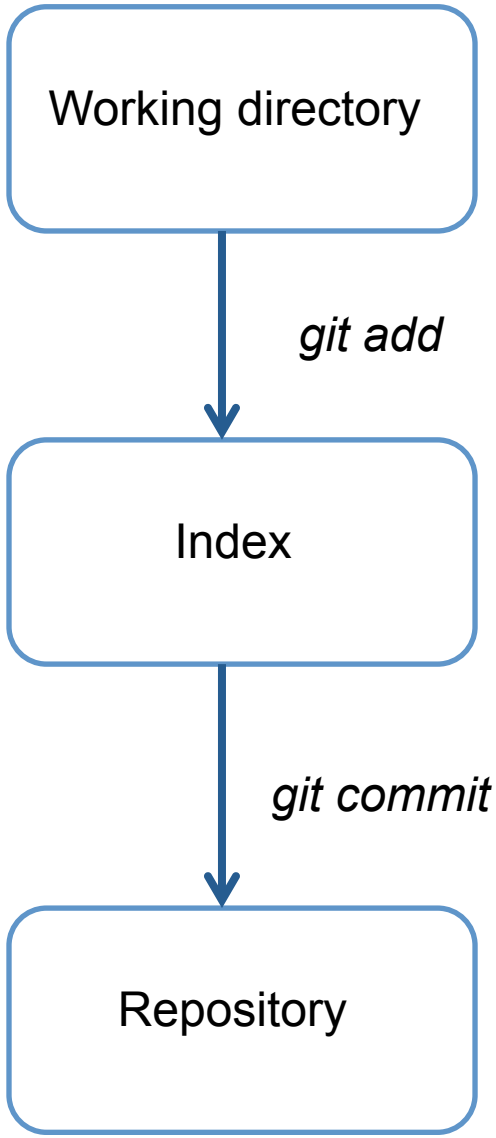
Where you make changes →



'Archived' version(s) →

Local projects with git

Where you make changes →



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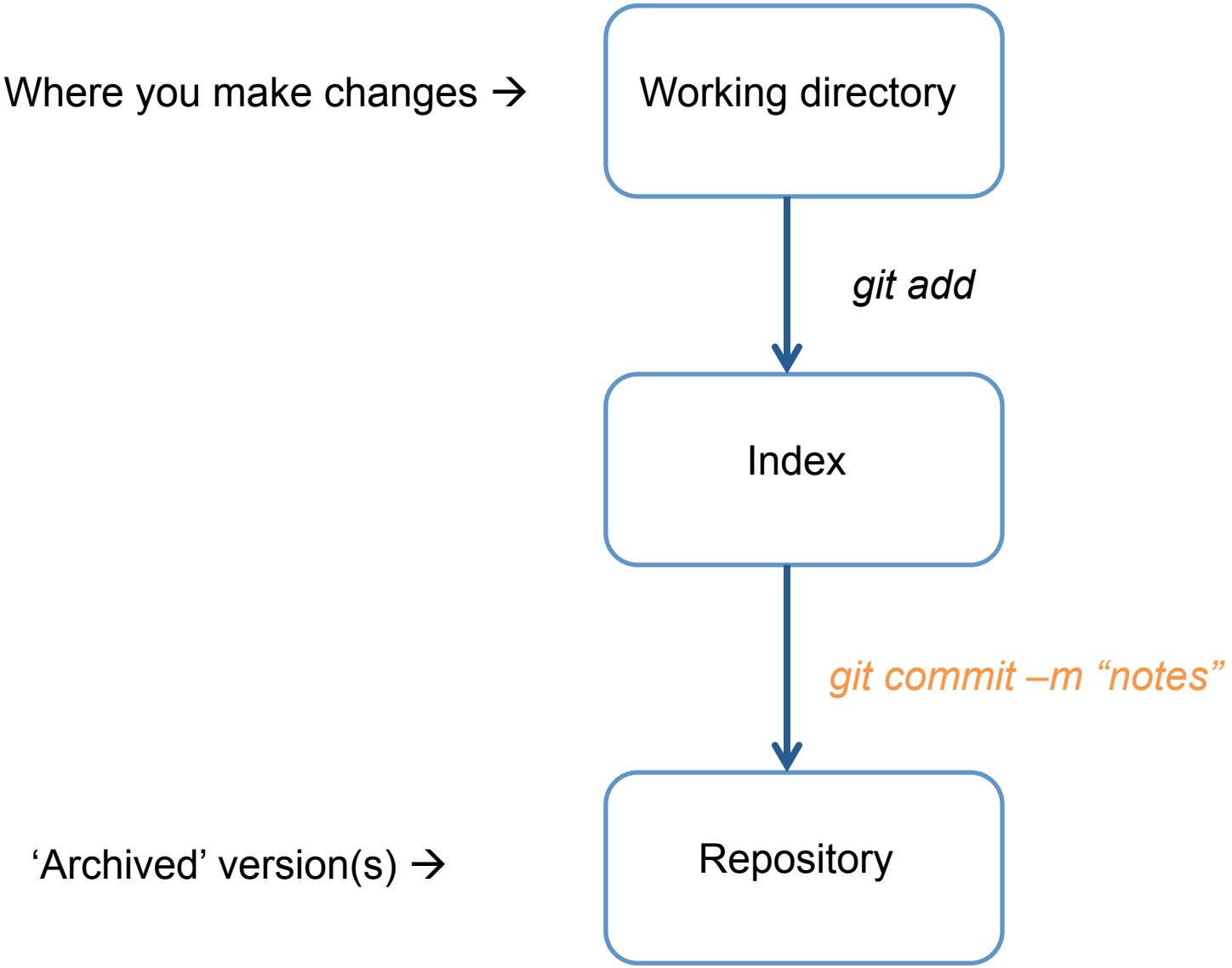
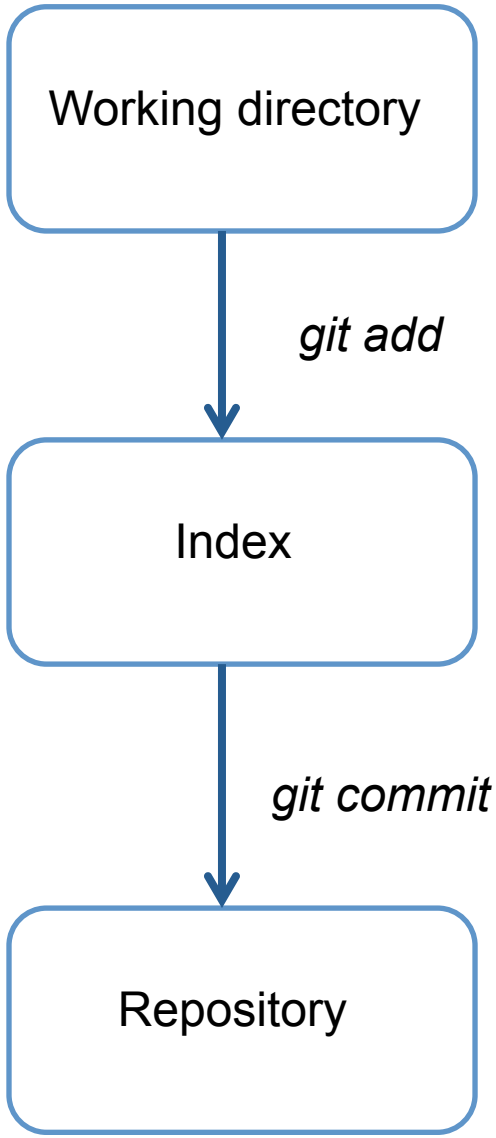
Local projects with git



Local projects with git

Where you make changes →



git status tells you at which stage files are placed

‘Archived’ version(s) →

Example: Creating a local git repository

Initialize

1st step: make directory and initialize as a repo:

```
$ mkdir git_example

$ cd git_example

$ git init
Initialized empty Git repository in /Users/prasun/Documents/
repos/git_example/.git/

$ ls –a
.   ..  .git
```

History of changes will be stored in hidden directory .git

Create file, add and commit

1. **Open text editor and make file,** *scientists.txt*
2. **Check status**

```
$ cat scientists.txt
Issac Newton
Albert Einstein

$ git status
On branch master

Initial commit

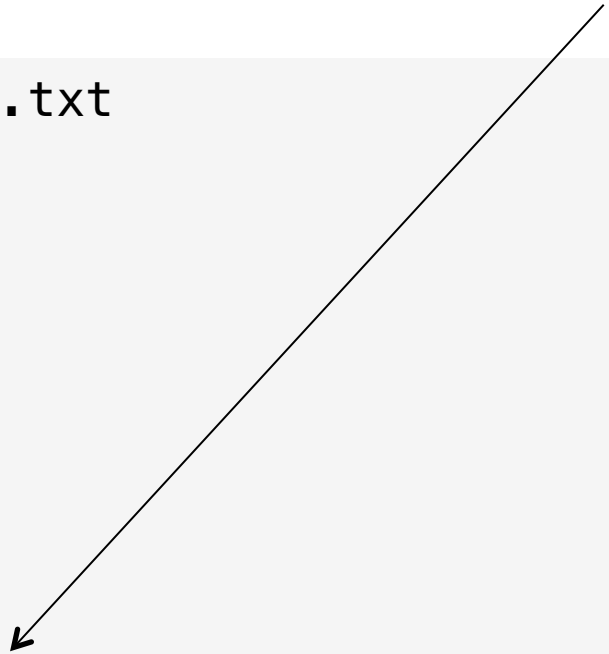
Untracked files:
  (use "git add <file>..." to include in what will be committed)

    scientists.txt

nothing added to commit but untracked files present (use "git
add" to track)
```

Create file, add and commit

Note: *git* tells you what to do next



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On branch master

Initial commit

Untracked files:
  (use "git add <file>..." to include in what will be committed)

    scientists.txt

nothing added to commit but untracked files present (use "git
add" to track)
```

Create file, add and commit

3. Add file to index

```
$ git add scientists.txt
$ git status
On branch master

Initial commit

Changes to be committed:
  (use "git rm --cached <file>..." to unstage)

    new file:   scientists.txt
```

Create file, add and commit

4. Commit file to repository

```
$ git commit -m "initial commit, scientists.txt added to repo"
scientists.txt
[master (root-commit) 6e74cfc] initial commit, scientists.txt
added to repo
 Committer: Prasun Ray

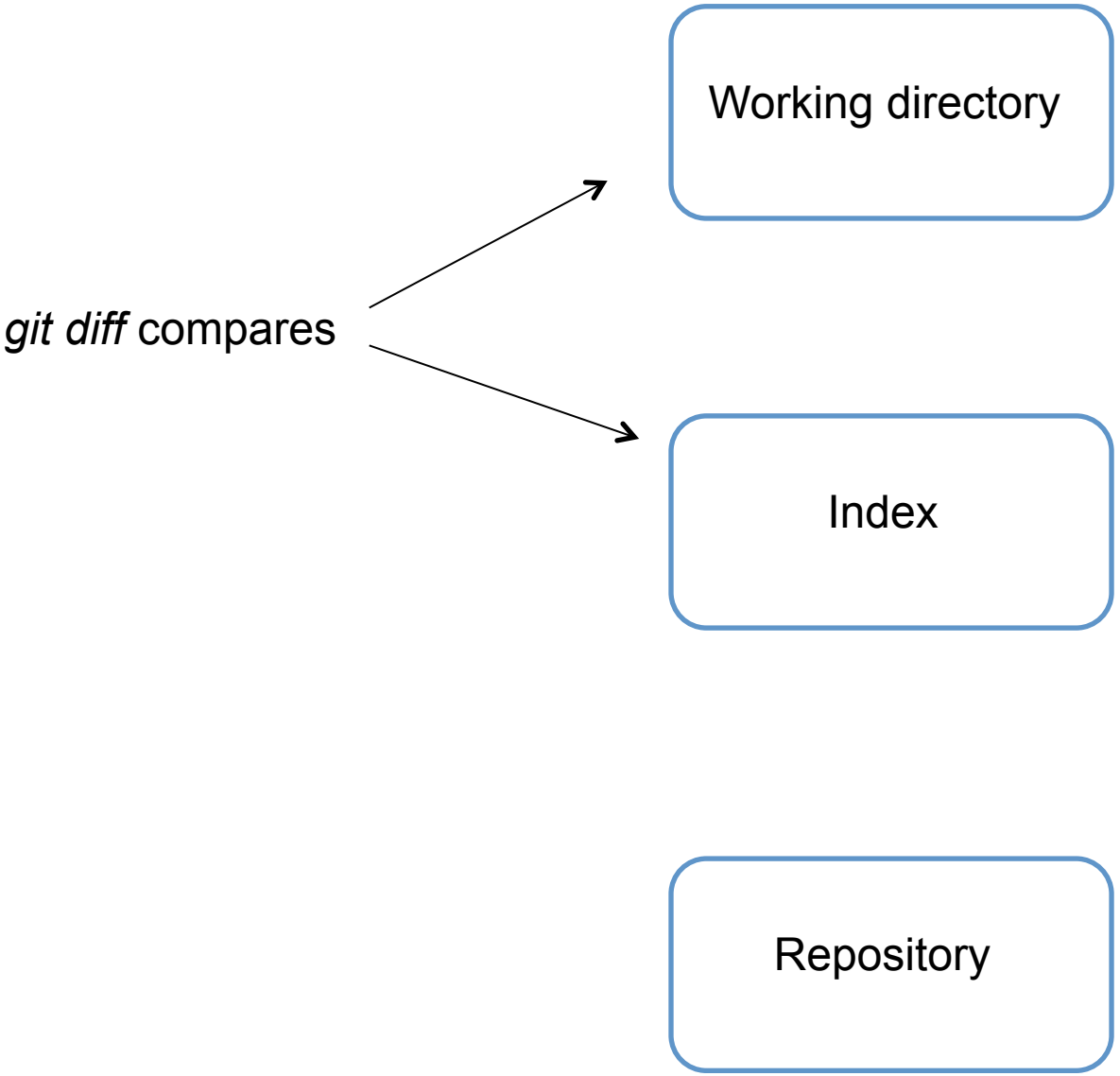
 1 file changed, 2 insertions(+)
 create mode 100644 scientists.txt
```

Now try *git status:*

```
$ git status
On branch master
nothing to commit, working directory clean
```

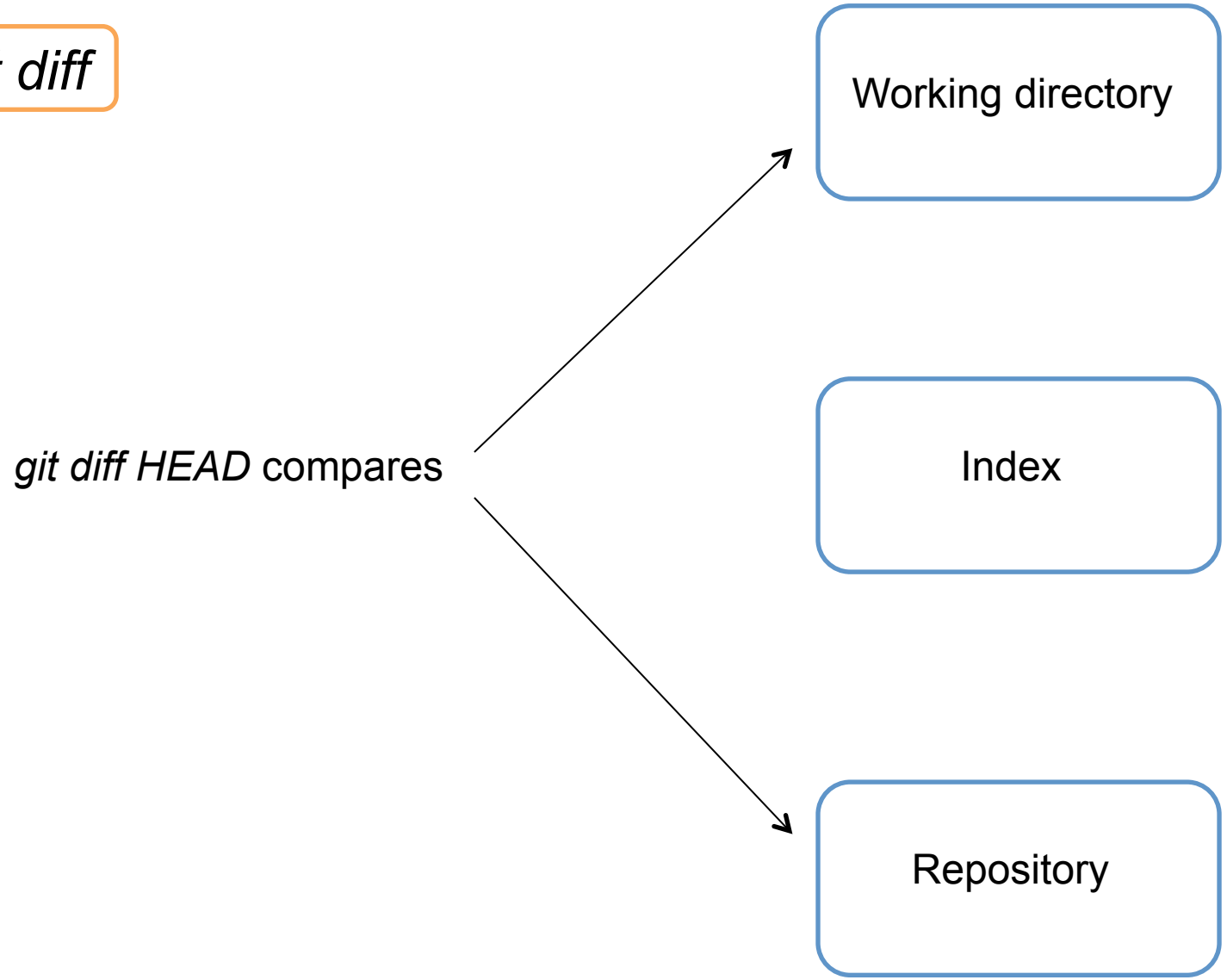
Local projects with git

git diff



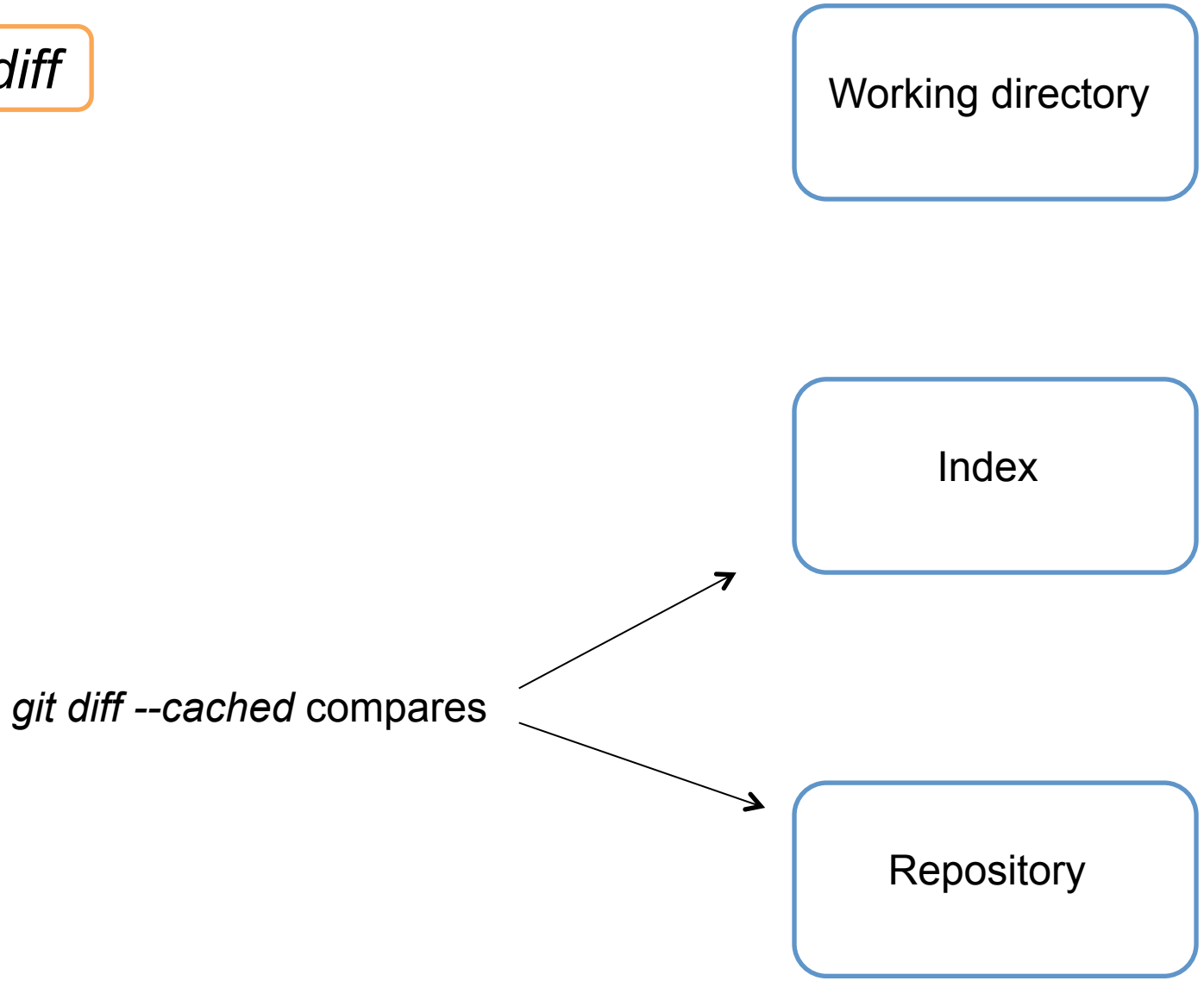
Local projects with git

git diff



Local projects with git

git diff



diff example

Make change to *scientists.txt* and compare to “official” version

```
$ cat scientists.txt
Issac Newton
Albert Einstein
Galileo Galilei
$
$ git diff HEAD
diff --git a/scientists.txt b/scientists.txt
index 9079fe8..efc1584 100644
--- a/scientists.txt
+++ b/scientists.txt
@@ -1,2 +1,3 @@
 Issac Newton
 Albert Einstein
+Galileo Galilei
```

Visiting previous versions

- *git log* provides project history

```
$ git log
commit aa47da5b74ab89a7929100d62679c2c5b81b2674
Author: Prasun Ray <p.ray@imperial.ac.uk>
Date:   Sun Oct 4 14:49:13 2015 +0100

    added Galileo

commit 6e74cfc8cf12191558751e610d80b76cb321a58c
Author: Prasun Ray <prasun@Prasuns-Air.home>
Date:   Sun Oct 4 14:34:22 2015 +0100

    initial commit, scientists.txt added to repo
```

Visiting previous versions

- *git log* provides project history
- *git checkout* lets you examine previous versions
- *git checkout master* returns to current version

```
$ git checkout 6e74cfc8c
Note: checking out '6e74cfc8c'.

You are in 'detached HEAD' state. You can look around, make experimental
changes and commit them, and you can discard any commits you make in this
state without impacting any branches by performing another checkout.

If you want to create a new branch to retain commits you create, you may
do so (now or later) by using -b with the checkout command again.
Example:

  git checkout -b new_branch_name

HEAD is now at 6e74cfc... initial commit, scientists.txt added to repo
```

```
$ cat scientists.txt
Issac Newton
Albert Einstein
```

Local projects with git

List of commands (so far):

git add
commit
status
diff
log
checkout

Local projects with git

List of commands (so far):

git add
commit
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Getting help:
git add --help
or
git log --help

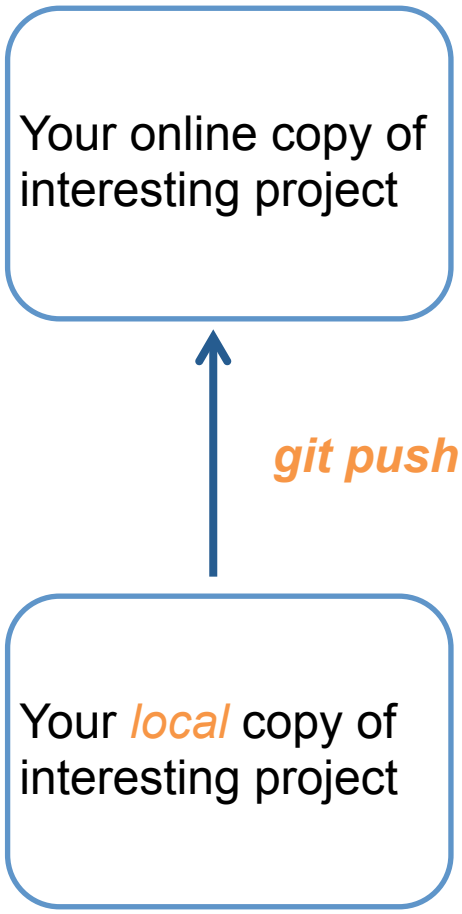
Laptop → cloud

1. **Create online repo in bitbucket:**
   Create → Create repository

2. **After creation, bitbucket takes you to "Repository setup"**

3. **Choose either "I'm starting from scratch" or "I have an existing project" and follow instructions.**

Copying & pasting instructions for pre-existing project…



Laptop → cloud

```
$ git remote add origin https://ImperialHPSC@bitbucket.org/
ImperialHPSC/git-example.git

$ git push -u origin --all # pushes up the repo and its refs for
the first time
Counting objects: 6, done.
Delta compression using up to 4 threads.
Compressing objects: 100% (2/2), done.
Writing objects: 100% (6/6), 531 bytes | 0 bytes/s, done.
Total 6 (delta 0), reused 0 (delta 0)
To https://ImperialHPSC@bitbucket.org/ImperialHPSC/git-
example.git
 * [new branch]      master -> master
Branch master set up to track remote branch master from origin.

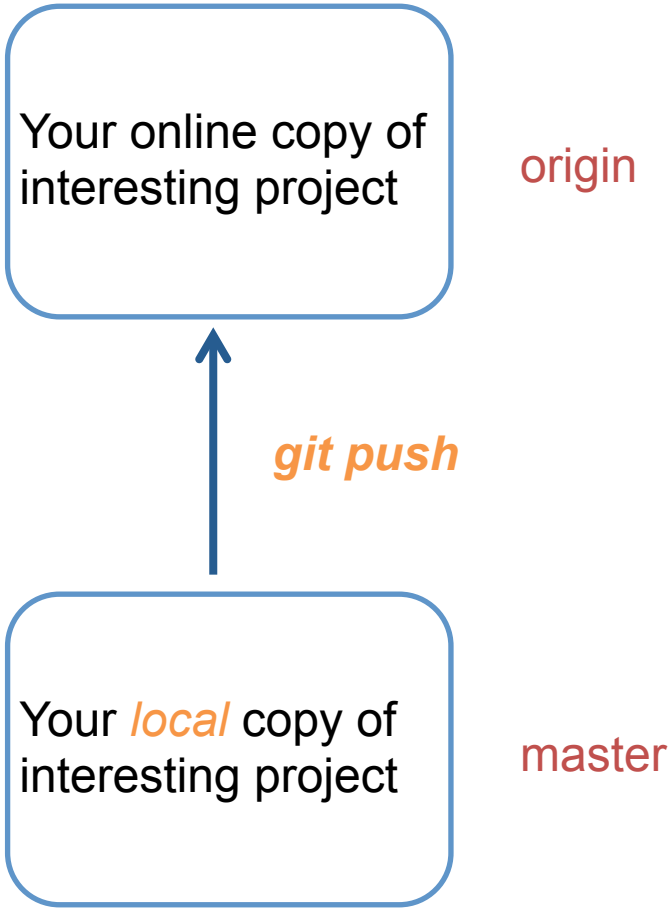
$ git push -u origin --tags # pushes up any tags
Everything up-to-date
```

Online repo is named *origin* and the local repo is *pushed* to *origin*

Laptop → cloud

Push your local repo online for:

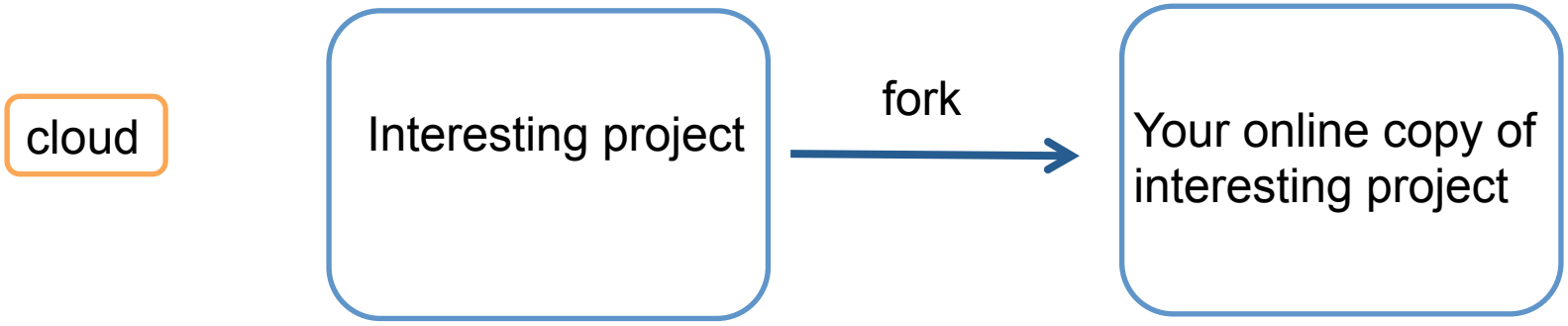
- **backup**
- **access to files from other machines**
- **sharing files**



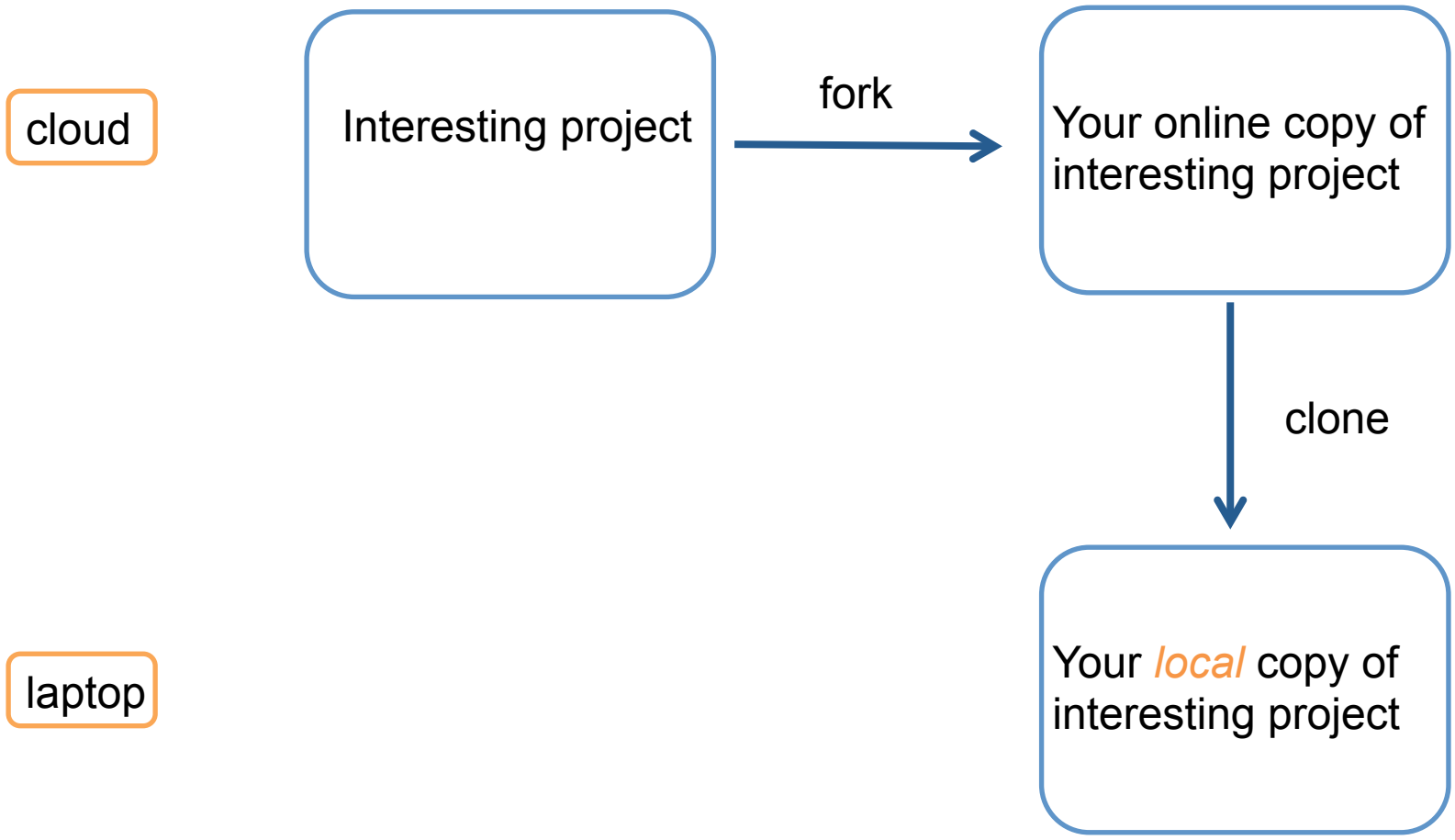
Online projects

- We've seen how to make local projects and *push* them online
- But how do we work on projects that are already online?
  - Will need to *fork* and then *clone* the project

Online project

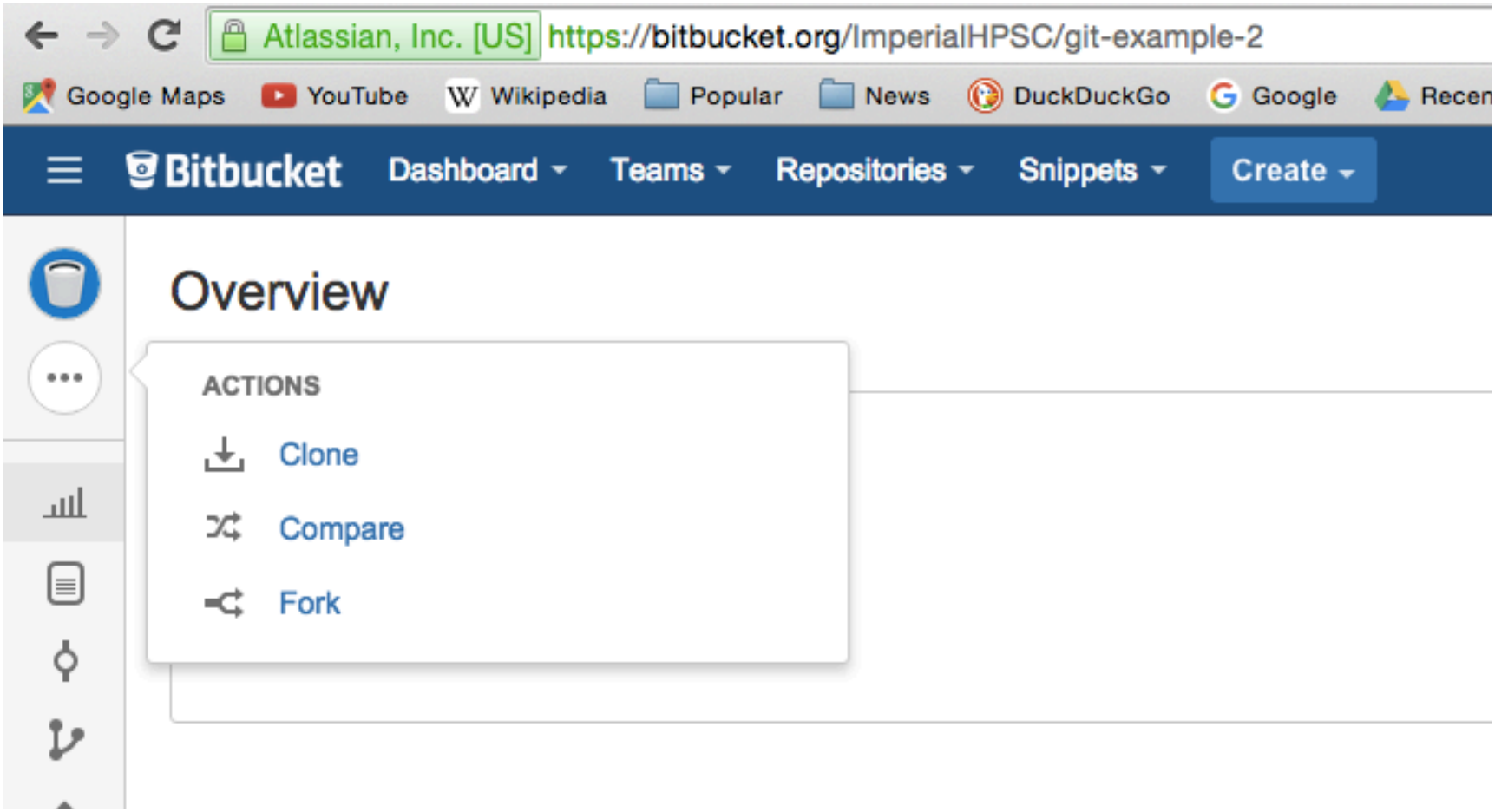


Cloud → laptop



Online projects: Example

1. Go to *bitbucket.org/ImperialHPSC/git-example-2* and fork the repo:



Online projects: Example

2. Use *git clone* to make local copy of your fork:

```
$ git clone https://username@bitbucket.org/username/git-
example-2.git
Cloning into 'git-example-2'...
remote: Counting objects: 3, done.
remote: Total 3 (delta 0), reused 0 (delta 0)
Unpacking objects: 100% (3/3), done.
Checking connectivity... done.

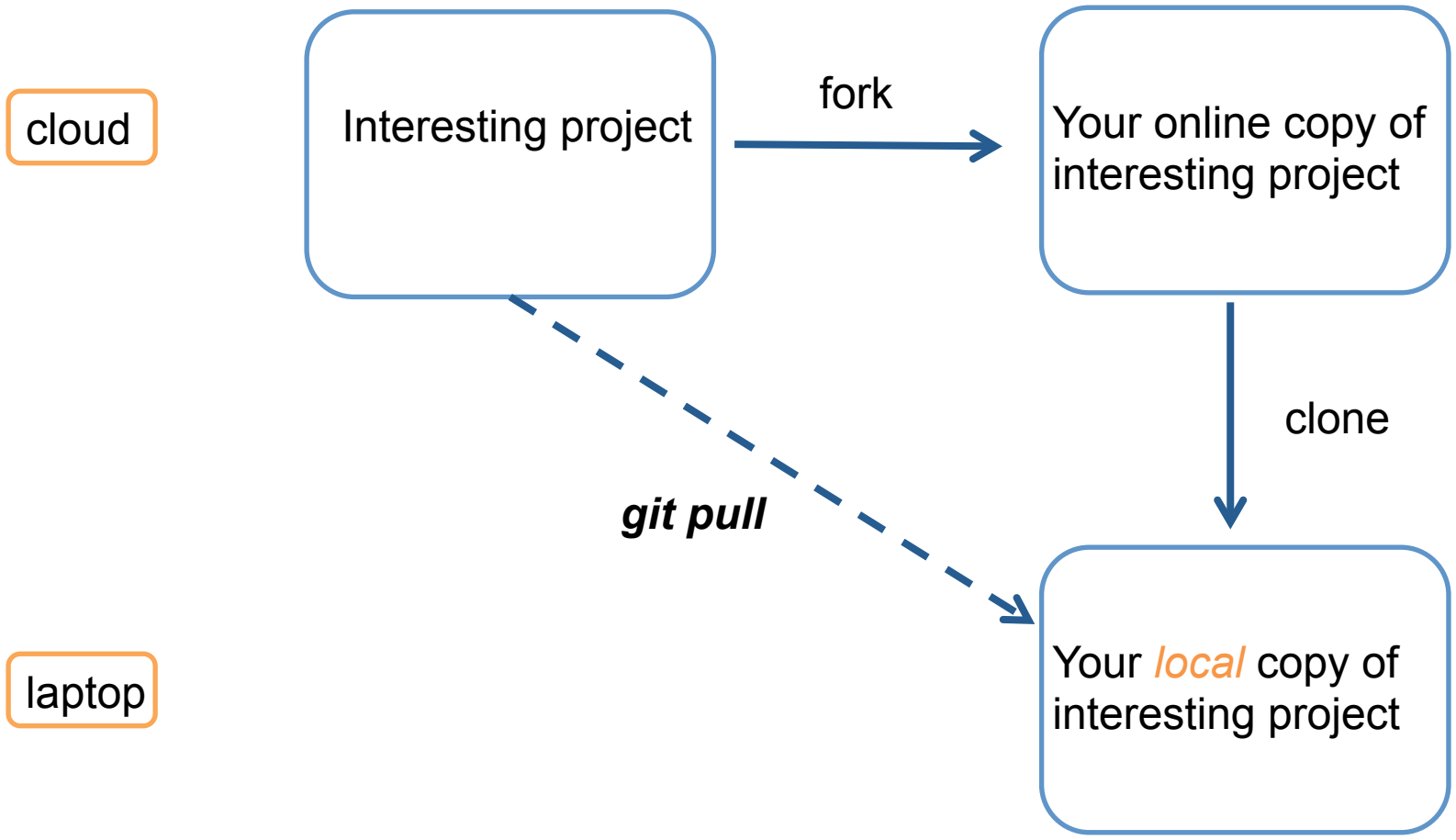
$ cd git-example-2/
$ ls
mathematicians.txt
```

Now you have your own copy to play with!

Note: If the original repo is updated, bitbucket will tell you and give you the option of syncing your fork

or, you can directly pull the updated original repo to your local repo…

Cloud → laptop



Cloud → laptop

Procedure: pull from online repo to local branch

1st, specify online repo:

git remote add IHPSC https://username@bitbucket.org/ImperialHPSC/git-example-2.git

Here IHPSC is the online repo name

Cloud → laptop

Procedure: pull from online repo to local branch

1st, specify online repo:

git remote add IHPSC https://username@bitbucket.org/ImperialHPSC/git-example-2.git

Here IHPSC is the online repo name

Check which local branch you want to use:

- ***git branch*** **tells you which branch you are on**
- ***git branch –a*** **lists all branches**
- ***git checkout branch_name*** **switches to branch_name**

Cloud → laptop

Procedure: pull from online repo to local branch

1st, specify online repo:

git remote add IHPSC https://username@bitbucket.org/ImperialHPSC/git-example-2.git

Here IHPSC is the online repo name

Check which local branch you want to use:

git branch **tells you which branch you are on**

git branch –a **lists all branches**

git checkout branch_name **switches to branch_name**

For example,

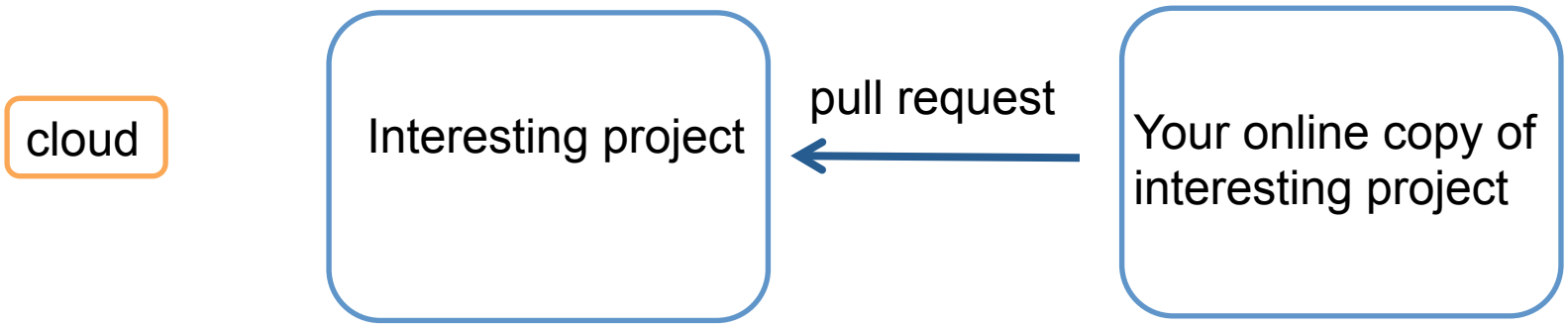
git pull IHPSC master

will pull from the IHPSC online repo to your local master branch

Finally, push your local repo to your fork:

git push origin master

Pull requests



Can ‘suggest’ improvements to original project with pull requests on bitbucket

Essential for collaborative work