



GIT FOR LAMMPS CONTRIBUTION

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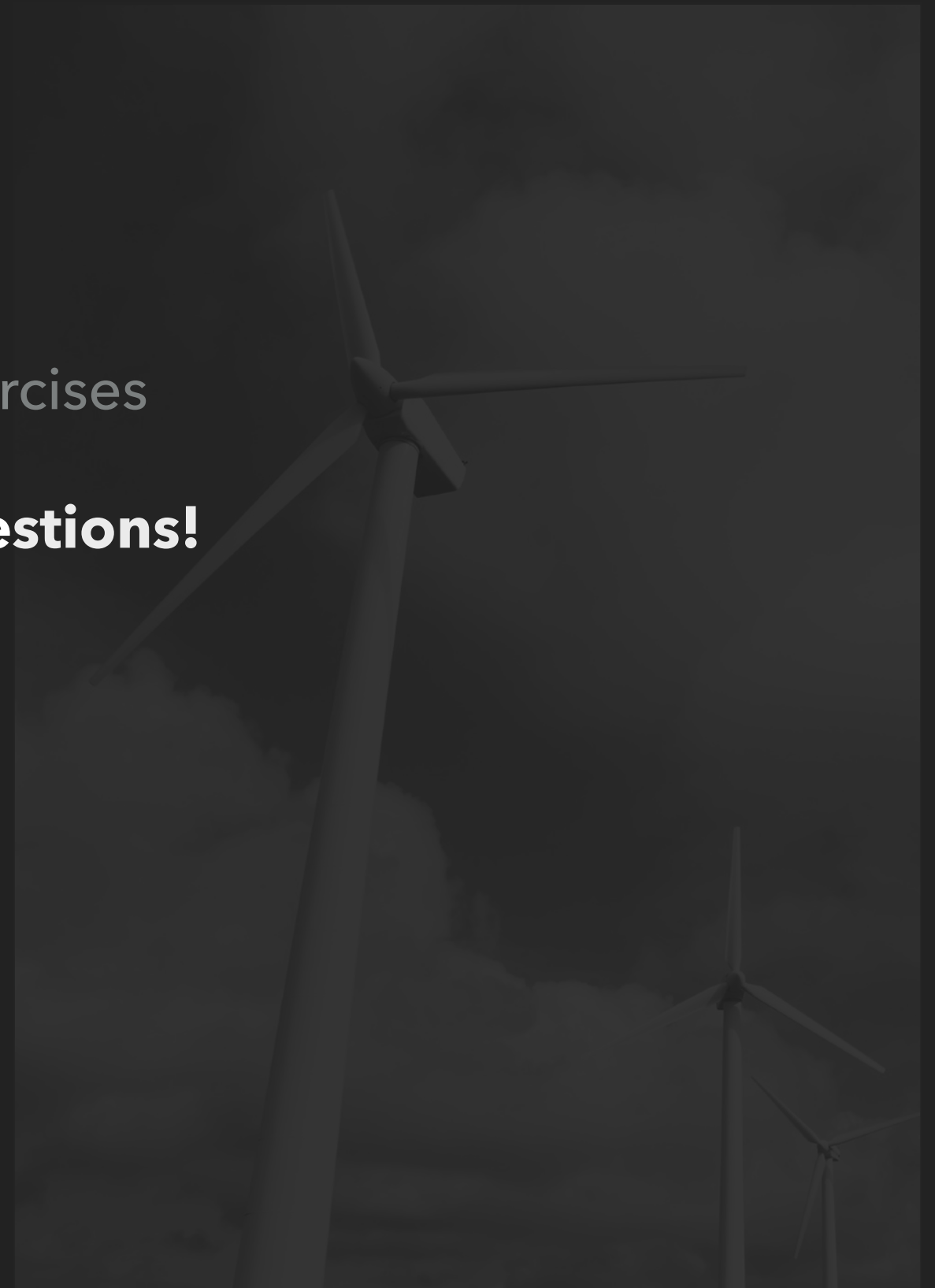
YOU WILL....

- ▶ Understand git basics
- ▶ Create GitHub account
- ▶ Clone LAMMPS
- ▶ Add a compute
- ▶ Commit changes to your own branch
- ▶ Add a pull request for our approval

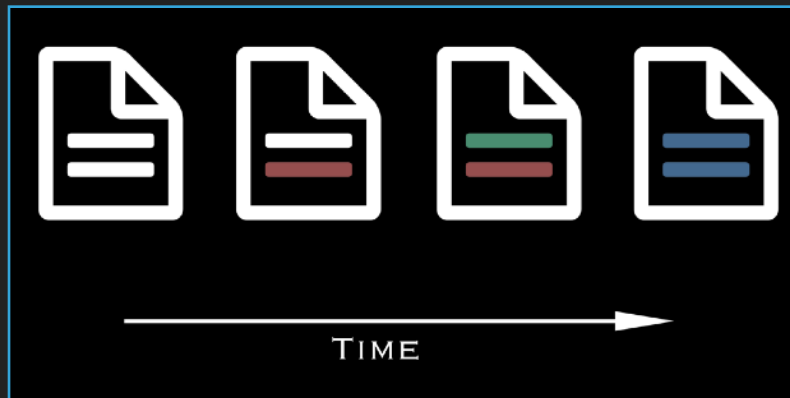


DEMO FIRST

- ▶ I do everything while I explain
- ▶ You will repeat all the steps in the exercises
- ▶ **Please interrupt if you have any questions!**



WHAT IS GIT?



Version control system (VCS)



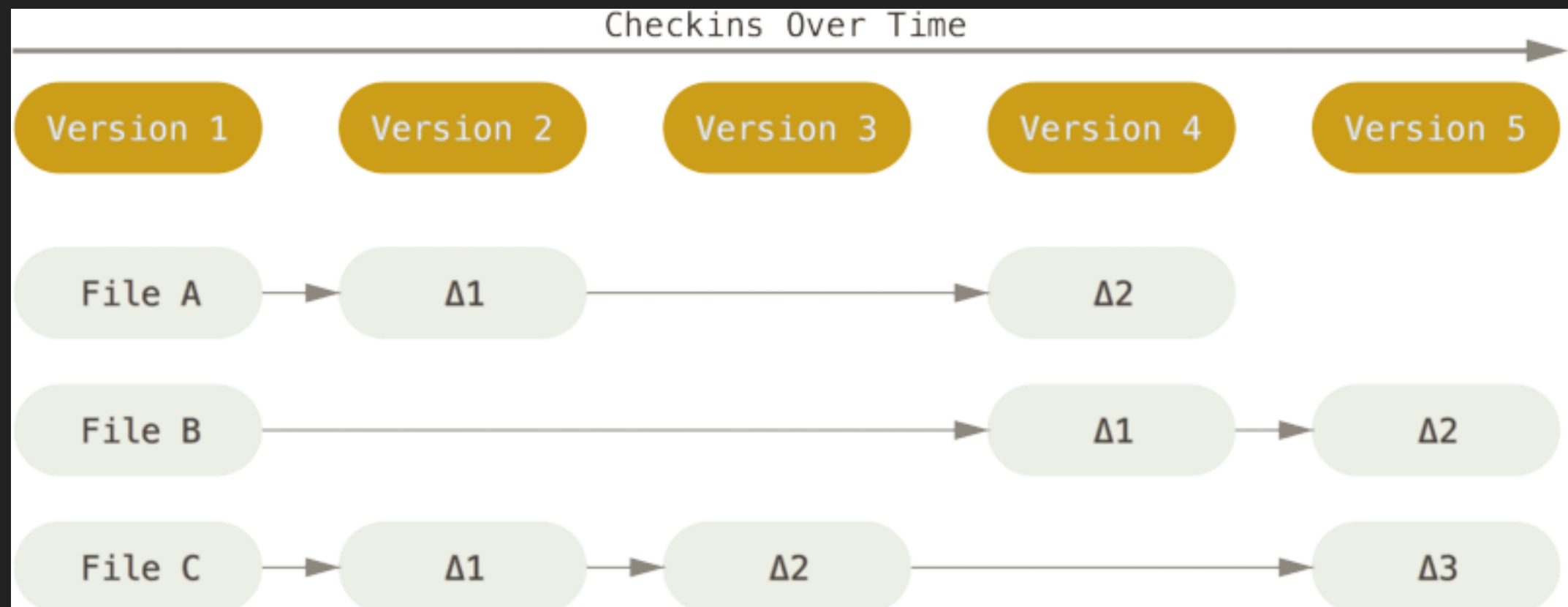
Keeps track of
who/when/what changed files



Work very well offline
and across machines

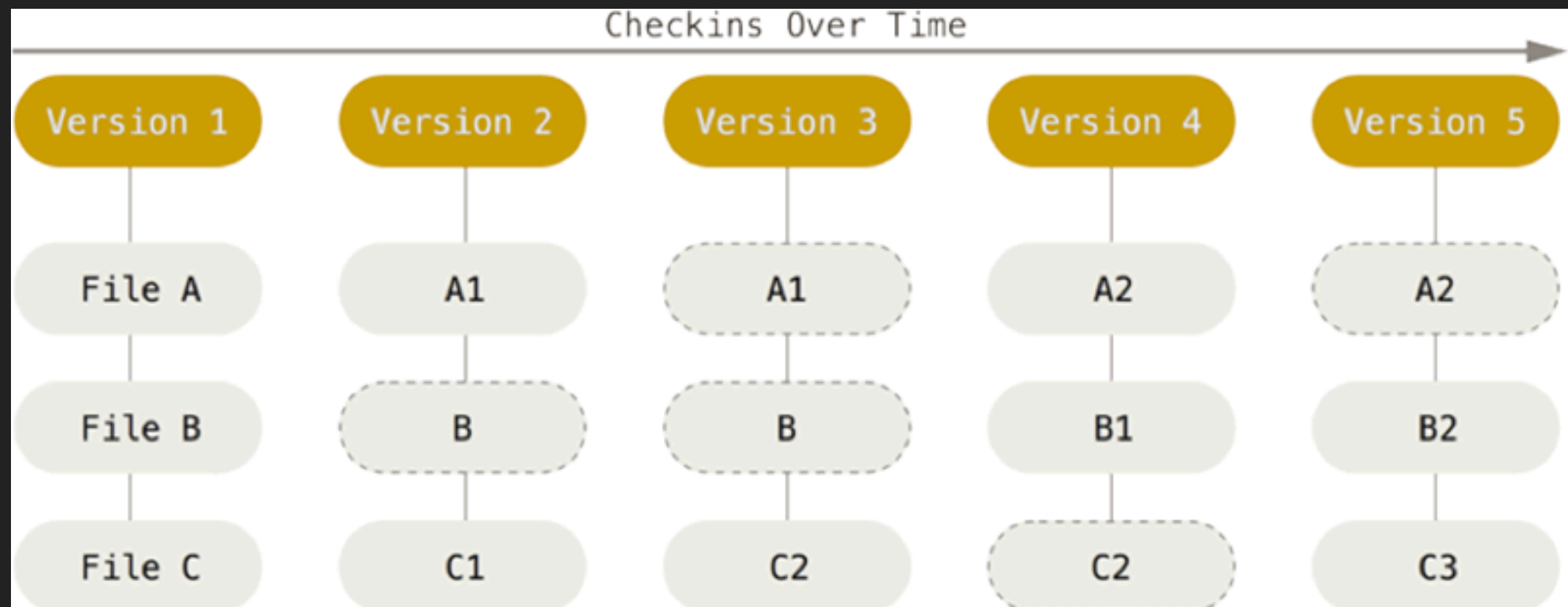
HOW DOES IT WORK?

- ▶ git stores snapshots of all your files
- ▶ All file changes stores the full file, not diffs
- ▶ If file has not changed, it stores a reference

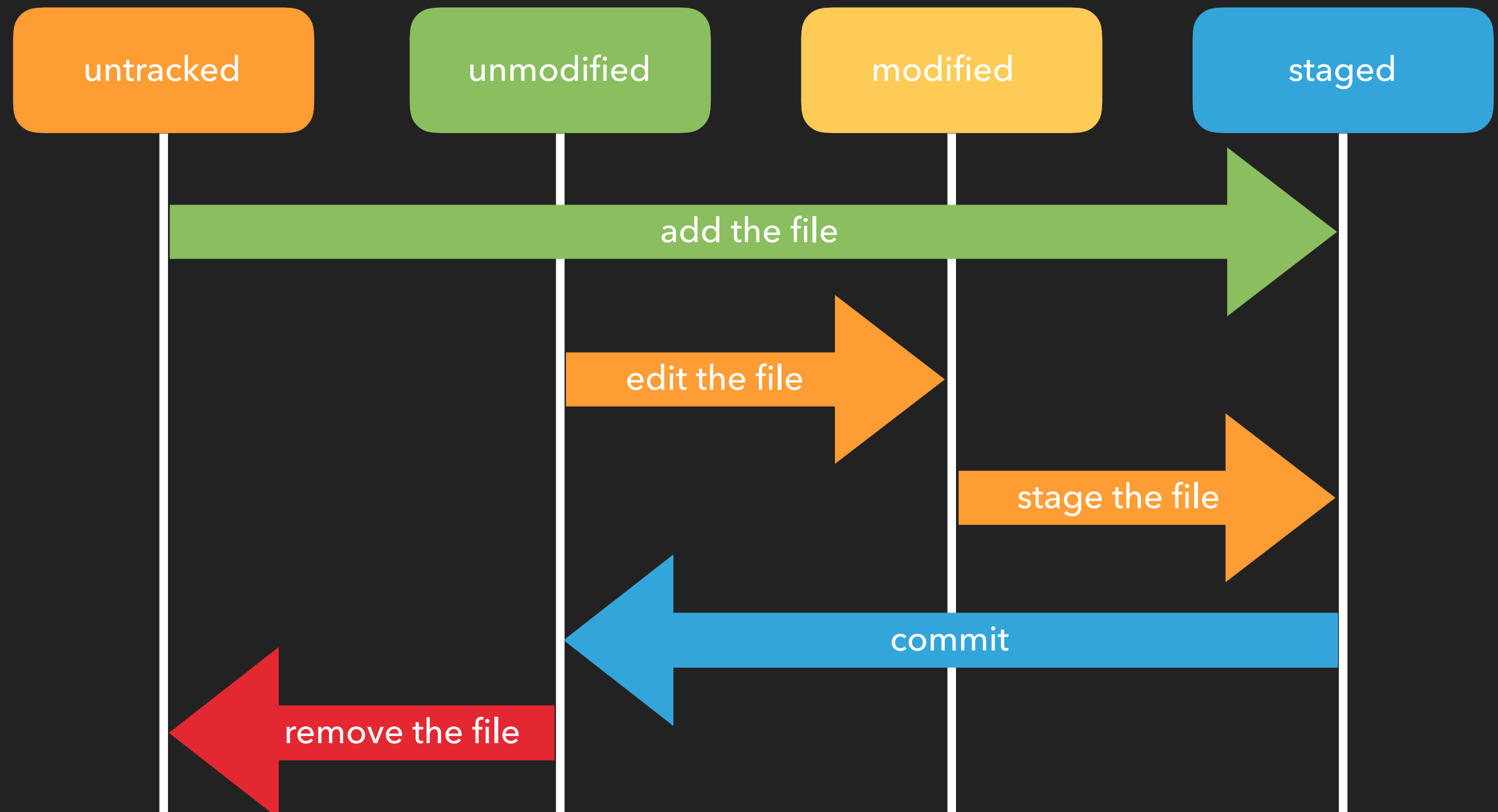


HOW DOES IT WORK?

- ▶ git stores snapshots of all your files
- ▶ All file changes stores the full file, not diffs
- ▶ If file has not changed, it stores a reference



FILE LIFE CYCLE IN GIT



INSTALL GIT

macOS: Installed with command line tools (Xcode)

Linux:

```
$ sudo apt-get install git
```

or

```
$ sudo yum install git
```

Windows: Cygwin / Ubuntu bash

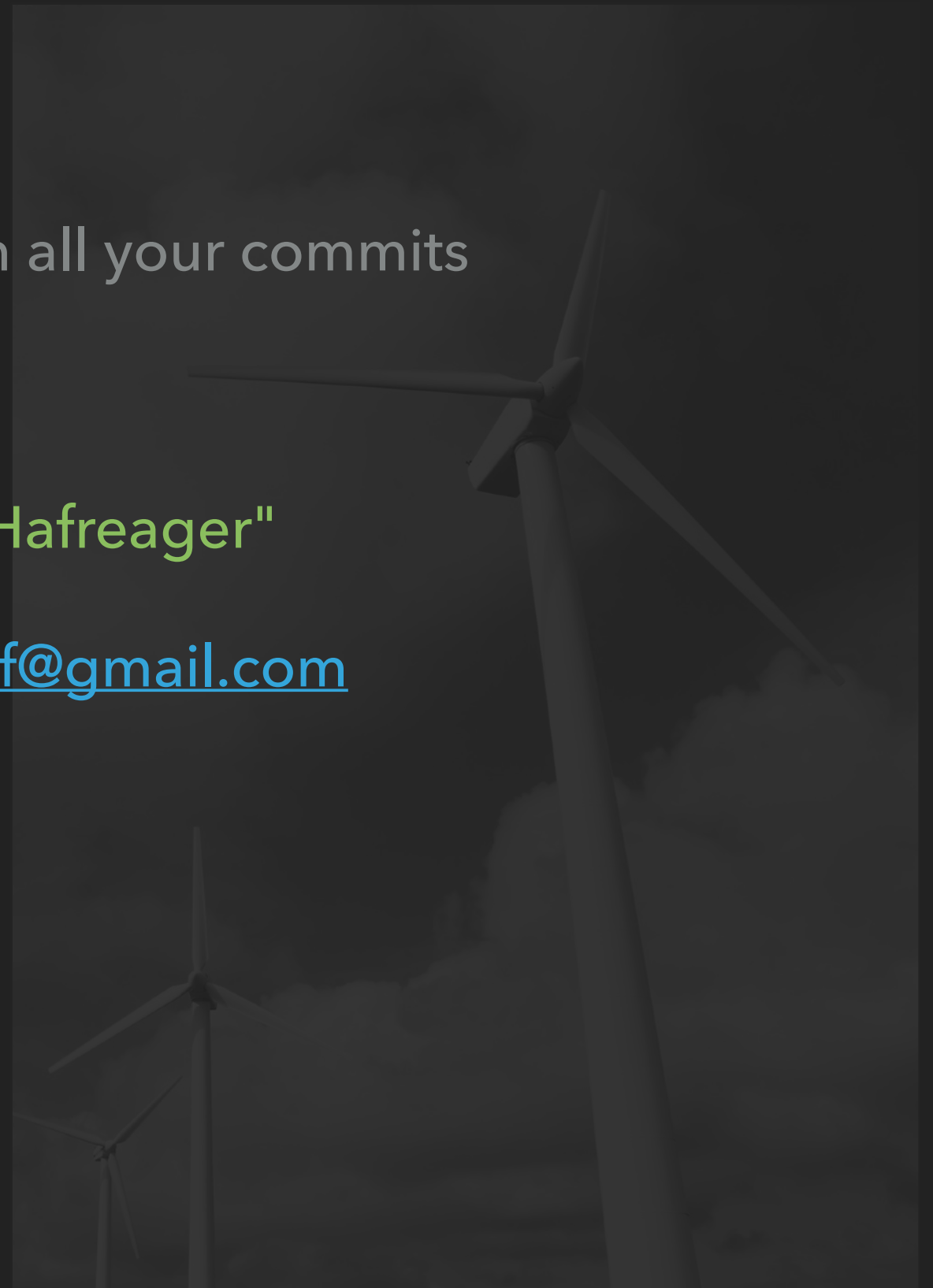


GIT CONFIG

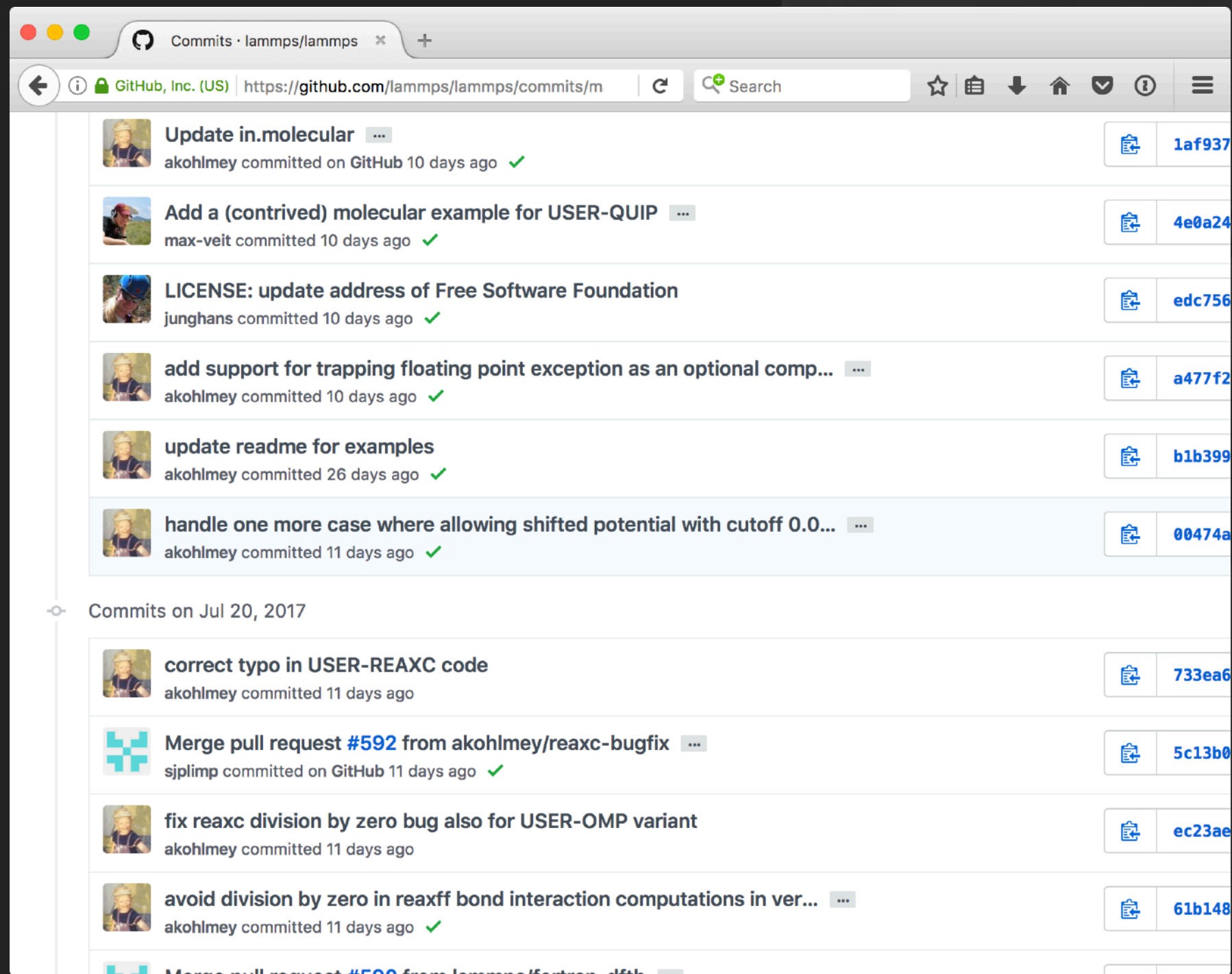
Tell git who you are. This identifies you in all your commits

```
$ git config --global user.name "Anders Hafreager"
```

```
$ git config --global user.email andershaf@gmail.com
```



GIT CONFIG



The screenshot shows the commit history of the `lammps/lammps` repository on GitHub. The browser address bar indicates the URL `https://github.com/lammps/lammps/commits/m`. The commit list includes:

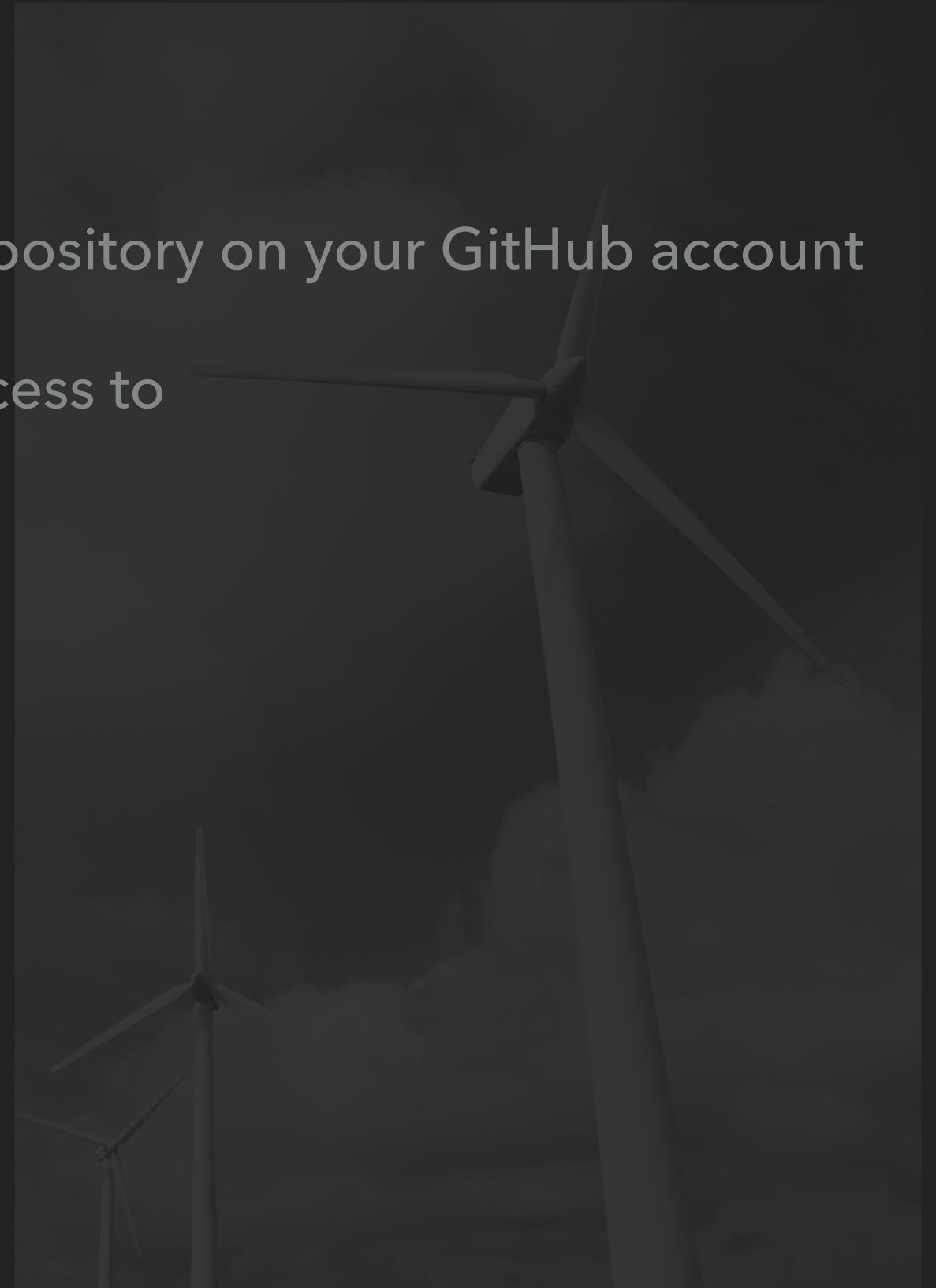
- Update in.molecular** by akohlmey, committed 10 days ago. Commit hash: `1af937`.
- Add a (contrived) molecular example for USER-QUIP** by max-veit, committed 10 days ago. Commit hash: `4e0a24`.
- LICENSE: update address of Free Software Foundation** by junghans, committed 10 days ago. Commit hash: `edc756`.
- add support for trapping floating point exception as an optional comp...** by akohlmey, committed 10 days ago. Commit hash: `a477f2`.
- update readme for examples** by akohlmey, committed 26 days ago. Commit hash: `b1b399`.
- handle one more case where allowing shifted potential with cutoff 0.0...** by akohlmey, committed 11 days ago. Commit hash: `00474a`.

A section separator indicates "Commits on Jul 20, 2017". The subsequent commits are:

- correct typo in USER-REAXC code** by akohlmey, committed 11 days ago. Commit hash: `733ea6`.
- Merge pull request #592 from akohlmey/reaxc-bugfix** by sjplimp, committed 11 days ago. Commit hash: `5c13b0`.
- fix reaxc division by zero bug also for USER-OMP variant** by akohlmey, committed 11 days ago. Commit hash: `ec23ae`.
- avoid division by zero in reaxff bond interaction computations in ver...** by akohlmey, committed 11 days ago. Commit hash: `61b148`.
- Merge pull request #590 from lammps/fortran_dftb** (partially visible).

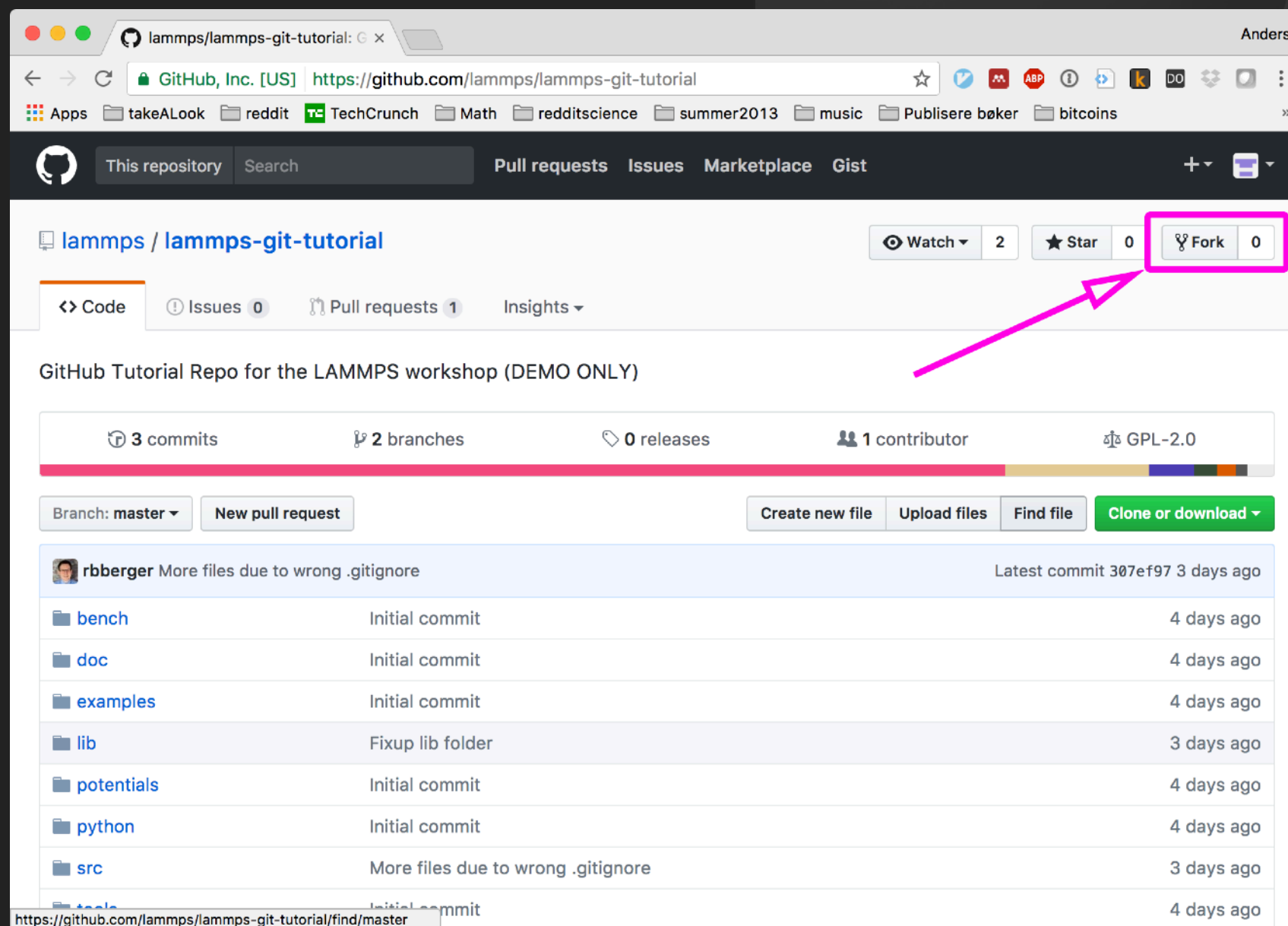
FORK LAMMPS ON GITHUB

- ▶ Fork means get a copy of LAMMPS repository on your GitHub account
- ▶ This is a full copy that you have full access to

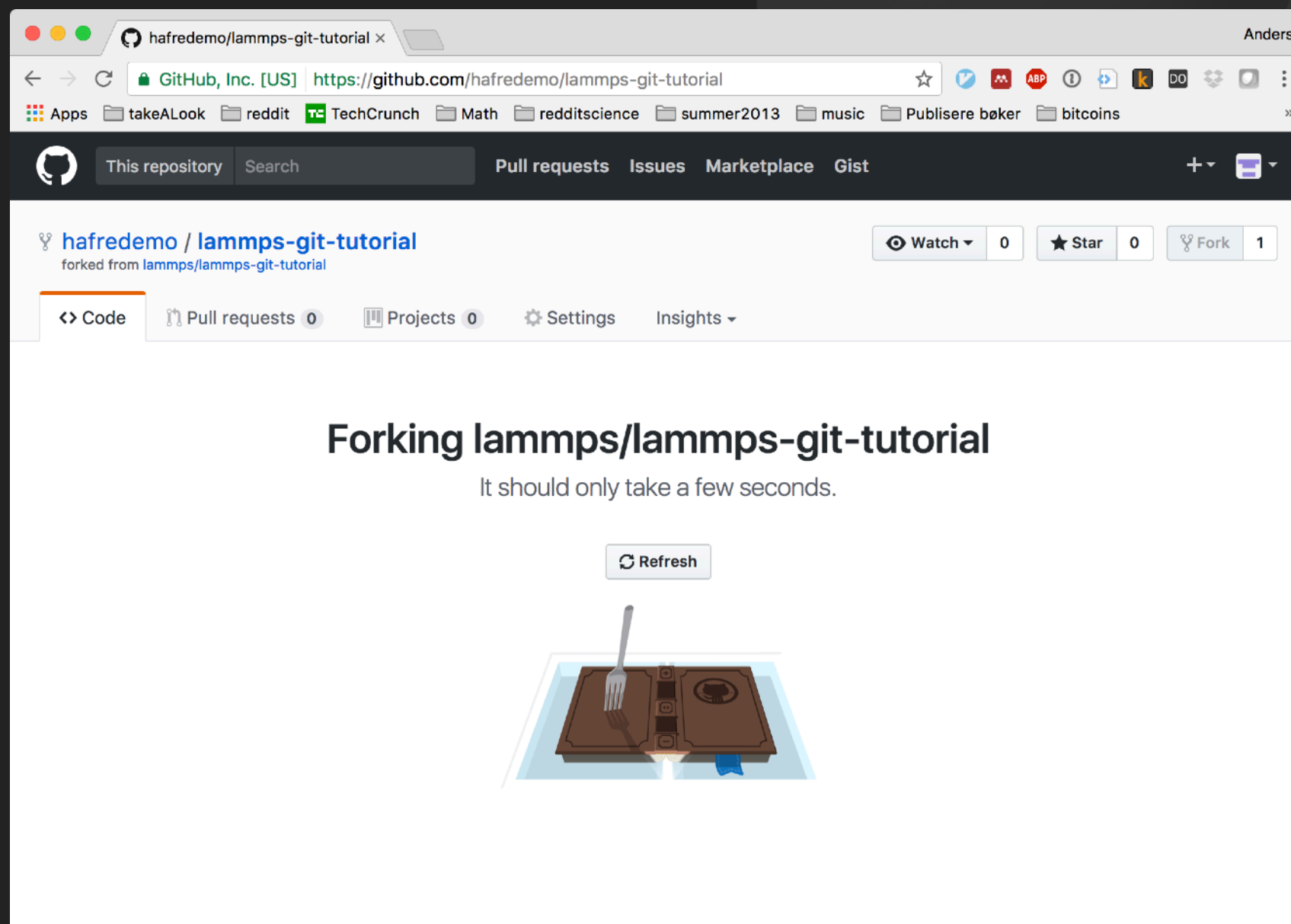


FORK LAMMPS ON GITHUB

- Go to <https://github.com/lammps/lammps-git-tutorial>



FORK LAMMPS ON GITHUB



FORK LAMMPS ON GITHUB

Notice that the copy is now under your account

The screenshot shows a web browser window displaying a GitHub repository page. The browser's address bar shows the URL <https://github.com/hafredemo/lammps-git-tutorial>. The repository name **hafredemo / lammps-git-tutorial** is highlighted with a pink box. Below the repository name, it says "forked from lammps/lammps-git-tutorial". The page shows the repository's metadata: 3 commits, 2 branches, 0 releases, and 1 contributor. There are buttons for "Watch", "Star", and "Fork". The "Code" tab is selected, showing the repository's description: "GitHub Tutorial Repo for the LAMMPS workshop (DEMO ONLY)". Below this, there are buttons for "Branch: master", "New pull request", "Create new file", "Upload files", "Find file", and "Clone or download". A list of files is shown, including `bench`, `doc`, `examples`, `lib`, `potentials`, and `python`, each with its commit history and the time since the last commit.

hafredemo / lammps-git-tutorial
forked from lammps/lammps-git-tutorial

Watch 0 Star 0 Fork 1

Code Pull requests 0 Projects 0 Settings Insights

GitHub Tutorial Repo for the LAMMPS workshop (DEMO ONLY) Edit

Add topics

3 commits 2 branches 0 releases 1 contributor

Branch: master New pull request Create new file Upload files Find file Clone or download

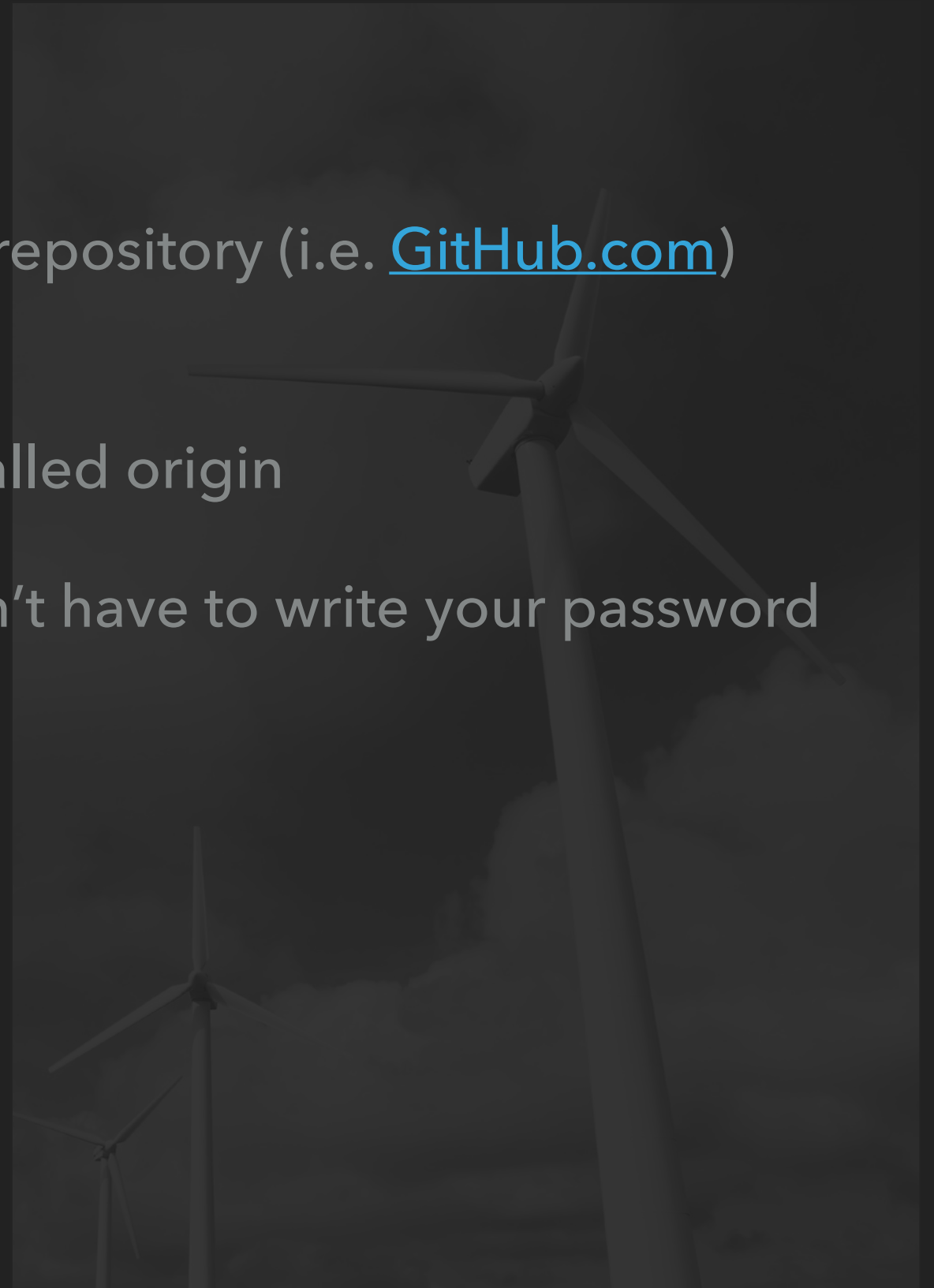
This branch is even with lammps:master. Pull request Compare

rbberger More files due to wrong .gitignore Latest commit 307ef97 3 days ago

bench	Initial commit	4 days ago
doc	Initial commit	4 days ago
examples	Initial commit	4 days ago
lib	Fixup lib folder	3 days ago
potentials	Initial commit	4 days ago
python	Initial commit	4 days ago

CLONE YOUR LAMMPS FORK

- ▶ Clone means get a copy from remote repository (i.e. [GitHub.com](https://github.com)) to your local machine
- ▶ It is connected to GitHub repository called origin
- ▶ But first, we need SSH keys so you don't have to write your password

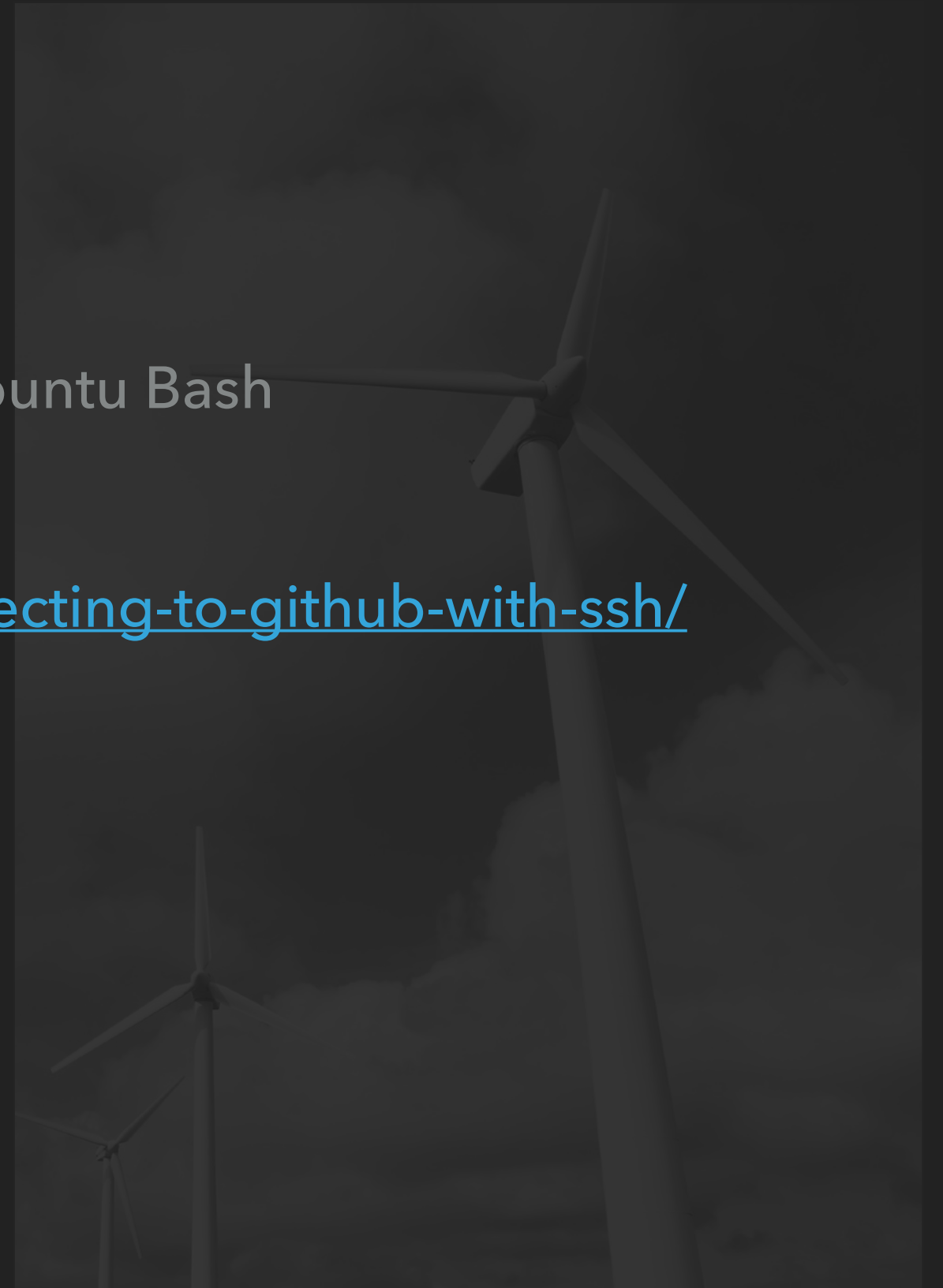


ONE DOES NOT SIMPLY

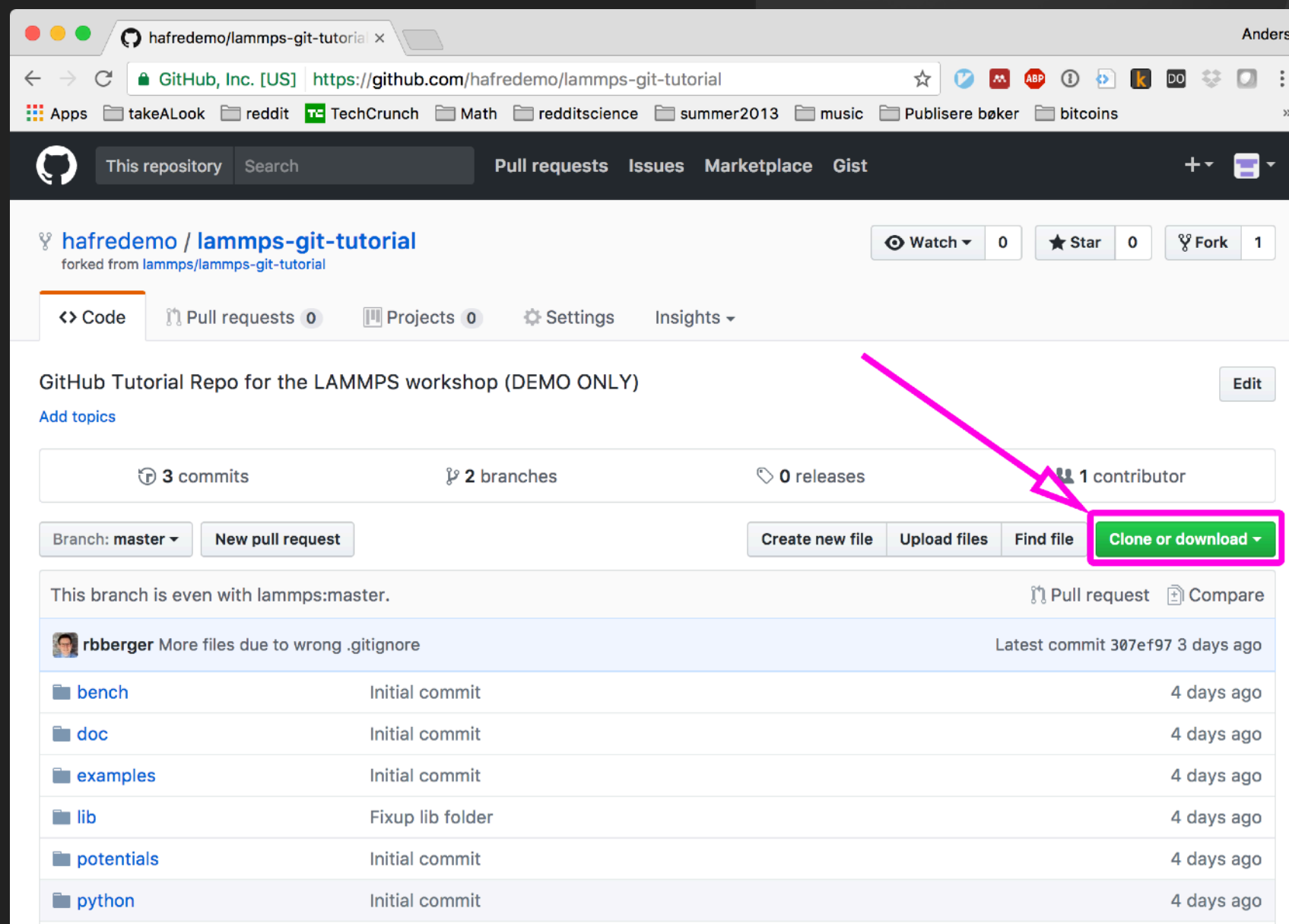
**REMEMBER PASSWORDS TO ALL THE
SERVERS**

GENERATE SSH-KEY

- ▶ Works on macOS, Linux
- ▶ Works on Windows with Cygwin or Ubuntu Bash
- ▶ Follow instructions on <https://help.github.com/articles/connecting-to-github-with-ssh/>

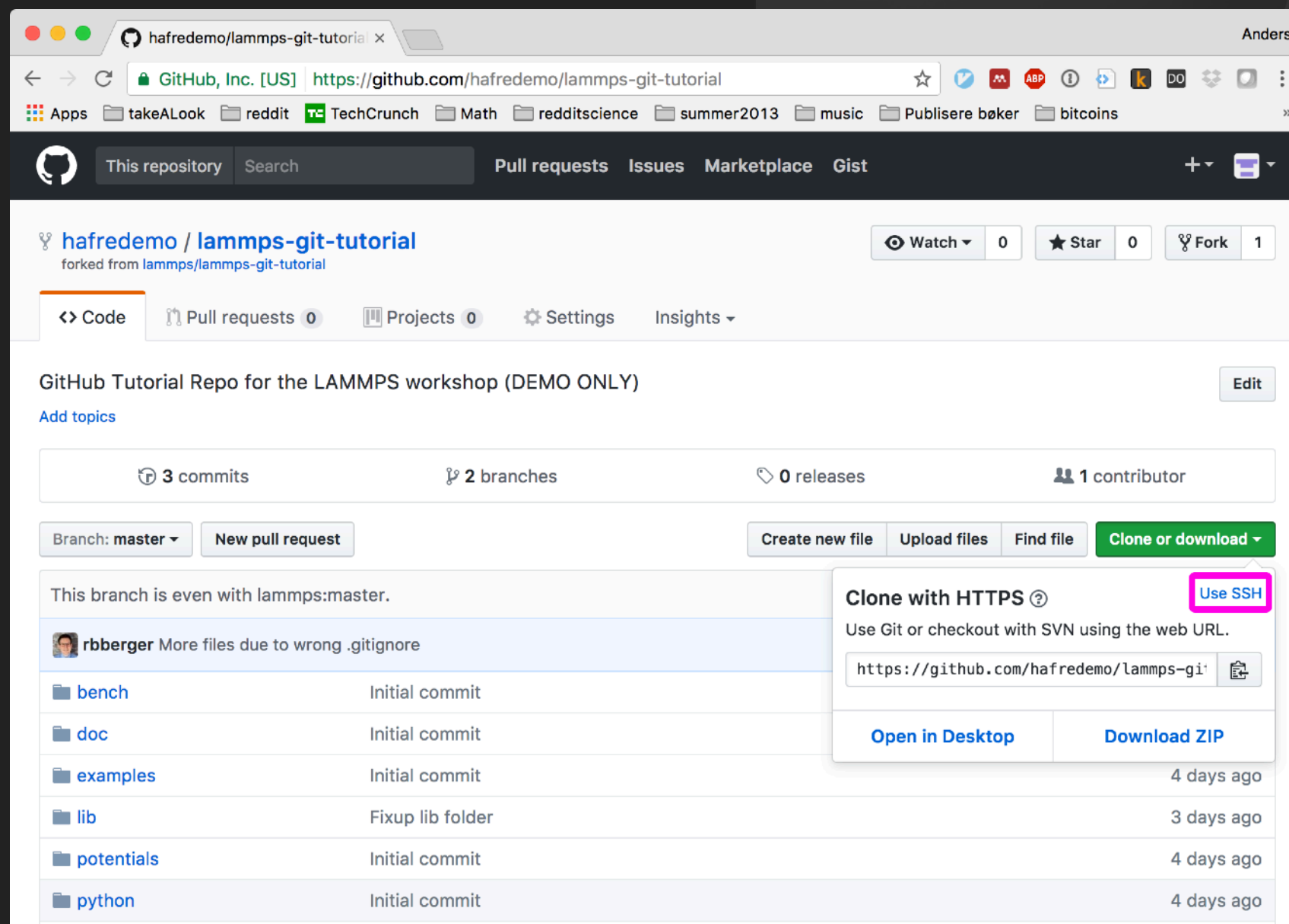


CLONE YOUR LAMMPS FORK



CLONE YOUR LAMMPS FORK

If you have set up SSH keys, make sure you click [Use SSH](#) click it so the text field starts with git@github.com. If not, click [Use HTTPS](#) (requires password more often).



CLONE YOUR LAMMPS FORK

Copy the contents of the text field

The screenshot shows a web browser window displaying a GitHub repository page for 'hafredemo/lammps-git-tutorial'. The repository is a fork of 'lammps/lammps-git-tutorial'. The page shows the repository name, a description 'GitHub Tutorial Repo for the LAMMPS workshop (DEMO ONLY)', and statistics: 3 commits, 2 branches, 0 releases, and 1 contributor. The 'Clone or download' button is highlighted, and a dropdown menu is open showing the 'Clone with SSH' option. The SSH clone command is displayed in a text field: `git@github.com:hafredemo/lammps-git-tu`. Below the clone command, there are buttons for 'Open in Desktop' and 'Download ZIP'. The repository files list includes 'bench', 'doc', 'examples', 'lib', 'potentials', and 'python', each with an 'Initial commit' status and a timestamp.

hafredemo / lammps-git-tutorial
forked from lammps/lammps-git-tutorial

Watch 0 Star 0 Fork 1

Code Pull requests 0 Projects 0 Settings Insights

GitHub Tutorial Repo for the LAMMPS workshop (DEMO ONLY) Edit

Add topics

3 commits 2 branches 0 releases 1 contributor

Branch: master New pull request Create new file Upload files Find file Clone or download

This branch is even with lammps:master.

rbberger More files due to wrong .gitignore

Clone with SSH Use HTTPS

Use an SSH key and passphrase from account.

git@github.com:hafredemo/lammps-git-tu

Open in Desktop Download ZIP

4 days ago

3 days ago

4 days ago

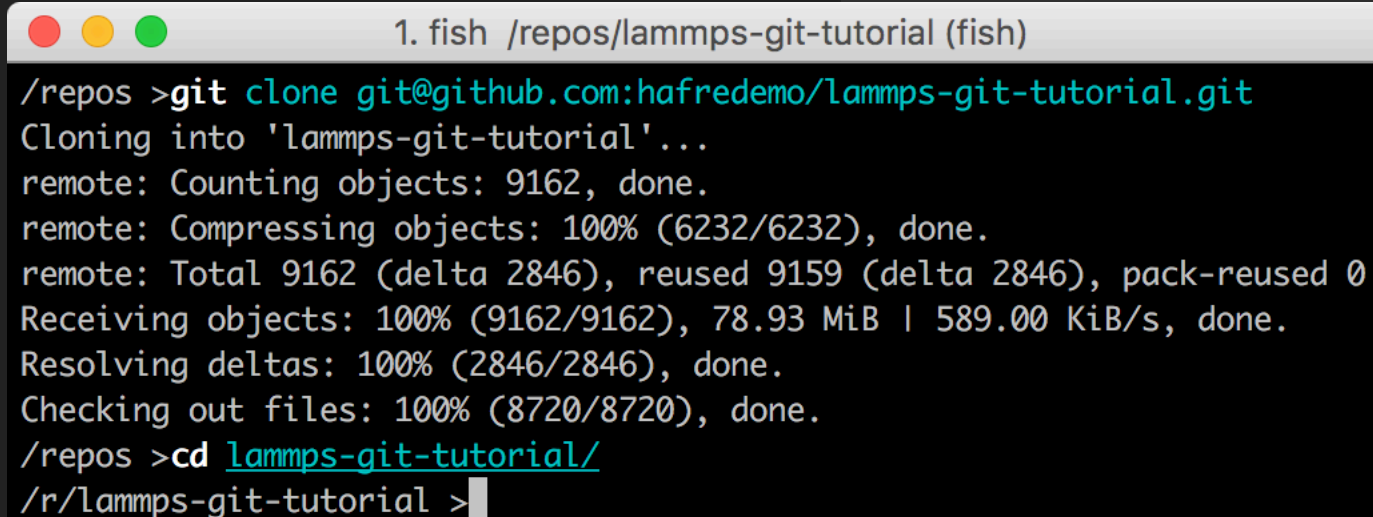
4 days ago

File	Commit	Time
bench	Initial commit	4 days ago
doc	Initial commit	3 days ago
examples	Initial commit	4 days ago
lib	Fixup lib folder	4 days ago
potentials	Initial commit	4 days ago
python	Initial commit	4 days ago

CLONE YOUR LAMMPS FORK

\$ git clone [git@github.com:yourusername/lammps-git-tutorial.git](https://github.com:yourusername/lammps-git-tutorial.git) (few mins)

\$ cd lammps-git-tutorial

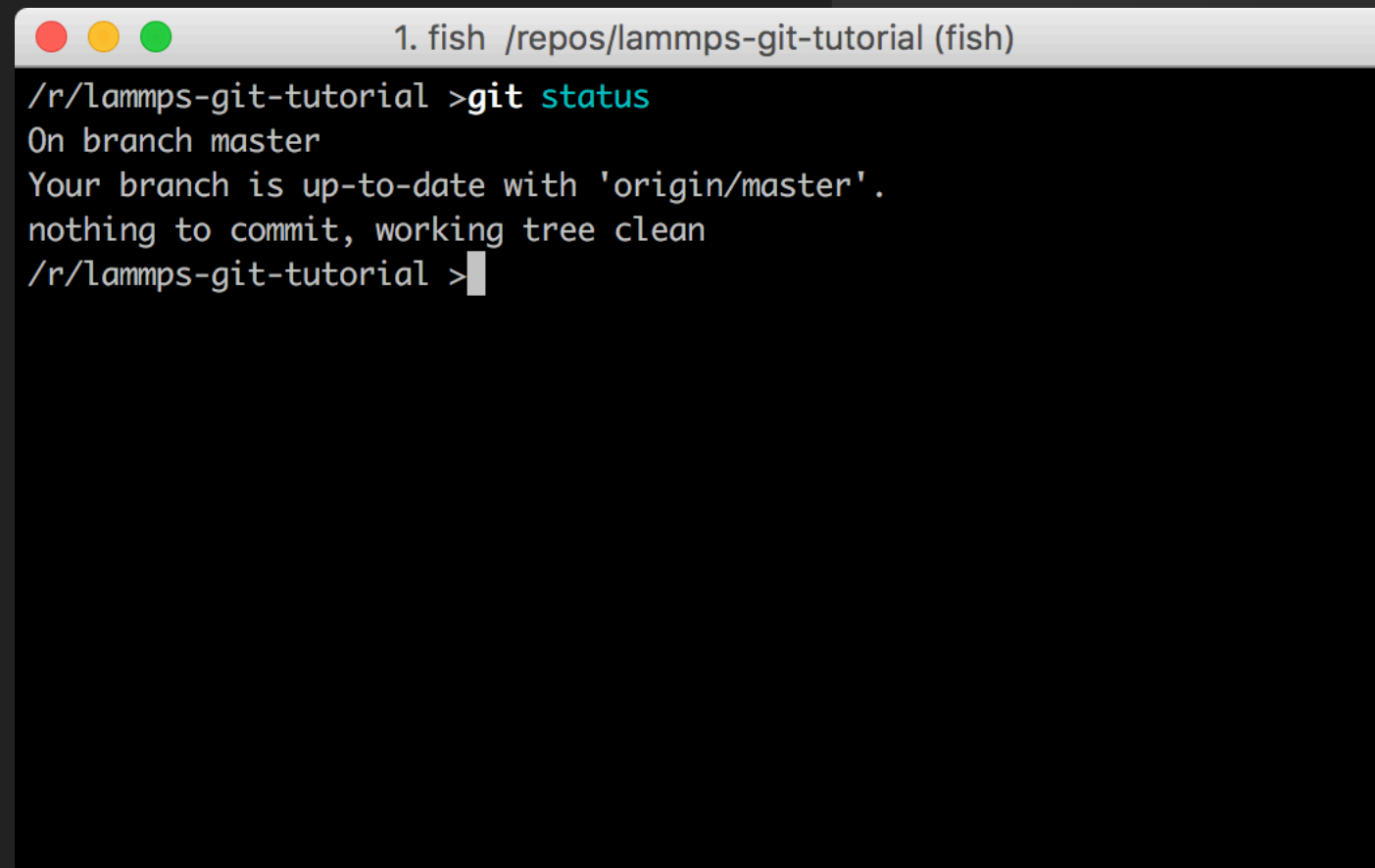


```
1. fish /repos/lammps-git-tutorial (fish)
/repos >git clone git@github.com:hafredemo/lammps-git-tutorial.git
Cloning into 'lammps-git-tutorial'...
remote: Counting objects: 9162, done.
remote: Compressing objects: 100% (6232/6232), done.
remote: Total 9162 (delta 2846), reused 9159 (delta 2846), pack-reused 0
Receiving objects: 100% (9162/9162), 78.93 MiB | 589.00 KiB/s, done.
Resolving deltas: 100% (2846/2846), done.
Checking out files: 100% (8720/8720), done.
/repos >cd lammps-git-tutorial/
/r/lammps-git-tutorial >
```

CHECK STATUS OF REPOSITORY

Check git status (you can never do this too often!)

\$ git status

A terminal window with a dark background and light text. The title bar shows three colored circles (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial (fish)". The terminal content shows the command "git status" being executed, with the output: "On branch master", "Your branch is up-to-date with 'origin/master'.", and "nothing to commit, working tree clean". The prompt "/r/lammps-git-tutorial >" is visible at the end of the output.

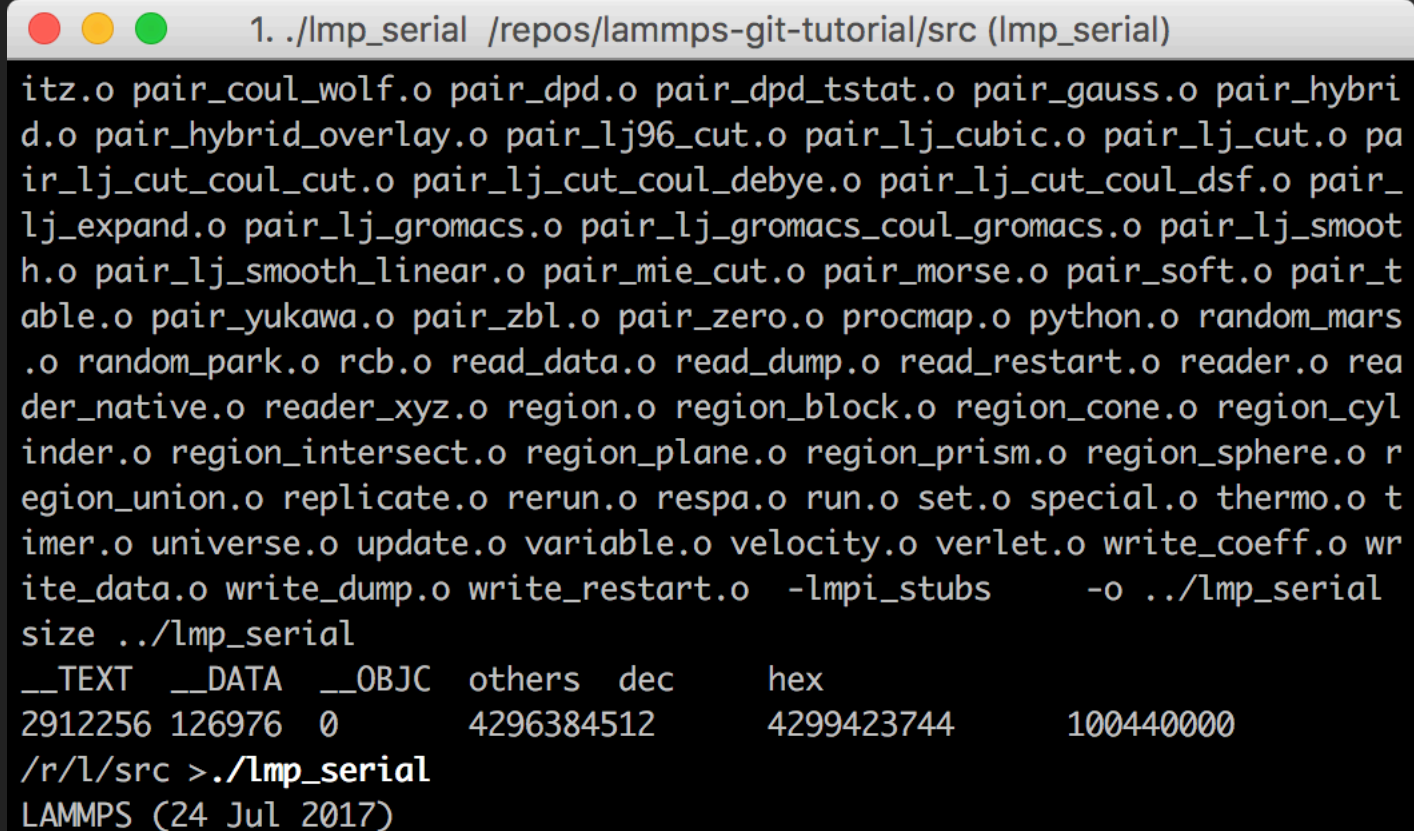
```
1. fish /repos/lammps-git-tutorial (fish)
/r/lammps-git-tutorial >git status
On branch master
Your branch is up-to-date with 'origin/master'.
nothing to commit, working tree clean
/r/lammps-git-tutorial >
```

TEST THAT LAMMPS WORKS

```
$ cd src
```

```
$ make -j4 serial
```

```
$ ./lmp_serial
```

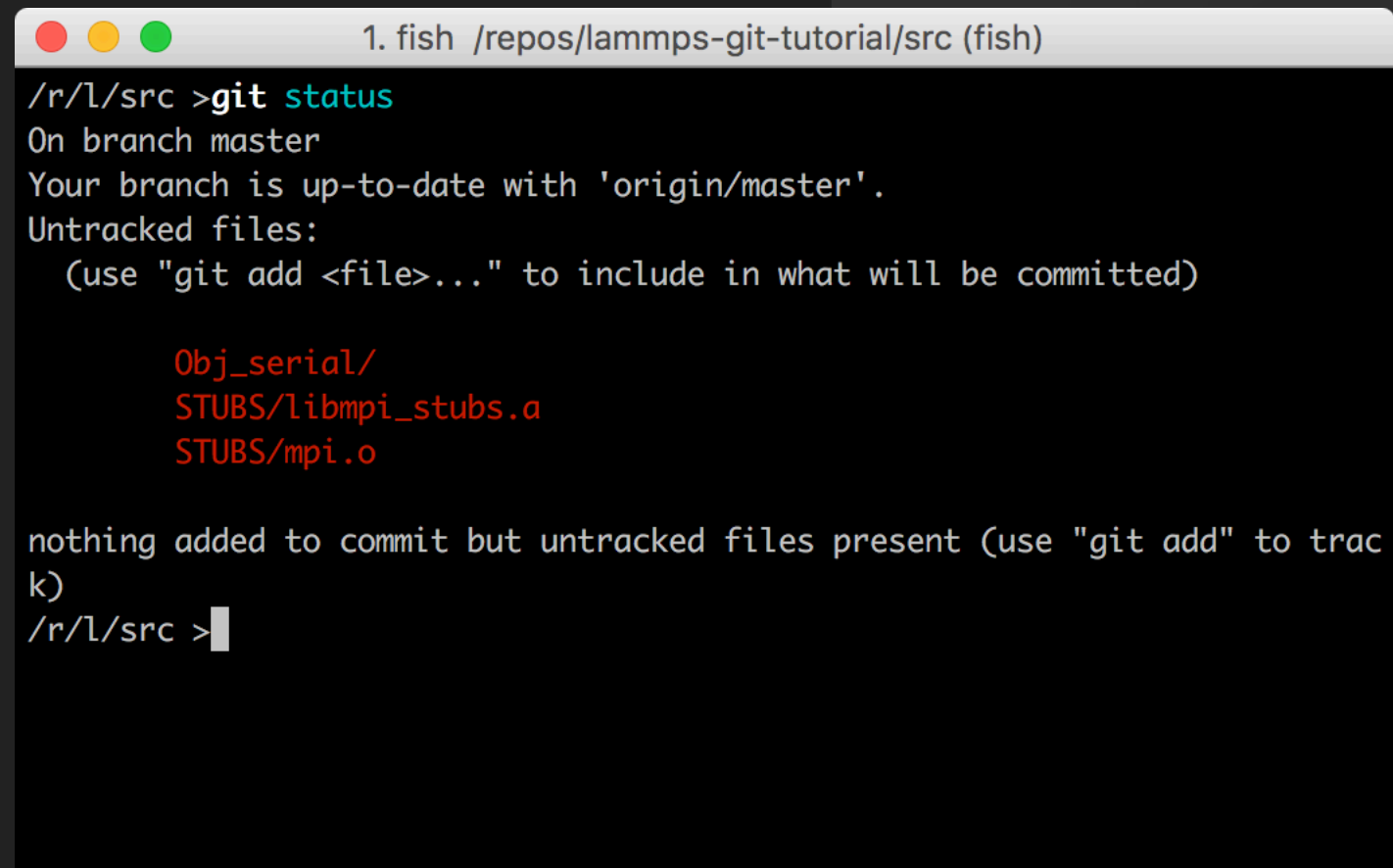
A terminal window titled "1. ./lmp_serial /repos/lammps-git-tutorial/src (lmp_serial)" displays the output of the LAMMPS serial executable. The output lists various modules and their sizes, followed by a summary table and the version information.

```
itz.o pair_coul_wolf.o pair_dpd.o pair_dpd_tstat.o pair_gauss.o pair_hybri
d.o pair_hybrid_overlay.o pair_lj96_cut.o pair_lj_cubic.o pair_lj_cut.o pa
ir_lj_cut_coul_cut.o pair_lj_cut_coul_debye.o pair_lj_cut_coul_dsf.o pair_
lj_expand.o pair_lj_gromacs.o pair_lj_gromacs_coul_gromacs.o pair_lj_smoot
h.o pair_lj_smooth_linear.o pair_mie_cut.o pair_morse.o pair_soft.o pair_t
able.o pair_yukawa.o pair_zbl.o pair_zero.o procmap.o python.o random_mars
.o random_park.o rcb.o read_data.o read_dump.o read_restart.o reader.o rea
der_native.o reader_xyz.o region.o region_block.o region_cone.o region_cyl
inder.o region_intersect.o region_plane.o region_prism.o region_sphere.o r
egion_union.o replicate.o rerun.o respa.o run.o set.o special.o thermo.o t
imer.o universe.o update.o variable.o velocity.o verlet.o write_coeff.o wr
ite_data.o write_dump.o write_restart.o -lmpi_stubs      -o ../lmp_serial
size ../lmp_serial
__TEXT __DATA __OBJC  others  dec      hex
2912256 126976  0      4296384512  4299423744  100440000
/r/l/src > ./lmp_serial
LAMMPS (24 Jul 2017)
```

CHECK STATUS OF REPOSITORY

Check git status (you can never do this too often!)

\$ git status

A terminal window with a title bar showing three colored circles (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial/src (fish)". The terminal output shows the command "git status" being executed in the directory "/r/l/src". The output indicates the user is on the "master" branch, which is up-to-date with "origin/master". It lists three untracked files: "Obj_serial/", "STUBS/libmpi_stubs.a", and "STUBS/mpi.o". A message at the bottom states "nothing added to commit but untracked files present (use 'git add' to track)" and the prompt "/r/l/src >" is shown with a cursor.

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git status
On branch master
Your branch is up-to-date with 'origin/master'.
Untracked files:
  (use "git add <file>..." to include in what will be committed)

        Obj_serial/
        STUBS/libmpi_stubs.a
        STUBS/mpi.o

nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```


CHECK STATUS OF REPOSITORY

untracked

unmodified

modified

staged

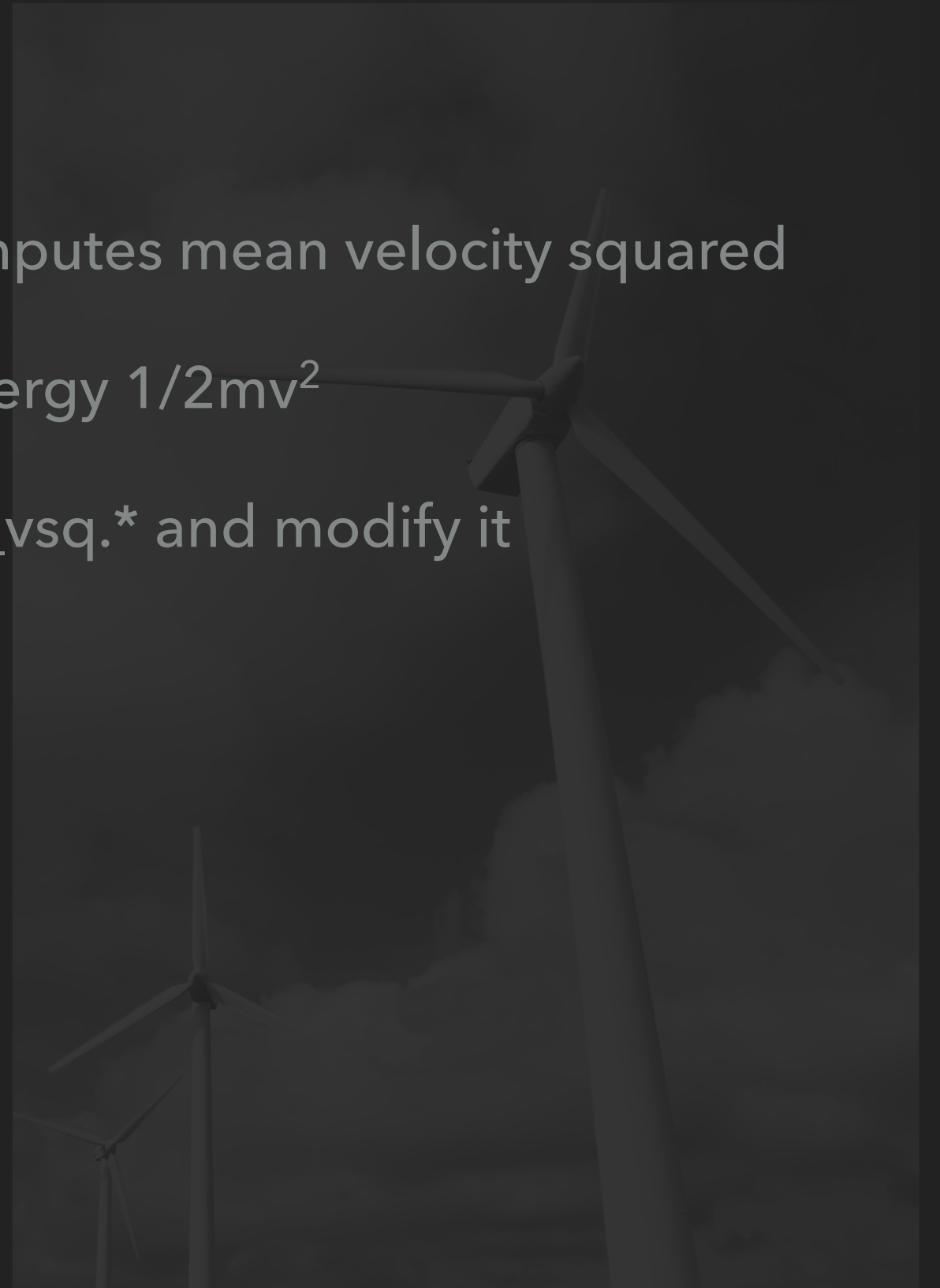
```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git status
On branch master
Your branch is up-to-date with 'origin/master'.
Untracked files:
  (use "git add <file>..." to include in what will be committed)

    Obj_serial/
    STUBS/libmpi_stubs.a
    STUBS/mpi.o

nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```

CREATE NEW COMPUTE

- ▶ We want to create a compute that computes mean velocity squared
- ▶ This is closely related to the kinetic energy $1/2mv^2$
- ▶ We copy `compute_ke.*` into `compute_vsq.*` and modify it

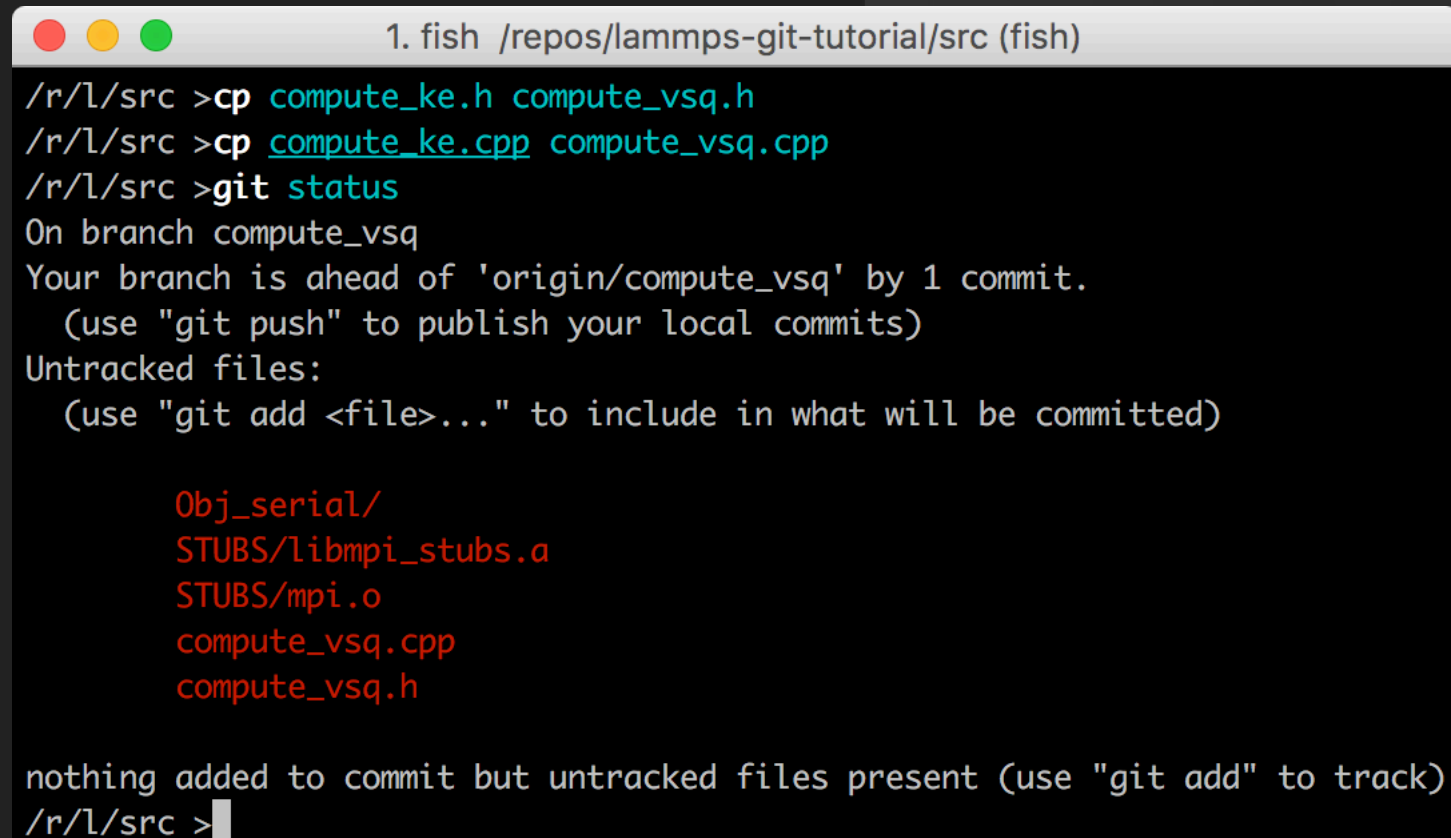


CREATE NEW COMPUTE

\$ cp compute_ke.cpp compute_vsq.cpp (add your username in the filename)

\$ cp compute_ke.h compute_vsq.h (add your username in the filename)

\$ git status

A terminal window with a title bar showing three colored circles (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial/src (fish)". The terminal content shows the execution of several commands: "cp compute_ke.h compute_vsq.h", "cp compute_ke.cpp compute_vsq.cpp", and "git status". The output of "git status" indicates the current branch is "compute_vsq", which is ahead of the origin by one commit. It lists untracked files: "Obj_serial/", "STUBS/libmpi_stubs.a", "STUBS/mpi.o", "compute_vsq.cpp", and "compute_vsq.h". At the bottom, it states "nothing added to commit but untracked files present (use 'git add' to track)".

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >cp compute_ke.h compute_vsq.h
/r/l/src >cp compute_ke.cpp compute_vsq.cpp
/r/l/src >git status
On branch compute_vsq
Your branch is ahead of 'origin/compute_vsq' by 1 commit.
  (use "git push" to publish your local commits)
Untracked files:
  (use "git add <file>..." to include in what will be committed)

        Obj_serial/
        STUBS/libmpi_stubs.a
        STUBS/mpi.o
        compute_vsq.cpp
        compute_vsq.h

nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```

CHECK STATUS OF REPOSITORY

untracked

unmodified

modified

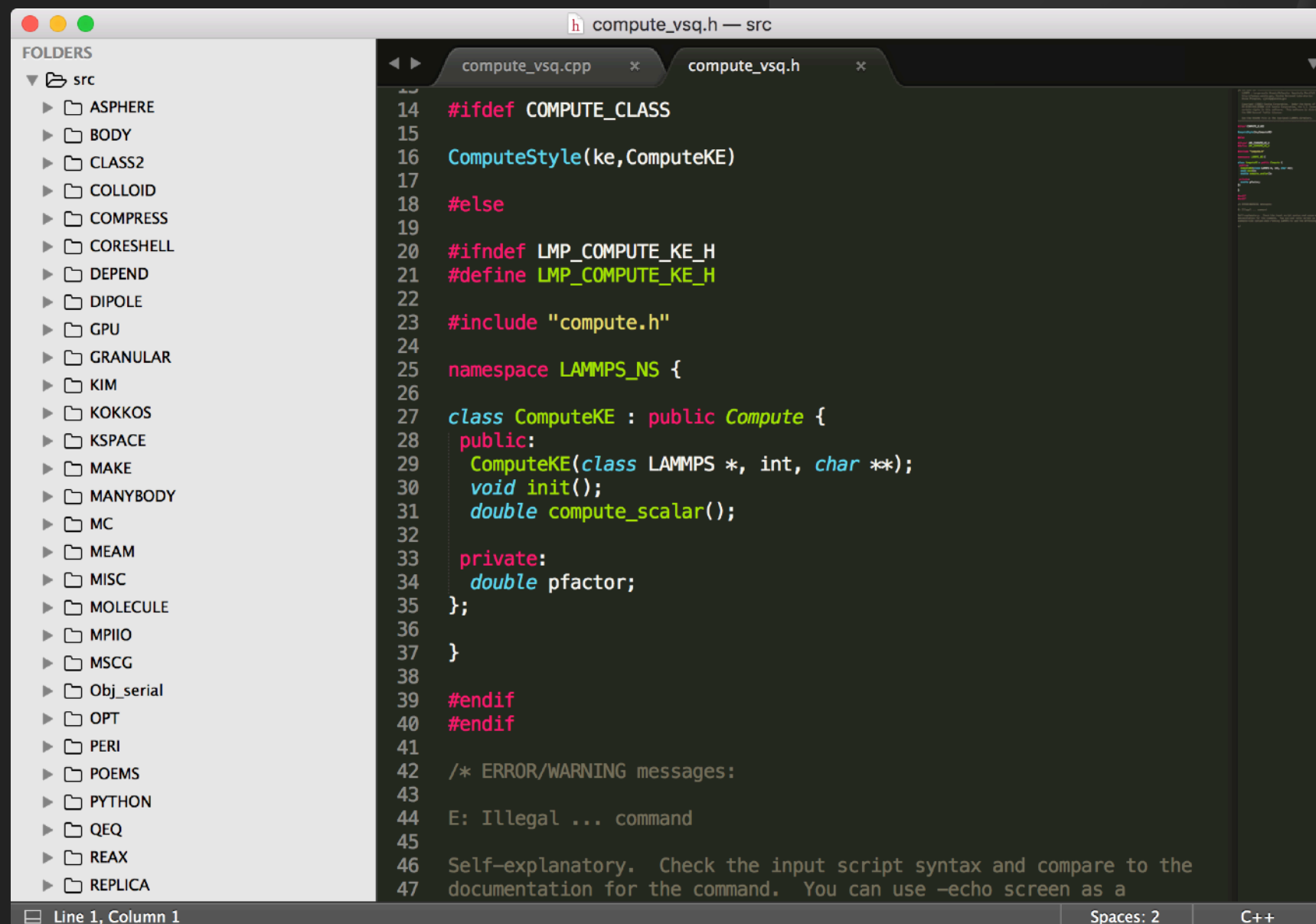
staged

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >cp compute_ke.h compute_vsq.h
/r/l/src >cp compute_ke.cpp compute_vsq.cpp
/r/l/src >git status
On branch compute_vsq
Your branch is ahead of 'origin/compute_vsq' by 1 commit.
(use "git push" to publish your local commits)
Untracked files:
(use "git add <file>..." to include in what will be committed)

  Obj_serial/
  STUBS/libmpi_stubs.a
  STUBS/mpi.o
  compute_vsq.cpp
  compute_vsq.h

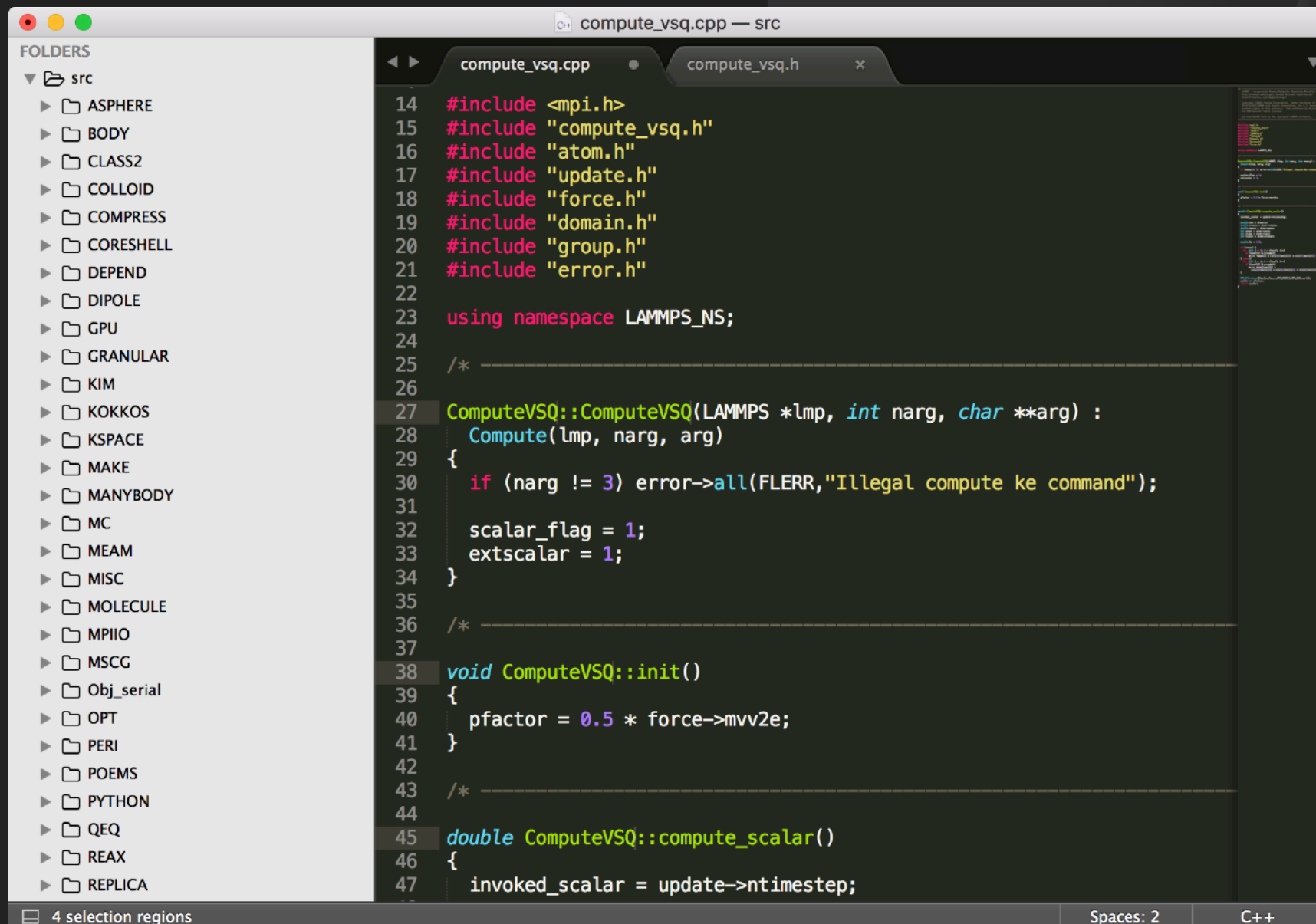
nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```

OPEN SRC FOLDER IN YOUR FAVOURITE EDITOR



RENAME COMPUTE TO ComputeVSQ

Remember to rename all c++-references from ke to vsq

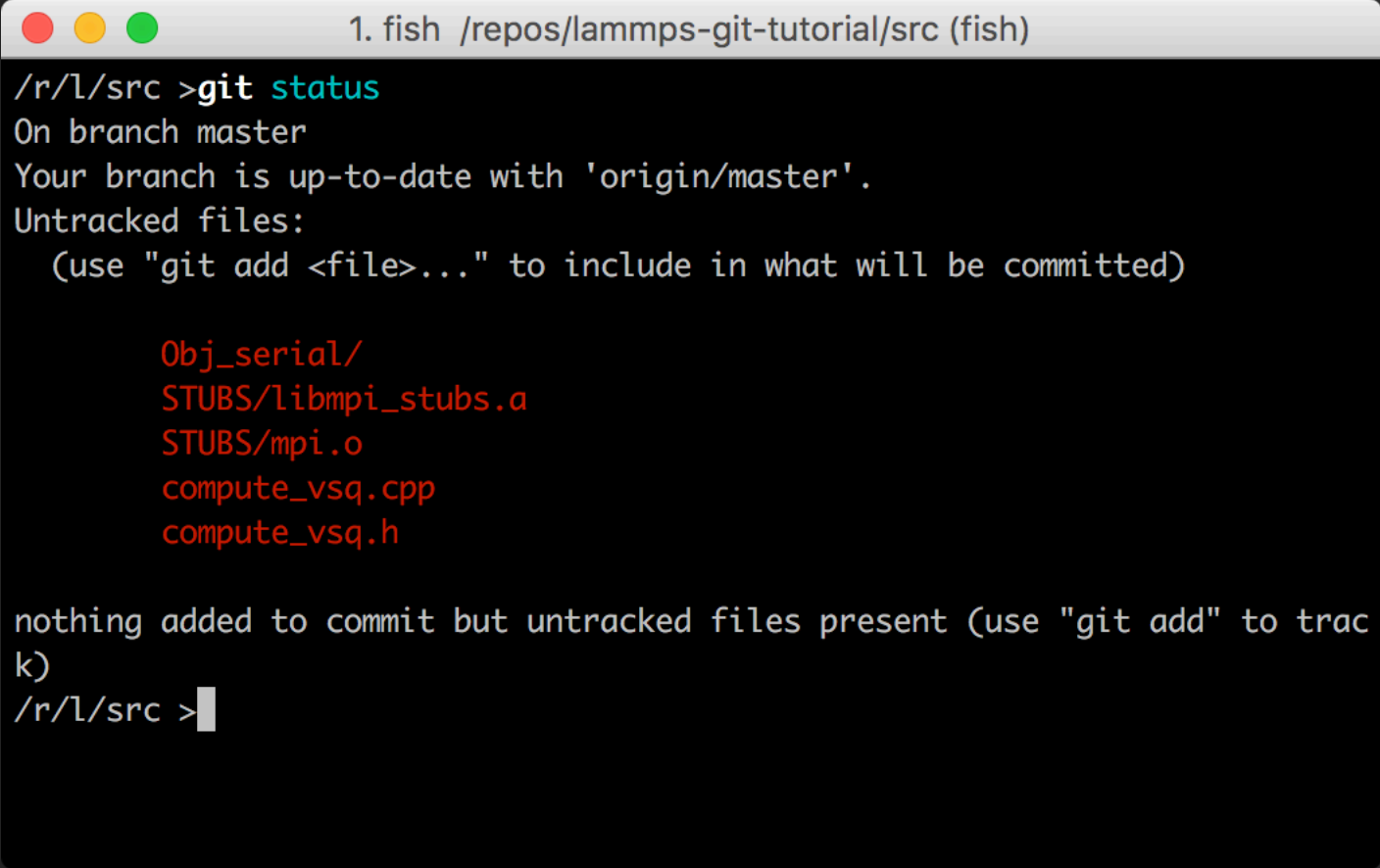


The screenshot shows a code editor window titled "compute_vsq.cpp — src". The left sidebar displays a "FOLDERS" list with various subdirectories under "src", including ASPHERE, BODY, CLASS2, COLLOID, COMPRESS, CORESHELL, DEPEND, DIPOLE, GPU, GRANULAR, KIM, KOKKOS, KSPACE, MAKE, MANYBODY, MC, MEAM, MISC, MOLECULE, MPIIO, MSCG, Obj_serial, OPT, PERI, POEMS, PYTHON, QEQ, REAX, and REPLICA. The main editor area shows the code for "compute_vsq.cpp". The code includes headers for mpi.h, compute_vsq.h, atom.h, update.h, force.h, domain.h, group.h, and error.h. It uses the LAMMPS namespace and defines a ComputeVSQ class. The class has a ComputeVSQ method that checks the number of arguments and sets scalar and extscalar flags. It also has an init method that sets the pfactor. The compute_scalar method is partially visible at the bottom.

```
14 #include <mpi.h>
15 #include "compute_vsq.h"
16 #include "atom.h"
17 #include "update.h"
18 #include "force.h"
19 #include "domain.h"
20 #include "group.h"
21 #include "error.h"
22
23 using namespace LAMMPS_NS;
24
25 /* -----
26
27 ComputeVSQ::ComputeVSQ(LAMMPS *lmp, int narg, char **arg) :
28   Compute(lmp, narg, arg)
29 {
30   if (narg != 3) error->all(FLError, "Illegal compute ke command");
31
32   scalar_flag = 1;
33   extscalar = 1;
34 }
35
36 /* -----
37
38 void ComputeVSQ::init()
39 {
40   pfactor = 0.5 * force->mvv2e;
41 }
42
43 /* -----
44
45 double ComputeVSQ::compute_scalar()
46 {
47   invoked_scalar = update->ntimestep;
```

CHECK GIT STATUS

\$ git status



```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git status
On branch master
Your branch is up-to-date with 'origin/master'.
Untracked files:
  (use "git add <file>..." to include in what will be committed)

    Obj_serial/
    STUBS/libmpi_stubs.a
    STUBS/mpi.o
    compute_vsq.cpp
    compute_vsq.h

nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```

CHECK GIT STATUS AGAIN

untracked

unmodified

modified

staged

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git status
On branch master
Your branch is up-to-date with 'origin/master'.
Untracked files:
  (use "git add <file>..." to include in what will be committed)

    Obj_serial/
    STUBS/libmpi_stubs.a
    STUBS/mpi.o
    compute_vsq.cpp
    compute_vsq.h

nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```


TEST COMPILATION

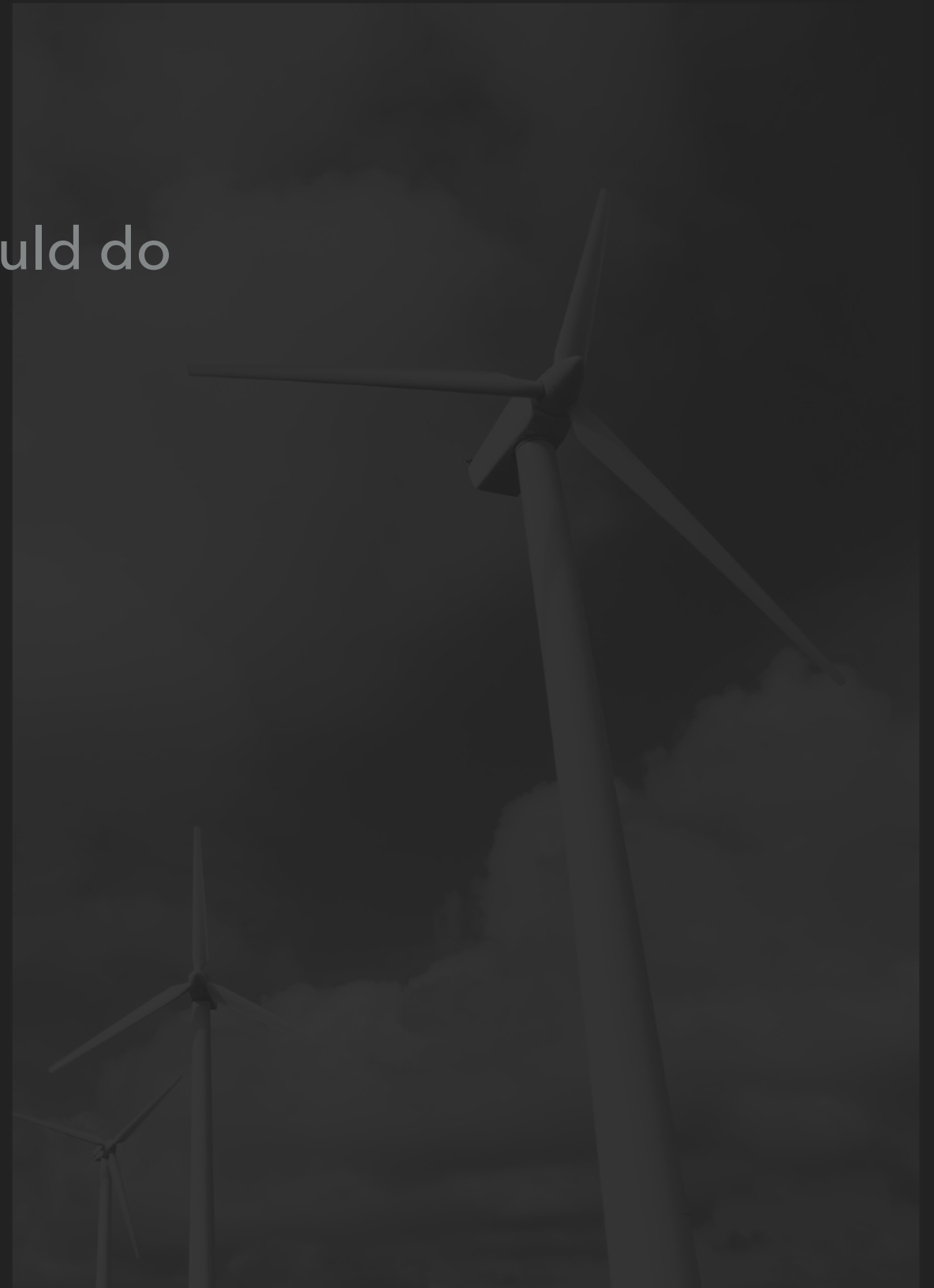
\$ make serial

Your new compute would now work as a command in LAMMPS

```
1. fish /repos/lammps-git-tutorial/src (fish)
.o pair_buck_coul_cut.o pair_coul_cut.o pair_coul_debye.o pair_coul_dsf.o
pair_coul_streitz.o pair_coul_wolf.o pair_dpd.o pair_dpd_tstat.o pair_gaus
s.o pair_hybrid.o pair_hybrid_overlay.o pair_lj96_cut.o pair_lj_cubic.o pa
ir_lj_cut.o pair_lj_cut_coul_cut.o pair_lj_cut_coul_debye.o pair_lj_cut_co
ul_dsf.o pair_lj_expand.o pair_lj_gromacs.o pair_lj_gromacs_coul_gromacs.o
pair_lj_smooth.o pair_lj_smooth_linear.o pair_mie_cut.o pair_morse.o pair
_soft.o pair_table.o pair_yukawa.o pair_zbl.o pair_zero.o procmmap.o python
.o random_mars.o random_park.o rcb.o read_data.o read_dump.o read_restart.
o reader.o reader_native.o reader_xyz.o region.o region_block.o region_con
e.o region_cylinder.o region_intersect.o region_plane.o region_prism.o reg
ion_sphere.o region_union.o replicate.o rerun.o respa.o run.o set.o specia
l.o thermo.o timer.o universe.o update.o variable.o velocity.o verlet.o wr
ite_coeff.o write_data.o write_dump.o write_restart.o -lmpi_stubs -o
../lmp_serial
size ../lmp_serial
__TEXT __DATA __OBJC others dec hex
2916352 126976 0 4296388608 4299431936 100442000
/r/l/src >
```

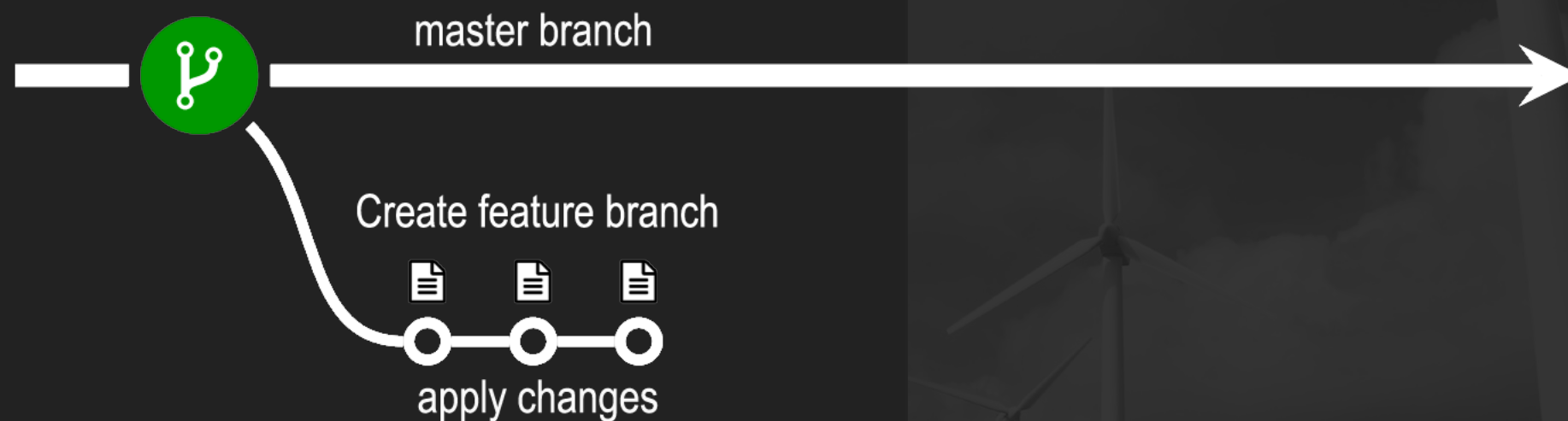
MODIFY COMPUTE

- ▶ Modify compute so it does what it should do



COMMIT TO FEATURE BRANCH

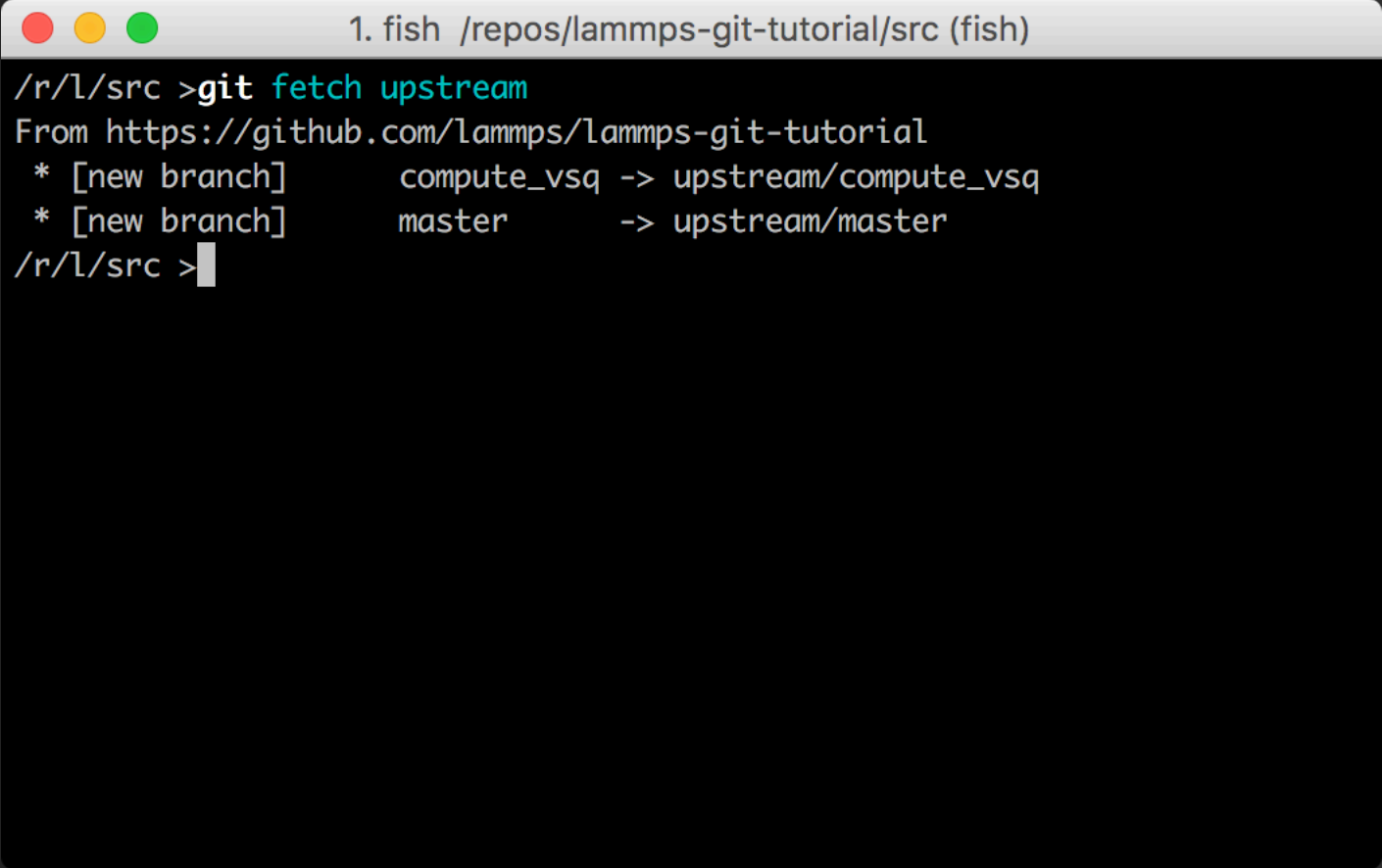
- ▶ We want to branch out so master branch is not affected
- ▶ This is often called a feature branch
- ▶ We will eventually create a pull request to LAMMPS repository
- ▶ We will branch out from main repository master branch



ADD LAMMPS REPOSITORY AS REMOTE

\$ git remote add upstream <https://github.com/lammps/lammps-git-tutorial.git>

\$ git fetch upstream

A terminal window with a title bar containing three colored circles (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial/src (fish)". The terminal content shows the command "git fetch upstream" being executed. The output indicates that two new branches were fetched from the upstream repository: "compute_vsq" and "master".

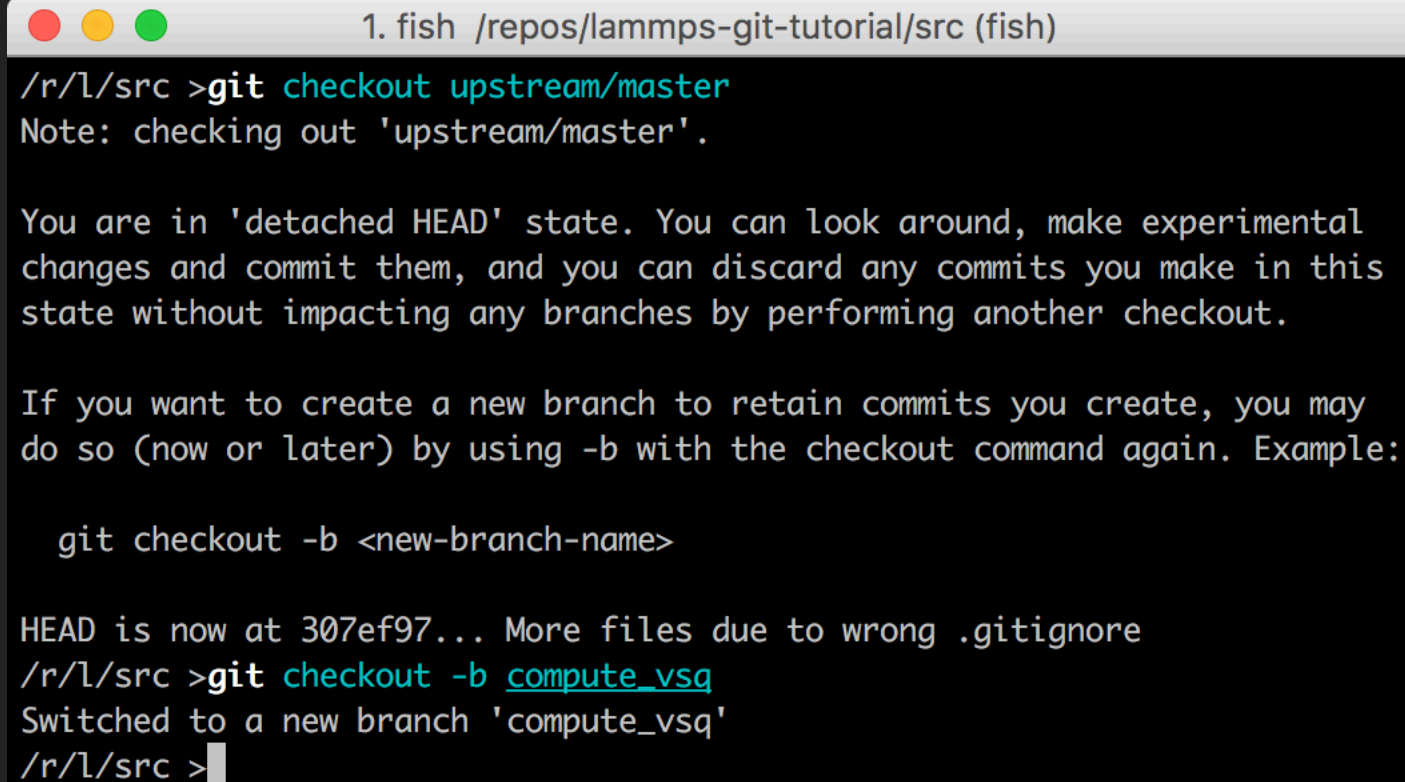
```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git fetch upstream
From https://github.com/lammps/lammps-git-tutorial
 * [new branch]      compute_vsq -> upstream/compute_vsq
 * [new branch]      master    -> upstream/master
/r/l/src >
```

CREATE FEATURE BRANCH

\$ `git fetch upstream` (ALWAYS fetch upstream to be sure we are up to date)

\$ `git checkout upstream/master`

\$ `git checkout -b compute_vsq` (branch name should be somewhat informative)

A terminal window with a title bar showing three colored circles (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial/src (fish)". The terminal content shows the execution of "git checkout upstream/master", a note about the detached HEAD state, and instructions on how to create a new branch. It then shows the execution of "git checkout -b compute_vsq", which switches to a new branch.

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git checkout upstream/master
Note: checking out 'upstream/master'.

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:

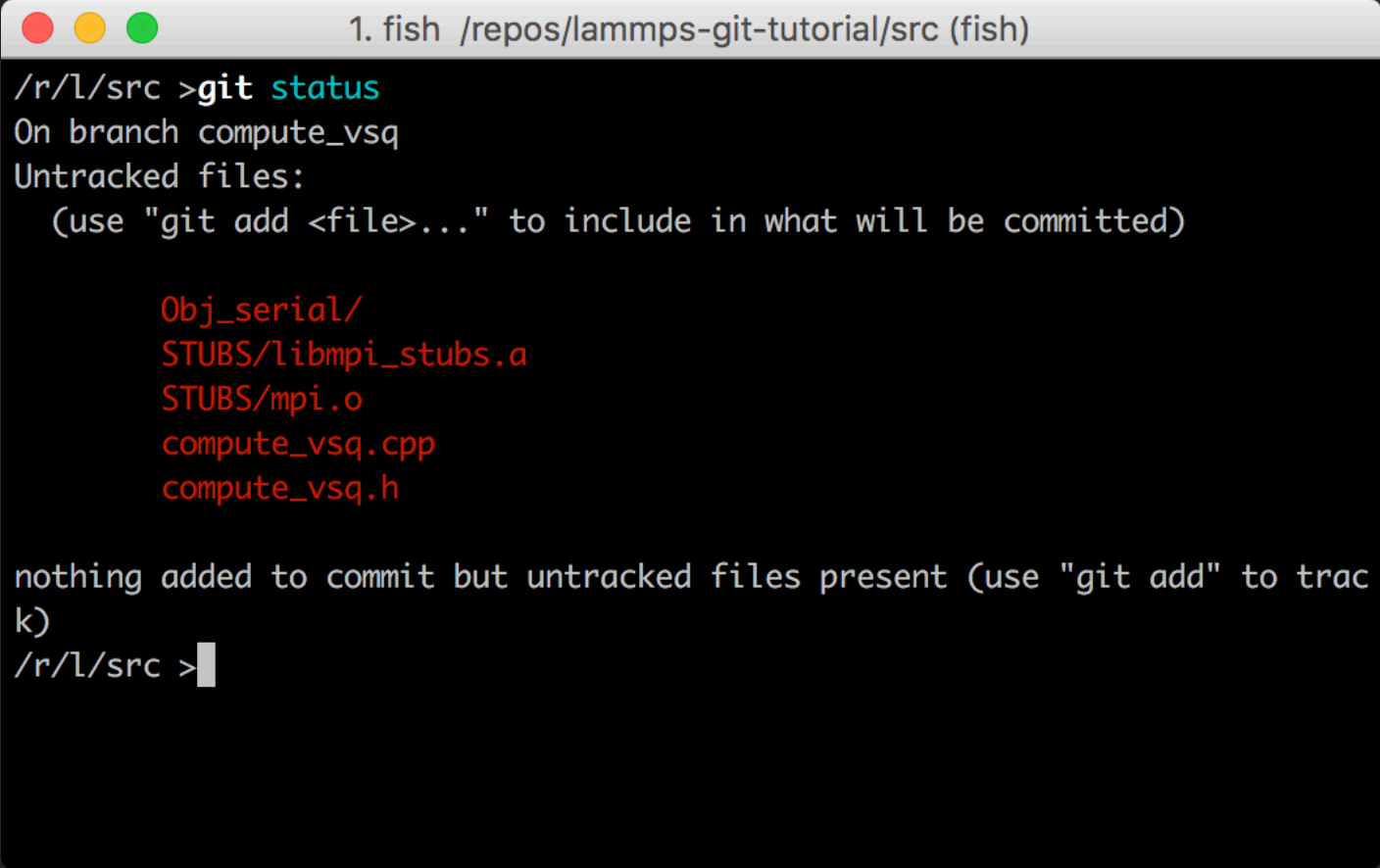
    git checkout -b <new-branch-name>

HEAD is now at 307ef97... More files due to wrong .gitignore
/r/l/src >git checkout -b compute_vsq
Switched to a new branch 'compute_vsq'
/r/l/src >
```

GIT STATUS

\$ git status

Notice that we now are on the new branch `compute_vsq`

A terminal window with a title bar showing three colored circles (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial/src (fish)". The terminal content shows the command "git status" being executed in the directory "/r/l/src". The output indicates the current branch is "compute_vsq" and lists several untracked files: "Obj_serial/", "STUBS/libmpi_stubs.a", "STUBS/mpi.o", "compute_vsq.cpp", and "compute_vsq.h". A message at the bottom states "nothing added to commit but untracked files present (use 'git add' to track)" and the prompt "/r/l/src >" is followed by a cursor.

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git status
On branch compute_vsq
Untracked files:
  (use "git add <file>..." to include in what will be committed)

        Obj_serial/
        STUBS/libmpi_stubs.a
        STUBS/mpi.o
        compute_vsq.cpp
        compute_vsq.h

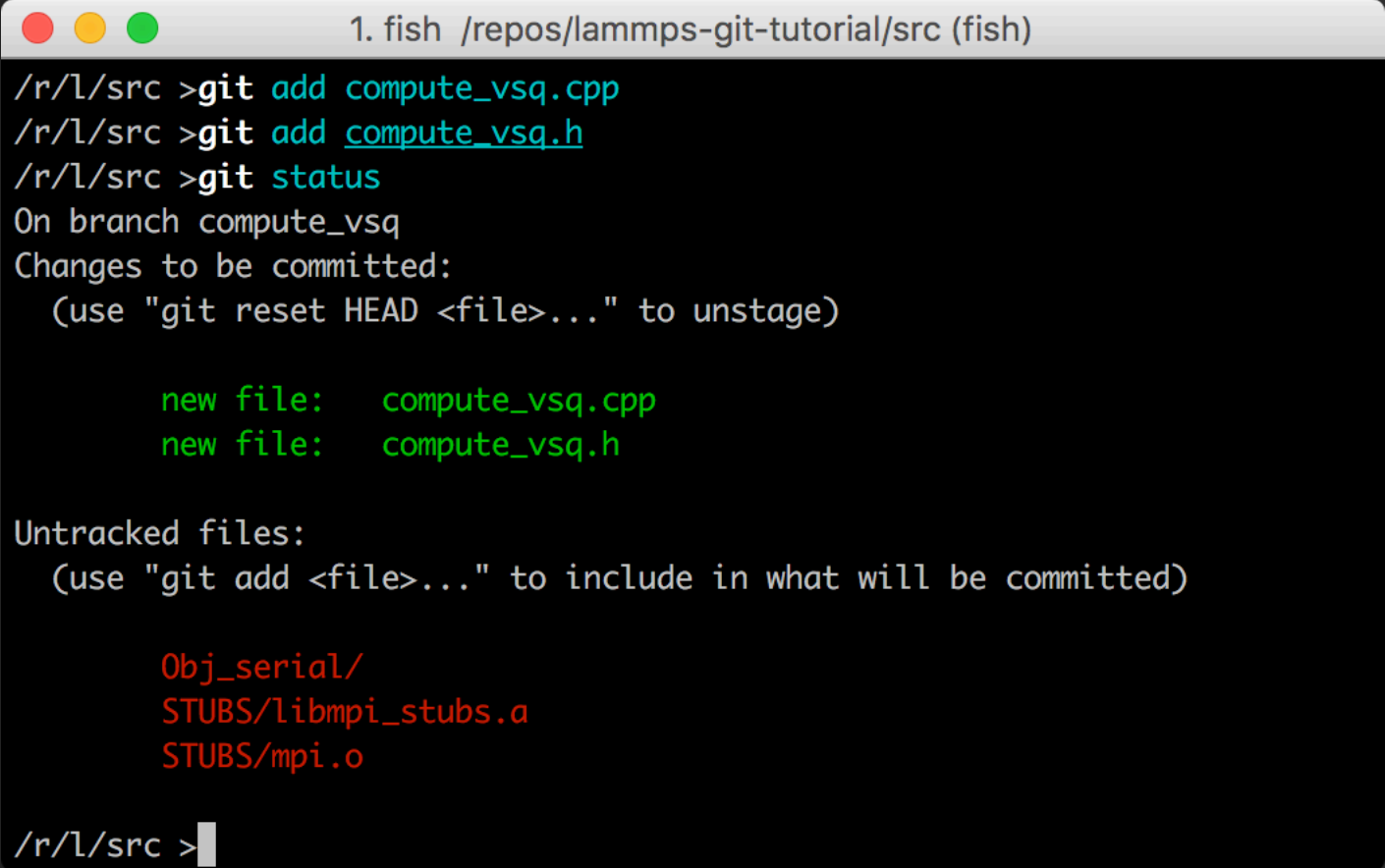
nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```

ADD CHANGES TO STAGED AREA

```
$ git add compute_vsq.cpp
```

```
$ git add compute_vsq.h
```

```
$ git status
```

A terminal window with a title bar showing three colored circles (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial/src (fish)". The terminal content shows the execution of git commands and their output. The output for "git status" indicates that two new files are staged for commit, while three other files remain untracked.

```
/r/l/src >git add compute_vsq.cpp
/r/l/src >git add compute_vsq.h
/r/l/src >git status
On branch compute_vsq
Changes to be committed:
  (use "git reset HEAD <file>..." to unstage)

        new file:   compute_vsq.cpp
        new file:   compute_vsq.h

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

        Obj_serial/
        STUBS/libmpi_stubs.a
        STUBS/mpi.o

/r/l/src >
```

ADD CHANGES TO STAGED AREA

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git add compute_vsq.cpp
/r/l/src >git add compute_vsq.h
/r/l/src >git status
On branch compute_vsq
Changes to be committed:
  (use "git reset HEAD <file>..." to unstage)

    new file:   compute_vsq.cpp
    new file:   compute_vsq.h

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

    Obj_serial/
    STUBS/libmpi_stubs.a
    STUBS/mpi.o

/r/l/src >
```

untracked

unmodified

modified

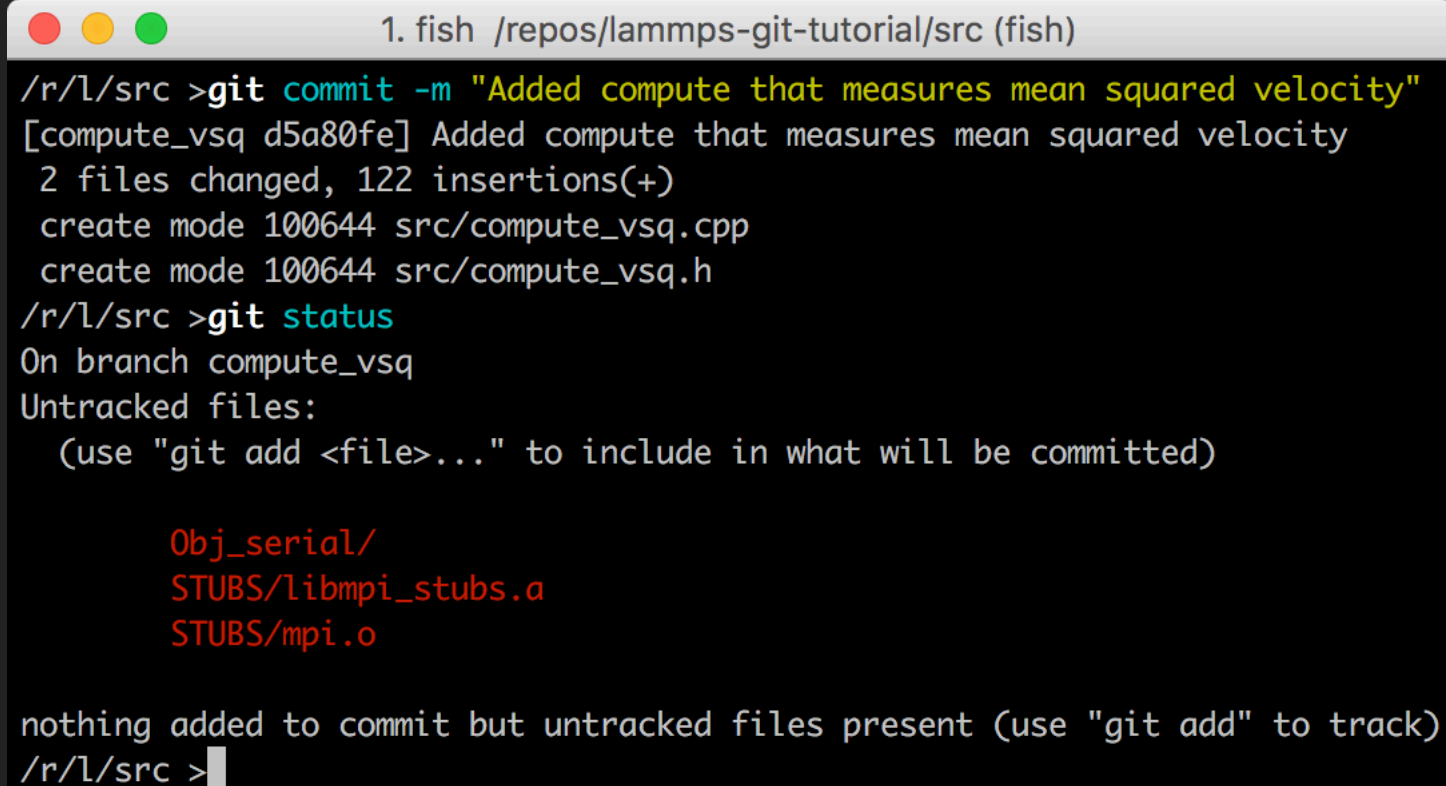
staged

add the file

COMMIT CHANGES (WITH GOOD MESSAGE)

\$ git commit -m "Added compute that measures mean squared velocity"

\$ git status

A terminal window with a title bar showing three colored circles (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial/src (fish)". The terminal output shows the execution of "git commit -m 'Added compute that measures mean squared velocity'", followed by the commit hash "[compute_vsq d5a80fe]", the commit message, and details about the files changed. Then, "git status" is run, showing the current branch and untracked files. Finally, a message states that nothing was added to the commit but untracked files are present.

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git commit -m "Added compute that measures mean squared velocity"
[compute_vsq d5a80fe] Added compute that measures mean squared velocity
2 files changed, 122 insertions(+)
create mode 100644 src/compute_vsq.cpp
create mode 100644 src/compute_vsq.h
/r/l/src >git status
On branch compute_vsq
Untracked files:
  (use "git add <file>..." to include in what will be committed)

    Obj_serial/
    STUBS/libmpi_stubs.a
    STUBS/mpi.o

nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```

COMMIT CHANGES

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git commit -m "Added compute that measures mean squared velocity"
[compute_vsqa d5a80fe] Added compute that measures mean squared velocity
2 files changed, 122 insertions(+)
create mode 100644 src/compute_vsqa.cpp
create mode 100644 src/compute_vsqa.h
/r/l/src >git status
On branch compute_vsqa
Untracked files:
  (use "git add <file>..." to include in what will be committed)

    Obj_serial/
    STUBS/libmpi_stubs.a
    STUBS/mpi.o

nothing added to commit but untracked files present (use "git add" to track)
/r/l/src >
```

untracked

unmodified

modified

staged

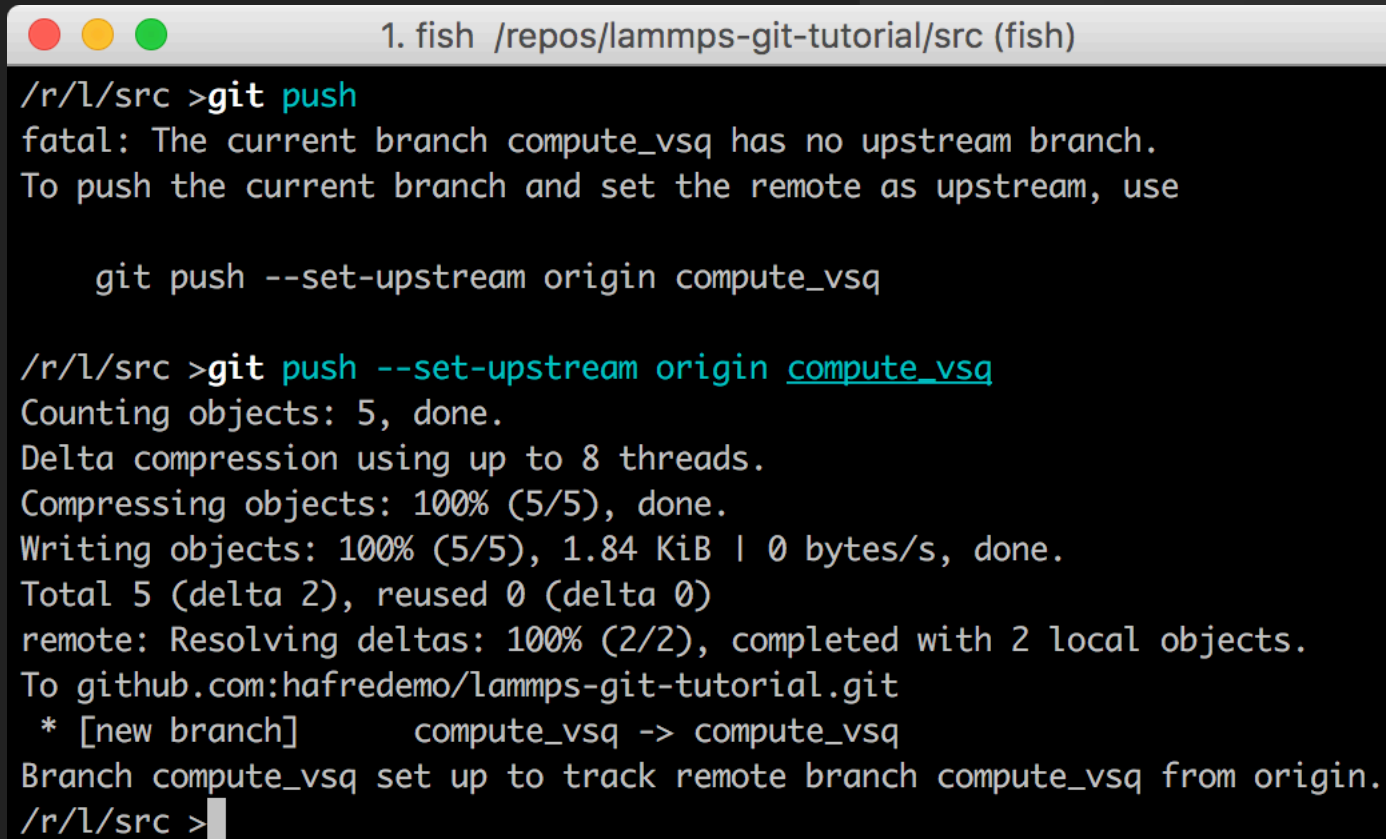
add the file

commit

PUSH COMMIT TO YOUR FORK

\$ `git push` (won't work so we follow the instructions)

\$ `git push --set-upstream origin compute_vsq`

A terminal window with a title bar showing three colored window control buttons (red, yellow, green) and the text "1. fish /repos/lammps-git-tutorial/src (fish)". The terminal content shows a failed `git push` command followed by the successful execution of `git push --set-upstream origin compute_vsq`. The output includes details about object counting, compression, and the successful push to the remote repository, setting up the local branch to track the remote one.

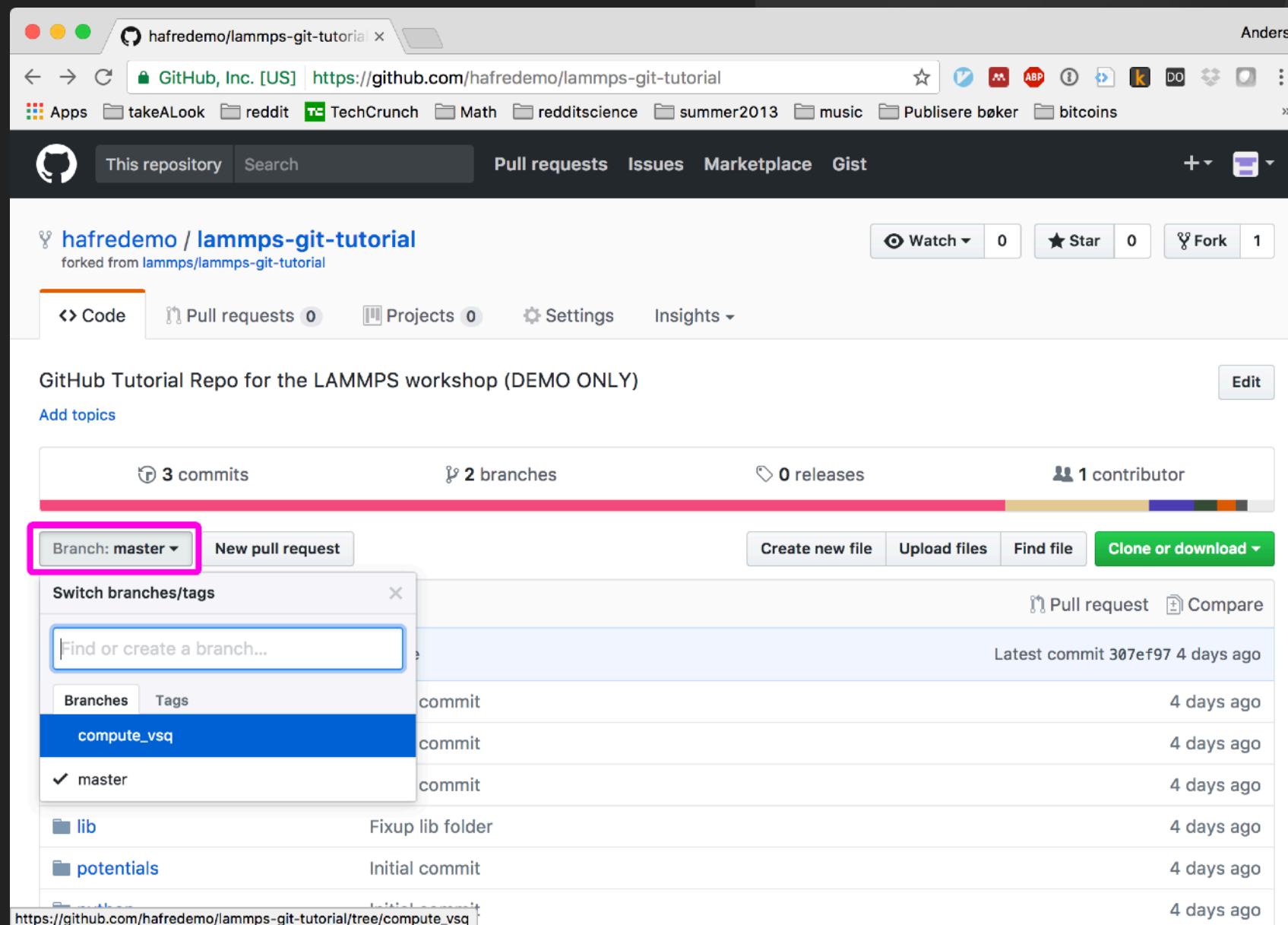
```
/r/l/src >git push
fatal: The current branch compute_vsq has no upstream branch.
To push the current branch and set the remote as upstream, use

    git push --set-upstream origin compute_vsq

/r/l/src >git push --set-upstream origin compute_vsq
Counting objects: 5, done.
Delta compression using up to 8 threads.
Compressing objects: 100% (5/5), done.
Writing objects: 100% (5/5), 1.84 KiB | 0 bytes/s, done.
Total 5 (delta 2), reused 0 (delta 0)
remote: Resolving deltas: 100% (2/2), completed with 2 local objects.
To github.com:hafredemo/lammps-git-tutorial.git
 * [new branch]      compute_vsq -> compute_vsq
Branch compute_vsq set up to track remote branch compute_vsq from origin.
/r/l/src >
```

GO TO YOUR FORK ON GITHUB

Select the new branch we just created



CLICK PULL REQUEST

Also notice that this branch is 1 commit ahead of lammps:master

The screenshot shows a web browser window displaying the GitHub repository page for 'hafredemo/lammps-git-tutorial'. The browser's address bar shows the URL 'https://github.com/hafredemo/lammps-git-tutorial/tree/compute_vsq'. The repository page includes a header with the repository name, a search bar, and navigation links for 'Pull requests', 'Issues', 'Marketplace', and 'Gist'. Below the header, the repository is identified as 'hafredemo / lammps-git-tutorial' and 'forked from lammps/lammps-git-tutorial'. The page shows 4 commits, 2 branches, 0 releases, and 1 contributor. A pink arrow points to the 'Pull request' button, which is highlighted with a pink box. The text 'This branch is 1 commit ahead of lammps:master.' is also highlighted with a pink underline. Below the pull request button, a list of commits is shown, including 'Initial commit' for folders like 'bench', 'doc', 'examples', 'lib', 'potentials', and 'python'.

hafredemo / lammps-git-tutorial
forked from lammps/lammps-git-tutorial

4 commits 2 branches 0 releases 1 contributor

Branch: compute_vsq New pull request Create new file Upload files Find file Clone or download

This branch is 1 commit ahead of lammps:master.

Pull request Compare

Latest commit d5a80fe 14 minutes ago

File	Commit	Time
bench	Initial commit	4 days ago
doc	Initial commit	4 days ago
examples	Initial commit	4 days ago
lib	Fixup lib folder	4 days ago
potentials	Initial commit	4 days ago
python	Initial commit	4 days ago

WRITE PULL REQUEST (PR) INFO TO MAINTAINERS

Pull request template is automatically filled in
Allow edits from maintainers lets them push directly to your branch if needed

Comparing lammps:master...hafr... x https://raw.githubusercontent.com x Anders

GitHub, Inc. [US] https://github.com/lammps/lammps-git-tutorial/compare/master...hafredemo/lammps-git-tuto... ☆

Apps takeALook reddit TechCrunch Math redditscience summer2013 music Publisere bøker bitcoins »

<> Code 1 Issues 0 Pull requests 0 Insights ▼

Open a pull request

Create a new pull request by comparing changes across two branches. If you need to, you can also [compare across forks](#).

base fork: lammps/lammps-git-tutorial base: master ... head fork: hafredemo/lammps-git-tuto... compare: compute_vsqs

✓ Able to merge. These branches can be automatically merged.

Added compute that measures mean squared velocity

Write Preview AA B i “ <> ☰ ☷ ☹ ↩ @ ★

Purpose

Added new compute that measures the mean squared velocity.

Author(s)

Anders Hafreager

Backward Compatibility

Attach files by dragging & dropping, [selecting them](#), or pasting from the clipboard.

☒ Allow edits from maintainers. [Learn more](#)

Create pull request

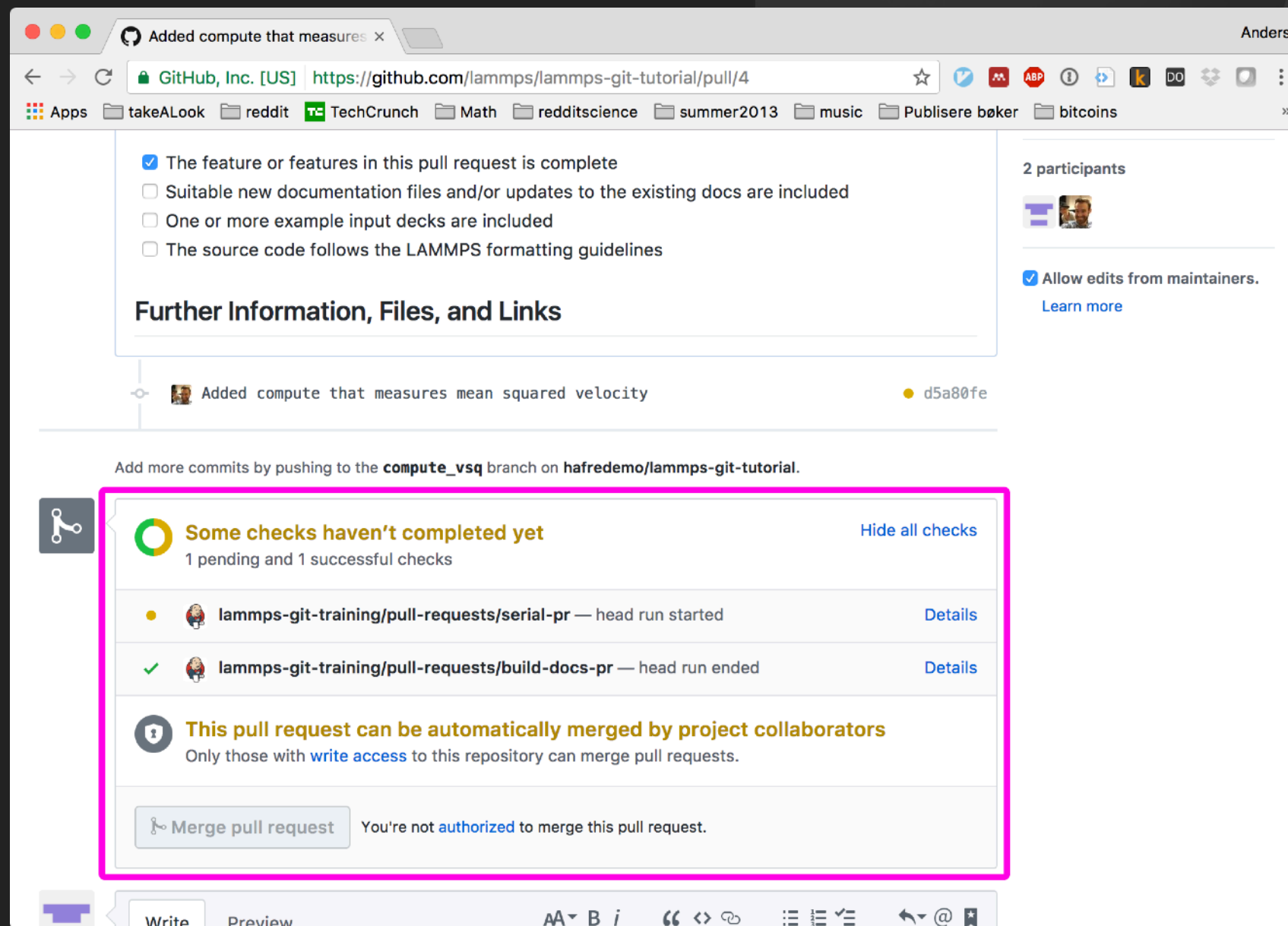
WRITE PULL REQUEST (PR) INFO TO MAINTAINERS

- ▶ You don't have to fill in every field if it's not relevant, it's just a template
- ▶ Not all changes require new documentation / new examples (i.e. bug fixes)
- ▶ You will get good feedback from maintainers
- ▶ When you're ready, press

Create pull request

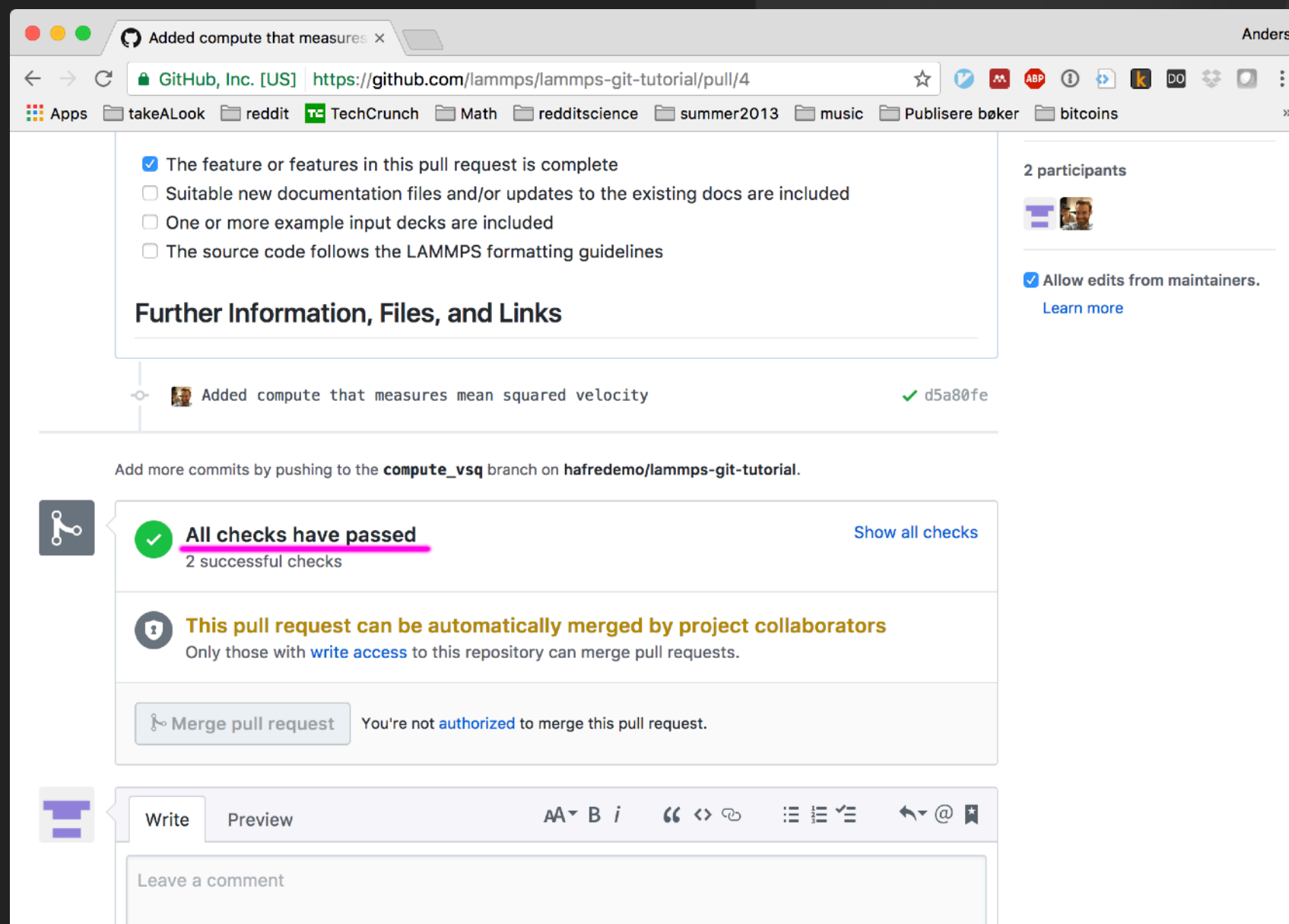
NOW WAIT

- ▶ We have Jenkins, and automated build system testing all PR's
- ▶ It builds the documentation and source code



NOW WAIT

- ▶ Jenkins typically spends a few minutes per build

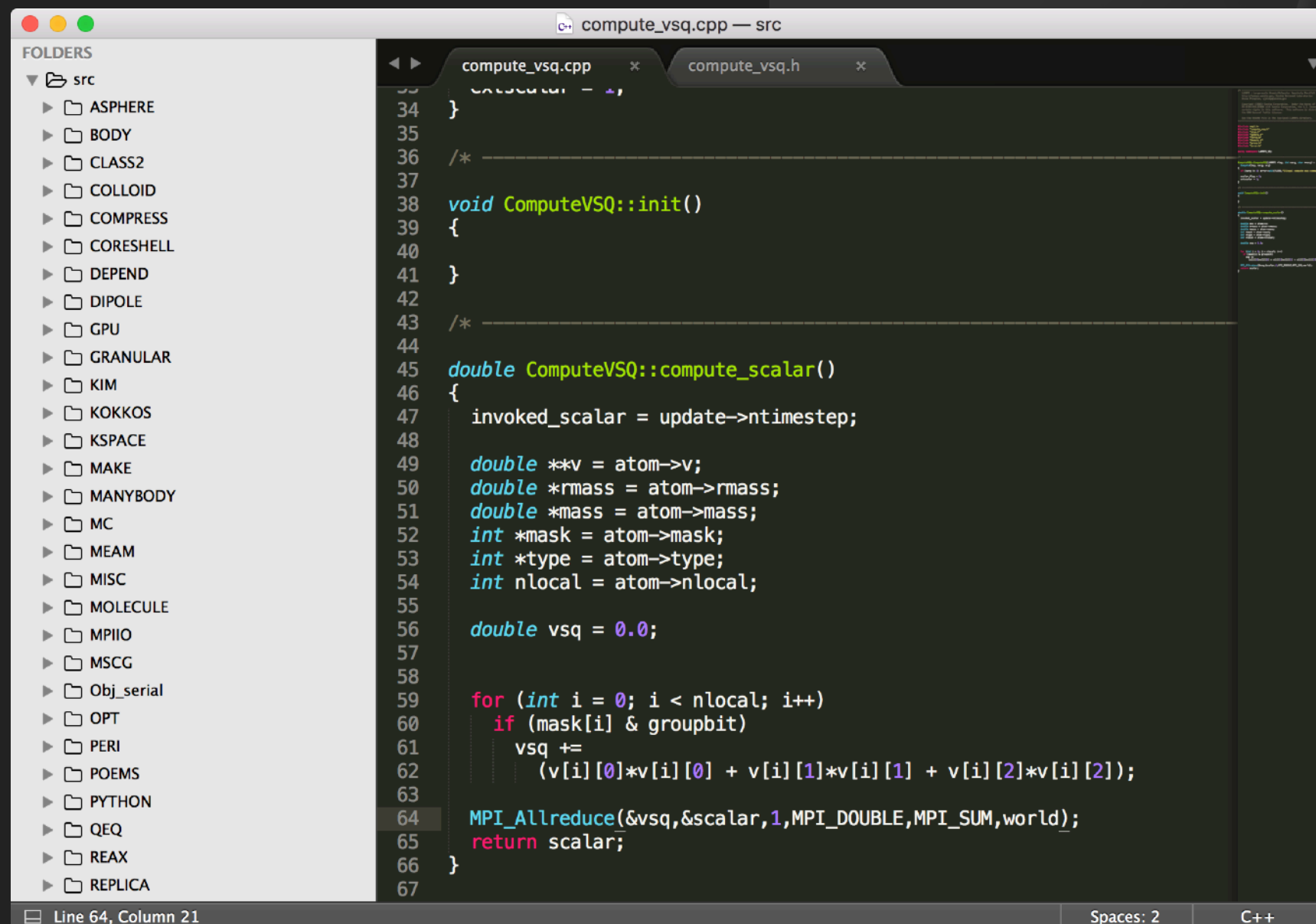


NOW WAIT

- ▶ Maintainers will label the pull request and give feedback
- ▶ Here it seems like I made a programming mistake, and I haven't added doc pages

The screenshot shows a GitHub pull request interface. At the top, the browser address bar displays the URL `https://github.com/lammps/lammps-git-tutorial/pull/4`. The pull request title is "Added compute that measures mean squared velocity". The status is "d5a80fe" with a green checkmark. The pull request is labeled with "enhancement" and "needswork" tags, added 3 minutes ago by "andeplane". A comment from "andeplane" (Collaborator) states: "Hi, I looked through the code. It seems like you have forgotten the `MPI_Allreduce` to synchronize across processes. Also could you add a doc page explaining the usage of this new compute?". The pull request has 2 participants. The "Further Information, Files, and Links" section shows a list of checkboxes: "The feature or features in this pull request is complete" (checked), "Suitable new documentation files and/or updates to the existing docs are included" (unchecked), "One or more example input decks are included" (unchecked), and "The source code follows the LAMMPS formatting guidelines" (unchecked). The bottom section shows a status bar with a green checkmark and the text "All checks have passed" (2 successful checks), a link to "Show all checks", and a message: "This pull request can be automatically merged by project collaborators".

MAKE THE CHANGES



```
compute_vsq.cpp — src
compute_vsq.cpp  compute_vsq.h
33
34 }
35
36 /* -----
37
38 void ComputeVSQ::init()
39 {
40 }
41
42 /* -----
43
44 double ComputeVSQ::compute_scalar()
45 {
46     invoked_scalar = update->ntimestep;
47
48     double **v = atom->v;
49     double *rmass = atom->rmass;
50     double *mass = atom->mass;
51     int *mask = atom->mask;
52     int *type = atom->type;
53     int nlocal = atom->nlocal;
54
55     double vsq = 0.0;
56
57     for (int i = 0; i < nlocal; i++)
58         if (mask[i] & groupbit)
59             vsq +=
60                 (v[i][0]*v[i][0] + v[i][1]*v[i][1] + v[i][2]*v[i][2]);
61
62     MPI_Allreduce(&vsq,&scalar,1,MPI_DOUBLE,MPI_SUM,world);
63     return scalar;
64 }
65
66
67
```

Line 64, Column 21 Spaces: 2 C++

MAKE THE CHANGES

\$ git status

```
1. fish /repos/lammps-git-tutorial/src (fish)
Your branch is up-to-date with 'origin/compute_vsq'.
Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git checkout -- <file>..." to discard changes in working directory)

        modified:   compute_vsq.cpp
        modified:   compute_vsq.h

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

        Obj_serial/
        STUBS/libmpi_stubs.a
        STUBS/mpi.o

no changes added to commit (use "git add" and/or "git commit -a")
/r/l/src >
```

MAKE THE CHANGES

untracked

unmodified

modified

staged

edit the file

```
1. fish /repos/lammps-git-tutorial/src (fish)
Your branch is up-to-date with 'origin/compute_vsq'.
Changes not staged for commit:
  (use "git add <file>..." to update what will be committed)
  (use "git checkout -- <file>..." to discard changes in working directory)

        modified:   compute_vsq.cpp
        modified:   compute_vsq.h

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

        Obj_serial/
        STUBS/libmpi_stubs.a
        STUBS/mpi.o

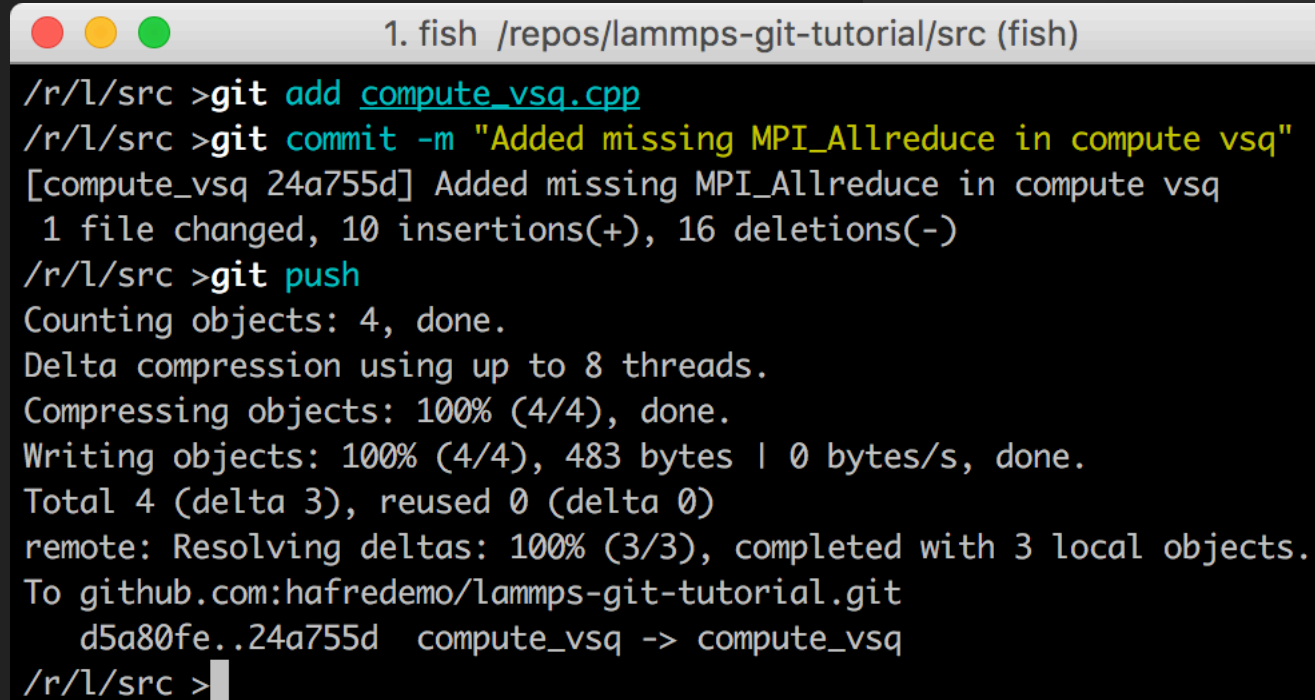
no changes added to commit (use "git add" and/or "git commit -a")
/r/l/src >
```

COMMIT CHANGES

```
$ git add compute_vsq.cpp
```

```
$ git commit -m "Added missing MPI_Allreduce in compute vsq"
```

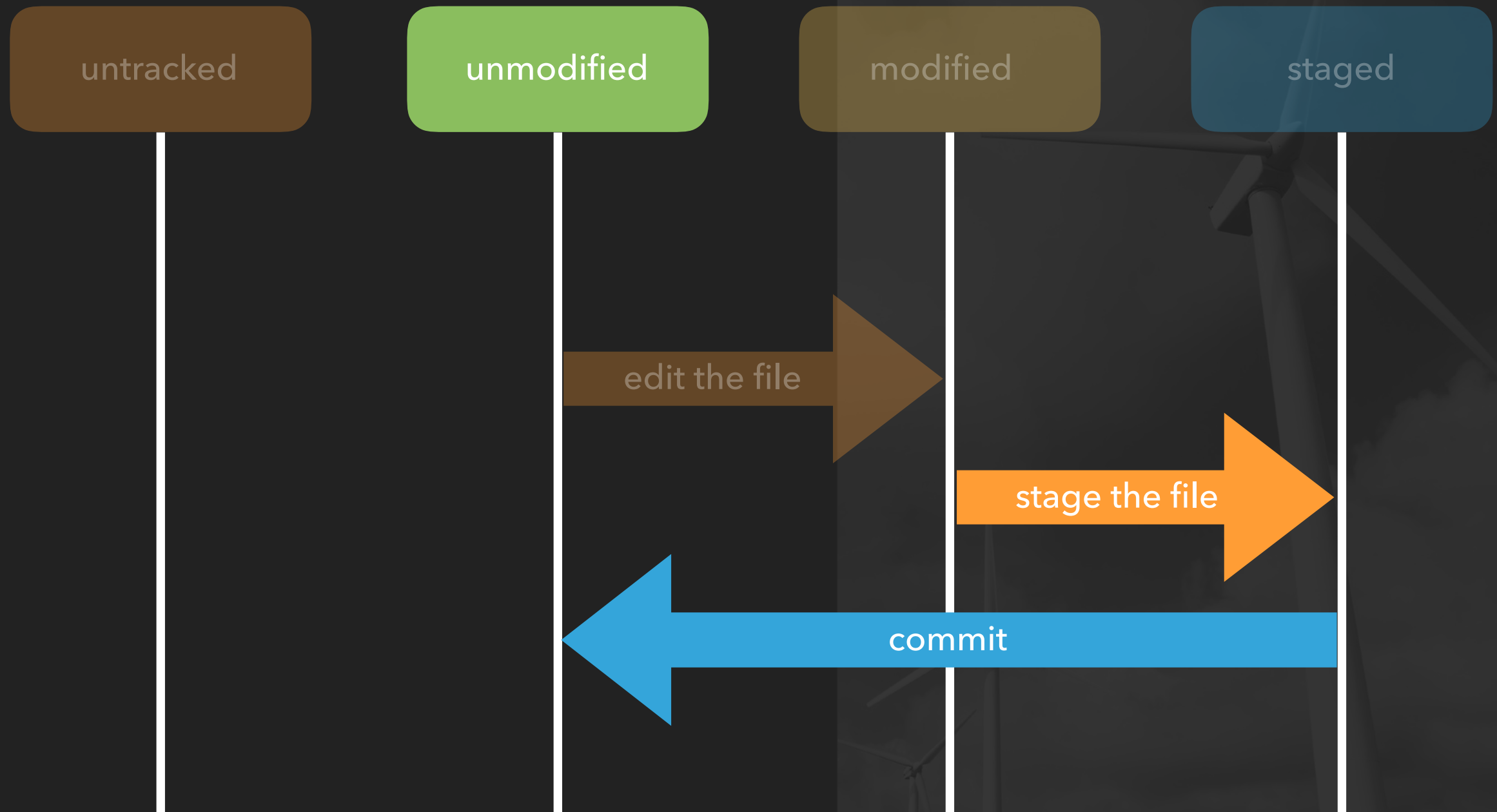
```
$ git push
```

A terminal window titled "1. fish /repos/lammps-git-tutorial/src (fish)" showing the execution of git commands. The output shows the file being added, the commit message, the commit hash, the number of files changed, and the push operation details including object counting, compression, and writing to the remote repository.

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git add compute_vsq.cpp
/r/l/src >git commit -m "Added missing MPI_Allreduce in compute vsq"
[compute_vsq 24a755d] Added missing MPI_Allreduce in compute vsq
1 file changed, 10 insertions(+), 16 deletions(-)
/r/l/src >git push
Counting objects: 4, done.
Delta compression using up to 8 threads.
Compressing objects: 100% (4/4), done.
Writing objects: 100% (4/4), 483 bytes | 0 bytes/s, done.
Total 4 (delta 3), reused 0 (delta 0)
remote: Resolving deltas: 100% (3/3), completed with 3 local objects.
To github.com:hafredemo/lammps-git-tutorial.git
d5a80fe..24a755d compute_vsq -> compute_vsq
/r/l/src >
```

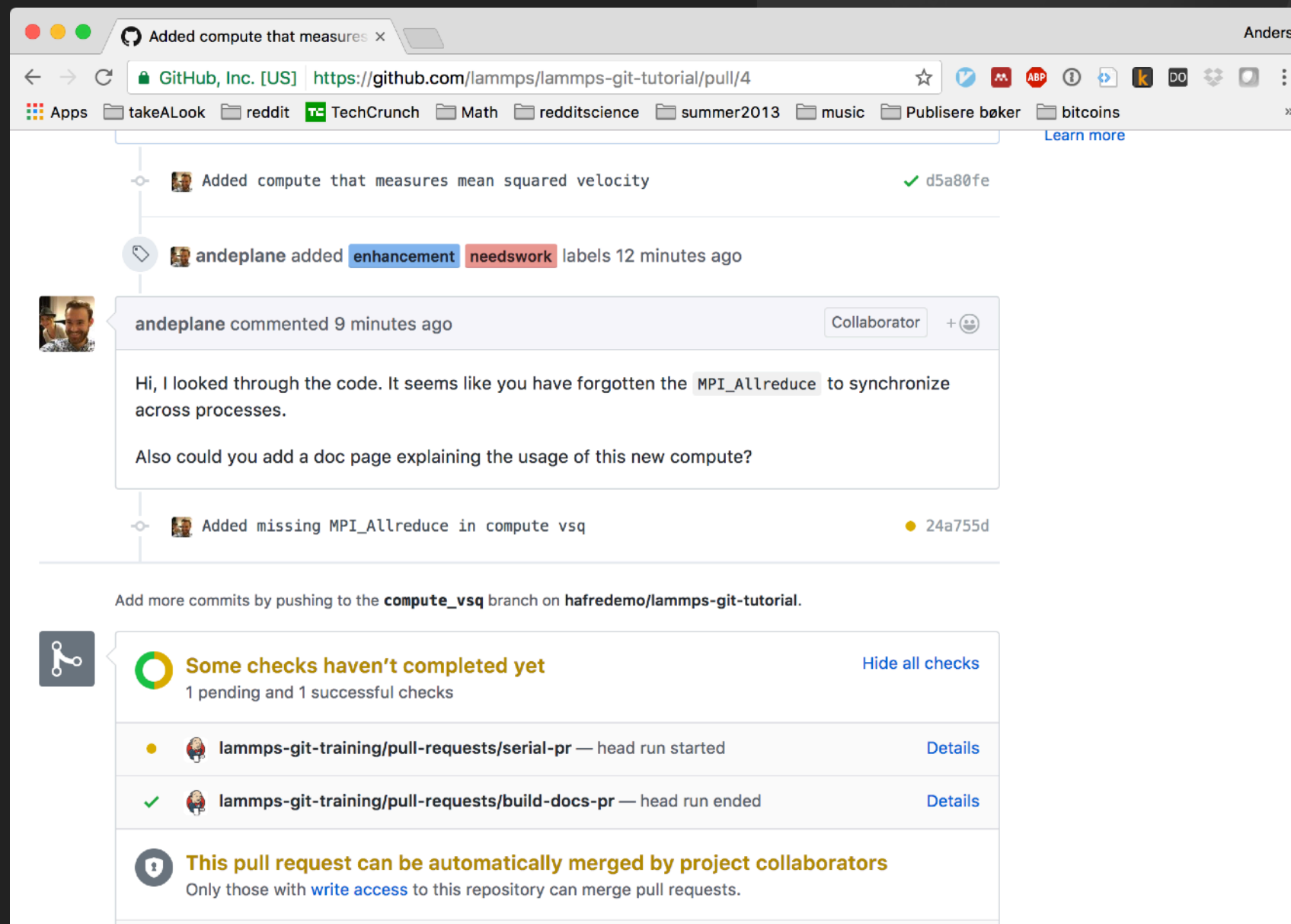
COMMIT CHANGES

```
1. fish /repos/lammps-git-tutorial/src (fish)
/r/l/src >git add compute_vsq.cpp
/r/l/src >git commit -m "Added missing MPI_Allreduce in compute vsq"
[compute_vsq 24a755d] Added missing MPI_Allreduce in compute vsq
1 file changed, 10 insertions(+), 16 deletions(-)
/r/l/src >git push
Counting objects: 4, done.
Delta compression using up to 8 threads.
Compressing objects: 100% (4/4), done.
Writing objects: 100% (4/4), 483 bytes | 0 bytes/s, done.
Total 4 (delta 3), reused 0 (delta 0)
remote: Resolving deltas: 100% (3/3), completed with 3 local objects.
To github.com:hafredemo/lammps-git-tutorial.git
d5a80fe..24a755d compute_vsq -> compute_vsq
/r/l/src >
```



NOW WAIT AGAIN

- ▶ New commit is automatically added to PR
- ▶ Jenkins will build after the new commit



MERGE IS DONE BY STEVE

- ▶ When PR is ready to be merged, Steve is assigned
- ▶ You can delete the branch after merge (GitHub shows a button for that)

The screenshot shows a GitHub pull request (PR) for the repository lammps/lammps. The PR is titled "Bugfix for USER-REAXC and re x" and is currently open. The PR is assigned to Steve (sjplimp) by Anders (akohlmey) 11 days ago. The PR includes two commits: "avoid division by zero in reaxff bond interaction computations in ver..." (61b1487) and "fix reaxc division by zero bug also for USER-OMP variant" (ec23aef). The PR is labeled with "bugfix", "kokkos_package", "user_omp_package", and "user_reaxc_package". The PR is merged into the lammps:master branch 11 days ago. The PR is closed by akohlmey 10 days ago. The PR is assigned to Steve (sjplimp) by Anders (akohlmey) 11 days ago. The PR is labeled with "bugfix", "kokkos_package", "user_omp_package", and "user_reaxc_package". The PR is merged into the lammps:master branch 11 days ago. The PR is closed by akohlmey 10 days ago.

The interface includes a sidebar with navigation links (Apps, takeALook, reddit, TechCrunch, Math, redditscience, summer2013, music, Publisere bøker, bitcoins) and a right-hand sidebar with sections: Labels (bugfix, kokkos_package, user_omp_package, user_reaxc_package), Projects (None yet), Milestone (No milestone), Notifications (Subscribe button, "You're not receiving notifications from this thread."), and 2 participants (akohlmey, sjplimp).

At the bottom, there is a "Write" and "Preview" tab for comments, with a text area for "Leave a comment" and a "Subscribe" button.



EXERCISES

(15 minute break first)

EXERCISE 0 – GITHUB ACCOUNT

- ▶ Go to github.com and create an account
- ▶ Verify that you have git. If not, install it (see [slide 8](#))
- ▶ (Optional) Add an SSH key to your GitHub account
<https://help.github.com/articles/connecting-to-github-with-ssh>

EXERCISE 1 – ISSUES

- ▶ Create a new issue on the tutorial [git repository](#) to track your progress on the exercises
- ▶ State your name and affiliation in the description and add a task list for each exercise
- ▶ As you progress, check the exercises you've completed

EXERCISE 2: CREATE A FORK

- ▶ Fork the [lammps/lammps-git-tutorial](#) repository into your GitHub account
- ▶ Clone your fork into a working directory on your computer
- ▶ Add upstream as remote and fetch it

Steps are explained from [slide 11](#)

EXERCISE 3: CREATE A FEATURE BRANCH

- ▶ Copy files `src/XYZ` to `src/ABC`
- ▶ **Use your GitHub username as part of the filename to avoid conflicts when we merge**
- ▶ Edit file and implement the new compute
- ▶ Create a new feature branch
- ▶ Push your new branch to your fork (origin)

Steps are explained from [slide 26](#)

EXERCISE 4: CREATE A PULL REQUEST

- ▶ Go to GitHub and create a new pull request (your branch to master)
- ▶ Fix any compilation errors and update your branch

Steps are explained from [slide 44](#)

EXERCISE 5: WAIT FOR FEEDBACK AND FOLLOW INSTRUCTIONS

- ▶ You will have to make changes and push your updates again
- ▶ Continue until we merge into master

BONUS EXERCISE: TRY TO BUILD DOCUMENTATION

- ▶ Go into the doc/ folder and run "make -j 4 html"
- ▶ This will download dependencies and generate the documentation (requires Python 3, pip and virtualenv)
- ▶ Verify that you can view the documentation by opening doc/html/Manual.html