PHY604 Lecture 2

August 31, 2023

Review: Memory determines largest number that can be stored

- E.g., 1 byte: | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $= 1x2^6 + 1x2^5 + 1x2^4 + 1x2^3 + 1x2^2 + 1x2^1 + 1x2^0 = 127_{10}$

  Sign bit; 0 if positive integer
  1 if negative integer

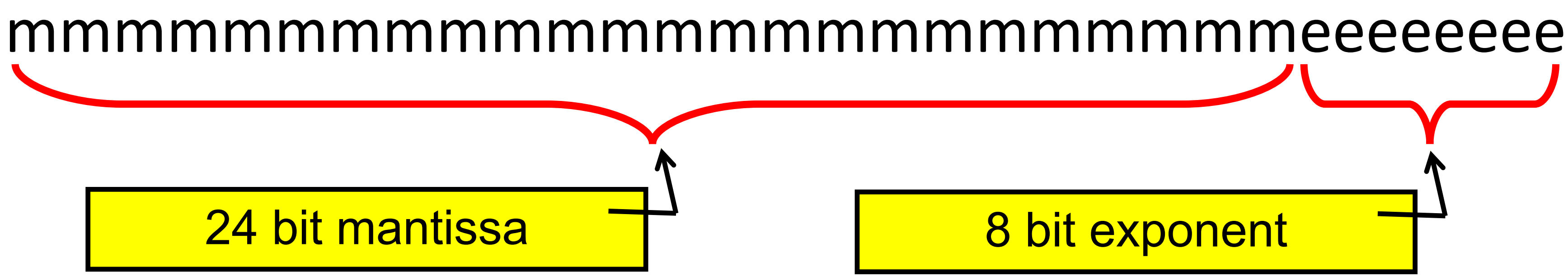
- 2-byte:
  - This can store 2^{15}-1 distinct values: -32,768 to 32,767 (signed)
  - Or it can store 2^{16} values: 0 to 65,535 (unsigned)

- Standard in many languages is 4-bytes
  - This can store 2^{31}-1 distinct values: -2,147,483,648 to 2,147,483,647 (signed)
    - C/C++: int (usually) or int32_t
    - Fortran: integer or integer(4)
  - Or it can store 2^{32} distinct values : 0 to 4,294,967,295 (unsigned)
    - C/C++: uint or uint32_t
    - Fortran (as of 95): unsigned

- For very big integers, 8-byte allows for 2^{64}
  - Fotran: integer(8)
  - C++: long

Review: Storing floating point data

- IEEE 754 mantissa-exponent form:



- Value = mantissa x 2 ^{exponent}
- Single precision:
  - Sign: 1 bit; exponent: 8 bits; significand: 24 bits (23 stored) = 32 bits
  - Range: 2^7-1 in exponent (because of sign) = 2^{127} multiplier ~ 10^{38}
  - Decimal precision: ~6 significant digits
- Double precision:
  - Sign: 1 bit; exponent: 11 bits; significand: 53 bits (52 stored) = 64 bits
  - Range: 2^{10}-1 in exponent = 2^{1023} multiplier ~ 10^{308}
  - Decimal precision: ~15 significant digits

Review: Real/Floating point numbers are more complicated

- Infinite real numbers on the number line need to be represented by a finite number of bits

- Finite memory results in limited **size and precision** of floating point numbers
  - Not all real numbers (even simple ones) can be stored in a finite number of digits in a base-2 representation
  - Example: $1/10 = 0.1_{10} = 0.0001100110011..._2$ does not have a finite representation in base 2 just as $1/3 = 0.333333..._{10}$ has no finite representation in base 10

- This means that even simple floating point numbers are often approximated with some small error
  - This means that floating point arithmetic is not exact! (on all computers and programming languages)

- Errors can compound if not treated carefully!

Review: Epsilon check for comparing floats

- Take two real numbers `a` and `b`
- We take `a==b` if `abs(a-b) < epsilon`

- Have to be very careful with this!!! We should think about:
  - The choice of `epsilon` based on the precision we require/expect for `a` and `b`
  - The choice of `epsilon` based on the magnitude of `a` and `b`
  - What will happen in special cases (`0, NaN, inf`)
  - …

Today’s lecture:

- Roundoff and truncation errors

- Good programming practices:
  - Version control

  - Testing

  - Misc. good practices

OTB: Round-off error example

- Imagine that we can only keep track of 4 significant digits
- Compute $\sqrt{x+1} - \sqrt{x}$
- Take *x* = 1984. Keeping only 4 digits each step of the way:

$$\sqrt{x+1} - \sqrt{x} = 44.55 - 44.54 = 0.01$$

- We've lost a lot of precision
- Instead, consider:

$$\sqrt{x+1} - \sqrt{x} = (\sqrt{x+1} - \sqrt{x}) \left(\frac{\sqrt{x+1} + \sqrt{x}}{\sqrt{x+1} + \sqrt{x}} \right) = \frac{1}{\sqrt{x+1} + \sqrt{x}}$$

- Then

$$\sqrt{1985} - \sqrt{1984} = \frac{1}{\sqrt{1985} + \sqrt{1984}} = \frac{1}{44.55 + 44.54} = 0.01122$$

Roundoff error: Another example

- Consider computing exp(-24) via a truncated Taylor series:

$$e^x \simeq S(x) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + ... + \frac{x^n}{n!}$$

- Error in the approximation (**i.e., truncation error**) is less than:

$$\frac{|x|^{n+1}}{(n+1)!} \max\{1, e^x\}$$

- But if we compute S(-24) by adding terms until they are less than machine precision (8 byte):
  - S(-24)=3.7814382919759864E-007
  - Exp(-24)=3.7751345442790977E-011
  - Error is larger than the result (much larger than truncation error)!!
  - Looking at terms, we see we are relying on cancellations of terms

How can we make is more accurate? Choose a different algorithm

- Realize that:

$$e^{-24} = (e^{-1})^{24} \Rightarrow S(-24) = S(-1)^{24}$$

- $S(-1)^{24}$ = 3.7751345442791294E-011
- exp(-24) = 3.7751345442790977E-011

Truncation errors are different from roundoff

- Translating continuous mathematical expressions into discrete forms introduces truncation error
- For example: $e^x \simeq S(x) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + ... + \frac{x^n}{n!}$
- Error: $\frac{|x|^{n+1}}{(n+1)!} \max\{1, e^x\}$
- Or $f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$ vs. $D_h(x) = \frac{f(x+h) - f(x)}{h}$

Floating point arithmetic not associative

- Adding lots of numbers together can compound round-off error
- One solution: sort and add starting with the smallest numbers
- Kahan summation (see reading list)
  - Algorithm for adding sequence of numbers while minimizing roundoff accumulation
  - Keeps a separate variable that accumulates small errors
  - Requires that the compiler obey parenthesis

Floating point arithmetic not associative:

$$(1.0 - 1.0) + 10^{-9} \stackrel{?}{=} 1.0 + (-1.0 + 10^{-9})$$

```
! Purpose:  Test the precision of reals
! Author:    Cyrus Dreyer
! Date:        2/4/2019
program test_prec_reals
  implicit none         ! Turn off implicit typing
  ! Variable dictionary
  real :: factor1     ! Variable for factor 1
  real :: factor2     ! Variable for factor 2
  real :: prec_test_lhs ! Variable for result
  real :: prec_test_rhs ! Variable for result

  factor1 = 1.0           ! Assign a value to factor1
  factor2 = 1.0d-9        ! Assign a value to factor2

  prec_test_lhs = (factor1-factor1) + factor2 ! LHS of inequality on slide
  prec_test_rhs = factor1 + (-factor1 + factor2) ! RHS of inequality on slide

  ! Output
  write(*,'(a20,e20.12e2,a20,e20.12e2)') "Prec_test_lhs:",prec_test_lhs, &
       "Prec_test_rhs:", prec_test_rhs

  stop 0                ! Stop execution of the program
end program test_prec_reals
```

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- Good programming practices:
  - Version control
  - Testing
  - Misc. good practices

Software engineering practices

- Some basic practices that can *greatly* enhance your ability to write maintainable code
  - Version control
  - Build environments
  - Testing procedures
  - Automatic code error checking
  - Profiling
  - Documentation
- There are many tools that will help you write safe code and find bugs as they are introduced. These let you focus more on the science.
- Main goal of this lecture is to just show you what kind of tools are out there and how they can help your workflow

Coding experiences to try and avoid

- *You swear that the code worked perfectly 6 months ago*, but today it doesn't, and you can't figure out what changed
- *Your research group is all working on the same code*, and you need to sync up with everyone's changes, and make sure no one breaks the code
- *Your code always worked fine on machine X*, but now you switch to a new system/architecture, and you code gives errors, crashes, ...
- *Your code ties together lots of code*: legacy code from your advisor's advisor, new stuff you wrote, all tied together by a driver. The code is giving funny behavior sometime—how do you go about debugging such a beast?

Version control

- What is it?
  - A system that records changes to a file or set of files over time so that you can recall specific versions late
- Why is it important?
  - So that if the code stops working, you can go back to specific previous versions to see what changes broke it
  - Allows you to compare changes over time
  - If multiple people are working on a file, see who last modified something that might be causing a problem, who introduced an issue and when, etc.

Types of version control: Local

- Previous versions (or patch sets) stored elsewhere on local machine

- Can be as simple as copying files into a different folder to store them before making changes
  - Will take up a lot of memory if not done in a smart way

- There are some tools to make this more consistent such as GNU RCS

- Pros: Simplicity
- Cons: Single point of failure

Types of version control: Centralized

- Have a single server that contains all the versioned files, stores history and changes

- User communicates with the server to:
  - Checkout source
  - Commit changes back to the source
  - Request a log (history) of a file from the server
  - Diff your local version with the version on the server

- Has advantages over local version control:
  - Everyone knows what everyone else is doing on a project
  - Administrators have control over who can do what

- Cons: Does not scale well for large projects, single point of failure

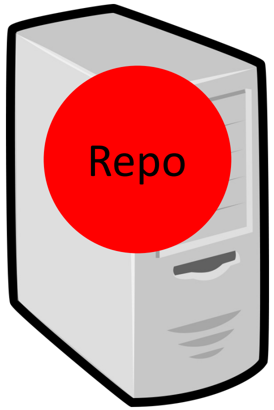
Types of version control: Distributed

- Clients fully mirror (i.e., clone) the repository and its history on their local machine
  - Not just the latest snapshot of the files
  - No single point of failure: if any server dies, any client repository can be copied back to restore it

- Deals well with multiple different groups simultaneously working on a project
  - Easy to “fork”

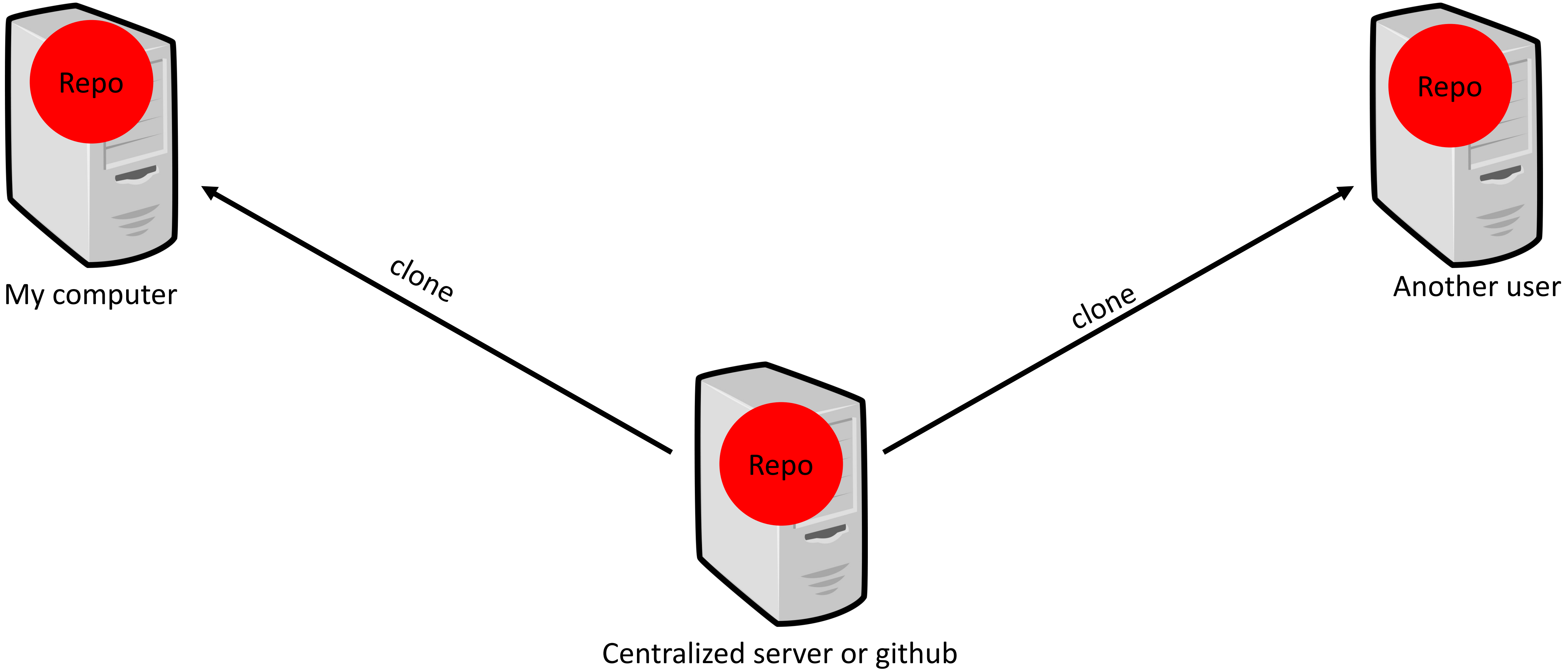
- Common DVCS: **Git**, Mercurial, Bazaar

Distributed version control

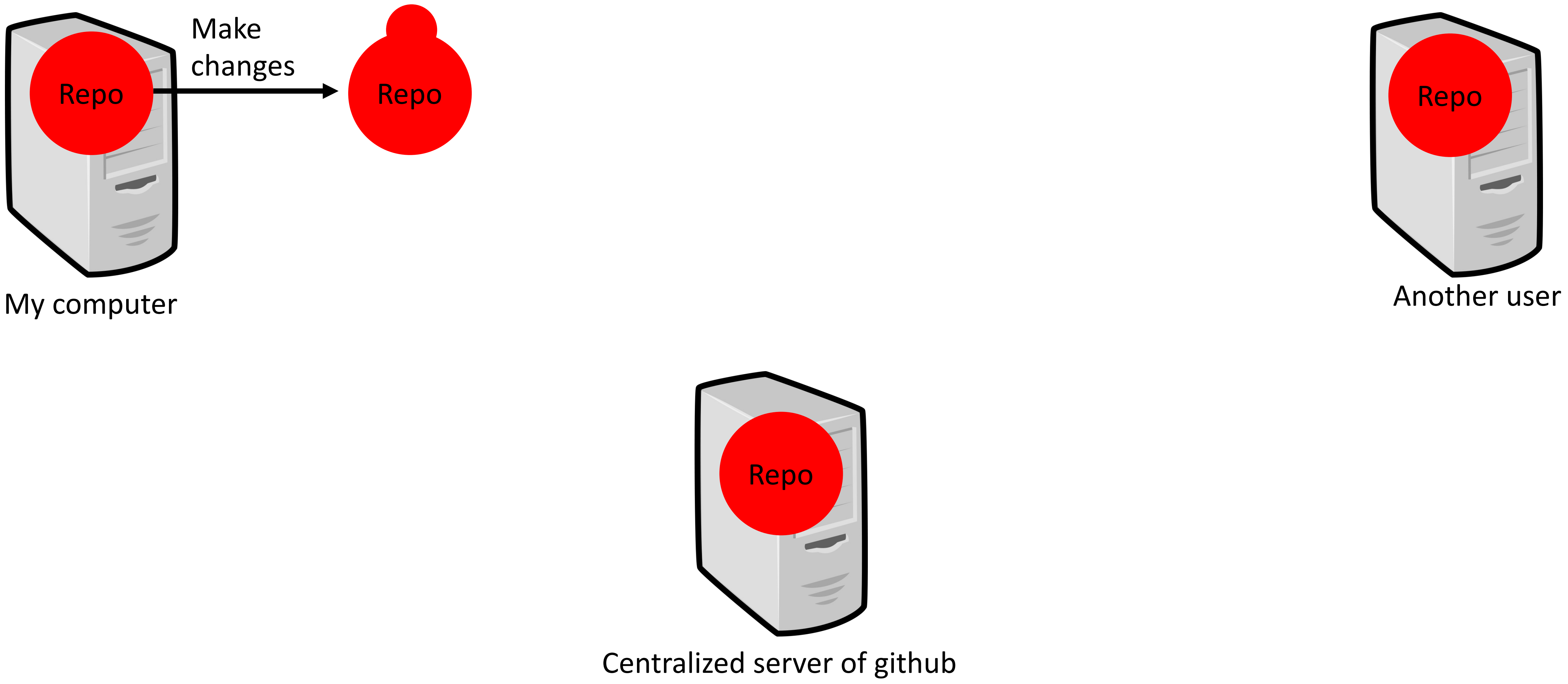


Centralized server or github

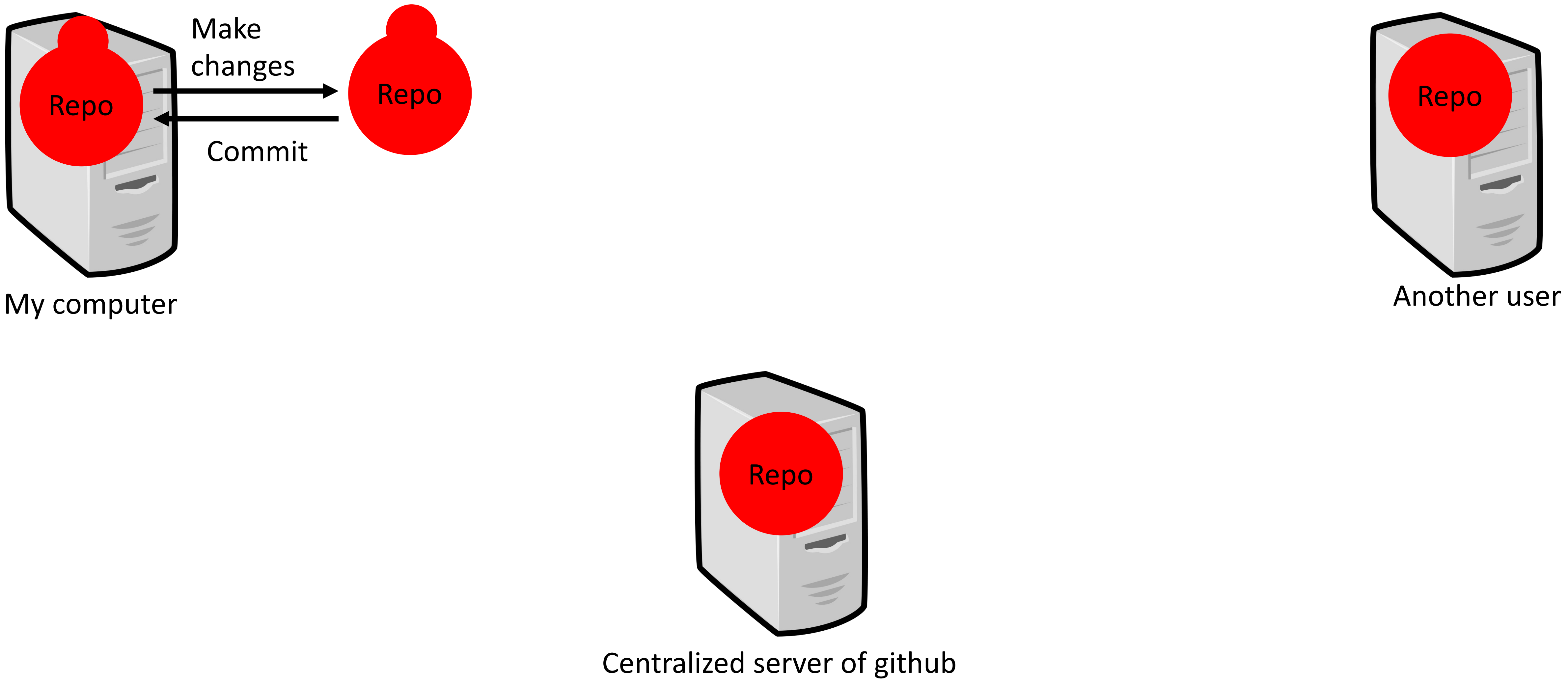
Distributed version control



Distributed version control



Distributed version control



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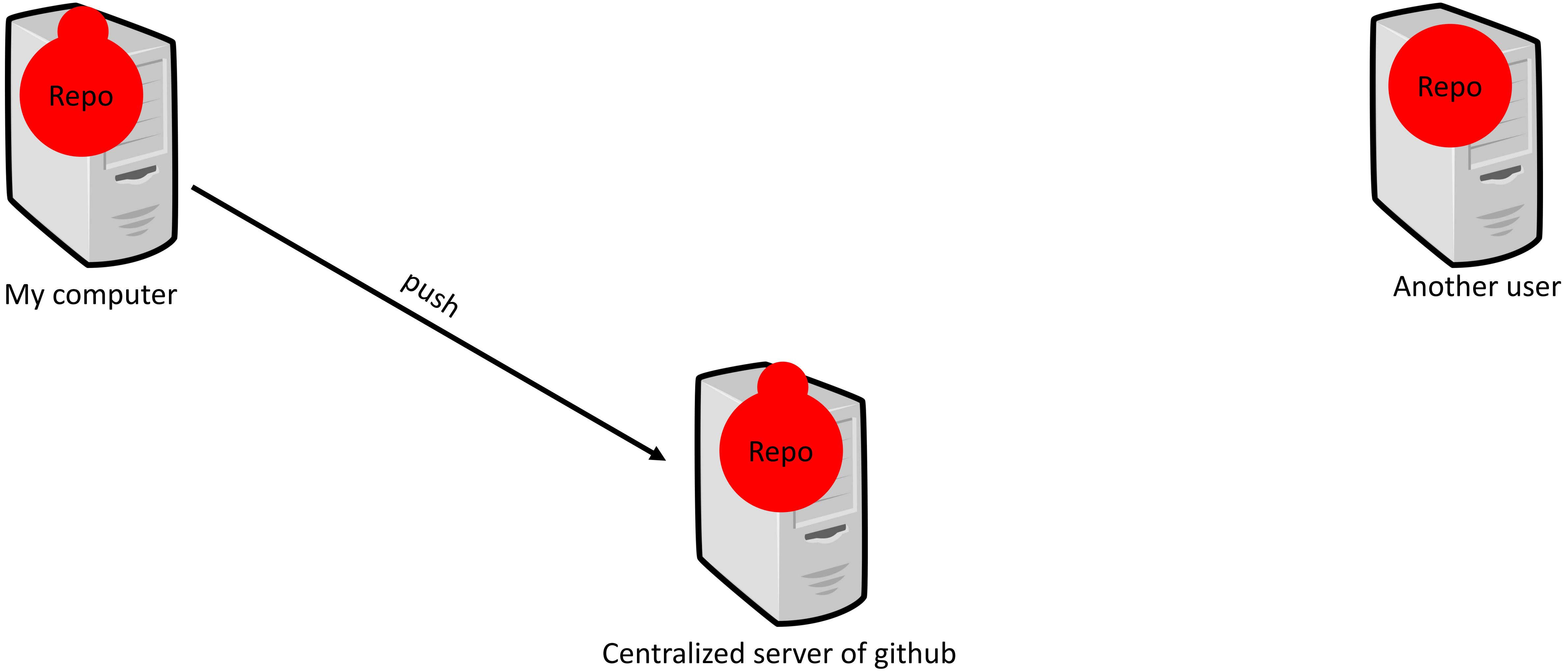

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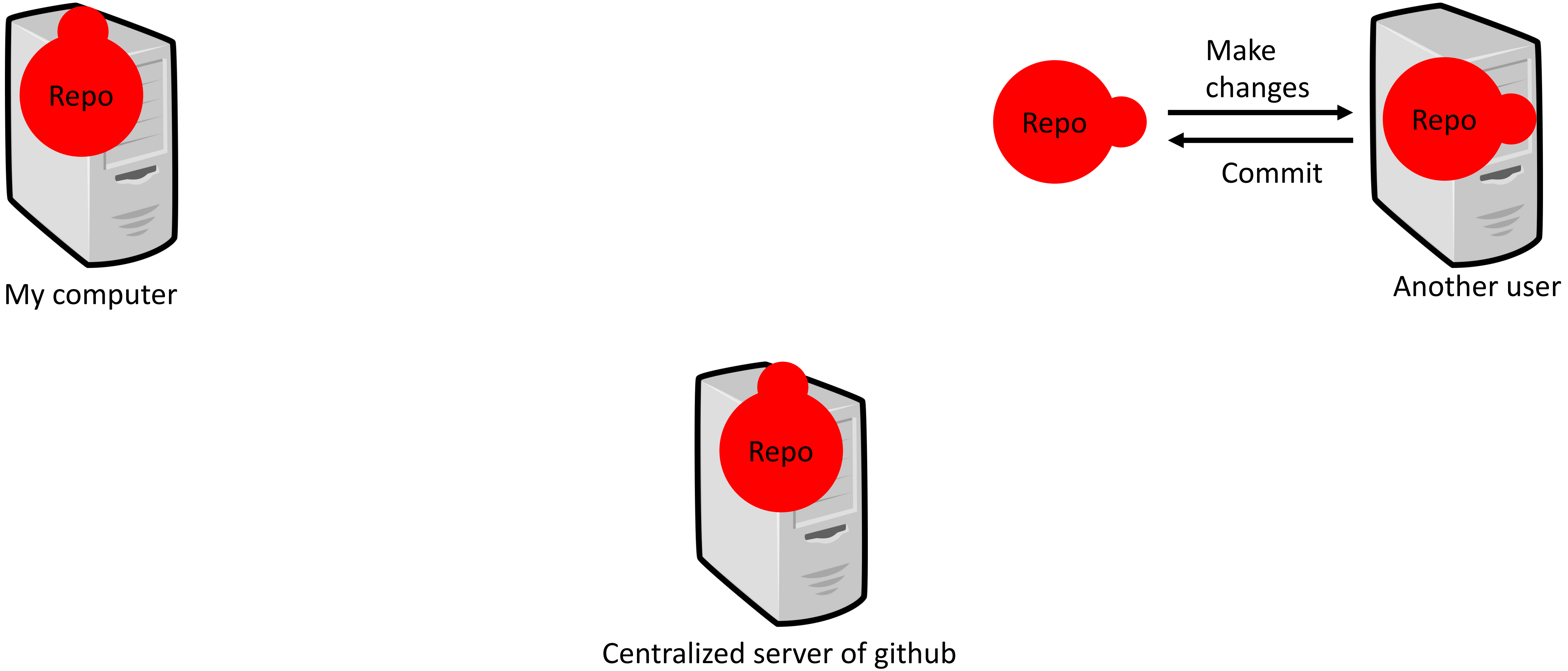

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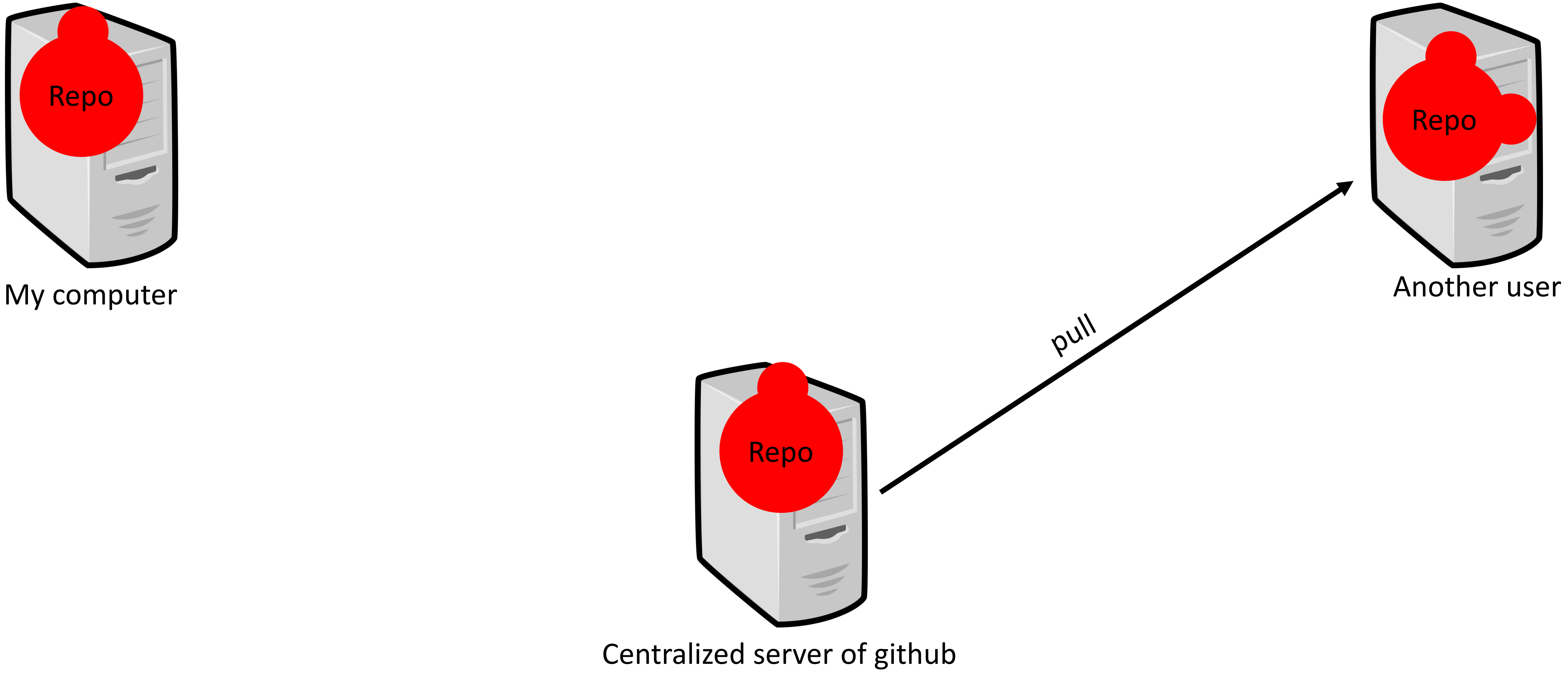

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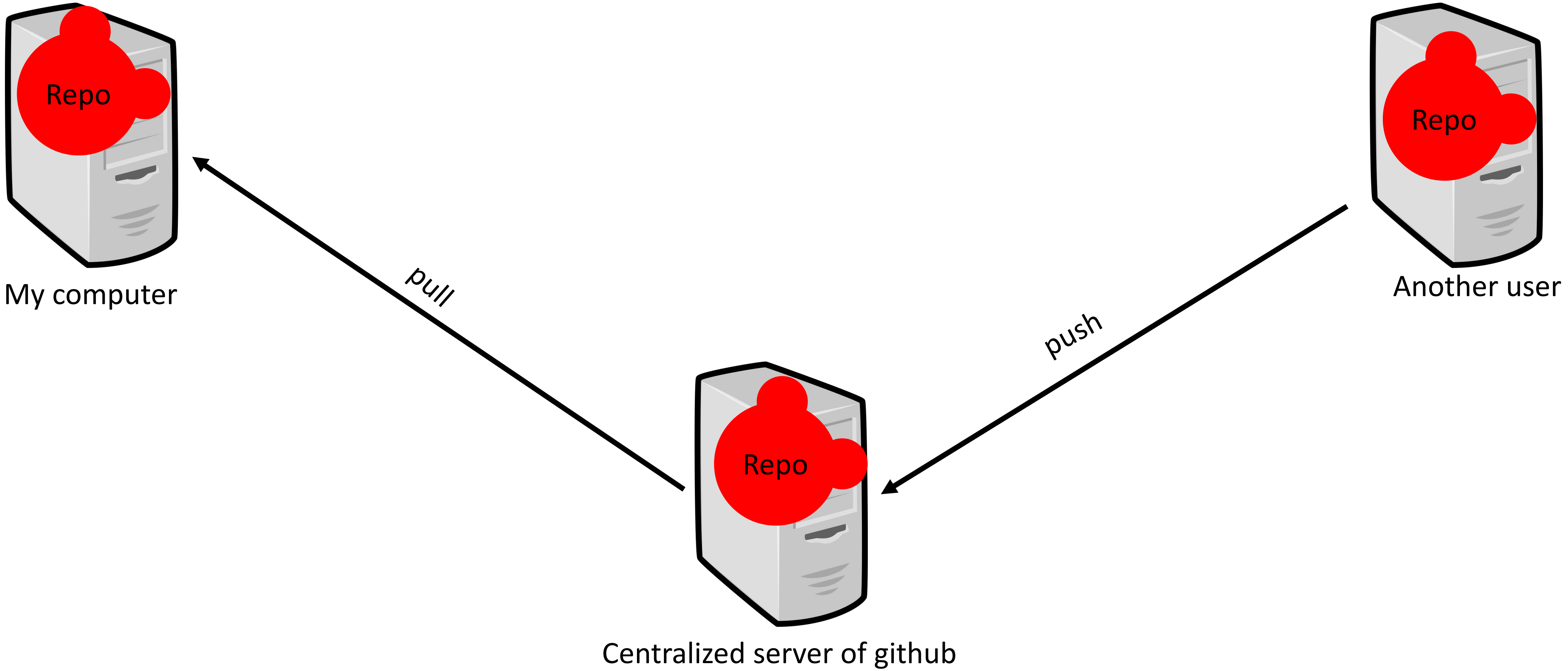

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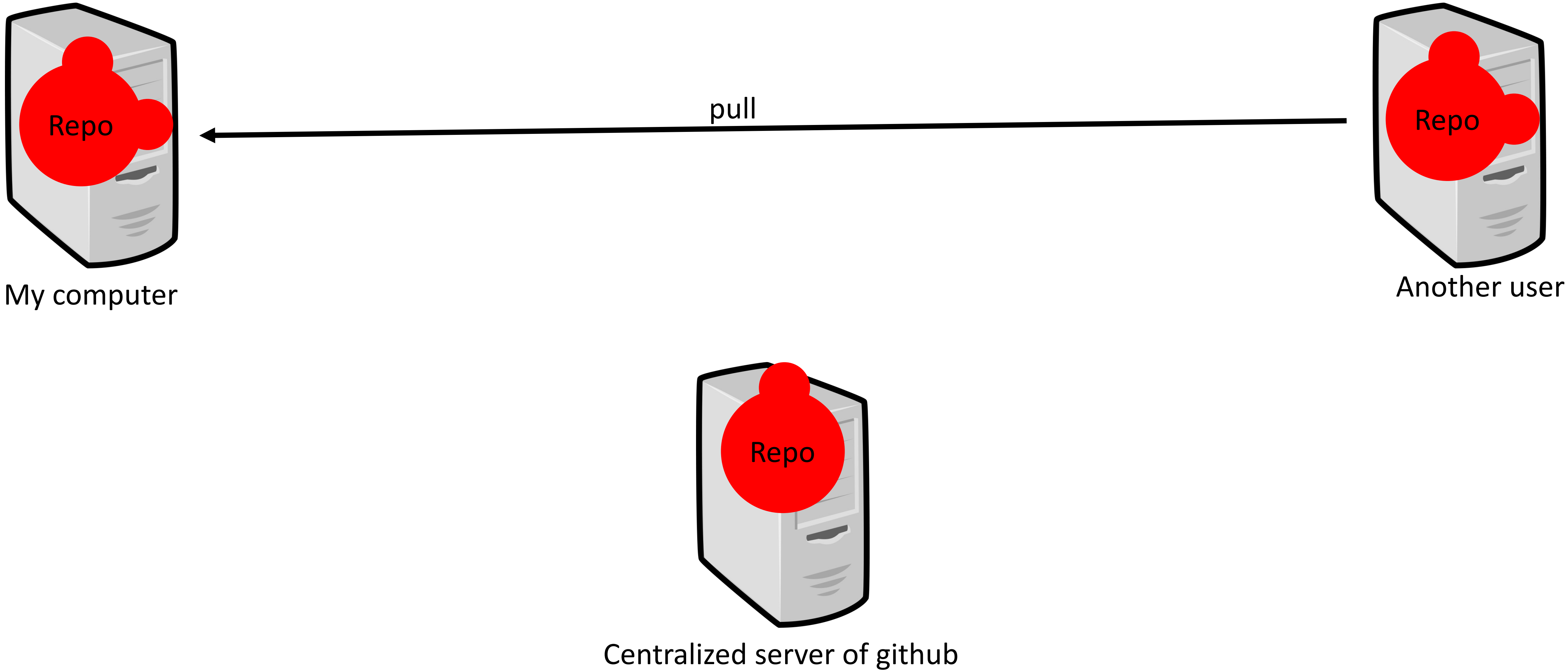

Comments about Git

- Note that with git, every change generates a new “hash” that identifies the entire collection of source.
  - You cannot update just a single sub-directory—it's all or nothing.
- Branches in a repo allow you to work on changes in a separate are from the main source.
  - You can perfect them, then merge back to the main branch, and then push back to the remote.
  - Overall, very light weight!!
- LOTS of resources on the web (see readings)
  - Best way to learn is to practice.
  - There is more than one way to do most things

Example: “Local” version control with Git

- You can use Git to do local version control on your computer:

- **`git init`** to create a new git repository
- **`git add`** to add file contents to the index
- **`git commit`** to record changes to the repository
- **`git log`** to show previous commits
- …

Branching with git

- One of the killer apps of git is lightweight "branching"
  - Creates a different line of development which can be merged back into the main one
  - Does not require making multiple copies of source code, etc.

- Allows you to work in different directions and later merge together as you wish

- Git will help if there are conflicting changes

After class tasks

- No office hours today
- If you do not already have one, make an account on github: https://github.com/
- Readings:
  - What every computer scientist should know about floating-point arithmetic
  - Wikipedia page on the Floating Point
  - Wikipedia page on the Kahan Summation Algorithm

  - Pro Git online book