Software management and HPC computing

marco milanesio, paola goatin, regis duvigneau

11-12 / 3 / 2024

part II: Collaborating

UNIVERSITÉ CÔTE D'AZUR

UNIVERSITÉ CÔTE D'AZUR
MAISON DE LA MODÉLISATION, DE LA SIMULATION ET DES INTERACTIONS

Inria

Agenda

- 11 - 3 - 2024
  - Scientific software
  - Design and development
  - Data structures
  - **Collaborating**
  - Open science

- 12 - 3 - 2024
  - Parallelisation and HPC
  - Documentation

Versioning

Version control

Version control is a system that records changes to a file or set of files over time so that you can recall specific versions later.

- Local (you should do it (and call it backup))
- Central (you don't have to)
- Fully distributed (you should really do it)

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- TFS (central)
- Mercurial (distributed)
- Git (distributed)

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Git

- Speed
- Simple design
- Strong support for non-linear development (thousands of parallel branches)
- Fully distributed
- Able to handle large projects like the Linux kernel efficiently (speed and data size)

- GitLab: repository management software
- GitHub: platform to upload copies of the repositories

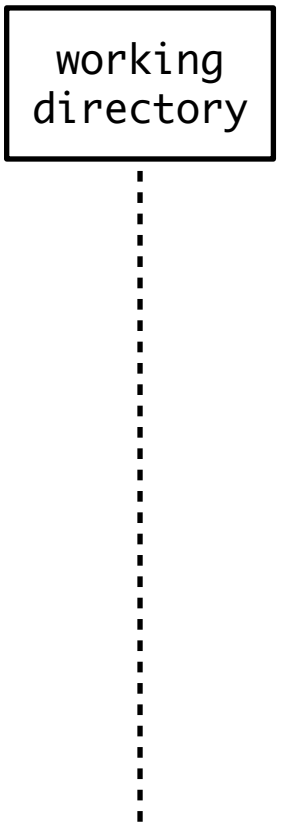
Git

- Use it every time there's development
- Just type: `git init`
- You're versioning, on branch `main` (`master`)
- https://git-scm.com/book/en/v2

Hands on

Workflow

Workflow



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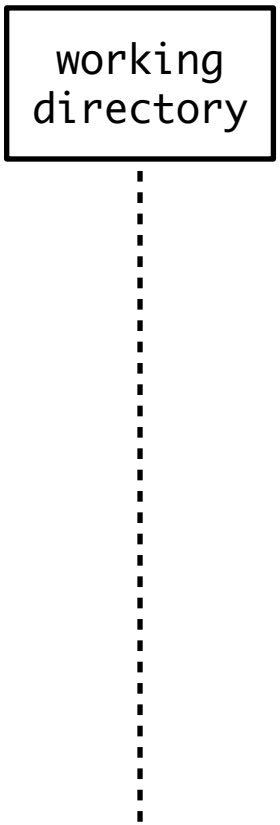

file.txt

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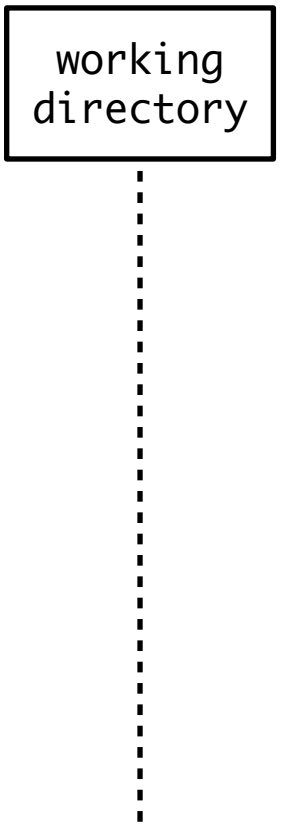

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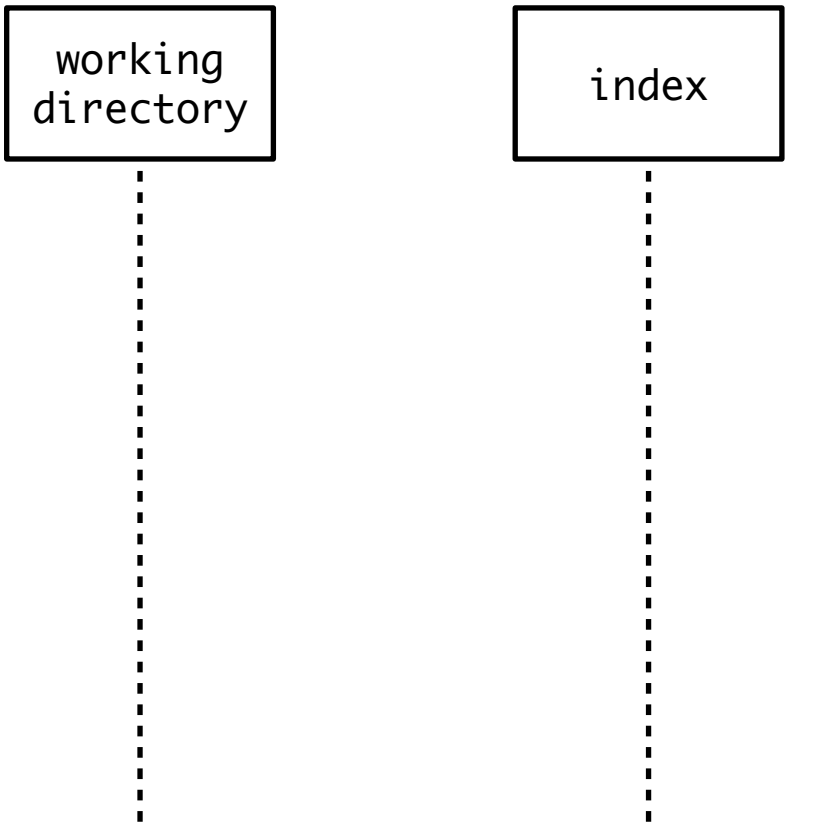
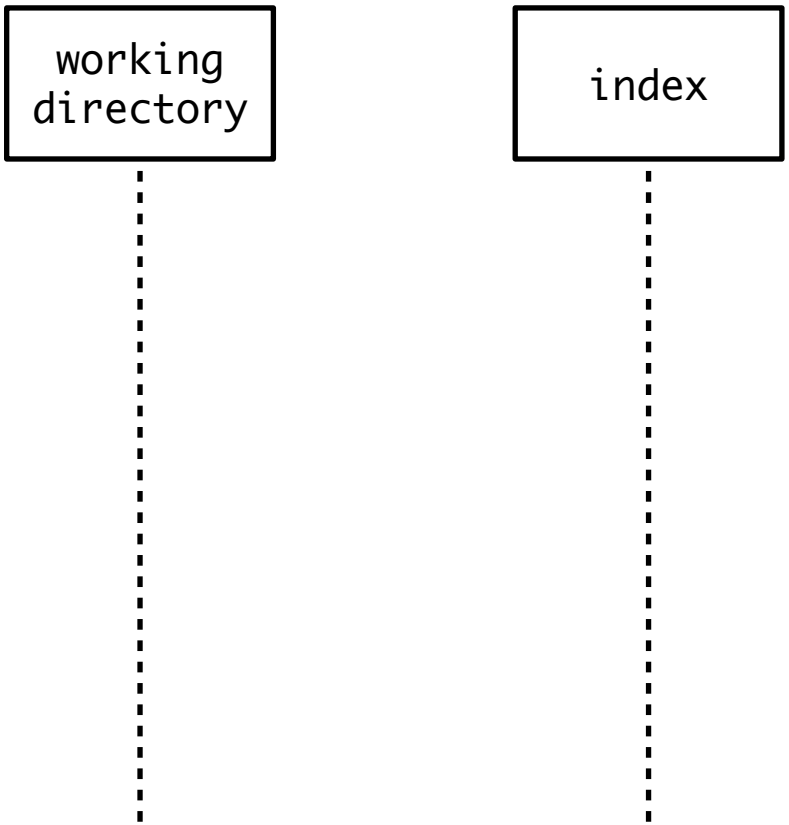


`git init`

`file.txt`

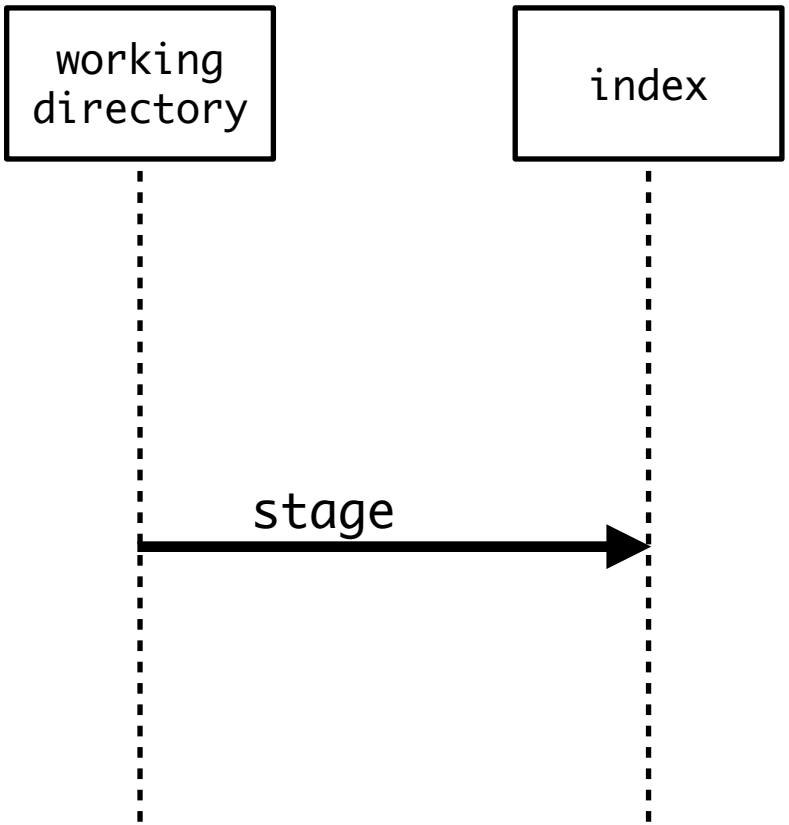
Workflow




```
git init
git add file.txt
```

file.txt

Workflow

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file.txt file.txt

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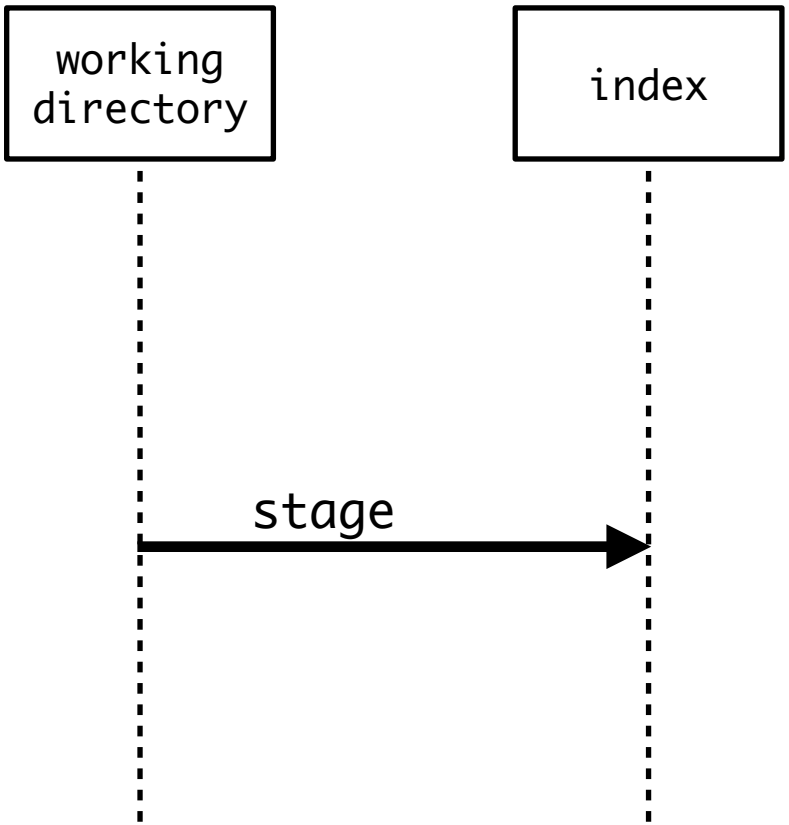


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git init
git add file.txt
git commit -m "1st"
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file.txt file.txt

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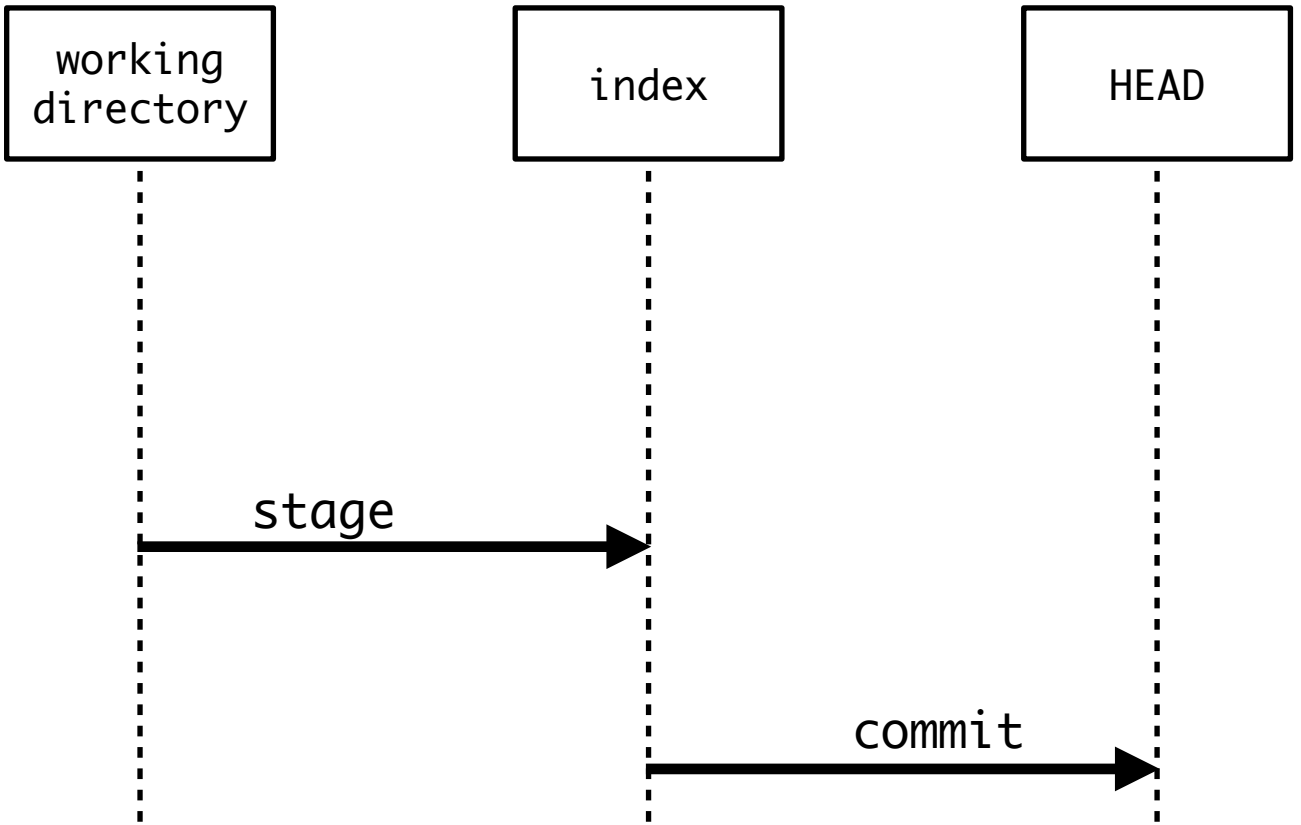


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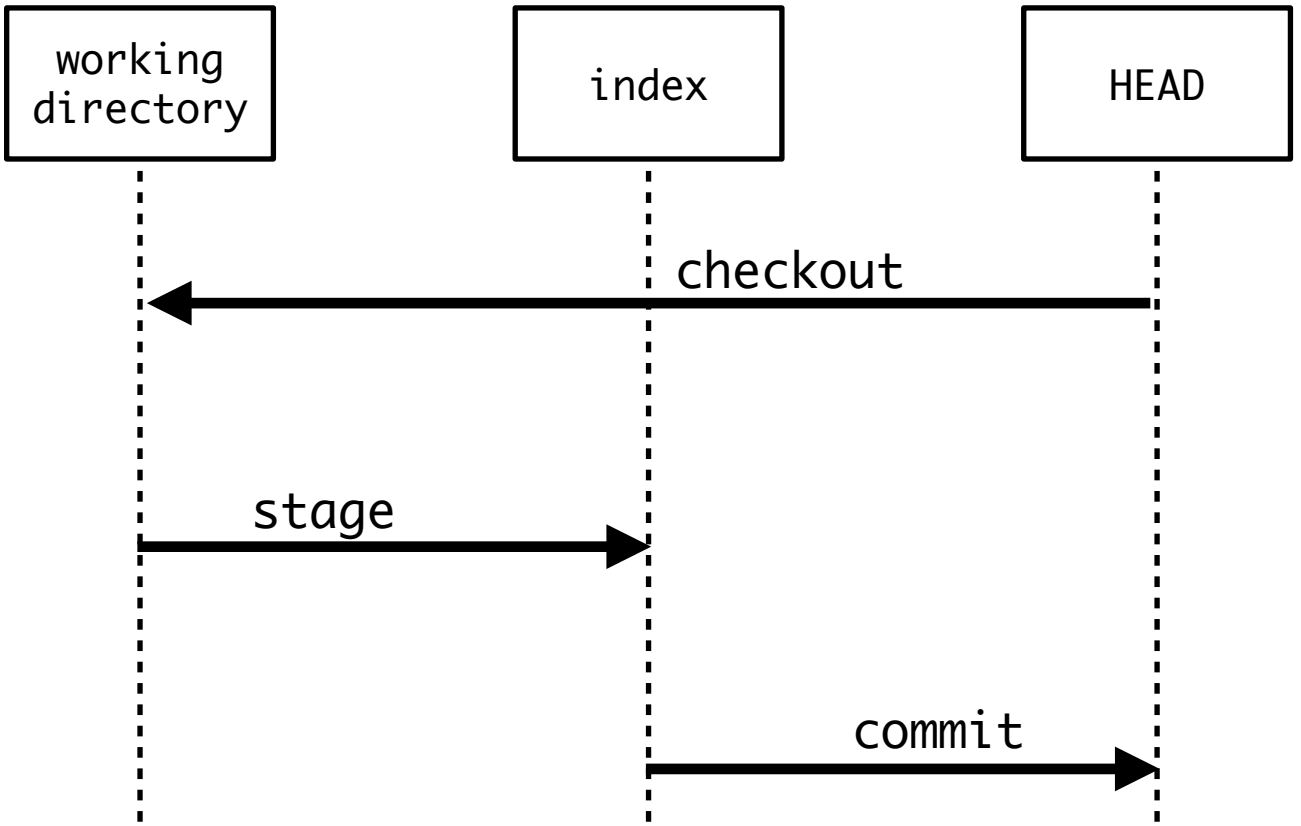


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Branching

- Explore new ideas
- Bug fix
- Add new features

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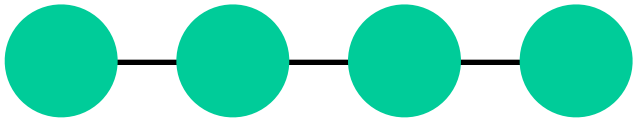

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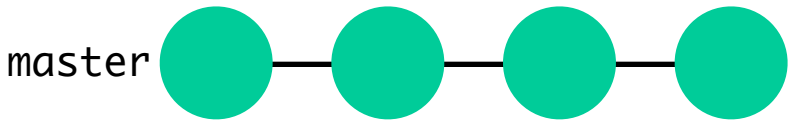

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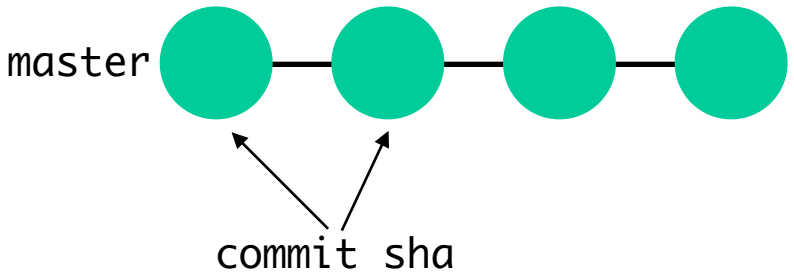

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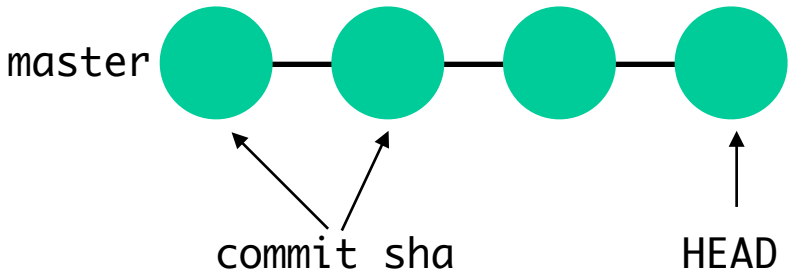

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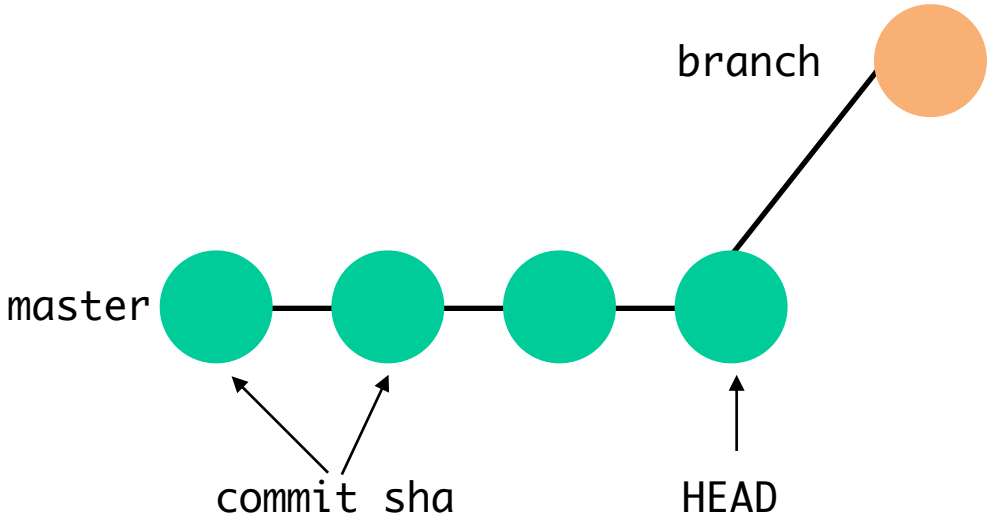

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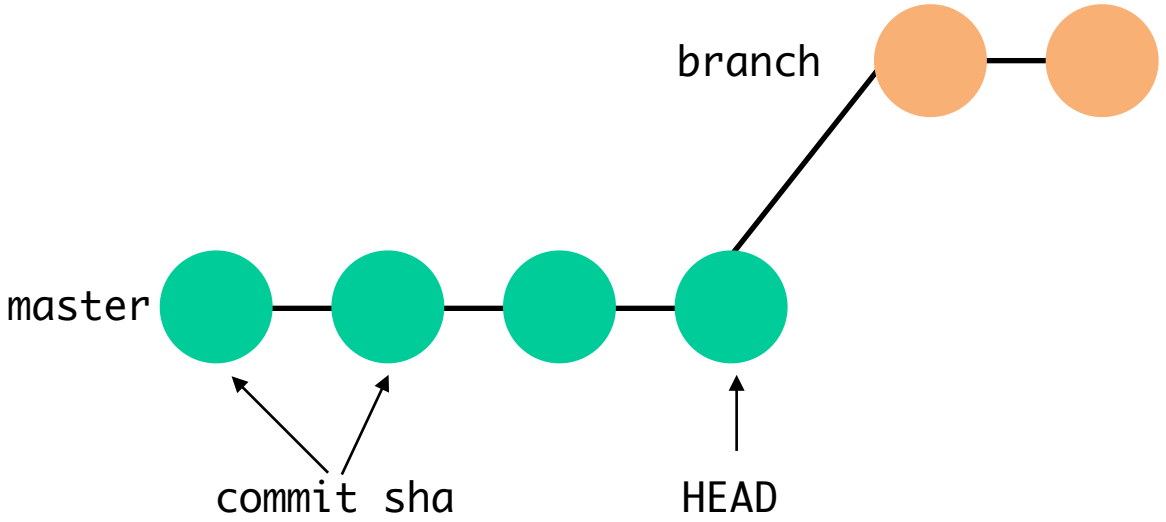

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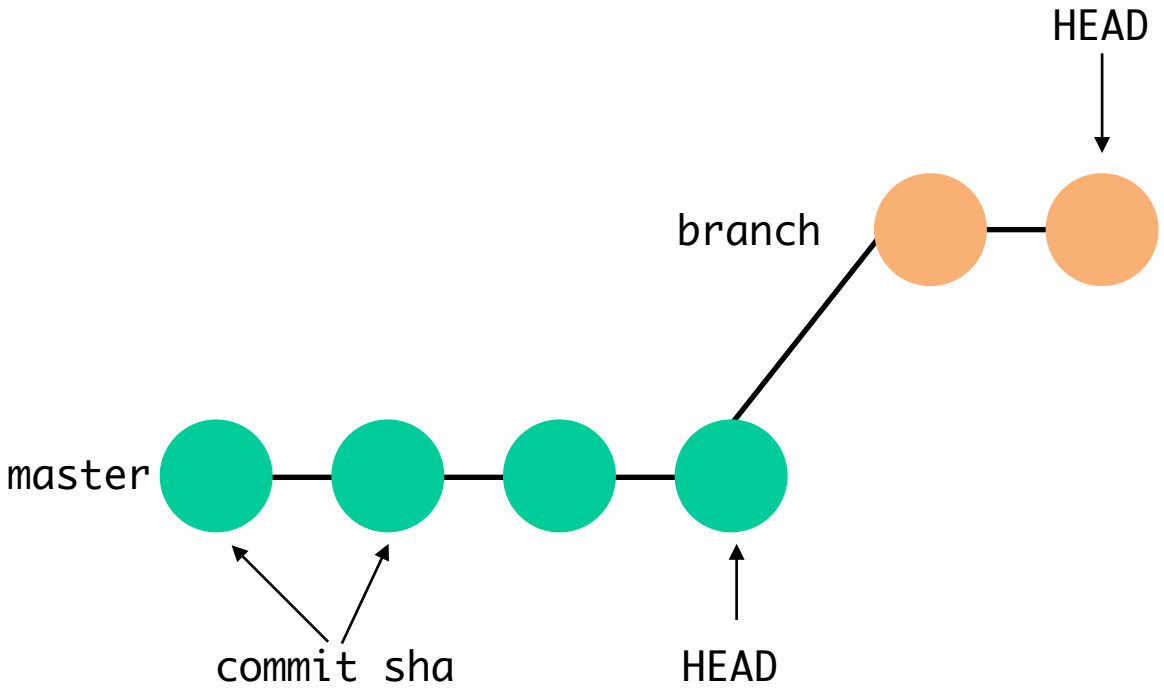

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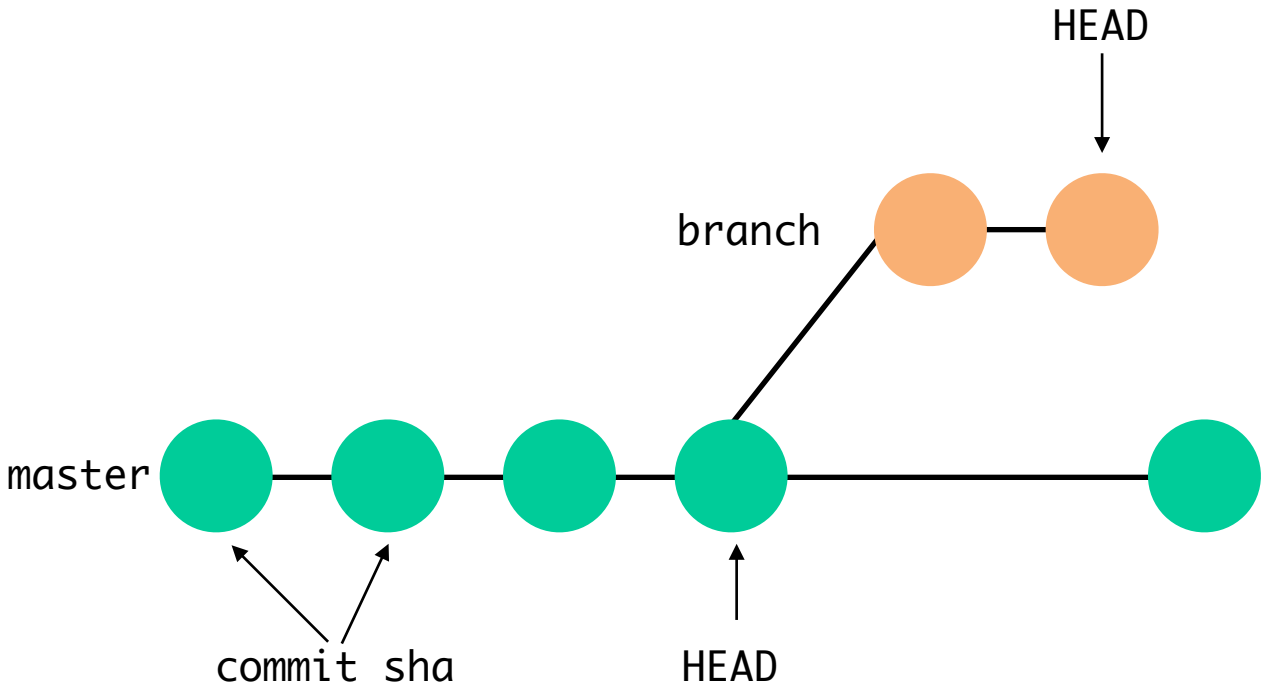

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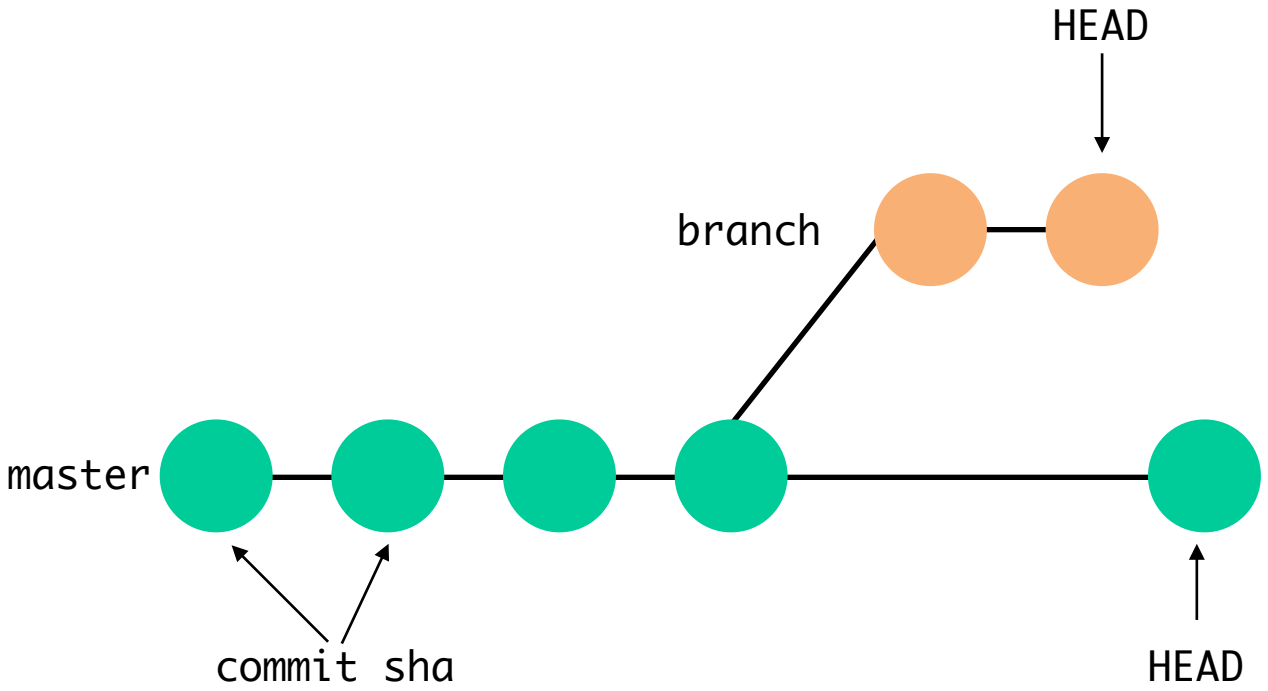

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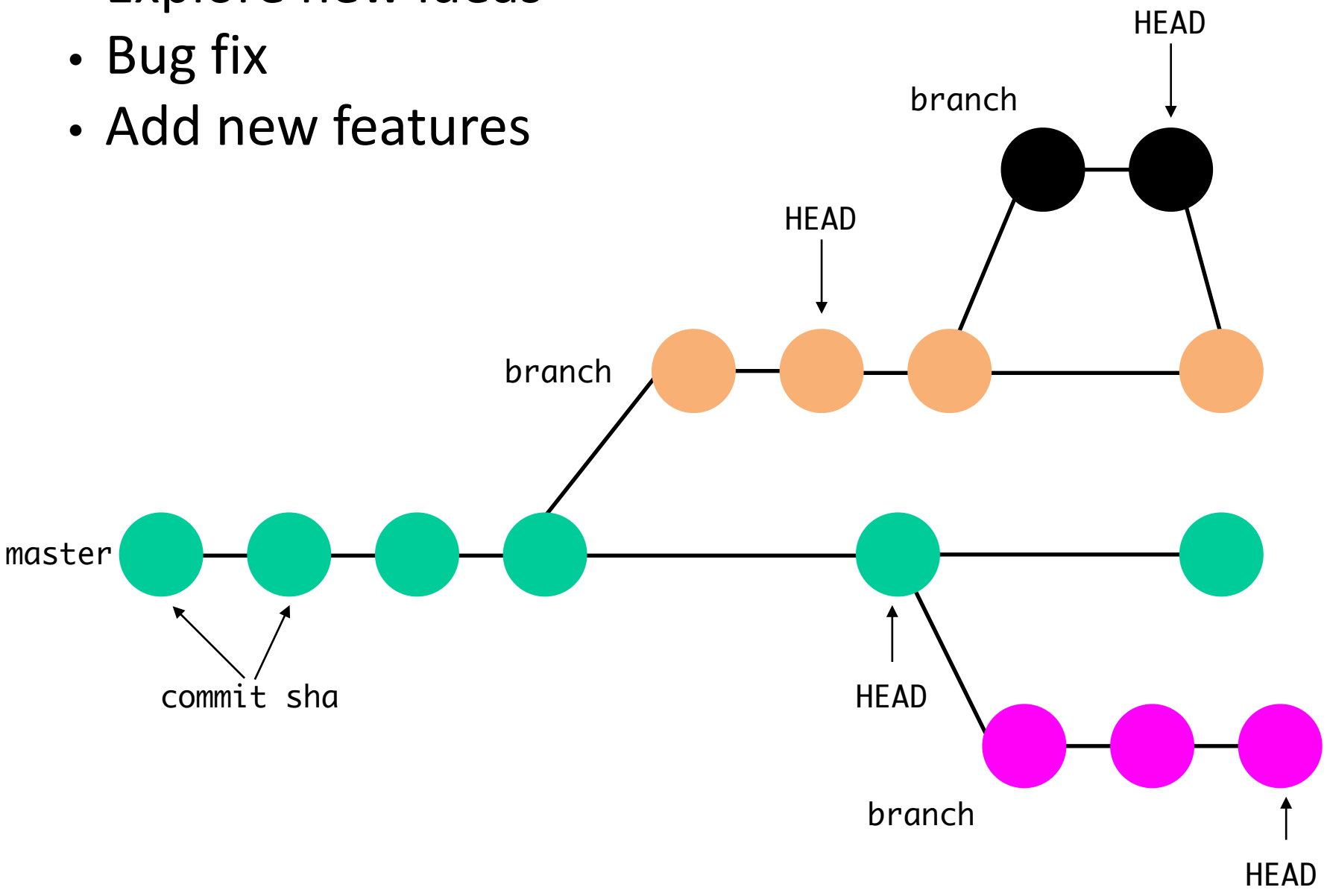

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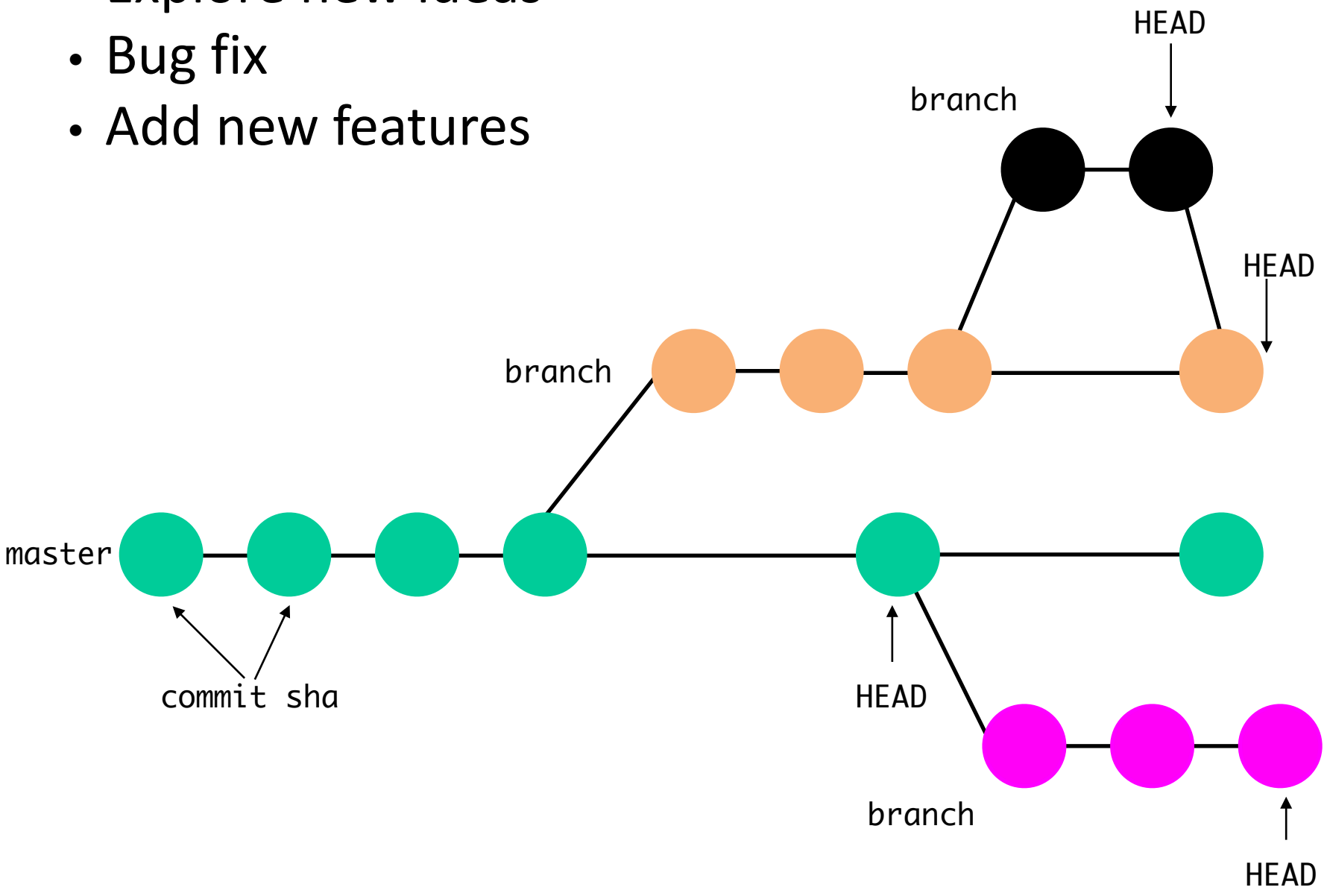

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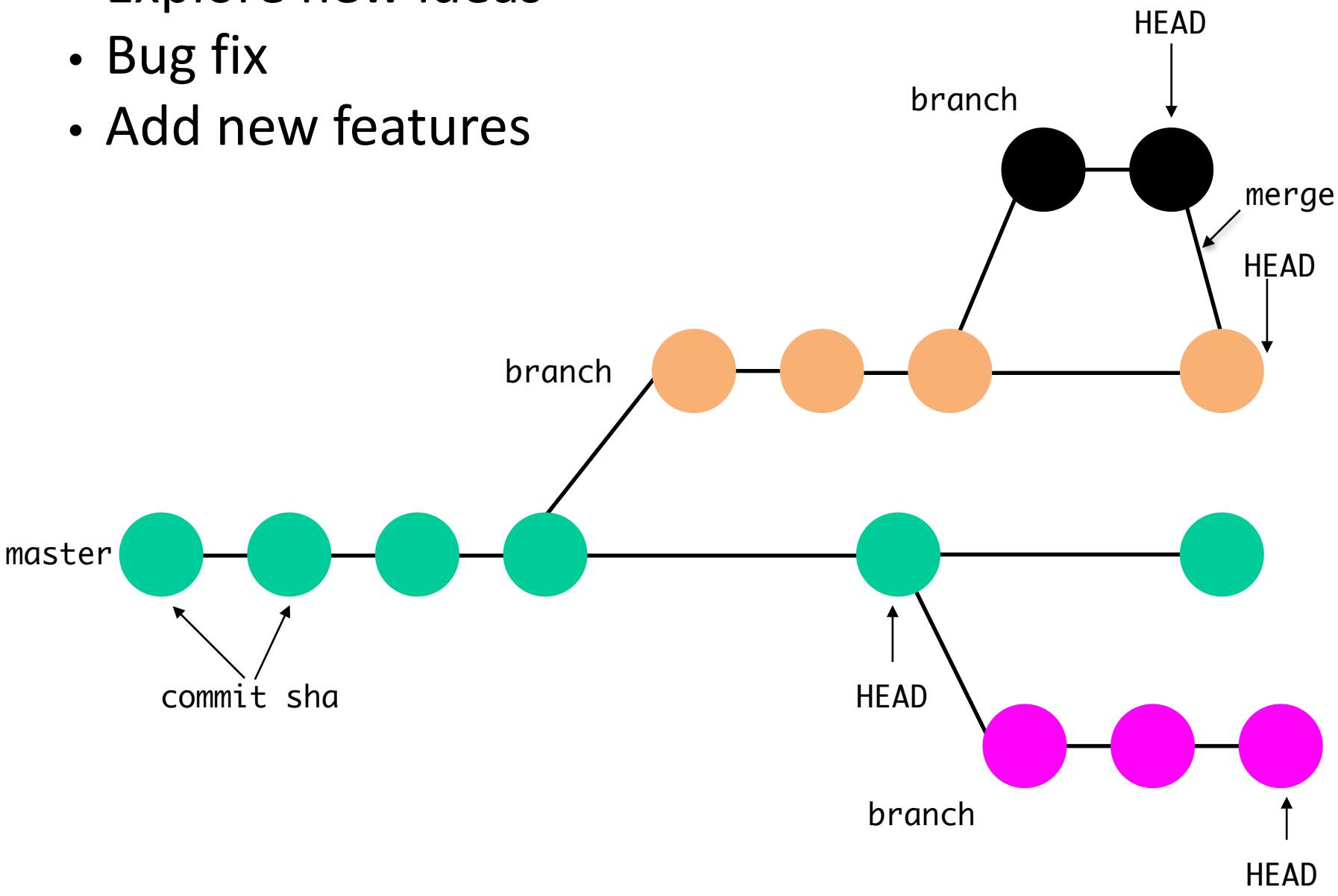
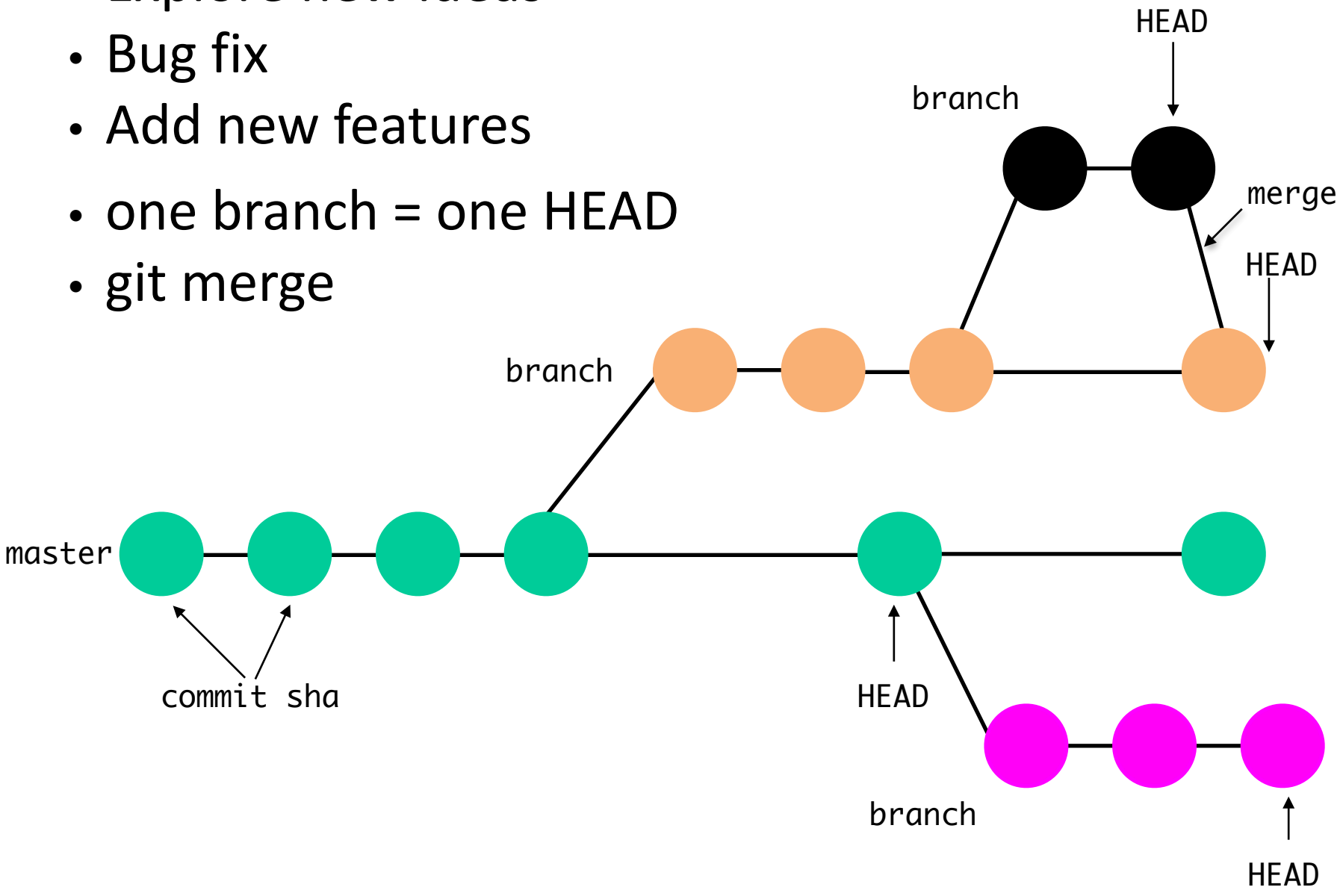


Branching

- Explore new ideas
- Bug fix
- Add new features
- one branch = one HEAD
- git merge

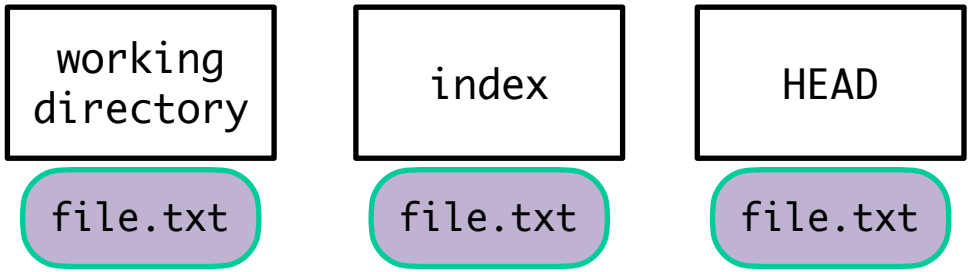


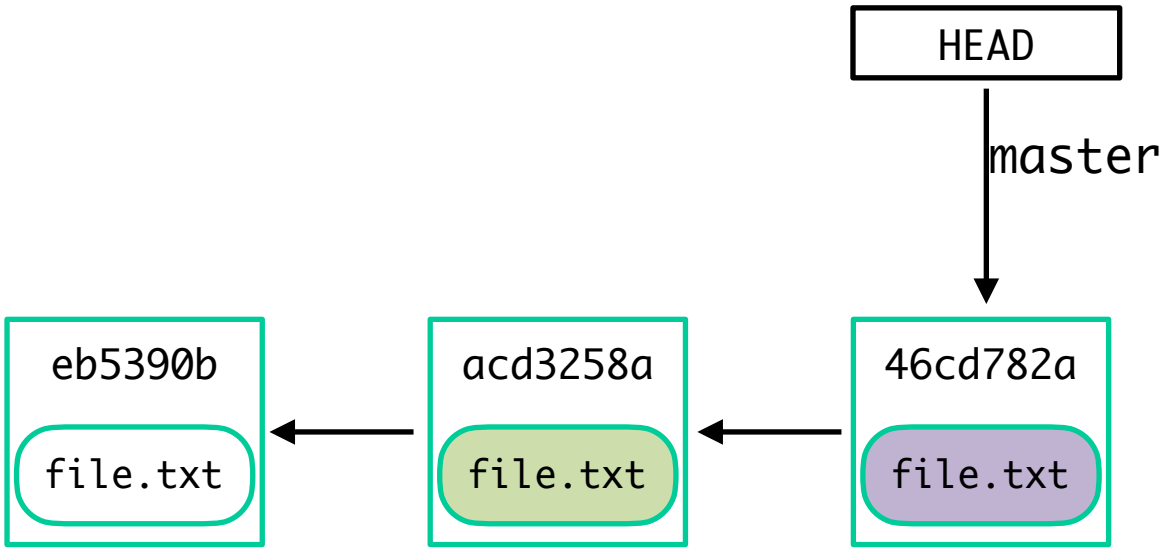
Git merge

- Update another branch
- Easy: if target branch hasn’t "moved"
- Hard: if target branch has "moved"
- merge conflicts

Git reset

- Most feared command
- Really not scary





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```
git reset acd3258a
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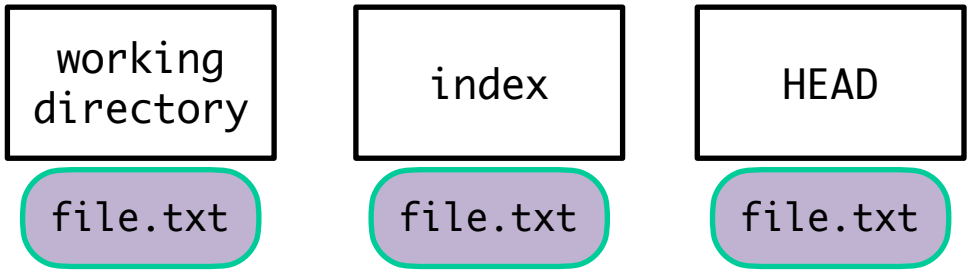

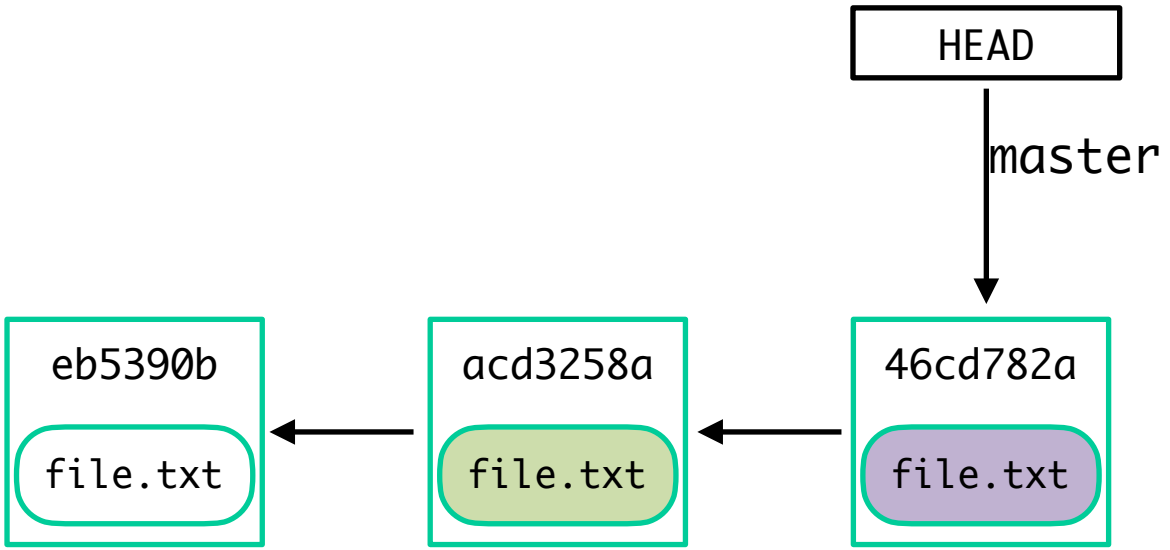

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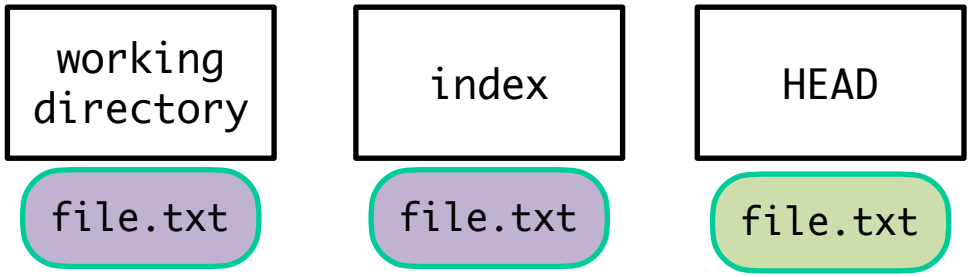

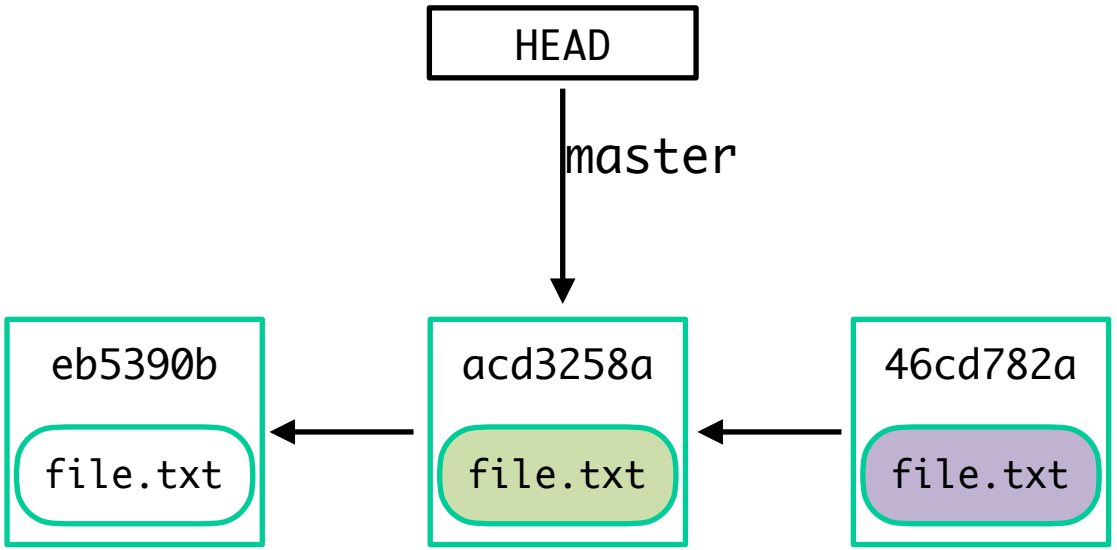

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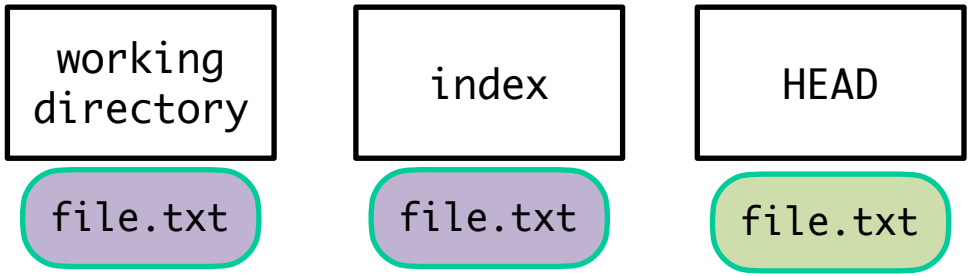
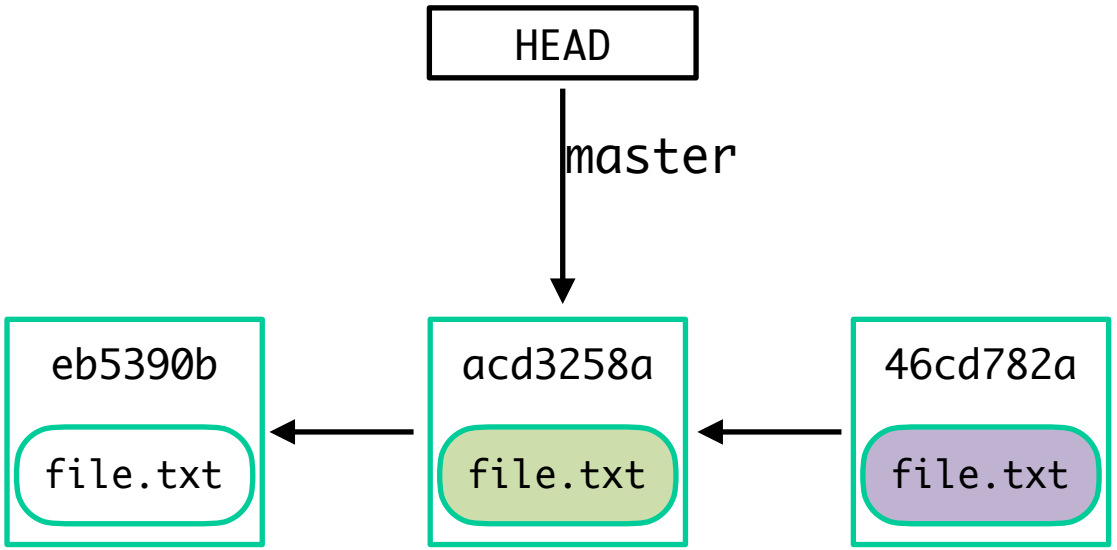
```
git reset --soft HEAD~
```





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git reset [--mixed] HEAD~
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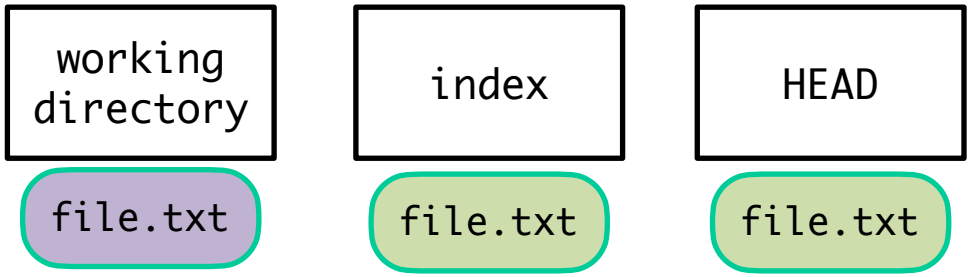

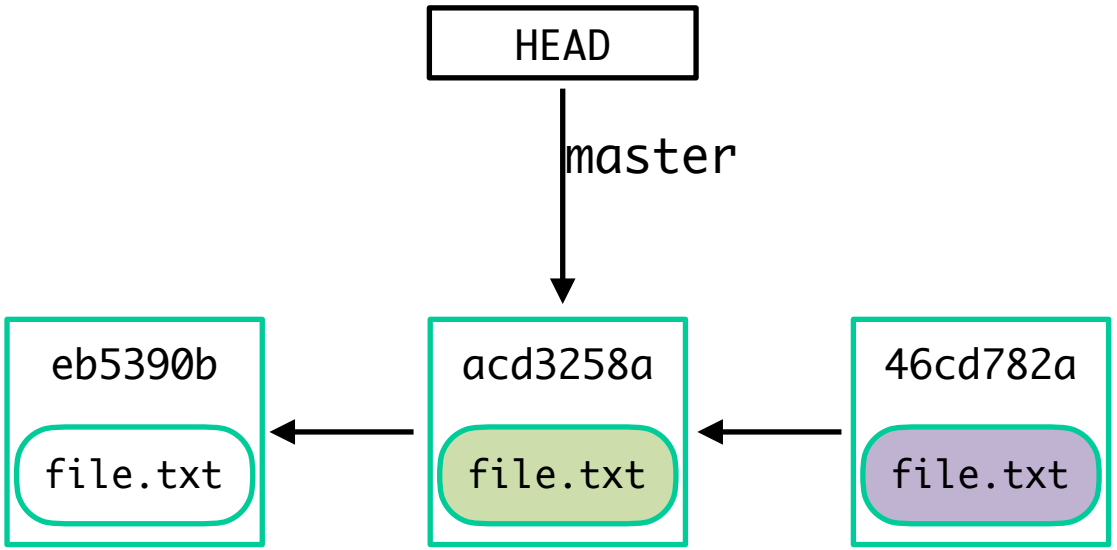

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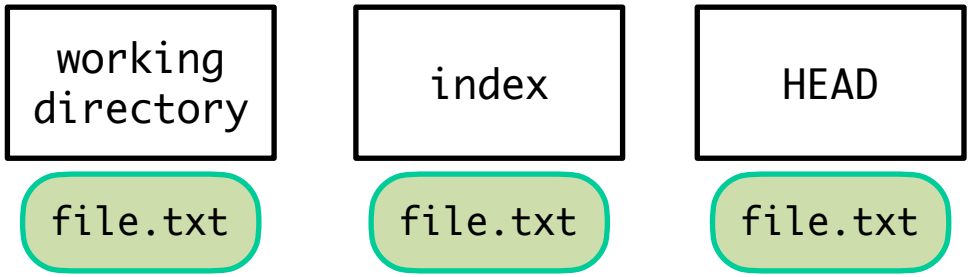

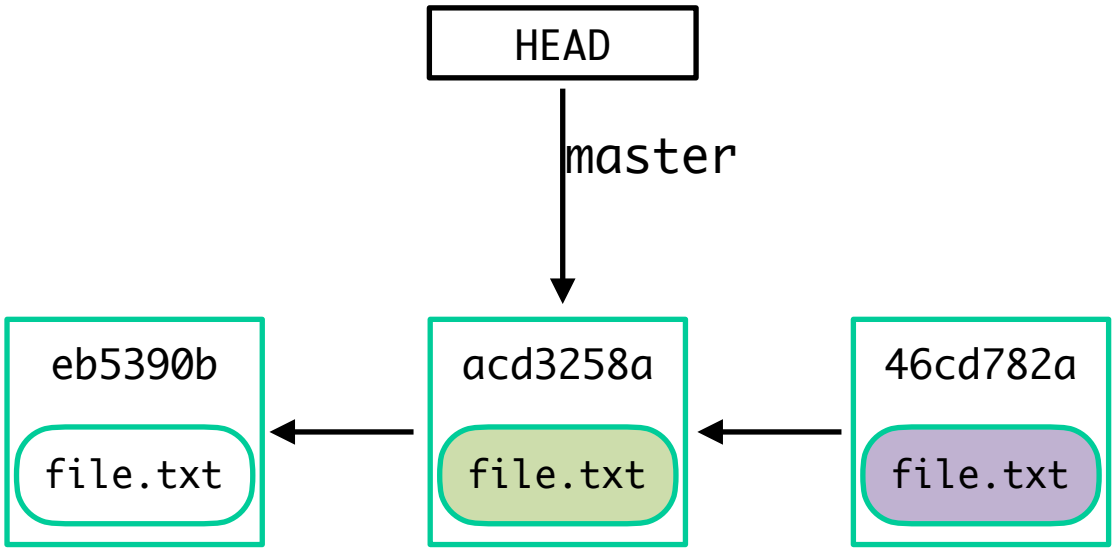

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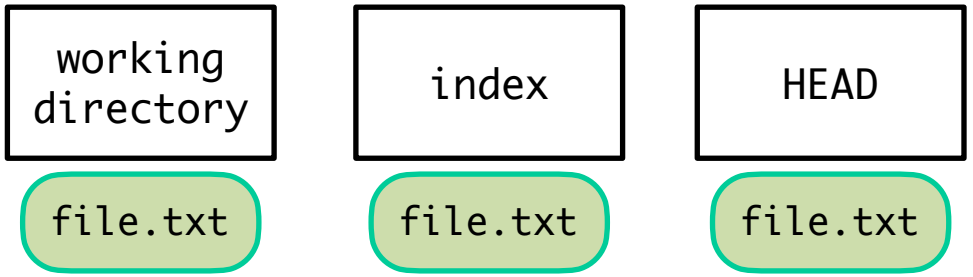

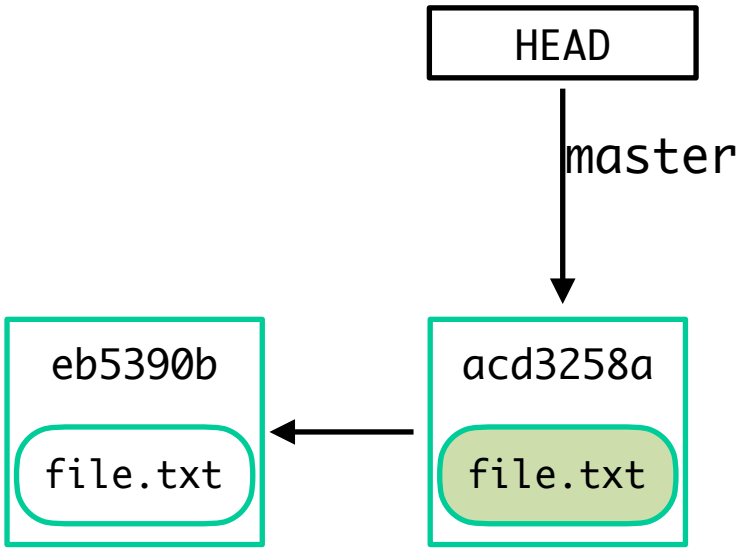

GitHub

- github.com
- "push" HEAD to the cloud
- That’s it.

- No, there’s more
- Team collaboration
- github actions
- CI/CD

Testing

Testing

- The fundamental skill
- Not only for being nice to others
- It’s for you!

- Testing rocks
- Debugging sucks
- There is no compiler to help you out there
- Make sure your code does what you want

Testing

- assertions / contracts
  - to validate program invariants
- unittest Module
  - builtin
  - used in standard library
  - can grow quite dramatically
- pytest an alternative

Test Driven Development

- Write a "single" unit test for a new feature
- Run the test(s): fail
- Write "just enough" code just to make it pass
- Run the test(s): success
- Refactor your code
- Run the test(s): success
- Repeat (new feature, new tests)

Hands on

Unit test vs Integration test

- *Misleading*
- Can be done in the same class (unittest.TestCase)
  - Not a good idea, though
- Different scopes:
  - single module
  - between modules
- White Box vs Black Box

CI / CD

- Continuous Integration / Continuous Delivery
- Github actions
- Integration testing
- Automatic test execution
  - before pull req / merge
  - after each commit / push
  - fully customisable

Agenda

- 11 - 3 - 2024
  - Scientific software
  - Design and development
  - Data structures
  - Collaborating
  - **Open science**

- 12 - 3 - 2024
  - Parallelisation and HPC
  - Documentation

Open Science

Open source

- Community contribution
- Code quality
- Collaboration
- Source code availability
- Licenses

Licences

- Legal instruments governing the distribution
- Two common categories
  - Proprietary software
  - Free and Open Source
- Many types:
  - Public domain
  - FOSS
  - Copyleft
  - Freeware / Shareware
  - Proprietary
  - Secret
- It’s a matter of rights

Rights

- Copyright retainment
- Right to perform
- Right to display
- Right to copy
- Right to modify
- Right to distribute
- Right to sublicense
- Right to sell

Choose a license

- **University policies or requirements**
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GPL v3

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GPL v3

```
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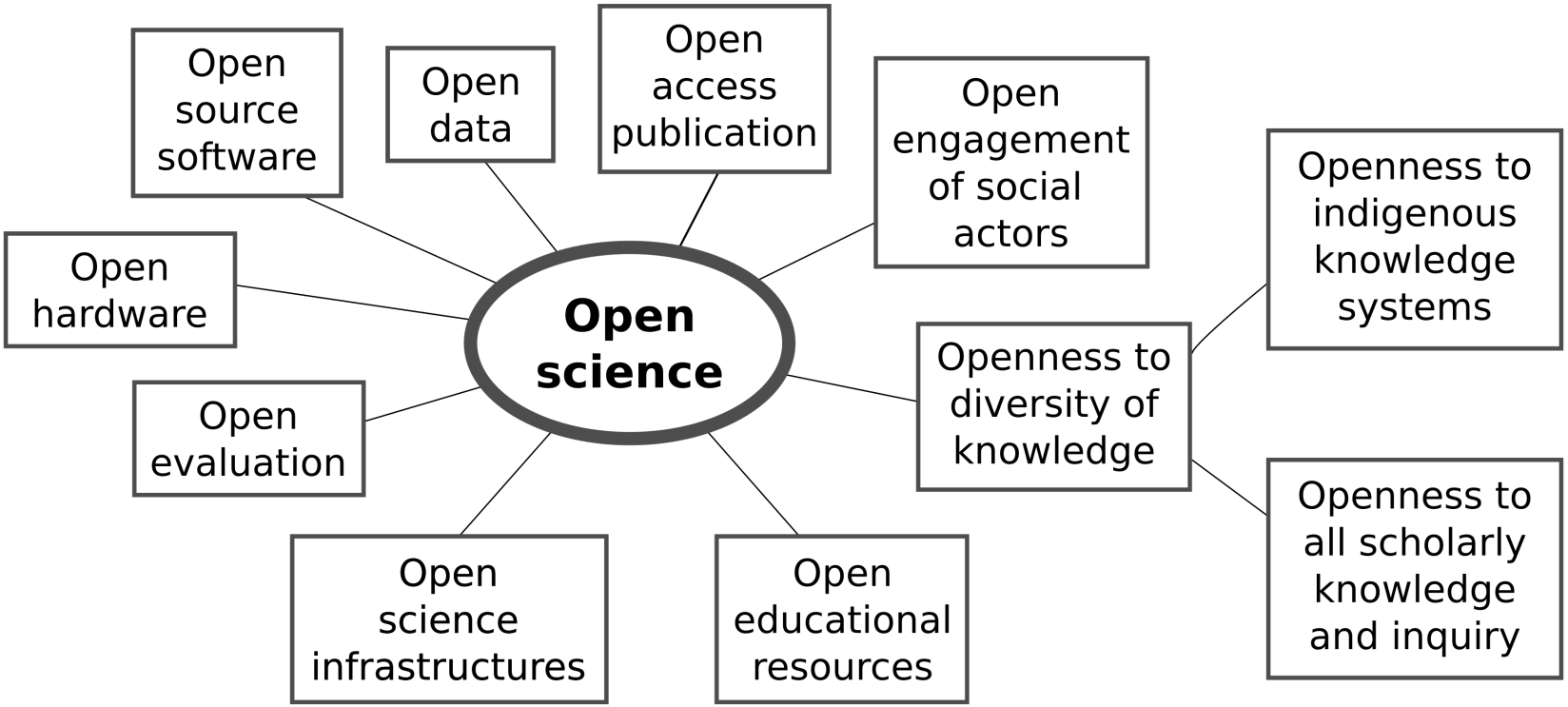
```

Enforcing

- Self governance and community enforcement
  - OSS communities
  - License compliance tools
- Legal system and Copyright Law
  - in case of blatant violation
  - CC is a nice middle ground here
- Public advocacy and Education
  - OSS organisations and foundations (e.g., GNU)
  - Universities
- It’s a collective effort: go out there and participate!

Open Science



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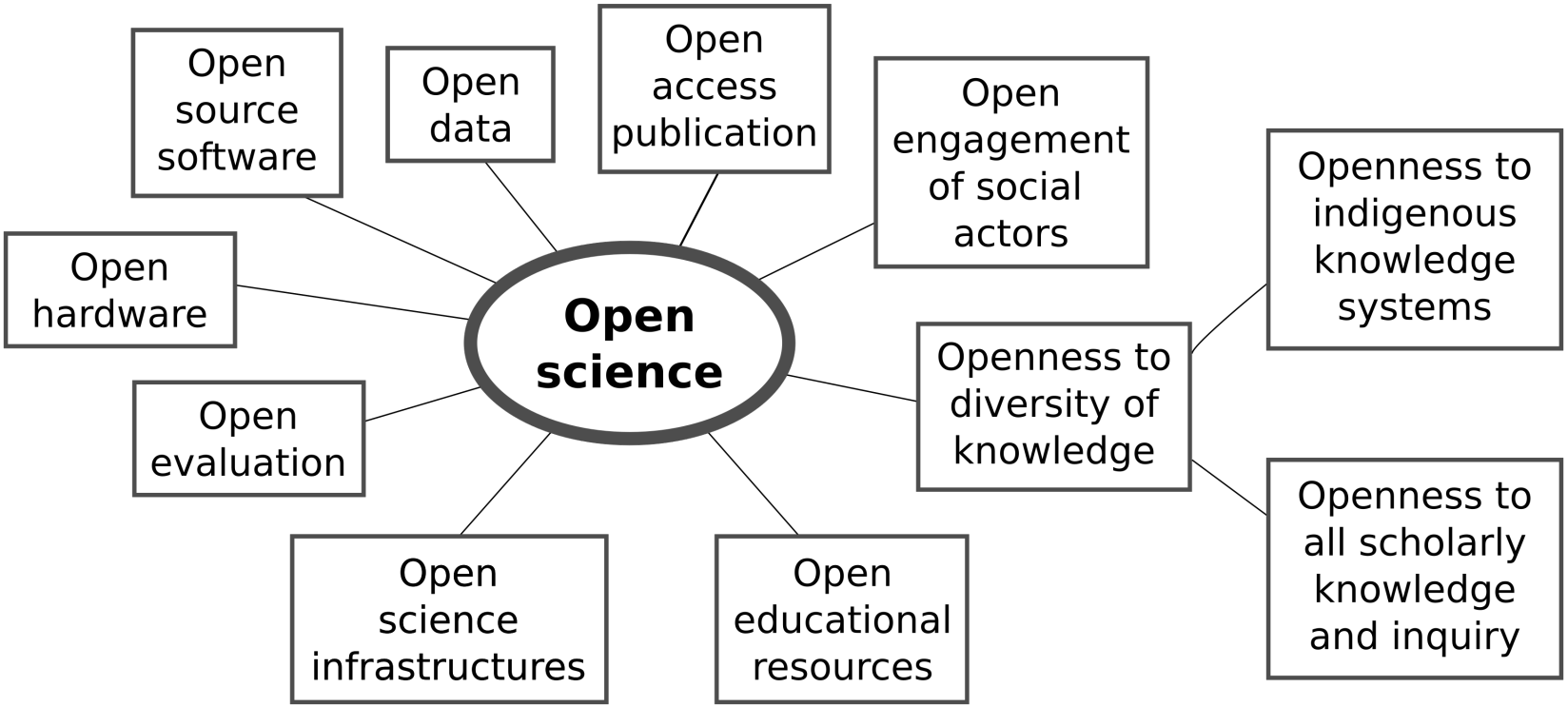
Open Science



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Inria

Open science/Open Access

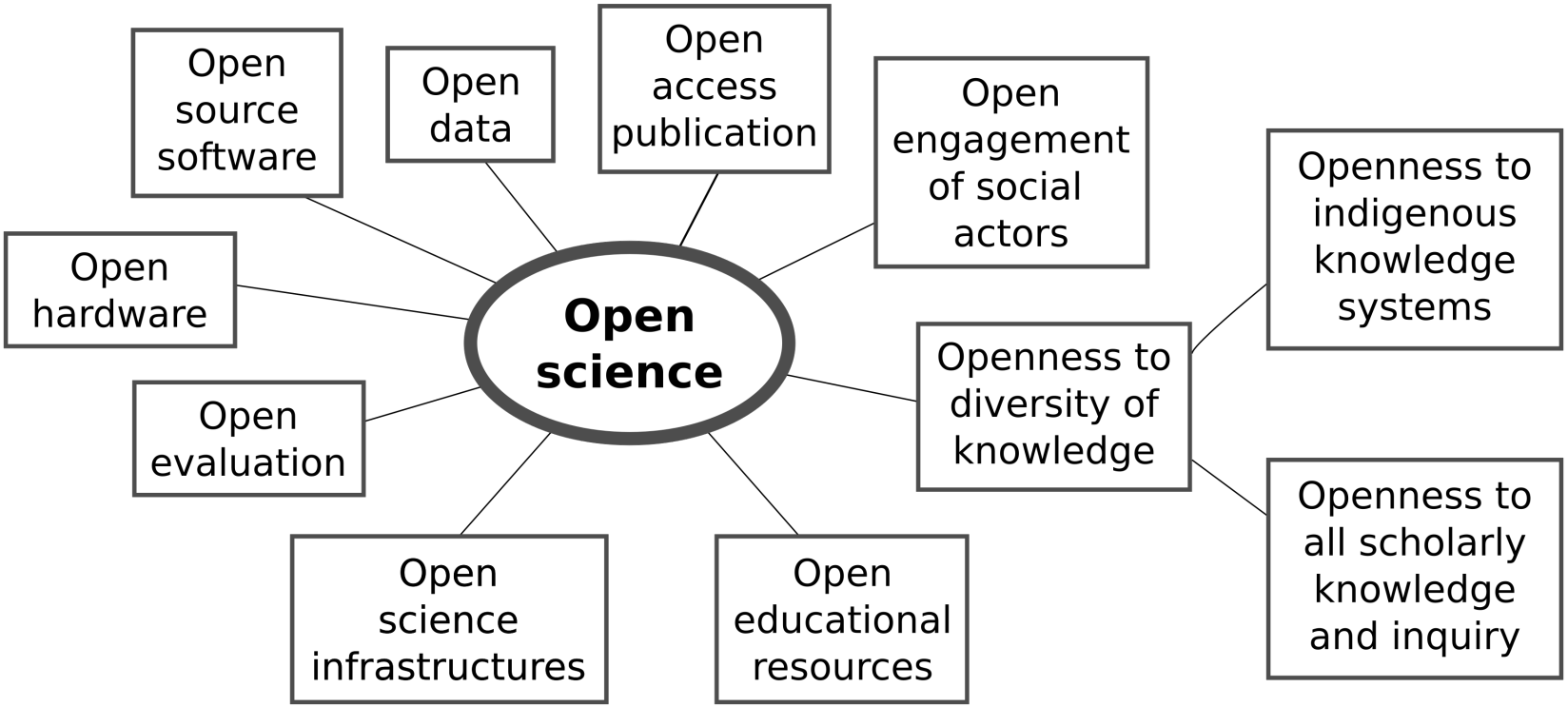
What role does Inria play when it comes to Open Science?

Date: 10 Feb. 2022

Home > News and events > What role does Inria play when it comes to Open Science?

https://www.inria.fr/en/open-science-inria-role

Open Science



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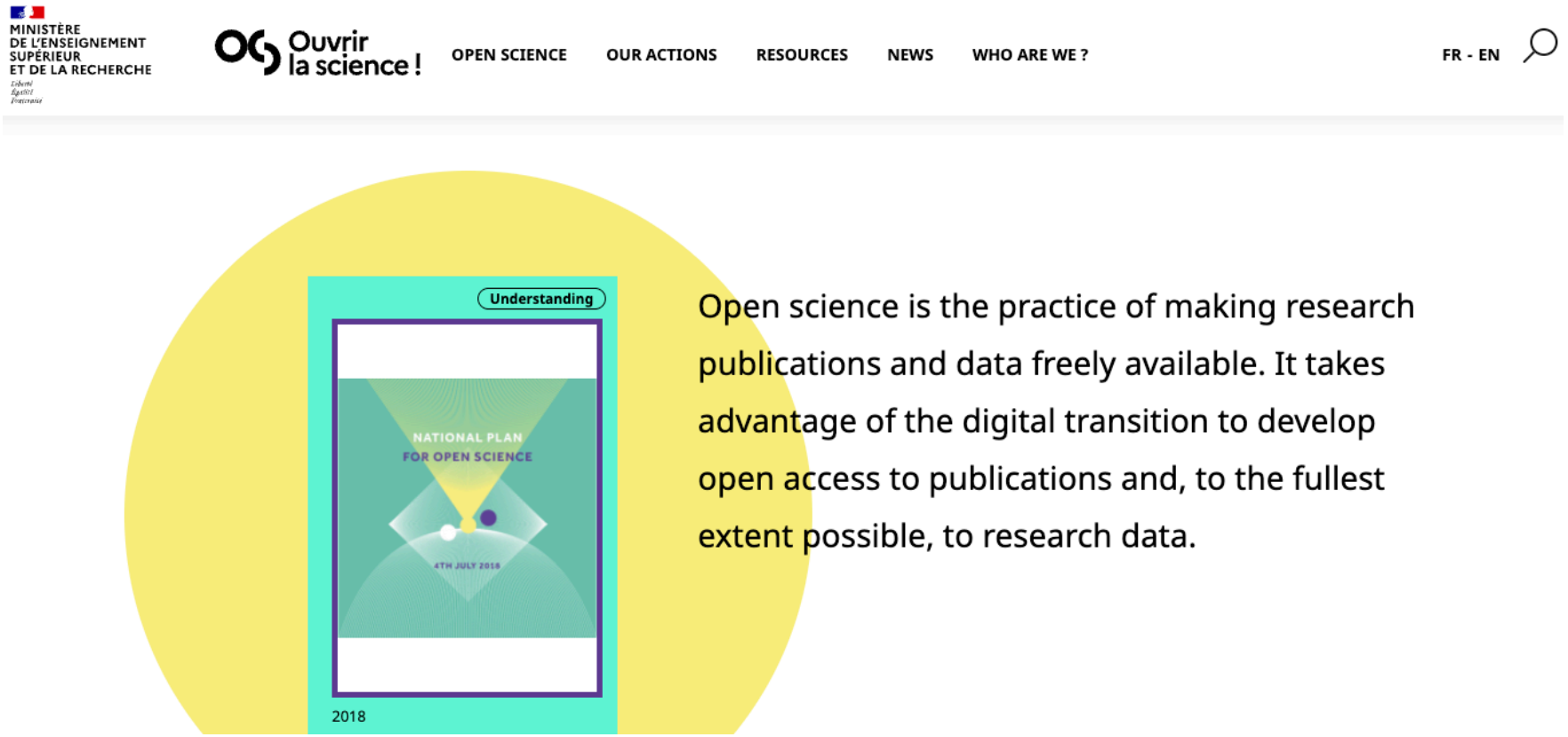
SCIENCE OUVERTE

La science ouverte est la diffusion sans entrave des résultats, des méthodes et des produits de la recherche scientifique. Cette démarche globale s'oppose à la privatisation du savoir scientifique et aux limitations induites à sa diffusion pour restaurer son rôle sociétal, démocratique et rétablir les conditions de son fonctionnement comme science efficace et de qualité.

Université Côte d'Azur soutient fermement cette dynamique en proposant un panel de services destinés à favoriser l'ouverture des publications et des données produites par ses chercheurs.

https://univ-cotedazur.fr/recherche-innovation/science-ouverte

Open Science



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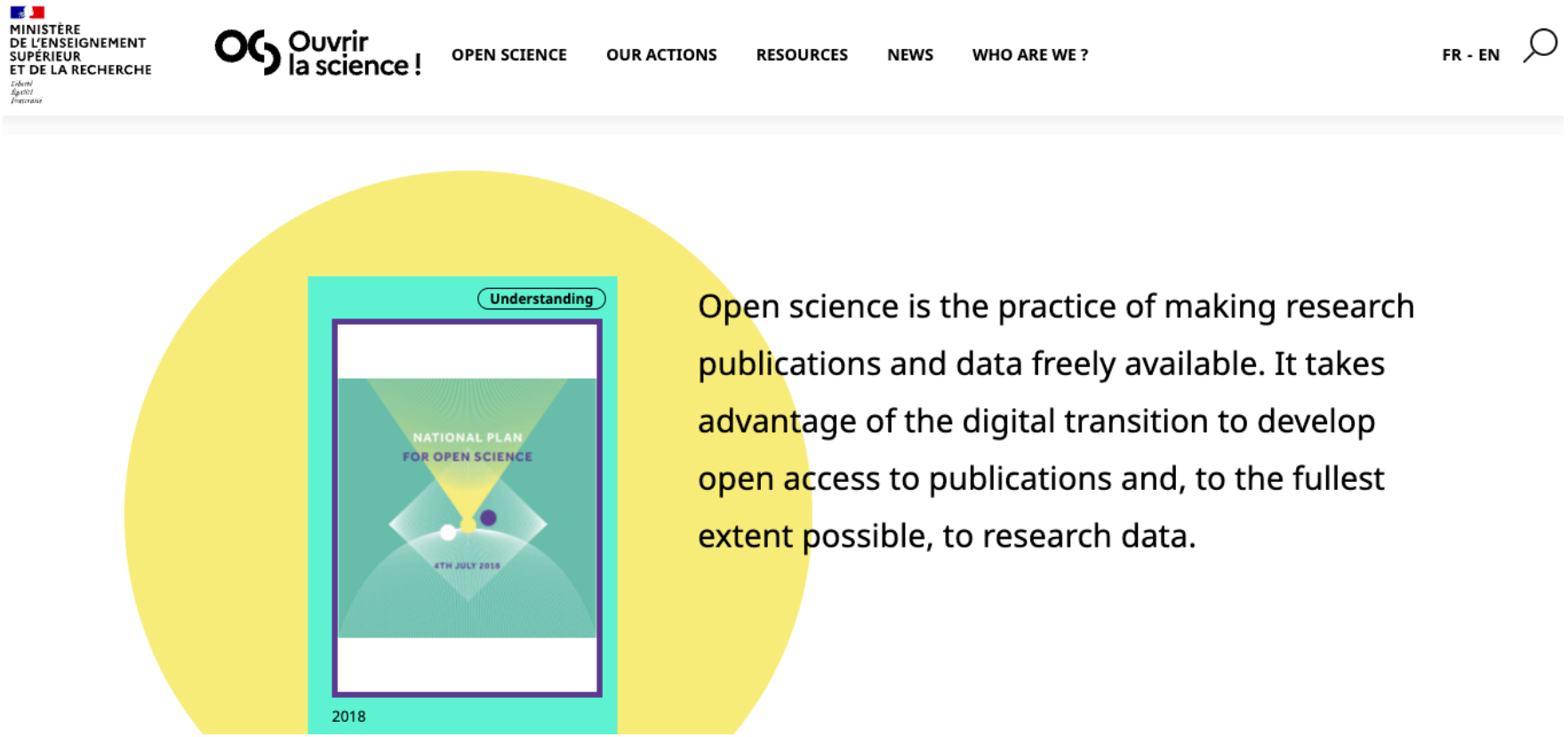
Open Science



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research.data.gouv.fr

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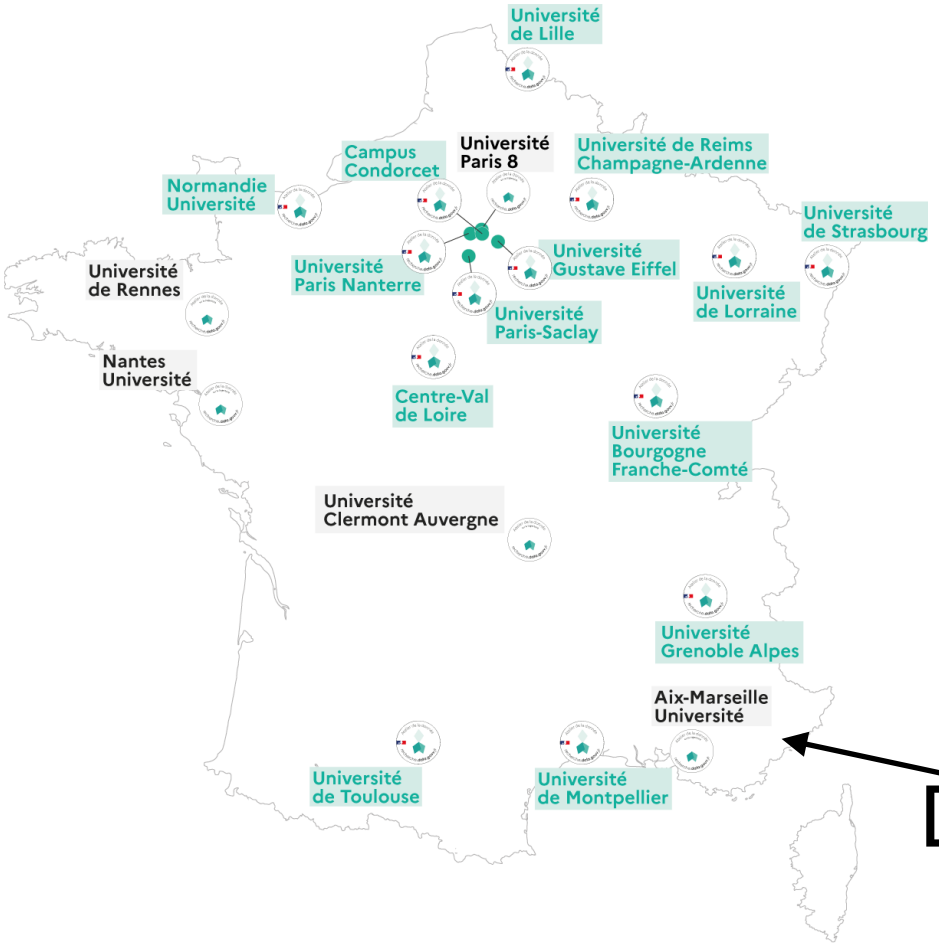

EOSC

What the European Open Science Cloud is

The ambition of the European Open Science Cloud (EOSC) is to provide European researchers, innovators, companies and citizens with a federated and open multi-disciplinary environment where they can publish, find and reuse data, tools and services for research, innovation and educational purposes.

This environment will operate under well-defined conditions to ensure trust and safeguard the public interest.

The EOSC enables a step change across scientific communities and research infrastructures towards

- seamless access
- FAIR (Findability, Accessibility, Interoperability and Reusability) management
- reliable reuse of research data and all other digital objects produced along the research life cycle (e.g. methods, software and publications)

The European Open Science Cloud (EOSC) ultimately aims to develop a 'Web of FAIR Data and services' for science in Europe upon which a wide range of value-added services can be built. These range from visualisation and analytics to long-term information preservation or the monitoring of the uptake of open science practices.

The EOSC is recognised by the Council of the European Union among the 20 actions of the policy agenda 2022-2024 of the European Research Area (ERA) with the specific objective to deepen open science practices in Europe. It is also recognised as the "science, research and innovation data space" which will be fully articulated with the other sectoral data spaces defined in the European strategy for data.

Full deployment of the EOSC will lead to higher research productivity, new insights and innovations, as well as improved reproducibility and trust in science.

bit.ly/eosc

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Problems

- Ultimately: data sharing
- "Easy"
  - experiments and results
    - publications
  - HAL
  - journals
  - arxiv
- "Hard"
  - software
- "Harder"
  - data

Problems: Hard

- Publish software
- License
- Tests
- Installation / configuration
- [multi]platform

Problems: Harder

- Data and databases
- License
- Management
  - storage
  - access
- Documentation
- Format

Your role

- Try to publish your data
  - Ask your institution
  - Ask your supervisor
  - Find a data center for your data domain
    - Human and social science
    - Astrophysics
    - Chemistry
    - Environment
    - …
- And ask Datazur for help in publishing a data paper
  - and the data too