

Introduction to Conda

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- Notebooks let you analyze your data and describe your analyses at the same time
- Notebooks support real-time data visualization
- Interactive sections can be included within a notebook
- Notebooks support the principles of reproducibility in analysis

But

- Notebooks requires a JupyterLab server
- Notebooks don't include <u>external dependencies</u>







Tool	Version
fastqc	0.12.1
hisat2	2.2.1
htseq	0.13.5
samtools	1.15.1
r-base	4.2.3
deseq2	
zenodo_get	
bash_kernel	

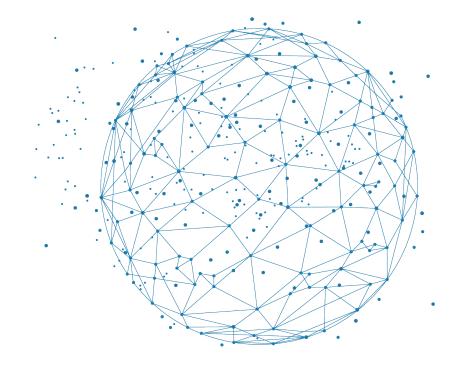
During this course we will discover how to use **conda** to simplify the installation of these tools for any users







Installing software is hard

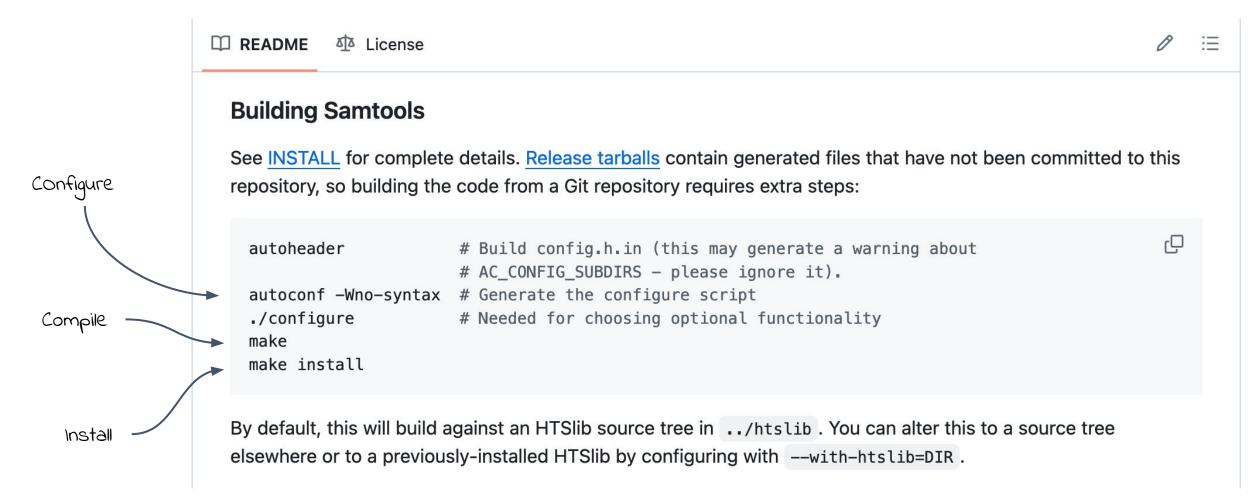








Installing software can be a tricky operation:









To facilitate software deployment, a number of package systems are available:

- offers pre-compiled software versions
- automatically manages dependencies
- offers updatés

Most Linux distributions offer a package system for easy installation of :

However, these package systems have a number of drawbacks:

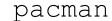
- require administrative rights
- often only one version of a tool can be installed (sometimes without choice)
- poor support of scientific software
- hard to contribute











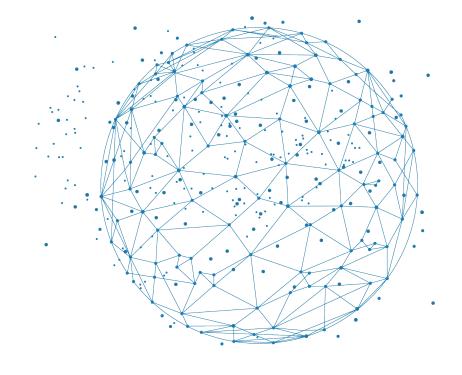








Introducing Conda









CONDA is a multi-platform package management system designed for users







Conda's strengths:

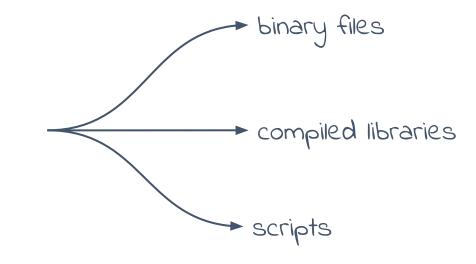
- Does not require administrator rights
- Allows you to choose the version of the tool you want to install
- Allows multiple versions of the same tool to coexist (through environments)
- Many tools in the scientific field (bioconda)
- A very open contribution model
- Compatible with any Linux distribution
- Also compatible with MacOS and Windows (in theory)







- Each software and library is available in the form of a package (a tar bz2 archive).
- A package contains the compiled version of the software and the list of packages on which it depends.







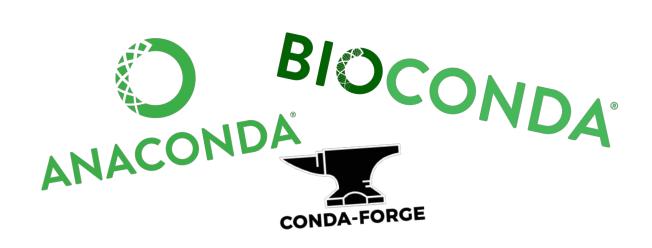


tar bz2 archive

The packages are hosted on a central server: anaconda.org



Free



Organised by channel







By the way, what is a channel?

A channel is a set of packages available on the conda repositories and managed by the same organisation.

The creators of conda offer a set of packages in the ANACONDA channel.

For several years, two main channels have grouped together most of the packages:

- CONDA-FORGE: for all user tools, languages and libraries
- BIOCONDA: for bioinformatics tools and libraries.

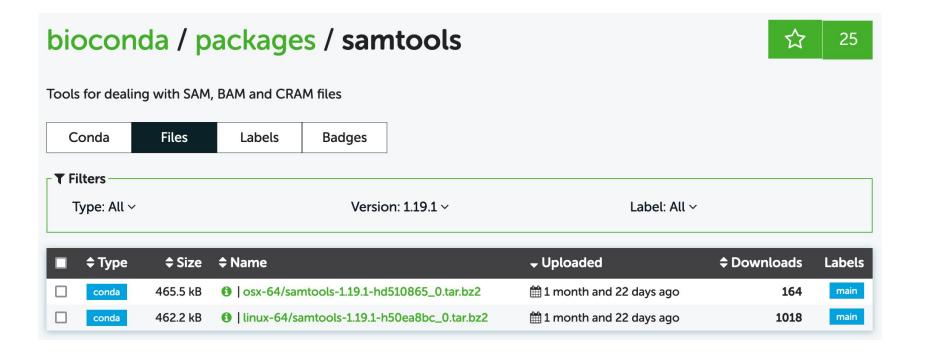
There are also numerous channels proposed by conda users. On these channels you can sometimes find tools in more recent versions, **but reliability is not guaranteed**.







 For a given software version, there are several archives corresponding to the different OS and CPU architectures for which the software is available.









- The conda tool allows you to install packages from the command line.
- For each package, it determines the list of dependencies (other packages) required, downloads the packages and installs them.

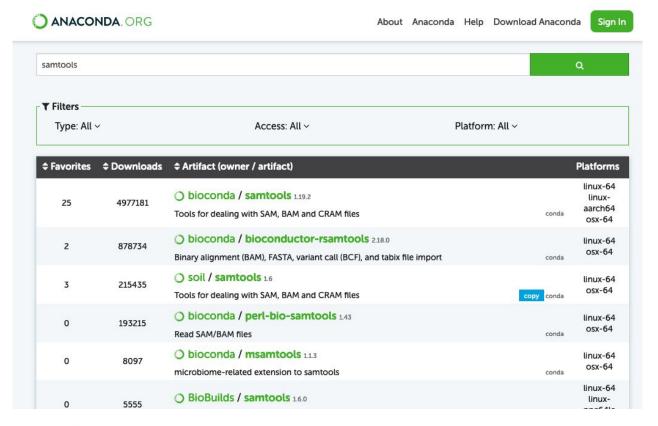
```
(base) $ conda install samtools=1.19.1
```







 The anaconda.org website has a search engine that lets you look for packages across all the channels.

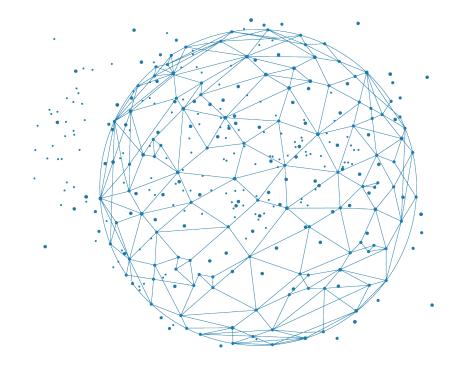








Installing Conda

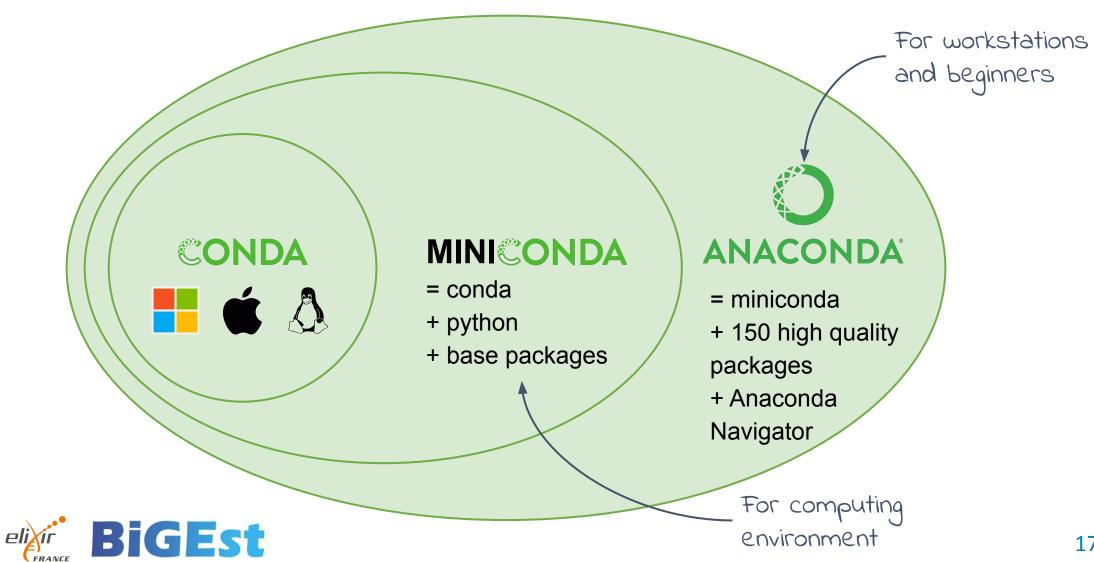








Conda is available in three different flavors









Conda is already available on the IFB Core Cluster so you don't need to install it.

```
$ module load conda
$ conda --version
conda 22.9.0
```







Installing Conda

Conda can run natively on many operating systems without the need to install special system packages. Conda can therefore be used as a non-administrator user.

Similarly, the same installation of Conda can run on several OS. This is the case on the Core cluster where some of the compute nodes are running Centos and others Ubuntu.

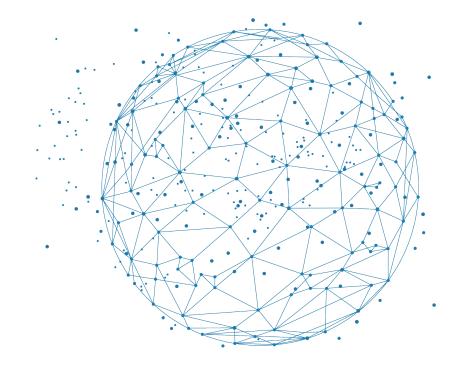
Conda also supports OS updates very well.







First steps with Conda











Let's load conda in our shell session:

```
$ module load conda
$ conda --version
conda 22.9.0
```









Conda needs to be initialized in your shell if you want to use its full power.

Try the following command to check if conda is already initialized:

```
$ conda activate --help
CommandNotFoundError: Your shell has not been properly configured to use 'conda activate'.
To initialize your shell, run
   $ conda init <SHELL NAME>
Currently supported shells are:
  - bash
  - fish
  - tcsh
  - xonsh
  - zsh
  - powershell
See 'conda init --help' for more information and options.
IMPORTANT: You may need to close and restart your shell after running 'conda init'.
```









If you get the CommandNotFoundError message it means that conda is not initialized for your shell yet

Run:

```
$ conda init bash
```

Now close and relaunch your terminal



You will now see the indication (base) in your prompt:

```
(base) ~$
```

This means that conda has loaded the base conda environment by default.









Configuration

Before installing a package, you need to determine which package sources or channels you want to use and their order of priority.

```
(base) $ conda config --add channels defaults
(base) $ conda config --add channels bioconda
(base) $ conda config --add channels conda-forge
(base) $ conda config --set channel_priority strict
(base) $ conda config --set notify_outdated_conda false
```

What does it mean?

Specify the channel order in which conda will search for packages Conda will first search the **conda-forge** channel, then **bioconda** and finally **defaults**.

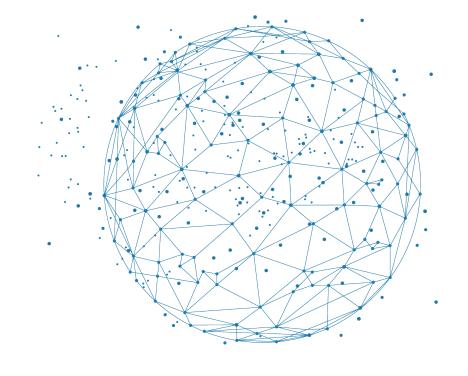
Ask conda not to inform us if it is out of date (notify outdated conda false).







Conda environments









With conda, each piece of software must be installed in an environment.

An environment is a folder containing all the files needed for the software to work.

This folder looks like a miniature operating system.

You can install multiple software in an environment but **only one version of a** software in a given environment.

By default, environments are created in the .conda/envs folder in your home directory.







Conda environments

Each package provides files which are installed in an environment through hard links.

The package files are stored in a central location in order to limit the space occupied by the environments.

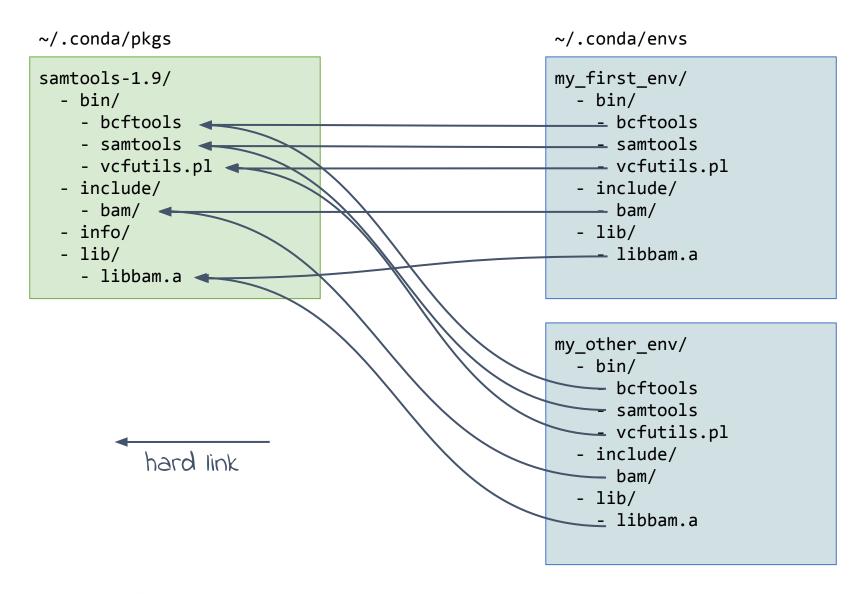
This means that if the same package is installed in two different environments, the space occupied by that package will only be used once.

By default, packages are unzipped into the .conda/pkgs folder in your home directory.

















Let's try installing a tool

(base) \$ conda install fastqc







Let's try installing a tool...

```
Collecting package metadata (current repodata.json): done
Solving environment: done
## Package Plan ##
 environment location: /shared/ifbstor1/software/miniconda
 added / updated specs:
      fastqc
The following NEW packages will be INSTALLED:
                  bioconda/noarch::fastqc-0.12.1-hdfd78af 0 None
 fastqc
 font-ttf-dejavu-s~ conda-forge/noarch::font-ttf-dejavu-sans-mono-2.37-hab24e00_0 None
                  conda-forge/linux-64::fontconfig-2.14.2-h14ed4e7_0 None
 fontconfig
                  conda-forge/linux-64::freetype-2.12.1-h267a509_2 None
 freetype
                  conda-forge/linux-64::libpng-1.6.43-h2797004_0 None
 libpng
                  conda-forge/linux-64::libuuid-2.38.1-h0b41bf4 0 None
 libuuid
                                                                                                   what's wrong?
                  conda-forge/linux-64::libxcrypt-4.4.36-hd590300_1 None
 libxcrypt
                  conda-forge/linux-64::openjdk-8.0.382-hd590300 0 None
 openjdk
                  conda-forge/linux-64::perl-5.32.1-7_hd590300_perl5 None
 perl
Proceed ([y]/n)?
Preparing transaction: done
Verifying transaction: failed
EnvironmentNotWritableError: The current user does not have write permissions to the target environment.
  environment location: /shared/ifbstor1/software/miniconda
  uid: 100002
  gid: 100002
```







Let's try installing a tool...

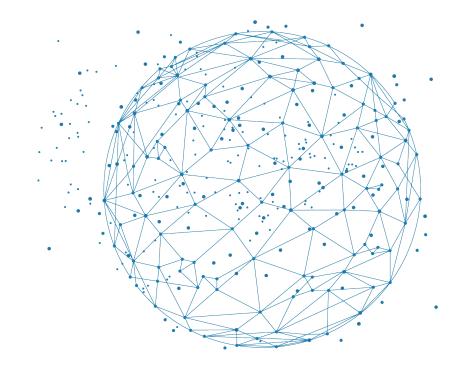
```
Collecting package metadata (current repodata.json): done
Solving environment: done
## Package Plan ##
 environment location: /shared/ifbstor1/software/miniconda
 added / updated specs:
     - fastqc
                                                                   Conda tells us that it cannot run the installation
The following NEW packages will be INSTALLED:
                                                                   because it cannot write to the environment
                bioconda/noarch::fastgc-0.12.1-hdfd78af 0 None
 fastqc
 font-ttf-dejavu-s~ conda-forge/noarch::font-ttf-dejavu-sans-mono-2.37-hab24e00_0
                                                                   (/shared/ifbstor1/software/miniconda).
                conda-forge/linux-64::fontconfig-2.14.2-h14ed4e7 0 None
 fontconfig
                conda-forge/linux-64::freetype-2.12.1-h267a509_2 None
 freetype
                conda-forge/linux-64::libpng-1.6.43-h2797004 0 None
 libpng
                conda-forge/linux-64::libuuid-2.38.1-h0b41bf4 0 None
 libuuid
                                                                   This is because the base environment has
                conda-forge/linux-64::libxcrypt-4.4.36-hd590300_1 None
 libxcrvpt
                conda-forge/linux-64::openjdk-8.0.382-hd590300 0 None
 openjdk
                                                                   been created by the cluster administrator
 perl
                conda-forge/linux-64::perl-5.32.1-7_hd590300_perl5 None
                                                                   and cannot be modified by users.
Proceed ([y]/n)?
Preparing transaction: done
Verifying transaction: failed
EnvironmentNotWritableError: The current user does not have write permissions to the target environment.
  environment location: /shared/ifbstor1/software/miniconda
  uid: 100002
  gid: 100002
```







Creating an environment for our pipeline











Let's create an environment for our pipeline:

```
(base) $ conda create -n pipeline
```

The -n option is used to specify the name of the environment.

The environment is created in the ~/.conda/envs/pipeline folder

Alternatively, you can use the -p option to indicate a path rather than a name.









We can now activate our new environment:

```
(base) $ conda activate pipeline
(pipeline) $
```

From now on, you will see the indication (pipeline) in your prompt.

Conda has set up environment variables to indicate the current environment. He has also modified your shell's \$PATH so that it can give priority access to tools (executables) installed in the environment.









The conda list command is used to list the packages installed in the environment

For the moment there are none.









Let's install the first tool we need

(pipeline) \$ conda install fastqc=0.12.1







Creating an environment for our pipeline



Conda proposes a large list of packages to install.

These are all dependencies required to run fastqc.

For each package it indicates the source channel and the version it will deploy.

We can see that it has found fastqc in the bioconda channel but that most of the dependencies come from the conda-forge channel.

The bioconda channel offers tools specifically for bioinformatics.

The conda-forge channel offers genetic tools and libraries.







Creating an environment for our pipeline



fastqc is now available

(pipeline)\$ fastqc --version FastQC v0.12.1









Now let's install hisat2 version 2.2.1

We can explicitly specify the channel we want to use to speed up dependency resolution

```
(pipeline)$ conda install -c bioconda hisat2=2.2.1
```

Solving dependencies takes a loooooooong time.

Conda's dependencies solver algorithm is notoriously inefficient.

The conda solver will make several attempts to find a solution to match the dependencies of fastqc and hisat2.







What is dependency resolution?

Each conda package is dependent on other packages. These may be libraries (openssl, jpeg, etc.), interpreters (python, java, perl, etc.) or tools (bzip2, pip, etc.).

Each of these dependencies may itself require a number of sub-dependencies.

A dependency tree can therefore be created for each package.

For example, we can consult the direct dependencies of the fastqc tool using the conda search command:

```
(pipeline)$ conda search fastqc=0.12.1 --info
(pipeline)$ conda search hisat2=2.2.1 --info
```







Creating an environment for our pipeline

```
hisat2 2.2.1 hdbdd923 6
            : hisat2-2.2.1-hdbdd923 6.tar.bz2
        : hisat2
name
version : 2.2.1
       : hdbdd923 6
build
build number: 6
size
        : 16.2 MB
license : GPL-3.0
subdir : linux-64
url
https://conda.anaconda.org/bioconda/linux-64/hisat2
-2.2.1-hdbdd923 6.tar.bz2
        : 98bb9f67fee33c105f41a9f86c3f8c23
md5
timestamp
            : 2023-05-16 08:44:56 UTC
dependencies:
  - libgcc-ng >=12
  - libstdcxx-ng >=12
  - perl
                                  other conda packages
```

We can see that **several revisions** have been proposed **for the same version of hisat2**.

Revision 6 has been installed in our environment.

Dependencies are not defined precisely.

A tool can therefore work with several different versions of a library or tool. This allows the solver to adjust the dependency versions in order to find a dependency tree common to several tools.





- python >3.5





We can use the conda remove command to uninstall a package from our environment:

(pipeline)\$ conda remove hisat2

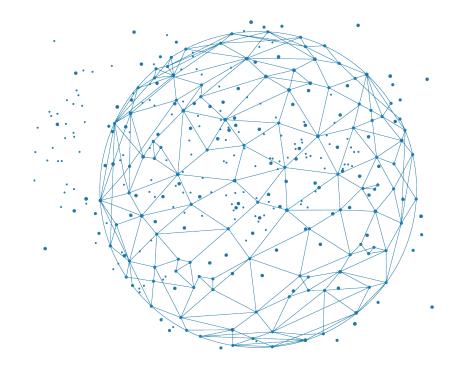
Conda resolves dependencies to ensure that the environment is as up-to-date as possible.







mamba, the super powered solver







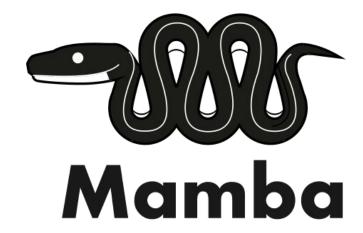


A faster solver as been developed for conda : libmamba

This library has been developed by a french company called QuantStack



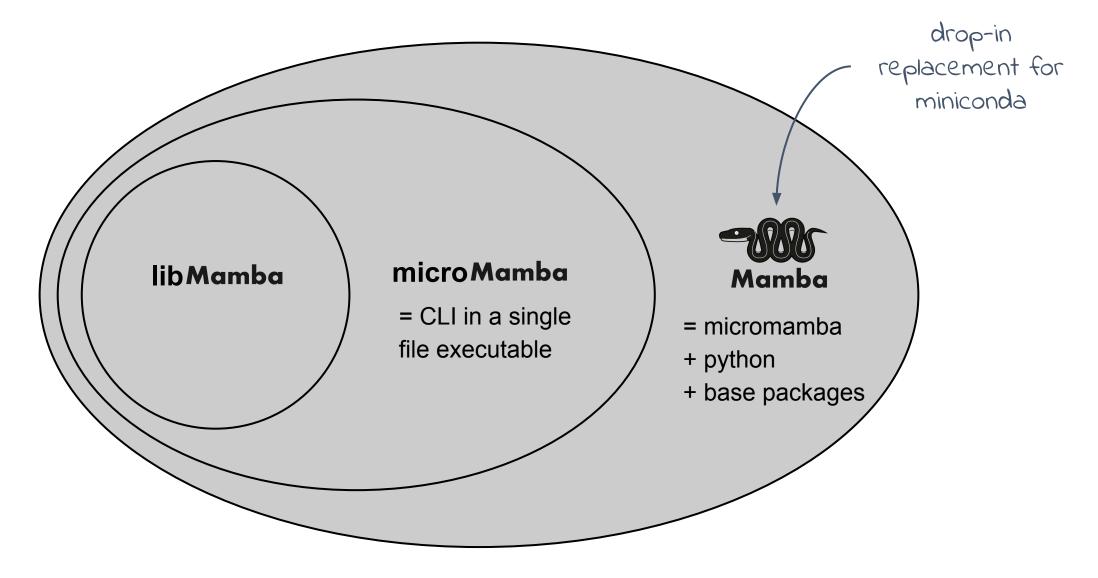
A new package manager based on libmamba is now available : mamba It uses the same channels as conda.









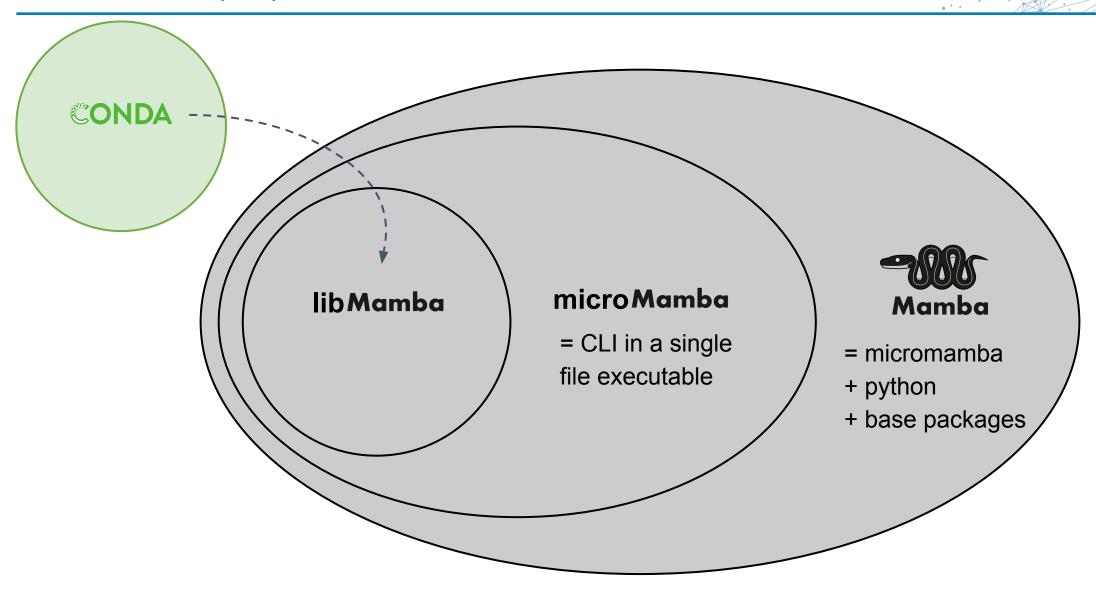








mamba, the super powered solver











Let's install hisat2 again using the mamba solver.

```
(pipeline)$ conda install --experimental-solver=libmamba -c bioconda hisat2=2.2.1
```

In the latest conda version, libmamba is no more considered as "experimental":

conda install --solver=libmamba

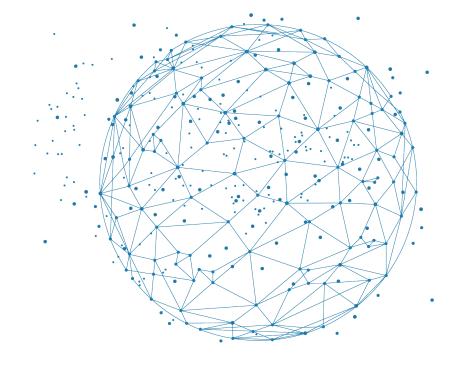
Solving should be much faster!







Sharing your environment











We can't share our environment directly, which is an assembly of hard links, but we can describe its dependencies in a YAML file.

Create a new file called environment.yml:

name: pipeline channels: - conda-forge - bioconda - defaults dependencies: - fastqc - hisat2 - htseq - samtools - r-base

This file gives the direct dependencies of our pipeline. It does not indicate the libraries and other tools required, i.e. the dependencies of dependencies.





zenodo_get

bash_kernel

- bioconductor-deseq2





We can easily deploy our conda environment with this file

```
(pipeline)$ conda deactivate
(base)$ conda env remove -n pipeline
(base)$ conda env create --experimental-solver=libmamba -f environment.yml
```







If we install this environment today, conda will install the requested tools in the following versions:

fastqc: 0.12.1

hisat2: 2.2.1

htseq: 2.0.5

samtools: 1.19.2

If we need to recreate the environment in a few months' time, it is possible that conda will propose us new versions of certain tools.

So we have an environment that is easy to update but not reproducible.









To improve reproducibility, you can specify the desired versions for each direct dependency:

```
name: pipeline
channels:
  - conda-forge
  - bioconda
  - defaults
dependencies:
  - fastqc=0.12.1
  - hisat2=2.2.1
  - htseq=2.0.5
  - samtools=1.19.2
  - r-base=4.2.3
  - bioconductor-deseq2
  zenodo_get
  - bash_kernel
```

We have made an improvement in terms of **reproducibility**, however, when we install this environment a number of additional dependencies will be installed without us having fine control over their versions.

These dependencies can therefore change over the course of the installations and have an impact on the result of our workflow.









Conda can be used to generate a YAML file from the contents of an environment.

```
(pipeline)$ conda env export > environment.lock.yml
```

This time we have a complete and precise list of dependencies. It is highly reproducible.

However, we lose our ability to easily update our direct dependencies.

By changing the version of one of our direct dependencies, it is highly likely that conda will no longer be able to find a functional dependency tree.







In brief

Dependencies specification	Reproducibility	Upgradability
Direct	Awful	Automatic
Versionned direct	Okish	Good
Through env export	Perfect	Awful







Sharing your environment

In order to ensure perfect reproducibility of our environment, while at the same time being able to upgrade it if necessary, we need to keep two files:

- a file with direct versioned dependencies
- an environment lock file to create the identical environment each time we want to install it



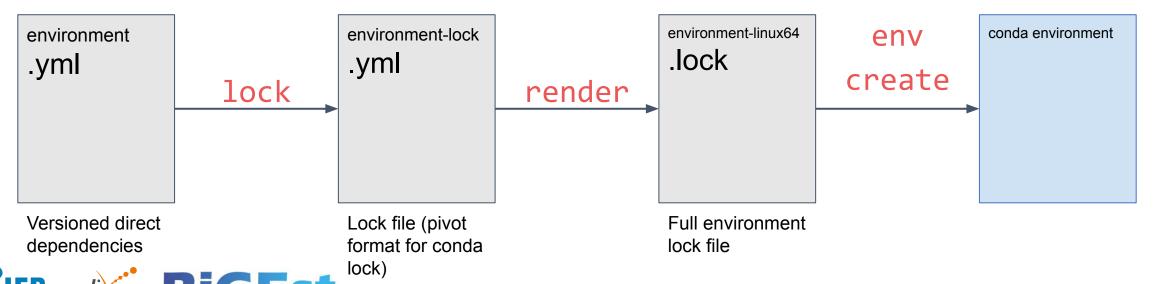




The conda lock tool generates an environment lock file from a conda environment file in YAML format.

Whereas conda env export creates a precise list of dependencies, conda lock creates a list of package URLs to download. This avoids the dependency resolution stage when you want to install the environment.

In addition, conda lock can be used to generate lock files for any operating system.





Create a lock file for linux:

```
(base)$ conda <u>lock lock</u> --mamba -p linux-64 --lockfile environment-lock.yml -f environment.yml

Not a mistype;)
```

Render a lock environment file for linux:

(base)\$ conda lock render -p linux-64 --filename-template environment-{platform}.lock environment-lock.yml

Create the environment:

```
(base)$ conda env remove -n pipeline
(base)$ conda create -n pipeline -f environment-linux-64.lock
```

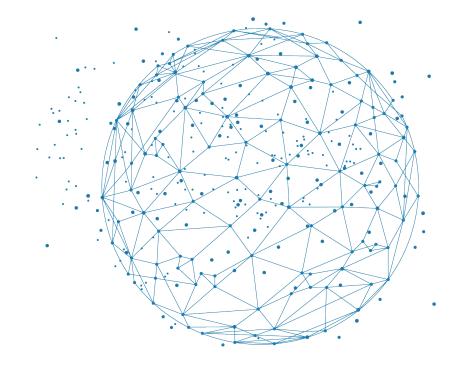
conda doesn't need to do any solving!







About package building









Creating a package is "easy"

- 1. Create a meta.yml file to describe your package and its dependencies
- 2. Create a build.sh script to describe the compilation workflow

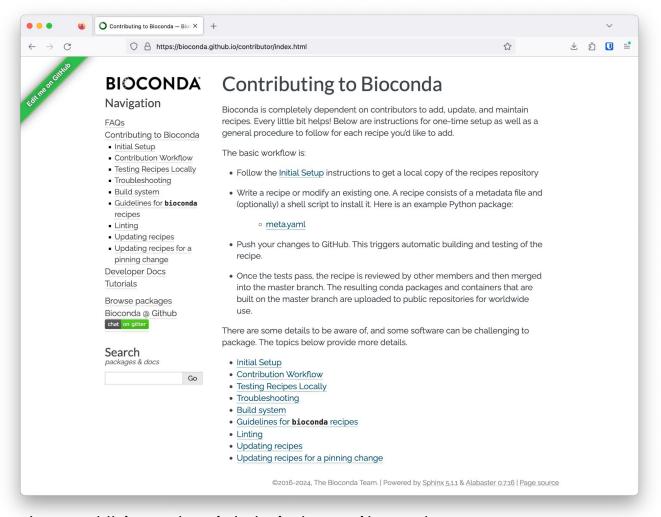
conda build let you build your package and publish it

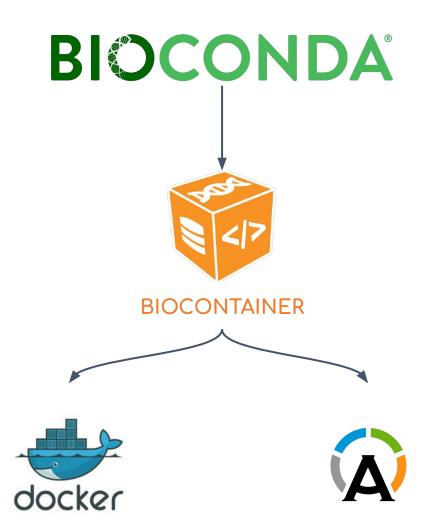






Contribute to BIOCONDA





https://bioconda.github.io/contributor/





