



ELIXIR Webinar

Bioconda and BioContainers

Tool deployment and sustainability in science

Björn Grüning

Bioconda/BioContainer community



www.elixir-europe.org

Tool deployment & sustainability in science

Question → Development of code → Deployment



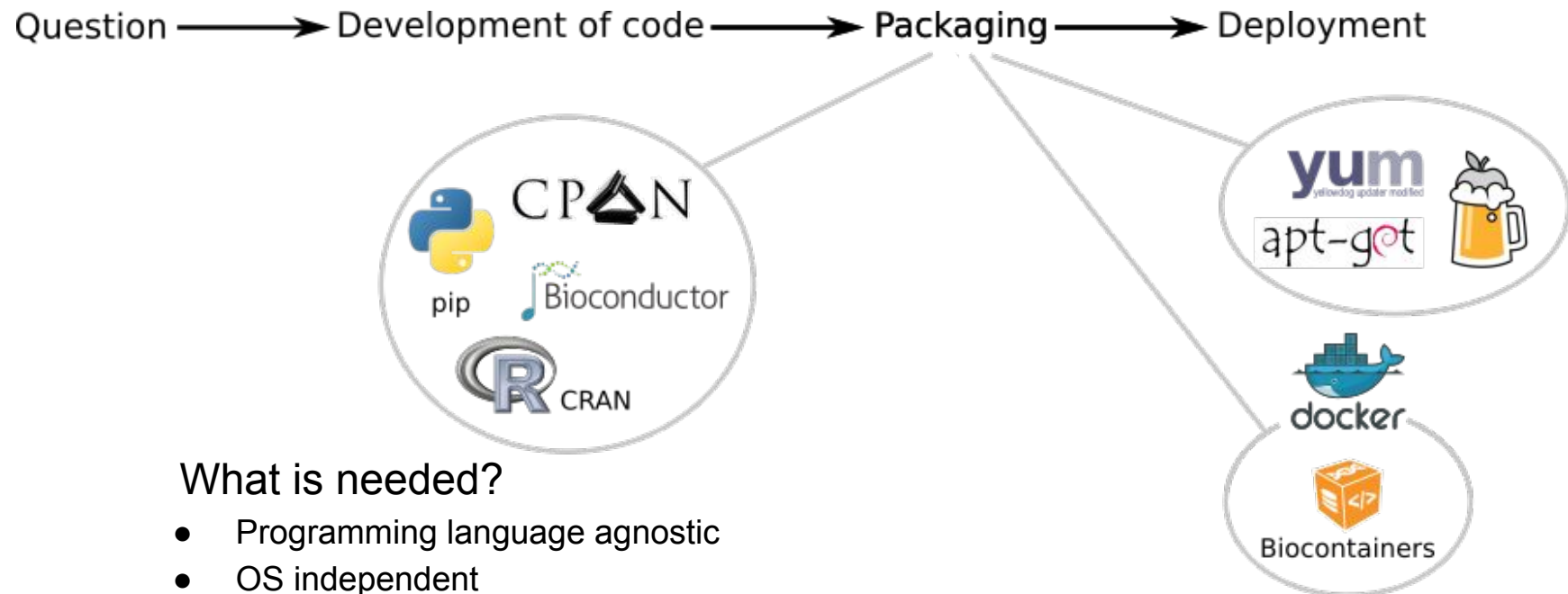
Tool deployment & sustainability in science

Question → Development of code → Packaging → Deployment

***Package managers** are charged with the task of **finding, installing, maintaining** or **uninstalling** software packages upon the **user's** command.*



Tool deployment & sustainability in science



What is needed?

- Programming language agnostic
- OS independent
- No root privileges needed
- Management of multiple version
- HPC and Cloud compatible
- easy to maintain

CONDA

- Open Source package manager
- Independent of any programming language and OS
- Fast, robust and easy package installation

```
$ conda install deeptools
```

- Installation and management of multiple versions



```
package:
  name: deeptools
  version: '2.4.3'
```

meta.yaml

```
source:
  fn: deepTools-2.4.3.tar.gz
  url: https://pypi.python.org/packages/40/4b/2f443a9d0d4201d3f152c3a9f291075f4b2cd5322d29c796/deepTools-2.4.3.tar.gz
  md5: 1751e860c5436d1973d7621ebdf00c6a
```

```
requirements:
```

```
  build:
```

- python
- setuptools
- numpy >=1.9.0
- scipy >=0.17.0
- matplotlib >=1.4.0
- pysam >=0.8.2
- py2bit >=0.2.0
- gcc

```
  run:
```

- python
- pybigwig >=0.2.3
- numpy >=1.9.0
- scipy >=0.17.0
- matplotlib >=1.4.0
- pysam >=0.8.2
- py2bit >=0.2.0

```
test:
```

```
  imports:
```

- deeptools

```
  commands:
```

- bamCompare --version

```
about:
```

```
  home: https://github.com/fidelram/deepTools
```

```
  license: GPL3
```

```
  summary: A set of user-friendly tools for normalization and visualization of deep-sequencing data
```

```
#!/bin/bash
```

```
$PYTHON setup.py install
```

build.sh





- Build packages

```
$ conda build packages/deeptools/
```

- building a scientific community

BIOCONDA®

- using a unified build environment

```
$ ./simulate-travis.py --docker --package deeptools
```

- joining other Conda communities



CONDA-FORGE

<https://bioconda.github.io> | <https://conda.io/docs>



Bioconda is a channel for the [conda](#) package manager specializing in bioinformatics software. Bioconda consists of:

- a [repository of recipes](#) hosted on GitHub
- a [build system](#) that turns these recipes into conda packages
- a [repository of >1500 bioinformatics packages](#) ready to use with `conda install`
- Over 130 contributors that add, modify, update and maintain the recipes

Browse packages in the bioconda channel: [Available packages](#)

The conda package manager has recently made installing software a vastly more streamlined process. Conda is a combination of other package managers you may have encountered, such as pip, CPAN, CRAN, Bioconductor, apt-get, and homebrew. Conda is both language- and OS-agnostic, and can be used to install C/C++, Fortran, Go, R, Python, Java etc programs on Linux, Mac OSX, and Windows.

Conda allows separation of packages into separate repositories, or *channels*. The main *defaults* channel has a large number of common packages. Users can add additional channels from which to install software packages not available in the defaults channel. Bioconda is one such channel specializing in bioinformatics software.

Using bioconda

bioconda supports only 64-bit Linux and Mac OSX.

<https://bioconda.github.io>
<https://conda.io/docs>

1. Install conda

Bioconda requires the conda package manager to be installed. If you have an Anaconda Python installation, you already have it. Otherwise, the best way to install it is with the [Miniconda](#) package. The Python 3 version is recommended.

See also:

- [What's the difference between Anaconda, conda, and Miniconda?](#)
- The conda [FAQs](#) explain how it's easy to use with existing Python installations.





BIOCONDA[®]

Navigation

[Available packages](#)

[Contributing](#)

- [One-time setup](#)
- [Contributing a recipe](#)
- [Troubleshooting failed recipes](#)
- [Build system](#)
- [Guidelines for **bioconda** recipes](#)

[Linting](#)

[FAQs](#)

Contributing

Bioconda is completely dependent on contributors to add, update, and maintain recipes. Every little bit helps! Below are instructions for one-time setup as well as a general procedure to follow for each recipe you'd like to add.

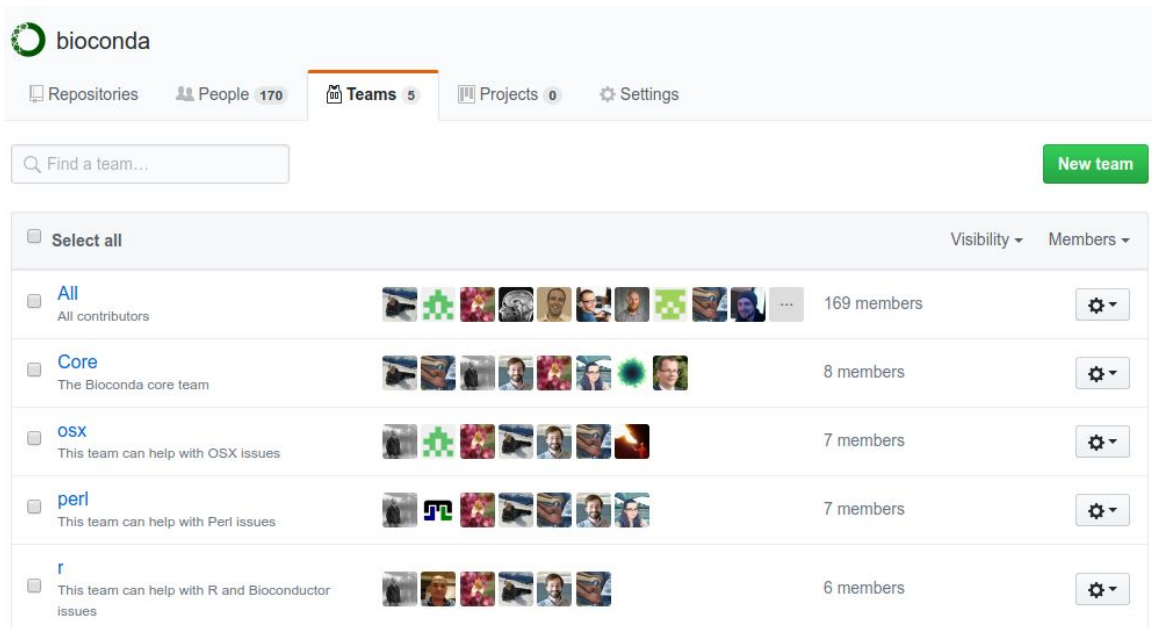
- [One-time setup](#)
 - [Git and GitHub \(one-time setup\)](#)
 - [Install conda and Docker \(one-time setup\)](#)
 - [Request to be added to the bioconda team](#)
- [Contributing a recipe](#)
 - [Update repo and requirements](#)
 - [Write a recipe](#)
 - [Test locally](#)
 - [Push changes, wait for tests to pass, submit pull request](#)
 - [Use your new recipe](#)
- [Troubleshooting failed recipes](#)
 - [Reading bioconda-utils logs on Travis-CI](#)
 - [HTTP 500 errors](#)
 - [HTTP 404 errors](#)
 - [ZLIB errors](#)
 - [/usr/bin/perl or /usr/bin/python not found](#)
 - [Troubleshooting failed **mulled-build** tests](#)
- [Build system](#)
- [Guidelines for **bioconda** recipes](#)
 - [bioconda recipe checklist](#)
 - [Python](#)
 - [R \(CRAN\)](#)
 - [R \(Bioconductor\)](#)
 - [Java](#)
 - [Perl](#)
 - [C/C++](#)
 - [General command-line tools](#)
 - [Metapackages](#)
 - [Other examples of interest](#)
 - [Name collisions](#)
 - [Tests](#)
 - [Link and unlink scripts \(pre- and post- install hooks\)](#)
 - [Versions](#)

<https://bioconda.github.io>
<https://conda.io/docs>



BIOCONDA®

- 2245 package (2017.03)
- contribute at <https://github.com/bioconda/bioconda-recipes>
- community driven



The screenshot shows the bioconda GitHub organization page. At the top, there's a navigation bar with links for Repositories, People (170), Teams (5), Projects (0), and Settings. Below this is a search bar labeled "Find a team..." and a green "New team" button. The main content area displays a list of teams, each with a checkbox, a name, a description, a row of member avatars, the number of members, and a settings gear icon. The teams listed are:

Team Name	Description	Members
All	All contributors	169 members
Core	The Bioconda core team	8 members
OSX	This team can help with OSX issues	7 members
perl	This team can help with Perl issues	7 members
r	This team can help with R and Bioconductor issues	6 members

Community

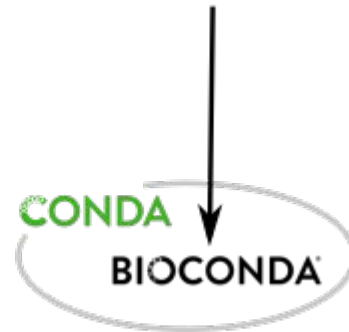


208 Contributors **3700 merged PR**
in 1.5 years



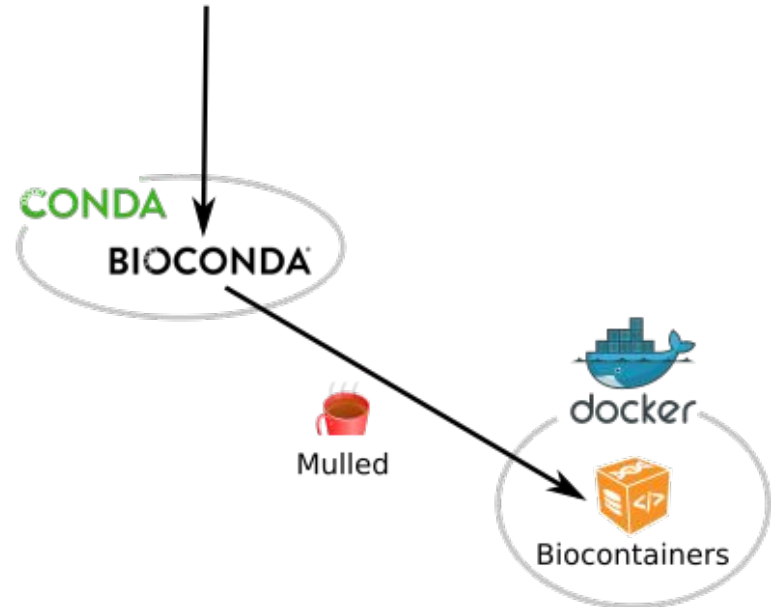
But the new cool kid is called **Containers**

Question → Development of code → Packaging → Deployment




But the new cool kid is called Containers

Question → Development of code → Packaging → Deployment



Mulled

- A layer donning approach to build containers
- without Dockerfile
- completely automatised
- powered by  Travis CI



Biocontainers

<http://biocontainers.pro>

The screenshot shows the BioContainers website homepage. At the top, there is a navigation bar with the BioContainers logo on the left and links for 'REGISTRY', 'GITHUB', and 'DOCUMENTATION' on the right. The main content area has a dark background. On the left, there are four colored squares (yellow, green, red, blue) arranged in a 2x2 grid. In the center, the text 'BIOINFORMATICS MORE ACCESSIBLE & REPRODUCIBLE' is displayed in large, white, bold letters. Below this, a paragraph describes BioContainers as an open source and community-driven framework for bioinformatics software. On the right, there is a large blue DNA helix icon. At the bottom, there are four colored buttons: 'DOCS' (red), 'FIND MORE' (green), 'COMMUNITY' (blue), and 'GITHUB' (yellow).

BIOCONTAINERS

REGISTRY GITHUB DOCUMENTATION

BIOINFORMATICS MORE ACCESSIBLE & REPRODUCIBLE

BioContainers is an open source and community-driven framework which provides system-agnostic executable environments for bioinformatics software. BioContainers framework allows software to be installed and executed under an isolated and controllable environment.

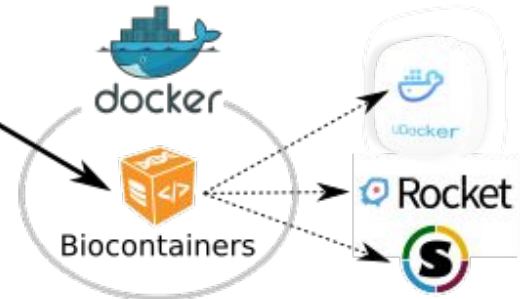
DOCS FIND MORE COMMUNITY GITHUB

- defining standards and best practises for containers
- developing training material
- developing documentation



But the new cool kid is called Containers

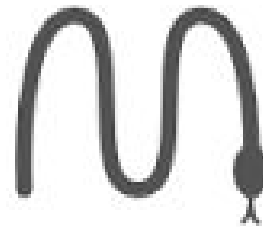
Question → Development of code → Packaging → Deployment



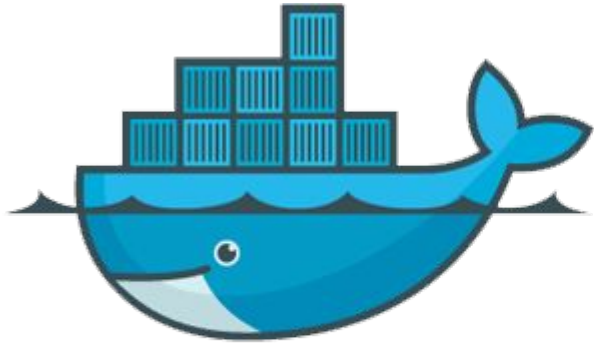
Get all the other nice technologies for free

- rkt
- singularity
- modules

Who is using it?



Thanks!



docker



TRAVIS



Yasset Perez-Riverol
Felipe Leprevost ...



Rolf Backofen and the RBC

GitHub

BIOCONDA[®]

Johannes Köster
Ryan Dale ...

