The Conda package manager

MANCHESTER 1824
The University of Manchester

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Overview of Conda

- Language agnostic (Python/R/C++/Julia)
- Multi-platform: (Windows/macOS/Linux)
- Multi-architecture: (`i386`/`x86_64`/`POWER8`/`POWER9` and I think `arm64` is coming))
- Installs binaries (No install from source support)
- Very popular in the academic and commercial “Data Science” community
  - Many popular libraries list it as the recommended install method
- Has changed a lot in the last two years

Installation

- Conda can be into any location in three lines: (similar for macOS, GUI installer for windows)

```
wget http://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
sh Miniconda3-latest-Linux-x86_64.sh "${HOME}/miniconda"
# Add to you shell rc file:
source "${HOME}/miniconda/etc/profile.d/conda.sh"      # For bash-like shells
source "${HOME}/miniconda/etc/profile.d/conda.csh"     # For csh-like shells
source "${HOME}/miniconda/etc/fish/conf.d/conda.fish"  # For fish
```

- This used to be done with `export PATH=$CONDA_DIR/bin:$PATH`
  - Now uses a function instead
    - Prevents bad interactions with other software
    - Allows conda environments to modify the shell environment
  - The “root” environment can be set up with conda activate root

- Use of the base “root” environment is discouraged

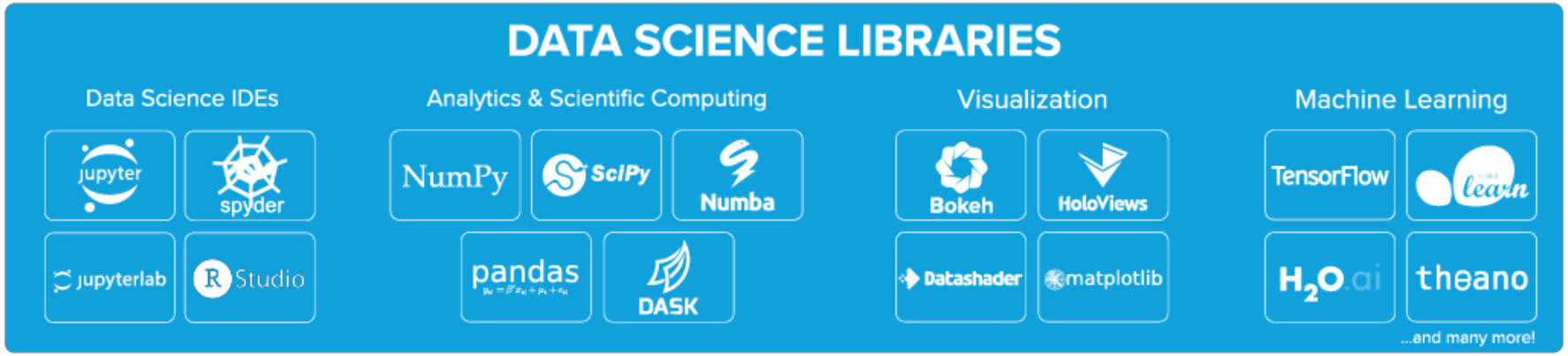
Environments

- A conda "environment" is just a folder in `$CONDA_DIR/envs/`
  - Switch between them using `conda [de]activate $ENV_NAME`
  - Activating sets PATH and sources scripts in `$CONDA_DIR/etc/conda/activate.d`
- Create an environment with `conda create --name $ENV_NAME python=3.7 matplotlib pandas`
- When activated packages are installed with `conda install scikit-learn`
- Behind the scenes:
  - Packages are kept in `$CONDA_DIR/pkgs/`
  - Both a tarball-like file and it's extracted contents
  - Mixture of copying, hard links and symlinks to the environment's directory

Sources of packages

Anaconda distribution

- The default source is the Anaconda Distribution
- Mostly Python/R packages for Data Science
  - Contains over 1,400 packages
  - Includes proprietary software: Intel MKL and CUDA
- Freely available and the build recipes are open source
  - Enterprise support is available (see right)
- Even provides a GUI for managing environments



Sources of packages

- Packages are installed from “channels”
- Anaconda Distribution
- Anaconda.org
  - Provides 3GB of storage **(soft limit, hard limit isn’t clear but 5-10GB)**
  - “Contact us for additional storage”
- Custom repositories
  - Any HTTP(S) url can be used as a channel provided the correct structure is present

conda-forge

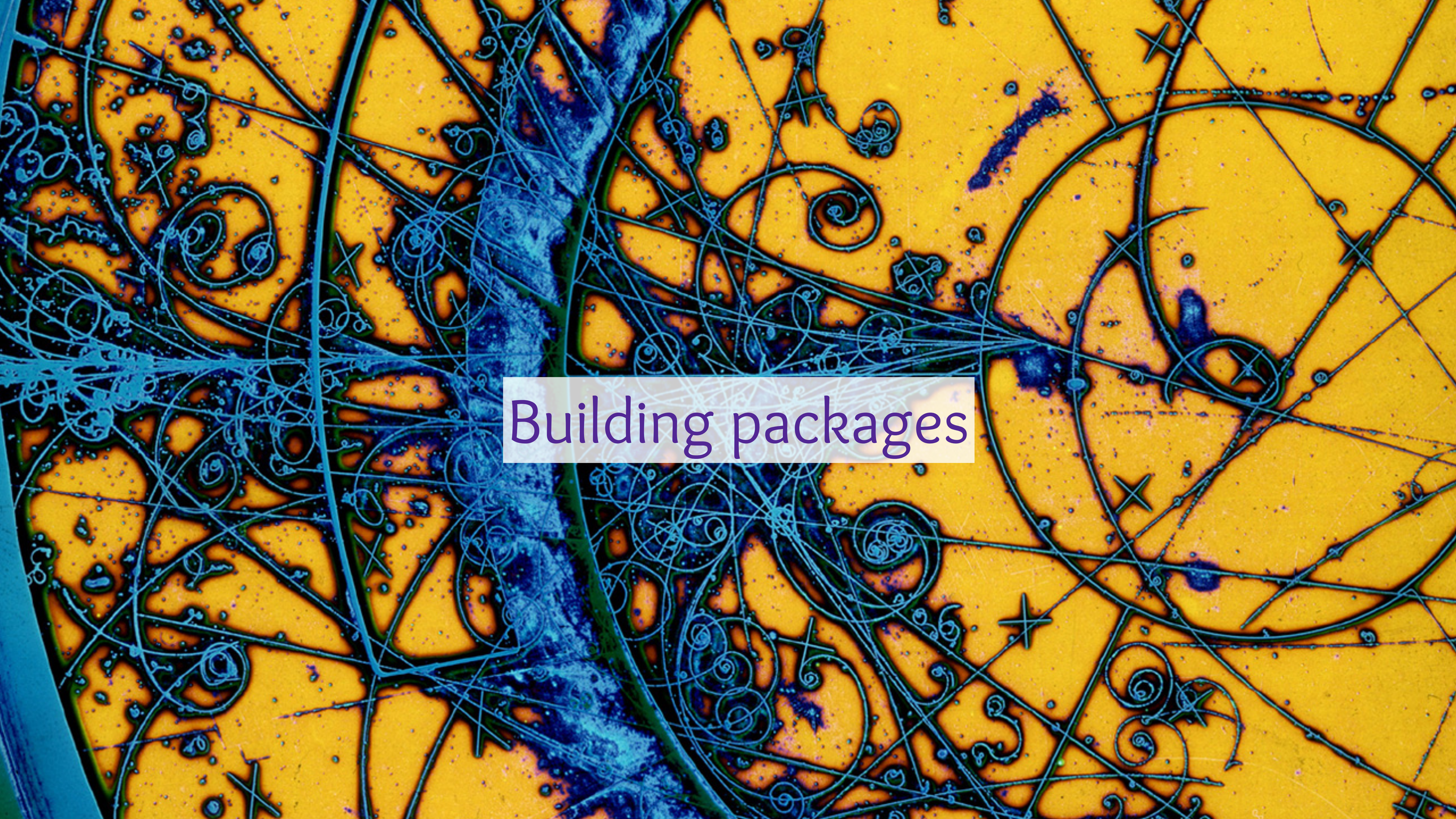
- Community maintained channel https://conda-forge.org
  - Based around a GitHub organisation (over 1,100 members)
  - Various CI providers are used for builds
  - Anaconda Inc. provides storage, bandwidth and general support
- Contains over 6,000 packages
  - One Git repository per package
  - Maintainers are listed in the recipe
  - New packages are added by making a pull request
- Lots of automation
  - General maintenance
  - Monitor for new releases and make pull requests

CONDA-FORGE

Other third party channels

- Bioconda https://bioconda.github.io
  - Builds on top of conda-forge
  - Contains over 6,000 packages for bioinformatics research
  - Around 600 contributors and 450 GitHub organisation members
  - Similar to conda-forge (Anaconda Inc. provide hosting, use CI to build packages)
  - Publication about the initiative doi:10.1038/s41592-018-0046-7
- AstroConda https://astroconda.readthedocs.io
  - Maintained by Space Telescope Science Institute in Baltimore, Maryland
  - Only depends on the default Anaconda channel
  - Contains over 1,500 packages
  - Hosted independtly of Anaconda Inc. - http://ssb.stsci.edu/astroconda
- AstroPy seem to be setting up something similar

  https://github.com/astropy/conda-channel-astropy



Building packages

Recipes

- A package is built from a “recipe” which is a folder containing a file `meta.yaml`
  - Jinja2 templates are used for fancy features
- Defined with cross-compilation in mind
  - Build, Host and Run sections of the dependencies
  - Runtime dependencies can be propagated
    - These can be explicitly ignored if needed
- Builds are normally run a script: `build.[sh|bat]`
  - Creates “build” and “install” conda environments
  - Package is then tested by installing to a new environment
- Various check made afterwards
  - Overlinking, undefined dependencies, RPATH patching, …
- Metadata (conda-forge uses this to set the GitHub access rights)

```yaml
{% set name = "vdt" %}
{% set version = "0.4.2" %}

package:
  name: {{ name|lower }}
  version: {{ version }}

source:
  url: https://github.com/dpiparo/{{ name }}/archive/v{{ version }}.tar.gz
  sha256: 643136a38d6890c1cf18074bd494f99a4f269429ac552c57907e28c0091df8e6

build:
  number: 1002
  skip: True  # [win]
  run_exports:
    - {{ pin_subpackage('vdt', max_pin='x.x.x') }}

requirements:
  build:
    - {{ compiler('c') }}
    - {{ compiler('cxx') }}
    - cmake
  host:
  run:

test:
  # Some package might need a `test/commands` key to check CLI.
  # List all the packages/modules that `run_test.py` imports.
  imports:

about:
  home: https://svnweb.cern.ch/trac/vdt
  license: GPL-3.0
  license_family: GPL
  license_file: Licence.txt
  summary: 'VectoriseD maTh C++ Library for Fast Math'

  description: |
    VDT is a library of mathematical functions, implemented in double and
    single precision. The implementation is fast and with the aid of modern
    compilers (e.g. gcc 4.7) autovectorisable.
  dev_url: https://github.com/drbenmorgan/vdt

extra:
  recipe-maintainers:
    - chrisburr
```

Compilers

- Originally relied on compilers installed on the system*
  - Use CentOS 5 for builds and rely on ABI versioning
  - Eventually packaged gcc 4.8.5 because C++11 support was needed
- Took a long time to figure out a proper solution
  - In October 2017 Anaconda 5.0 fixed this situation
  - conda-forge only finished their migration 2 weeks ago
  - Anaconda Distribution and conda-forge are harmonising
- Now much more maintainable for future updates
  - First release included gcc 7.3.0
  - gcc 8.2.0 is already available
- Based around cross-compiling

*This slide might get the details wrong

Host dependencies

- Since conda-build 3 the Anaconda distribution has used CDTs
  - Repackage libraries from CentOS 6 and move them to the sysroot of conda's pseudo-cross compilers
  - Used at build time for linking
  - Use libraries from the host at run time
  - Rely on ABI symbol versioning
- Why?
  - Lack of resources to create a recipe for a robust binary
  - Some libraries might have better performance when taken from the host
- conda-forge prefers to use it's own libraries
  - I think they're currently trying to harmonise
  - OpenGL is a library where performance is a consideration
    - Currently waiting for someone to find enough time to test if it makes a difference

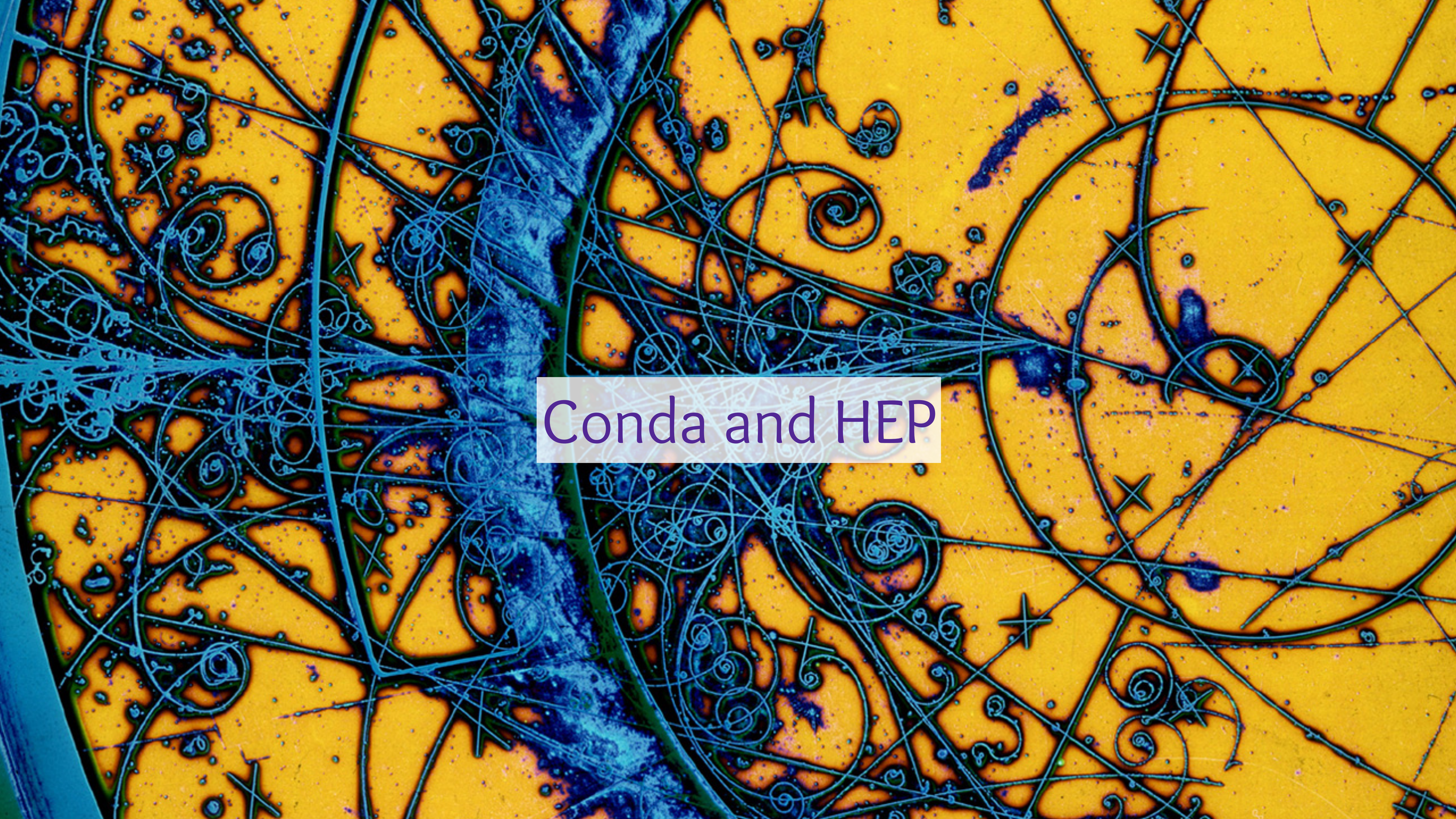
Prefix replacement

- Builds MUST be relocatable for conda
- Achieved by:
  - The usual RPATH tricks
  - Build and install to an environment with a very long path (255 characters)
  - When installing:
    - Text files: Effectively run sed on each file
    - Binary files: Effectively run sed on each file and append null bytes
- Mostly works, but occasionally needs some extra work
  - Example from patching ROOT's fork of clang:
    - Returning a constant path as a std::string doesn't work for different string lengths
    - Example from clang:

```
std::string Linux::computeSysRoot() const {
  return "/conda/conda-bld/clangdev-1234534/x86_64-conda_cos6-linux-gnu/sysroot";
}
```

```
std::string Linux::computeSysRoot() const {
  return conda_sysroot_directory();
}

extern "C"
{
  const char *conda_sysroot_directory();
}
```



Conda and HEP

Use in HEP

- A huge number of people in HEP already use conda
- It has even been by some experiments
  - XENON1T: https://indico.cern.ch/event/694818/contributions/2986393/
  - NEXT: https://indico.cern.ch/event/694818/contributions/2985799/
  - This was with the old compilers
- Lack of a ROOT package is inconvenient
  - Netherlands eScience Center built a package a few years ago
    - Stopped being maintained a while ago
    - Never worked reliably outside of RHEL 6 based distributions
- There is already a cling package inside conda-forge
  - Completely independent of HEP, used for the xeus-cling Jupyter kernel

ROOT in conda-forge

https://github.com/conda-forge/root-feedstock

- The day before conda-forge moved to the new compilers ROOT was added!

  Includes XRootD and its Python bindings

- Everything should work on any Linux distribution (macOS is a WIP)

```
wget http://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
sh miniconda.sh -b -p "${CONDA_INSTALL_LOCATION}"
# Add one of these to your shell rc file
source "${CONDA_INSTALL_LOCATION}/etc/profile.d/conda.sh"
source "${CONDA_INSTALL_LOCATION}/etc/profile.d/conda.csh"
source "${CONDA_INSTALL_LOCATION}/etc/fish/conf.d/conda.fish"
# Run it, source the rc file or open a new window
conda config --add channels conda-forge  # Make sure you don't already have a file called ~/.condarc

conda create --name root-example python=3.7 root scipy pandas
conda activate root-example
```

- GCC 7.3.0 included when installing (For now: Binaries are prefixed so $CC, $CXX, $LD... must be used)

- ROOT 6.16.00 was added today for Python 2.7, 3.6 and 3.7
  - Was delayed due to making some changes to the clang recipe
  - Release day updates are reasonable in future

Developed by Chris Burr, Enrico Guiraud, Henry Schreiner with help from Axel Naumann, Danilo Piparo, Guilherme Amadio and probably others whom I apologise for forgetting

Providing nightly binaries

- conda-forge doesn't support unreleased versions
  - Already struggle for CI resources sometimes (Travis CI, Circle CI, Appveyor and soon Azure)
- Builds of the conda package will be added to ROOT's nightlies soon
- Distributing the nightly builds of ROOT is potentially useful
  - Will likely upload the binaries from Jenkins to a dedicated channel
  - Anaconda.org channels cannot contain the word "root"
  - Have set up a "HEP" channel will probably be used instead

Conclusions

- Conda is very young
  - Lots of low hanging fruit to work on
  - Hacks that were used to get Anaconda working are being replaced with better solutions
    - Compiler infrastructure already replaced
    - Package file format: Version 2 proposal
  - Anaconda Inc. is investing heavily in conda-forge and is very open to external contributions
  - NUMFOCUS sponsors conda-forge
- Ultimately it doesn't matter…
  - The wider community has already decided to use conda
  - Later stages of HEP analysis are going to keep using it
- Also supports: **build variants, flexible version pinning, exporting/importing environments, …**

Questions?

The macOS SDK

- Conda builds everything* for macOS 10.9
- The macOS SDK cannot be distributed (legally)
- What should compilers distributed with conda use?
  - Especially now the SDK isn't available at / (macOS 10.14+)
- I've patched clang to
  - Look in common SDK locations
  - Set `MACOSX_DEPLOYMENT_TARGET=10.9`
  - See here and here for details

*A handful of recipes force a newer SDK when 10.9 isn't supported anymore