Hashdist – A tool for building and managing your scientific software distribution(s)

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`http://github.com/hashdist`

Acknowledgements

- Dag Sverre Seljebotn, Ondřej Čertík, Aron Ahmadia, Robert Maynord, Jimmy Tang, Lane Wittgen,...
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- Problem: You don't have root access to your machine.
- Solution: I need to add my software to a distribution that can handle all these cases.

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- Web apps (still needs good distribution)
- Matlab environment (a kind of distribution)
- Modules on HPC machines.

Background

- Proteus toolkit for PDE's was building its own stack with custom scripts, makefiles, and config files
- FENICS toolkit for PDE's had its own system (Dorsal)
- Various other DoD groups had their own Python distributions
- Could possibly have added to sage or enthough distributions but would require many new packages

Requirments for new system

- Must support mixing source and "host" packages (e.g. vendor MPI)
- Must support version control and reproducibility across users
- Must support many kinds of packages (Python, C++, Fortran,...)
- Must support needs of developers (building from git repos, trying new packages,...)

Scientific code

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- Dependencies are good: Can build on works of others
- Often happens: "Large frameworks" bundling things together
  - PETSc and Trilinos for solving PDEs
  - As soon as you want to push boundaries there's a lot of dirty work ahead

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- Sometimes you **need** the very latest version
- Fortran/C++ instead of C/Java/.NET
- Intersection of “need speed” and “do not pay dedicated application sysadmins”

Combinatorial explosion

```
/cluster/software/VERSIONS/hdf5-1.6.1/lib/libhdf5.so
/cluster/software/VERSIONS/hdf5-1.6.1_intel/lib/libhdf5.so
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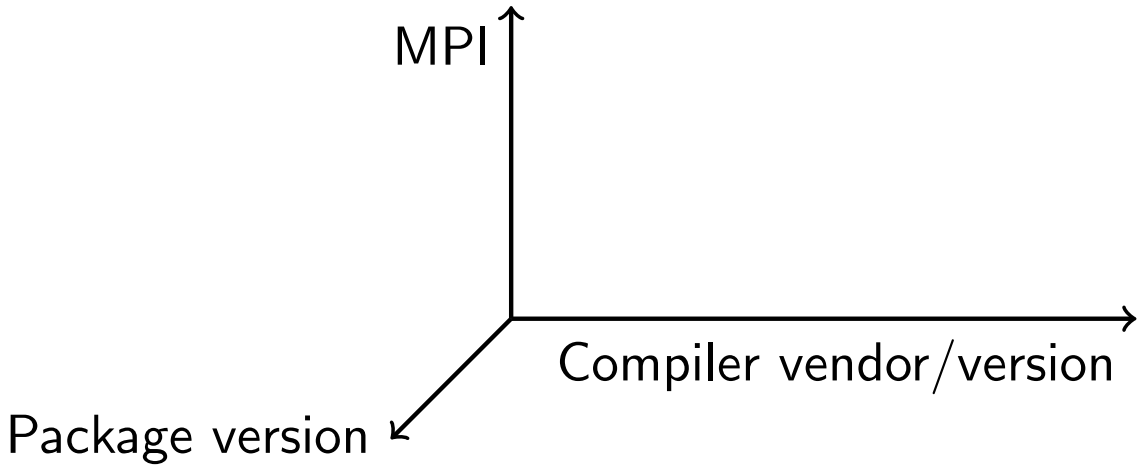

$\times$ LAPACK $\times$ FFT library $\times$ IDL/Python version...

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  - The sysadmins hate them
  - The users need newer/their own libraries

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  - 5 different within DoD (incl. python-hpcmp)
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- The details are different for everybody

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- Debian, RedHat, cluster sysadmins, dorsal is all about curated software stacks
- Perhaps you want 60% curated, 20% bleeding edge or manually tweaked, 20% your own code...
- The community using and supporting a distribution is as important as most of the other details.

HashDist Theory

Stateful vs. Functional

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- Main idea: create build artifact coordinates by hashing the input state and store the build artifacts in a "database" keyed on those hashes.
- Using the hash idea we can treat package building in a functional manner rather than a stateful manner (idea comes from Eelco Doltstra/Nix)

Cryptographic/secure hashing

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$h(\texttt{'The dark fox'}) = h(\texttt{54686520646172b20666f78}\text{ hex})$
$= \texttt{b6589fc6ab0dc82cf12099d1c2d40ab994e8410c}\text{ hex}$

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Example: git

```
$ (cd code/hashdist/.git/objects; find)
./59/5a2f8e3890d0ece24514f3e32ae874f1f03ac2
./2f/780151688e1f122a5b9072d42009c80c36140c
./2f/4b2eef40b51bc2d46027d1864653b37dd05f8f
./2f/237d74e3f81f498212629ac0b96bedac4b0b36
./2f/dff799c54fed6fe96a91e1d5f1593996228ebc
./2f/27bd4efa5f8521fb98eb82181a67aae97b7f1a
./2f/3fedf882f1b28905199961356f4e00281ddf76
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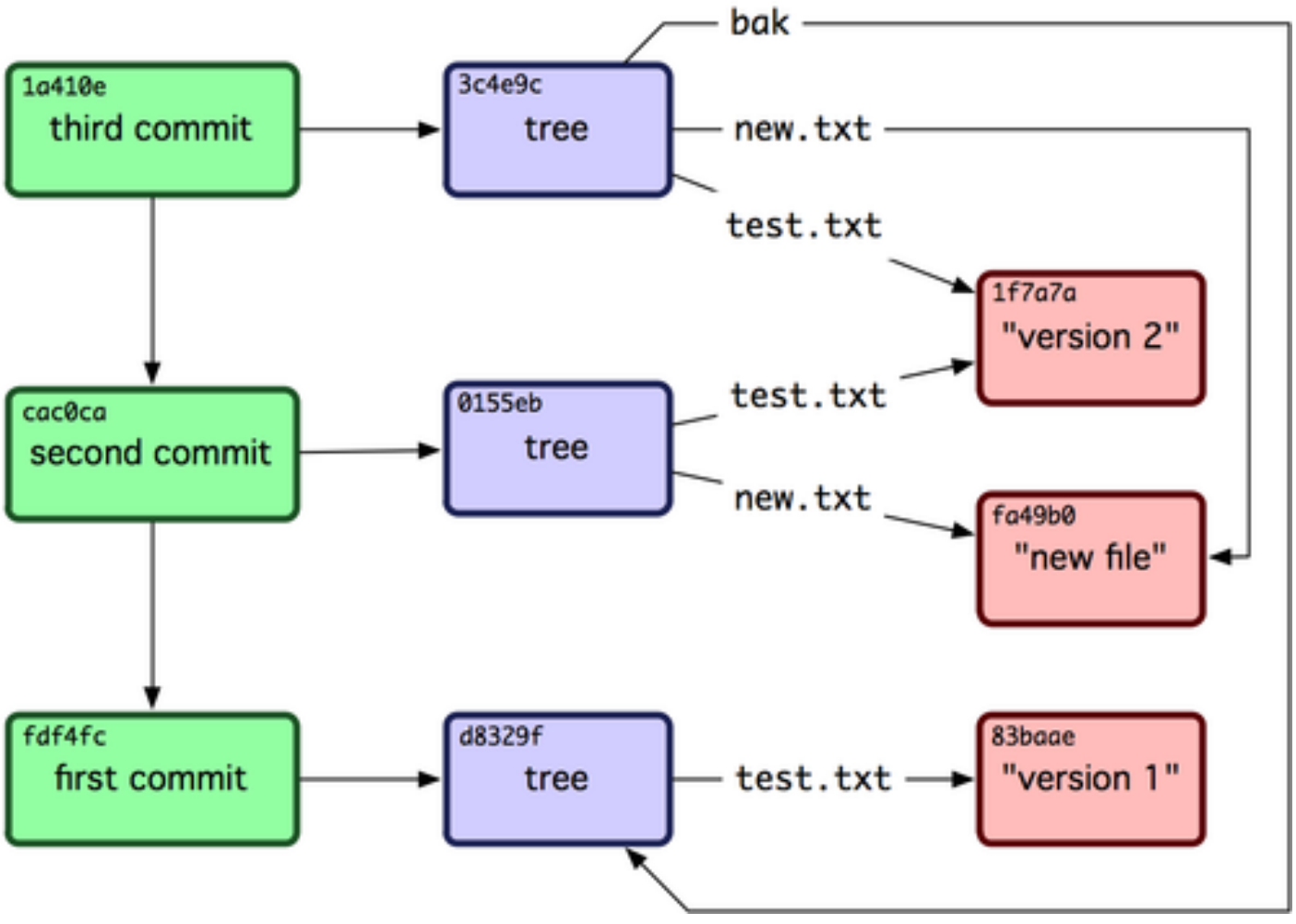

1a410e
third commit
3c4e9c
tree
bak
new.txt
test.txt
1f7a7a
"version 2"
cac0ca
second commit
0155eb
tree
test.txt
new.txt
fa49b0
"new file"
fdf4fc
first commit
d8329f
tree
test.txt
83baae
"version 1"

cython / cython

Pull Request | Unwatch | Unstar 310 | Fork 113

Code | Network | Pull Requests 14 | Wiki | Graphs | Settings

Graph | Members

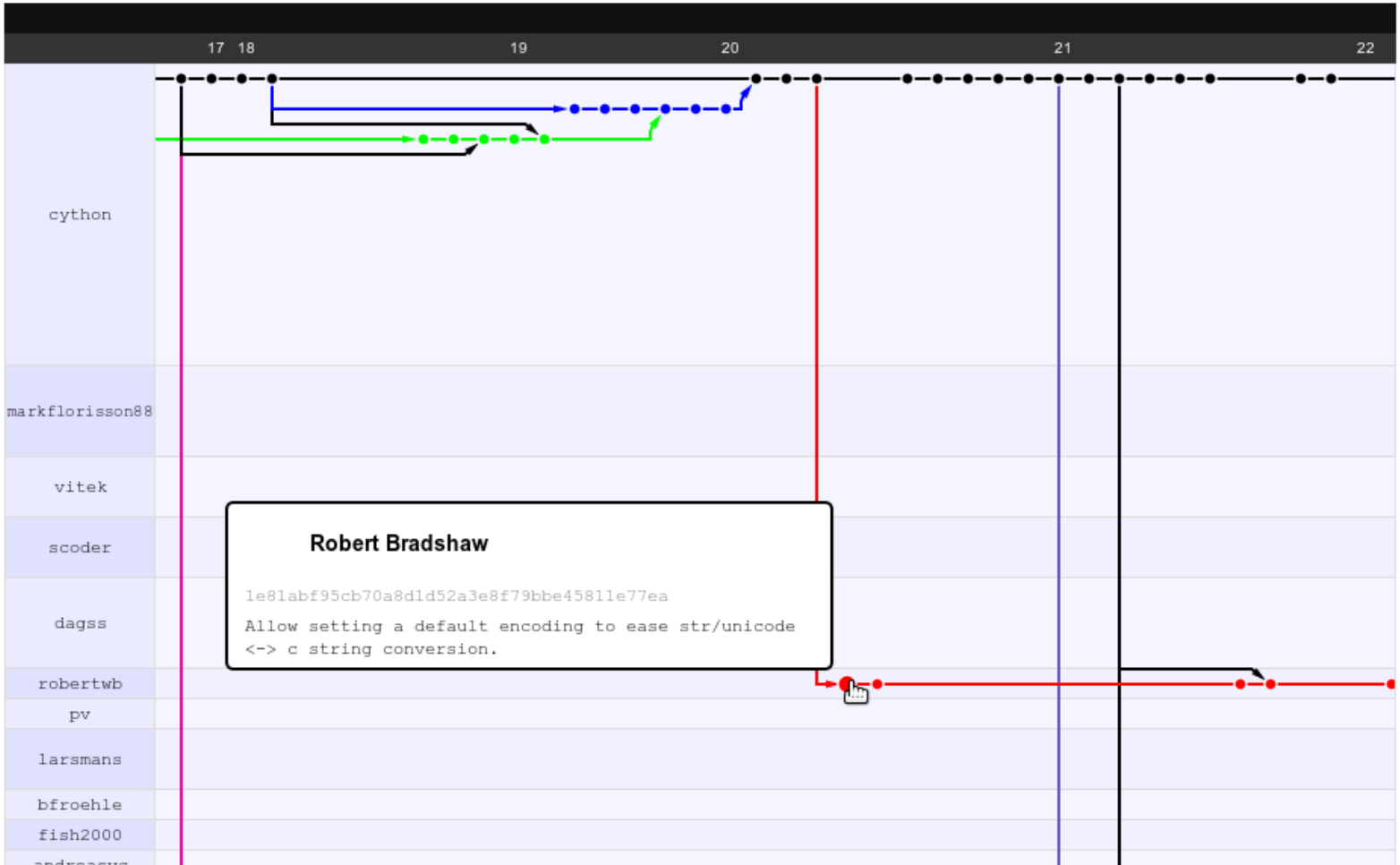
The cython network graph

Keyboard shortcuts available

*All branches in the network using **cython/cython** as the reference point. Read our blog post about how it works.*

Show Help

Last updated: 12 minutes ago



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- Hashdist:

  `~/.hashdist/bld/hdf5/pe7l56vsgg43`
  `~/.hashdist/bld/hdf5/tkiwsppxzc3r`

  (really `hdf5/tkiwsppxzc3ro3q7pyjjxq45jgh3wwcd`)

Step 1: Hash the build

Internal protocol!

```
{
  "build" : {
    "commands" : [
      {
        "cmd" : [
          "$BASH",
          "_hashdist/build.sh"
        ]
      },
    ],
    "import" : [
      {
        "id" : "zlib/3vq2jgzdjakdhpzvpvtrbzbcrtg6etrh",
        "ref" : "ZLIB"
      }
    ]
  },
  "name" : "hdf5",
  "sources" : [
    {
      "key" : "tar.bz2:l2q3vax4o42q5zriw6k243w6ax7ov4og",
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Step 2: Every build installs to separate location

Same as with the “module load“ system:

```
$ echo bld/*/* bld/adh/hwz2wmrcnbj7 bld/adh/lvpjelejrldo
bld/bzip2/zuo2tlurm7ez bld/cython/bidpqe4yx6gl bld/cython/pb
bld/cython/xoju62amg7pm bld/daetk/dpoolktbk3si
bld/docutils/ckp3lhso6vek bld/docutils/uv2667zawv7v
bld/docutils/yekwczohjna7

$ ls bld/zmq/x7ogmtwtkola/lib
pkgconfig  libzmq.a  libzmq.so  libzmq.so.3  libzmq.so.3.0.0
```

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Unlike "module load" we don't need LD_LIBRARY_PATH:

```
$ ldd bld/hdf5/tkiwsppxzc3r/lib/libhdf5.so
linux-vdso.so.1 =>  (0x00007fffe21fe000)
libpthread.so.0 => /lib/x86_64-linux-gnu/libpthread.so.0 (0x
libz.so.1 => /home/cekees/.hashdist/bld/zlib/3vq2jgzdjakd/li
libdl.so.2 => /lib/x86_64-linux-gnu/libdl.so.2 (0x00007f9d0c
libm.so.6 => /lib/x86_64-linux-gnu/libm.so.6 (0x00007f9d0cb8
libmpich.so.10 => /home/cekees/.hashdist/bld/mpich/4ztabf2u2
libc.so.6 => /lib/x86_64-linux-gnu/libc.so.6 (0x00007f9d0c35
/lib64/ld-linux-x86-64.so.2 (0x00007f9d0d9dc000)
libmpl.so.1 => /home/cekees/.hashdist/bld/mpich/4ztabf2u23u2
librt.so.1 => /lib/x86_64-linux-gnu/librt.so.1 (0x00007f9d0b
libgcc_s.so.1 => /lib/x86_64-linux-gnu/libgcc_s.so.1 (0x000
```

Step 3: Make a profile with links

```
$ ls -la bld/profile/ycz6e4bztfgd/bin
bunzip2 -> ../../../bzip2/zuo2tlurm7ez/bin/bunzip2
bzcat -> ../../../bzip2/zuo2tlurm7ez/bin/bzcat
bzcmp -> ../../../bzip2/zuo2tlurm7ez/bin/bzcmp
...
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- ```
  ~/mystack $ git fetch from-someone-else
  ~/mystack $ git checkout someone-elses-branch
  ~/mystack $ hit build # pause for extra builds
  ~/mystack $ ~/local/bin/python --version
  Python 2.7.3
  ```

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  ~/mystack $ ls
  default.yml sources.yml build.yml abel-cluster.yml
  ```
- ```
  ~/mystack $ hit build # takes some time
  ~/mystack $ ~/local/bin/python --version
  Python 2.7.2
  ```
- ```
  ~/mystack $ hit build # instant
  ```
- ```
  ~/mystack $ git fetch from-someone-else
  ~/mystack $ git checkout someone-elses-branch
  ~/mystack $ hit build # pause for extra builds
  ~/mystack $ ~/local/bin/python --version
  Python 2.7.3
  ```
- ```
  ~/mystack $ git checkout paper-from-2010
  ~/mystack $ hit build # instant
  ~/mystack $ ~/local/bin/python --version
  Python 2.6.3
  ```
  ```

Consequences of hash-based installation

1. More dimensions! Even
   `.../h5py-hdf5_1.8.9_pgi-python2.7-numpy1.6.3_debug_ubuntu12.10`
   is not exhaustive; "`h5py/5ffg...`" caters for everything

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Sophisticated features with simple implementation

Prior art: Eelco Dolstra's PhD thesis/the Nix project

Demo

- Show a stack/distribution profile spec
- Show package spec and modify source hash (to build new artifact)
- Show package spec and modify build options (to build new artifact)
- Revert package spec to show no rebuild occurs
- Show 'hit develop' to build a "virtual env"

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- Soon: relocatable builds, ipython notebook integration, flexible constraints