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 Maynard, 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 PDEs was building its own stack with custom scripts, makefiles, and config files
- FENICS toolkit for PDEs had its own system (Dorsal)
- Various other DoD groups had their own Python distributions
- Could possibly have added to Sage or Enthought distributions but would require many new packages and modifications to reuse “host“ packages (e.g. vendor MPI)

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,...)

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- 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
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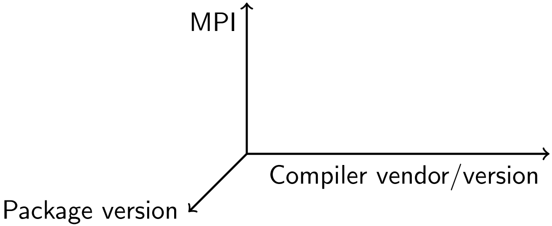

MPI

Compiler vendor/version

Package version

× LAPACK × FFT library × 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)
  - Sage
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- The details are different for everybody

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- Debian, RedHat, cluster sysadmins, dorsal are 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.

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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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$h(\texttt{'The dark fox'}) = h(\texttt{546865206461726b20666f78}\text{ hex})$
$= \texttt{b6589fc6ab0dc82cf12099d1c2d40ab994e8410c}\text{ hex}$

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$=$ `da4b9237bacccdf19c0760cab7aec4a8359010b0` hex

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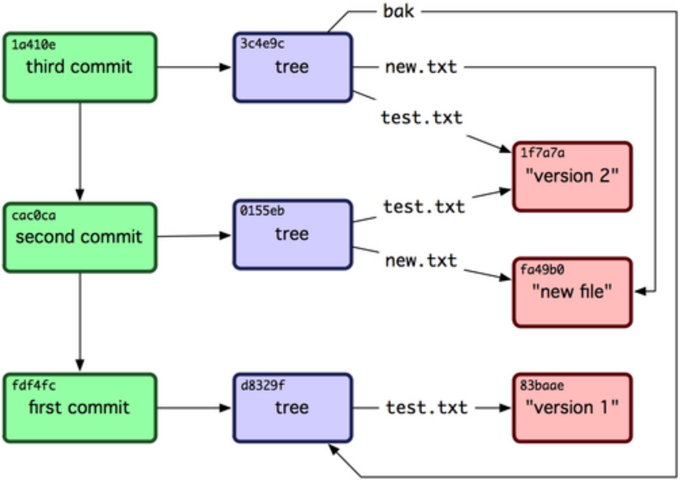
bak
1a410e
third commit
3c4e9c
tree
new.txt
test.txt
1f7a7a
"version 2"
cac0ca
second commit
0155eb
tree
test.txt
new.txt
fa49b0
"new file"
fdf4fc
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d8329f
tree
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83baae
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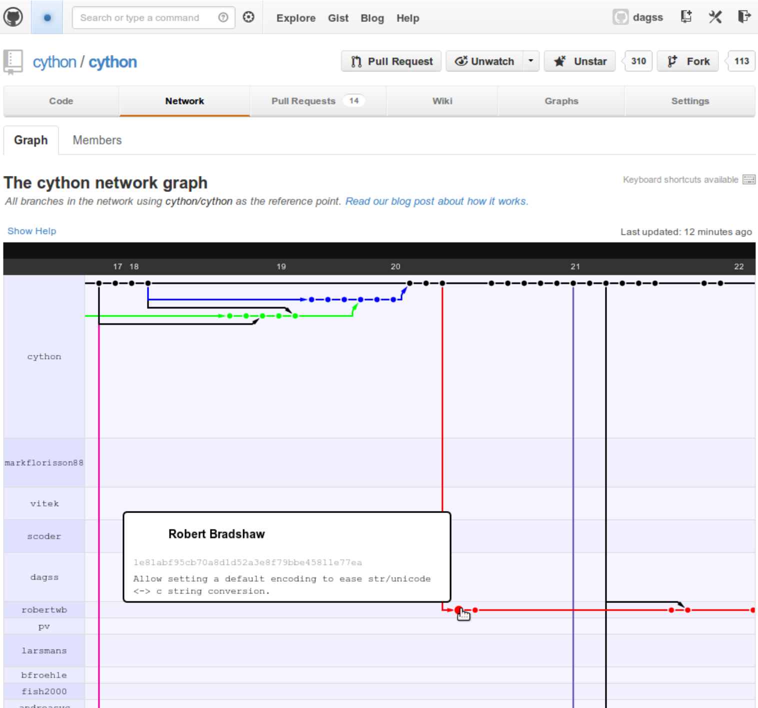

The cython network graph

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

Last updated: 12 minutes ago

Robert Bradshaw

1e81abf95cb70a8d1d52a3e8f79bbe45811e77ea

Allow setting a default encoding to ease str/unicode
<-> c string conversion.

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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",
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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 (0x0000
```

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
...
```

Branchable software stack

-
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  default.yml sources.yml build.yml abel-cluster.yml
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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
  ```

Branchable software stack

-
  ```
  ~/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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   $ hit build
   # ...then power shuts down, but you're good
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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