Hashdist – Yet Another Desperate Attempt at Fixing Scientific Software Distribution

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Simula, January 24, 2013

`http://github.com/hashdist`

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The Problem

HPC software distribution

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-
  ```
  $ ls /usr/mpi/*
  /usr/mpi/gcc:
  mvapich-1.2.0  mvapich-1.2.0-qlc  mvapich2-1.7
  mvapich2-1.7-qlc  openmpi-1.4.3  openmpi-1.4.3-qlc
  /usr/mpi/intel:
  mvapich-1.2.0-qlc  mvapich2-1.7-qlc  openmpi-1.4.3-qlc
  /usr/mpi/pgi:
  mvapich-1.2.0-qlc  mvapich2-1.7-qlc  openmpi-1.4.3-qlc
  ```

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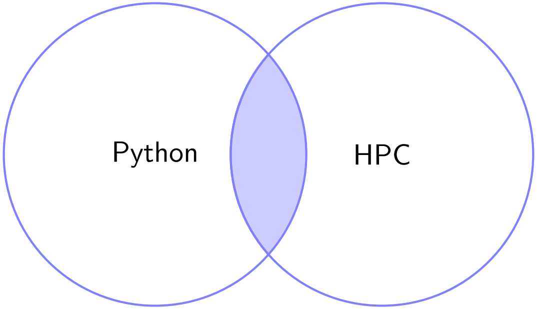

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- Python environment provided by sysadmins: Outdated

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Sage, python-hpcmp, dorsal, EasyBuild, Hans Petter's Python script:

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- The details are different for everybody
  - Best LAPACK for Sage is not best LAPACK for EPD/Anaconda

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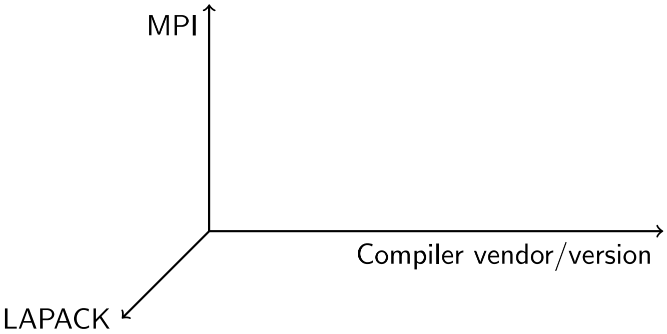
- Reproducibility

The real knot

Combinatorial explosion:



$\times$ Python version $\times$ NumPy version $\times$ FFT library...

Curation

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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 configured, 20% your own code...

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- Ubuntu + root access: Make your own PPA
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- dorsal, EasyBuild: Contribute your own configuration
  - `dolfin.package` vs. `dolfin-intel.package`

Hashdist

Hash-based installation

- Linux laptop:
  `/usr/lib/libhdf5.so`

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- HPC environment modules:

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

  ```
  ~/.hdist/opt/hdf5/efn3/lib/libhdf5.so
  ~/.hdist/opt/hdf5/i7ni/lib/libhdf5.so
  ~/.hdist/opt/hdf5/qgpd/lib/libhdf5.so
  ```

  (really `hdf5/efn3i7ni7lbtik4frlb5wcnqgpdmi3ql`)

(demo)

Using a hash-based software store

(1) Describe the build (**internal protocol!**)

```
{ "import" : [{ "id" : "gcc/apyicmxgafb564zz7rwhwvon7padvxdx"},
                { "id" : "virtual:unix"},
                { "id" : "zlib/wbg27phinbgwjg4nasb4xzf3ypo72otn"}],
   "sources" : [{ "key" : "tar.bz2:7jxgwn5xs5xnvsdaomvypridodr35or2"}],
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(3) If not found, do an *isolated* build on the fly

Using a hash-based software store

(4) When all packages are built create symbolic links to package contents in a *profile*:

```
$ ls -l ~/local
local -> /home/dagss/.hdist/opt/profile/w6gp

$ ls -l /home/dagss/.hdist/opt/profile/w6gp/bin
h5copy -> /home/dagss/.hdist/opt/hdf5/whfk/bin/h5copy
h5ls -> /home/dagss/.hdist/opt/hdf5/whfk/bin/h5ls
...

$ ldd /home/dagss/.hdist/opt/hdf5/whfk/lib/libhdf5.so
linux-vdso.so.1 => (0x00007fffeb3ff000)
libsz.so.2 => /home/dagss/.hdist/opt/szip/5a5t/lib/libsz.so.2
libz.so.1 => /home/dagss/.hdist/opt/zlib/cl16/lib/libz.so.1
libm.so.6 => /lib/x86_64-linux-gnu/libm.so.6
libc.so.6 => /lib/x86_64-linux-gnu/libc.so.6
/lib64/ld-linux-x86-64.so.2
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1. More dimensions! Even
   `.../h5py-hdf5_1.8.9_pgi-python2.7-numpy1.6.3_debug_ubuntu12.10`
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Sophisticated features with simple implementation

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

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-
  ```
  ~/mystack $ rm -rf ~/.hdist/opt/*
  ~/mystack $ hdist shell . # takes quite some time
  ~/mystack $ python --version
  Python 2.6.3
  ```

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Some help:

- Integrate with host system (Debian, environment modules, “generic”) to specify dependencies on package on host system
- “hdist-jail” can issue warnings if a build process accesses files it shouldn’t (or hide them)

User-facing software stack definitions

Declarative approach (because you can git it and share it):

```
include:
  - sources # pull in ./sources.yml
  - build
  - when cluster == "abel":
    - abel-overrides
profiles:
  - name: "default"
    configuration:
      lapack_type: "openblas"
      cluster: "hexagon"
    select:
      - project: "hdf5"
        version: 1.8.2
      - project: "h5py"
        ...
```

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        version: 1.8.2 to 1.8.5 # with integer linear programming
      - project: "h5py"
        ...
```

For stack developers: DSL focused on overrides

Manage the combinatorial explosion without creating packages for `hdf5_intel_mpich`, `hdf5_gcc_openmpi`, ...:

```
rules:
  ...
  CFLAGS: ["-g", "-O$optlevel"]
  when recipe == "configure-make-install":
    optlevel: 2
  when project == "hdf5":
    recipe: "configure-make-install"
    when version == 1.5.2:
      optlevel: 0
    build_deps:
      - project: "zlib"
        version: 1.2.5 to 1.2.7
  ...
```

Temporary internal representation in Hashdist

```
dict(
 package='hdf5',
 version='1.8.10',
 recipe='configure-make-install',
 downloads=['http://www.hdfgroup.org/ftp/HDF5/current/'
            'src/hdf5-1.8.10.tar.bz2'],
 sources=['tar.bz2:7jxgwn5xs5xnvsdaomvypridodr35or2'],
 configure=['--prefix=$ARTIFACT', '--with-pic'],
 CFLAGS=['-O2'],
 jail='warn',
 build_deps=[zlib, unix, gcc]
)
```

For Hashdist developers

Feed it through a Python pipeline:

```
@pipeline.add_recipe('configure-make-install')
def configure_make_install_recipe(ctx, cfg, build):
    build['build']['script'].extend([
        ["LDFLAGS=$(hdist", "build-ldflags", ")"],
        ["CFLAGS=$(hdist", "build-cflags", ")"],
        ["CFLAGS+= " + " ".join(cfg.CFLAGS)],
        ['./configure'] + cfg.configure,
        ['make'],
        ['make', 'install']
        ])
```

Generated, read by Hashdist developers while debugging

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