

# reproducible and user-controlled software management in HPC

with **GNU Guix**

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# System Admins

prefer **mature** software,  
no variants, only apply  
unavoidable updates

use **stable** software  
for **systems**

# Users

want **fresh** software,  
multiple variants, latest  
tools, **flexibility**

manage **user software**  
stack on their own

ad-hoc

There is no way to **reproduce** the environment, even on the same machine at a different point in time.

volatile

Due to a **lack of isolation**, the environment will change or even break when the host system changes.

primitive

**No safe upgrades or roll-backs.**  
No separation for different workflows.  
**Unportable.**

?



easybuild

CONDA



**Spack**

# Installing software is easy now!

## ...but reproducibility is still out of reach

 Open boegel opened this issue on Nov 5, 2013 · 0 comments



boegel commented on Nov 5, 2013

Member



It *seems* like the GCC libraries (e.g. `libiberty.a`) sometimes end up being built with `-fPIC` (e.g. on SL5), and sometimes not (e.g. on SL6), while `eb` is performing the exact same build procedure.

This causes problems for `cairo` (see ) and `ExtraE` (part of UNITE), which require `libiberty.a` to be built with `-fPIC`. The `cairo` builds works fine on SL5, but doesn't work on SL6 (see also [hpcugent/easybuild-easyconfigs#494](#) (comment)).

# Installing software is easy now!

## ...but reproducibility is still out of reach



**citibeth** commented on Oct 23, 2016

Collaborator



Good news, I ran into this problem too. But only on SOME computers... I don't yet know why some but not all. Anyway... look in the generated `spconfig.py` files, I see the following:

```
env['PATH'] = ":".join(cmdlist("""
/gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/cmake-3.6.1-xfzr
/gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/python-3.5.2-d5i
/gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/netcdf-cxx4-4.3.
/gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/py-numpy-1.11.1-
/gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/udunits2-2.2.20-
/gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/proj-4.9.2-f6543
/gpfsm/dnb53/rpfische/spack3/lib/spack/env
/gpfsm/dnb53/rpfische/spack3/lib/spack/env/case-insensitive
/gpfsm/dnb53/rpfische/spack3/lib/spack/env/gcc
/gpfsm/dnb53/rpfische/spack3/opt/spack/linux-SuSE11-x86_64/gcc-5.3.0/binutils-2.27-vd
/home/rpfische/git/modele-control/bin
/usr/local/other/SLES11.3/openmpi/1.10.1/gcc-5.3/bin
/usr/local/other/SLES11.3/gcc/5.3.0/bin
/usr/local/other/SLES11.3/git/2.7.4/libexec/git-core
/usr/local/other/SLES11.3/git/2.7.4/bin
```



seibert commented on May 13, 2015

There can be non-trivial issues with glibc that make it hard to distribute truly portable packages. I've been in situations where I couldn't easily deal with the range of Linux distributions that my colleagues were using.

## After activating an environment `libs/linux.so.1: cannot open shared object file` #5640

[Open](#) Nagasaki45 opened this issue 16 days ago · 1 comment



Nagasaki45 commented 16 days ago · edited

I have an `environment.yml` file as pasted below. When I create an environment from it, and activate it, I see some weird bugs:

```
(myenv) $ vim
vim: error while loading shared libraries: libs/linux.so.1: cannot open shared object file: No such file or directory

(myenv) $ /bin/python
Could not find platform architecture
Could not find platform architecture
Consider setting $PYTHONARCH to a platform architecture
Fatal Python error: Py_Initialize: ModuleNotFoundError: No module named 'platform'

Current thread 0x0000000000000000 (most recent call first):
  [1] 7891 abort ()
```

## libgfortran broken? #686

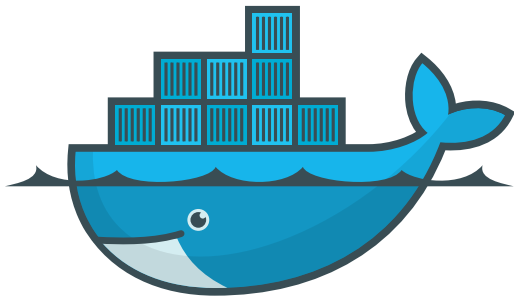
[Open](#) swryan opened this issue on Mar 7, 2016 · 35 comments



swryan commented on Mar 7, 2016

Started getting this error a couple days ago:

```
ImportError: /home/travis/miniconda/lib/python2.7/site-packages/scipy/special/../../..
/libgfortran.so.3: version GFORTRAN_1.4' not found (required by /usr/lib/liblapack.so.3gf)
```



docker



**100% reproducible**

**We have all the bits!**

**100% reproducible**

**We have all the bits!**

**100% stateful**

**We only have the bits!**

# App bundles are convenient

lack means of  
abstraction

don't compose well

are like giant statically  
linked binaries

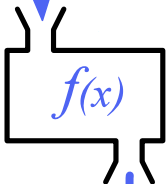


The logo for VGuix features a stylized lowercase 'v' on the left, rendered as a thick, flowing ribbon with a yellow-to-orange gradient. To the right of the 'v' is the word 'Guix' in a bold, black, sans-serif font.

**vGuix**

# Functional packaging

headers  
sources  
build tools  
libraries  
...



```
cabba9e-emacs-24.5/  
├─ bin  
│   └─ emacs  
├─ lib  
│   └─ ...
```

# Functional packaging

Same inputs?  
Same output!

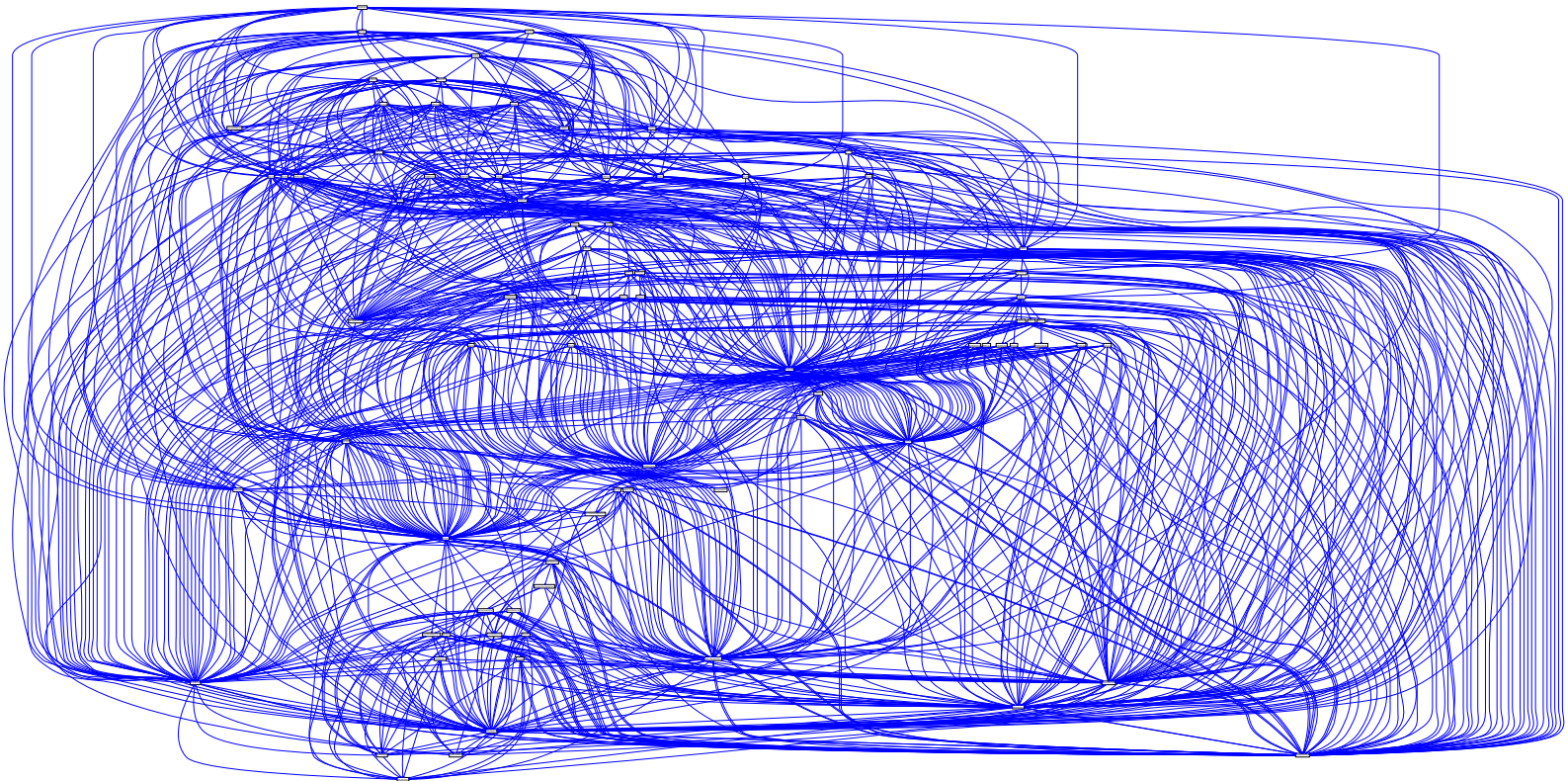
```
cabba9e-emacs-24.5/
```

```
| bin  
|  └─ emacs  
└─ lib  
    └─ ...
```

Different inputs?  
Different outputs.

```
dedbeef-emacs-24.5/
```

```
| bin  
|  └─ emacs  
└─ lib  
    └─ ...
```



```
guix gc --references  
  /gnu/store/...-foo-0.9
```

```
/gnu/store/...-glibc-2.25  
/gnu/store/...-gcc-4.9.3-lib  
/gnu/store/...-bar-0.7b  
/gnu/store/...-baz-1.4.9  
/gnu/store/...-foo-0.9
```



```
guix package -i baz  
  --with-input=foo=bar
```

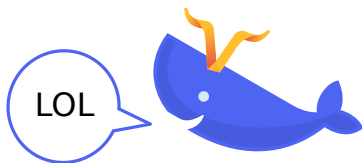
```
guix package -i baz  
  --with-source=baz-1.0.tgz
```

```
guix pack  
  samtools bedtools
```

```
/gnu/store/...-pack.tar.gz
```

```
guix pack -f docker  
          samtools bedtools
```

```
/gnu/store/  
...-docker-pack.tar.gz
```



```
guix package  
  --manifest=GeneNetwork
```

All you need is:

Guix version + package manifest

(+ source code)

- 1.** The level of abstraction matters
- 2.** Guix enables reproducible and safe experimentation
- 3.** Guix makes environment sharing easy
- 4.** There are ways to use Guix without root access
- 5.** Like Conda?  
`guix package -i conda`

# Learn more!

Poster A-142

#guix on [irc.freenode.net](http://irc.freenode.net)

<http://gnu.org/s/guix>

[ricardo.wurmus@mdc-berlin.de](mailto:ricardo.wurmus@mdc-berlin.de)

[pjotr.public34@thebird.nl](mailto:pjotr.public34@thebird.nl)

/home/rekado/.guix-profile

/var/guix/...

guix-profile

42

/gnu/store

hscq14x...-profile

bin

samtools

bowtie2

rhrdst11m...-samtools-1.2

bin

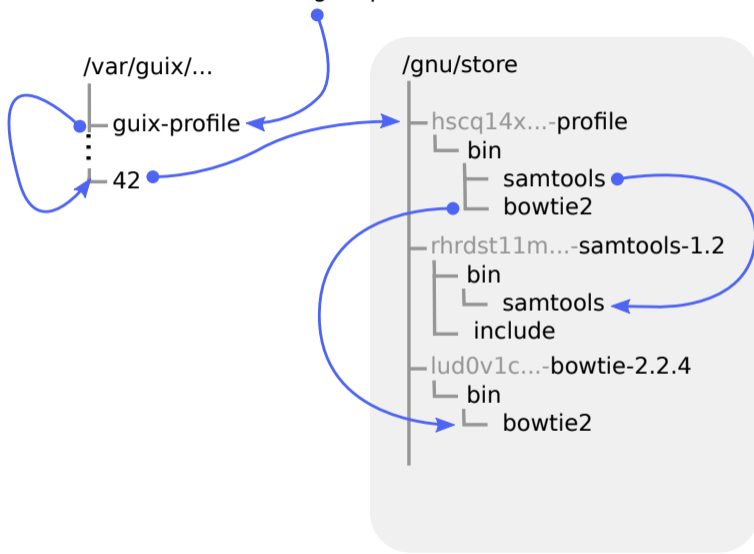
samtools

include

lud0v1c...-bowtie-2.2.4

bin

bowtie2



/home/rekado/.guix-profile

/var/guix/...

guix-profile

42

43

/gnu/store

hscq14x...-profile

bin

samtools

bowtie2

rhrdst11m...-samtools-1.2

bin

samtools

include

lud0v1c...-bowtie-2.2.4

bin

bowtie2

z3braf1sh...-profile

bin

samtools



/home/rekado/.guix-profile

/var/guix/...

guix-profile

42

43

/gnu/store

hscq14x...-profile

└─ bin

└─ samtools

└─ bowtie2

rhrdst11m...-samtools-1.2

└─ bin

└─ samtools

└─ include

lud0v1c...-bowtie-2.2.4

└─ bin

└─ bowtie2

z3braf1sh...-profile

└─ bin

└─ samtools

/home/rekado/.guix-profile

/var/guix/...

guix-profile

43

/gnu/store

hscq14x...-profile

└─ bin

└─ samtools

└─ bowtie2

rhrdst11m...-samtools-1.2

└─ bin

└─ samtools

└─ include

lud0v1c...-bowtie-2.2.4

└─ bin

└─ bowtie2

z3braf1sh...-profile

└─ bin

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└─ samtools

└─ include

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└─ bin

└─ samtools

