



# Dependable Software Deployment with Guix

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InPEx Workshop, Sitges, Catalunya

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*Inria*

- 
- ▶ **Guix since 2012**
  - ▶ **Guix-HPC since 2017 (Inria, MDC, UBC, UTHSC)**
  - ▶ **tools for reproducible software deployment**
  - ▶ **50,000+ packages**
  - ▶ **100 monthly contributors**

<https://hpc.guix.info>

- ▶ **PlaFRIM** (FR): Inria Bordeaux (3,000+ cores)
- ▶ **GriCAD** (FR): Grenoble (1,000+ cores)
- ▶ **GLICID** (FR): Nantes (4,000+ cores)
- ▶ **Grid'5000** (FR): 8 sites (12,000+ cores)
- ▶ **Max Delbrück Center** (DE): 250-node cluster + workstations
- ▶ **UMC Utrecht** (NL): 68-node cluster (1,000+ cores)
- ▶ ...

# **1. Robust deployment.**

## Redeploy environments: 2 files, 2 commands

1. `guix describe -f channels > channels.scm`
2. `guix time-machine -C channels.scm -- \`  
`shell -m manifest.scm`

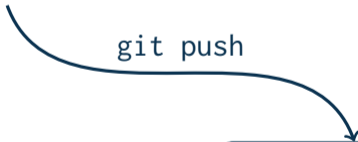
```
(define python  
  (package ...))
```

test



```
guix build python  
/gnu/store/...-python-3.9.6
```

git push



**Git repository**

(define python  
(package ...))

test

guix build python  
/gnu/store/...-python-3.9.6

git push

**Git repository**

*guix pull*

**user**

(define python  
(package ...))

test

guix build python  
/gnu/store/...-python-3.9.6

git push

guix pull

**Git repository**

user

get binaries

build farm

pull



## **build processes**

chroot, separate UIDs

**build daemon**

## **client commands**

```
guix build hello
```

## **build processes**

chroot, separate UIDs

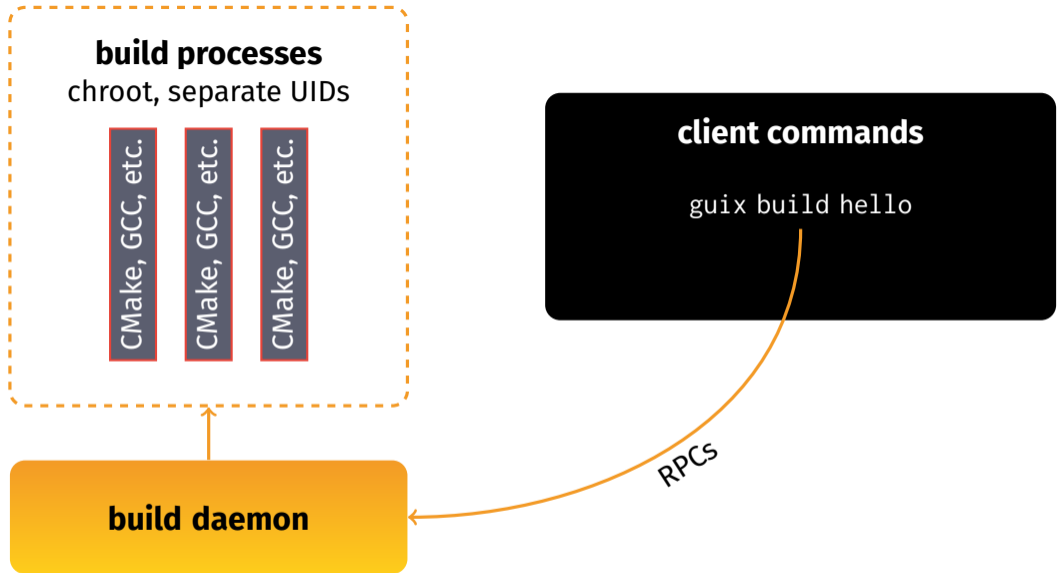
## **client commands**

```
guix build hello
```

**build daemon**

RPCs






















```
graph TD; A[client commands] -- RPCs --> B[build daemon];
```



Channel	Commit
<a href="https://gitlab.inria.fr/guix-hpc/guix-hpc.git">https://gitlab.inria.fr/guix-hpc/guix-hpc.git</a>	<a href="#">f002aad7b66cd215b6a1720c48f08ed73f2661d5</a>
<a href="https://git.savannah.gnu.org/git/guix.git">↑ https://git.savannah.gnu.org/git/guix.git</a>	<a href="#">7b0f145802f0c2c785014293d748721678fef824</a>

## Builds

All 36  Scheduled 0  Succeeded 32  Failed 4

ID 	Completion time 	Job 	Name 	System 
  <a href="#">714970</a>	1 Jun 18:19 +0200	rochpl.x86_64-linux	rochpl-5.7.1	x86_64-linux
  <a href="#">714967</a>	1 Jun 18:17 +0200	rocbblas.x86_64-linux	rocbblas-5.7.1	x86_64-linux
  <a href="#">714971</a>	27 May 13:48 +0200	rochpl.x86_64-linux	rochpl-5.6.1	x86_64-linux
  <a href="#">714964</a>	27 May 13:44 +0200	rocbblas.x86_64-linux	rocbblas-5.6.1	x86_64-linux
  <a href="#">714973</a>	27 May 11:30 +0200	rochpl.x86_64-linux	rochpl-5.4.4	x86_64-linux
  <a href="#">714972</a>	27 May 11:06 +0200	rochpl.x86_64-linux	rochpl-5.5.1	x86_64-linux
  <a href="#">714966</a>	27 May 11:04 +0200	rocbblas.x86_64-linux	rocbblas-5.5.1	x86_64-linux
  <a href="#">714948</a>	27 May 09:50 +0200	py-melissa-core.x86_64-linux	py-melissa-core-1.0.0-2.d8de4d5	x86_64-linux

<https://hpc.guix.info/blog/2023/03/contiguous-integration-and-continuous-delivery-for-hpc/>

## **2. Flexibility.**

- ▶ <https://github.com/guix-science/guix-science>
  - ▶ RStudio Server, JupyterLab, Grid Engine, ...
- ▶ <https://github.com/guix-science/guix-science-nonfree>
  - ▶ CUDA, PyTorch with CUDA, oneAPI MKL, ...
- ▶ <https://gitlab.inria.fr/guix-hpc/guix-hpc>
  - ▶ ROCm/HIP, StarPU, Chameleon, Maphys, Simgrid, ...
- ▶ ...

<https://hpc.guix.info/channels>

```
guix install hwloc \  
  --with-source=./hwloc-2.1rc1.tar.gz
```

```
guix shell intel-mpi-benchmarks \  
  --with-input=openmpi=mpich
```

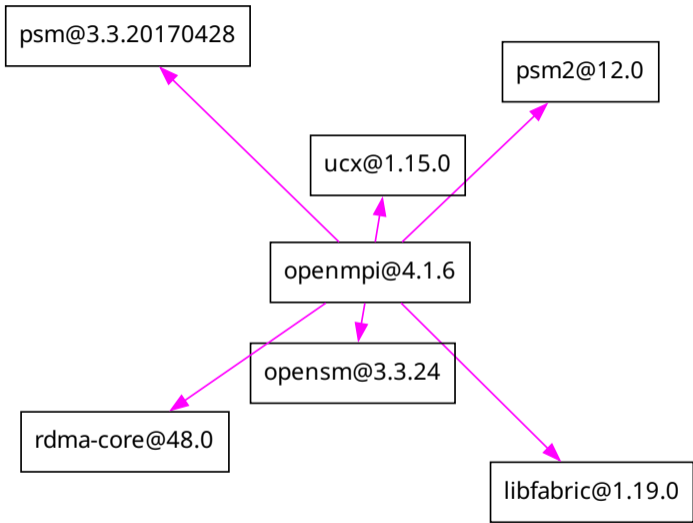
```
guix build dealii \  
  --with-branch=kokkos=master
```

- ▶ `--with-commit`
- ▶ `--with-patch`
- ▶ `--with-input`
- ▶ `--with-c-toolchain`
- ▶ `--with-graft`
- ▶ ...

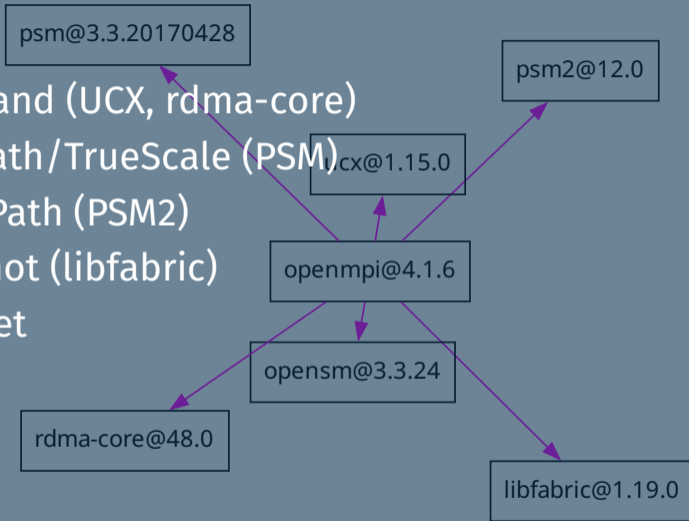
[https://guix.gnu.org/manual/en/html\\_node/  
Package-Transformation-Options.html](https://guix.gnu.org/manual/en/html_node/Package-Transformation-Options.html)



### **3. Performance portability.**



- ▶ InfiniBand (UCX, rdma-core)
- ▶ InfiniPath/TrueScale (PSM)
- ▶ Omni-Path (PSM2)
- ▶ Slingshot (libfabric)
- ▶ Ethernet
- ▶ ...



```
$ guix shell eigen-benchmarks -- \
    benchBlasGemm 240 240 240
240 x 240 x 240
cblas: 0.20367 (16.289 GFlops/s)
eigen : 0.285149 (11.635 GFlops/s)
```

```
$ guix shell eigen-benchmarks -- \
    benchBlasGemm 240 240 240
240 x 240 x 240
cblas: 0.20367 (16.289 GFlops/s)
eigen : 0.285149 (11.635 GFlops/s)
```

**Package  
multi-versioning**

```
$ guix shell --tune eigen-benchmarks -- \
    benchBlasGemm 240 240 240
guix shell: tuning for CPU micro-architecture skylake
240 x 240 x 240
cblas: 0.203131 (16.333 GFlops/s)
eigen : 0.0929638 (35.688 GFlops/s)
```

<https://hpc.guix.info/blog/2022/01/tuning-packages-for-a-cpu-micro-architecture/>



<https://hpc.guix.info/blog/2024/01/hip-and-rocm-come-to-guix/>

## **4. Interoperability.**

```
$ guix pack \  
python python-numpy python-scipy  
...  
/gnu/store/...-pack.tar.gz
```



```
$ guix pack --relocatable \  
python python-numpy python-scipy  
...  
/gnu/store/...-pack.tar.gz
```

<https://hpc.guix.info/blog/2020/05/faster-relocatable-packs-with-fakechroot/>

```
$ guix pack --format=squashfs \  
    python python-numpy python-scipy  
...  
/gnu/store/...-singularity-image.tar.gz
```

```
$ guix pack --format=docker \  
    python python-numpy python-scipy  
...  
/gnu/store/...-docker-image.tar.gz
```



ENVIRONMENT

**MODULES**

```
guix module create -o /opt/modules \  
gcc-toolchain openmpi netcdf gromacs
```

<https://hpc.guix.info/blog/2022/05/back-to-the-future-modules-for-guix-packages/>

```
guix module create -o /opt/modules \  
  --tune=skylake-avx512 \  
  gcc-toolchain openmpi netcdf gromacs
```

<https://hpc.guix.info/blog/2022/05/back-to-the-future-modules-for-guix-packages/>

```
guix module create -o /opt/modules \  
  --manifest=manifest.scm
```

<https://hpc.guix.info/blog/2022/05/back-to-the-future-modules-for-guix-packages/>

## **5. Open science & reproducible research.**

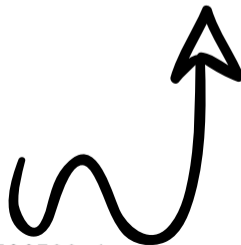




Software Heritage



 **Guix**



<https://hal.science/hal-04586520v1>

- ▶ P. Swartvagher, *On the Interactions between HPC Task-based Runtime Systems and Communication Libraries*, PhD thesis, Dec. 2022
- ▶ M. Felšöci, *Fast Solvers for High-Frequency Aeroacoustics*, PhD thesis, Feb. 2023
- ▶ N. Vallet *et al.*, *Toward practical transparent verifiable and long-term reproducible research using Guix*, Nature Scientific Data, Oct. 2022

**Wrapping up.**

- 1. robustness**
- 2. flexibility**
- 3. performance portability**
- 4. interoperability**
- 5. reproducible research**



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<https://hpc.guix.info>

**Bonus slides!**

guix **shell** python python-numpy

guix **shell** python python-numpy



```
guix shell --manifest=my-packages.scm
```

```
(specifications->manifest  
  ("gcc-toolchain" "openmpi"  
   "petsc" "hipblas"))
```

```
guix shell --container \  
  --manifest=my-packages.scm
```

```
(specifications->manifest  
  '("gcc-toolchain" "openmpi"  
    "petsc" "hipblas"))
```

```
bob@laptop$ guix shell --manifest=my-packages.scm ...
```

```
bob@laptop$ guix describe
```

```
guix cabba9e
```

```
repository URL: https://git.sv.gnu.org/git/guix.git
```

```
commit: cabba9e15900d20927c1f69c6c87d7d2a62040fe
```

```
bob@laptop$ guix shell --manifest=my-packages.scm ...
```

```
bob@laptop$ guix describe
```

```
guix cabba9e
```

```
repository URL: https://git.sv.gnu.org/git/guix.git
```

```
commit: cabba9e15900d20927c1f69c6c87d7d2a62040fe
```

```
alice@supercomp$ guix pull --commit=cabba9e
```

```
alice@supercomp$ guix shell --manifest=my-packages.scm ...
```




**travel in space *and* time!**

```
$ guix build hwloc
```

**isolated build:** chroot, separate name spaces, etc.

```
$ guix build hwloc  
/gnu/store/ h2g4sf72... -hwloc-1.11.2
```

hash of **all** the dependencies



```
$ guix build hwloc  
/gnu/store/h2g4sf72...-hwloc-1.11.2
```

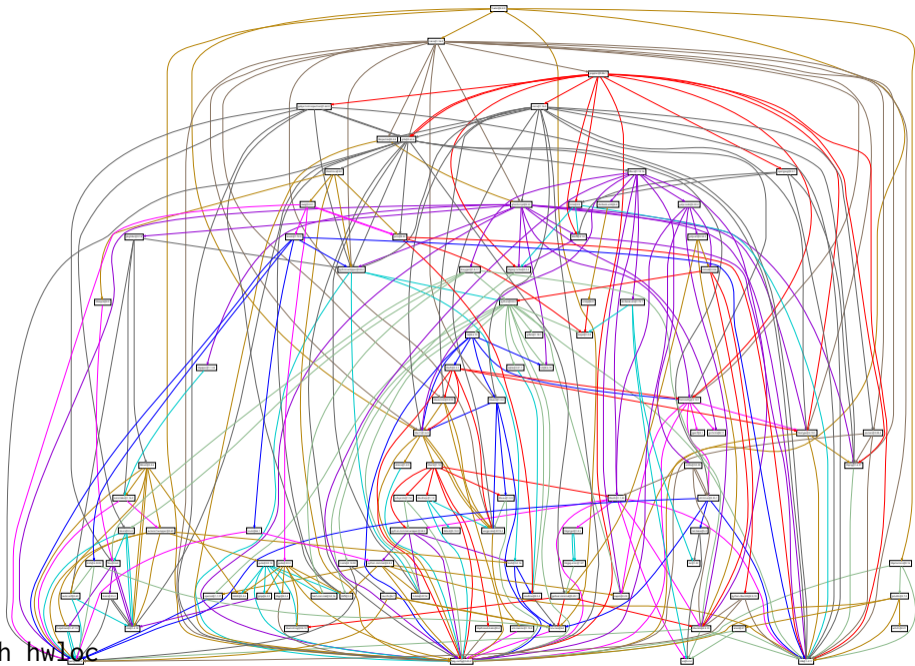
```
$ guix gc --references /gnu/store/...-hwloc-1.11.2  
/gnu/store/...-glibc-2.33  
/gnu/store/...-gcc-10.3.0-lib  
/gnu/store/...-hwloc-2.9.0
```



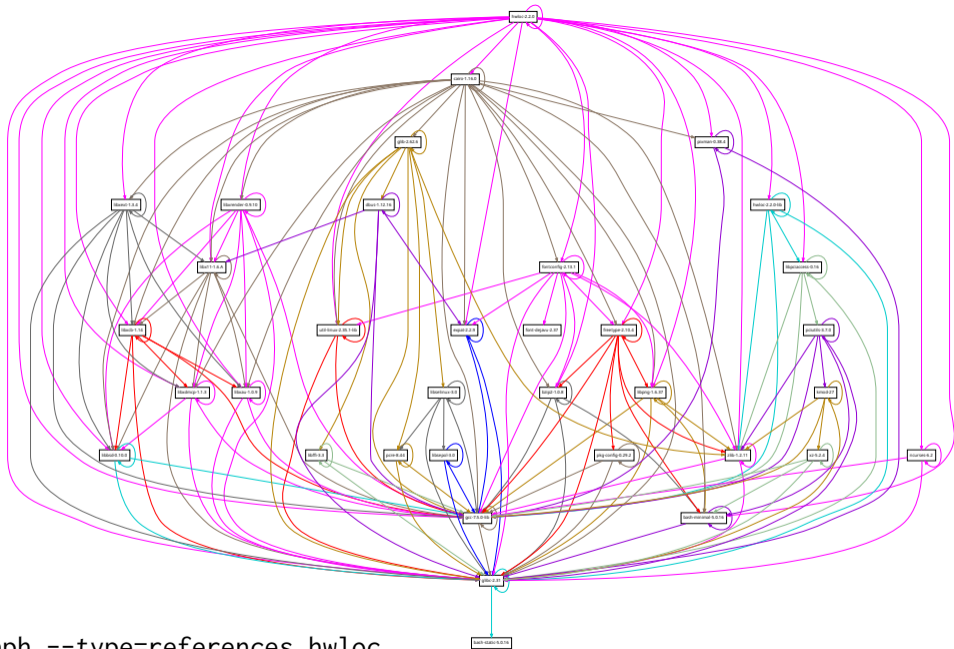
```
$ guix build hwloc  
/gnu/store/h2g4sf72... -hwloc-1.11.2
```

```
$ guix gc --references /gnu/store/...-hwloc-1.11.2  
/gnu/store/...-glibc-2.33  
/gnu/store/...-gcc-10.3.0-lib  
/gnu/store/...-hwloc-1.11.2
```

**(nearly) bit-identical for everyone**



guix graph hwloc



`guix graph --type=references hwloc`

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DeLorean time machine picture © 2014 Oto Godfrey and Justin Morton, CC-BY-SA 4.0,  
[https://commons.wikimedia.org/wiki/File:TeamTimeCar.com-BTTF\\_DeLorean\\_Time\\_Machine-OtoGodfrey.com-JMortonPhoto.com-07.jpg](https://commons.wikimedia.org/wiki/File:TeamTimeCar.com-BTTF_DeLorean_Time_Machine-OtoGodfrey.com-JMortonPhoto.com-07.jpg).

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