# Using Guix for scientific, reproducible, and publishable experiments

Ten Years of Guix – September 16, 2022

Philippe SWARTVAGHER
Inria Bordeaux – Sud-Ouest

# Few words about me

- PhD Student @ Inria Bordeaux
- HPC : interactions between task-based runtime systems and communication libraries
- Occasional Guix user
  - For my experiments
  - Maintainer of several packages in Guix-HPC channel

# Agenda

1. Software environment
2. Experiments without Guix
3. Experiments *with* Guix
4. Reproducible experiments

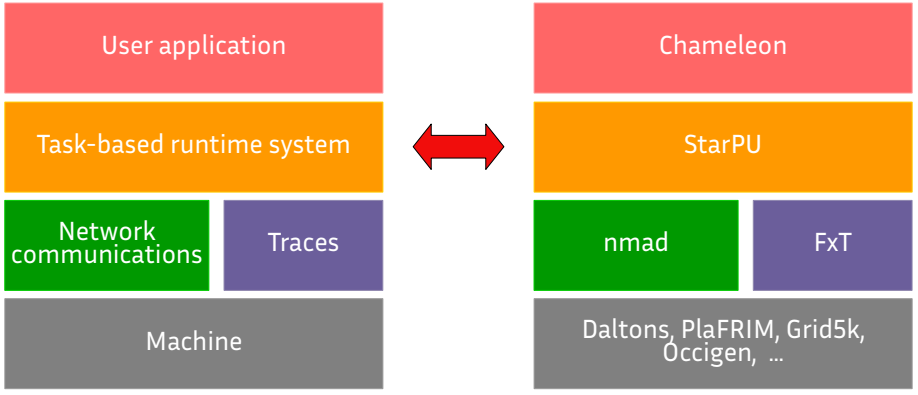
# Experimental protocol

1. Development, tries and failures on my laptop

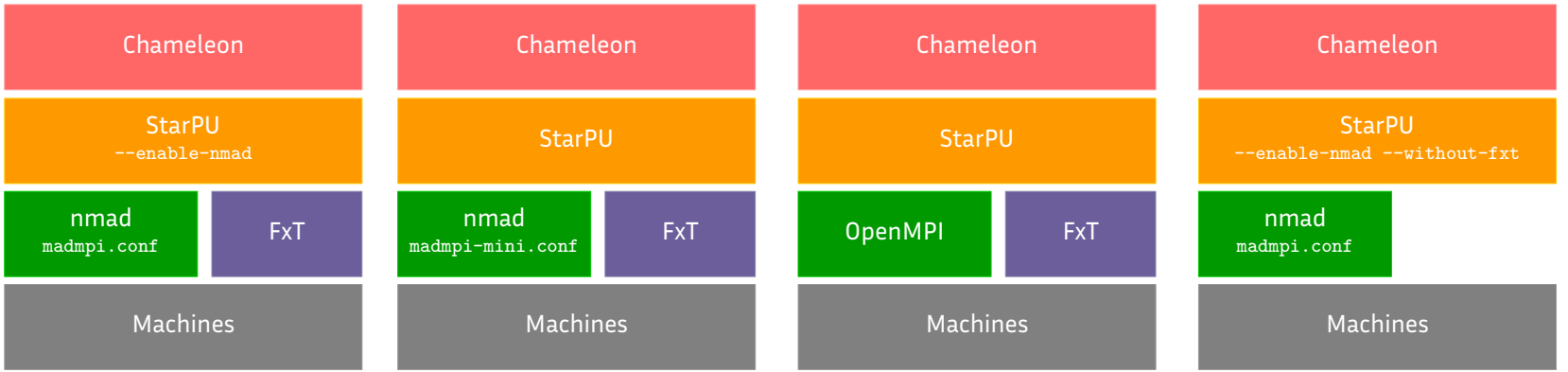
2. Experiments on clusters

   - Job scheduler (SLURM, OAR, …)
   - Non-interactive: submit a job executing a script, wait for its execution
   - At one point: experiments whose results will be published

# My software stack



# My software stack**s**!




- Several possible combinations of building parameters
- Rebuild the whole stack!

# Experimental protocol and variants

1. Development, tries and failure on my laptop

A main variant

2. Experiments on clusters

   - Job scheduler (SLURM, OAR, …)
   - Non-interactive: submit a job executing a script, wait for its execution
   - At one point : experiments whose results will be published

Comparaison of several variants of the same stack :

- `nmad`
- `madmpi`
- `openmpi`

# Several variants simultaneously

**How to switch from a variant to another one?**

- Rebuild everything?
  - Too long
  - Prevent using simultaneously different variants

# Level 0: `PATH`, `LD_LIBRARY_PATH`, *etc*

**Each variants installed in its own folder hierarchy**

- `--prefix=$HOME/builds/nmad/` at compile-time
  - Small script to wrap all these commands: `./build.sh nmad && ./build.sh madmpi`
- `PATH=$HOME/builds/nmad/bin LD_LIBRARY_PATH=$HOME/builds/nmad/lib` to run

- OK in scripts for non-interactive jobs
- But in interactive jobs: need to remember all variables and paths to define, need to type them...

# Level 1: modules

Very common on HPC clusters

**Each variants installed in its own folder hierarchy**

- `--prefix=$HOME/builds/nmad/` at compile time
  - Small script to wrap all these commands: `./build.sh nmad && ./build.sh madmpi`
- `PATH`, `LD_LIBRARY_PATH`, … defined in **modules files**

```
module load nmad
module unload nmad
module load madmpi
```

```
set     name            nmad
set     prefix          $HOME/builds/nmad/

prepend-path    PATH                $prefix/bin
prepend-path    LIBRARY_PATH        $prefix/lib
prepend-path    LD_LIBRARY_PATH     $prefix/lib
prepend-path    INCLUDE             $prefix/include
prepend-path    C_INCLUDE_PATH      $prefix/include
prepend-path    CPLUS_INCLUDE_PATH  $prefix/include
prepend-path    PKG_CONFIG_PATH     $prefix/lib/pkgconfig
```

- OK in scripts for non-interactive jobs
- OK in interactive scripts

# Final boss of level 1

Harder :

- Comparaisons between branches of the same library
- Comparaisons between commits of the same library
- Comparaisons with and without a patch applied to a library

- Different folders, module files, … again?
  - In this case, source code is modified, not the result of its compilation!

- How to know which source code was used to build the software we are using...
  - Right now?
  - 6 months ago?

# Guix!


- No package installed with Guix (no `guix install`)
- Use of `guix shell` instead
  - Required packages are built on-the-fly

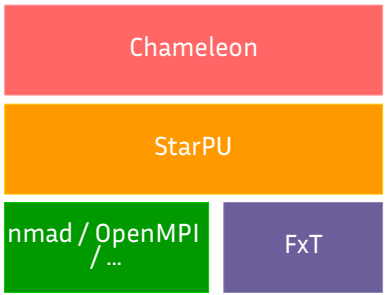
```
./build.sh --starpu --chameleon openmpi
module load openmpi
module load starpu-openmpi
module load chameleon-openmpi
mpirun ...
```

```
guix shell --pure chameleon -- mpirun ...
```

# Several variants simultaneously

**with Guix !**

- `openmpi` variant:
  - `guix shell --pure chameleon -- mpirun …`
  - Chameleon depends on StarPU, which depends on OpenMPI
  - *Default* variant
- `nmad` variant:
  - `guix shell --pure chameleon` **`--with-input=openmpi=nmad`** `-- mpirun …`
- `madmpi` variant:
  - `guix shell --pure chameleon --with-input=openmpi=`**`nmad-mini`** `-- mpirun …`
- Variant with `fxt` :
  - `guix shell --pure chameleon --with-input=`**`starpu=starpu+fxt`** `-- mpirun …`



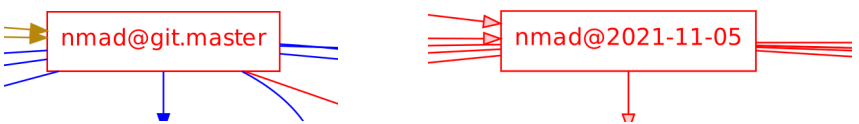

Existing packages in Guix-HPC

# Package transformations

- https://guix.gnu.org/en/manual/devel/en/html_node/Package-Transformation-Options.html
- Simple package substitution:
  - `guix shell --pure chameleon` **`--with-input=openmpi=nmad`** `-- mpirun …`
  - `guix shell --pure chameleon` **`--with-input=openblas=mkl`** `-- mpirun …`
- Use a specific upstream Git branch:
  - `guix shell --pure chameleon` **`--with-branch=starpu=coop-mcast`** `-- mpirun …`
- Use a specific upstream commit:
  - `guix shell --pure chameleon` **`--with-commit=starpu=acae6e78df7a9475bbfbd26e33fe324b1f7bedce`** `-- mpirun …`
- Apply a patch to package source code:
  - `guix shell --pure chameleon` **`--with-patch=chameleon=./wait-graph.patch`** `-- mpirun …`

# Package transformations

- Combinations of several transformations!
  - Be careful to transformation order:
    - `--with-input=openmpi=nmad --with-branch=nmad=master` : OK, `master` branch of `nmad`
    - `--with-branch=nmad=master --with-input=openmpi=nmad` : version specified in `nmad` package
  - Visualize applied transformations with:
    - `guix graph -M 4 chameleon --with-input=openmpi=nmad --with-branch=nmad=master | xdot -`



# Final boss of level 1

**with Guix !**

Harder :

- Comparaisons between branches of the same library
- Comparaisons between commits of the same library
- Comparaisons with and without a patch applied to a library

- Different folders, module files, … again?
  - In this case, source code is modified, not the result of its compilation!

- How to know which source code was used to build the software we are using...
  - Right now?
  - 6 months ago?

# Final boss of level 1

with Guix !

Harder :

- Comparaisons between branches of the same library
- Comparaisons between commits of the same library
- Comparaisons with and without a patch applied to a library

Very easy!

- Different folders, module files, … again?
  - In this case, source code is modified, not the result of its compilation!

- How to know which source code was used to build the software we are using...
  - Right now?
  - 6 months ago?

# Final boss of level 1

with Guix !

Harder :

- Comparaisons between branches of the same library
- Comparaisons between commits of the same library
- Comparaisons with and without a patch applied to a library

Very easy!

- Different folders, module files, … again?
  - In this case, source code is modified, not the result of its compilation!

Not needed!

- How to know which source code was used to build the software we are using...
  - Right now?
  - 6 months ago?

# Reproducibility: the problem

```
guix shell --pure chameleon -- mpirun …
```

… 6 months later …

```
guix pull
guix shell --pure chameleon -- mpirun …
```

- `chameleon` != `chameleon`
  - Different package version of `chameleon`
  - Different versions of `chameleon`'s dependencies

# Reproducibility: the solution

- Export currently used channels (**and their versions**):

  `guix describe -f channels > channels.scm`

- Explicitly use pinned channels:

  ```
  guix time-machine --channels=./channels.scm --
      shell --pure chameleon -- mpirun …
  ```

- Backup `channels.scm` : to be sure to execute the same code, even 6 months later

```
(list (channel
        (name 'guix)
        (url "https://git.savannah.gnu.org/git/guix.git")
        (branch "master")
        (commit
          "ec66f84824198f380d20126d3e4b2ea795fd205a")
        (introduction
          (make-channel-introduction
            "9edb3f66fd807b096b48283debdcddccfea34bad"
            (openpgp-fingerprint
              "BBB0 2DDF 2CEA F6A8 0D1D  E643 A2A0 6DF2 A33A 54FA"))))
      (channel
        (name 'guix-hpc-non-free)
        (url "https://gitlab.inria.fr/guix-hpc/guix-hpc-non-free.git")
        (branch "master")
        (commit
          "58aaac8c18773d900511d441e935145d73cdfc5e"))
      (channel
        (name 'guix-hpc)
        (url "https://gitlab.inria.fr/guix-hpc/guix-hpc.git")
        (branch "master")
        (commit
          "74840c47b744ad7342e7a86852831009a2831630")))
```

# Reproducibility: making scripts available

- Making experiments (scripts) with reproducibility in mind
- Public Git repository with scripts and instructions for reproducibility:
  - Detailed `README` to understand what is done, how, where, ...
  - Contains `channels.scm`
  - *Instructions to use also without Guix*
- Examples :
  - https://gitlab.inria.fr/pswartva/paper-model-memory-contention-r13y
  - https://gitlab.inria.fr/pswartva/paper-starpu-traces-r13y

# Reproducibility: in papers

- Ask SoftwareHeritage for a snapshot of your repository
  - Repository available forever
  - https://archive.softwareheritage.org/save/
  - Provide a unique identifier, to find the saved repository
- In the paper:

> A public companion contains the instructions to reproduce our study: https://gitlab.inria.fr/pswartva/paper-model-memory-contention-r13y, archived on https://www.softwareheritage.org/ with the ID `swh:1:snp:306f7c10cf69a5860587e5aad62b76070b798ecd`.

# Conclusion: Guix’s advantages

- Very easy to move from a machine to another one*,**
  - No wasted time to reinstall, recompile, look for appropriate modules, ...
  - **As long as the job scheduler is the same*
  - ***Require to parametrize/factorize scripts from the beginning*
- More confidence in experiment executions
  - Especially if I need to run them again (with different parameter, ...)

# Conclusion: future work

- Use manifest files
  - Put all parameters of `guix shell` in a file
  - Good way to factorize code?
- Use on a machine without Guix
  - `guix pack`