Reproductibilité & Portabilité des performances

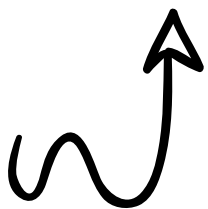
Ludovic Courtès

Journées calcul et données (JCAD)

14 décembre 2021

Inria

Software Heritage



The ReScience Journal

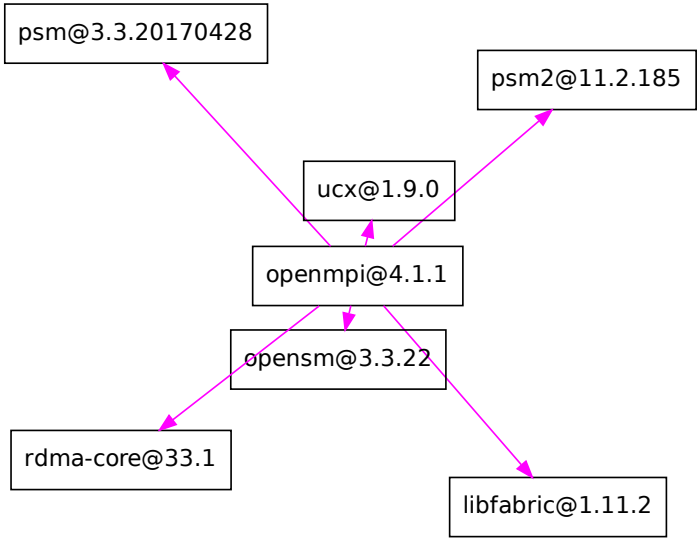
Deux obsessions : MPI et AVX

Some fairly common (but questionable) assumptions made by package managers (conda, pip, apt, etc.)

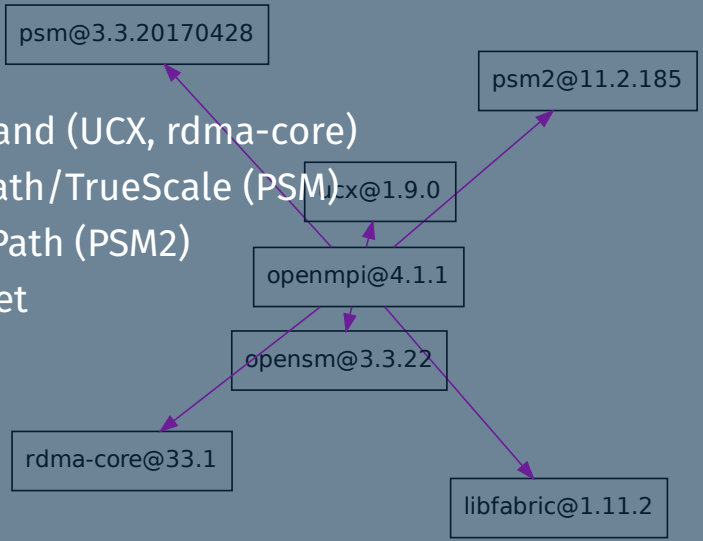
- **1:1 relationship between source code and binary (per platform)**
  - Good for reproducibility (e.g., Debian)
  - Bad for performance optimization
- **Binaries should be as portable as possible**
  - What most distributions do
  - Again, bad for performance
- **Toolchain is the same across the ecosystem**
  - One compiler, one set of runtime libraries
  - Or, no compiler (for interpreted languages)

Todd Gamblin (Spack)

https://trex-coe.eu/events/trex-build-system-hackathon-8-12-nov-2021

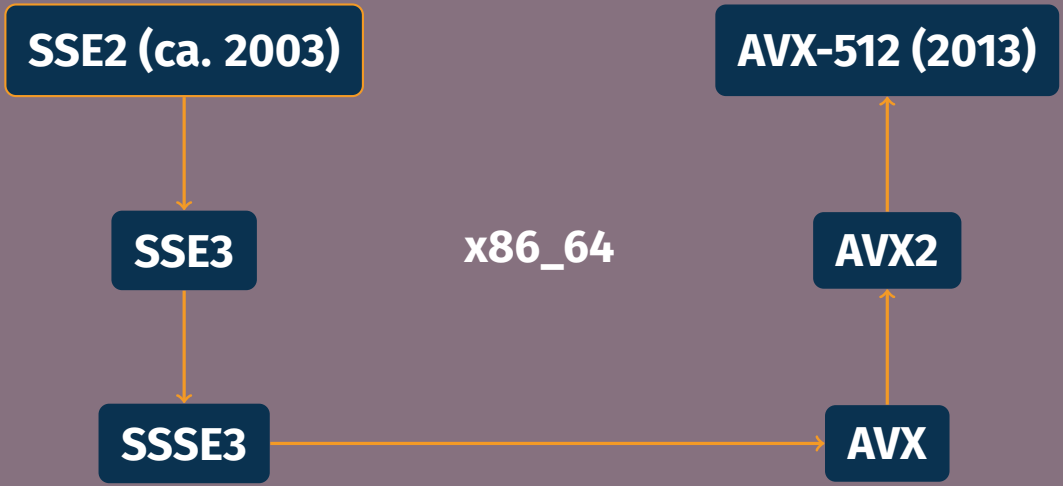

psm@3.3.20170428
psm2@11.2.185
ucx@1.9.0
openmpi@4.1.1
opensm@3.3.22
rdma-core@33.1
libfabric@1.11.2

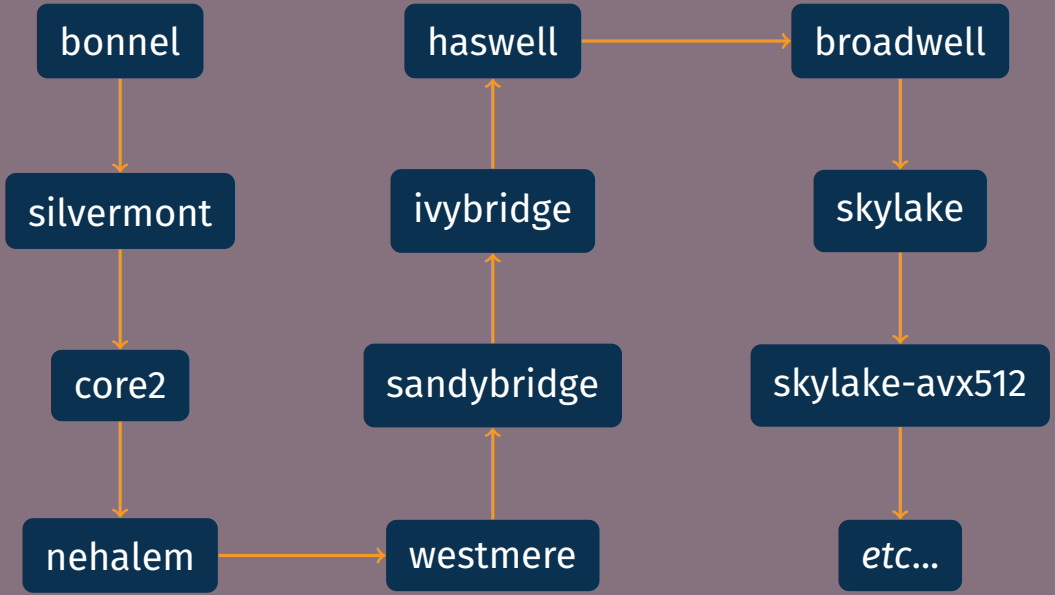
- InfiniBand (UCX, rdma-core)
- InfiniPath/TrueScale (PSM)
- Omni-Path (PSM2)
- Ethernet
- …



https://hpc.guix.info/blog/2019/12/optimized-and-portable-open-mpi-packaging/

La jungle
des extensions vectorielles


SSE2 (ca. 2003)
SSE3
SSSE3
x86_64
AVX
AVX2
AVX-512 (2013)


bonnel
haswell
broadwell
silvermont
ivybridge
skylake
core2
sandybridge
skylake-avx512
nehalem
westmere
etc...

code	GEMM 240x240x240
Eigen (x86_64 baseline)	11 Gflops/s
Eigen `-march=westmere`	12 Gflops/s
Eigen `-march=sandybridge`	20 Gflops/s
Eigen `-march=skylake`	**36** Gflops/s
OpenBLAS	16 Gflops/s

`guix shell eigen-benchmarks -- benchBlasGemm 240 240 240`, Intel CORE i7

```
$ ls /cm/shared/modules/intel/
broadwell       haswell  ivybridge
knightslanding  knl      skylake

$ ls /cm/shared/modules/intel/skylake/modulefiles/
compiler  linalg  tools
```

```
$ spack spec netcdf-c
Concretized
--------------------------------
netcdf-c@4.8.1… arch=linux-ubuntu18.04-skylake_avx512
    ^hdf5@1.10.7… arch=linux-ubuntu18.04-skylake_avx512
        ^cmake@3.21.4… arch=linux-ubuntu18.04-skylake_avx512
            ^ncurses@6.2… arch=linux-ubuntu18.04-skylake_avx512
                ^pkgconf@1.8.0… arch=linux-ubuntu18.04-skylake_avx512
            ^openssl@1.1.1l… arch=linux-ubuntu18.04-skylake_avx512
                ^perl@5.34.0… arch=linux-ubuntu18.04-skylake_avx512
             ^berkeley-db@18.1.40… arch=linux-ubuntu18.04-skylake_avx512
                    ^bzip2@1.0.8… arch=linux-ubuntu18.04-skylake_avx512
                   ^diffutils@3.8… arch=linux-ubuntu18.04-skylake_avx512
                   ^libiconv@1.16… arch=linux-ubuntu18.04-skylake_avx512
                    ^gdbm@1.19… arch=linux-ubuntu18.04-skylake_avx512
                     ^readline@8.1… arch=linux-ubuntu18.04-skylake_avx512
                    ^zlib@1.2.11… arch=linux-ubuntu18.04-skylake_avx512
```

```
$ spack spec netcdf-c
Concretized
--------------------------------
netcdf-c@4.8.1… arch=linux-ubuntu18.04-skylake_avx512
    ^hdf5@1.10.7… arch=linux-ubuntu18.04-skylake_avx512
        ^cmake@3.21.4… arch=linux-ubuntu18.04-skylake_avx512
            ^ncurses@6.2… arch=linux-ubuntu18.04-skylake_avx512
                ^pkgconf@1.8.0… arch=linux-ubuntu18.04-skylake_avx512
            ^openssl@1.1.1l… arch=linux-ubuntu18.04-skylake_avx512
                ^perl@5.34.0… arch=linux-ubuntu18.04-skylake_avx512
             ^berkeley-db@18.1.40… arch=linux-ubuntu18.04-skylake_avx512
                    ^bzip2@1.0.8… arch=linux-ubuntu18.04-skylake_avx512
                   ^diffutils@3.8… arch=linux-ubuntu18.04-skylake_avx512
                   ^libiconv@1.16… arch=linux-ubuntu18.04-skylake_avx512
                    ^gdbm@1.19… arch=linux-ubuntu18.04-skylake_avx512
                     ^readline@8.1… arch=linux-ubuntu18.04-skylake_avx512
                    ^zlib@1.2.11… arch=linux-ubuntu18.04-skylake_avx512
```

```
$ spack spec netcdf-c
Concretized
--------------------------------
netcdf-c@4.8.1… arch=linux-ubuntu18.04-skylake_avx512
    ^hdf5@1.10.7… arch=linux-ubuntu18.04-skylake_avx512
        ^cmake@3.21.4… arch=linux-ubuntu18.04-skylake_avx512
            ^ncurses@6.2… arch=linux-ubuntu18.04-skylake_avx512
                ^pkgconf@1.8.0… arch=linux-ubuntu18.04-skylake_avx512
            ^openssl@1.1.1l… arch=linux-ubuntu18.04-skylake_avx512
                ^perl@5.34.0… arch=linux-ubuntu18.04-skylake_avx512
             ^berkeley-db@18.1.40… arch=linux-ubuntu18.04-skylake_avx512
                    ^bzip2@1.0.8… arch=linux-ubuntu18.04-skylake_avx512
                   ^diffutils@3.8… arch=linux-ubuntu18.04-skylake_avx512
                   ^libiconv@1.16… arch=linux-ubuntu18.04-skylake_avx512
                    ^gdbm@1.19… arch=linux-ubuntu18.04-skylake_avx512
                     ^readline@8.1… arch=linux-ubuntu18.04-skylake_avx512
                    ^zlib@1.2.11… arch=linux-ubuntu18.04-skylake_avx512
```

```
$ spack spec netcdf-c
Concretized
--------------------------------
netcdf-c@4.8.1… arch=linux-ubuntu18.04-skylake_avx512
    ^hdf5@1.10.7… arch=linux-ubuntu18.04-skylake_avx512
        ^cmake@3.21.4… arch=linux-ubuntu18.04-skylake_avx512
            ^ncurses@6.2… arch=linux-ubuntu18.04-skylake_avx512
                ^pkgconf@1.8.0… arch=linux-ubuntu18.04-skylake_avx512
            ^openssl@1.1.1l… arch=linux-ubuntu18.04-skylake_avx512
                ^perl@5.34.0… arch=linux-ubuntu18.04-skylake_avx512
             ^berkeley-db@18.1.40… arch=linux-ubuntu18.04-skylake_avx512
                    ^bzip2@1.0.8… arch=linux-ubuntu18.04-skylake_avx512
                   ^diffutils@3.8… arch=linux-ubuntu18.04-skylake_avx512
                   ^libiconv@1.16… arch=linux-ubuntu18.04-skylake_avx512
                    ^gdbm@1.19… arch=linux-ubuntu18.04-skylake_avx512
                     ^readline@8.1… arch=linux-ubuntu18.04-skylake_avx512
                     ^zlib@1.2.11… arch=linux-ubuntu18.04-skylake_avx512
```

https://spack.readthedocs.io/en/latest/getting_started.html

```
$ spack spec netcdf-c
Concretized
-------------
netcdf-c@4.8.
    ^hdf5@1.1
        ^cmak
```

https://xkcd.com/303/

Function multi-versioning!

GNU libc

Libgcrypt

Nettle

OpenBLAS

BLIS

FFTW

GMP

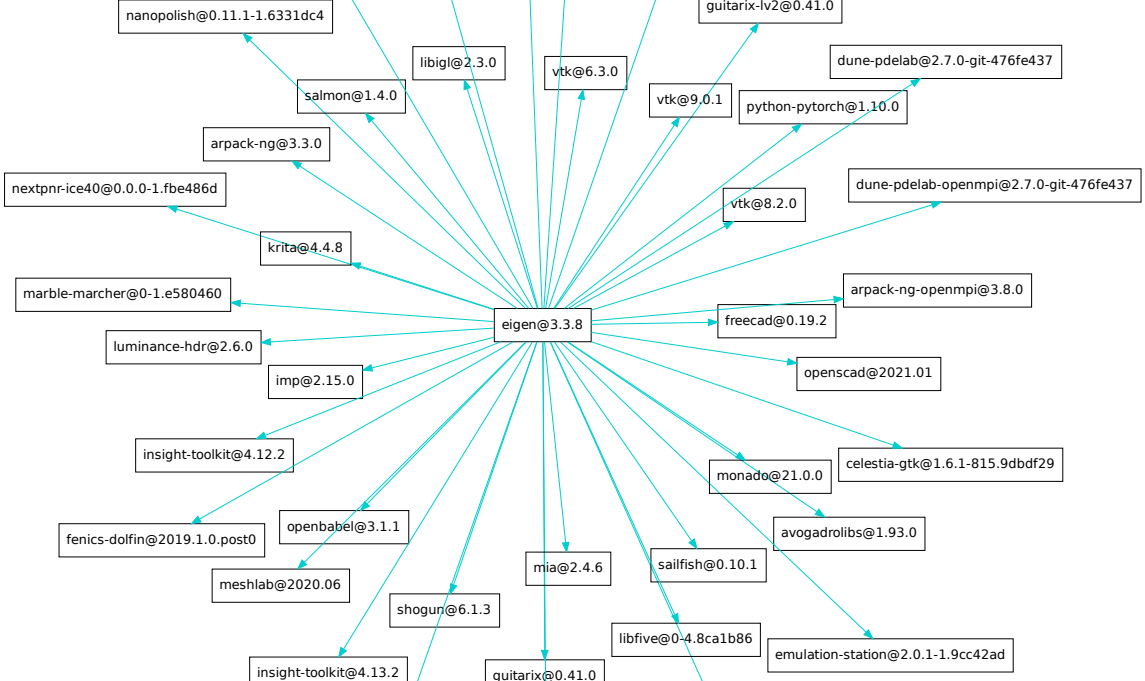
Julia

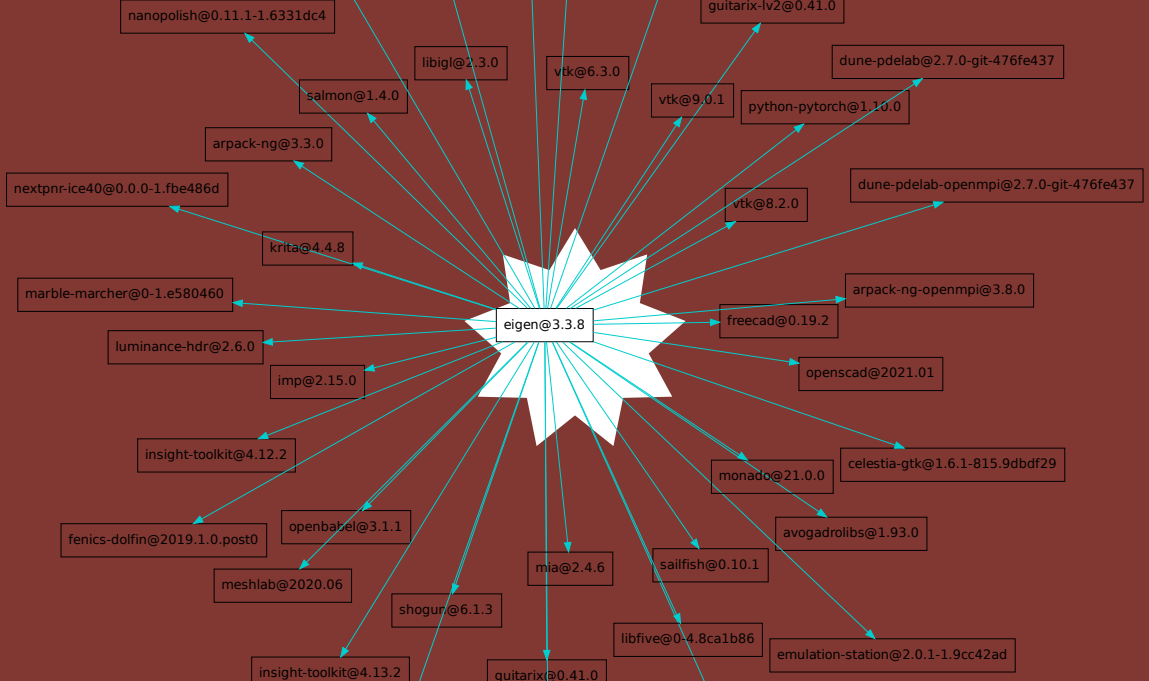
Rust

```
void my_func (double *array)
  __attribute__ ((target_clones ("arch=skylake", "default")))

void my_func (double *array)
{
  …
}
```

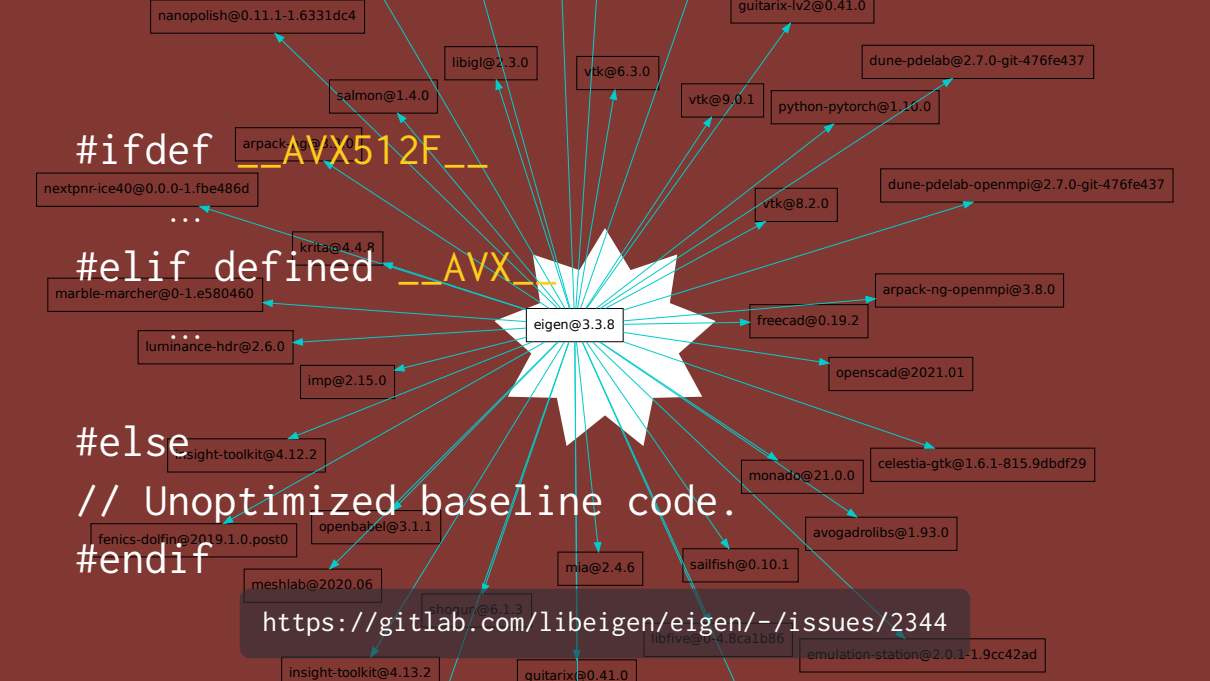
```
void my_func (double *array)
  __attribute__ ((target_clones ("arch=skylake", "default")))

void my_func (double *array)
{
  …
}
```

https://hpc.guix.info/blog/2018/01/pre-built-binaries-vs-performance/


nanopolish@0.11.1-1.6331dc4
guitarix-lv2@0.41.0
libigl@2.3.0
vtk@6.3.0
dune-pdelab@2.7.0-git-476fe437
salmon@1.4.0
vtk@9.0.1
python-pytorch@1.10.0
arpack-ng@3.3.0
nextpnr-ice40@0.0.0-1.fbe486d
dune-pdelab-openmpi@2.7.0-git-476fe437
vtk@8.2.0
krita@4.4.8
marble-marcher@0-1.e580460
arpack-ng-openmpi@3.8.0
eigen@3.3.8
freecad@0.19.2
luminance-hdr@2.6.0
openscad@2021.01
imp@2.15.0
insight-toolkit@4.12.2
celestia-gtk@1.6.1-815.9dbdf29
monado@21.0.0
fenics-dolfin@2019.1.0.post0
openbabel@3.1.1
avogadrolibs@1.93.0
meshlab@2020.06
mia@2.4.6
sailfish@0.10.1
shogun@6.1.3
libfive@0-4.8ca1b86
emulation-station@2.0.1-1.9cc42ad
insight-toolkit@4.13.2
guitarix@0.41.0


nanopolish@0.11.1-1.6331dc4
guitarix-lv2@0.41.0
libigl@2.3.0
vtk@6.3.0
dune-pdelab@2.7.0-git-476fe437
salmon@1.4.0
vtk@9.0.1
python-pytorch@1.10.0
arpack-ng@3.3.0
nextpnr-ice40@0.0.0-1.fbe486d
dune-pdelab-openmpi@2.7.0-git-476fe437
vtk@8.2.0
krita@4.4.8
marble-marcher@0-1.e580460
arpack-ng-openmpi@3.8.0
eigen@3.3.8
freecad@0.19.2
luminance-hdr@2.6.0
openscad@2021.01
imp@2.15.0
insight-toolkit@4.12.2
celestia-gtk@1.6.1-815.9dbdf29
monado@21.0.0
fenics-dolfin@2019.1.0.post0
openbabel@3.1.1
avogadrolibs@1.93.0
mia@2.4.6
sailfish@0.10.1
meshlab@2020.06
shogun@6.1.3
libfive@0-4.8ca1b86
emulation-station@2.0.1-1.9cc42ad
insight-toolkit@4.13.2
guitarix@0.41.0

```
#ifdef __AVX512F__
...
#elif defined __AVX__
...
#else
// Unoptimized baseline code.
#endif
```



https://gitlab.com/libeigen/eigen/-/issues/2344

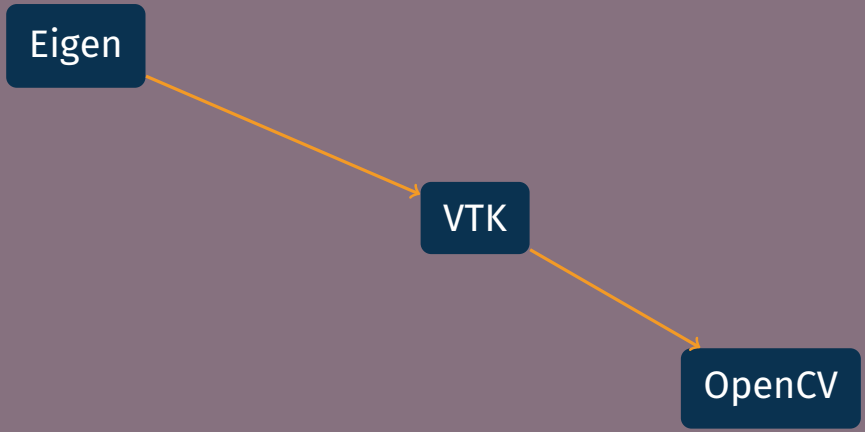
Package multi-versioning!

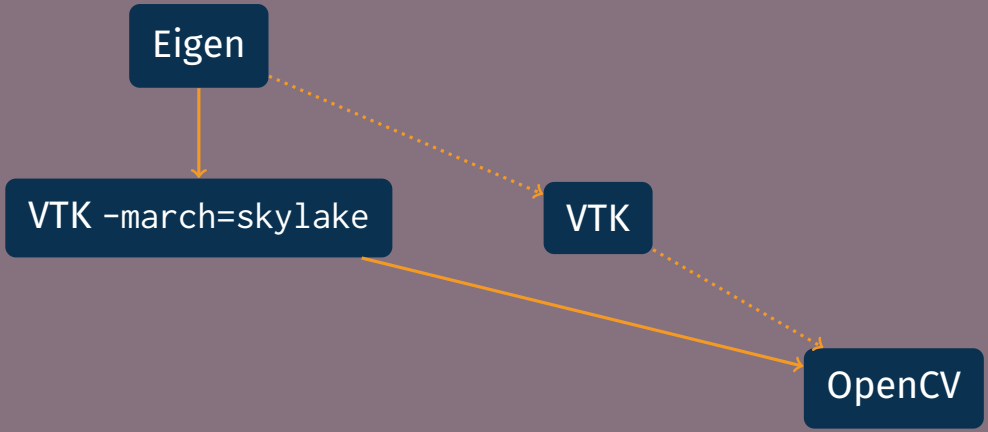
```
$ guix shell eigen-benchmarks -- \
    benchBlasGemm 240 240 240
240 x 240 x 240
cblas: 0.20367 (16.289 GFlops/s)
eigen : 0.285149 (11.635 GFlops/s)
```

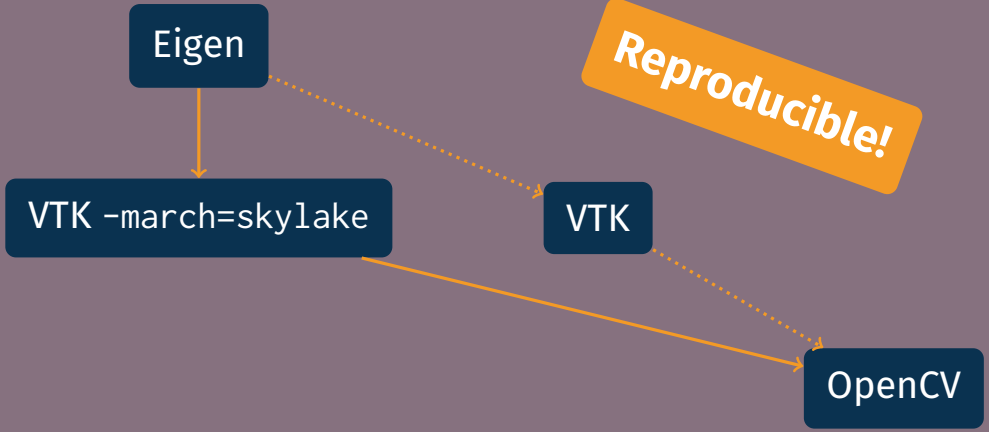
```
$ guix shell eigen-benchmarks -- \
    benchBlasGemm 240 240 240
240 x 240 x 240
cblas: 0.20367 (16.289 GFlops/s)
eigen : 0.285149 (11.635 GFlops/s)

$ guix shell --tune eigen-benchmarks -- \
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)
```

```
$ 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 --tune eigen-benchmarks -- \
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://issues.guix.gnu.org/52283


Eigen
VTK
OpenCV


Eigen
VTK -march=skylake
VTK
OpenCV


Eigen
Reproducible!
VTK -march=skylake
VTK
OpenCV

MPI, OPA, UCX, SSE, AVX, NEON...

MPI, OPA, UCX, SSE, AVX, NEON…

Portabilité, performance
***et* reproductibilité.**

https://hpc.guix.info

ludovic.courtes@inria.fr | @GuixHPC

Copyright © 2010, 2012–2021 Ludovic Courtès ludo@gnu.org.

GNU Guix logo, CC-BY-SA 4.0, https://gnu.org/s/guix/graphics.

Tandem picture by Jules Beau, public domain, https://images.bnf.fr/#/detail/1535157/9

LLNL supercomputer picture by US DoE, public domain,
https://commons.wikimedia.org/wiki/File:U.S._Department_of_Energy_-_Science_-_477_018_010_(9563440651).jpg

Copyright of other images included in this document is held by their respective owners.

This work is licensed under the Creative Commons Attribution-Share Alike 3.0 License. To view a copy of this license, visit https://creativecommons.org/licenses/by-sa/3.0/ or send a letter to Creative Commons, 171 Second Street, Suite 300, San Francisco, California, 94105, USA.

At your option, you may instead copy, distribute and/or modify this document under the terms of the GNU Free Documentation License, Version 1.3 or any later version published by the Free Software Foundation; with no Invariant Sections, no Front-Cover Texts, and no Back-Cover Texts. A copy of the license is available at https://www.gnu.org/licenses/gfdl.html.

The source of this document is available from https://git.sv.gnu.org/cgit/guix/maintenance.git.