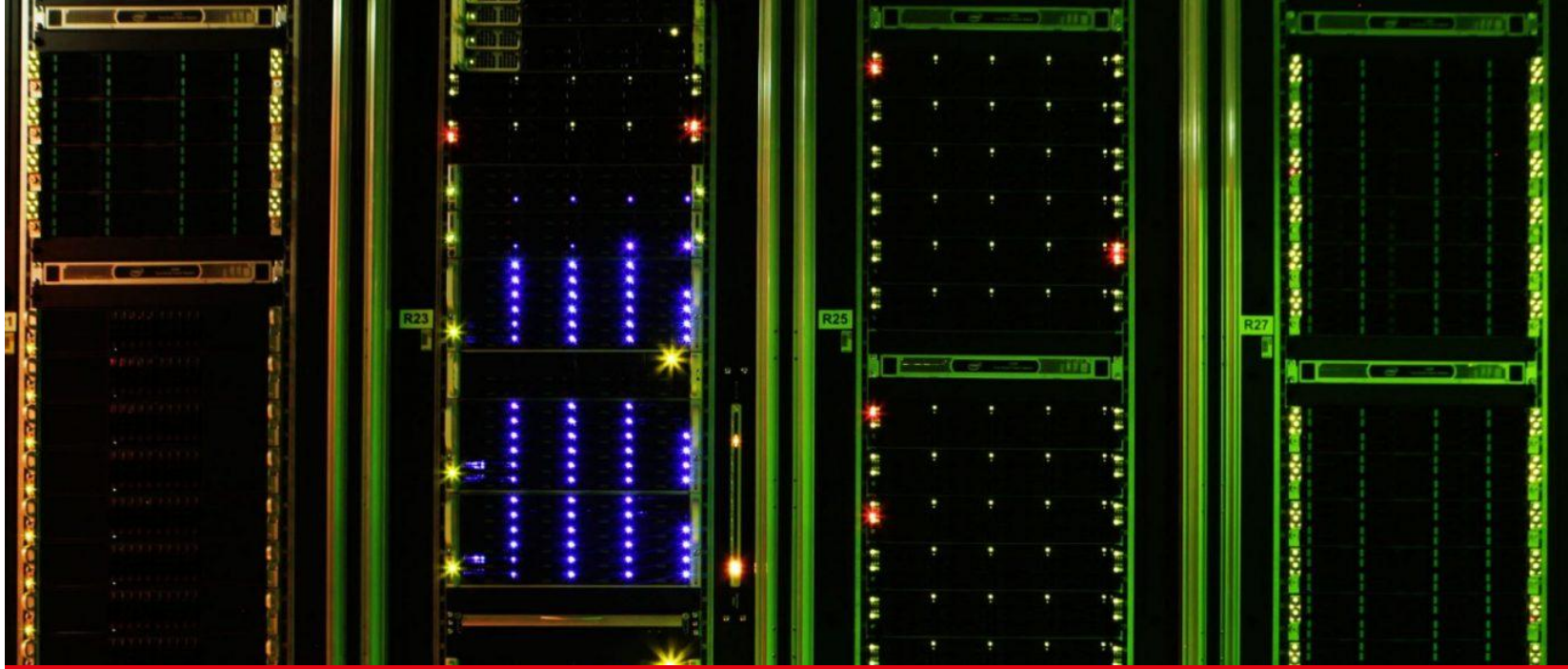
EPFL



Spack - a package manager for HPC that can be used on any machine

Informatique Scientifique & Support Applicatif
SCITAS
Scientific IT and Application Support

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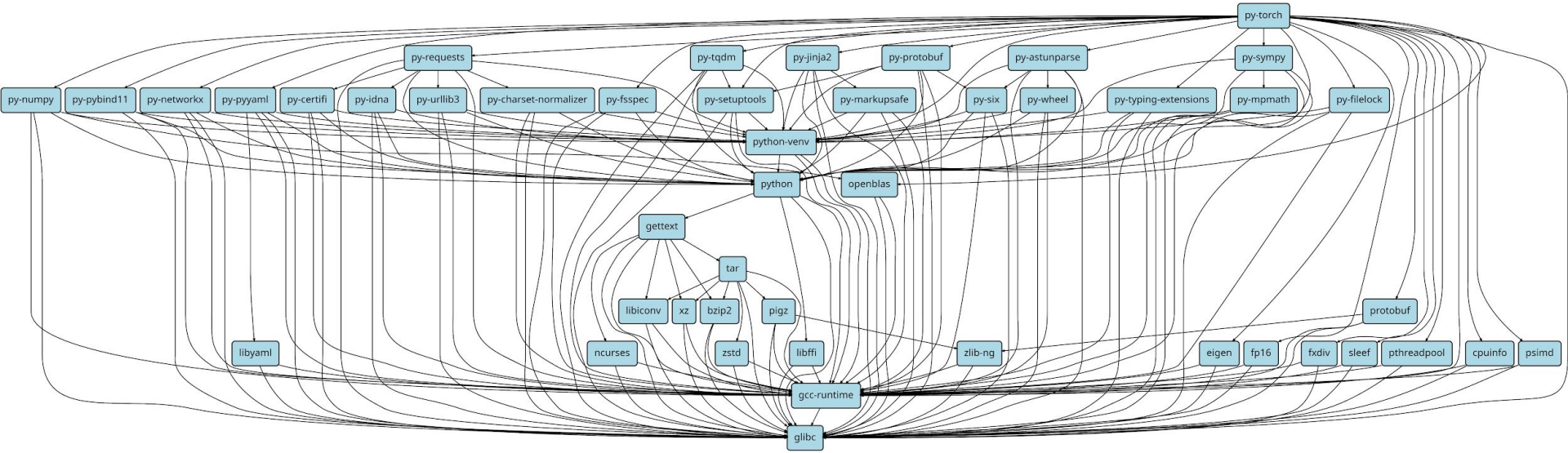
What problem do we try to solve ?



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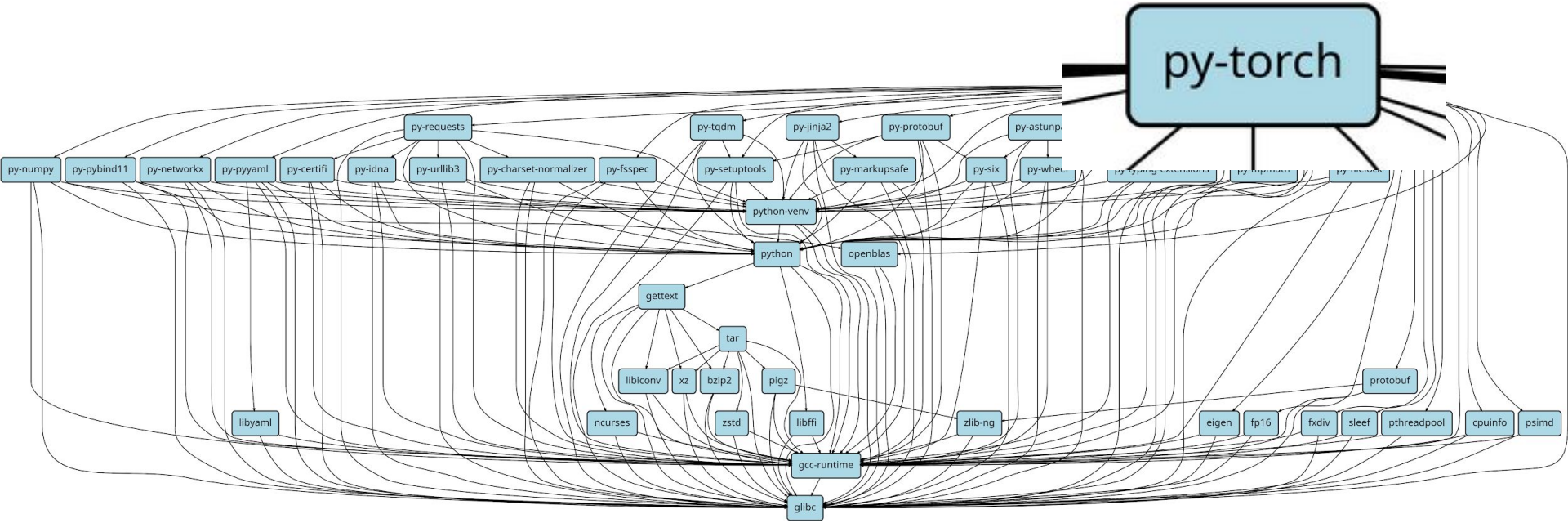

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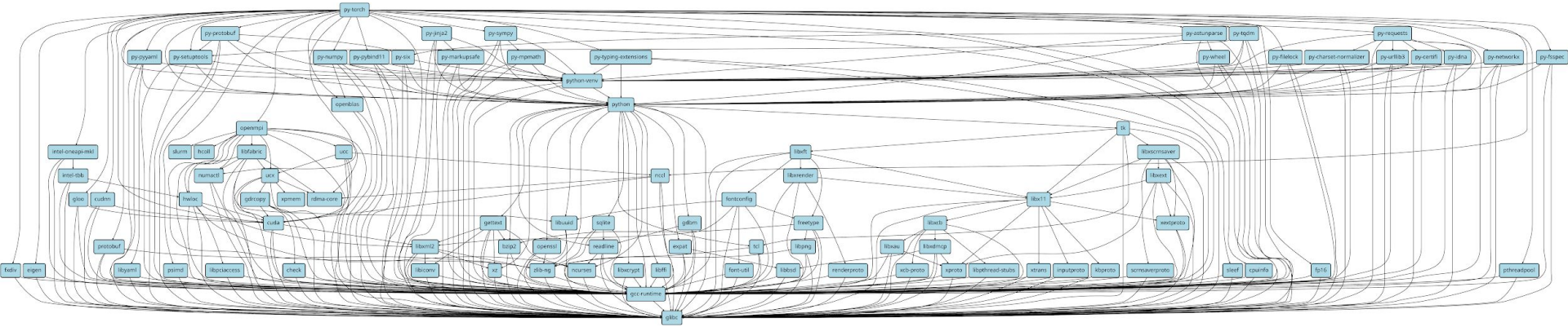


Package managers to the rescue

Package managers comes in different flavors:

- OS specific: `apt`, `yum`, `pacman`, `port`, `brew` …
- Language specific: `pip`, `cargo`, `npm`, `conan`, …
- Generic-ish: `spack`, `nix`, `guix`, `easy-build`, …

How does spack work ?

- Spack works with specs:
  - `$> spack spec -Il libfabric`

```
Input spec
--------------------------------
 -   libfabric

Concretized
--------------------------------
 -   nvd4apb  libfabric@1.21.0%gcc@14.2.0~debug~kdreg~uring build_system=autotools fabrics=sockets,tcp,udp arch=linux-debiann-skylake
 -   ugwr2kf      ^gcc-runtime@14.2.0%gcc@14.2.0 build_system=generic arch=linux-debiann-skylake
[e]  trd2mmn      ^glibc@2.40%gcc@14.2.0 build_system=autotools arch=linux-debiann-skylake
 -   5vxhodu      ^gmake@4.4.1%gcc@14.2.0~guile build_system=generic arch=linux-debiann-skylake
```

How does spack work ?

- Spack works with specs:
  - `$> spack spec -Il libfabric%gcc@12 fabrics=sockets,psm target=x86_64`

```
Input spec
--------------------------------
 -   libfabric%gcc@12 fabrics=psm,sockets arch=None-None-x86_64

Concretized
--------------------------------
 -   2p3tqre  libfabric@1.21.0%gcc@12.4.0~debug~kdreg~uring build_system=autotools fabrics=psm,sockets arch=linux-debiann-x86_64
 -   xm6eikd      ^gcc-runtime@12.4.0%gcc@12.4.0 build_system=generic arch=linux-debiann-x86_64
[e]  hflbnif      ^glibc@2.40%gcc@12.4.0 build_system=autotools arch=linux-debiann-x86_64
 -   5ski5sv      ^gmake@4.4.1%gcc@12.4.0~guile build_system=generic arch=linux-debiann-x86_64
 -   hj42t6a      ^psm@2017-04-28%gcc@12.4.0 build_system=makefile arch=linux-debiann-x86_64
 -   wlztzsi          ^util-linux-uuid@2.38.1%gcc@12.4.0 build_system=autotools arch=linux-debiann-x86_64
 -   ge6ygx7              ^pkgconf@2.2.0%gcc@12.4.0 build_system=autotools arch=linux-debiann-x86_64
```

How can I use it ?

- With spack environments
  - YAML file
  - Define which compiler to use
  - What to install
  - What to reuse from the system
  - Where to create the “view”
- Advantages:
  - Generates a “lock” file
  - Installed version and options saved
  - Can be redeployed
- Possible usage:
  - CI environments
  - Development environment
  - Replacement of brew
  - Test different versions

```
spack:
  compilers:
    - compiler:
        paths:
          cc: /opt/rh/devtoolset-10/root/usr/bin/gcc
          cxx: /opt/rh/devtoolset-10/root/usr/bin/g++
          ...

        operating_system: centos7
        target: x86_64
        spec: gcc@10.2.1
        ...

  include:
    - /softs/spack/etc/spack/packages.yaml

  specs:
    - openblas +pic threads=none
    - eigen
    - mumps ~mpi ~complex ~float
    - hdf5 ~mpi +szip +threadsafe +hl
    ...

  packages:
    cmake:
      externals:
      - spec: cmake@3.27.7
        prefix: /usr/local
    openssl:
      externals:
      - spec: openssl@1.0.2k-fips
        prefix: /usr
    perl:
      externals:
      - spec: perl@5.16.3
        prefix: /usr
    ...

  view: /softs/view
```

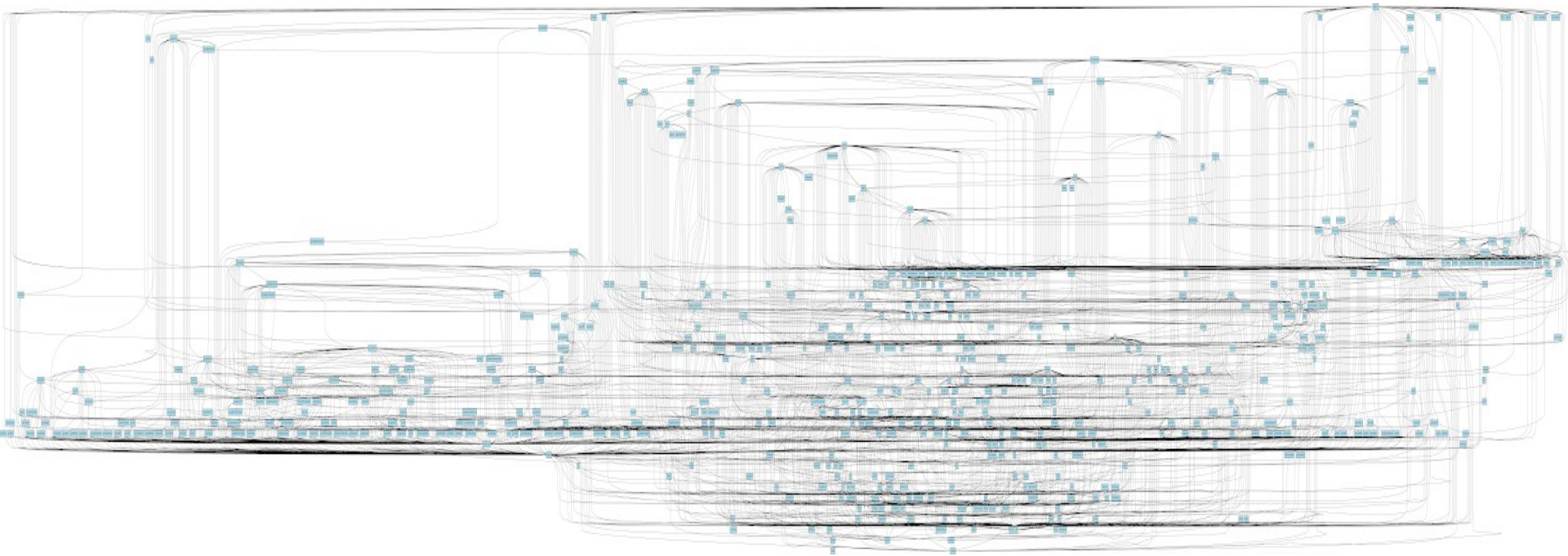
HPC usage of spack

- Virtual packages: `mpi, blas, lapack, fft-api`
- Automatic generation of `modules`
- Supports many compilers
- Compiles for the CPU architecture (can cross compile)
- Supports many accelerators
- Vendors help to develop recipes
  - AMD
  - Cray
  - Intel
  - Nvidia

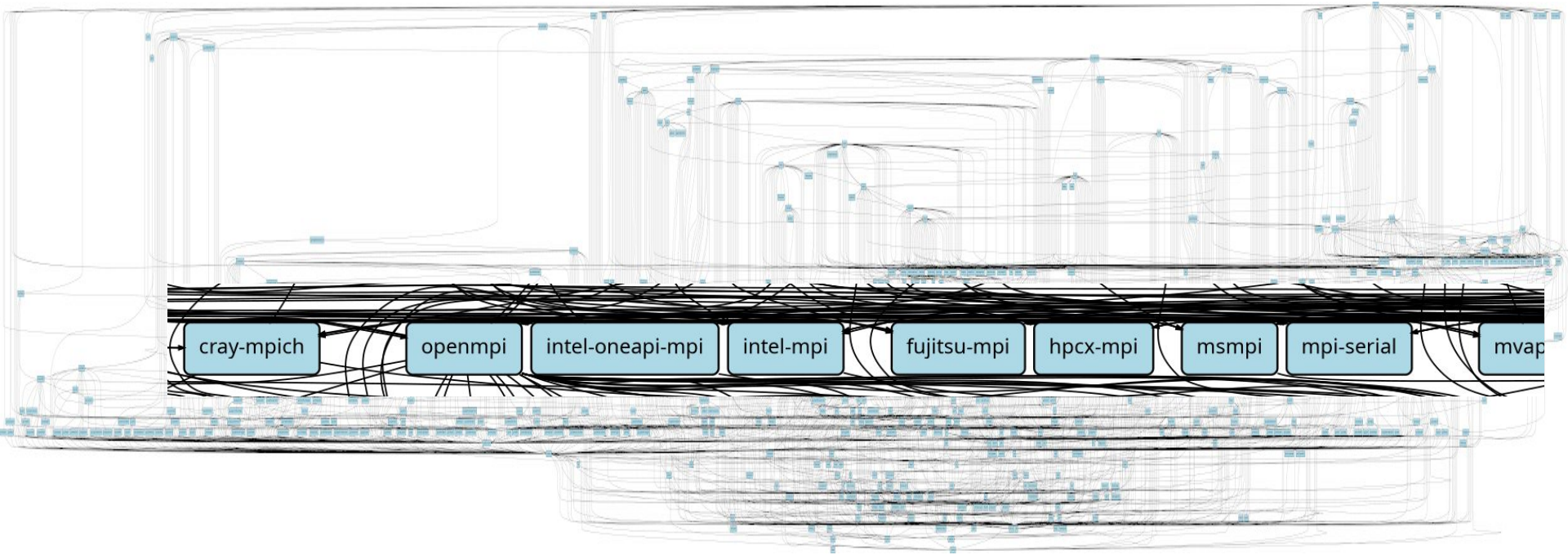
SCITAS usage of spack

- 4 clusters on-site:
  - 4 cpu architecture:
    - skylake_avx512
    - cascadelake
    - icelake
    - zen4
  - 3 gpu architecture:
    - Volta
    - Lovelace
    - Hopper
  - 2 type of network:
    - ethernet + roce
    - infiniband
  - 3 compilers:
    - gcc
    - intel-oneapi
    - nvhpc
  - ~250 packages to install
- Total amount of package compiled: 12’652

Spack view of py-torch



Spack view of py-torch



Spack view of py-torch