



Building a library: from Autotools to Guix

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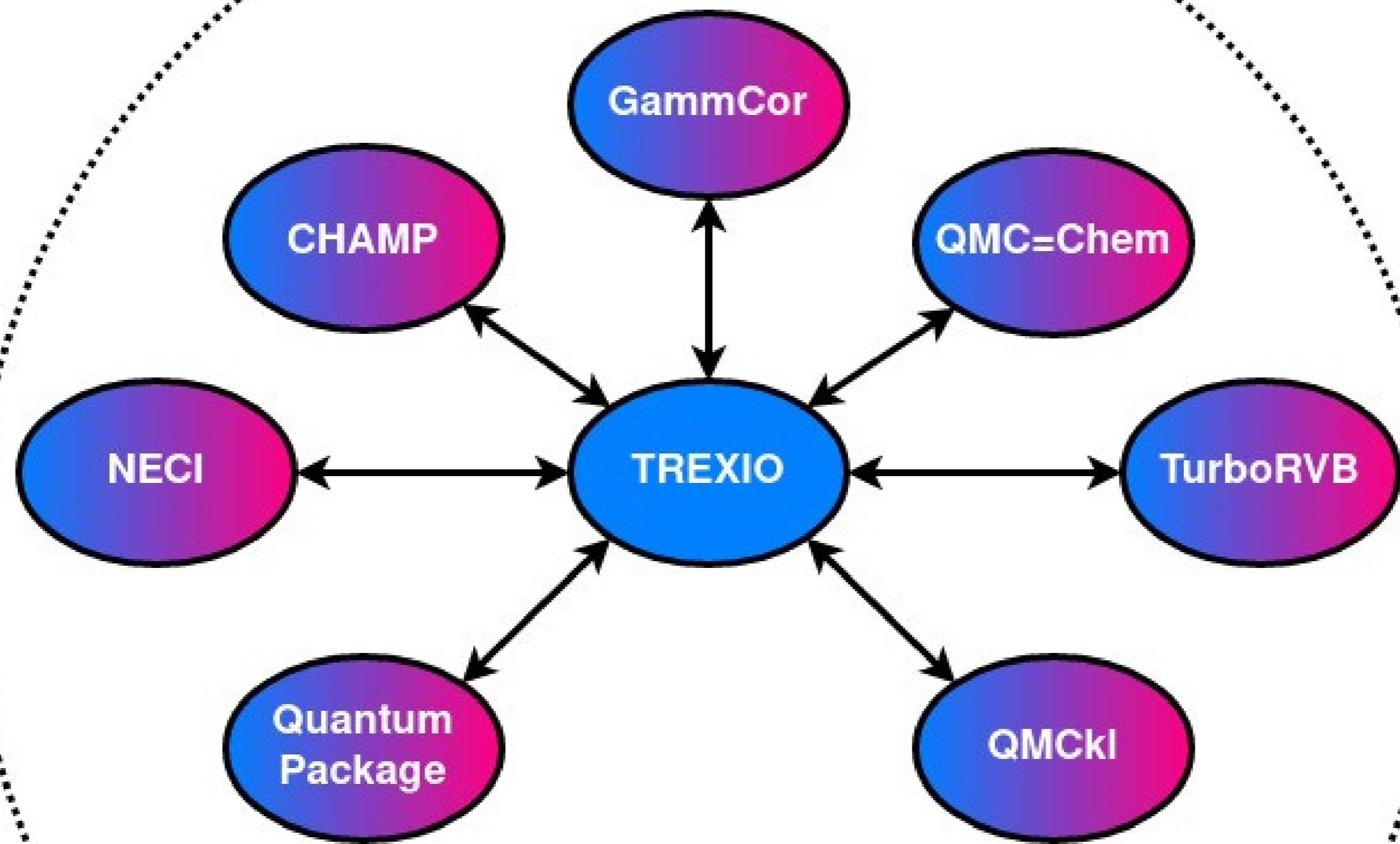
Laboratoire de Chimie et Physique Quantiques (LCPQ)

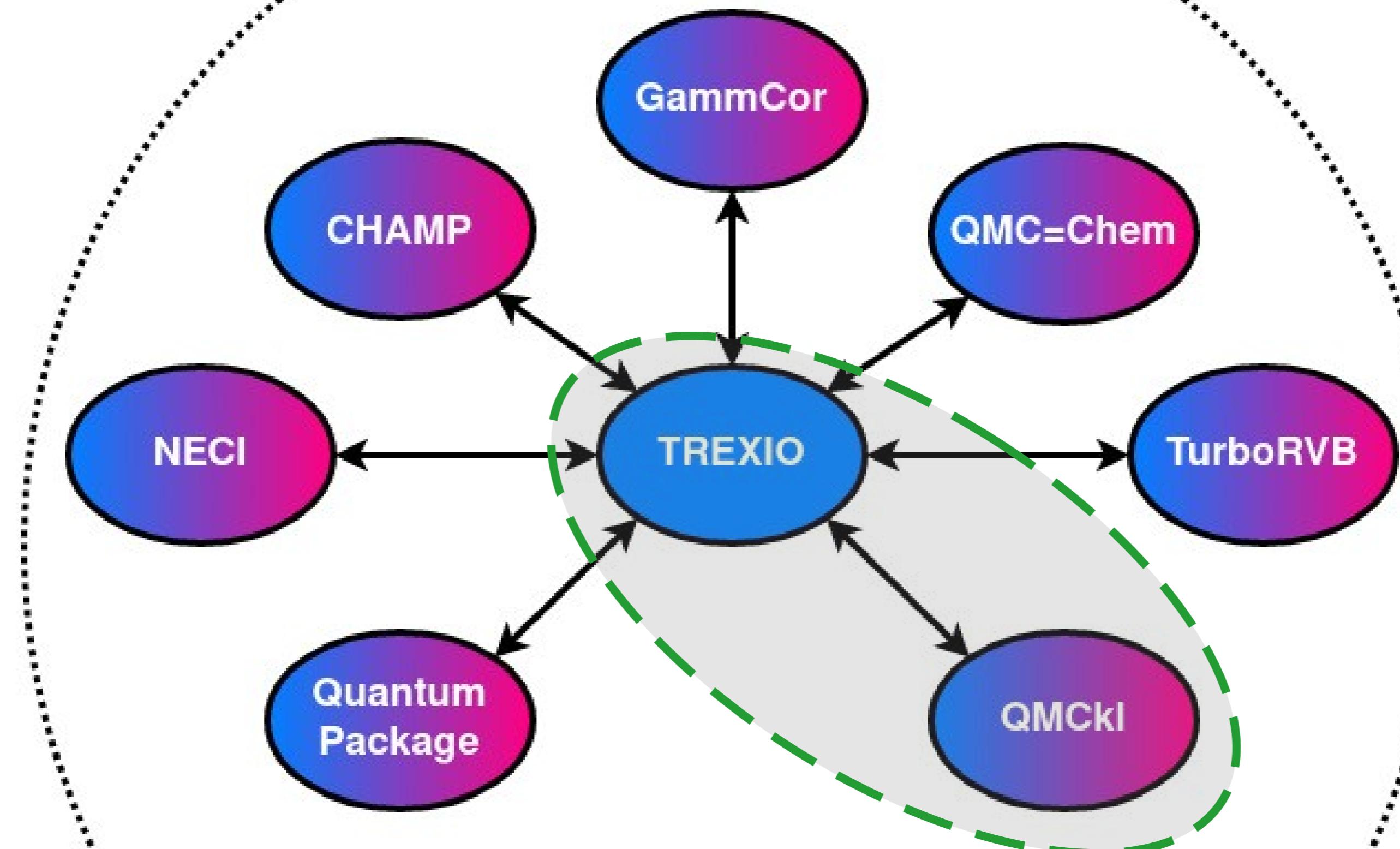
@ CNRS and University of Toulouse, France

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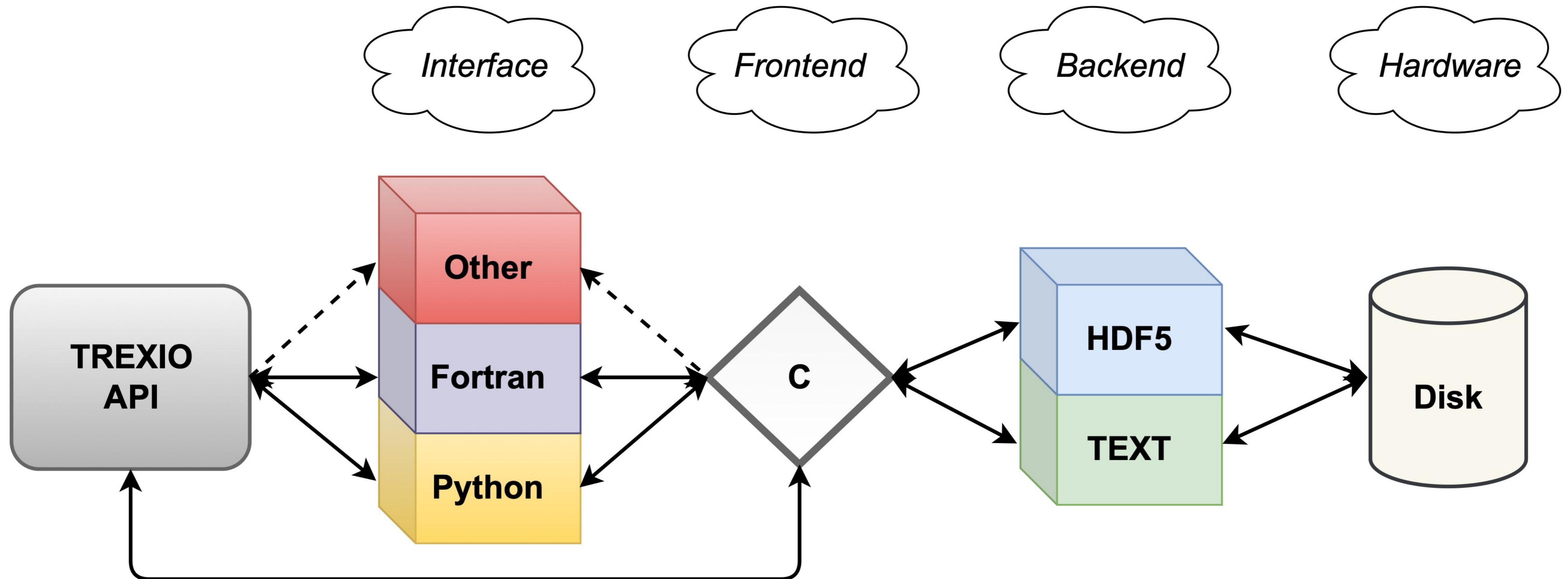
Open-source libraries for Quantum Monte Carlo :

TREXIO & QMCKI





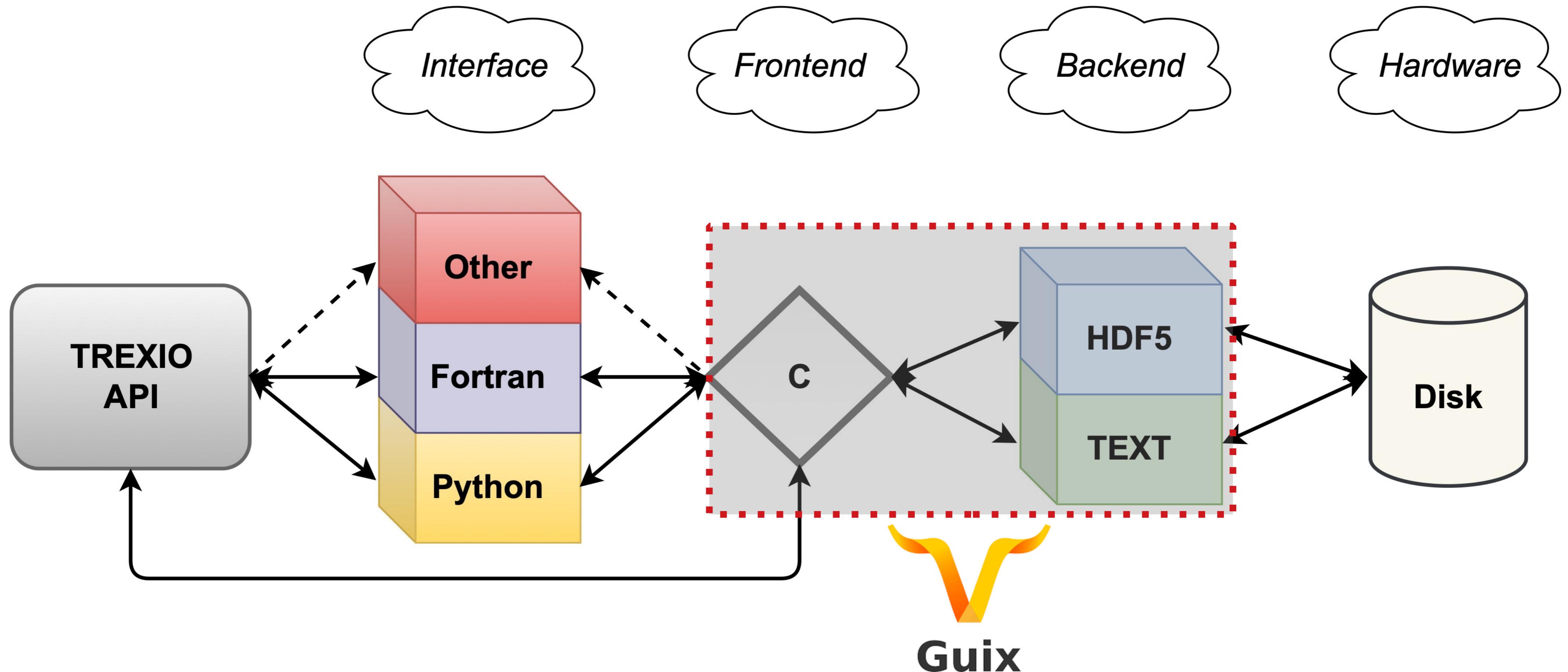
TREX
Targeting Real chemical accuracy at the EXascale



Source code in pure **C** (C99) for the best performance and interoperability

Bindings in **Fortran** (ISO_C_BINDING), **Python** (SWIG), **OCaml**

Easy to install (Autotools/CMake, conda, Spack, Guix, pip, opam)



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From Autotools to Guix

TREXIO package for Guix ([trexio.scm](#))

```
(define-public trexio-2.0
  (package
    (name "trexio")
    (version "2.0")
    (source (origin
              (method url-fetch)
              (uri (string-append "https://github.com/TREX-CoE/trexio/releases/download/v" version
                                  "/trexio-" version ".0"
                                  ".tar.gz")))
              (sha256
               (base32
                 ;; the hash below is produced by guix download <url>
                 "1d2cn4w2r9gfid5b9wrq9q290kqdnbjdmvli76sli5r58kdg5vkf"
                 ))))
    (build-system gnu-build-system)
    (arguments `(#:configure-flags '("--enable-silent-rules")))
    (inputs `(("hdf5" ,hdf5) ("gfortran", gfortran)))
    (synopsis "TREX I/O library")
    (description "The TREXIO library defines a standard format for storing wave functions,
                  together with a C-compatible API such that it can be easily used in any programming language.")
    (home-page "https://trex-coe.github.io/trexio")
    (license bsd-3)))
```

QMCKl package for Guix ([qmckl.scm](#))

```
(define-public qmckl-hpc-0.2.1
  (package
    (name "qmckl-hpc")
    (version "0.2.1")
    (source (origin
              (method url-fetch)
              (uri (string-append "https://github.com/TREX-CoE/qmckl/releases/download/v" version
                                  "/qmckl-" version ".tar.gz"))
              (sha256
               (base32
                ;; the hash below is produced by guix download <url>
                "18100fd4vp41saxiji734mq5lckjplbnmm1nz29da4azhxzbzki9"
                ))))
    (build-system gnu-build-system)
    (arguments
      `(#:configure-flags
        '(" --enable-silent-rules"
          " --enable-hpc"
          " --with-openmp")))
    (inputs
      `(("trexio", trexio)
        ("gfortran", gfortran)
        ("openblas", openblas)
        ("lapack", lapack)
      )))
    (synopsis "QMCKl: Quantum Monte Carlo Kernel Library")
    (description "The main QMC algorithms are exposed in a simple language and provided a standard
                  API to enable the high-performance implementations taking advantage of modern hardware.")
    (home-page "https://trex-coe.github.io/qmckl/index.html")
    (license bsd-3))))
```

QMCKl package for Guix ([qmckl.scm](#))

```
(define-public qmckl-hpc-0.2.1
  (package
    (name "qmckl-hpc")
    (version "0.2.1")
    (source (origin
              (method url-fetch)
              (uri (string-append "https://github.com/TREX-CoE/qmckl/releases/download/v" version
                                  "/qmckl-" version ".tar.gz"))
              (sha256
               (base32
                ;; the hash below is produced by guix download <url>
                "18100fd4vp41saxiji734mq5lckjplbnmm1nz29da4azhxzbzki9"
                ))))
    (build-system gnu-build-system)
    (arguments
      `(#:configure-flags
        '("--enable-silent-rules"
          "--enable-hpc"
          "--with-openmp")))
    (inputs
      `(("trexio", trexio)
        ("gfortran", gfortran)
        ("openblas", openblas)
        ("lapack", lapack)))
    )
  (synopsis "QMCKl: Quantum Monte Carlo Kernel Library")
  (description "The main QMC algorithms are exposed in a simple language and provided a standard API to enable the high-performance implementations taking advantage of modern hardware.")
  (home-page "https://trex-coe.github.io/qmckl/index.html")
  (license bsd-3)))
.....$ guix package      \
      -P "$GUIX_PROFILE" \
      -L ~/trexio/tools \
      -f ~/qmckl/tools/qmckl.scm
.....
```

QMCKL package for Guix (qmckl.scm)

```
(define-public qmckl-dev
  (let ((commit "26f8a1b906c329fa92adc2480e1769b8a90347de")
        (revision "1"))
    (package
      (name "qmckl-dev")
      (version (git-version "0.2.2" revision commit))
      (source (origin
                  (method git-fetch)
                  (uri (git-reference
                            (url "https://github.com/TREX-CoE/qmckl")
                            (commit commit)
                            (recursive? #t)))
                  (file-name (git-file-name name version)))
                  (sha256
                    (base32
                      ;; the hash below is produced by `guix hash -rx .`
                      "0px3880bnciky8mwivll56108j9ncxri3ic2bhavcwn1z12z7lcb"
                    )))
                )
      (build-system gnu-build-system)
      (arguments
        '(#:configure-flags
          '("--enable-hpc"
            "--with-openmp")
        #:phases
        ';; this is a workaround to activate QMCKL_DEVEL mode
        ' (modify-phases %standard-phases
          (add-after 'unpack 'set-devel
            (lambda
              (mkdir-p ".git")))))
        ))))
```

Reproducing and sharing the environment

```
$ guix package      \
-p "$GUIX_PROFILE" \
--export-manifest > manifest.scm
```

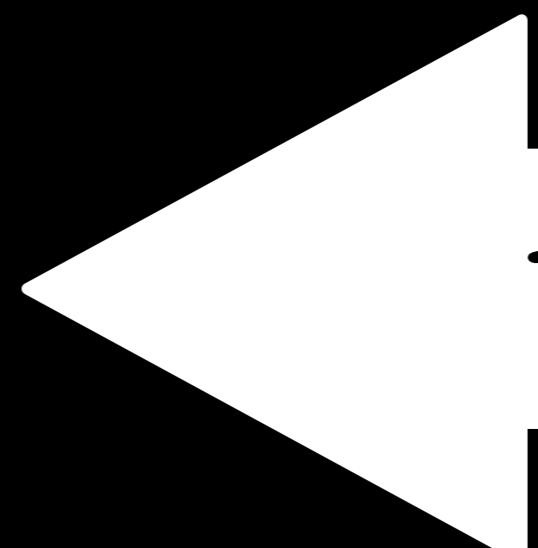
```
(specifications->manifest
  (list "qmckl-hpc"
        "trexio"
        "gcc-toolchain@9"
        "hdf5@1.10" ))
```

Reproducing and sharing the environment

```
$ guix package      \
-p "$GUIX_PROFILE" \
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```

```
(specifications->manifest
  (list "qmckl-hpc"
        "trexio"
        "gcc-toolchain@9"
        "hdf5@1.10" ))
```

```
$ guix pack      \
-f tarball      \
-L ~/trexio/tools \
-L ~/qmckl/tools \
-m manifest.scm
```



To Be Continued

139M 7cc1xav6bnv2al7kkwxainbbby7xy938i-qmckl-hpc-trexio-gcc-toolchain-hdf5-tarball-pack.tar.gz

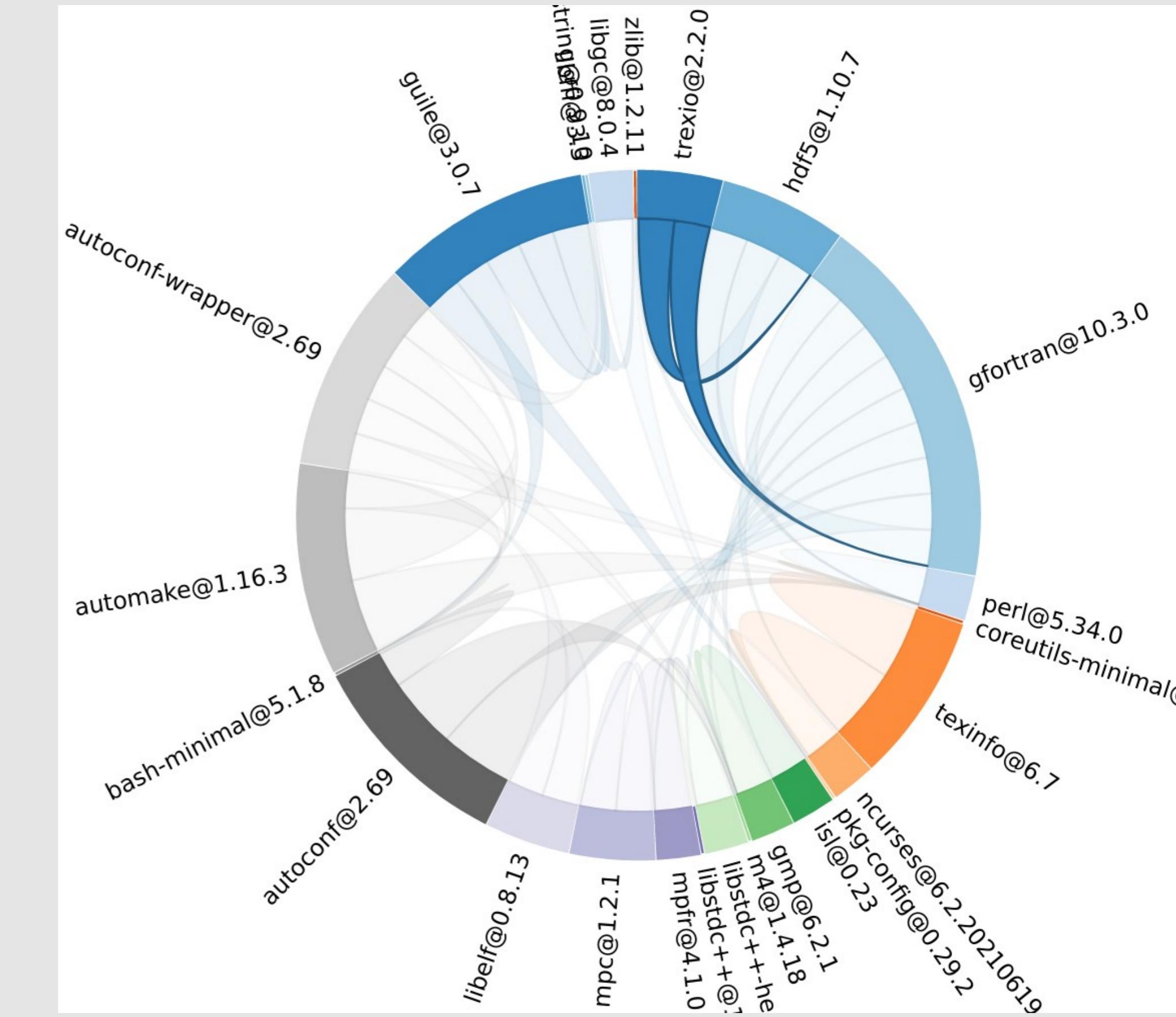


trexio : <https://github.com/TREX-CoE/trexio>

qmckl : <https://github.com/TREX-CoE/qmckl>

Thank you!

TREX-CoE : <https://trex-coe.eu>



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