Building a library: from Autotools to Guix

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Open-source libraries for Quantum Monte Carlo:

TREXIO & QMCKI
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)

[https://github.com/TREX-CoE/trexio](https://github.com/TREX-CoE/trexio)
Source code in pure C (C99) for the best performance and interoperability

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

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https://github.com/TREX-CoE/trexio
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>
              "1d2cn4w2r9gfid5b9wrg9q290kqdnbjdmvli76s1i5r58kdg5vkg"
             )))
   (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>
               "l8100fd4vp4lsaxiji73mq5lckjpblnmmlnz29da4ahxzbzki9"
              ))))
   (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
                           "81100fd4vp41saxiji734mq5lckjplbnmml1nz29da4azhxzbzki9"
                           )))
             (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)

```scheme
(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 -r x`
                  "0px3880bnciky8mwiwll56108j9ncxri3ic2bhavcw1n1z12z7lcb"
                  )))
      (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"  \
   --export-manifest > manifest.scm

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

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