Molpro 2025.1.0

ウェブページ

https://www.molpro.net/

バージョン

2025.1.0

ビルド環境

- GCC 13.1.1 (gcc-toolset-13)
- Intel MPI 2021.14.1
- Eigen 3.4.0
- MKL 2025.0

ビルドに必要なファイル

- molpro-2025.1.0.tar.gz
- ga-5.9.tar.gz
- work.patch
- patch-argos-binput.F
- patch-cic-ItfFortranInt.h
- patch-common_modules-common_cconf
    - 大きな CI 計算のためのパラメータの変更と、一時ディレクトリのデフォルトパスの変更をしています。
    - パッチファイル本体は /apl/molpro/2025.1.0/patches 以下に置いています。
- token

ビルド手順

```
#!/bin/sh

# Exit script if any error occurs
set -e

# Variable definitions
GA_VERSION=5.9
GA_ARCHIVE=/home/users/${USER}/Software/GlobalArrays/${GA_VERSION}/ga-${GA_VERSION}.tar.gz
MOLPRO_VERSION=2025.1.0
MOLPRO_DIRNAME=molpro-${MOLPRO_VERSION}
BASEDIR=/home/users/${USER}/Software/Molpro/${MOLPRO_VERSION}
MOLPRO_TARBALL=${BASEDIR}/${MOLPRO_DIRNAME}.tar.gz
PATCH0=${BASEDIR}/work.patch
PATCH1=${BASEDIR}/patch-argos-binput.F
PATCH2=${BASEDIR}/patch-cic-ItfFortranInt.h
PATCH3=${BASEDIR}/patch-common_modules-common_cconf
TOKEN=${BASEDIR}/token
WORKDIR=/gwork/users/${USER}
GA_INSTALLDIR=${WORKDIR}/ga-temporary
INSTALLDIR=/apl/molpro/${MOLPRO_VERSION}
PARALLEL=12

# Common environment setup function
setup_environment() {
  umask 0022
  ulimit -s unlimited

  export LANG=
  export LC_ALL=C
  export OMP_NUM_THREADS=1
}

# Directory cleanup function
```

```
cleanup_directory() {
  local dir_name=$1
  if [ -d "$dir_name" ]; then
    local temp_name="${dir_name}_tmp"
    mv "$dir_name" "$temp_name"
    rm -rf "$temp_name"
  fi
}

# Compiler and flags setup function
setup_compiler_flags() {
  # Compiler flags configuration
  export CFLAGS="-mpc80"
  export FFLAGS="-mpc80"
  export FCFLAGS="-mpc80"
  export CXXFLAGS="-mpc80"

  # Compiler settings
  export F77=mpif90
  export F90=mpif90
  export FC=mpif90
  export CC=mpicc
  export CXX=mpicxx
  export MPIF77=mpif90
  export MPICC=mpicc
  export MPICXX=mpicxx
  export GA_FOPT="-O3"
  export GA_COPT="-O3"
  export GA_CXXOPT="-O3"
}

# Patch application function
apply_patches() {
  local patch_files=("$@")
  for patch_file in "${patch_files[@]}"; do
    echo "Applying patch: $patch_file"
    patch -p0 < "$patch_file"
  done
}

# Build execution function
run_make() {
  local target=$1
  local options=$2

  if [ -z "$options" ]; then
    make -j ${PARALLEL} $target
  else
    make -j ${PARALLEL} $target $options
  fi
}

# Main processing
main() {
  # Environment setup
  setup_environment

  # Change to working directory
  cd $WORKDIR

  # Cleanup old directories
  cleanup_directory "ga-${GA_VERSION}"
  cleanup_directory "ga-temporary"
  cleanup_directory "${MOLPRO_DIRNAME}"
```

```
    # Load modules
    module -s purge
    module -s load gcc-toolset/13
    module -s load intelmpi/2021.14.1
    module -s load eigen/3.4.0

    # Building Global Arrays
    echo "Building Global Arrays ${GA_VERSION}..."
    tar zxf ${GA_ARCHIVE}
    cd ga-${GA_VERSION}

    setup_compiler_flags

    ./autogen.sh
    ./configure --enable-i8 \
                --with-mpi-pr \
                --prefix=${GA_INSTALLDIR}

    run_make
    make check
    make install

    # Building Molpro
    echo "Building Molpro ${MOLPRO_VERSION}..."
    module -s load mkl/2025.0.0.1

    cd ${WORKDIR}
    tar zxf ${MOLPRO_TARBALL}
    cd ${MOLPRO_DIRNAME}

    # Apply patches
    apply_patches "$PATCH0" "$PATCH1" "$PATCH2" "$PATCH3"

    export PATH="${GA_INSTALLDIR}/bin:$PATH"

    # Check GA library directory
    GA_LIBDIR="lib64"
    if [ ! -d "${GA_INSTALLDIR}/${GA_LIBDIR}" ]; then
        GA_LIBDIR="lib"
    fi

    # Molpro configuration and build
    CPPFLAGS="-I${GA_INSTALLDIR}/include" \
    LDFLAGS="-L${GA_INSTALLDIR}/${GA_LIBDIR}" \
    ./configure --prefix=${INSTALLDIR} \
                --enable-slater

    run_make

    # Copy token
    cp $TOKEN "$(pwd)/lib/.token"

    # Run tests
    make quicktest MOLPRO_OPTIONS="-n2"
    make test

    # Installation
    make install
    cp -a testjobs ${INSTALLDIR}/molpro*
    cp -a bench ${INSTALLDIR}/molpro*

    echo "Installation of Molpro ${MOLPRO_VERSION} completed successfully!"

}

# Execute main processing
```

```
main
```

テスト

全てパスしています。

メモ

- make tuningが無くなったので削除