

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