

PSI 4.0b5

ウェブページ

<http://www.psicode.org/index.php>

バージョン

4.0b5

ビルド環境

- gcc version 4.3.4
- Intel Compiler 13.1.1.163

ビルドに必要なファイル

- psi4.0b5.tar.gz

ビルド手順

```
#!/bin/csh -f
umask 022
set file_psi=/home/users/${USER}/build/psi40b5/psi4.0b5.tar.gz
set work=/work/users/${USER}
set prefix=/local/apl/uv/psi40b5
#-----
# "Make sure that ${prefix} directory exists and is writable for install."
#-----
# mkdir ${prefix}
#-----
if (! -d ${work}) then
  mkdir -p ${work}
endif
cd ${work}
if (-d psi4.0b5) then
  mv psi4.0b5 psi4.0b5-erase
  rm -rf psi4.0b5-erase &
endif
tar xzf ${file_psi}
cd psi4.0b5
mkdir obj
cd obj
../configure --prefix=${prefix} --with-blas='-mkl' \
  --with-cc=icc --with-cxx=icpc --with-fc=ifort \
  --with-opt='-O2 -static -no-prec-div' --with-incdirs=-mkl
make
make tests
make install
cd ..
cp -r tests ${prefix}
```