aenet-tinker-tutorial

June 20, 2021

Example usage of the ænet-Tinker interface for molecular dynamics simulations with artificial neural network (ANN) potentials.

[1]:
```
import os
```

The following lines might have to be adjusted for your ssystem. `intel_init` sets the command used to initialize the Intel compilers. `num_cores` is the number of cores to be used for MD simulations.

[2]:
```
intel_init = "source /opt/intel/bin/compilervars.sh intel64 2> /dev/null"
num_cores = 1
```

1 1. Compiling ænet

The following instructions download ænet and compile the ænet library version 2.0.4

[3]:
```
if not os.path.exists('aenet'):
  !! git clone https://github.com/atomisticnet/aenet.git --branch v2.0.4
```

Now, ænet can be compiled. We build both the `aenet` executables and the library (`libaenet.a`), since the Fortran code Tinker can also make use of the ænet module files .

[4]:
```
cmd = """\
{}
cd aenet/lib/
sed -i "s/FC *= *.*$/FC = ifort -c/" Makefile
make
cd ../..
cd aenet/src/
make -f makefiles/Makefile.ifort_serial
make -f makefiles/Makefile.ifort_serial lib
cd ../../
""".format(intel_init)
!{cmd}
```

```
tar xfvz Lbfgsb.3.0.tar.gz
./._Lbfgsb.3.0
Lbfgsb.3.0/
Lbfgsb.3.0/._algorithm.pdf
Lbfgsb.3.0/algorithm.pdf
Lbfgsb.3.0/blas.f
Lbfgsb.3.0/._code.pdf
Lbfgsb.3.0/code.pdf
Lbfgsb.3.0/driver1.f
Lbfgsb.3.0/driver1.f90
Lbfgsb.3.0/driver2.f
Lbfgsb.3.0/driver2.f90
Lbfgsb.3.0/driver3.f
Lbfgsb.3.0/driver3.f90
Lbfgsb.3.0/._iterate.dat
Lbfgsb.3.0/iterate.dat
Lbfgsb.3.0/lbfgsb.f
Lbfgsb.3.0/License.txt
Lbfgsb.3.0/linpack.f
Lbfgsb.3.0/._Makefile
Lbfgsb.3.0/Makefile
Lbfgsb.3.0/._OUTPUTS
Lbfgsb.3.0/OUTPUTS/
Lbfgsb.3.0/README
Lbfgsb.3.0/timer.f
Lbfgsb.3.0/x.lbfgsb_77_1
Lbfgsb.3.0/x.lbfgsb_77_2
Lbfgsb.3.0/x.lbfgsb_77_3
Lbfgsb.3.0/x.lbfgsb_90_1
Lbfgsb.3.0/x.lbfgsb_90_2
Lbfgsb.3.0/x.lbfgsb_90_3
Lbfgsb.3.0/OUTPUTS/._output_77_1
Lbfgsb.3.0/OUTPUTS/output_77_1
Lbfgsb.3.0/OUTPUTS/._output_77_2
Lbfgsb.3.0/OUTPUTS/output_77_2
Lbfgsb.3.0/OUTPUTS/._output_77_3
Lbfgsb.3.0/OUTPUTS/output_77_3
Lbfgsb.3.0/OUTPUTS/._output_90_1
Lbfgsb.3.0/OUTPUTS/output_90_1
Lbfgsb.3.0/OUTPUTS/._output_90_2
Lbfgsb.3.0/OUTPUTS/output_90_2
Lbfgsb.3.0/OUTPUTS/._output_90_3
Lbfgsb.3.0/OUTPUTS/output_90_3
ifort -c -O2 Lbfgsb.3.0/blas.f -o Lbfgsb.3.0/blas.o
ifort -c -O2 Lbfgsb.3.0/lbfgsb.f -o Lbfgsb.3.0/lbfgsb.o
Lbfgsb.3.0/lbfgsb.f(2802): remark #8291: Recommended relationship between field
width 'W' and the number of fractional digits 'D' in this edit descriptor is
'W>=D+7'.
```

```
 3001 format(2(1x,i4),2(1x,i5),2x,a3,1x,i4,1p,2(2x,d7.1),1p,2(1x,d10.3))
-----------------------------------------------------^
Lbfgsb.3.0/lbfgsb.f(2893): remark #8291: Recommended relationship between field
width 'W' and the number of fractional digits 'D' in this edit descriptor is
'W>=D+7'.
 3002 format(2(1x,i4),2(1x,i5),2x,a3,1x,i4,1p,2(2x,d7.1),6x,'-',10x,'-')
-----------------------------------------------------^
ifort -c -O2 Lbfgsb.3.0/linpack.f -o Lbfgsb.3.0/linpack.o
ifort -c -O2 Lbfgsb.3.0/timer.f -o Lbfgsb.3.0/timer.o
ar -crusv liblbfgsb.a Lbfgsb.3.0/blas.o    Lbfgsb.3.0/lbfgsb.o
Lbfgsb.3.0/linpack.o Lbfgsb.3.0/timer.o
ar: `u' modifier ignored since `D' is the default (see `U')
a - Lbfgsb.3.0/blas.o
a - Lbfgsb.3.0/lbfgsb.o
a - Lbfgsb.3.0/linpack.o
a - Lbfgsb.3.0/timer.o
ifort -c -O2 -fPIC -o Lbfgsb.3.0/blas_pic.o Lbfgsb.3.0/blas.f
ifort -c -O2 -fPIC -o Lbfgsb.3.0/lbfgsb_pic.o Lbfgsb.3.0/lbfgsb.f
Lbfgsb.3.0/lbfgsb.f(2802): remark #8291: Recommended relationship between field
width 'W' and the number of fractional digits 'D' in this edit descriptor is
'W>=D+7'.
 3001 format(2(1x,i4),2(1x,i5),2x,a3,1x,i4,1p,2(2x,d7.1),1p,2(1x,d10.3))
-----------------------------------------------------^
Lbfgsb.3.0/lbfgsb.f(2893): remark #8291: Recommended relationship between field
width 'W' and the number of fractional digits 'D' in this edit descriptor is
'W>=D+7'.
 3002 format(2(1x,i4),2(1x,i5),2x,a3,1x,i4,1p,2(2x,d7.1),6x,'-',10x,'-')
-----------------------------------------------------^
ifort -c -O2 -fPIC -o Lbfgsb.3.0/linpack_pic.o Lbfgsb.3.0/linpack.f
ifort -c -O2 -fPIC -o Lbfgsb.3.0/timer_pic.o Lbfgsb.3.0/timer.f
gcc -shared Lbfgsb.3.0/blas_pic.o    Lbfgsb.3.0/lbfgsb_pic.o
Lbfgsb.3.0/linpack_pic.o Lbfgsb.3.0/timer_pic.o -lm -lgfortran -o liblbfgsb.so
ifort -c -O2 -g -warn all -check bounds ext/io.f90 -o io.o
ifort -c -O2 -g -warn all -check bounds aeio.f90 -o aeio.o
ifort -c -O2 -g -warn all -check bounds ext/chebyshev.f90 -o chebyshev.o
ifort -c -O2 -g -warn all -check bounds constants.f90 -o constants.o
ifort -c -O2 -g -warn all -check bounds ext/xsflib.f90 -o xsflib.o
ifort -c -O2 -g -warn all -check bounds geometry.f90 -o geometry.o
ifort -c -O2 -g -warn all -check bounds ext/sortlib.f90 -o sortlib.o
ifort -c -O2 -g -warn all -check bounds ext/lclist.f90 -o lclist.o
ext/lclist.f90(1250): remark #7712: This variable has not been used.   [V1]
    double precision, dimension(3) :: v1, v2
--------------------------------------^
ext/lclist.f90(1249): remark #7712: This variable has not been used.
[CELL_DIST]
    double precision               :: cell_dist
--------------------------------------^
ext/lclist.f90(1251): remark #7712: This variable has not been used.   [VNORM]
```

```
    double precision               :: vnorm
-------------------------------------^
ifort -c -O2 -g -warn all -check bounds ext/feedforward.f90 -o feedforward.o
ifort -c -O2 -g -warn all -check bounds ext/sfbasis.f90 -o sfbasis.o
ext/sfbasis.f90(433): remark #7712: This variable has not been used.   [ITYPE0]
  subroutine sfb_eval(sfb, itype0, coo0, nat, itype1, coo1, nv, &
--------------------------^
ifort -c -O2 -g -warn all -check bounds ext/symmfunc.f90 -o symmfunc.o
ifort -c -O2 -g -warn all -check bounds sfsetup.f90 -o sfsetup.o
ifort -c -O2 -g -warn all -check bounds trainset.f90 -o trainset.o
ifort -c -O2 -g -warn all -check bounds potential.f90 -o potential.o
ifort -c -O2 -g -warn all -check bounds ext/timing.f90 -o timing.o
ifort -c -O2 -g -warn all -check bounds aenet.f90 -o aenet.o
aenet.f90(631): remark #7712: This variable has not been used.   [NNB_HERE]
    integer :: nnb_here
---------------^
ifort -c -O2 -g -warn all -check bounds input.f90 -o input.o
ifort -c -O2 -g -warn all -check bounds parallel.F90 -o parallel.o
ifort -c -O2 -g -warn all -check bounds random.f90 -o random.o
ifort -c -O2 -g -warn all -check bounds optimize.f90 -o optimize.o
optimize.f90(976): remark #8291: Recommended relationship between field width
'W' and the number of fractional digits 'D' in this edit descriptor is 'W>=D+7'.
    write(*,'(1x,"Learning rate               : ",ES9.3)') adam_learnrate
-----------------------------------------------------^
optimize.f90(979): remark #8291: Recommended relationship between field width
'W' and the number of fractional digits 'D' in this edit descriptor is 'W>=D+7'.
    write(*,'(1x,"Epsilon                     : ",ES9.3)') adam_eps
-----------------------------------------------------^
optimize.f90(1538): warning #8889: Explicit declaration of the EXTERNAL
attribute is required.   [DPOTRF]
          call DPOTRF('U', opt_nw_tot, A, opt_nw_tot, info)
---------------^
optimize.f90(1542): warning #8889: Explicit declaration of the EXTERNAL
attribute is required.   [DPOTRS]
             call DPOTRS('U', opt_nw_tot, 1, A, opt_nw_tot, lm_Wup, &
------------------^
ifort -static-intel -g -warn all -check bounds -o
../bin/generate.x-2.0.4-ifort_serial generate.f90 aenet.o aeio.o chebyshev.o
constants.o feedforward.o geometry.o input.o io.o lclist.o optimize.o parallel.o
potential.o random.o sfbasis.o sfsetup.o sortlib.o symmfunc.o timing.o
trainset.o xsflib.o ../lib/liblbfgsb.a -mkl
ifort -static-intel -g -warn all -check bounds -o
../bin/train.x-2.0.4-ifort_serial train.f90 aenet.o aeio.o chebyshev.o
constants.o feedforward.o geometry.o input.o io.o lclist.o optimize.o parallel.o
potential.o random.o sfbasis.o sfsetup.o sortlib.o symmfunc.o timing.o
trainset.o xsflib.o ../lib/liblbfgsb.a -mkl
train.f90(199): remark #7712: This variable has not been used.   [BATCHSIZE]
  integer                                          :: batchsize
```

```
-----------------------------------------------------^
ifort -static-intel -g -warn all -check bounds -o
../bin/predict.x-2.0.4-ifort_serial predict.F90 aenet.o aeio.o chebyshev.o
constants.o feedforward.o geometry.o input.o io.o lclist.o optimize.o parallel.o
potential.o random.o sfbasis.o sfsetup.o sortlib.o symmfunc.o timing.o
trainset.o xsflib.o ../lib/liblbfgsb.a -mkl
ar -crusv libaenet.a aenet.o aeio.o chebyshev.o constants.o feedforward.o
geometry.o input.o io.o lclist.o optimize.o parallel.o potential.o random.o
sfbasis.o sfsetup.o sortlib.o symmfunc.o timing.o trainset.o xsflib.o
ar: `u' modifier ignored since `D' is the default (see `U')
a - aenet.o
a - aeio.o
a - chebyshev.o
a - constants.o
a - feedforward.o
a - geometry.o
a - input.o
a - io.o
a - lclist.o
a - optimize.o
a - parallel.o
a - potential.o
a - random.o
a - sfbasis.o
a - sfsetup.o
a - sortlib.o
a - symmfunc.o
a - timing.o
a - trainset.o
a - xsflib.o
ifort -c -O2 -g -warn all -check bounds -fPIC -o aenet_pic.o aenet.f90
aenet.f90(631): remark #7712: This variable has not been used.   [NNB_HERE]
    integer :: nnb_here
---------------^
ifort -c -O2 -g -warn all -check bounds -fPIC -o aeio_pic.o aeio.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o chebyshev_pic.o
ext/chebyshev.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o constants_pic.o constants.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o feedforward_pic.o
ext/feedforward.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o geometry_pic.o geometry.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o input_pic.o input.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o io_pic.o ext/io.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o lclist_pic.o ext/lclist.f90
ext/lclist.f90(1250): remark #7712: This variable has not been used.   [V1]
    double precision, dimension(3) :: v1, v2
-------------------------------------^
ext/lclist.f90(1249): remark #7712: This variable has not been used.
```

```
[CELL_DIST]
    double precision               :: cell_dist
-------------------------------------^
ext/lclist.f90(1251): remark #7712: This variable has not been used.   [VNORM]
    double precision               :: vnorm
-------------------------------------^
ifort -c -O2 -g -warn all -check bounds -fPIC -o optimize_pic.o optimize.f90
optimize.f90(976): remark #8291: Recommended relationship between field width
'W' and the number of fractional digits 'D' in this edit descriptor is 'W>=D+7'.
    write(*,'(1x,"Learning rate               : ",ES9.3)') adam_learnrate
-----------------------------------------------------^
optimize.f90(979): remark #8291: Recommended relationship between field width
'W' and the number of fractional digits 'D' in this edit descriptor is 'W>=D+7'.
    write(*,'(1x,"Epsilon                     : ",ES9.3)') adam_eps
-----------------------------------------------------^
optimize.f90(1538): warning #8889: Explicit declaration of the EXTERNAL
attribute is required.   [DPOTRF]
          call DPOTRF('U', opt_nw_tot, A, opt_nw_tot, info)
---------------^
optimize.f90(1542): warning #8889: Explicit declaration of the EXTERNAL
attribute is required.   [DPOTRS]
             call DPOTRS('U', opt_nw_tot, 1, A, opt_nw_tot, lm_Wup, &
------------------^
ifort -c -O2 -g -warn all -check bounds -fPIC -o parallel_pic.o parallel.F90
ifort -c -O2 -g -warn all -check bounds -fPIC -o potential_pic.o potential.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o random_pic.o random.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o sfbasis_pic.o ext/sfbasis.f90
ext/sfbasis.f90(433): remark #7712: This variable has not been used.   [ITYPE0]
  subroutine sfb_eval(sfb, itype0, coo0, nat, itype1, coo1, nv, &
---------------------------^
ifort -c -O2 -g -warn all -check bounds -fPIC -o sfsetup_pic.o sfsetup.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o sortlib_pic.o ext/sortlib.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o symmfunc_pic.o ext/symmfunc.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o timing_pic.o ext/timing.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o trainset_pic.o trainset.f90
ifort -c -O2 -g -warn all -check bounds -fPIC -o xsflib_pic.o ext/xsflib.f90
gcc -shared aenet_pic.o aeio_pic.o chebyshev_pic.o constants_pic.o
feedforward_pic.o geometry_pic.o input_pic.o io_pic.o lclist_pic.o
optimize_pic.o parallel_pic.o potential_pic.o random_pic.o sfbasis_pic.o
sfsetup_pic.o sortlib_pic.o symmfunc_pic.o timing_pic.o trainset_pic.o
xsflib_pic.o -lgfortran -o libaenet.so
```

2 2. Download the `aenet-tinker` interface

The ænet-Tinker interface is separately maintained and distributed. We download it here.

[5]:
```
if not os.path.exists('aenet-tinker'):
  !! git clone https://github.com/atomisticnet/aenet-tinker.git
```

3 3. Compiling Tinker with ænet support

Now, we download and compile Tinker version 8.9.1, using the ænet library that we built above.

Note: The links on the Tinker website are not permanent, and you might have to update the address to the current version (or latest revision of version 8).

Tinker website: https://dasher.wustl.edu/tinker/

[6]:
```
if not os.path.exists('tinker'):
  !! wget https://dasher.wustl.edu/tinker/downloads/tinker-8.9.1.tar.gz
  !! tar xfvz tinker-8.9.1.tar.gz
```

Some files from the `aenet-tinker` directory simply need to be copied over to the Tinker `source` directory.

- `aenettinker.f90`
- `extra.f`
- `extra1.f`

Additionally, the `aenet.mod` module file from the main aenet source directory also needs to be copied over.

[7]:
```
! cp aenet-tinker/src/*.f* tinker/source/
! cp aenet/src/aenet.* tinker/source/
```

If a Makefile for your version of Tinker is available in `aenet-tinker/src/makefiles`, then we recommend using this file directly. If the precise version is not available, start with Tinker's own Makefile (`tinker/make/Makefile`) and apply the patch in `aenet-tinker/src/makefiles` that is closest in version number.

In our example case, we can copy the available Makefile:

[8]:
```
! cp aenet-tinker/src/makefiles/Makefile.aenetlib_ifort.tinker-8.9.1 tinker/
↪source/Makefile
```

Now, the `Makefile` still might have to be edited to ensure that compiler settings are paths are correct. In our case, the paths to `aenet` and `tinker` need to be updated:

[9]:
```
%cd tinker/source/
!sed -i 's|TINKERDIR *= *.*$|TINKERDIR = ../../tinker|g' Makefile
!sed -i 's|AENETDIR *= *.*$|AENETDIR = ../../aenet|g' Makefile
%cd ../..
```

```
/data/home/na2782/aenet-tinker-test-2/tinker/source
/data/home/na2782/aenet-tinker-test-2
```

The rest of the Makefile should be fine for a generic Linux. So, Tinker can now be compiled.

Note: This can take a few minutes!

[10]:
```
cmd = """\
{}
cd tinker/source/
make
chmod a+x ./dynamic.x
cd ../..
""".format(intel_init)
!{cmd}
```

```
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
analyz.f -o analyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
sizes.f -o sizes.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
atoms.f -o atoms.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
energi.f -o energi.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
files.f -o files.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
inform.f -o inform.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
iounit.f -o iounit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
katoms.f -o katoms.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mutant.f -o mutant.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
potent.f -o potent.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
units.f -o units.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
usage.f -o usage.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
alchemy.f -o alchemy.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
action.f -o action.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
keys.f -o keys.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
active.f -o active.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
atomid.f -o atomid.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
bound.f -o bound.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
boxes.f -o boxes.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
deriv.f -o deriv.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
neigh.f -o neigh.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
aenettinker.f90 -o aenettinker.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
align.f -o align.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
angbnd.f -o angbnd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
atmlst.f -o atmlst.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bndstr.f -o bndstr.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
cflux.f -o cflux.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
charge.f -o charge.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
chgpen.f -o chgpen.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
math.f -o math.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mplpot.f -o mplpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mpole.f -o mpole.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
alterchg.f -o alterchg.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
group.f -o group.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
inter.f -o inter.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
limits.f -o limits.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
vdwpot.f -o vdwpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
analysis.f -o analysis.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
angang.f -o angang.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
angpot.f -o angpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
angtor.f -o angtor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
bath.f -o bath.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bitor.f -o bitor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
chgpot.f -o chgpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
chgtrn.f -o chgtrn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
couple.f -o couple.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
dipole.f -o dipole.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
disp.f -o disp.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ewald.f -o ewald.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
fields.f -o fields.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
improp.f -o improp.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
imptor.f -o imptor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
korbs.f -o korbs.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ktrtor.f -o ktrtor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kvdws.f -o kvdws.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
molcul.f -o molcul.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
moment.f -o moment.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
opbend.f -o opbend.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
opdist.f -o opdist.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
output.f -o output.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
piorbs.f -o piorbs.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pistuf.f -o pistuf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pitors.f -o pitors.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pme.f -o pme.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
polar.f -o polar.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
polgrp.f -o polgrp.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
polpot.f -o polpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
repel.f -o repel.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
solute.f -o solute.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
strbnd.f -o strbnd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
strtor.f -o strtor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
titles.f -o titles.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
tors.f -o tors.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
tortor.f -o tortor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
urey.f -o urey.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
vdw.f -o vdw.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
virial.f -o virial.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
analyze.f -o analyze.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
angles.f -o angles.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mdstuf.f -o mdstuf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
warp.f -o warp.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
anneal.f -o anneal.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
archive.f -o archive.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
argue.f -o argue.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ascii.f -o ascii.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
attach.f -o attach.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
freeze.f -o freeze.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
moldyn.f -o moldyn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
stodyn.f -o stodyn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
baoab.f -o baoab.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bar.f -o bar.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
basefile.f -o basefile.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ielscf.f -o ielscf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
beeman.f -o beeman.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bicubic.f -o bicubic.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bitors.f -o bitors.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bndpot.f -o bndpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bonds.f -o bonds.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pbstuf.f -o pbstuf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
solpot.f -o solpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
born.f -o born.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bounds.f -o bounds.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
bussi.f -o bussi.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
calendar.f -o calendar.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
cell.f -o cell.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
center.f -o center.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
chkpole.f -o chkpole.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
chkring.f -o chkring.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
chkxyz.f -o chkxyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
cholesky.f -o cholesky.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
chrono.f -o chrono.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
chunks.f -o chunks.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
clock.f -o clock.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
cluster.f -o cluster.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
column.f -o column.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
command.f -o command.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
zclose.f -o zclose.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
zcoord.f -o zcoord.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
connect.f -o connect.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
faces.f -o faces.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
connolly.f -o connolly.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
control.f -o control.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
correlate.f -o correlate.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
minima.f -o minima.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
critical.f -o critical.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
crystal.f -o crystal.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
cspline.f -o cspline.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ctrpot.f -o ctrpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
hescut.f -o hescut.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
tarray.f -o tarray.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
cutoffs.f -o cutoffs.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
damping.f -o damping.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
dcflux.f -o dcflux.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
deflate.f -o deflate.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
delete.f -o delete.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
diagq.f -o diagq.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
diffeq.f -o diffeq.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
diffuse.f -o diffuse.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
disgeo.f -o disgeo.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
refer.f -o refer.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
restrn.f -o restrn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
distgeom.f -o distgeom.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
dma.f -o dma.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
document.f -o document.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
domega.f -o domega.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
dsppot.f -o dsppot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
dynamic.f -o dynamic.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangang.f -o eangang.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangang1.f -o eangang1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
hessn.f -o hessn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangang2.f -o eangang2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangang3.f -o eangang3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangle.f -o eangle.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangle1.f -o eangle1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangle2.f -o eangle2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangle3.f -o eangle3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
torpot.f -o torpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangtor.f -o eangtor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangtor1.f -o eangtor1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangtor2.f -o eangtor2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eangtor3.f -o eangtor3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
ebond.f -o ebond.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ebond1.f -o ebond1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ebond2.f -o ebond2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ebond3.f -o ebond3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
light.f -o light.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
shunt.f -o shunt.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ebuck.f -o ebuck.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ebuck1.f -o ebuck1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ebuck2.f -o ebuck2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ebuck3.f -o ebuck3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echarge.f -o echarge.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echarge1.f -o echarge1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echarge2.f -o echarge2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echarge3.f -o echarge3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echgdpl.f -o echgdpl.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echgdpl1.f -o echgdpl1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echgdpl2.f -o echgdpl2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echgdpl3.f -o echgdpl3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echgtrn.f -o echgtrn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echgtrn1.f -o echgtrn1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echgtrn2.f -o echgtrn2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
echgtrn3.f -o echgtrn3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
edipole.f -o edipole.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
edipole1.f -o edipole1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
edipole2.f -o edipole2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
edipole3.f -o edipole3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
edisp.f -o edisp.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
edisp1.f -o edisp1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
edisp2.f -o edisp2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
edisp3.f -o edisp3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
egauss.f -o egauss.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
egauss1.f -o egauss1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
egauss2.f -o egauss2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
egauss3.f -o egauss3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
egeom.f -o egeom.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
egeom1.f -o egeom1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
egeom2.f -o egeom2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
egeom3.f -o egeom3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ehal.f -o ehal.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ehal1.f -o ehal1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ehal2.f -o ehal2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ehal3.f -o ehal3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eimprop.f -o eimprop.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eimprop1.f -o eimprop1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eimprop2.f -o eimprop2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eimprop3.f -o eimprop3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eimptor.f -o eimptor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eimptor1.f -o eimptor1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
eimptor2.f -o eimptor2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eimptor3.f -o eimptor3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
elj.f -o elj.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
elj1.f -o elj1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
elj2.f -o elj2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
elj3.f -o elj3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
embed.f -o embed.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kchrge.f -o kchrge.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
emetal.f -o emetal.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
emetal1.f -o emetal1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
emetal2.f -o emetal2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
emetal3.f -o emetal3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
emm3hb.f -o emm3hb.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
emm3hb1.f -o emm3hb1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
emm3hb2.f -o emm3hb2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
emm3hb3.f -o emm3hb3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mrecip.f -o mrecip.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
empole.f -o empole.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
empole1.f -o empole1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
empole2.f -o empole2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
empole3.f -o empole3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rigid.f -o rigid.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
energy.f -o energy.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eopbend.f -o eopbend.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
eopbend1.f -o eopbend1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eopbend2.f -o eopbend2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eopbend3.f -o eopbend3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eopdist.f -o eopdist.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eopdist1.f -o eopdist1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eopdist2.f -o eopdist2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eopdist3.f -o eopdist3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
epitors.f -o epitors.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
epitors1.f -o epitors1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
epitors2.f -o epitors2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
epitors3.f -o epitors3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
epolar.f -o epolar.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
polopt.f -o polopt.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
poltcg.f -o poltcg.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
epolar1.f -o epolar1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
epolar2.f -o epolar2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
epolar3.f -o epolar3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
reppot.f -o reppot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erepel.f -o erepel.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erepel1.f -o erepel1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erepel2.f -o erepel2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erepel3.f -o erepel3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erf.f -o erf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rxnfld.f -o rxnfld.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
rxnpot.f -o rxnpot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erxnfld.f -o erxnfld.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erxnfld1.f -o erxnfld1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erxnfld2.f -o erxnfld2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
erxnfld3.f -o erxnfld3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
gkstuf.f -o gkstuf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
hpmf.f -o hpmf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
nonpol.f -o nonpol.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
esolv.f -o esolv.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
esolv1.f -o esolv1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
esolv2.f -o esolv2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
esolv3.f -o esolv3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
estrbnd.f -o estrbnd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
estrbnd1.f -o estrbnd1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
estrbnd2.f -o estrbnd2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
estrbnd3.f -o estrbnd3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
estrtor.f -o estrtor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
estrtor1.f -o estrtor1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
estrtor2.f -o estrtor2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
estrtor3.f -o estrtor3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
etors.f -o etors.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
etors1.f -o etors1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
etors2.f -o etors2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
etors3.f -o etors3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
etortor.f -o etortor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
etortor1.f -o etortor1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
etortor2.f -o etortor2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
etortor3.f -o etortor3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
urypot.f -o urypot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eurey.f -o eurey.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eurey1.f -o eurey1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eurey2.f -o eurey2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
eurey3.f -o eurey3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kdsp.f -o kdsp.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
evcorr.f -o evcorr.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
extra.f -o extra.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
extra1.f -o extra1.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
extra2.f -o extra2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
extra3.f -o extra3.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
fatal.f -o fatal.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
fft.f -o fft.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
openmp.f -o openmp.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
fft3d.f -o fft3d.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
fftpack.f -o fftpack.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
field.f -o field.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
fracs.f -o fracs.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kanang.f -o kanang.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kcpen.f -o kcpen.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
kctrn.f -o kctrn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kpolr.f -o kpolr.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
krepl.f -o krepl.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ksolut.f -o ksolut.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
merck.f -o merck.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
omega.f -o omega.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
orbits.f -o orbits.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
paths.f -o paths.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pdb.f -o pdb.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
polpcg.f -o polpcg.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
potfit.f -o potfit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
qmstuf.f -o qmstuf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rgddyn.f -o rgddyn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ring.f -o ring.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rotbnd.f -o rotbnd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
socket.f -o socket.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
syntrn.f -o syntrn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
uprior.f -o uprior.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
vibs.f -o vibs.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
final.f -o final.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
flatten.f -o flatten.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
freeunit.f -o freeunit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
gda.f -o gda.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
geometry.f -o geometry.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
getarc.f -o getarc.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getint.f -o getint.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getkey.f -o getkey.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getmol.f -o getmol.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getmol2.f -o getmol2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getnumb.f -o getnumb.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getpdb.f -o getpdb.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
params.f -o params.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getprm.f -o getprm.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getref.f -o getref.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getstring.f -o getstring.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
gettext.f -o gettext.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getword.f -o getword.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
getxyz.f -o getxyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ghmcstep.f -o ghmcstep.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
gradient.f -o gradient.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
gradrgd.f -o gradrgd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
gradrot.f -o gradrot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
groups.f -o groups.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
grpline.f -o grpline.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
gyrate.f -o gyrate.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
hessian.f -o hessian.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
hessrgd.f -o hessrgd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
hessrot.f -o hessrot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
kangs.f -o kangs.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kbonds.f -o kbonds.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kdipol.f -o kdipol.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kitors.f -o kitors.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kstbnd.f -o kstbnd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ksttor.f -o ksttor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ktorsn.f -o ktorsn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
hybrid.f -o hybrid.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
image.f -o image.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
impose.f -o impose.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
induce.f -o induce.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
inertia.f -o inertia.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ptable.f -o ptable.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
initatom.f -o initatom.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
linmin.f -o linmin.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
scales.f -o scales.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
sequen.f -o sequen.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
initial.f -o initial.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kantor.f -o kantor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kcflux.f -o kcflux.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
khbond.f -o khbond.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kiprop.f -o kiprop.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kmulti.f -o kmulti.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kopbnd.f -o kopbnd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
kopdst.f -o kopdst.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kpitor.f -o kpitor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kurybr.f -o kurybr.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kvdwpr.f -o kvdwpr.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
initprm.f -o initprm.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
resdue.f -o resdue.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
initres.f -o initres.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
initrot.f -o initrot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
insert.f -o insert.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
intedit.f -o intedit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
intxyz.f -o intxyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
invbeta.f -o invbeta.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
invert.f -o invert.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
jacobi.f -o jacobi.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kangang.f -o kangang.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kangle.f -o kangle.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kangtor.f -o kangtor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
katom.f -o katom.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kbond.f -o kbond.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kcharge.f -o kcharge.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kchgflx.f -o kchgflx.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kchgtrn.f -o kchgtrn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kdipole.f -o kdipole.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kdisp.f -o kdisp.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
kewald.f -o kewald.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kextra.f -o kextra.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kgeom.f -o kgeom.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kimprop.f -o kimprop.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kimptor.f -o kimptor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kinetic.f -o kinetic.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kmetal.f -o kmetal.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kmpole.f -o kmpole.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kopbend.f -o kopbend.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kopdist.f -o kopdist.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
korbit.f -o korbit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kpitors.f -o kpitors.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kpolar.f -o kpolar.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
krepel.f -o krepel.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ksolv.f -o ksolv.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kstrbnd.f -o kstrbnd.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kstrtor.f -o kstrtor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ktors.f -o ktors.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ktortor.f -o ktortor.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kurey.f -o kurey.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
kvdw.f -o kvdw.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
lattice.f -o lattice.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
lbfgs.f -o lbfgs.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
lights.f -o lights.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
lusolve.f -o lusolve.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
makeint.f -o makeint.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
makeref.f -o makeref.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
makexyz.f -o makexyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
maxwell.f -o maxwell.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mdinit.f -o mdinit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mdrest.f -o mdrest.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mdsave.f -o mdsave.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mdstat.f -o mdstat.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mechanic.f -o mechanic.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
merge.f -o merge.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
minimize.f -o minimize.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
minirot.f -o minirot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
minrigid.f -o minrigid.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mol2xyz.f -o mol2xyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
molecule.f -o molecule.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
molxyz.f -o molxyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
moments.f -o moments.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
monte.f -o monte.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
mutate.f -o mutate.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
nblist.f -o nblist.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
newton.f -o newton.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
newtrot.f -o newtrot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
nextarg.f -o nextarg.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
nexttext.f -o nexttext.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
nose.f -o nose.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
nspline.f -o nspline.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
nucleo.f -o nucleo.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
nucleic.f -o nucleic.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
number.f -o number.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
numeral.f -o numeral.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
numgrad.f -o numgrad.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
ocvm.f -o ocvm.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
openend.f -o openend.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
optimize.f -o optimize.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
optinit.f -o optinit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
optirot.f -o optirot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
optrigid.f -o optrigid.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
optsave.f -o optsave.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
orbital.f -o orbital.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
orient.f -o orient.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
orthog.f -o orthog.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
overlap.f -o overlap.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
path.f -o path.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pdbxyz.f -o pdbxyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
phipsi.f -o phipsi.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
picalc.f -o picalc.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pmestuf.f -o pmestuf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
pmpb.f -o pmpb.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
polarize.f -o polarize.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
poledit.f -o poledit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
polymer.f -o polymer.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
potential.f -o potential.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
predict.f -o predict.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pressure.f -o pressure.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prmedit.f -o prmedit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prmkey.f -o prmkey.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
promo.f -o promo.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
protein.f -o protein.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prtdyn.f -o prtdyn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prterr.f -o prterr.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prtint.f -o prtint.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prtmol2.f -o prtmol2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prtpdb.f -o prtpdb.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prtprm.f -o prtprm.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prtseq.f -o prtseq.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
prtxyz.f -o prtxyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
tree.f -o tree.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pss.f -o pss.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pssrigid.f -o pssrigid.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
pssrot.f -o pssrot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
qrsolve.f -o qrsolve.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
quatfit.f -o quatfit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
radial.f -o radial.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
random.f -o random.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rattle.f -o rattle.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readdyn.f -o readdyn.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readgau.f -o readgau.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readgdma.f -o readgdma.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readint.f -o readint.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readmol.f -o readmol.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readmol2.f -o readmol2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readpdb.f -o readpdb.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readprm.f -o readprm.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readseq.f -o readseq.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
readxyz.f -o readxyz.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
replica.f -o replica.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
respa.f -o respa.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rgdstep.f -o rgdstep.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rings.f -o rings.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rmsfit.f -o rmsfit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rotlist.f -o rotlist.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
rotpole.f -o rotpole.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
saddle.f -o saddle.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
scan.f -o scan.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
sdstep.f -o sdstep.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
search.f -o search.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
server.f -o server.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
shakeup.f -o shakeup.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
sigmoid.f -o sigmoid.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
simplex.f -o simplex.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
sktstuf.f -o sktstuf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
sniffer.f -o sniffer.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
sort.f -o sort.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
spacefill.f -o spacefill.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
spectrum.f -o spectrum.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
square.f -o square.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
suffix.f -o suffix.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
superpose.f -o superpose.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
surface.f -o surface.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
surfatom.f -o surfatom.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
switch.f -o switch.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
tcgstuf.f -o tcgstuf.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
temper.f -o temper.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
testgrad.f -o testgrad.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
testhess.f -o testhess.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
testpair.f -o testpair.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
testpol.f -o testpol.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
testrot.f -o testrot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
testvir.f -o testvir.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
timer.f -o timer.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
timerot.f -o timerot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
tncg.f -o tncg.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
torphase.f -o torphase.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
torque.f -o torque.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
torsfit.f -o torsfit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
torsions.f -o torsions.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
trimtext.f -o trimtext.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
unitcell.f -o unitcell.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
valfit.f -o valfit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
valence.f -o valence.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
verlet.f -o verlet.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
version.f -o version.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
vibbig.f -o vibbig.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
vibrate.f -o vibrate.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
vibrot.f -o vibrot.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
volume.f -o volume.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
xtals.f -o xtals.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
xtalfit.f -o xtalfit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
xtalmin.f -o xtalmin.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
xyzatm.f -o xyzatm.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
xyzedit.f -o xyzedit.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
xyzint.f -o xyzint.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
xyzmol2.f -o xyzmol2.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
```

```
xyzpdb.f -o xyzpdb.o
ifort -c -xHost -I../../aenet/src  -O3 -no-ipo -no-prec-div -recursive -qopenmp
zatom.f -o zatom.o
ar -crusv libtinker.a \
action.o \
active.o \
aenettinker.o \
align.o \
alterchg.o \
analysis.o \
analyz.o \
angang.o \
angbnd.o \
angles.o \
angpot.o \
angtor.o \
argue.o \
ascii.o \
atmlst.o \
atomid.o \
atoms.o \
attach.o \
baoab.o \
basefile.o \
bath.o \
beeman.o \
bicubic.o \
bitor.o \
bitors.o \
bndpot.o \
bndstr.o \
bonds.o \
born.o \
bound.o \
bounds.o \
boxes.o \
bussi.o \
calendar.o \
cell.o \
center.o \
cflux.o \
charge.o \
chgpen.o \
chgpot.o \
chgtrn.o \
chkpole.o \
chkring.o \
chkxyz.o \
```

```
cholesky.o \
chrono.o \
chunks.o \
clock.o \
cluster.o \
column.o \
command.o \
connect.o \
connolly.o \
control.o \
couple.o \
cspline.o \
ctrpot.o \
cutoffs.o \
damping.o \
dcflux.o \
deflate.o \
delete.o \
deriv.o \
diagq.o \
diffeq.o \
dipole.o \
disgeo.o \
disp.o \
dma.o \
domega.o \
dsppot.o \
eangang.o \
eangang1.o \
eangang2.o \
eangang3.o \
eangle.o \
eangle1.o \
eangle2.o \
eangle3.o \
eangtor.o \
eangtor1.o \
eangtor2.o \
eangtor3.o \
ebond.o \
ebond1.o \
ebond2.o \
ebond3.o \
ebuck.o \
ebuck1.o \
ebuck2.o \
ebuck3.o \
echarge.o \
```

```
echarge1.o \
echarge2.o \
echarge3.o \
echgdpl.o \
echgdpl1.o \
echgdpl2.o \
echgdpl3.o \
echgtrn.o \
echgtrn1.o \
echgtrn2.o \
echgtrn3.o \
edipole.o \
edipole1.o \
edipole2.o \
edipole3.o \
edisp.o \
edisp1.o \
edisp2.o \
edisp3.o \
egauss.o \
egauss1.o \
egauss2.o \
egauss3.o \
egeom.o \
egeom1.o \
egeom2.o \
egeom3.o \
ehal.o \
ehal1.o \
ehal2.o \
ehal3.o \
eimprop.o \
eimprop1.o \
eimprop2.o \
eimprop3.o \
eimptor.o \
eimptor1.o \
eimptor2.o \
eimptor3.o \
elj.o \
elj1.o \
elj2.o \
elj3.o \
embed.o \
emetal.o \
emetal1.o \
emetal2.o \
emetal3.o \
```

```
emm3hb.o \
emm3hb1.o \
emm3hb2.o \
emm3hb3.o \
empole.o \
empole1.o \
empole2.o \
empole3.o \
energi.o \
energy.o \
eopbend.o \
eopbend1.o \
eopbend2.o \
eopbend3.o \
eopdist.o \
eopdist1.o \
eopdist2.o \
eopdist3.o \
epitors.o \
epitors1.o \
epitors2.o \
epitors3.o \
epolar.o \
epolar1.o \
epolar2.o \
epolar3.o \
erepel.o \
erepel1.o \
erepel2.o \
erepel3.o \
erf.o \
erxnfld.o \
erxnfld1.o \
erxnfld2.o \
erxnfld3.o \
esolv.o \
esolv1.o \
esolv2.o \
esolv3.o \
estrbnd.o \
estrbnd1.o \
estrbnd2.o \
estrbnd3.o \
estrtor.o \
estrtor1.o \
estrtor2.o \
estrtor3.o \
etors.o \
```

```
etors1.o \
etors2.o \
etors3.o \
etortor.o \
etortor1.o \
etortor2.o \
etortor3.o \
eurey.o \
eurey1.o \
eurey2.o \
eurey3.o \
evcorr.o \
ewald.o \
extra.o \
extra1.o \
extra2.o \
extra3.o \
faces.o \
fatal.o \
fft.o \
fft3d.o \
fftpack.o \
field.o \
fields.o \
files.o \
final.o \
flatten.o \
fracs.o \
freeunit.o \
freeze.o \
geometry.o \
getarc.o \
getint.o \
getkey.o \
getmol.o \
getmol2.o \
getnumb.o \
getpdb.o \
getprm.o \
getref.o \
getstring.o \
gettext.o \
getword.o \
getxyz.o \
ghmcstep.o \
gkstuf.o \
gradient.o \
gradrgd.o \
```

```
gradrot.o \
group.o \
groups.o \
grpline.o \
gyrate.o \
hescut.o \
hessian.o \
hessn.o \
hessrgd.o \
hessrot.o \
hpmf.o \
hybrid.o \
ielscf.o \
image.o \
impose.o \
improp.o \
imptor.o \
induce.o \
inertia.o \
inform.o \
initatom.o \
initial.o \
initprm.o \
initres.o \
initrot.o \
insert.o \
inter.o \
invbeta.o \
invert.o \
iounit.o \
jacobi.o \
kanang.o \
kangang.o \
kangle.o \
kangs.o \
kangtor.o \
kantor.o \
katom.o \
katoms.o \
kbond.o \
kbonds.o \
kcflux.o \
kcharge.o \
kchgflx.o \
kchgtrn.o \
kchrge.o \
kcpen.o \
kctrn.o \
```

```
kdipol.o \
kdipole.o \
kdisp.o \
kdsp.o \
kewald.o \
kextra.o \
keys.o \
kgeom.o \
khbond.o \
kimprop.o \
kimptor.o \
kinetic.o \
kiprop.o \
kitors.o \
kmetal.o \
kmpole.o \
kmulti.o \
kopbend.o \
kopbnd.o \
kopdist.o \
kopdst.o \
korbit.o \
korbs.o \
kpitor.o \
kpitors.o \
kpolar.o \
kpolr.o \
krepel.o \
krepl.o \
ksolut.o \
ksolv.o \
kstbnd.o \
kstrbnd.o \
kstrtor.o \
ksttor.o \
ktors.o \
ktorsn.o \
ktortor.o \
ktrtor.o \
kurey.o \
kurybr.o \
kvdw.o \
kvdwpr.o \
kvdws.o \
lattice.o \
lbfgs.o \
light.o \
lights.o \
```

```
limits.o \
linmin.o \
lusolve.o \
makeint.o \
makeref.o \
makexyz.o \
math.o \
maxwell.o \
mdinit.o \
mdrest.o \
mdsave.o \
mdstat.o \
mdstuf.o \
mechanic.o \
merck.o \
merge.o \
minima.o \
molcul.o \
moldyn.o \
molecule.o \
moment.o \
moments.o \
mplpot.o \
mpole.o \
mrecip.o \
mutant.o \
mutate.o \
nblist.o \
neigh.o \
nextarg.o \
nexttext.o \
nonpol.o \
nose.o \
nspline.o \
nucleo.o \
number.o \
numeral.o \
numgrad.o \
ocvm.o \
omega.o \
opbend.o \
opdist.o \
openend.o \
openmp.o \
optinit.o \
optsave.o \
orbital.o \
orbits.o \
```

```
orient.o \
orthog.o \
output.o \
overlap.o \
params.o \
paths.o \
pbstuf.o \
pdb.o \
phipsi.o \
picalc.o \
piorbs.o \
pistuf.o \
pitors.o \
pme.o \
pmestuf.o \
pmpb.o \
polar.o \
polgrp.o \
polopt.o \
polpcg.o \
polpot.o \
poltcg.o \
polymer.o \
potent.o \
potfit.o \
predict.o \
pressure.o \
prmkey.o \
promo.o \
prtdyn.o \
prterr.o \
prtint.o \
prtmol2.o \
prtpdb.o \
prtprm.o \
prtseq.o \
prtxyz.o \
ptable.o \
qmstuf.o \
qrsolve.o \
quatfit.o \
random.o \
rattle.o \
readdyn.o \
readgau.o \
readgdma.o \
readint.o \
readmol.o \
```

```
readmol2.o \
readpdb.o \
readprm.o \
readseq.o \
readxyz.o \
refer.o \
repel.o \
replica.o \
reppot.o \
resdue.o \
respa.o \
restrn.o \
rgddyn.o \
rgdstep.o \
rigid.o \
ring.o \
rings.o \
rmsfit.o \
rotbnd.o \
rotlist.o \
rotpole.o \
rxnfld.o \
rxnpot.o \
scales.o \
sdstep.o \
search.o \
sequen.o \
server.o \
shakeup.o \
shunt.o \
sigmoid.o \
simplex.o \
sizes.o \
sktstuf.o \
socket.o \
solpot.o \
solute.o \
sort.o \
square.o \
stodyn.o \
strbnd.o \
strtor.o \
suffix.o \
surface.o \
surfatom.o \
switch.o \
syntrn.o \
tarray.o \
```

```
tcgstuf.o \
temper.o \
titles.o \
tncg.o \
torphase.o \
torpot.o \
torque.o \
tors.o \
torsions.o \
tortor.o \
tree.o \
trimtext.o \
unitcell.o \
units.o \
uprior.o \
urey.o \
urypot.o \
usage.o \
valfit.o \
vdw.o \
vdwpot.o \
verlet.o \
version.o \
vibs.o \
virial.o \
volume.o \
warp.o \
xtals.o \
xyzatm.o \
zatom.o \
zclose.o \
zcoord.o
ar: `u' modifier ignored since `D' is the default (see `U')
a - action.o
a - active.o
a - aenettinker.o
a - align.o
a - alterchg.o
a - analysis.o
a - analyz.o
a - angang.o
a - angbnd.o
a - angles.o
a - angpot.o
a - angtor.o
a - argue.o
a - ascii.o
a - atmlst.o
```

```
a - atomid.o
a - atoms.o
a - attach.o
a - baoab.o
a - basefile.o
a - bath.o
a - beeman.o
a - bicubic.o
a - bitor.o
a - bitors.o
a - bndpot.o
a - bndstr.o
a - bonds.o
a - born.o
a - bound.o
a - bounds.o
a - boxes.o
a - bussi.o
a - calendar.o
a - cell.o
a - center.o
a - cflux.o
a - charge.o
a - chgpen.o
a - chgpot.o
a - chgtrn.o
a - chkpole.o
a - chkring.o
a - chkxyz.o
a - cholesky.o
a - chrono.o
a - chunks.o
a - clock.o
a - cluster.o
a - column.o
a - command.o
a - connect.o
a - connolly.o
a - control.o
a - couple.o
a - cspline.o
a - ctrpot.o
a - cutoffs.o
a - damping.o
a - dcflux.o
a - deflate.o
a - delete.o
a - deriv.o
```

```
a - diagq.o
a - diffeq.o
a - dipole.o
a - disgeo.o
a - disp.o
a - dma.o
a - domega.o
a - dsppot.o
a - eangang.o
a - eangang1.o
a - eangang2.o
a - eangang3.o
a - eangle.o
a - eangle1.o
a - eangle2.o
a - eangle3.o
a - eangtor.o
a - eangtor1.o
a - eangtor2.o
a - eangtor3.o
a - ebond.o
a - ebond1.o
a - ebond2.o
a - ebond3.o
a - ebuck.o
a - ebuck1.o
a - ebuck2.o
a - ebuck3.o
a - echarge.o
a - echarge1.o
a - echarge2.o
a - echarge3.o
a - echgdpl.o
a - echgdpl1.o
a - echgdpl2.o
a - echgdpl3.o
a - echgtrn.o
a - echgtrn1.o
a - echgtrn2.o
a - echgtrn3.o
a - edipole.o
a - edipole1.o
a - edipole2.o
a - edipole3.o
a - edisp.o
a - edisp1.o
a - edisp2.o
a - edisp3.o
```

```
a - egauss.o
a - egauss1.o
a - egauss2.o
a - egauss3.o
a - egeom.o
a - egeom1.o
a - egeom2.o
a - egeom3.o
a - ehal.o
a - ehal1.o
a - ehal2.o
a - ehal3.o
a - eimprop.o
a - eimprop1.o
a - eimprop2.o
a - eimprop3.o
a - eimptor.o
a - eimptor1.o
a - eimptor2.o
a - eimptor3.o
a - elj.o
a - elj1.o
a - elj2.o
a - elj3.o
a - embed.o
a - emetal.o
a - emetal1.o
a - emetal2.o
a - emetal3.o
a - emm3hb.o
a - emm3hb1.o
a - emm3hb2.o
a - emm3hb3.o
a - empole.o
a - empole1.o
a - empole2.o
a - empole3.o
a - energi.o
a - energy.o
a - eopbend.o
a - eopbend1.o
a - eopbend2.o
a - eopbend3.o
a - eopdist.o
a - eopdist1.o
a - eopdist2.o
a - eopdist3.o
a - epitors.o
```

```
a - epitors1.o
a - epitors2.o
a - epitors3.o
a - epolar.o
a - epolar1.o
a - epolar2.o
a - epolar3.o
a - erepel.o
a - erepel1.o
a - erepel2.o
a - erepel3.o
a - erf.o
a - erxnfld.o
a - erxnfld1.o
a - erxnfld2.o
a - erxnfld3.o
a - esolv.o
a - esolv1.o
a - esolv2.o
a - esolv3.o
a - estrbnd.o
a - estrbnd1.o
a - estrbnd2.o
a - estrbnd3.o
a - estrtor.o
a - estrtor1.o
a - estrtor2.o
a - estrtor3.o
a - etors.o
a - etors1.o
a - etors2.o
a - etors3.o
a - etortor.o
a - etortor1.o
a - etortor2.o
a - etortor3.o
a - eurey.o
a - eurey1.o
a - eurey2.o
a - eurey3.o
a - evcorr.o
a - ewald.o
a - extra.o
a - extra1.o
a - extra2.o
a - extra3.o
a - faces.o
a - fatal.o
```

```
a - fft.o
a - fft3d.o
a - fftpack.o
a - field.o
a - fields.o
a - files.o
a - final.o
a - flatten.o
a - fracs.o
a - freeunit.o
a - freeze.o
a - geometry.o
a - getarc.o
a - getint.o
a - getkey.o
a - getmol.o
a - getmol2.o
a - getnumb.o
a - getpdb.o
a - getprm.o
a - getref.o
a - getstring.o
a - gettext.o
a - getword.o
a - getxyz.o
a - ghmcstep.o
a - gkstuf.o
a - gradient.o
a - gradrgd.o
a - gradrot.o
a - group.o
a - groups.o
a - grpline.o
a - gyrate.o
a - hescut.o
a - hessian.o
a - hessn.o
a - hessrgd.o
a - hessrot.o
a - hpmf.o
a - hybrid.o
a - ielscf.o
a - image.o
a - impose.o
a - improp.o
a - imptor.o
a - induce.o
a - inertia.o
```

```
a - inform.o
a - initatom.o
a - initial.o
a - initprm.o
a - initres.o
a - initrot.o
a - insert.o
a - inter.o
a - invbeta.o
a - invert.o
a - iounit.o
a - jacobi.o
a - kanang.o
a - kangang.o
a - kangle.o
a - kangs.o
a - kangtor.o
a - kantor.o
a - katom.o
a - katoms.o
a - kbond.o
a - kbonds.o
a - kcflux.o
a - kcharge.o
a - kchgflx.o
a - kchgtrn.o
a - kchrge.o
a - kcpen.o
a - kctrn.o
a - kdipol.o
a - kdipole.o
a - kdisp.o
a - kdsp.o
a - kewald.o
a - kextra.o
a - keys.o
a - kgeom.o
a - khbond.o
a - kimprop.o
a - kimptor.o
a - kinetic.o
a - kiprop.o
a - kitors.o
a - kmetal.o
a - kmpole.o
a - kmulti.o
a - kopbend.o
a - kopbnd.o
```

```
a - kopdist.o
a - kopdst.o
a - korbit.o
a - korbs.o
a - kpitor.o
a - kpitors.o
a - kpolar.o
a - kpolr.o
a - krepel.o
a - krepl.o
a - ksolut.o
a - ksolv.o
a - kstbnd.o
a - kstrbnd.o
a - kstrtor.o
a - ksttor.o
a - ktors.o
a - ktorsn.o
a - ktortor.o
a - ktrtor.o
a - kurey.o
a - kurybr.o
a - kvdw.o
a - kvdwpr.o
a - kvdws.o
a - lattice.o
a - lbfgs.o
a - light.o
a - lights.o
a - limits.o
a - linmin.o
a - lusolve.o
a - makeint.o
a - makeref.o
a - makexyz.o
a - math.o
a - maxwell.o
a - mdinit.o
a - mdrest.o
a - mdsave.o
a - mdstat.o
a - mdstuf.o
a - mechanic.o
a - merck.o
a - merge.o
a - minima.o
a - molcul.o
a - moldyn.o
```

```
a - molecule.o
a - moment.o
a - moments.o
a - mplpot.o
a - mpole.o
a - mrecip.o
a - mutant.o
a - mutate.o
a - nblist.o
a - neigh.o
a - nextarg.o
a - nexttext.o
a - nonpol.o
a - nose.o
a - nspline.o
a - nucleo.o
a - number.o
a - numeral.o
a - numgrad.o
a - ocvm.o
a - omega.o
a - opbend.o
a - opdist.o
a - openend.o
a - openmp.o
a - optinit.o
a - optsave.o
a - orbital.o
a - orbits.o
a - orient.o
a - orthog.o
a - output.o
a - overlap.o
a - params.o
a - paths.o
a - pbstuf.o
a - pdb.o
a - phipsi.o
a - picalc.o
a - piorbs.o
a - pistuf.o
a - pitors.o
a - pme.o
a - pmestuf.o
a - pmpb.o
a - polar.o
a - polgrp.o
a - polopt.o
```

```
a - polpcg.o
a - polpot.o
a - poltcg.o
a - polymer.o
a - potent.o
a - potfit.o
a - predict.o
a - pressure.o
a - prmkey.o
a - promo.o
a - prtdyn.o
a - prterr.o
a - prtint.o
a - prtmol2.o
a - prtpdb.o
a - prtprm.o
a - prtseq.o
a - prtxyz.o
a - ptable.o
a - qmstuf.o
a - qrsolve.o
a - quatfit.o
a - random.o
a - rattle.o
a - readdyn.o
a - readgau.o
a - readgdma.o
a - readint.o
a - readmol.o
a - readmol2.o
a - readpdb.o
a - readprm.o
a - readseq.o
a - readxyz.o
a - refer.o
a - repel.o
a - replica.o
a - reppot.o
a - resdue.o
a - respa.o
a - restrn.o
a - rgddyn.o
a - rgdstep.o
a - rigid.o
a - ring.o
a - rings.o
a - rmsfit.o
a - rotbnd.o
```

```
a - rotlist.o
a - rotpole.o
a - rxnfld.o
a - rxnpot.o
a - scales.o
a - sdstep.o
a - search.o
a - sequen.o
a - server.o
a - shakeup.o
a - shunt.o
a - sigmoid.o
a - simplex.o
a - sizes.o
a - sktstuf.o
a - socket.o
a - solpot.o
a - solute.o
a - sort.o
a - square.o
a - stodyn.o
a - strbnd.o
a - strtor.o
a - suffix.o
a - surface.o
a - surfatom.o
a - switch.o
a - syntrn.o
a - tarray.o
a - tcgstuf.o
a - temper.o
a - titles.o
a - tncg.o
a - torphase.o
a - torpot.o
a - torque.o
a - tors.o
a - torsions.o
a - tortor.o
a - tree.o
a - trimtext.o
a - unitcell.o
a - units.o
a - uprior.o
a - urey.o
a - urypot.o
a - usage.o
a - valfit.o
```

```
a - vdw.o
a - vdwpot.o
a - verlet.o
a - version.o
a - vibs.o
a - virial.o
a - volume.o
a - warp.o
a - xtals.o
a - xyzatm.o
a - zatom.o
a - zclose.o
a - zcoord.o
echo libtinker.a
libtinker.a
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o alchemy.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib alchemy.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
alchemy.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o analyze.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib analyze.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
analyze.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o anneal.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib anneal.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
anneal.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o archive.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib archive.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
archive.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o bar.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib bar.o libtinker.a
../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip bar.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o correlate.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib correlate.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
correlate.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o critical.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib critical.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
critical.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o crystal.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib crystal.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
crystal.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o diffuse.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib diffuse.o
```

```
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
diffuse.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o distgeom.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib distgeom.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
distgeom.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o document.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib document.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
document.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o dynamic.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib dynamic.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
dynamic.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o gda.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib gda.o libtinker.a
../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip gda.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o intedit.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib intedit.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
intedit.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o intxyz.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib intxyz.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
intxyz.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o minimize.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib minimize.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
minimize.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o minirot.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib minirot.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
minirot.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o minrigid.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib minrigid.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
minrigid.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o mol2xyz.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib mol2xyz.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
mol2xyz.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o molxyz.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib molxyz.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
molxyz.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o monte.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib monte.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
```

```
monte.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o newton.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib newton.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
newton.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o newtrot.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib newtrot.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
newtrot.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o nucleic.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib nucleic.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
nucleic.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o optimize.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib optimize.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
optimize.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o optirot.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib optirot.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
optirot.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o optrigid.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib optrigid.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
optrigid.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o path.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib path.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
path.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o pdbxyz.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib pdbxyz.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
pdbxyz.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o polarize.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib polarize.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
polarize.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o poledit.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib poledit.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
poledit.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o potential.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib potential.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
potential.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o prmedit.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib prmedit.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
```

```
prmedit.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o protein.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib protein.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
protein.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o pss.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib pss.o libtinker.a
../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip pss.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o pssrigid.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib pssrigid.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
pssrigid.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o pssrot.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib pssrot.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
pssrot.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o radial.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib radial.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
radial.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o saddle.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib saddle.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
saddle.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o scan.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib scan.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
scan.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o sniffer.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib sniffer.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
sniffer.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o spacefill.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib spacefill.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
spacefill.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o spectrum.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib spectrum.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
spectrum.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o superpose.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib superpose.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
superpose.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o testgrad.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib testgrad.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
testgrad.x
```

```
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o testhess.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib testhess.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
testhess.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o testpair.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib testpair.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
testpair.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o testpol.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib testpol.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
testpol.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o testrot.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib testrot.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
testrot.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o testvir.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib testvir.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
testvir.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o timer.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib timer.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
timer.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o timerot.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib timerot.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
timerot.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o torsfit.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib torsfit.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
torsfit.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o valence.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib valence.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
valence.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o vibbig.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib vibbig.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
vibbig.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o vibrate.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib vibrate.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
vibrate.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o vibrot.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib vibrot.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
vibrot.x
```

```
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o xtalfit.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib xtalfit.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
xtalfit.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o xtalmin.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib xtalmin.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
xtalmin.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o xyzedit.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib xyzedit.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
xyzedit.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o xyzint.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib xyzint.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
xyzint.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o xyzmol2.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib xyzmol2.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
xyzmol2.x
ifort -O3 -no-ipo -no-prec-div -recursive -qopenmp -static-libgcc -static-intel
-o xyzpdb.x -L. -L../../tinker/lib/linux -L../../tinker/fftw/lib xyzpdb.o
libtinker.a ../../aenet/src/libaenet.a -mkl -lfftw3_threads -lfftw3; strip
xyzpdb.x
```

4 4. Running Tinker with aenet ANN potentials

An example Tinker molecular dynamics simulation of amorphous LiSi with an ænet ANN potential is provided in the directory `aenet-tinker/examples/01-ANN-MD-aLiSi`.

In short: (1) the file `aenet.prm` needs to be present to define the masses of all atomic species. (2) all ANN potentials need to be provided in files named `<symbol>.ann`, where `<symbol>` is the chemical symbol. And, (3) the Tinker *key* file has to contain the following line:

```
EXTRATERM only
```

[11]:
```
if not os.path.exists('md-example'):
  ! mkdir md-example
  ! cp aenet-tinker/examples/02-ANN-MD-aLiSi-aenet-2.0.4-tinker-8.9.1/* ./
 ↪md-example/
```

We can now run an example MD simulation with Tinker's `dynamic.x` tool.

The meaning of the command-line options to `dynamic.x` after `-k md.key` are:

- initial atomic structure: "md.xyz"
- MD steps: 100
- time step in fs: 2.0
- time between write out in ps: 0.002

- MD type: 2 (= NVT)
- temperature in Kelvin: 800

[12]:
```
%cd md-example/
cmd = """\
{}
../tinker/source/dynamic.x -k md.key md.xyz 100 2.0 0.002 2 800 | tee dynamic.
 ↪out
""".format(intel_init)
!{cmd}
%cd ..
```

```
/data/home/na2782/aenet-tinker-test-2/md-example

     ##############################################################################
   ##############################################################################
  ###                                                                          ###
 ###            Tinker  ---  Software Tools for Molecular Design                ###
 ##                                                                            ##
 ##                          Version 8.9.1  June 2021                          ##
 ##                                                                            ##
 ##                Copyright (c)  Jay William Ponder  1990-2021                ##
 ###                            All Rights Reserved                           ###
  ###                                                                        ###
   ##############################################################################
     ##############################################################################

OMP: Info #274: omp_set_nested routine deprecated, please use
omp_set_max_active_levels instead.
 Atomic species : Li
 File name      : Li.ann

 ------------------------------------------------------------------------
                          Training set info.
 ------------------------------------------------------------------------

 Training set file                   : LiSi.train.scaled
 Number of structures in the data set: 41894

 Atomic species in training set      : 2
   Species : Li Si

 Average energy (eV/atom) : 0.078108
 Minimum energy (eV/atom) : -1.000000
 Maximum energy (eV/atom) : 1.000951

 The input and output values have been normalized to [-1.0, 1.0].
 Structures outside of this interval will not be used for training.
```

```
  Energy scaling factor: 2.598642
  Atomic energy shift  : 0.115184

Number of layers :   4

Number of nodes (without bias)
and activation type per layer :

      1 :    44
      2 :    15  hyperbolic tangent (tanh)
      3 :    15  hyperbolic tangent (tanh)
      4 :     1  linear function (linear)

Required memory (words) :     194491 (   1519.46 KB)

Total number of weights (incl. bias) :      931

Structural fingerprint (SF) set-up for Li

  N. Artrith and A. Urban, Comput. Mater. Sci. 114 (2016) 135-150.
  N Artrith, A Urban, G Ceder, Physical Review B 96 (2017), 014112.

environment types: Li Si
minimal distance : 0.75 Angstrom
maximal cut-off  : 8.00 Angstrom
size of basis    : 44
evaluations      : 3708517

Basis function type Chebyshev
[N. Artrith and A. Urban (2016)]

Radial Rc     : 8.00
Angular Rc    : 3.00
Radial order  : 16
Angular order : 4

Atomic species : Si
File name      : Si.ann

--------------------------------------------------------------------
                        Training set info.
--------------------------------------------------------------------

Training set file                   : LiSi.train.scaled
Number of structures in the data set: 41894

Atomic species in training set      : 2
  Species : Li Si
```

```
Average energy (eV/atom) : 0.078108
Minimum energy (eV/atom) : -1.000000
Maximum energy (eV/atom) : 1.000951

The input and output values have been normalized to [-1.0, 1.0].
Structures outside of this interval will not be used for training.
  Energy scaling factor: 2.598642
  Atomic energy shift  : 0.115184

Number of layers :   4

Number of nodes (without bias)
and activation type per layer :

      1 :    44
      2 :    15  hyperbolic tangent (tanh)
      3 :    15  hyperbolic tangent (tanh)
      4 :     1  linear function (linear)

Required memory (words) :     194491 (   1519.46 KB)

Total number of weights (incl. bias) :      931

Structural fingerprint (SF) set-up for Si

  N. Artrith and A. Urban, Comput. Mater. Sci. 114 (2016) 135-150.
  N Artrith, A Urban, G Ceder, Physical Review B 96 (2017), 014112.

environment types: Li Si
minimal distance : 0.75 Angstrom
maximal cut-off  : 8.00 Angstrom
size of basis    : 44
evaluations      : 2204626

Basis function type Chebyshev
[N. Artrith and A. Urban (2016)]

Radial Rc     : 8.00
Angular Rc    : 3.00
Radial order  : 16
Angular order : 4


Random Number Generator Initialized with SEED :         122058

Molecular Dynamics Trajectory via Modified Beeman Algorithm
```

```
   MD Step       E Total    E Potential      E Kinetic       Temp       Pres

         1    -20576.3057    -21158.2400       581.9343     765.60    6136.74

Instantaneous Values for Frame Saved at         1 Dynamics Steps

Current Time                 0.0020 Picosecond
Current Potential       -21158.2400 Kcal/mole
Current Kinetic            581.9343 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     1
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

         2    -20584.0650    -21180.6998       596.6347     784.94    6291.76

Instantaneous Values for Frame Saved at         2 Dynamics Steps

Current Time                 0.0040 Picosecond
Current Potential       -21180.6998 Kcal/mole
Current Kinetic            596.6347 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     2
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

         3    -20583.3156    -21217.5635       634.2480     834.42    6688.41

Instantaneous Values for Frame Saved at         3 Dynamics Steps

Current Time                 0.0060 Picosecond
Current Potential       -21217.5635 Kcal/mole
Current Kinetic            634.2480 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     3
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

         4    -20593.0145    -21262.6956       669.6811     881.04    7062.06

Instantaneous Values for Frame Saved at         4 Dynamics Steps
```

```
Current Time                0.0080 Picosecond
Current Potential       -21262.6956 Kcal/mole
Current Kinetic            669.6811 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                      4
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

        5    -20595.4286    -21308.5664       713.1377     938.21    7520.33

Instantaneous Values for Frame Saved at         5 Dynamics Steps

Current Time                0.0100 Picosecond
Current Potential       -21308.5664 Kcal/mole
Current Kinetic            713.1377 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                      5
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

        6    -20595.2153    -21348.9068       753.6915     991.56    7947.99

Instantaneous Values for Frame Saved at         6 Dynamics Steps

Current Time                0.0120 Picosecond
Current Potential       -21348.9068 Kcal/mole
Current Kinetic            753.6915 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                      6
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

        7    -20595.1661    -21378.3021       783.1360    1030.30    8258.49

Instantaneous Values for Frame Saved at         7 Dynamics Steps

Current Time                0.0140 Picosecond
Current Potential       -21378.3021 Kcal/mole
Current Kinetic            783.1360 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                      7
```

```
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

        8    -20594.9196    -21393.7283       798.8088    1050.92    8423.77

Instantaneous Values for Frame Saved at         8 Dynamics Steps

Current Time                 0.0160 Picosecond
Current Potential       -21393.7283 Kcal/mole
Current Kinetic            798.8088 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     8
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

        9    -20604.4242    -21396.0244       791.6003    1041.43    8347.75

Instantaneous Values for Frame Saved at         9 Dynamics Steps

Current Time                 0.0180 Picosecond
Current Potential       -21396.0244 Kcal/mole
Current Kinetic            791.6003 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     9
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       10    -20605.7005    -21388.5822       782.8817    1029.96    8255.81

Instantaneous Values for Frame Saved at        10 Dynamics Steps

Current Time                 0.0200 Picosecond
Current Potential       -21388.5822 Kcal/mole
Current Kinetic            782.8817 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    10
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       11    -20609.7940    -21376.0481       766.2542    1008.09    8080.47
```

```
Instantaneous Values for Frame Saved at        11 Dynamics Steps

Current Time                0.0220 Picosecond
Current Potential       -21376.0481 Kcal/mole
Current Kinetic            766.2542 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    11
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       12    -20609.7416    -21363.7880       754.0464     992.03    7951.73

Instantaneous Values for Frame Saved at        12 Dynamics Steps

Current Time                0.0240 Picosecond
Current Potential       -21363.7880 Kcal/mole
Current Kinetic            754.0464 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    12
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       13    -20606.3984    -21355.3445       748.9461     985.32    7897.94

Instantaneous Values for Frame Saved at        13 Dynamics Steps

Current Time                0.0260 Picosecond
Current Potential       -21355.3445 Kcal/mole
Current Kinetic            748.9461 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    13
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       14    -20608.6916    -21351.7452       743.0535     977.57    7835.81

Instantaneous Values for Frame Saved at        14 Dynamics Steps

Current Time                0.0280 Picosecond
Current Potential       -21351.7452 Kcal/mole
Current Kinetic            743.0535 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
```

```
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    14
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       15    -20613.1141    -21352.5752       739.4611     972.84    7797.92

Instantaneous Values for Frame Saved at        15 Dynamics Steps

Current Time                 0.0300 Picosecond
Current Potential       -21352.5752 Kcal/mole
Current Kinetic            739.4611 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    15
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       16    -20619.7525    -21356.9514       737.1989     969.86    7774.07

Instantaneous Values for Frame Saved at        16 Dynamics Steps

Current Time                 0.0320 Picosecond
Current Potential       -21356.9514 Kcal/mole
Current Kinetic            737.1989 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    16
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       17    -20621.0081    -21364.5318       743.5238     978.18    7840.76

Instantaneous Values for Frame Saved at        17 Dynamics Steps

Current Time                 0.0340 Picosecond
Current Potential       -21364.5318 Kcal/mole
Current Kinetic            743.5238 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    17
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc
```

```
       18    -20611.9359    -21375.1163       763.1804    1004.05    8048.05

Instantaneous Values for Frame Saved at        18 Dynamics Steps

Current Time                0.0360 Picosecond
Current Potential       -21375.1163 Kcal/mole
Current Kinetic            763.1804 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    18
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       19    -20609.7492    -21388.0182       778.2691    1023.90    8207.17

Instantaneous Values for Frame Saved at        19 Dynamics Steps

Current Time                0.0380 Picosecond
Current Potential       -21388.0182 Kcal/mole
Current Kinetic            778.2691 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    19
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       20    -20607.3082    -21401.8850       794.5769    1045.35    8379.14

Instantaneous Values for Frame Saved at        20 Dynamics Steps

Current Time                0.0400 Picosecond
Current Potential       -21401.8850 Kcal/mole
Current Kinetic            794.5769 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    20
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       21    -20615.5296    -21415.2476       799.7180    1052.11    8433.36

Instantaneous Values for Frame Saved at        21 Dynamics Steps

Current Time                0.0420 Picosecond
Current Potential       -21415.2476 Kcal/mole
```

```
Current Kinetic            799.7180 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    21
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       22    -20621.7513    -21426.1809       804.4296    1058.31    8483.04

Instantaneous Values for Frame Saved at        22 Dynamics Steps

Current Time                0.0440 Picosecond
Current Potential       -21426.1809 Kcal/mole
Current Kinetic            804.4296 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    22
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       23    -20620.9391    -21432.9041       811.9650    1068.23    8562.51

Instantaneous Values for Frame Saved at        23 Dynamics Steps

Current Time                0.0460 Picosecond
Current Potential       -21432.9041 Kcal/mole
Current Kinetic            811.9650 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    23
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       24    -20618.3490    -21433.1482       814.7993    1071.96    8592.39

Instantaneous Values for Frame Saved at        24 Dynamics Steps

Current Time                0.0480 Picosecond
Current Potential       -21433.1482 Kcal/mole
Current Kinetic            814.7993 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    24
Coordinate File            md.arc
Velocity File              md.vel
```

```
Force Vector File           md.frc

       25    -20613.9945    -21425.6014       811.6070    1067.76    8558.73

Instantaneous Values for Frame Saved at        25 Dynamics Steps

Current Time                 0.0500 Picosecond
Current Potential       -21425.6014 Kcal/mole
Current Kinetic            811.6070 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    25
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       26    -20611.1675    -21411.5391       800.3716    1052.97    8440.25

Instantaneous Values for Frame Saved at        26 Dynamics Steps

Current Time                 0.0520 Picosecond
Current Potential       -21411.5391 Kcal/mole
Current Kinetic            800.3716 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    26
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       27    -20614.8265    -21395.7672       780.9408    1027.41    8235.34

Instantaneous Values for Frame Saved at        27 Dynamics Steps

Current Time                 0.0540 Picosecond
Current Potential       -21395.7672 Kcal/mole
Current Kinetic            780.9408 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    27
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       28    -20615.3102    -21383.6525       768.3423    1010.84    8102.49

Instantaneous Values for Frame Saved at        28 Dynamics Steps
```

```
Current Time                0.0560 Picosecond
Current Potential       -21383.6525 Kcal/mole
Current Kinetic            768.3423 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     28
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       29    -20618.5448    -21378.0054       759.4605     999.15    8008.82

Instantaneous Values for Frame Saved at        29 Dynamics Steps

Current Time                0.0580 Picosecond
Current Potential       -21378.0054 Kcal/mole
Current Kinetic            759.4605 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     29
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       30    -20628.5417    -21378.5748       750.0331     986.75    7909.41

Instantaneous Values for Frame Saved at        30 Dynamics Steps

Current Time                0.0600 Picosecond
Current Potential       -21378.5748 Kcal/mole
Current Kinetic            750.0331 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     30
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       31    -20633.7200    -21381.9761       748.2561     984.41    7890.67

Instantaneous Values for Frame Saved at        31 Dynamics Steps

Current Time                0.0620 Picosecond
Current Potential       -21381.9761 Kcal/mole
Current Kinetic            748.2561 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     31
```

```
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       32    -20631.4932    -21384.2556       752.7623     990.34    7938.19

Instantaneous Values for Frame Saved at        32 Dynamics Steps

Current Time                 0.0640 Picosecond
Current Potential       -21384.2556 Kcal/mole
Current Kinetic            752.7623 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    32
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       33    -20635.4992    -21383.9183       748.4191     984.63    7892.39

Instantaneous Values for Frame Saved at        33 Dynamics Steps

Current Time                 0.0660 Picosecond
Current Potential       -21383.9183 Kcal/mole
Current Kinetic            748.4191 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    33
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       34    -20643.2335    -21380.8543       737.6208     970.42    7778.51

Instantaneous Values for Frame Saved at        34 Dynamics Steps

Current Time                 0.0680 Picosecond
Current Potential       -21380.8543 Kcal/mole
Current Kinetic            737.6208 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    34
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       35    -20648.8861    -21374.7286       725.8425     954.92    7654.31
```

```
Instantaneous Values for Frame Saved at        35 Dynamics Steps

Current Time                0.0700 Picosecond
Current Potential       -21374.7286 Kcal/mole
Current Kinetic            725.8425 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    35
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       36    -20651.6714    -21365.8152       714.1439     939.53    7530.94

Instantaneous Values for Frame Saved at        36 Dynamics Steps

Current Time                0.0720 Picosecond
Current Potential       -21365.8152 Kcal/mole
Current Kinetic            714.1439 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    36
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       37    -20657.0960    -21355.9017       698.8057     919.35    7369.19

Instantaneous Values for Frame Saved at        37 Dynamics Steps

Current Time                0.0740 Picosecond
Current Potential       -21355.9017 Kcal/mole
Current Kinetic            698.8057 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    37
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       38    -20663.4468    -21347.5628       684.1159     900.03    7214.28

Instantaneous Values for Frame Saved at        38 Dynamics Steps

Current Time                0.0760 Picosecond
Current Potential       -21347.5628 Kcal/mole
Current Kinetic            684.1159 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
```

```
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    38
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       39    -20669.6557    -21343.5971       673.9414     886.64    7106.99

Instantaneous Values for Frame Saved at        39 Dynamics Steps

Current Time                 0.0780 Picosecond
Current Potential       -21343.5971 Kcal/mole
Current Kinetic             673.9414 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    39
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       40    -20668.1672    -21346.3305       678.1633     892.20    7151.51

Instantaneous Values for Frame Saved at        40 Dynamics Steps

Current Time                 0.0800 Picosecond
Current Potential       -21346.3305 Kcal/mole
Current Kinetic             678.1633 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    40
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       41    -20668.0009    -21356.7115       688.7105     906.07    7262.74

Instantaneous Values for Frame Saved at        41 Dynamics Steps

Current Time                 0.0820 Picosecond
Current Potential       -21356.7115 Kcal/mole
Current Kinetic             688.7105 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    41
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc
```

```
       42    -20667.0128    -21373.2323       706.2195     929.11    7447.38

 Instantaneous Values for Frame Saved at        42 Dynamics Steps

 Current Time                0.0840 Picosecond
 Current Potential       -21373.2323 Kcal/mole
 Current Kinetic            706.2195 Kcal/mole
 Lattice Lengths           17.045000     17.481000     14.704000
 Lattice Angles            95.830000     86.110000     94.920000
 Frame Number                     42
 Coordinate File               md.arc
 Velocity File                 md.vel
 Force Vector File             md.frc

       43    -20670.0764    -21391.6580       721.5816     949.32    7609.38

 Instantaneous Values for Frame Saved at        43 Dynamics Steps

 Current Time                0.0860 Picosecond
 Current Potential       -21391.6580 Kcal/mole
 Current Kinetic            721.5816 Kcal/mole
 Lattice Lengths           17.045000     17.481000     14.704000
 Lattice Angles            95.830000     86.110000     94.920000
 Frame Number                     43
 Coordinate File               md.arc
 Velocity File                 md.vel
 Force Vector File             md.frc

       44    -20659.7576    -21406.8619       747.1043     982.90    7878.52

 Instantaneous Values for Frame Saved at        44 Dynamics Steps

 Current Time                0.0880 Picosecond
 Current Potential       -21406.8619 Kcal/mole
 Current Kinetic            747.1043 Kcal/mole
 Lattice Lengths           17.045000     17.481000     14.704000
 Lattice Angles            95.830000     86.110000     94.920000
 Frame Number                     44
 Coordinate File               md.arc
 Velocity File                 md.vel
 Force Vector File             md.frc

       45    -20665.0729    -21415.3330       750.2601     987.05    7911.80

 Instantaneous Values for Frame Saved at        45 Dynamics Steps

 Current Time                0.0900 Picosecond
 Current Potential       -21415.3330 Kcal/mole
```

```
Current Kinetic            750.2601 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    45
Coordinate File           md.arc
Velocity File             md.vel
Force Vector File         md.frc

       46    -20670.0576    -21415.8544       745.7968     981.18    7864.73

Instantaneous Values for Frame Saved at        46 Dynamics Steps

Current Time                0.0920 Picosecond
Current Potential       -21415.8544 Kcal/mole
Current Kinetic           745.7968 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    46
Coordinate File           md.arc
Velocity File             md.vel
Force Vector File         md.frc

       47    -20672.6226    -21410.2982       737.6756     970.49    7779.09

Instantaneous Values for Frame Saved at        47 Dynamics Steps

Current Time                0.0940 Picosecond
Current Potential       -21410.2982 Kcal/mole
Current Kinetic           737.6756 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    47
Coordinate File           md.arc
Velocity File             md.vel
Force Vector File         md.frc

       48    -20675.0688    -21401.2573       726.1885     955.38    7657.96

Instantaneous Values for Frame Saved at        48 Dynamics Steps

Current Time                0.0960 Picosecond
Current Potential       -21401.2573 Kcal/mole
Current Kinetic           726.1885 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    48
Coordinate File           md.arc
Velocity File             md.vel
```

```
Force Vector File           md.frc

       49    -20677.0777    -21391.1824       714.1046     939.48    7530.53

Instantaneous Values for Frame Saved at        49 Dynamics Steps

Current Time                 0.0980 Picosecond
Current Potential       -21391.1824 Kcal/mole
Current Kinetic            714.1046 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    49
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       50    -20673.4709    -21383.7727       710.3018     934.48    7490.43

Instantaneous Values for Frame Saved at        50 Dynamics Steps

Current Time                 0.1000 Picosecond
Current Potential       -21383.7727 Kcal/mole
Current Kinetic            710.3018 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    50
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       51    -20670.7018    -21381.3350       710.6332     934.91    7493.92

Instantaneous Values for Frame Saved at        51 Dynamics Steps

Current Time                 0.1020 Picosecond
Current Potential       -21381.3350 Kcal/mole
Current Kinetic            710.6332 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    51
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       52    -20666.3383    -21384.5230       718.1847     944.85    7573.55

Instantaneous Values for Frame Saved at        52 Dynamics Steps
```

```
Current Time                0.1040 Picosecond
Current Potential       -21384.5230 Kcal/mole
Current Kinetic            718.1847 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     52
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       53    -20672.6590    -21391.8945       719.2355     946.23    7584.63

Instantaneous Values for Frame Saved at        53 Dynamics Steps

Current Time                0.1060 Picosecond
Current Potential       -21391.8945 Kcal/mole
Current Kinetic            719.2355 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     53
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       54    -20672.3002    -21400.3681       728.0679     957.85    7677.78

Instantaneous Values for Frame Saved at        54 Dynamics Steps

Current Time                0.1080 Picosecond
Current Potential       -21400.3681 Kcal/mole
Current Kinetic            728.0679 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     54
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       55    -20669.7209    -21408.7278       739.0069     972.24    7793.13

Instantaneous Values for Frame Saved at        55 Dynamics Steps

Current Time                0.1100 Picosecond
Current Potential       -21408.7278 Kcal/mole
Current Kinetic            739.0069 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     55
```

```
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       56    -20673.9003    -21417.1302       743.2300     977.80    7837.67

Instantaneous Values for Frame Saved at        56 Dynamics Steps

Current Time                 0.1120 Picosecond
Current Potential       -21417.1302 Kcal/mole
Current Kinetic            743.2300 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    56
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       57    -20671.4461    -21424.2800       752.8339     990.43    7938.94

Instantaneous Values for Frame Saved at        57 Dynamics Steps

Current Time                 0.1140 Picosecond
Current Potential       -21424.2800 Kcal/mole
Current Kinetic            752.8339 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    57
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       58    -20684.0649    -21430.5501       746.4853     982.08    7871.99

Instantaneous Values for Frame Saved at        58 Dynamics Steps

Current Time                 0.1160 Picosecond
Current Potential       -21430.5501 Kcal/mole
Current Kinetic            746.4853 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    58
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       59    -20685.7654    -21436.2073       750.4419     987.29    7913.72
```

```
Instantaneous Values for Frame Saved at        59 Dynamics Steps

Current Time                0.1180 Picosecond
Current Potential       -21436.2073 Kcal/mole
Current Kinetic           750.4419 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    59
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       60    -20692.8086    -21437.6755       744.8669     979.95    7854.93

Instantaneous Values for Frame Saved at        60 Dynamics Steps

Current Time                0.1200 Picosecond
Current Potential       -21437.6755 Kcal/mole
Current Kinetic           744.8669 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    60
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       61    -20695.0944    -21433.5486       738.4541     971.52    7787.30

Instantaneous Values for Frame Saved at        61 Dynamics Steps

Current Time                0.1220 Picosecond
Current Potential       -21433.5486 Kcal/mole
Current Kinetic           738.4541 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    61
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       62    -20702.0744    -21426.3493       724.2749     952.86    7637.78

Instantaneous Values for Frame Saved at        62 Dynamics Steps

Current Time                0.1240 Picosecond
Current Potential       -21426.3493 Kcal/mole
Current Kinetic           724.2749 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
```

```
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    62
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       63    -20711.3259    -21419.5636       708.2377     931.76    7468.66

Instantaneous Values for Frame Saved at        63 Dynamics Steps

Current Time                 0.1260 Picosecond
Current Potential       -21419.5636 Kcal/mole
Current Kinetic            708.2377 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    63
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       64    -20714.6217    -21415.9791       701.3574     922.71    7396.10

Instantaneous Values for Frame Saved at        64 Dynamics Steps

Current Time                 0.1280 Picosecond
Current Potential       -21415.9791 Kcal/mole
Current Kinetic            701.3574 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    64
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc

       65    -20721.4717    -21416.4019       694.9301     914.25    7328.32

Instantaneous Values for Frame Saved at        65 Dynamics Steps

Current Time                 0.1300 Picosecond
Current Potential       -21416.4019 Kcal/mole
Current Kinetic            694.9301 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    65
Coordinate File              md.arc
Velocity File                md.vel
Force Vector File            md.frc
```

```
       66    -20717.8628    -21420.6203       702.7576     924.55    7410.87

 Instantaneous Values for Frame Saved at        66 Dynamics Steps

 Current Time                0.1320 Picosecond
 Current Potential       -21420.6203 Kcal/mole
 Current Kinetic            702.7576 Kcal/mole
 Lattice Lengths          17.045000     17.481000     14.704000
 Lattice Angles           95.830000     86.110000     94.920000
 Frame Number                    66
 Coordinate File              md.arc
 Velocity File                md.vel
 Force Vector File            md.frc

       67    -20709.3847    -21428.0348       718.6501     945.46    7578.46

 Instantaneous Values for Frame Saved at        67 Dynamics Steps

 Current Time                0.1340 Picosecond
 Current Potential       -21428.0348 Kcal/mole
 Current Kinetic            718.6501 Kcal/mole
 Lattice Lengths          17.045000     17.481000     14.704000
 Lattice Angles           95.830000     86.110000     94.920000
 Frame Number                    67
 Coordinate File              md.arc
 Velocity File                md.vel
 Force Vector File            md.frc

       68    -20709.5624    -21437.5561       727.9936     957.75    7676.99

 Instantaneous Values for Frame Saved at        68 Dynamics Steps

 Current Time                0.1360 Picosecond
 Current Potential       -21437.5561 Kcal/mole
 Current Kinetic            727.9936 Kcal/mole
 Lattice Lengths          17.045000     17.481000     14.704000
 Lattice Angles           95.830000     86.110000     94.920000
 Frame Number                    68
 Coordinate File              md.arc
 Velocity File                md.vel
 Force Vector File            md.frc

       69    -20710.5568    -21447.5258       736.9690     969.56    7771.64

 Instantaneous Values for Frame Saved at        69 Dynamics Steps

 Current Time                0.1380 Picosecond
 Current Potential       -21447.5258 Kcal/mole
```

```
Current Kinetic            736.9690 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    69
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       70    -20718.5704    -21456.3518       737.7814     970.63    7780.21

Instantaneous Values for Frame Saved at        70 Dynamics Steps

Current Time                0.1400 Picosecond
Current Potential       -21456.3518 Kcal/mole
Current Kinetic            737.7814 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    70
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       71    -20706.7510    -21463.0712       756.3202     995.02    7975.71

Instantaneous Values for Frame Saved at        71 Dynamics Steps

Current Time                0.1420 Picosecond
Current Potential       -21463.0712 Kcal/mole
Current Kinetic            756.3202 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    71
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       72    -20703.5916    -21466.8472       763.2556    1004.14    8048.85

Instantaneous Values for Frame Saved at        72 Dynamics Steps

Current Time                0.1440 Picosecond
Current Potential       -21466.8472 Kcal/mole
Current Kinetic            763.2556 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    72
Coordinate File            md.arc
Velocity File              md.vel
```

```
Force Vector File           md.frc

       73    -20707.7983    -21466.2810       758.4827     997.86    7998.51

Instantaneous Values for Frame Saved at        73 Dynamics Steps

Current Time                 0.1460 Picosecond
Current Potential       -21466.2810 Kcal/mole
Current Kinetic            758.4827 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    73
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       74    -20699.3257    -21461.4475       762.1218    1002.65    8036.89

Instantaneous Values for Frame Saved at        74 Dynamics Steps

Current Time                 0.1480 Picosecond
Current Potential       -21461.4475 Kcal/mole
Current Kinetic            762.1218 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    74
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       75    -20698.7505    -21453.3985       754.6480     992.82    7958.07

Instantaneous Values for Frame Saved at        75 Dynamics Steps

Current Time                 0.1500 Picosecond
Current Potential       -21453.3985 Kcal/mole
Current Kinetic            754.6480 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    75
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       76    -20699.3008    -21444.1039       744.8032     979.87    7854.26

Instantaneous Values for Frame Saved at        76 Dynamics Steps
```

```
Current Time                0.1520 Picosecond
Current Potential       -21444.1039 Kcal/mole
Current Kinetic            744.8032 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    76
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       77    -20702.6698    -21436.4543       733.7845     965.37    7738.06

Instantaneous Values for Frame Saved at        77 Dynamics Steps

Current Time                0.1540 Picosecond
Current Potential       -21436.4543 Kcal/mole
Current Kinetic            733.7845 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    77
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       78    -20703.0092    -21433.3066       730.2974     960.78    7701.29

Instantaneous Values for Frame Saved at        78 Dynamics Steps

Current Time                0.1560 Picosecond
Current Potential       -21433.3066 Kcal/mole
Current Kinetic            730.2974 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    78
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       79    -20707.0737    -21436.3106       729.2369     959.39    7690.10

Instantaneous Values for Frame Saved at        79 Dynamics Steps

Current Time                0.1580 Picosecond
Current Potential       -21436.3106 Kcal/mole
Current Kinetic            729.2369 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    79
```

```
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       80    -20705.9033    -21444.9003       738.9971     972.23    7793.03

Instantaneous Values for Frame Saved at        80 Dynamics Steps

Current Time                 0.1600 Picosecond
Current Potential       -21444.9003 Kcal/mole
Current Kinetic            738.9971 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    80
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       81    -20702.5966    -21456.7491       754.1525     992.17    7952.85

Instantaneous Values for Frame Saved at        81 Dynamics Steps

Current Time                 0.1620 Picosecond
Current Potential       -21456.7491 Kcal/mole
Current Kinetic            754.1525 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    81
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       82    -20698.4929    -21469.2897       770.7968    1014.07    8128.37

Instantaneous Values for Frame Saved at        82 Dynamics Steps

Current Time                 0.1640 Picosecond
Current Potential       -21469.2897 Kcal/mole
Current Kinetic            770.7968 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    82
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       83    -20704.4031    -21480.2077       775.8047    1020.65    8181.18
```

```
Instantaneous Values for Frame Saved at        83 Dynamics Steps

Current Time                  0.1660 Picosecond
Current Potential       -21480.2077 Kcal/mole
Current Kinetic            775.8047 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    83
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       84    -20705.7512    -21487.8307       782.0794    1028.91    8247.35

Instantaneous Values for Frame Saved at        84 Dynamics Steps

Current Time                  0.1680 Picosecond
Current Potential       -21487.8307 Kcal/mole
Current Kinetic            782.0794 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    84
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       85    -20698.9730    -21490.9850       792.0120    1041.98    8352.09

Instantaneous Values for Frame Saved at        85 Dynamics Steps

Current Time                  0.1700 Picosecond
Current Potential       -21490.9850 Kcal/mole
Current Kinetic            792.0120 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    85
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       86    -20698.9586    -21488.8682       789.9096    1039.21    8329.92

Instantaneous Values for Frame Saved at        86 Dynamics Steps

Current Time                  0.1720 Picosecond
Current Potential       -21488.8682 Kcal/mole
Current Kinetic            789.9096 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
```

```
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    86
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       87    -20707.9530    -21481.6148       773.6618    1017.83    8158.58

Instantaneous Values for Frame Saved at        87 Dynamics Steps

Current Time                 0.1740 Picosecond
Current Potential       -21481.6148 Kcal/mole
Current Kinetic             773.6618 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    87
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       88    -20713.9364    -21470.5065       756.5701     995.35    7978.34

Instantaneous Values for Frame Saved at        88 Dynamics Steps

Current Time                 0.1760 Picosecond
Current Potential       -21470.5065 Kcal/mole
Current Kinetic             756.5701 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    88
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       89    -20713.8865    -21457.9796       744.0931     978.93    7846.77

Instantaneous Values for Frame Saved at        89 Dynamics Steps

Current Time                 0.1780 Picosecond
Current Potential       -21457.9796 Kcal/mole
Current Kinetic             744.0931 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    89
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc
```

```
       90    -20717.4099    -21446.4304       729.0205     959.10    7687.82

Instantaneous Values for Frame Saved at        90 Dynamics Steps

Current Time                0.1800 Picosecond
Current Potential       -21446.4304 Kcal/mole
Current Kinetic            729.0205 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     90
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       91    -20714.0327    -21437.0387       723.0060     951.19    7624.40

Instantaneous Values for Frame Saved at        91 Dynamics Steps

Current Time                0.1820 Picosecond
Current Potential       -21437.0387 Kcal/mole
Current Kinetic            723.0060 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     91
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       92    -20719.6526    -21430.0128       710.3602     934.55    7491.04

Instantaneous Values for Frame Saved at        92 Dynamics Steps

Current Time                0.1840 Picosecond
Current Potential       -21430.0128 Kcal/mole
Current Kinetic            710.3602 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     92
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       93    -20721.7867    -21425.2440       703.4573     925.47    7418.25

Instantaneous Values for Frame Saved at        93 Dynamics Steps

Current Time                0.1860 Picosecond
Current Potential       -21425.2440 Kcal/mole
```

```
Current Kinetic            703.4573 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    93
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       94    -20723.5667    -21422.8379       699.2712     919.97    7374.10

Instantaneous Values for Frame Saved at        94 Dynamics Steps

Current Time                0.1880 Picosecond
Current Potential       -21422.8379 Kcal/mole
Current Kinetic            699.2712 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    94
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       95    -20724.9063    -21421.6819       696.7756     916.68    7347.79

Instantaneous Values for Frame Saved at        95 Dynamics Steps

Current Time                0.1900 Picosecond
Current Potential       -21421.6819 Kcal/mole
Current Kinetic            696.7756 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    95
Coordinate File            md.arc
Velocity File              md.vel
Force Vector File          md.frc

       96    -20725.7699    -21420.1896       694.4197     913.58    7322.94

Instantaneous Values for Frame Saved at        96 Dynamics Steps

Current Time                0.1920 Picosecond
Current Potential       -21420.1896 Kcal/mole
Current Kinetic            694.4197 Kcal/mole
Lattice Lengths          17.045000     17.481000     14.704000
Lattice Angles           95.830000     86.110000     94.920000
Frame Number                    96
Coordinate File            md.arc
Velocity File              md.vel
```

```
Force Vector File           md.frc

       97    -20731.8499    -21417.5711       685.7211     902.14    7231.21

Instantaneous Values for Frame Saved at        97 Dynamics Steps

Current Time                 0.1940 Picosecond
Current Potential       -21417.5711 Kcal/mole
Current Kinetic            685.7211 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     97
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       98    -20720.9397    -21413.9073       692.9676     911.67    7307.63

Instantaneous Values for Frame Saved at        98 Dynamics Steps

Current Time                 0.1960 Picosecond
Current Potential       -21413.9073 Kcal/mole
Current Kinetic            692.9676 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     98
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

       99    -20716.1987    -21409.2943       693.0956     911.84    7308.98

Instantaneous Values for Frame Saved at        99 Dynamics Steps

Current Time                 0.1980 Picosecond
Current Potential       -21409.2943 Kcal/mole
Current Kinetic            693.0956 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                     99
Coordinate File             md.arc
Velocity File               md.vel
Force Vector File           md.frc

      100    -20713.7640    -21403.5341       689.7700     907.47    7273.91

Instantaneous Values for Frame Saved at       100 Dynamics Steps
```

```
Current Time                  0.2000 Picosecond
Current Potential        -21403.5341 Kcal/mole
Current Kinetic             689.7700 Kcal/mole
Lattice Lengths           17.045000     17.481000     14.704000
Lattice Angles            95.830000     86.110000     94.920000
Frame Number                    100
Coordinate File               md.arc
Velocity File                 md.vel
Force Vector File             md.frc
```

```
/data/home/na2782/aenet-tinker-test-2
```

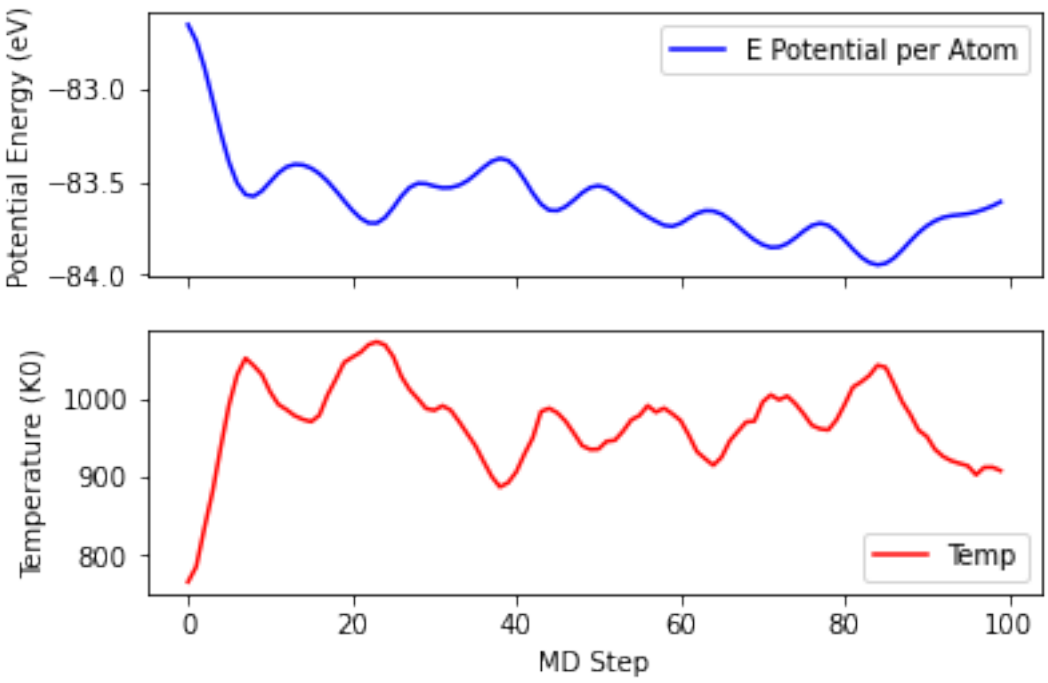
Visualization of some key data from the MD trajectory:

[13]:
```
import matplotlib.pyplot as plt
import pandas as pd
import re

data = []
with open('md-example/dynamic.out') as fp:
    for line in fp:
        if re.match(r"^ *[0-9]", line):
            try:
                fields = line.split()
                data.append([float(f) for f in fields[1:]])
            except ValueError:
                pass

df = pd.DataFrame(data=data,
                  columns=["E Total", "E Potential",
                           "E Kinetic", "Temp", "Pres"])

fig, ax = plt.subplots(2, 1, sharex=True)
df['E Potential per Atom'] = df['E Potential']/256
df.plot(y="E Potential per Atom", color='blue', ax=ax[0])
ax[0].set_ylabel("Potential Energy (eV)")
df.plot(y="Temp", color='red', ax=ax[1])
ax[1].set_xlabel("MD Step")
ax[1].set_ylabel("Temperature (K0)")
plt.show()
```


Potential Energy (eV)
−83.0
−83.5
−84.0
E Potential per Atom
Temperature (K0)
1000
900
800
Temp
0
20
40
60
80
100
MD Step

[ ]: