Q
Version 5.7
Developers Manual

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Contents

1 Introduction

This is the developers manual for **Q**, the free enegies from molecular dynamics program. Q is entirely written in modern Fortran. Its initial development was in Fortran 90, but the incorporation of object oriented paradigms into modern Fortran have seen the code evolve to take advantage of the evolution of the language. Currently the program incorporporates elements of the Fortran 2008 standard and it is developing the use of the OpenMP 4.0 standard[i] for in-node parallelization.

1.1 Makefile

1.2 Cluster Architectures

1.3 Debugging

1.4 Profiling

[i] which is now fully implemented into gnu Fortran version 5.1

1.5 Best Practices

`http://www.fortran90.org/src/best-practices.html`

2 ChangeLog

3 Release Schedule

4 qprep

qprep is the utility which allows the translation of pdb files into a format which the dynamics engine can understand. The main file generated by **qprep** is refered to as the topology.

```
qprep generate.inp >& generate.out &
```

5 qdum

6 qdyn

qdyn is compiled using the following explicit rules:

```
-ffree-line-length-none
-fcray-pointer
-fall-intrinsics
-std=legacy
-Wall
-Wtabs
-fstack-protector
-O3
-DG95=1 -c
```

Development flags recommended from fortran90.org:
-Wall -Wextra -Wimplicit-interface -fPIC -fmax-errors=1 -g -fcheck=all -fbacktrace
Production flags recommended from fortran90.org:
-Wall -Wextra -Wimplicit-interface -fPIC -Werror -fmax-errors=1 -O3 -march=native -ffast-math -funroll-loops
sizes: Specifies data storage for all Q programs.
Modules used= NONE
nrgy: Input/Output for energy data and energy file.
Modules used= sizes
Subroutines:
nrgy_startup = empty
put_ene =
Functions:
mpiglob: Declares global variables for MPI parallelization of qdyn Modules used = nrgy Subroutines:
Functions:
misc:
Modules used = sizes
Subroutines:
Functions:
prmfile: Data files parser. Modules used = misc Subroutines: prmfile_startup = EMPTY ? WTF
Functions:
index: Modules used = NONE
topo: Modules used = sizes, misc Subroutines: topo_startup = EMPTY ? WTF
Functions:
qatom: Modules used = sizes, nrgy, misc, prmfile, indexer, topo
mask: Modules used = topo
trj: Modules used = atom_mask, misc
-DG95=1 -cpp -c
md: This is the main molecular dynamics *module*. Modules used =
qdyn: This file contains the main **qdyn** *program* code. Modules used =

7 qfep

8 qcalc

9 Tricks

A very convenient trick for cleaning up the code is:
emacs –batch md.f90 -f mark-whole-buffer -f f90-indent-subprogram -f save-buffer

10 Links

The following is a collection of reference links useful for fotran programers.
- The description of the GNU Compiler Collection (gcc) version 5.1.0
https://gcc.gnu.org/onlinedocs/gcc-5.1.0/gfortran.pdf

10.1 Doxygen

To automatically document fortran code the only current available option is doxygen. To use doxygen a configuration file is necessary. This has been downloaded from:

https://modelingguru.nasa.gov/docs/DOC-1811
And modified to our needs.
Just doing:

```
doxygen DoxygenConfigFortran
```

Generates html code which we make available at:
doxygen.qdyn.org
A mainfile document is included in the file maintext.txt

10.2 Fortran codes available online

These projects are a good resource to check-out development and practices on coding.
Gyro-Kinetics at Warwick. A program for turbulence study in plasmas.
https://bitbucket.org/gkw/gkw/wiki/Home
OpenMC. A Monte Carlo code.
https://github.com/mit-crpg/openmc
A collection of generic Fortran routines. https://github.com/astrofrog/fortranlib