Q DEVELOPERS MANUAL

Mauricio Esguerra
mauricio.esguerra@gmail.com

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1 Introduction

This is the developers manual for Q, the free enegies from molecular dynamics program. Q is entirely writen in Fortran. It's 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.

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

1.1 makefile

1.2 Cluster Architectures

1.3 Debugging

1.4 profiling

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.

```
bash-3.1\$ qprep generate.inp >& generate.out &
```

```
bash-3.1\$ pwd
/home/username
bash-3.1\$ cd Desktop
bash-3.1\$ ls
Trash
```

5 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: Does this. Modules used= NONE

nrgy: Does this. 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 =

5.1 subsection 1

Make sure to have the location of the binaries on your path.

Make sure to modify rungms to have the path to the gamess binary and also the location of scratch.

Make a symbolic link to the mac executable which comes with a funky name.

6 qfep

7 qcalc

8 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`

8.1 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

8.2 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`