The MOM semimicroscopic optical model potential program

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v1.01

Chapter 1

Introduction

MOM is a program which implements the semimicroscopic nucleon-nucleus spherical optical model potential as described in [1], in an easy to use package that needs only a minimal number of input and produces observables. The optical model potential of [1] and its extension to deformed and unstable nuclei has been widely tested [1, 2, 3, 4, 5] and produces predictions from A=30 to 240 and for energies ranging from 10 keV up to 200 MeV. MOM stands for “Modèle Optique Microscopique” in French, or “Microscopic Optical Model” in English.

1.1 Code Structure

The MOM code system (MOMCS) is actually a chain of different programs linked by a c-shell script. The MOMCS uses two main modules (as well as a few auxiliary modules that handle file format translation etc...). The first main module of the MOMCS is the MOM program that reads the target A, Z, and radial densities, the projectile type (p or n) and energy, and the folding ranges, and performs the folding of the Nuclear Matter (NM) optical model potential described in [1] with the densities to obtain a local optical model potential (OMP). This is then put in the ECIS95 [6] code to compute observables by solving the Schrödinger equation for the interaction of the projectile with the aforementioned OMP. ECIS95 is the second main module of the MOMCS and should be obtained separately. The user can also chose to run only the MOM program and then feed the resultant OMP into his favorite Schrödinger OMP program (SCAT2, FOP, ...), in this case the user is responsible for translating from the MOM output file format to his OMP program input file format. Figure 1.1 illustrates the MOMCS.

1.2 Physical content

The MOMCS calculates the OMP by folding the target radial matter density with an OMP in nuclear matter based on the Brückner-Hartree-Fock work of

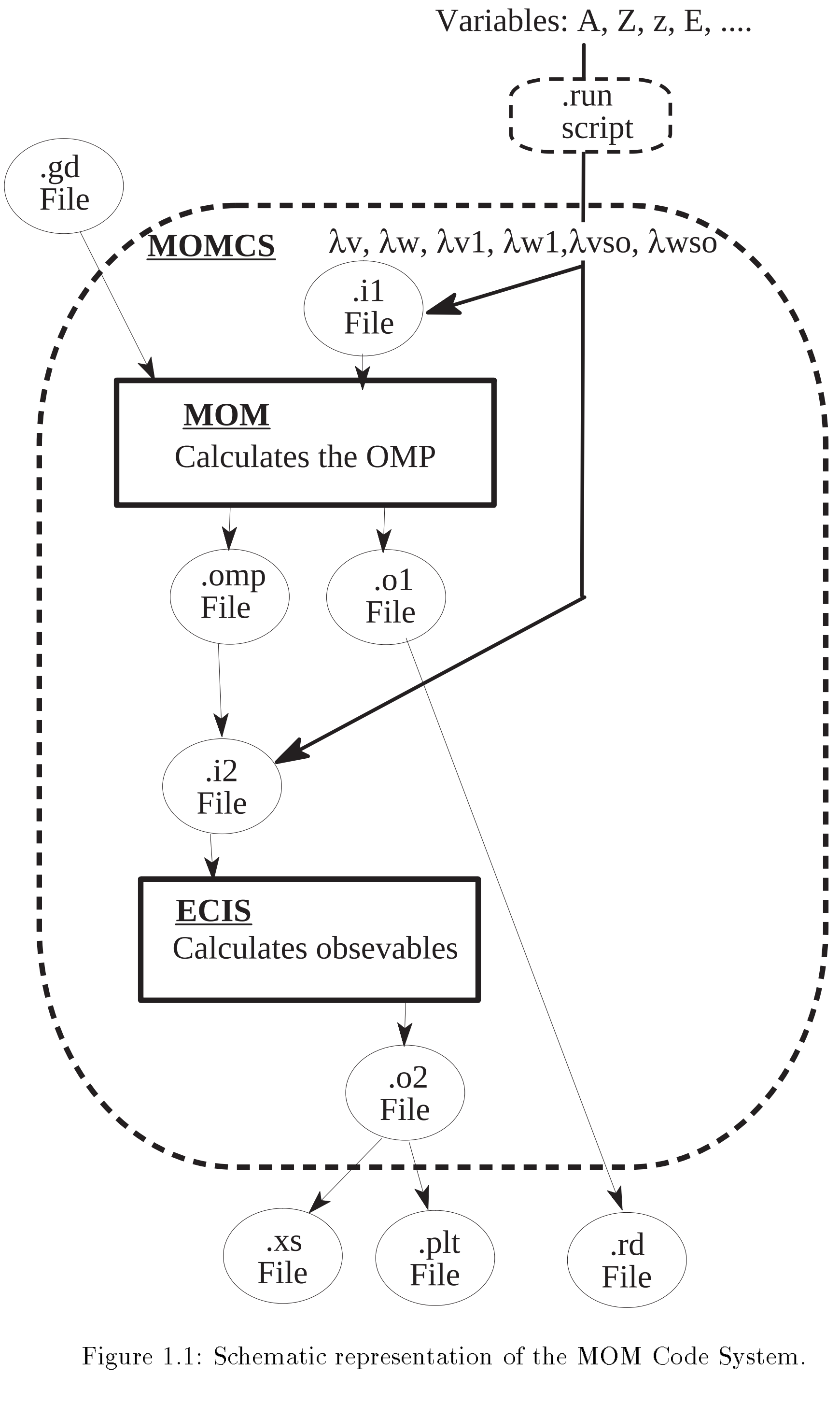

Figure 1.1: Schematic representation of the MOM Code System.

Jeukenne, Lejeune and Mahaux [7, 8, 9, 10]. This NM OMP was then phenomenologically altered in [1, 11] in order to improve the agreement of predicted finite nuclei observables with a large set of experimental data. These improvements consist in unifying the low and high energy parameterizations of the NM interaction in [11], and in studying the energy variations of the potential depth normalization factors in [1]. These factors now include non-negligible renormalizations of isovector components [1] that are needed in order to account simultaneously for (p,p) and (n,n) elastic scattering as well as $(\mathrm{p,n})_{IAS}$ quasi-elastic scattering. The final NM potential for a given nuclear matter density $\rho = \rho_n - \rho_p$ and asymmetry $\alpha = (\rho_n + \rho_p)/\rho$ reads

$$\begin{aligned} U_{NM}(E)_{\rho,\alpha} = \quad & \lambda_V(E)\left[V_0(\tilde{E}) \pm \lambda_{V1}(E)\alpha V_1(\tilde{E})\right] \\ + \quad & i\lambda_W(E)\left[W_0(\tilde{E}) \pm \lambda_{W1}(E)\alpha W_1(\tilde{E})\right], \end{aligned} \tag{1.1}$$

with E the incident nucleon energy, $\tilde{E} = E - V_c$ (where V_c is the Coulomb field), V_0, V_1, W_0, and W_1 the real isoscalar, real isovector, imaginary isoscalar, and imaginary isovector NM OMP components respectively, and λ_V, λ_{V1}, λ_W, and λ_{W1} the real (isoscalar+isovector), real isovector, imaginary, and imaginary isovector normalization factors respectively. The values of λ_V, λ_{V1}, λ_W, and λ_{W1} given in [1] read

$$\lambda_V(E) = 0.951 + 0.0008\ \ln(1000E) + 0.00018\ [\ln(1000E)]^2 \tag{1.2}$$

$$\begin{aligned} \lambda_W(E) = \quad & \left[1.24 - \left[1 + e^{\left(\frac{E-4.5}{2.9}\right)}\right]^{-1}\right]\left[1 + 0.06\ e^{-\left(\frac{E-14}{3.7}\right)^2}\right] \\ \times \quad & \left[1 - 0.09\ e^{-\left(\frac{E-80}{78}\right)^2}\right]\left[1 + \left(\frac{E-80}{400}\right)\Theta(E-80)\right] \end{aligned} \tag{1.3}$$

$$\lambda_{V1}(E) = 1.5 - 0.65\left[1 + e^{\frac{E-1.3}{3}}\right]^{-1} \tag{1.4}$$

$$\begin{aligned} \lambda_{W1}(E) = \quad & \left[1.1 + 0.44\left[1 + \left(e^{\frac{E-40}{50.9}}\right)^4\right]^{-1}\right] \\ \times \quad & \left[1 - 0.065\ e^{-\left(\frac{E-40}{13}\right)^2}\right]\left[1 - 0.083\ e^{-\left(\frac{E-200}{80}\right)^2}\right]. \end{aligned} \tag{1.5}$$

with the energy E expressed in MeV. As stated in [1], in the 20 to 50 MeV range, the uncertainties related to λ_V, λ_{V1}, λ_W, and λ_{W1} are estimated to be 1.5%, 10%, 10%, and 10%, respectively. Outside this energy range, uncertainties are estimated to be 1.5 times larger.

Moreover in order to apply the NM OMP to finite nuclei an approximation hat to be performed. This is the Local Density Approximation (LDA) where the local value of the finite nucleus OMP is taken to be the NM OMP value for the local finite nucleus density: $U_{FN}(r) = U_{NM}(\rho(r))$. Since this LDA produces potentials with too small rms radii, the improved LDA, which broadens the OMP with a Gaussian form factor (1.6), is introduced. In [11, 1] different prescription for the improved Local Density approximation are compared and LDA range parameters are optimized.

$$U_{FN}(r,E) = (t\sqrt{\pi})^{-3} \int \frac{U_{NM}(\rho(r'),E)}{\rho(r')} \exp(-|\vec{r}-\vec{r'}|^2/t_r^2)\rho(r')d\vec{r'}, \tag{1.6}$$

with t the range of the Gaussian form factor. The $t_r = 1.25$ fm and $t_i = 1.35$ fm values were found [1] to be global optimal values for the real and imaginary ranges, respectively.

Finally, since no spin-orbit (SO) potential exists between a nucleon and NM, the Scheerbaum [12] prescription was selected in [11], coupled with the phenomenological complex potential depths $\lambda_{v_{so}}$, and $\lambda_{w_{so}}$. The SO potential reads

$$U^{so}_{n(p)}(r) = (\lambda_{v_{so}}(E) + i\lambda_{v_{so}}(E)) \frac{1}{r}\frac{d}{dr}\left(\frac{2}{3}\rho_{p(n)} + \frac{1}{3}\rho_{n(p)}\right), \tag{1.7}$$

with

$$\lambda_{v_{so}} = 130 \exp(-0.013\,E) + 40 \tag{1.8}$$

and

$$\lambda_{w_{so}} = -0.2\,(E-20). \tag{1.9}$$

Chapter 2

Input description for MOM

2.1 Overall presentation

Running MOM by hand is achieved by typing the command:

```
 MOMR> momf/mom
```

MOM then asks for the name of the input file, output file, and radial density file.

```
 MOMR/test> ../momf/mom
  Input file name:
test.i1
  Output file name (or c.r. for screen):
test.o1
  Ground-state density file name (or c.r. if none):
pb208.hfbu.gd
 MOMR/test>
```

2.2 Input and output files

Let us first have a look at the `test.i1` file. It looks like:

```
hfb 26.00000 MeV 208Pb (n,n) jlm
test.omp
b0.
c82,208
d26.00000
e1.
o1.,1.,1.5
p1.,1.,1.399
u1.25,1.35,2.,0.,1.,1.
v1.
```

After mom terminates files named `test.o1` (output file of mom) and `test.omp` (OMP file) should be written to disk.

2.2.1 .i1 file description

The first line is a string used to describe the run.

The second line specifies the name of the .omp file which contains the OMP on the calculation mesh.

The following lines are identified by the first letter (`b`,`c`,`d`,`e`,`o`,`p`,`u`,`v`,`w`) which tags the cards. This first letter is then followed by one or more real numerical values (free format) separated by commas. If a line is omitted then its values take on default values defined in the MOM code. The user can also chose to omit the final values of a card, in this case these will also take on the default values.

The line identified by `b` (line `b`) holds one variable `zp`: the charge number of the projectile (default `zp=0`).

Line `c` holds `z` and `a` the target charge and mass number (default `z=0 a=0`).

Line `d` holds `einc0` the projectile incident energy in MeV (default `einc=0`).

Line `e` holds `irel` which switches between relativistic (`irel`=1) or classical (`irel`=0) kinematics (default `irel=0`).

Line `o` holds `al0r`, `dum`, and `alti` the real potential depth normalization for the isoscalar (`al0r`) and isovector (`altr`) components of the OMP. `dum` is a dummy value that is not used and kept for compatibility with older codes (defaults `al0r=1 altr=1`).

Line `p` holds `al0i`, `dum`, and `alti` the imaginary potential depth normalization for the isoscalar (`al0i`) and isovector (`alti`) components of the OMP. `dum` is a dummy value that is not used and kept for compatibility with older codes (defaults `al0i=1, alti=1`).

Line `u` holds `tjlmr`, `tjlmi`, `dum`, `dum`, `icorv` and `icorw`. `tjlmr` and `tjlmi` are the improved LDA ranges (in fm) of the real and imaginary OMP components, respectively. `dum` are dummy values kept for compatibility reasons. `icorv` and `icorw` control the Coulomb corrections: if `icorv=1` (resp. `icorw`) the real (resp. imaginary) potential component is evaluated at `einc0`-V_c otherwise it is evaluated at `einc` (defaults `tjlmr=1.0 tjlmi=1.0 icorv=1 icorw=1`).

Line `v` holds `kmw` which controls whether the imaginary OMP components are multiplied by the effective mass (default `kmw=0`). According to [13, 14] the imaginary OMP components *should* be multiplied by the effective mass, so `kmw` should be set to `1`. If MOM is run through the MOMCS scripts, `kmw` is set to `1`.

Line `w` holds `xlw` and `xlw` the potential depth normalization factors for the real and imaginary OMP components respectively (default `xlv=1.0 xlw=1.0`).

The .i1 file ends by a blank line.

2.2.2 .gd file description

The .gd file which holds the radial density information is built as follows: every line contains r, $p0$, $p2$, $p4$, $p6$, $p8$, $n0$, $n2$, $n4$, $n6$, $n8$, in free format, where r is the radial distance (in fm), $p0$ and $n0$ are the proton and neutron densities (in fm^{-3}) respectively, and $p2$, $p4$, $p6$, $p8$, $n2$, $n4$, $n6$, $n8$ are not used but are kept for compatibility reasons. The densities are read every 0.1 fm starting with 0.1 fm, and with at least 122 values (i.e. at least to 12.2 fm).

Note: the `pb208.hfbu.gd` density file found in the `tests` is a Hartree-Fock calculation for ^{208}Pb performed with the Gogny D1S interaction.

2.2.3 .o1 file format description

The .o1 file is meant to be human-readable, an is used to check both the input and output of a MOM run. In a first part this file summarizes the inputs read in from the console (.i1, .o1, .gd file names), from the .i1 file (.omp file name, b,c,d,e,h,o,p,u,v,z,A lines, and the read values), from the .gd file (proton and neutron densities on the 0.1, to 12.2 fm mesh with a 0.1 fm step).

The second part of the .o1 file holds the calculated OMP components (on the same mesh as the densities).

2.2.4 .omp file format description

The .omp file holds the OMP on the usual mesh (0.1 to 12.2 fm mesh with a 0.1 fm step). The first line should be 122, this value represent the number of points on the mesh. Then, for each radial position on the mesh there are 2 lines of 3 real values. The first line holding $V(r)$, dum, dum and the second line holds $W(r)$, dum, dum. V is the real potential, W is the imaginary potential , and dum are dummy values that are retained for historical reasons. After 244 such lines comes a single integer value that should be 122. Then come 122 pairs of lines that hold alternatively $V_{so}(r)$ and $W_{so}(r)$, the un-normalized real and imaginary spin-orbit potential components on the calculation mesh.

Chapter 3

Input description for scripts

3.1 Presentation

Here is an example of a MOMCS script that automatically calculate the OMP for the 10 MeV n+^{208}Pb reaction (using MOM), then prepares an ECIS input for that case using the calculated OMP, runs ECIS and generates report files.

```
#!/bin/csh -f
#################################
# begining of user editable part#
#################################
######### variables #############
#################################
####### mom & ecis   ############
set sym = Pb
set en = 10.00000
set ee = 10
set aa = 208
set ca = 08
set zz = 82
set ap = 1.
set zp = 0.
set rel = 1.
set lab = d
#################################
#### variable parameters      ###
####  as a fct of en       ######
#################################
set pv = 2
set pw = 4
set pvso = 2
set pwso = 1
```

```
set v1n = a
set w1n = a
##### ecis only    #############
set lv = 0.96
set lw = 1.1
set lvs = 150.
set lws = -2.
##### mom only      ############
set tjr = 1.25
set tji = 1.35
set fgd = pb208.hfbu.gd
##################################
### end of user editable part ###
##################################
source ${MOMDIR}/scripts/runscript
```

This script is named `pb10.run` and when run it produces the following output:

```
MOMR/test>./pb10d.run
mu -0.0000      rc 1.18832
10.00000 MeV
lv=0.9736 lw=1.0847 lvso=154.15241 lwso=2.00000 v1n=1.466 w1n=1.501
 10.00000 5208.913086 2677.631592 2531.281494
MOMR/test>
```

3.2 Input/script file

The `pb10.run` script is a c-shell script that runs on unixes and unix-like systems, and as such it must follow the c-shell syntax (type `man csh` on a unix-like system for more information). The section of the file between the `beginning of user editable part` and `end of user editable part` tags can be edited by the user to describe the calculation.

Let us go through all the variables set in the example file:

The `sym` variable is the chemical symbol for the target (Lead in this example). This variable is used only to generate names for the output files. Note that for some files the lowercase translation of the symbols is used (i.e. pb instead of Pb).

The `en` variable is the projectile energy in MeV. It should be given with 5 digits past the decimal point.

The `ee` variable is the projectile energy as is should appear in the generated file names (2 characters).

The `aa` variable is A the mass number of the target.

The `ca` is the mass number of the target as is should appear in the generated file names (2 characters).

The `zz` variable is Z the charge number of the target.

The ap variable is a the mass of the projectile (always 1. in this version that supports only proton and neutron projectiles).

The zp variable is z the charge number of the projectile (1. for proton, 0. for neutron).

The rel variable switches between relativistic (1.) and non-relativistic (0.) kinematics in MOM (see irel in MOM input description) and ECIS.

The lab is a label that is used in generating the output file names (1 or 2 characters). The output file names then are generated by concatenation of sym, ee, ca, lab and a file extension. In the current example the files will be named Pb0810d.* or pb0810d.*.

The next section in the script file deals with the control of the normalization factors. The pv variable is either 0 or 2. If it is 2 the real potential depth normalization factor λ_v is calculated using formula (1.2), otherwise the value of variable lv is used.

The pw variable is either 0 or 4. If it is 4 the imaginary potential depth normalization factor λ_w is calculated using formula (1.3)[1], otherwise the value of variable lw is used.

The pvso variable is either 0 or 2. If it is 2 the real s.o. potential depth normalization factor $\lambda_{v_{so}}$ is calculated using formula (1.8), otherwise the value of variable lvs is used.

The pwso variable is either 0 or 2. If it is 2 the imaginary s.o. potential depth normalization factor $\lambda_{w_{so}}$ is calculated using formula (1.9), otherwise the value of variable lws is used.

The v1n variable is either a or a real value. If it is a the real isovector potential depth normalization factor λ_{V1} is calculated using formula (1.4), if it is a real value this value is used for λ_{V1}.

The w1n variable is either a or a real value. If it is a the imaginary isovector potential depth normalization factor λ_{W1} is calculated using formula (1.5), if it is a real value this value is used for λ_{W1}.

The lv, lw, lvs and lws have been described above.

The tjr and tji variables hold t_r and t_i the Gaussian form factors used in (1.6) for the real and imaginary potential respectively (see also tjlmr and tjlmi in MOM input description).

The fgd variable holds the name of the .gd file.

3.3 Output files

After the run several files are created:

```
MOMR/test>ls
 Pb0810d.i1
```

[1]Since the (1.3) expression was optimized with a different program (FLIT from Frank S. Dietrich of LLNL) that treats the densities a little differently from MOM, (1.3) does not produce an optimal fit with MOM. In order to obtain a better fit, equ. (1.3) should be multiplied by a 0.95 factor. This re-normalization is performed in MOMCS scripts if the pw = 4 option is activated.

```
 Pb0810d.i2
 Pb0810d.o1
 Pb0810d.o2
 Pb0810d.omp
 pb0810d.plt
 pb0810d.rd
 pb0810d.xs
MOMR/test>
```

Among these files the .i1, .o1, and .omp files are described above. The .i2 and .o2 are the ECIS input and output files respectively (refer to the ECIS description and [6] for more information).

3.3.1 .plt file

The .plt file holds the angular distribution extracted from the ECIS output from 0.5 to 180.0 degrees c.m. If the projectile is a neutron, this file has three columns: θ (degrees), $d\sigma/d\Omega$ (mb/sr), A_y. If the projectile is a proton, the file has four columns: θ (degrees), $d\sigma/d\Omega$ (mb/sr), $\sigma(\theta)/\sigma_{Ruth}$, A_y.

3.3.2 .xs file

The .xs file holds the angle integrated cross sections, depending on the projectile it is made of two or three columns. If the projectile is a proton the two columns are the projectile energy in MeV, and the reaction cross section in mb. If the projectile is a neutron the three columns are the projectile energy in MeV, the total cross section (mb), the reaction cross section (mb), and the shape elastic cross section (mb). Note that successive runs of the script appends to the end of this file adding a line for each run.

3.3.3 .rd file

The .rd repeats the potential volume integrals, rms, and sharp cut-off radii from the .o1 file. This file is made of 7 columns: the projectile energy (MeV), the real potential volume integral (fm$^3/A$), rms radius (fm) and sharp cut-off radius (fm), and the imaginary potential volume integral (fm$^3/A$), rms radius (fm) and sharp cut-off radius (fm). As with the .xs file, successive runs of the script appends to the end of this file adding a line for each run.

Chapter 4

Installation and tests

4.1 Installation

The installation package comes in the form of a gziped tar file: `mom.tgz`.

First, `cd` to the directory where MOM will be installed, uncompress `mom.tgz` with the command `gzip -d mom.tgz` (on unix), then untar the file with the command `tar xf mom.tar`. A `MOMR` directory should be created with four subdirectories: `manual`, `momf`, `scripts`, and `test`.

Go to the `momf` directory and type `make` at the command line. (Note: if your FORTRAN compiler is not invoked by the `f77` command you will have to edit the `Makefile` to change the `CC` and `LD` variables). Alternatively, the `mom` program can be compiled with the `f77 -o mom *.f` command. Hopefully, there will be no errors or warnings at the compilation.

Then go to the scripts directory and type `make` (Note: if your FORTRAN compiler is not invoked by the `f77` command, or your c compiler is not invoked by the `cc` command , you will have to edit the `Makefile` to change the `CC` and `FF` variables). Alternatively, you can compile programs by hand by typing `cc -o col2vec col2vec.c` ,`cc -o calcpar calcpar.c -lm`, and `f77 -o pot2ecis2 pot2ecis.f`.

Edit the `runscript` file in the `scripts` directory and change the `MOMBASE` variable so that is provides the full path to your `MOMR` directory. Also, change the `ECIS` variable so that it gives the full path to your ECIS executable.

4.2 Tests

Go to the test directory, type `../momf/mom` and answer the questions as follows:

```
 MOMR/test> ../momf/mom
  Input file name:
test.i1
  Output file name (or c.r. for screen):
```

```
test.o1
  Ground-state density file name (or c.r. if none):
pb208.hfbu.gd
 MOMR/test>
```

A `test.omp` and a `test.o1` file should be written on disk. Compare with the files stored in the `outputs` directory (for example with the `diff test.o1 outputs/test.o1` command) if no difference appears then the `mom` program has passed the test.

Now type `pb10d.run`, the following output should be written to the screen

```
MOMR/test>./pb10d.run
mu -0.0000      rc 1.18832
10.00000 MeV
lv=0.9736 lw=1.0847 lvso=154.15241 lwso=2.00000 v1n=1.466 w1n=1.501
 10.00000 5208.913086 2677.631592 2531.281494
MOMR/test>
```

Compare the generated `Pb0810d.i1`, `Pb0810d.i2`, `Pb0810d.o1`, `Pb0810d.o2`, `Pb0810d.omp`, `pb0810d.plt`, `pb0810d.rd`, and `pb0810d.xs` with their respective counterparts in the `outputs` directory. If no difference appears then MOMCS has passed the test. (Note: the `Pb0810d.o2` file should include one difference since the running time of the program is written in `Pb0810d.o2`.)

If MOMCS passed the test you can now edit the `template.run` to change the `../scripts/runscript` path on the last line of the file to the full path of the `scripts/runscript` script file. This `template.run` file can now be used as a template for other runs, and run from anywhere on the disk (as long as the .gd file is in the current directory).

4.2.1 What if some differences occur during the tests ?

If the differences are very small (last decimal figure) they are likely due to minor differences in the treatment or the rounding of floating point values between the computer system you use and the one that I used to generate the test cases (Sparc Ultra5 with Solaris).

If large differences (> last decimal) appear at the first testing stage then they are likely to be due to important differences in the compiler/libraries and the MOM code should not be used to calculate cross sections in this un-validated state. If you encounter such a problem please contact the author (see section 5 “Contact and help”). Note that if there are small (last decimal figure) differences in the first testing stage (`./momf`) these will likely propagate to larger differences in the second testing stage (`./pb10d.run`) ; if that occurs, a more detailed analysis of the differences must be performed.

Finally differences can occur in the formatting of the outputs (extra spaces, 0.0, 0. or .0, ...) that do not affect the results at all.

As of now, the MOM code has been successfully compiled and tested on the following systems:

Sun Sparc Ultra5 with Solaris 7
sgi MIPS with IRIX 6
Compaq Alpha with TruUnix
Pentium with Linux
PPC with MacOS X.

Chapter 5

Contact and help

If you have problems with the MOM code that you cannot solve easily, if you have questions that are not adressed in the manual, or if you have more remarks regarding MOM, MOMCS, this manual, or the physics behind the codes, feel free to contact the author:

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Chapter 6

Acknowledgments

I wish to thank F.S. Dietrich of LLNL whose FLIT code got me started in the field of JLM OMPs. Note that the .i1 file format of the present MOM code is actually a subset of the FLIT input file format and should be compatible with it. The .omp, and .o1 file formats are also very close to their FLIT conterparts.

I also wish to acknowledge J. Raynal for is efforts in maintaning and updating the ECIS code to the highest standards.

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