MODULE 7
Calculating fundamental atomic structure and electron impact cross-section data - Autostructure and R-Matrix.

Demonstration script

Hugh Summers, Nigel Badnell, Martin O'Mullane and Alessandra Giunta

September 27, 2013

Contents

1 Demo (a) Introducing the Cowan code

```
------------------------------
DEMO A: Introducing the Cowan code
------------------------------
PURPOSE: To calculate excitation cross section using Plane Wave Born (PWB)
approximation, as implemented within ADAS801 using the Cowan code.

The input file is in the adf34 format.
This gives the set of configurations according to the parity for each ionisation
stage.
The format is fixed. It requires the element symbol, the atomic number, the
ionisation stage  charge +1 and the configurations to build up the appropriate
atomic structure.

The output is a Type 1 or 3 adf04 data file (See Module 1 Demo c).. .


EXAMPLE: For this demo Be-like Fe (Fe22+) is considered.
The input file in the adf34 format for the ADAS801 run is fe22.dat.
For adas8#1 offline run, the executable is
/home/adas/offline_adas/adas8#1/scripts/run_adas8#1.
It requires the input file adf34, fe22.dat, together with two other files,
fe22.inst and fe22.pp, which set up the type of transition (electric dipole,
magnetic dipole etc.), the temperature range requested for calculating the cross
sections, scale factors and the other parameter nedded for the run.
Type 3 adf04 in ic resolution has been established as output for this demo:
- for the interactive run the output adf04 is ic#fe22.dat;
- for the offile run he output adf04 is fe22_offline.dat.


COMMENTS: Note that the configurations must be grouped according to their
parity.
For example for F22+, 15 configurations are included in the adf34 fe22.dat as
follows:
 2s2             1s2  2s2
 2s1 3s1         1s2  2s1  3s1
 2s1 4s1         1s2  2s1  4s1
 2s1 3d1         1s2  2s1  3d1
 2s1 4d1         1s2  2s1  4d1
 2p2             1s2  2p2
 2p1 3p1         1s2  2p1  3p1
 2p1 4p1         1s2  2p1  4p1
 2s1 2p1         1s2  2s1  2p1
 2s1 3p1         1s2  2s1  3p1
 2s1 4p1         1s2  2s1  4p1
 2s1 4f1         1s2  2s1  4f1
 2p1 3s1         1s2  2p1  3s1
 2p1 3d1         1s2  2p1  3d1
 2p1 4d1         1s2  2p1  4d1
```

```
According to the Parity (P=(-1)^sum(li)), the first group include only even
configurations:
 2s2             1s2  2s2
 2s1 3s1         1s2  2s1  3s1
 2s1 4s1         1s2  2s1  4s1
 2s1 3d1         1s2  2s1  3d1
 2s1 4d1         1s2  2s1  4d1
 2p2             1s2  2p2
 2p1 3p1         1s2  2p1  3p1
 2p1 4p1         1s2  2p1  4p1
while the second group includes only odd configurations:
 2s1 2p1         1s2  2s1  2p1
 2s1 3p1         1s2  2s1  3p1
 2s1 4p1         1s2  2s1  4p1
 2s1 4f1         1s2  2s1  4f1
 2p1 3s1         1s2  2p1  3s1
 2p1 3d1         1s2  2p1  3d1
 2p1 4d1         1s2  2p1  4d1


DEMO a1: Examine the adf34 driver file for Be-like Fe (Fe22+)
1. Open the adf34 file fe22.dat and explore it.
Sample of adf34 files: fe22.dat

DEMO a2: Use interactive ADAS801 to make Fe22+ adf04 file
1. Run ADAS801 interactively.
2. Set up Intermediate Coupling adf04 in the output window.
Output file: ic#fe22.dat

DEMO a3: Use offline_adas/adas8#1 for same Fe22+
1. Look at the input files fe22.inst and fe22.pp.
2. Type /home/adas/offline_adas/adas8#1/scripts/run_adas8#1 fe22.dat fe22.inst
   fe22.pp from the command line.
Sample of script: demo_a_3.sh
Input files: fe22.dat, fe22.inst, fe22.pp
Ouptup file: fe22_offline.dat
```

1.1 Demo (a) Figures

1.2 Demo (a) Procedures

1.2.1 Demo (a-1) demo_d/fe22.dat

```
2  -5    2   10  1.0    5.d-09    5.d-11-2  0130    1.0 0.65  0.0  0.5
   26   23   Fe  2s2              1s2  2s2
   26   23   Fe  2s1 3s1          1s2  2s1  3s1
   26   23   Fe  2s1 4s1          1s2  2s1  4s1
   26   23   Fe  2s1 3d1          1s2  2s1  3d1
   26   23   Fe  2s1 4d1          1s2  2s1  4d1
   26   23   Fe  2p2              1s2  2p2
   26   23   Fe  2p1 3p1          1s2  2p1  3p1
   26   23   Fe  2p1 4p1          1s2  2p1  4p1
   26   23   Fe  2s1 2p1          1s2  2s1  2p1
   26   23   Fe  2s1 3p1          1s2  2s1  3p1
   26   23   Fe  2s1 4p1          1s2  2s1  4p1
   26   23   Fe  2s1 4f1          1s2  2s1  4f1
   26   23   Fe  2p1 3s1          1s2  2p1  3s1
   26   23   Fe  2p1 3d1          1s2  2p1  3d1
   26   23   Fe  2p1 4d1          1s2  2p1  4d1
   -1
```

1.2.2 Demo (a-2) demo_a/ic#fe22.dat

```
FE+22        26        23      15730300.0
    1 1S2 2S2             (1)0( 0.0)            0.0
    2 1S2 2S1 2P1         (3)1( 0.0)       354118.2
    3 1S2 2S1 2P1         (3)1( 1.0)       382472.7
    4 1S2 2S1 2P1         (3)1( 2.0)       467040.0
    5 1S2 2S1 2P1         (1)1( 1.0)       696851.6
    6 1S2 2P2             (3)1( 0.0)       960656.6
    7 1S2 2P2             (3)1( 1.0)      1027340.8
     . . .
   81 1S2 2P1 4D1         (1)3( 3.0)     12617526.6
   82 1S2 2P1 4D1         (1)1( 1.0)     12620938.0
   -1    633.698 146.252 141.219 61.9155 60.3980 59.3358 34.3952 33.7317
 23.0    3       2.65+05 5.29+05 1.06+06 1.59+06 2.65+06 5.29+06 7.94+06
   3   1 7.04+07 9.66-03 1.01-02 1.09-02 1.15-02 1.24-02 1.37-02 1.46-02
   5   1 1.62+10 3.34-01 3.42-01 3.58-01 3.72-01 3.95-01 4.36-01 4.63-01
. . .
  82  79 1.27+00 2.11-02 2.55-02 2.88-02 3.02-02 3.14-02 3.24-02 3.27-02
  82  81 9.20-07 1.43-02 1.90-02 2.38-02 2.66-02 3.02-02 3.51-02 3.80-02
  -1
  -1  -1
C--------------------------------------------------------------------------------
C
C              Configuration
C        Eissner            == Standard           R  %   Parentage
C
```

```
C    1   521522            ==  1S2 2S2             97  1 1S  1S/
C    2   521512513         ==  1S2 2S1 2P1        100  1 2S  2S/ 1 2P  3P/
C    3   521512513         ==  1S2 2S1 2P1         97  1 2S  2S/ 1 2P  3P/
C    4   521512513         ==  1S2 2S1 2P1        100  1 2S  2S/ 1 2P  3P/
C    5   521512513         ==  1S2 2S1 2P1         97  1 2S  2S/ 1 2P  1P/
C    6   521523            ==  1S2 2P2             92  1 3P  3P/
. . .
C   77   521513519         ==  1S2 2P1 4D1         58  1 2P  2P/ 1 2D  3D/
C   78   521513519         ==  1S2 2P1 4D1         71  1 2P  2P/ 1 2D  3P/
C   79   521513519         ==  1S2 2P1 4D1         51  1 2P  2P/ 1 2D  3P/
C   80   521513519         ==  1S2 2P1 4D1        100  1 2P  2P/ 1 2D  3P/
C   81   521513519         ==  1S2 2P1 4D1         73  1 2P  2P/ 1 2D  1F/
C   82   521513519         ==  1S2 2P1 4D1         74  1 2P  2P/ 1 2D  1P/
C
C (R) - Levels (or levels within a term) have been reassigned
C       from their principal component.
C
C (excl) - Levels included in structure but no A-value or
C          collision strength calculated.
C
C-------------------------------------------------------------------------------
C
C   Generated from Cowan Atomic Structure Program
C
C   From IFG file : /home/mog/adas/pass/ifg#fe22.dat
C
C   Options in effect
C
C   Coupling    Avalue   numtemps   Lweight   Isonuclear   Comment Level
C   IC          YES      14         NO        NO           2
C
C
C   Cowan code options
C   ------------------
C
C         SCF method used                      :  HR
C
C         Scale factors for Slater Parameters  :  80 90 80 80 80
C
C         Optically allowed transitions        :  Yes
C
C         Optically forbidden transitions (M1) :  Both Parities
C
C         Optically forbidden transitions (E2) :  Both Parities
C
C         Born Collision-Strength  - forbidden :  0 ->  2
C
C         Born Collision-Strength  - allowed   :  1 ->  1
C
C
```

```
C   Parity 1    Parity 2    Allowed
C        550         753       1071     initially
C        550         753       1071     reduced
C
C   Note: The Born method does NOT calculate spin changing transitions
C   correctly. You should supplement for important transitions of this type.
C
C-----------------------------------------------------------------------------
C
C   Code     : ADAS801
C   Producer : Martin O'Mullane
C   Date     : 22/05/13
C
C-----------------------------------------------------------------------------
```

1.2.3 Demo (a-3) demo_a/demo_a_3.sh

```
/home/adas/offline_adas/adas8#1/scripts/run_adas8#1 fe22.dat fe22.inst fe22.pp
```

1.2.4 Demo (a-3) demo_a/fe22.inst

```
z0 26
zi 22
parity-1  8 : 8  1  2  3  4  5  6  7  8
parity-2  7 : 7  1  2  3  4  5  6  7
E2 3
M1 3
scale 80 90 80 80 80
temperature 25
 1.00e+03 1.47e+03 2.15e+03 3.16e+03 4.64e+03 6.81e+03 1.00e+04 1.47e+04
 2.15e+04 3.16e+04 4.64e+04 6.81e+04 1.00e+05 1.47e+05 2.15e+05 3.16e+05
 4.64e+05 6.81e+05 1.00e+06 1.47e+06 2.15e+06 3.16e+06 4.64e+06 6.81e+06
 1.00e+07
```

1.2.5 Demo (a-3) demo_a/fe22.pp

```
1
Martin O'Mullane
14-05-2014
5
C
C  Cowan plane wave Born method
C
C  Scale factors 80 90 80 80 80
C
 &FILES ifgfile = 'ifg#fe22.dat' , outfile = 'fe22_offline.dat' &END
 &OPTIONS  ip =  15730300.0, coupling = 'IC' ,  aval = 'YES' ,  isonuclear =
'NO', quantity = 'RATES', lweight = 'NO' ,  comments = 2,  numtemp = 14 , &END
  1  2  3  5  7  9 11 12 13 14 15 17 19 20
parity-1  8 : 8  1  2  3  4  5  6  7  8
```

```
parity-2  7 : 7  1  2  3  4  5  6  7
```

1.2.6 Demo (a-3) demo_a/fe22_offline.dat

```
FE+22        26        23      15730300.0
    1 1S2 2S2            (1)0( 0.0)            0.0
    2 1S2 2S1 2P1        (3)1( 0.0)       354118.2
    3 1S2 2S1 2P1        (3)1( 1.0)       382472.7
    4 1S2 2S1 2P1        (3)1( 2.0)       467040.0
    5 1S2 2S1 2P1        (1)1( 1.0)       696851.6
    . . .
   81 1S2 2P1 4D1        (1)3( 3.0)     12617526.6
   82 1S2 2P1 4D1        (1)1( 1.0)     12620938.0
   -1    633.698 146.252 141.219 61.9155 60.3980 59.3358 34.3952 33.7317
 23.0    3       5.29+05 7.78+05 1.14+06 2.45+06 5.29+06 1.14+07 2.45+07
   3   1 7.04+07 1.01-02 1.05-02 1.10-02 1.22-02 1.37-02 1.54-02 1.73-02
   5   1 1.62+10 3.42-01 3.50-01 3.60-01 3.91-01 4.36-01 4.90-01 5.52-01

  82  79 1.27+00 2.55-02 2.75-02 2.91-02 3.13-02 3.24-02 3.30-02 3.32-02
  82  81 9.20-07 1.90-02 2.16-02 2.43-02 2.97-02 3.51-02 4.06-02 4.60-02
  -1
  -1  -1
C-------------------------------------------------------------------------------
C
C              Configuration
C        Eissner            == Standard           R  %   Parentage
C
C    1   521522             ==  1S2 2S2             97  1 1S  1S/
C    2   521512513          ==  1S2 2S1 2P1        100  1 2S  2S/ 1 2P  3P/
. . .
C   81   521513519          ==  1S2 2P1 4D1         73  1 2P  2P/ 1 2D  1F/
C   82   521513519          ==  1S2 2P1 4D1         74  1 2P  2P/ 1 2D  1P/
C
C (R) - Levels (or levels within a term) have been reassigned
C       from their principal component.
C
C (excl) - Levels included in structure but no A-value or
C          collision strength calculated.
C
C-------------------------------------------------------------------------------
C
C   Generated from Cowan Atomic Structure Program
C
C   From IFG file : ifg#fe22.dat
C
C   Options in effect
C
C   Coupling    Avalue   numtemps   Lweight   Isonuclear   Comment Level
C   IC          YES      14         NO        NO           2
C
```

```
C
C   Cowan code options
C   ------------------
C
C      Cowan plane wave Born method
C
C      Scale factors 80 90 80 80 80
C
C   Parity 1    Parity 2    Allowed
C        550         753       1071     initially
C        550         753       1071     reduced
C
C   Note: The Born method does NOT calculate spin changing transitions
C   correctly. You should supplement for important transitions of this type.
C
C-------------------------------------------------------------------------------
C
C   Code     : ADAS801
C   Producer : Martin O'Mullane
C   Date     : 14-05-2014
C
C-------------------------------------------------------------------------------
```

2 Demo (b) Introducing the Autostructure code

```
------------------------------
DEMO B: Introducing the Autostructure code
------------------------------
PURPOSE: To calculate excitation cross section in the Distorted Wave (DW)
approximation using the ADAS  offline version adas7#1. The code is a full
implementation of the program AUTOSTRUCTURE, which  has been developed by N.R.
Badnell.

The input file for the AUTOSTRUCTURE run is in the adf27 format. This format is
different from the adf34 which drives the ADAS801 run. It contains a series of
parameters which regulate the type of calculation (RUN=''), coupling scheme
(CUP=''), free electron energy ranges (EMIN='', EMAX=''), the orbital
specification (e.g. 2 0  2 1  3 0  3 1  3 2  4 0  4 1  4 2  4 3) and the
occupation numbers (e.g. 1    0    0    0    1    0    0    0    0  means one
electron in 2s orbital and one electron in 3d orbital). See the ADAS manual for
further parameter specifications.


EXAMPLE: As for Demo a, Be-like Fe (Fe22+) is considered.
The input files in the adf27 format are the following:
- for ls resolution: ls#fe22_adf27.dat;
- for ic resolution: ic#fe22_adf27.dat
The executable is /home/adas/offline_adas/adas7#1/bin/as24.x.
The output are Type 5 adf04 (See Module 1 Demo c) data files in ls and ic
```

```
resolution.
They will be provided with Eissner configuration. In order to convert them from
Eissner to Standard configuration the program
/home/asg/adas_dev/idl/adaslib/proc_adf/trim_cophps_adf04.pro is used.
This program reduces the number of levels (and transitions) of an adf04 file to
those below 105% of the ionisation potential, changes the Eissner configuration
to standard and re-orders the transition list.

COMMENTS: Note that for this demo a restricted number of transitions has been
inlcuded in the cross section calculation. This has been done to constrain the
running time.



DEMO b1: Examine adf27 driver file for Fe22+
1. Open the adf27 files ic#fe22_adf27.dat and ls#fe22_adf27.dat and explore
them. Sample of adf27 files: ic#fe22_adf27.dat, ls#fe22_adf27



DEMO b2: Offline_adas/adas7#1 for Fe22+ distorted wave
1. Type /home/adas/offline_adas/adas7#1/bin/as24.x < ic#fe22_adf27.dat
   for producing a Type 5 adf04 in ic resolution.
   (Note thet this will take a few minutes.)
2. Type /home/adas/offline_adas/adas7#1/bin/as24.x < ls#fe22_adf27.dat
   for producing a Type 5 adf04 in ic resolution.
   (Note thet this will take a few minutes.)
Sample of script: demo_b_2.sh
Output files: adf04ic, adf04ls


DEMO b3: Use trim_cophps_adf04.pro to trim AS adf04 and
         get Standard Configurations
1. Use trim_cophps_adf04.pro to remove the levels above the ionisation
   potential and convert the configuration from Eissner to Standard notation.
Program: demo_b_3.pro
Output file: ic#fe22_as.dat
```

2.1 Demo (b) Figures

2.2 Demo (b) Procedures

2.2.1 Demo (b-1) demo_b/ic#fe22_adf27.dat

```
A.S. Be-like fe22 structure - energies + radiative rates + dw adf04 type 5
 &SALGEB RUN='DE' CUP='ICR' KCOR1=1 KCOR2=1 NMETA=2 MXCONF=9 MXVORB=9  &END
 2 0  2 1  3 0  3 1  3 2  4 0  4 1  4 2  4 3
  2    0    0    0    0    0    0    0    0
  1    1    0    0    0    0    0    0    0
  1    0    1    0    0    0    0    0    0
```

```
  1    0    0    1    0    0    0    0    0
  1    0    0    0    1    0    0    0    0
  1    0    0    0    0    1    0    0    0
  1    0    0    0    0    0    1    0    0
  1    0    0    0    0    0    0    1    0
  1    0    0    0    0    0    0    0    1
 &SMINIM NZION=26 ORTHOG='NO' JPRINT=-33 MAXE=719 MSTEP=12 &END
 &SRADCON MENG=-14 EMIN=0.719 EMAX=719 NDE=8 MENGI=-1  &END
  3.943264 6.866504 9.786447 10.75793 86.6706 89.10385 110.4799 122.3742
```

2.2.2 Demo (b-1) demo_b/ls#fe22_adf27.dat

```
A.S. Be-like fe22 structure - energies + radiative rates + dw adf04 type 5
 &SALGEB RUN='DE' CUP='LSR' KCOR1=1 KCOR2=1 NMETA=2 MXCONF=9 MXVORB=9  &END
 2 0  2 1  3 0  3 1  3 2  4 0  4 1  4 2  4 3
  2    0    0    0    0    0    0    0    0
  1    1    0    0    0    0    0    0    0
  1    0    1    0    0    0    0    0    0
  1    0    0    1    0    0    0    0    0
  1    0    0    0    1    0    0    0    0
  1    0    0    0    0    1    0    0    0
  1    0    0    0    0    0    1    0    0
  1    0    0    0    0    0    0    1    0
  1    0    0    0    0    0    0    0    1
 &SMINIM NZION=26 ORTHOG='NO' JPRINT=-33 MAXE=719 MSTEP=12 &END
 &SRADCON MENG=-14 EMIN=0.719 EMAX=719 NDE=8 MENGI=-1  &END
  3.943264 6.866504 9.786447 10.75793 86.6706 89.10385 110.4799 122.3742
```

2.2.3 Demo (b-2) demo_b/demo_b_2.sh

```
/home/adas/offline_adas/adas7#1/bin/as24.x < ic#fe22_adf27.dat
/home/adas/offline_adas/adas7#1/bin/as24.x < ls#fe22_adf27.dat
```

2.2.4 Demo (b-2) demo_b/adf04ic.dat

```
FE+22        26        23  15732424.0413
    1 522              (1)0( 0.0)              0.0000
    2 512513           (3)1( 0.0)          294125.9172
    3 512513           (3)1( 1.0)          325899.9255
    4 512513           (3)1( 2.0)          415988.7673
    5 512513           (1)1( 1.0)          707772.8090
    6 512514           (3)0( 1.0)         8870629.5839
    7 512514           (1)0( 0.0)         8951832.3306
    8 512515           (3)1( 0.0)         9033381.3395
    9 512515           (3)1( 1.0)         9039155.3069
   10 512515           (3)1( 2.0)         9069060.1402
   11 512515           (1)1( 1.0)         9091505.2370
   12 512516           (3)2( 1.0)         9158129.9078
   13 512516           (3)2( 2.0)         9162034.5349
   14 512516           (3)2( 3.0)         9168854.9245
```

```
   15 512516            (1)2( 2.0)         9234055.2919
   16 512517            (3)0( 1.0)        11914413.9492
   17 512517            (1)0( 0.0)        11938997.7345
   18 512518            (3)1( 0.0)        11978429.8706
   19 512518            (3)1( 1.0)        11980543.3733
   20 512518            (3)1( 2.0)        11993395.2560
   21 512518            (1)1( 1.0)        12000726.8394
   22 512519            (3)2( 1.0)        12030232.6316
   23 512519            (3)2( 2.0)        12031822.9851
   24 512519            (3)2( 3.0)        12034771.8869
   25 512519            (1)2( 2.0)        12053979.2430
   26 51251A            (3)3( 2.0)        12056986.4039
   27 51251A            (3)3( 3.0)        12057710.0117
   28 51251A            (3)3( 4.0)        12059219.6822
   29 51251A            (1)3( 3.0)        12063174.2569
   -1    610.369 141.144 135.886 61.3953 59.9111 58.9282 34.1663 33.5524
23.00    5       7.19-01 1.74+00 3.35+00 5.92+00 1.00+01 1.65+01 2.69+01
   2   1 1.00-30 1.26-03 1.25-03 1.23-03 1.20-03 1.16-03 1.09-03 9.94-04
   3   1 5.05+07 1.50-02 1.51-02 1.53-02 1.67-02 1.54-02 1.46-02 1.53-02
   4   1 1.00-30 6.27-03 6.21-03 6.12-03 5.98-03 5.76-03 5.43-03 4.95-03
   5   1 2.18+10 4.15-01 4.18-01 4.23-01 4.30-01 4.44-01 4.98-01 4.46-01
   6   1 1.00-30 1.25-03 1.23-03 1.20-03 1.16-03 1.09-03 1.00-03 8.76-04
   7   1 1.00-30 1.23-02 1.24-02 1.24-02 1.25-02 1.27-02 1.29-02 1.32-02
   8   1 1.00-30 2.92-04 2.87-04 2.82-04 2.73-04 2.61-04 2.42-04 2.15-04
   9   1 1.48+12 1.62-03 1.63-03 1.64-03 1.65-03 1.68-03 1.73-03 1.81-03
  10   1 1.00-30 1.45-03 1.43-03 1.40-03 1.36-03 1.30-03 1.21-03 1.07-03
  11   1 1.14+13 6.41-03 6.55-03 6.73-03 7.01-03 7.46-03 8.18-03 9.34-03
  12   1 1.00-30 1.81-03 1.78-03 1.75-03 1.69-03 1.60-03 1.47-03 1.29-03
  13   1 1.12+08 3.09-03 3.05-03 2.99-03 2.89-03 2.75-03 2.55-03 2.26-03
  14   1 1.00-30 4.22-03 4.16-03 4.07-03 3.93-03 3.73-03 3.43-03 3.02-03
  15   1 2.17+10 1.75-02 1.77-02 1.80-02 1.84-02 1.91-02 2.02-02 2.16-02
  16   1 1.00-30 4.23-04 4.16-04 4.07-04 3.92-04 3.70-04 3.39-04 2.96-04
  17   1 1.00-30 2.32-03 2.33-03 2.34-03 2.36-03 2.39-03 2.44-03 2.50-03
  18   1 1.00-30 1.09-04 1.08-04 1.06-04 1.03-04 9.80-05 9.11-05 8.08-05
  19   1 7.65+11 5.09-04 5.10-04 5.11-04 5.12-04 5.16-04 5.22-04 5.36-04
  20   1 1.00-30 5.46-04 5.39-04 5.29-04 5.13-04 4.90-04 4.55-04 4.04-04
  21   1 4.63+12 1.42-03 1.44-03 1.47-03 1.53-03 1.62-03 1.77-03 2.00-03
  22   1 1.00-30 5.18-04 5.12-04 5.02-04 4.86-04 4.63-04 4.29-04 3.81-04
  23   1 2.93+07 8.83-04 8.72-04 8.56-04 8.31-04 7.94-04 7.39-04 6.62-04
  24   1 1.00-30 1.21-03 1.19-03 1.17-03 1.13-03 1.08-03 1.00-03 8.89-04
  25   1 2.87+09 2.72-03 2.74-03 2.78-03 2.84-03 2.94-03 3.09-03 3.27-03
  26   1 1.00-30 4.38-04 4.30-04 4.19-04 4.01-04 3.75-04 3.38-04 2.88-04
  27   1 1.10+06 6.28-04 6.19-04 6.04-04 5.82-04 5.49-04 5.04-04 4.40-04
  28   1 1.00-30 7.88-04 7.75-04 7.54-04 7.22-04 6.75-04 6.09-04 5.19-04
  29   1 2.47+07 9.57-04 9.69-04 9.89-04 1.02-03 1.07-03 1.15-03 1.23-03
  -1
  -1  -1
```

2.2.5 Demo (b-2) demo_b/adf04ls.dat

```
FE+22        26        23  15732424.0413
    1 522               (1)0( 0.0)              0.0000
    2 512513            (3)1( 4.0)           375367.8485
    3 512513            (1)1( 1.0)           698925.8983
    4 512514            (3)0( 1.0)          8870629.5839
    5 512514            (1)0( 0.0)          8951832.3306
    6 512515            (3)1( 4.0)          9057167.1848
    7 512515            (1)1( 1.0)          9085386.2500
    8 512516            (3)2( 7.0)          9164564.9183
    9 512516            (1)2( 2.0)          9233669.9138
   10 512517            (3)0( 1.0)         11914413.9492
   11 512517            (1)0( 0.0)         11938997.7345
   12 512518            (3)1( 4.0)         11988406.7848
   13 512518            (1)1( 1.0)         11997851.8701
   14 512519            (3)2( 7.0)         12032956.1843
   15 512519            (1)2( 2.0)         12053753.8930
   16 51251A            (3)3(10.0)         12058262.5629
   17 51251A            (1)3( 3.0)         12062940.7455
   -1    610.369 141.144 135.886 61.3953 59.9111 58.9282 34.1663 33.5524
23.00    5       7.19-01 1.74+00 3.35+00 5.92+00 1.00+01 1.65+01 2.69+01
   2   1 1.00-30 1.13-02 1.12-02 1.10-02 1.08-02 1.04-02 9.78-03 8.92-03
   3   1 2.15+10 4.26-01 4.29-01 4.34-01 4.41-01 4.56-01 5.10-01 4.56-01
   3   2 1.00-30 3.37-02 3.33-02 3.26-02 3.15-02 2.99-02 2.76-02 2.44-02
   4   1 1.00-30 1.25-03 1.23-03 1.20-03 1.16-03 1.09-03 1.00-03 8.76-04
   4   2 2.28+12 3.83-03 3.82-03 3.81-03 3.80-03 3.81-03 3.81-03 3.85-03
   5   1 1.00-30 1.23-02 1.23-02 1.24-02 1.25-02 1.27-02 1.29-02 1.32-02
   5   2 1.00-30 1.03-03 1.02-03 1.00-03 9.74-04 9.35-04 8.77-04 7.94-04
   6   1 1.00-30 2.62-03 2.58-03 2.53-03 2.45-03 2.34-03 2.17-03 1.93-03
   6   2 4.21+09 8.07-02 8.07-02 8.07-02 8.05-02 8.03-02 8.03-02 8.01-02
   7   1 1.29+13 7.16-03 7.32-03 7.52-03 7.84-03 8.36-03 9.18-03 1.05-02
   7   2 1.00-30 7.42-03 7.32-03 7.17-03 6.92-03 6.56-03 6.05-03 5.34-03
   8   1 1.00-30 9.04-03 8.92-03 8.73-03 8.43-03 7.99-03 7.35-03 6.47-03
   8   2 2.04+13 2.37-01 2.38-01 2.40-01 2.42-01 2.47-01 2.55-01 2.68-01
   9   1 2.18+10 1.76-02 1.78-02 1.81-02 1.85-02 1.92-02 2.03-02 2.17-02
   9   2 1.00-30 1.82-02 1.79-02 1.74-02 1.68-02 1.58-02 1.44-02 1.24-02
  10   1 1.00-30 4.23-04 4.16-04 4.07-04 3.92-04 3.70-04 3.39-04 2.96-04
  10   2 7.08+11 1.16-03 1.15-03 1.14-03 1.13-03 1.11-03 1.08-03 1.05-03
  11   1 1.00-30 2.32-03 2.33-03 2.34-03 2.36-03 2.39-03 2.44-03 2.50-03
  11   2 1.00-30 3.91-04 3.87-04 3.80-04 3.71-04 3.56-04 3.34-04 3.03-04
  12   1 1.00-30 9.83-04 9.71-04 9.52-04 9.24-04 8.82-04 8.19-04 7.27-04
  12   2 1.19+09 1.78-02 1.77-02 1.76-02 1.75-02 1.74-02 1.72-02 1.69-02
  13   1 5.39+12 1.60-03 1.62-03 1.67-03 1.73-03 1.84-03 2.02-03 2.29-03
  13   2 1.00-30 2.67-03 2.63-03 2.58-03 2.49-03 2.36-03 2.18-03 1.93-03
  14   1 1.00-30 2.59-03 2.56-03 2.51-03 2.43-03 2.31-03 2.15-03 1.91-03
  14   2 6.34+12 4.71-02 4.72-02 4.73-02 4.76-02 4.79-02 4.87-02 4.99-02
  15   1 2.90+09 2.74-03 2.76-03 2.80-03 2.86-03 2.96-03 3.11-03 3.30-03
  15   2 1.00-30 6.50-03 6.40-03 6.25-03 6.02-03 5.67-03 5.18-03 4.51-03
  16   1 1.00-30 1.84-03 1.81-03 1.76-03 1.68-03 1.57-03 1.42-03 1.21-03
```

```
  16   2 1.02+10 9.84-03 9.80-03 9.73-03 9.63-03 9.51-03 9.40-03 9.34-03
  17   1 2.58+07 9.72-04 9.86-04 1.01-03 1.04-03 1.09-03 1.18-03 1.27-03
  17   2 1.00-30 2.54-03 2.49-03 2.42-03 2.30-03 2.14-03 1.90-03 1.60-03
  -1
  -1  -1
```

2.2.6 Demo (b-3) demo_b/demo_b3.pro

```
pro demo_b_3

trim_cophps_adf04, infile='adf04ic', outfile='ic#fe22_as.dat'

end
```

2.2.7 Demo (b-3) demo_b/ic#fe22_as.dat

```
FE+22        26        23 15732424.0(1s)
    1 1S2 2S2           (1)0( 0.0)            0.0000   {X}
    2 1S2 2S1 2P1       (3)1( 0.0)       294125.9172   {X}
    3 1S2 2S1 2P1       (3)1( 1.0)       325899.9255   {X}
    4 1S2 2S1 2P1       (3)1( 2.0)       415988.7673   {X}
    5 1S2 2S1 2P1       (1)1( 1.0)       707772.8090   {X}
    6 1S2 2S1 3S1       (3)0( 1.0)      8870629.5839   {X}
    7 1S2 2S1 3S1       (1)0( 0.0)      8951832.3306   {X}
    8 1S2 2S1 3P1       (3)1( 0.0)      9033381.3395   {X}
    9 1S2 2S1 3P1       (3)1( 1.0)      9039155.3069   {X}
   10 1S2 2S1 3P1       (3)1( 2.0)      9069060.1402   {X}
   11 1S2 2S1 3P1       (1)1( 1.0)      9091505.2370   {X}
   12 1S2 2S1 3D1       (3)2( 1.0)      9158129.9078   {X}
   13 1S2 2S1 3D1       (3)2( 2.0)      9162034.5349   {X}
   14 1S2 2S1 3D1       (3)2( 3.0)      9168854.9245   {X}
   15 1S2 2S1 3D1       (1)2( 2.0)      9234055.2919   {X}
   16 1S2 2S1 4S1       (3)0( 1.0)     11914413.9492   {X}
   17 1S2 2S1 4S1       (1)0( 0.0)     11938997.7345   {X}
   18 1S2 2S1 4P1       (3)1( 0.0)     11978429.8706   {X}
   19 1S2 2S1 4P1       (3)1( 1.0)     11980543.3733   {X}
   20 1S2 2S1 4P1       (3)1( 2.0)     11993395.2560   {X}
   21 1S2 2S1 4P1       (1)1( 1.0)     12000726.8394   {X}
   22 1S2 2S1 4D1       (3)2( 1.0)     12030232.6316   {X}
   23 1S2 2S1 4D1       (3)2( 2.0)     12031822.9851   {X}
   24 1S2 2S1 4D1       (3)2( 3.0)     12034771.8869   {X}
   25 1S2 2S1 4D1       (1)2( 2.0)     12053979.2430   {X}
   26 1S2 2S1 4F1       (3)3( 2.0)     12056986.4039   {X}
   27 1S2 2S1 4F1       (3)3( 3.0)     12057710.0117   {X}
   28 1S2 2S1 4F1       (3)3( 4.0)     12059219.6822   {X}
   29 1S2 2S1 4F1       (1)3( 3.0)     12063174.2569   {X}
   -1
 23.0    3       7.19-01 1.74+00 3.35+00 5.92+00 1.00+01 1.65+01 2.69+01
   2   1 1.00-30 1.26-03 1.25-03 1.23-03 1.20-03 1.16-03 1.09-03 9.94-04
   3   1 5.05+07 1.50-02 1.51-02 1.53-02 1.67-02 1.54-02 1.46-02 1.53-02
```

```
 4   1 1.00-30 6.27-03 6.21-03 6.12-03 5.98-03 5.76-03 5.43-03 4.95-03
 5   1 2.18+10 4.15-01 4.18-01 4.23-01 4.30-01 4.44-01 4.98-01 4.46-01
 6   1 1.00-30 1.25-03 1.23-03 1.20-03 1.16-03 1.09-03 1.00-03 8.76-04
 7   1 1.00-30 1.23-02 1.24-02 1.24-02 1.25-02 1.27-02 1.29-02 1.32-02
 8   1 1.00-30 2.92-04 2.87-04 2.82-04 2.73-04 2.61-04 2.42-04 2.15-04
 9   1 1.48+12 1.62-03 1.63-03 1.64-03 1.65-03 1.68-03 1.73-03 1.81-03
10   1 1.00-30 1.45-03 1.43-03 1.40-03 1.36-03 1.30-03 1.21-03 1.07-03
11   1 1.14+13 6.41-03 6.55-03 6.73-03 7.01-03 7.46-03 8.18-03 9.34-03
12   1 1.00-30 1.81-03 1.78-03 1.75-03 1.69-03 1.60-03 1.47-03 1.29-03
13   1 1.12+08 3.09-03 3.05-03 2.99-03 2.89-03 2.75-03 2.55-03 2.26-03
14   1 1.00-30 4.22-03 4.16-03 4.07-03 3.93-03 3.73-03 3.43-03 3.02-03
15   1 2.17+10 1.75-02 1.77-02 1.80-02 1.84-02 1.91-02 2.02-02 2.16-02
16   1 1.00-30 4.23-04 4.16-04 4.07-04 3.92-04 3.70-04 3.39-04 2.96-04
17   1 1.00-30 2.32-03 2.33-03 2.34-03 2.36-03 2.39-03 2.44-03 2.50-03
18   1 1.00-30 1.09-04 1.08-04 1.06-04 1.03-04 9.80-05 9.11-05 8.08-05
19   1 7.65+11 5.09-04 5.10-04 5.11-04 5.12-04 5.16-04 5.22-04 5.36-04
20   1 1.00-30 5.46-04 5.39-04 5.29-04 5.13-04 4.90-04 4.55-04 4.04-04
21   1 4.63+12 1.42-03 1.44-03 1.47-03 1.53-03 1.62-03 1.77-03 2.00-03
22   1 1.00-30 5.18-04 5.12-04 5.02-04 4.86-04 4.63-04 4.29-04 3.81-04
23   1 2.93+07 8.83-04 8.72-04 8.56-04 8.31-04 7.94-04 7.39-04 6.62-04
24   1 1.00-30 1.21-03 1.19-03 1.17-03 1.13-03 1.08-03 1.00-03 8.89-04
25   1 2.87+09 2.72-03 2.74-03 2.78-03 2.84-03 2.94-03 3.09-03 3.27-03
26   1 1.00-30 4.38-04 4.30-04 4.19-04 4.01-04 3.75-04 3.38-04 2.88-04
27   1 1.10+06 6.28-04 6.19-04 6.04-04 5.82-04 5.49-04 5.04-04 4.40-04
28   1 1.00-30 7.88-04 7.75-04 7.54-04 7.22-04 6.75-04 6.09-04 5.19-04
29   1 2.47+07 9.57-04 9.69-04 9.89-04 1.02-03 1.07-03 1.15-03 1.23-03
-1
-1  -1
```

3 Demo (c) Compare the resulting adf04 files

```
------------------------------
DEMO C: Compare the resulting adf04 files
------------------------------
PURPOSE: To compare different adf04 data files using ADAS811 interactively.

EXAMPLE: For this demo adf04 files generated using R-Matrix (from central ADAS),
Distorted Wave (DW), produced by AUTOSTRUCTURE (ADAS7#1 - Demo B), and Plane
Wave Born (PWB),produced  by Cowan (ADAS801 - Demo A)) are compared.
The program used is ADAS811.


COMMENTS: Note that the adf04 data files which have to be compared, must have
same configuration strings. For this demo, the three adf04 file used have been
edited in order to have the same configuration strings:
- R-Matrix: copied locally from central ADAS and edited (belike_nrb05#fe22.dat)
  Example:
  SOURCE          EDITED
  2s2             1s2 2s2
  2s1 2p1         1s2 2s1 2p1
 ..............................

- DW: copied locatty from Module 7 Demo B and edited (ic#fe22_as.dat)
  Example:
  SOURCE          EDITED
  522             1s2 2s2
  512513          1s2 2s1 2p1
 ..............................

- Cowan: taken from Module 7 Demo A, not edited.



DEMO c1: Examine common transitions between above datasets
         with interactive ADAS811

1.  Edit the adf04 files to be compared in order to have same
    configuration strings.
2.  Use ADAS811 interactively to compare the collision strengths
    for different transitions.
Input files: belike_nrb05#fe22.dat, ic#fe22_as.dat, ../demo_a/ic#fe22.dat
Sample of output files: adas811_plot_example1.ps, adas811_plot_example2.ps
```

3.1 Demo (c) Figures

3.1.1 Demo (c-1) demo_c/adas811_plot_example1.pdf

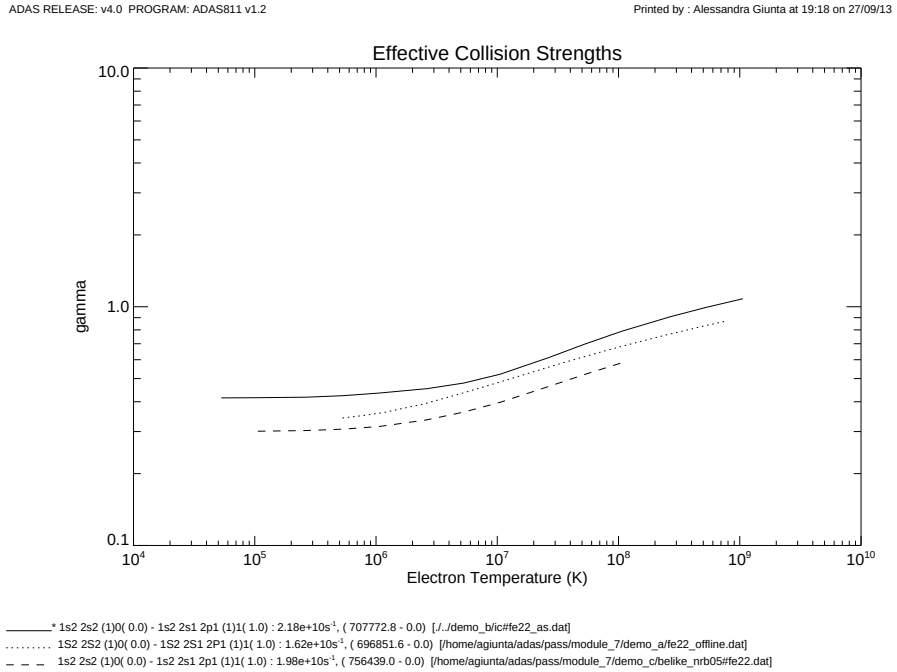

Figure 1:

3.1.2 Demo (c-1) demo_c/adas811_plot_example2.pdf

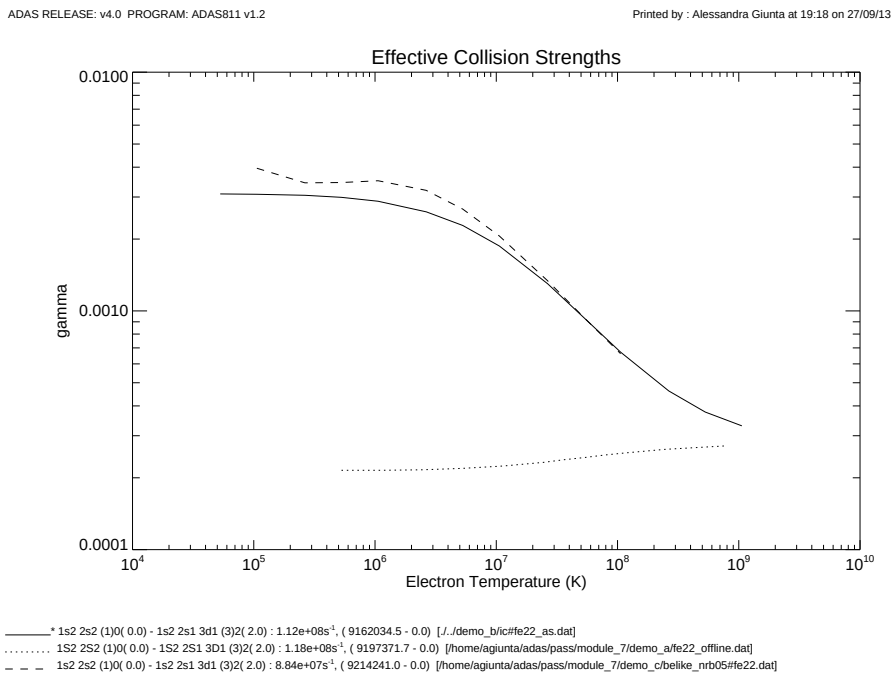

Figure 2:

3.2 Demo (c) Procedures

3.2.1 Demo (c-1) demo_c/belike_nrb05#fe22.dat

```
Fe+22        26        23      15730000.0
    1 1s2 2s2            (1)0( 0.0)              0.
    2 1s2 2s1 2p1        (3)1( 0.0)          345707.
    3 1s2 2s1 2p1        (3)1( 1.0)          377694.
    4 1s2 2s1 2p1        (3)1( 2.0)          469122.
    5 1s2 2s1 2p1        (1)1( 1.0)          756439.
. . .
   96 1s2 2p1 4f1        (3)2( 1.0)        12638336.
   97 1s2 2p1 4d1        (1)1( 1.0)        12641921.
   98 1s2 2p1 4f1        (1)2( 2.0)        12642691.
   -1
23.00    3       1.06+05 2.64+05 5.29+05 1.06+06 2.64+06 5.29+06 1.06+07
   2   1 0.00+00 4.75-03 3.77-03 3.05-03 2.61-03 2.66-03 2.57-03 2.11-03
   3   1 4.72+07 2.35-02 1.96-02 1.70-02 1.54-02 1.57-02 1.61-02 1.58-02
. . .

  97  96 8.34+01 3.06-02 3.19-02 3.35-02 3.55-02 3.85-02 4.10-02 4.37-02
  98  96 8.68-01 7.00-02 6.82-02 6.55-02 6.15-02 5.45-02 4.87-02 4.34-02
  98  97 1.32+02 6.55+00 7.44+00 8.45+00 9.63+00 1.13+01 1.24+01 1.36+01
  -1
  -1  -1
C-----------------------------------------------------------------------------
C
C
C Details of the calculations are in
C
C Chidichimo,M. C., Del Zanna, G., Mason, H.E.,
C Badnell,N. R., Tully, J.A., Berrington, K.A., 2005,
C Atomic Data from the IRON Project LVI. Electron excitation of Be-like Fe
C      XXIII, A\&A, 430, 331
C
C Complete OMEGA file from GDZ processed thru adasexj by NRB.
C
C A-values calculated with AUTOSTRUCTURE including all n=4 levels
C (RAD='ALL' CUP='ICM'  KUTSO=-17 KCUT=0).
C All A-values of the Ek and M1 transitions have been summed up and
C combined with M2, see next.
C
C M2 data have been calculated with SUPERSTRUCTURE for lower levels 1 thr 10
C and upper levels 2 thru 45 by GDZ.
C NAME: N R Badnell
C DATE: 05/05/05
C
C UPDATES
C
C Allan Whiteford, 09/05/05
```

```
C
C Fixed formatting
C Added element symbol
C
C Nigel Badnell and Allan Whiteford, 10/05/05
C
C Supplemented with more complete M2 data, also note that the previous M2
C data were incorrectly indexed.
C
C The M2 A-values are obtained from a 45-configuration SUPERSTRUCTURE run
C with term energy corrections and observed energies (whenever available),
C see Del Zanna, Chidichimo and Mason 2005 A&A 432, 1137 - produced by GDZ
C
C-----------------------------------------------------------------------
```

4 Demo (d) R-Matrix

```
------------------------------
DEMO D: R-Matrix
------------------------------
PURPOSE: To examine the driver files and instructions for an R-Matrix run.

EXAMPLE: The offline program dedicated to R-Matrix within ADAS is ADAS8#3.
For this demo the set of scripts and input files needed for an R-Matrix run
is shown.



DEMO d1: Examine driver file and computer configuration
         instructions to calulate R-Matrix cross sections
         for Fe22+.
Samples of scripts and input files: adas803.pl, Makefile, currentsite,
                                    parallel_procfile, input.dat
```

4.1 Demo (d) Figures

4.2 Demo (d) Procedures

4.2.1 Demo (d-1) demo_d/adas803.pl

```
#! /usr/bin/perl
   use List::Util qw[min max];
#-----------------------------------------------------------------------
#
# adas8#3    :  ADAS8#3 - Automated R-matrix calculations
#
# AUTHOR     :  Allan Whiteford, Mike Witthoeft, Stuart Loch and Connor Ballance
# DATE       :  26-09-2005
#
# MODIFIED:
#
#       1.1     Allan Whiteford
# 26-09-2005
#               First Release
#       1.2     Allan Whiteford
#               Fixed bug where the month was wrong by one.
#       1.3     Allan Whiteford
#               Allowed --outer=N for spefification of chunk.
# Only re-run structure if necessary.
#       1.4     Allan Whiteford
#               Fixed bug in maximum allowed occupation
# Added --example output
#       1.5     Allan Whiteford
#               Added --root option
# Made --archive option more sensible
#
#       2011 :
#
#       1.6     Mike Witthoeft, Stuart Loch and Connor Ballance
#               Added --dip option for calculation D- and B- matrices
#                for the general case
#               Added OMEGA filtering for numerical failures
#               Replaced omgmerge with arrange
#
#      2012
#
#       1.7     Connor Ballance and Stuart Loch
#               Now an 'accelerated' parallel approach in which
#               every partial wave and diagonalisation is carried
#               out concurrently.
#
#               Added utility codes : hfilter,dfilter (no input required)
#
#
# VERSION:
```

```
#       1.1    26-09-2005
#       1.2    22-01-2007
# 1.3    09-07-2007
# 1.4    11-08-2008
# 1.5    20-08-2008
#       1.6    19-09-2011
#-----------------------------------------------------------------------

sub auto_maxc
{
mkdir ("maxc", 0755);
chdir ("maxc");
symlink("../str/radout","radial");

# return;
. . .
if ($actionadf)
{
make_adf_file();
}

if ($actionarc)
{
        archive_output();
}
```

4.2.2 Demo (d-1) demo_d/Makefile

```
###############################################################################
#
#                                ADAS8#3 Makefile
#                                ----------------
#
# This makefile:
# * Compiles necessary R-matrix codes
# * Produces "proc" file for adas8#3 script
# * Downloads codes from the web
#
# Necessary modifications:
# * Define where your binary files should go
# * Specify if you want parallel of just serial
#   binaries.
# * Include (or write) an appropriate .def file.
# * Define a wget username/password (in def file)
#
# Usage:
# * "make" will build all codes
#
```

```
#                       * "make directories"
#                       * "make update_serial"
#                       * "make update_utility"
#                       * "make update_parallel"
#                       * "make clean"
#
# Updates:
# V1.0 Allan Whiteford, 26/09/05
#      First Release
#
#                       V1.1 MCW, SDL, CPB     1/6/10
#
#                       V1.2    Martin O'Mullane, Mike Witthoeft,
#                               Stuart Loch, Connor Ballance   (14/10/11)
#                             - Introduce REPOScode and REPOSparam
#                               which can be set to CB or NRB repositories
#                               for finer control over retrieving the code
#                               and parameter files.
#                             - radiation damping for the general case
#
##############################################################################


# Codes to make by default, options are any combination of
# serial, parallel and utility. This can be overridden at the
# command line by, e.g., "make parallel"

CODETYPE = serial utility parallel

# Include here machine dependent definitions and choose which repository
# from which to draw the code and dimensions.

include currentsite


BIN = $(BASE)/bin


# Where you want the automatically generated procfiles to go.
# Note that the main adas8#3 script expects the procfile to be
# in ~/.adas8#3proc unless you specify otherwise with --proc=
# you can specify /dev/null if you don't want a procfile

SPROCFILE = $(BIN)/serial_procfile
PPROCFILE = $(BIN)/parallel_procfile
. . .
$(p_stgfdamp): $(p_stgfdamp_src) $(p_stgfdamp_header)
@$(ECHO) 'Compiling outer region stage Fdamp...'
@$(CP) $(p_stgfdamp_header) $(p_stgfdamp_param)
@$(PFF) $(PFFLAGS) $(p_stgfdamp_src) -o $(p_stgfdamp) $(PLFLAGS)
```

```
@$(RM) $(p_stgfdamp_param) *.mod

$(p_stgicfdamp): $(p_stgicfdamp_src) $(p_stgicfdamp_header)
@$(ECHO) 'Compiling outer region stage ICFdamp...'
@$(CP) $(p_stgicfdamp_header) $(p_stgicfdamp_param)
@$(PFF) $(PFFLAGS) $(p_stgicfdamp_src) -o $(p_stgicfdamp) $(PLFLAGS)
@$(RM) $(p_stgicfdamp_param) *.mod
```

4.2.3 Demo (d-1) demo_d/parallel_procfile

```
GENERAL
chunk_size = 1000
internal_split = 10
adf00_path = /home/adas/adas/adf00
matrix_type = K

EXECUTABLE INFORMATION
auto            1 /home/mog/rmx_test/bin/autos.x
stg1_ex         4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstg1r.x
stg2_ex         4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstg2r.x
stg3_ex        50   /usr/lib64/openmpi/bin/mpirun -np 50 /home/mog/rmx_test/bin/pstg3r.x
stg1_dip        4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstg1r.x
stg2_dip       12  /usr/lib64/openmpi/bin/mpirun -np 12 /home/mog/rmx_test/bin/pstg2r_dip.
stg3_dip        4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstg3r_dip.x
stgd_dip        4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstgd_dip.x
stg1_tcc        1 /home/mog/rmx_test/bin/stg1r.x
stg2_tcc        1 /home/mog/rmx_test/bin/stg2r.x
stgjk_tcc       1 /home/mog/rmx_test/bin/stgjk.x
stgf_ex         4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstgf.x
stgicf_ex       4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstgicf.x
stgfdamp_ex     4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstgfdamp.x
stgicfdamp_ex   4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstgicfdamp.
stgb            1 /home/mog/rmx_test/bin/stgb.x
stg1_nx         1 /home/mog/rmx_test/bin/stg1r.x
stg2_nx         4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstg2r.x
stg3_nx         4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstg3r.x
stgf_nx         4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstgf.x
stgicf_nx       4  /usr/lib64/openmpi/bin/mpirun -np 4 /home/mog/rmx_test/bin/pstgicf.x
omadd           1 /home/mog/rmx_test/bin/omadd.x
om2omu          1 /home/mog/rmx_test/bin/om2omu.x
omr2omc         1 /home/mog/rmx_test/bin/omr2omc.x
adasexj         1 /home/mog/rmx_test/bin/adasexj.x
arrange         1 /home/mog/rmx_test/bin/arrange.x
dfilter         1 /home/mog/rmx_test/bin/dfilter.x
```

4.2.4 Demo (d-1) demo_d/input.dat

```
GENERAL
2Jmax_ex = 21
2Jmax_nx = 55
```

```
maxc = 42
mesh_fine = 0.0000015
mesh_coarse = 0.001
maxe/ionpot = 3
rdamp = 1
adamp = 0
accel = 0

CONFIGURATION LIST
1s1
2s1
2p1
3s1
3p1
3d1
4s1
4p1
4d1
4f1
5s1
5p1
5d1
5f1
5g1


SCALING PARAMETERS
1s = 1.0
2s = 1.0
2p = 1.0
3s = 1.0
3p = 1.0
3d = 1.0
4s = 1.0
4p = 1.0
4d = 1.0
4f = 1.0
```