Error sensitivity studies involving MonteCarlo R-matrix runs

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1. How do we implement this ? (easy question)

2. How do we vary the parameter space (A-values,effective collision strengths etc) within physically meaningful limits?

adas803.pl (continued)

- Following on from Mike Witthoeft's talk. This work is characterized as a 'sensitvity' study within chosen method, in this case R-matrix.

- Yesterday, we showed that the perl scripted R-matrix calculations were feasible along iso-electronic sequences, so yesterday during the adas steering commitee meeting, I calculated n=3 helium-like cases from Z=22 to 27..

```
File  Edit  View  Terminal  Help
connorb@zebedee:~/icftscript/adas$ ls -al 2*adf04
-rw-r--r-- 1 connorb connorb 18851 2011-10-06 17:22 2202.adf04
-rw-r--r-- 1 connorb connorb 18851 2011-10-06 17:35 2302.adf04
-rw-r--r-- 1 connorb connorb 18851 2011-10-06 17:48 2402.adf04
-rw-r--r-- 1 connorb connorb 18851 2011-10-06 18:01 2502.adf04
-rw-r--r-- 1 connorb connorb 18851 2011-10-06 18:15 2602.adf04
-rw-r--r-- 1 connorb connorb 18851 2011-10-06 18:28 2702.adf04
connorb@zebedee:~/icftscript/adas$
```

So even on a laptop , small sequences are possible with over 60,000 pts in each calculation

```
    27        2
    17    63753       136
     0        1         0         3         0        -1         0        -3         0      ....
```

adas803.pl (continued)

As Mike Witthoeft has highlighted in previous work, sequence calculations allow us to identify emerging trends, investigate anomalies of a particluar ion stage, and largely remove user error in the input decks.

For example 1s^2(J=0)-1s2p(J=1) strongest dipole transition from the groundstate

Though each ion stage is using a slightly different temperature grid for the Maxwellian (defined as the adas default)

```
connorb@zebedee:~/icftscript/adas$ grep   ' 7   1 '  2*02.adf04
2202.adf04:   7   1 2.44+14 2.98-03 2.99-03 3.02-03 3.12-03 3.37-03 3.63-03 4.02-03 5.05-03 6.43-03 8.32-03 1.16-02 1.49-02 1.88-02-8.54-03
2302.adf04:   7   1 2.91+14 2.72-03 2.73-03 2.76-03 2.85-03 3.07-03 3.30-03 3.66-03 4.62-03 5.99-03 8.12-03 1.20-02 1.55-02 1.94-02-7.73-03
2402.adf04:   7   1 3.43+14 2.49-03 2.50-03 2.52-03 2.61-03 2.81-03 3.02-03 3.34-03 4.21-03 5.46-03 7.39-03 1.09-02 1.40-02 1.76-02-7.01-03
2502.adf04:   7   1 4.01+14 2.28-03 2.29-03 2.31-03 2.39-03 2.58-03 2.77-03 3.06-03 3.85-03 4.98-03 6.72-03 9.88-03 1.28-02 1.60-02-6.37-03
2602.adf04:   7   1 4.66+14 2.10-03 2.11-03 2.13-03 2.20-03 2.37-03 2.55-03 2.81-03 3.53-03 4.56-03 6.15-03 9.04-03 1.17-02 1.46-02-5.80-03
2702.adf04:   7   1 5.37+14 1.93-03 1.94-03 1.96-03 2.03-03 2.18-03 2.34-03 2.58-03 3.24-03 4.18-03 5.62-03 8.24-03 1.06-02 1.33-02-5.30-03
```

A-values

Effective Collision Strengths

Bethe limits

•So, we intend to use the icftscript (adas803.pl) to carry out the 1000's of calculations required to build up meaningful statistics on the variation of R-matrix calculations.

- In answer to Randall's question posed yesterday : Can the script be used to run an isolated aspect of the calculation ?

(Yes .... and we rely on that fact for quick turnaround)

```
File  Edit  View  Terminal  Help
          ADAS8#3 - Automated R-matrix calculations
          ----------------------------------------
Usage: ./adas803.pl [options] input.dat [Z]

 input.dat     - ADF41 file to control calculation.
 Z             - Nuclear charge (or element symbol) for calculation.

                 Valid Options
                 +++++++++++++
 --help        - display this message
 --example     - print out example input file
 --report      - analyse directories for calculation progress
 --dir         - create directory structure
 --clean       - remove large (unnecssary) passing files
 --veryclean   - leave only inputs, collision strenths and adf04
 --delete      - delete all subdirectories
 --archive     - copy files to parent directory
 --inp         - generate input files (implies dir)
 --inner       - do only inner region (exchange)
 --tcc         - create TCCDW.DAT file
 --dip         - do only inner region (dipole, if damped)
 --stgbinp     - make input file for STGB (if inner finished)
 --stgb        - run STGB
 --outer       - do only outer region (exchange)
 --noninn      - do inner region non-exchange calculation
 --nonout      - do outer region non-exchange calculation
 --born        - calculate born limits and non-dipole A-values
 --merge       - merge collision strengths
 --adf04       - generate adf04 file
 --run         - run whole calculation (from inner to adf04)
 --all         - [default] '--inp' then '--run'
 --proc=file   - alternative excecutables file, defaults to ~/.adas803proc
 --root=path   - top level directory to run in, defaults to current
connorb@zebedee:~/icftscript$
```

Scripting adas803.pl

(below is an expression of our intent, rather than any final implementation)

In many cases the variation of the atomic structure, affects many aspects of collisional radiative modelling … A-values, energy levels, resonance positions , high energy behavio(u)r of collision strengths etc. => key parameter.

File Edit Search Preferences Shell Macro Windows Help

tmaster.uni | master.1311.uni

```
while ($I1_geom <= $N_last_geometry)
#
cat > input.dat << EOF
GENERAL
2Jmax_ex = 23
2Jmax_nx = 91
maxc = 55
mesh_fine = 0.0000025
mesh_coarse = 0.01
maxe/ionpot = 4
rdamp = 0
adamp = 0

CONFIGURATION LIST
1s2
1s1 2s1
1s1 2p1
1s1 3s1
1s1 3p1
1s1 3d1

SCALING PARAMETERS
1s = 1.0
2s = $M_position[$I1_geom]
2p = $N_position[$I1_geom]
3s = 1.0
3p = 1.0
3d = 1.0
EOF
./adas803.tester.pl --inp input.dat $O_position[$I1_geom]
./adas803.tester.pl --inner input.dat $O_position[$I1_geom]   &
./adas803.tester.pl --born input.dat $O_position[$I1_geom]    &
./adas803.tester.pl --tcc input.dat $O_position[$I1_geom]     &
./adas803.tester.pl --noninn input.dat $O_position[$I1_geom]
./adas803.tester.pl --outer input.dat $O_position[$I1_geom]
./adas803.tester.pl --nonout input.dat $O_position[$I1_geom]
./adas803.tester.pl --merge input.dat $O_position[$I1_geom]
./adas803.tester.pl --adf04 input.dat $O_position[$I1_geom]
#
mv /home/connorb/icftscript/adas/adf04 /home/connorb/icftscript/adas/$O_position[$I1_geom]02.adf04
@ I1_geom = $I1_geom + 1
```

Modified input : variation of the 2s & 2p

Notice : non-interacting parts of the calculations are running concurrently

1. Low angular mom. exchnage
2. High angular mom. Non-exchange
3. Infinite limit points

And now the more difficult question:

2. How do you vary the parameter space (A-values,effective collision strengths etc) within physically meaningful limits?

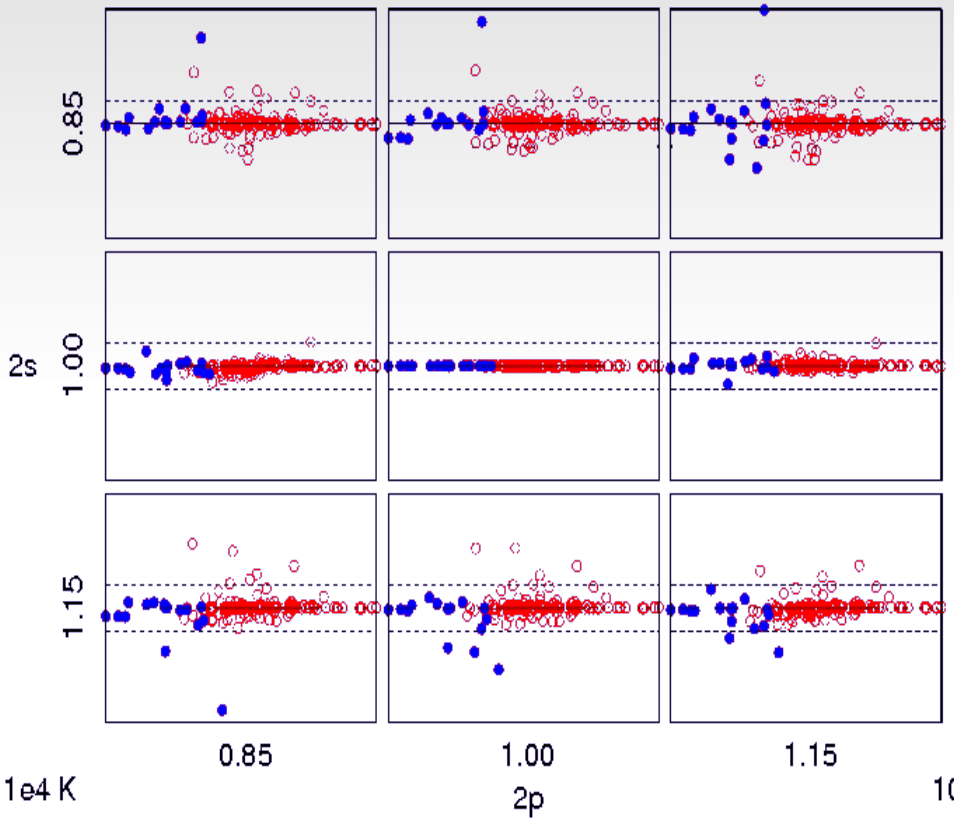
A possible way : varying orbitals between the eigen-energies of the neighbouring ion stages, for example consider He-like O case below

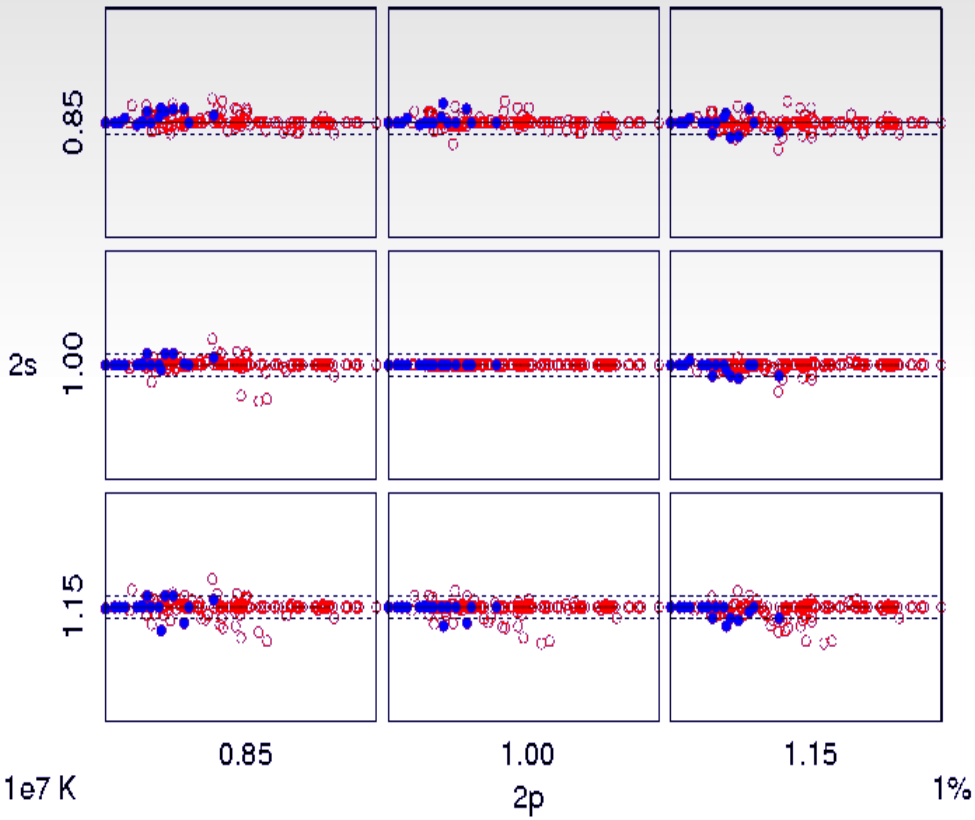
File Edit Search Preferences Shell Macro Windows Help

n	l	H-like O	He-like O	Li-like O
1	0	-32.000000	-31.947171	-31.887838
2	0	-8.000000	-7.932535	-7.762302
2	1	-8.000000	-7.898946	-7.651316
3	0	-3.555555	-3.517349	-3.412003
3	1	-3.555555	-3.507412	-3.377005
3	2	-3.555555	-3.500354	-3.336807
4	0	-2.000000	-1.976151	-1.908433
4	1	-2.000000	-1.971912	-1.893230
4	2	-2.000000	-1.968953	-1.876944
4	3	-2.000000	-1.968752	-1.875030
5	0	-1.280000	-1.263817	-1.217204
5	1	-1.280000	-1.261627	-1.209287
5	2	-1.280000	-1.260117	-1.201105
5	3	-1.280000	-1.260002	-1.200025
5	4	-1.280000	-1.260000	-1.200000

Simple preliminary H-like O , 17 level , n=3 model

Let me explain .....





Blue circles : transitions from the groundstate only
Red circles : all transtions