New developments in R-matrix (and older schemes revitalised)

Oct 6-8th , ADAS workshop 2011

Connor Ballance

Auburn University

Collaborators : S D Loch, M S Pindzola
: D Wu, R Rogers, J Pearce, N Alzate (AU)
: M Witthoeft (Goddard)
: N R Badnell (Strathclyde)

Supported by : US DoE Fusion Energy Sciences

Overview

1. Adaptive parallelism of the R-matrix suite

   -> Beyond the divide and conquer approach
   -> Reorganisation of the codes to address the 1000 term/level calculation

2. Revitalisation and new features of adas803

   (perl scripted Intermediate Coupling Frame Transformation R-matrix calculations)

3. Laying the groundwork for Monte-Carlo R-matrix calculations used in the method sensitivity part of error propagation. [Tomorrow]

This represents the current work, that extends beyond naively splitting the serial problem over more processors, to one in which the parallel code adapts to a particular problem

Hamiltonian formation

1. Serial : Each partial wave is calculated consecutively (50-100) .... a month

2. Naive parallelism : each partial wave is carried out concurrently .... 3 days
(remember a single partial wave > 200 Gbs) .... 100 procs

3. Adaptive parallelism : As well as each partial wave being carried out concurrently
the target terms are grouped into their L S Pi groups
(perhaps 20-40 unique groups) .... 2000-4000 procs … 4hrs

RESULT : Hamiltonian formation is reduced scattering from a set of target terms with the same L S Pi values.

Hamiltonian diagonalisation

1.Serial : Impossible ! Every eigenvalue of a 200 K by 200 K Hamiltonian

2. Naive parallelism : sequential parallel diagonalisation using Scalapack, possible,
but regardless of diagonalisation time, you must read 5 Tb .... 4 days

3.Adaptive parallelism : Each Hamiltonian is concurrently diagonalised in parallel , with
an n^3 scaling law controlling the distribution of processors … 5 hrs

Adaptive parallelism : Formation of the Hamiltonian

```
-rw-r--r-- 1 connorb connorb   1240 2011-04-20 13:34 STG2HBB000000
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HBB000001
-rw-r--r-- 1 connorb connorb    832 2011-04-20 13:34 STG2HBB000002
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HBB000003
-rw-r--r-- 1 connorb connorb  19248 2011-04-20 13:34 STG2HBC000000
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HBC000001
-rw-r--r-- 1 connorb connorb   7728 2011-04-20 13:34 STG2HBC000002
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HBC000003
-rw-r--r-- 1 connorb connorb  76972 2011-04-20 13:34 STG2HCC000000
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HCC000001
-rw-r--r-- 1 connorb connorb  76972 2011-04-20 13:34 STG2HCC000002
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HCC000003
-rw-r--r-- 1 connorb connorb 115272 2011-04-20 13:34 STG2HCC001000
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HCC001001
-rw-r--r-- 1 connorb connorb 115272 2011-04-20 13:34 STG2HCC001002
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HCC001003
-rw-r--r-- 1 connorb connorb  76848 2011-04-20 13:34 STG2HCC002000
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HCC002001
-rw-r--r-- 1 connorb connorb  76848 2011-04-20 13:34 STG2HCC002002
-rw-r--r-- 1 connorb connorb      0 2011-04-20 13:34 STG2HCC002003
-rw-r--r-- 1 connorb connorb   5124 2011-04-20 13:34 STG2H.DAT
```

bound-bound

bound-continuum

Continuum-continuum

Illustrates a simple case of multi-level parallelism, where as well as each partial LSPi partial wave being carried concurrently, there is a further subsequent divsion Into the bound-bound, bound-continuum and continuum-continuum Hamiltonians.

Let us use the high n shell ionisation problem as a representative case:

Consider boron-like system such as B I / C II (results of which M Pindzola will discuss in the next talk)

This will require ionisation from : 1s^2 2s^2 nl (where n=2-4, l=0-3)
: 1s^2 2s 2p^2
: 1s^2 2p^3 (for C II)

In addition to the above spectroscopic terms, we shall require minimum pseudostate expansions of the form:

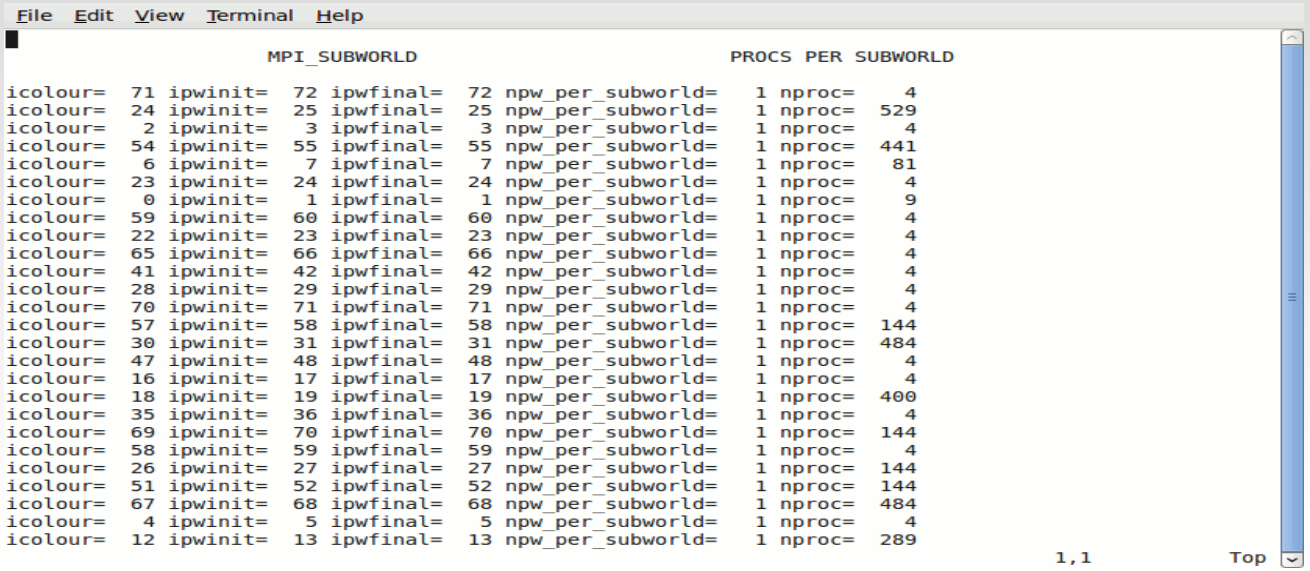
1. 1s^2 2s^2 *nl* (where n=5,14,l=0-6)
2. 1s^2 2s 2p *nl* (where n=5,14,l=0-6)
3. 1s^2 2p^2 *nl* (where n=5,14,l=0-6)

If you want to calculate

a) Direct ionisation of the outer shell electron
b) Direct ionisation of the 2s electron
c) All the excitation-autoionisations from every term ie. e + 1s^2 2s^2 3s
--> 1s^2 2s2p 3s

Well, 1444 terms , approximately 4-5000 close-coupled channels and 5 Tb of Hamiltonian matrices requiring diagonalisation poses an *interesting* challenge ...

RESULT : Adaptive diagonalisation ---> 1 Hamiltonian read, 1 diagonalisation



Better load balancing as processing power is distributed to where it is needed

- At the moment the codebase is two-tiered, with the advanced suite catering to to a large number of processor supercomputer environment, but with the regular online codecase catering to a small cluster.

History shows , one eventually becomes the other

adas803.pl : The R-matrix Intermediate Coupling Frame Transformation perl script

adas803.pl

- In recent years, EIE R-matrix calculations, have moved beyond the isolated, one-off serial calculations to parallel calculations along entire iso-nuclear/iso-electronic sequences

Witthoeft et al 2007 (J. Phys. B Vol 40)
Liang and Badnell 2010 (Astron. Astrophys. Vol 518 A64)

Perl-scripted calculations, **automatically** calculate tabulated **every** effective collision strength for **all** transitions from user given structure.

- This data is stored in a well-prescribed format that includes the atomic configurations, the energy levels, the A-Values for all E1,E2,M1,M2 transitions, Maxwellian averaged collision strengths for a range of temperatures and the Born/Bethe infinite energy limit points.

adas803.pl

- The goal is to systematically calculate effective collision strengths along iso-electronic sequences, once the user has decided upon an initial set of target configurations.

1. make update_serial
   make update_parallel
   make update_serial

'pulls' the most recent and most stable version of the scripted R-matrix codes from either Strathclyde or my website.

2. make (having specified the local fortran compiler)

3. Minimum : specify choice of orbitals and configurations

4 ./adas803.pl input.dat XX (will take the user from a structure calculation through to an effective collision strength file)

Once demanded a small parallel cluster, but now runs efficiently on a multi-core laptop

The minimum the user must supply is a single file : input.dat

File Edit Search Preferences Shell
Macro Windows Help

```
GENERAL
2Jmax_ex = 23
2Jmax_nx = 91
maxc = 55
mesh_fine = 0.0000125
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 = 1.00
2p = 1.00
3s = 1.0
3p = 1.0
3d = 1.0
```

Though the user may optimise the structure better with autostructure or indeed use other structure codes such as MCHF and CIV3 (with minor tweaking)

Atomic Structure to Effective Collision Strength (automatically)

New feature within adas803.pl : auger/radiationally damped EIE calculations

./adas803.pl –dip input.dat XX
./adas803.pl –stgb input.dat

Or if rdamp=1 within the input.dat file, this occurs transparently.

- It will analyse the target configurations that the user provides, identifying open shells, and internally determine a realistic set of bound states that Rydberg series can radiate to.

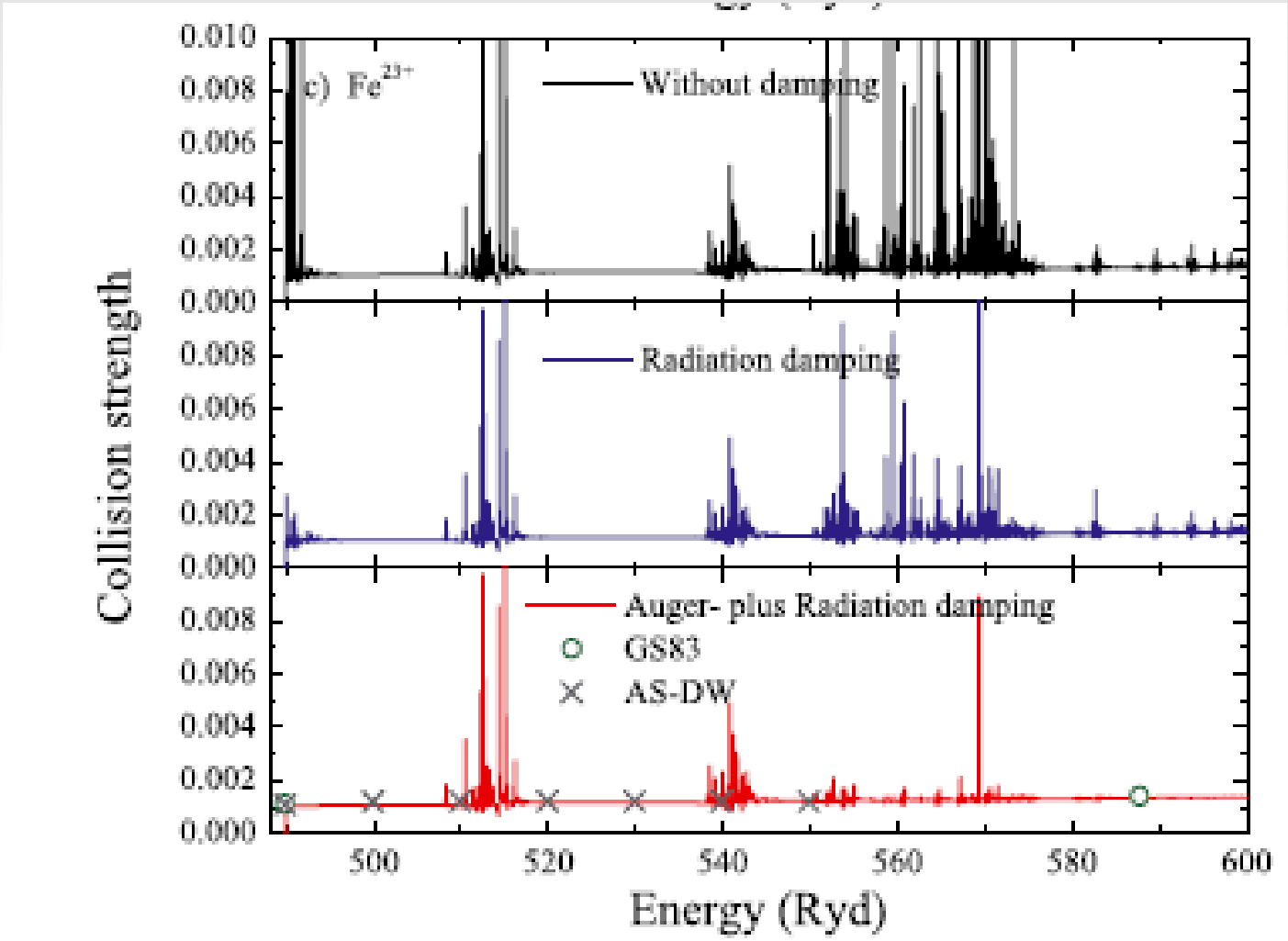
- Given this set of target configurations, and a range of angular momenta and spin multiplicities for the partial waves, the script uses dipole selection rules carry every dipole allowed pair of symmetries

- Finally utility codes remove symmetries for which they are no close coupled channels .... ie empty dipole files.

- The presence of bound-free dipole matrix files automatically causes pstgf, pstgicf or pstgfdamp,pstgicfdamp codes to be called in the outer region

Example : Inner shell excitation of Li-like Fe : 1s^22s(^2S 1/2) -- 1s2s2p(^2 P 1/2)

Ref : G Y Liang and N R Badnell (A & A 528, A68 (2011)



- A little more quality control, collision strength files are parsed for 'overt numerical failure'

- Hopefully over time, as all permutations are tried and tested this will provided better than 'baseline' comprehensive coverage over Plane Wave Born.

Future

- Having the radiation damping in place .... implementing photoionisation fairly strightforward

- ./adas803.pl --archive input XX (upload final omega files, adf04 files perhaps a tar file of the input decks)

- Error analysis (more details from Mike and myself tomorrow) but we must be able to systematically carry out 1000's of R-matrix calculations to build up meaningful statistics.