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New Version: GRASP2K Relativistic Atomic Structure Package

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Abstract

A revised version of GRASP2K [P. Jönsson, X. He, C. Froese Fischer, and I.P. Grant, Comput. Phys. Commun. 177 (2007) 597] is presented. It supports earlier non-block and block versions of codes as well as a new block version in which the `njgraf` library module [A. Bar-Shalom and M. Klapisch, Comput. Phys. Commun. 50 (1988) 375] has been replaced by the `librang` angular package developed by G. Gaigalas based on the theory of [G.A. Gaigalas, Z.B. Rudzikas, and C. Froese Fischer, J. Phys. B: At. Mol. Phys. 30 (1997) 3747, G. Gaigalas, S. Fritzsche, and I.P. Grant, Comput. Phys. Commun. 139 (2001) 263]. Tests have shown that errors encountered by `njgraf` do not occur with the new angular package. The three versions are denoted `v1`, `v2`, `v3`, respectively. In addition, in `v3`, the coefficients of fractional parentage have been extended to $j = 9/2$, making calculations feasible for the lanthanides and actinides. Changes in `v2` include minor improvements. For example, the new version of `rci2` may be used to compute QED corrections only from selected orbitals. In `v3` a new program, `jj2lsj`, reports the percentage composition of the wave function in LSJ and the program `rlevels` has been modified to report the CSF with the largest coefficient of an LSJ expansion. The `bioscl2` and `bioscl3` application programs have been modified to produce a file of transition data with one record for each transition in the same format as in ATSP2K [C. Froese Fischer, G. Tachiev, G. Gaigalas, and M.R. Godefroid, Comput. Phys. Commun. 176 (2007) 559], that identifies each atomic state by the total energy and a label for the CSF with the largest expansion coefficient in LSJ intermediate coupling. All versions of

the codes have been adapted for 64-bit computer architecture.

Key words: atomic structure calculations, Breit interaction, configuration interaction, correlation, Dirac-Fock theory, energy levels, hyperfine structure, isotope shift, jj coupling, LSJ intermediate coupling, multiconfiguration Dirac-Hartree-Fock, nuclear volume effects, QED, relativistic effects in atoms, specific mass shift, transverse photon interactions, transition probabilities, Zeeman effect
PACS: 2.70, 32.10.-f, 31.15Ne, 31.25.-v, 32.30.-r

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PROGRAM SUMMARY

Title of the Program: GRASP2K, version 1_1

Catalogue identifier:
ADZL_v1_1

Licensing provisions: no

Programming language: Fortran.

Computer: Intel Xeon, 2.66 GHz

Operating system: Suse, Ubuntu, and Debian Linux 64-bit

High-speed storage required: 500 MB or more

No. of bytes in distributed program, including test data, etc.: 51 Mbytes

Distribution format: tar gzip file

Nature of problem:
Prediction of atomic properties - atomic energy levels, oscillator strengths, radiative decay rates, hyperfine structure parameters, Landé g_J-factors, and specific mass shift parameters - using a multiconfiguration Dirac-Hartree-Fock approach.

Solution method:
The computational method is the same as in the previous GRASP2K [1] version except that for `v3` codes the `njgraf` library module [2] for recoupling has been replaced by `librang` [3,4].

Restrictions:
The packing algorithm restricts the maximum number of orbitals to be ≤ 214. The tables of reduced coefficients of fractional parentage used in this version are limited to subshells with $j \leq 9/2$ [5]; occupied subshells with $j > 9/2$ are, therefore, restricted to a maximum of two electrons. Some other parameters, such as the maximum number of subshells of a configuration state function (CSF) outside a common set of closed shells are determined by a `parameter.def` file that can be modified prior to compile time.

Unusual features:
The `biosc13` program reports transition data in the same format as in ATSP2K [6], and the data processing program `tables` of the latter package can be used. The `tables` program takes a `name.lsj` file, usually a concatenated file of all the `.lsj` transition files for a given atom or ion, and finds the energy structure of the levels and the multiplet transition arrays. The tables posted at the website

`http://atoms.vuse.vanderbilt.edu` are examples of tables produced by the `tables` program. With the extension of coefficients of fractional parentage to $j = 9/2$, calculations for the lanthanides and actinides become possible.

Running time:
CPU time required to execute test cases: 70.5 s.

References

[1] P. Jönsson, X. He, C. Froese Fischer, and I.P. Grant, Comput. Phys. Commun. **177** (2007) 597.

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1 Introduction

A revised version of GRASP2K [1] is presented. Some changes are in response to errors that have been reported, whereas others are modifications for improved reliability or extended capability. The previous version maintained the non-block format of GRASP92 [2] placing such codes in the directory `v1`. Versions for large-scale computation in block format were retained in the directory `v2`. In this spirit, we have placed versions using the new library based on the approach of reduced coefficients of fractional parentage [3,4] in directory `v3` along with a new `jj2lsj` program written in Fortran 90 and based on the LS-jj transformation matrices for a shell of equivalent electrons [5]. All versions are still included in this new GRASP2K release.

2 Installation

The installation of GRASP2K relies on environment variables. In the new version two environment variables have been added. The first is `NEWGRASPLIBS` that specifies the libraries to be searched for `v3` codes. The second is `GRASP_INCLUDES` as described below. The environment variables can be set by executing a shell script. Scripts for 64-bit Linux systems using the gfortran, ifort, and pgf95 compiler are available. We recommend the use of the GNU gfortran compiler. Extensive consistency checks of the code have been done with different versions of this compiler, the latest version being gcc 4.6.3. The full installation procedure of GRASP2K, including the use of shell scripts to set environment variables, is described in detail in the `README` file that resides in the main directory, `grasp2K_v1_1`, of the package.

3 Parameters in the package

The GRASP2K routines are designed around a number of parameters as shown in Table 1. These parameter values need to be defined in the `parameter.def` file prior to compilation. A default copy of the `parameter.def` file with the values shown in Table 1 is included in this distribution. The `makefiles` have been modified to search for this file in a directory specified by a new environment variable, `GRASP_INCLUDES`.

Increasing the values of parameters often extends the range of arrays and hence the memory that is required. For example, the parameter `NNNQN` defines the maximum number of sub-shells outside the common closed core. The parameter `NNNP` determines the number of points in a grid. Whereas some parameters are only limited by memory considerations, others like `NNNW` are limited by the packing algorithm.

3.1 The GRASP2K *radial grid*

The GRASP2K radial grid is determined by the value of `RNT`, the first non-zero point on the grid, a parameter `H`, and the number of grid points `NNNP`. The grid points are then

```
R(I) = RNT*(exp((I-1)*H)-1), I = 1, ...,NNNP
```

The present defaults are `RNT` $= 2.0 \times 10^{-6}$, `H` $= 5.0 \times 10^{-2}$, and `NNNP` $= 590$.

Table 1
Present parameter values. Except for KEYORB all names of parameters start with NNN.

Plant	Meaning or value	present value	maximum value
KEYORB	Integral index encoding key	121	215
NNNP	Maximum number of radial tabulation points	590	
NNN1	NNNP+10		
NNNW	Maximum number of relativistic subshells	120	214
NNNWM1	NNNW-1	119	213
NNNWM2	NNNW-2	118	212
NNNWP	INT(NNNW/4)	30	54
NNNQN	Maximum number of quantum numbers required to completely specify the coupling	10	
NNNTJV	Maximum number of different J values	10	

The grid defaults may be changed at run time entering n (no) in response to question about defaults. For Hg, RNT $= 1.0 \times 10^{-6}$ and H $= 1.0 \times 10^{-2}$ have been recommended. Many decisions in GRASP2K are based on the parameter ACCY = H**6 (set in the rscf routine getscd.f). For this value of H, ACCY would be 1.0×10^{-12}. Users should be aware that tests such as for convergence may be as small as $0.001 \times$ ACCY.

4 The rang angular library

In v3 programs the rang library for recoupling replaces the njgraf library module [6] used in earlier versions. The rang library is based on the combination of second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique [3], and is similar to the ANCO library [7]. In this theory the coefficients of fractional parentage are greatly reduced [4] and have been extended to include $j = 9/2$. Thus all open f-shells can be computed, but correlation subshells with higher j orbital quantum numbers are restricted in occupation to at most two.

Several codes are available that use the new and extended angular library. When compared with codes based on the `njgraf` library module there is a considerable speed up. Depending on the case and on the operator the new codes are up to 5 times faster.

4.1 The `jjreduce3` *program*

The `jjreduce3` program selects CSFs that have at least one non-zero matrix element with a CSF of a reference list. The program is in non-block form, but has been updated and now uses the `rang` library to compute the matrix elements.

4.2 The `mcp3` *program*

The `mcp3` program uses the `rang` library to generate the angular data needed by `rscf2`. No code modifications are needed. For consistency, the user may wish to define `rscf3` to be the same as that of `rscf2` (copy the executable `rscf2` to `rscf3`).

4.3 The `rci3` *program*

The `rci3` program is the version of `rci2` that uses the new `rang` library.

Relativistic corrections beyond the Dirac-Coulomb approximation for a many electron system are implemented using assumptions based on one-electron concepts. For example, the self-energy correction is computed from a screened-hydrogenic approximation, a model that does not apply well to correlation orbitals that are far from hydrogenic. To handle this the `rci2` and `rci3` codes now include an option that limits the self-energy correction to user specified orbitals.

The `rci3` includes an option in the non-default mode to shift diagonal energies in the interaction matrix to bring calculated eigenvalue differences in agreement with experimental spectra. This process is referred to as fine-tuning [8].

4.4 The `rhfs3` *program*

The `rhfs3` program is the version of `rhfs2` that uses the new `rang` library.

4.5 The `biotra3` *and* `bioscl3` *programs*

These are versions of the `biotra2` and `bioscl2` programs that use the `rang` library.

Additional modifications have been made in `bioscl3` to produce a `name1.name2.(c)t.lsj` file in the format of the output of `biotr` of ATSP2K [9]. This file contains a series of records, one for each transition, that can then be processed by the ATSP2K `tables` program to produce tables of energy levels and transition tables. These tables can then be used to post results to the MCHF/MCDHF Database [10]. A sample output file from `bioscl3`, taken from the included `examples` directory, see section 6, is given in Table 2.

Table 2
Sample output file from `bioscl3`. For electric multipole transitions parameters are given in both length form (fourth row of a record) and velocity form (fifth row of a record). `dT` is the absolute value of the fractional difference of the transition rate `AKI` in the two forms.

```
--------------------------------------------------------------------------------
 Transition between files:
 odd4
 odd4


   0  -50.89526010  1s(2).2s_2S.2p_3P
   4  -50.89425519  1s(2).2s_2S.2p_3P
     220.55 CM-1    453409.10 ANGS(VAC)    453362.23 ANGS(AIR)
E2  S =  7.66628D-01   GF =  1.38093D-15   AKI =  8.96114D-12   dT =  0.88435
         6.62879D+00         1.19404D-14          7.74841D-11


   2  -50.89495351  1s(2).2s_2S.2p_3P
   2  -50.60113912  1s(2).2s_2S.2p_1P
   64484.81 CM-1      1550.75 ANGS(VAC)      1550.75 ANGS(AIR)
E2  S =  1.05377D-05   GF =  4.74432D-13   AKI =  4.38642D-04   dT =  0.66018
         3.10094D-05         1.39612D-12          1.29080D-03


   2  -50.89495351  1s(2).2s_2S.2p_3P
   4  -50.89425519  1s(2).2s_2S.2p_3P
     153.26 CM-1    652469.10 ANGS(VAC)    652401.65 ANGS(AIR)
E2  S =  1.72618D+00   GF =  1.04343D-15   AKI =  3.26977D-12   dT =  0.87733
         1.40722D+01         8.50630D-15          2.66559D-11


   4  -50.89425519  1s(2).2s_2S.2p_3P
   2  -50.60113912  1s(2).2s_2S.2p_1P
   64331.54 CM-1      1554.45 ANGS(VAC)      1554.45 ANGS(AIR)
E2  S =  6.79066D-06   GF =  3.03557D-13   AKI =  2.79325D-04   dT =  0.95742
         2.89160D-07         1.29261D-14          1.18942D-05
 Transition between files:
 odd4
 odd4


   0  -50.89526010  1s(2).2s_2S.2p_3P
   2  -50.89495351  1s(2).2s_2S.2p_3P
      67.29 CM-1   1486162.12 ANGS(VAC)   1486008.49 ANGS(AIR)
M1  S =  1.99982D+00   GF =  5.44152D-09   AKI =  5.47783D-06


   0  -50.89526010  1s(2).2s_2S.2p_3P
   2  -50.60113912  1s(2).2s_2S.2p_1P
   64552.09 CM-1      1549.14 ANGS(VAC)      1549.14 ANGS(AIR)
M1  S =  6.40550D-06   GF =  1.67209D-11   AKI =  1.54917D-02


   2  -50.89495351  1s(2).2s_2S.2p_3P
   2  -50.60113912  1s(2).2s_2S.2p_1P
   64484.81 CM-1      1550.75 ANGS(VAC)      1550.75 ANGS(AIR)
M1  S =  5.27375D-06   GF =  1.37522D-11   AKI =  1.27147D-02


   2  -50.89495351  1s(2).2s_2S.2p_3P
   4  -50.89425519  1s(2).2s_2S.2p_3P
     153.26 CM-1    652469.10 ANGS(VAC)    652401.65 ANGS(AIR)
M1  S =  2.49953D+00   GF =  1.54915D-08   AKI =  4.85452D-05
```

```
   4  -50.89425519  1s(2).2s_2S.2p_3P
   2  -50.60113912  1s(2).2s_2S.2p_1P
   64331.54 CM-1      1554.45 ANGS(VAC)      1554.45 ANGS(AIR)
 M1  S =  8.15033D-06   GF =  2.12028D-11   AKI =  1.95103D-02

-------------------------------------------------------------------------------
```

5 New v3 programs

5.1 The `jj2lsj` *program*

Unlike the earlier `LSJ` program [11], that transforms a wave function expanded in a basis of jj-coupled configuration state functions (CSFs) to a basis of LSJ-coupled CSF's, the purpose of the present code is to transform only the most important components of large expansions. In the Atomic Spectra Database (ASD) [12] the composition of a level is frequently given by the two most important components, which in some cases may account for less than 90% of the wave function. The present code allows the user to select the maximum percentage of the wave function that can be omitted. From the latter information, it is easy to derive the smallest coefficient in the CSF expansion that *must* be included. However, with many components of about the same size, smaller values may be needed to meet the original objective. In this implementation, the user specifies the CSFs that can be omitted. The remaining CSFs define the basis that is to be transformed. By transforming this basis in decreasing order of importance, the desired percentage of the wave function can be transformed. A second parameter controls the printing of expansion coefficients in the LSJ basis and their contribution to the composition of the wave function. The default is to transform at least 99% of the wave function composition and print components in LSJ that contribute more than 0.1% to the composition. The cut-off for the jj-expansion has the value of 0.005 whereas the cut-off for printing is 0.001.

Table 3 Table showing the transformation of the wave function expansion from a jj-coupled basis to an LSJ-coupled basis for $2s2p\ ^{1,3}P_1$ in N^{+3}.

```
 ===============================================================================
   jj2lsj: Transformation of ASFs from a jj-coupled CSF basis
           into an LS-coupled CSF basis  (Fortran 95 version)
           (C) Copyright by   G. Gaigalas and Ch. F. Fischer (2011).

 Name of state
>>odd4.J=1
 Loading Configuration Symmetry List File ...
 There are 16 relativistic subshells;
 There are 840 relativistic CSFs;
  ... load complete;

 Mixing coefficients from a CI calc.?
```

```
>>y
    nelec  =            4
    ncftot =          840
    nw     =           16
    nblock =            1

   block     ncf     nev    2j+1  parity
       1     840       2       3      -1
 Default settings?  (y/n)
>>y

 Maximum % of omitted composition is    1.000
 Below  5.0E-03 the eigenvector component is to be neglected for calculating
 Below  1.0E-03 the eigenvector composition is to be neglected for printing


 . . . . . .
 Under investigation is the block:     1          The number of eigenvectors:  2
 The number of CSF (in jj-coupling):       840    The number of CSF (in LS-coupling): 78
 Weights of major contributors to ASF in jj-coupling:

  Level  J Parity      CSF contributions

    1    1   -      0.66674 of   2    0.33083 of   1    0.00095 of   9    0.00053 of   8
                    0.00030 of   14
              Total sum over  weight (in jj) is:   0.9997273477871375

 Definition of leading CSF:

            2) 1s ( 2)   2s ( 1)   2p-( 1)
                            1/2       1/2
                               1/2          1


 Weights of major contributors to ASF in LS-coupling:

  Level  J Parity      CSF contributions

    1    1   -      0.99756 of      2
              Total sum over  weight (in LSJ) is:   0.9976254987715388

 Definition of leading CSF:

         2)     1s( 2)   2s( 1)   2p( 1)
                   1S0      2S1      2P1      2S       3P          1

 . . . . . .
 The new level is under investigation.
 Weights of major contributors to ASF in jj-coupling:

  Level  J Parity      CSF contributions

    2    1   -      0.65799 of    1    0.32645 of  2    0.00823 of   8    0.00452 of  14
                    0.00090 of    9
              Total sum over  weight (in jj) is:   0.9996670582549905

 Definition of leading CSF:

            1) 1s ( 2)   2s ( 1)   2p ( 1)
                            1/2       3/2
                               1/2          1


 Weights of major contributors to ASF in LS-coupling:

  Level  J Parity      CSF contributions

    2    1   -      0.98444 of      1    0.01365 of      7
```

```
              Total sum over  weight (in LSJ) is:   0.9983605942917795

 Definition of leading CSF:

        1)     1s( 2)   2s( 1)   2p( 1)
                  1S0      2S1      2P1      2S       1P          1
        7)     1s( 2)   2p( 1)   3d( 1)
                  1S0      2P1      2D1      2P       1P          1
 ====================================================
       jj2lsj: Execution Finished ...
 ====================================================
 Wall time:
       13 seconds

 Finish Date and Time:
   Date (Yr/Mon/Day): 2011/06/03
   Time (Hr/Min/Sec): 13/59/45.009
```

```
Output file odd.J=1.lsj.lbl
-----------------------------------------------------
 Pos   J   Parity      Energy Total      Comp. of ASF
  1    1     -           -50.898218639      99.763%
         0.99878133    0.99756415   1s(2).2s_2S.2p_3P
  2    1     -           -50.604403556      99.836%
         0.99218733    0.98443570   1s(2).2s_2S.2p_1P
        -0.11684913    0.01365372   1s(2).2p_2P.3d_1P
-----------------------------------------------------
```

Table 3 shows the execution of the program for the $2s2p\ ^{1,3}P_1$ example for N^{+3}, built on a basis containing orbitals with principal quantum numbers up to $n = 4$, along with the contents of the `odd.J=1.lsj.lbl` output file. For each ASF, the position, J, parity, total energy (in hartrees), and percentage of the wave function compositions are provided, followed by a list of coefficients, their squares, and the CSF in LSJ-coupling.

In the non-default mode, the input queries are:

```
 Default settings?  (y/n)
>>n
 All levels (Y/N)
>>y

 Maximum % of omitted composition
>>1
 What is the value below which an eigenvector component
 is to be neglected in the determination of the LSJ expansion:
 should be smaller than: 0.01000
>>0.005
 What is the value below which an eigenvector composition
 is to be neglected for printing?
>>0.001
 Do you need the output file *.lsj.c?  (y/n)
>>y
 Do you need the output file *.lsj.j?  (y/n)
>>y
```

In particular, the user may request a complete transformation, with a list of CSFs in LS in `name.lsj.c` and their expansion coefficients in `name.lsj.j`. The two files have the same format as in ATSP2K [9]. Complete expansions

are feasible only for small expansions.

6 Modifications to v2 programs

Several codes contain minor changes.

(1) The `rscf2` has had a change that improves convergence. In variational calculations, the diagonal energy parameter may oscillate from one iteration to the next. In `getscd.f` the damping parameter `ODAMP(I)` has been changed to an initial value of 0.0 rather than `1.0` and `dampck.f` modified to change the damping factor only if the oscillations are sufficiently large.
(2) The `rci2` program includes the option in the non-default mode to shift diagonal energies in the interaction matrix. As described earlier for `rci3` it is now also possible to limit the self-energy correction to user specified orbitals.
(3) The format of `rlevels` has changed in that the field for the number of levels has been increased to allow for up to 100 levels. In addition, if the `name.lsj.lbl` files are available for each of the input files, the first label in the `name.lsj.lbl` files for the ASF will be appended to the former output.
(4) The `bioscl2` program has been modified to produce a file in the ATSP2K format as described earlier for `bioscl3`. The output format has been changed: the transition energy is reported in a fixed format to facilitate sorting using the Linux sort command, and the number of digits reported reduced to reflect possible accuracy.
(5) The outputs of the `rhfs2` and `sms2` programs have been shortened and the programs no longer print information on radial orbitals and energy eigenvalues. The `sms2` program is based on the non-relativistic form of the specific mass shift operator. The program is obsolete and is replaced by the RIS program [13], that implements operators to the lowest-order relativistic approximation and to first order in (m/M).

7 Example and manual

The distributed code includes the previously published example for forbidden E2 and M1 transitions between levels of $2s2p\ ^{1,3}P$ in N^{+3}. The script files in the `examples` directory have been modified to use the new codes, when appropriate. The outputs produced from the calculations are found in the `output` directory. The execution time for the test calculation is 70.5 s. For the new version a comprehensive manual in pdf-format has been prepared with instructions on how to run the codes and interpret the output files. The manual

is found in the `manual` directory and contains examples from calculations for $1s^2 2s\ ^2S$, $1s^2 2p\ ^2P$ in Li I, $2s2p\ ^{1,3}P$ in B II, and $2s^2 2p^3$ and $2p^5$ in Si VIII. In addition there is a larger case study of the $2s^2 2p$ and $2s2p^2$ states in Mo XXXVIII. The examples in the manual can also be run using script files. These reside in the `example1`, `example2`, `example3`, and `casestudy` directories. The outputs produced from the calculations described in the manual are found in the corresponding `output` directories.

8 Future releases

To make the GRASP2K package easier to maintain and update, future releases will be based on Fortran 2003 and a more modular structure such as the one found in RATIP [14]. Work along these lines have already begun.

Sample Disclaimer

Certain commercial equipment, instruments, software, or materials are identified in this paper in order to specify the computational procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

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