Reducing the Computational Load - Atomic Multiconfiguration Calculations based on Configuration State Function **G**enerators

(in Grasp2018)

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EMMI-SHE workshop, October 24, 2022

The CompAS International Collaboration

- `https://compas.github.io`

- C. Froese Fischer, I. Grant, A. Hibbert, T. Brage, J. Bieroń, **P. Jönsson, G. Gaigalas, C.Y. Chen, M. Godefroid**, S. Fritzsche, J. Marques, J. Ekman, J.E. Sienkiewicz, P. Syty, H. Hartman, Gustafsson, L. Radžiūtė, A. Papoulia, P. Rynkun, J. Grumer, **K. Wang, R. Si**, Wenxian Li, Jiguang Li, **Yanting Li**, ...

- **The General Relativistic Atomic Structure Package**

C. Froese Fischer, G. Gaigalas, P. Jönsson & J. Bieroń, J. CPC **237** (2018) 184.

Members of the CompAS core

- Department of Computer Science, University of British Columbia, Vancouver, Canada → NIST (USA)
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- Material Science and Applied Mathematics, Malmö University, Sweden.
- Division of Mathematical Physics, Lund University, Lund, Sweden.
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- Universidade de Lisboa, Lisboa, Portugal.
- Université libre de Bruxelles, Brussels, Belgium.
- Institute of Modern Physics, Fudan University, Shanghai, China.
- National Astronomical Observatories, Beijing, China.

CompAS meeting in Malmö (June 2016)

SHE Workshop Aims and Topics

May we contribute?
Paul's reply: "*Of course, look at our website!*"

- It is well known that even relatively light atoms like Ni have a complicated structure that we still cannot calculate accurately.
- If we go to heavy or super-heavy elements, with several open shells with high-l values, it is going to be even more difficult.

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Reducing the computational load – atomic multiconfiguration calculations based on configuration state function generators ☆

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ABSTRACT

In configuration interaction (CI) calculations the atomic wave functions are given as expansions over configuration state functions (CSFs) built on relativistic one-electron orbitals. The expansion coefficients of the configuration state functions are obtained by constructing and diagonalizing the Hamiltonian matrix. Here we show how a regrouping of the configuration state functions and the introduction of configuration state function generators (CSFGs) allow for a substantial reduction of the computational load in relativistic

Configuration Interaction calculations

Configuration Interaction (CI) calculations: the atomic wave function is expanded in CSFs

$$\Psi(\Gamma J M_J) = \sum_{i=1}^{M} c_{\gamma_i} \Phi(\gamma_i J M_J).$$

CSFs are **all-electron** antisymmetrized and symmetry-adapted functions constructed from products of relativistic one-electron orbitals.

Configuration Interaction calculations

Applying the variational condition on the expansion coefficients leads to an eigenvalue problem

$$(\boldsymbol{H} - E\boldsymbol{I})\boldsymbol{c}^T = \boldsymbol{0},$$

where $\boldsymbol{c} = (c_1, c_2, \ldots, c_M)$ is the vector of expansion coefficients

$\boldsymbol{H}$ is the Hamiltonian matrix with elements

$$H_{ij} = \langle \Phi(\gamma_i J M_J) | \mathcal{H}_{\mathrm{DCB}} | \Phi(\gamma_j J M_J) \rangle$$

of the Dirac-Coulomb-Breit (DCB) Hamiltonian.

Configuration Interaction calculations

A major part of the calculation is to construct the Hamiltonian matrix.

Spin-angular integration resolves the matrix element into a combination of radial integrals and interaction strengths

$$
\begin{aligned}
H_{ij} &= \langle \Phi(\gamma_i J M_J) | \mathcal{H}_{\mathrm{DCB}} | \Phi(\gamma_j J M_J) \rangle \\
&= \underbrace{\sum_{ab} t_{ab}^{ij} I(a,b) + \sum_{abcd;k} v_{abcd;k}^{ij} R^k(ab,cd)}_{\text{Dirac-Coulomb}} + \underbrace{\sum_{abcd;k} w_{abcd;k}^{ij} X^k(ab,cd)}_{\text{Breit}},
\end{aligned}
$$

t_{ab}^{ij}, $v_{abcd;k}^{ij}$ and $w_{abcd;k}^{ij}$ are the spin-angular coefficients, evaluated by methods and programs developed by **G. Gaigalas** (Vilnius U.)

Accuracy of CI calculations

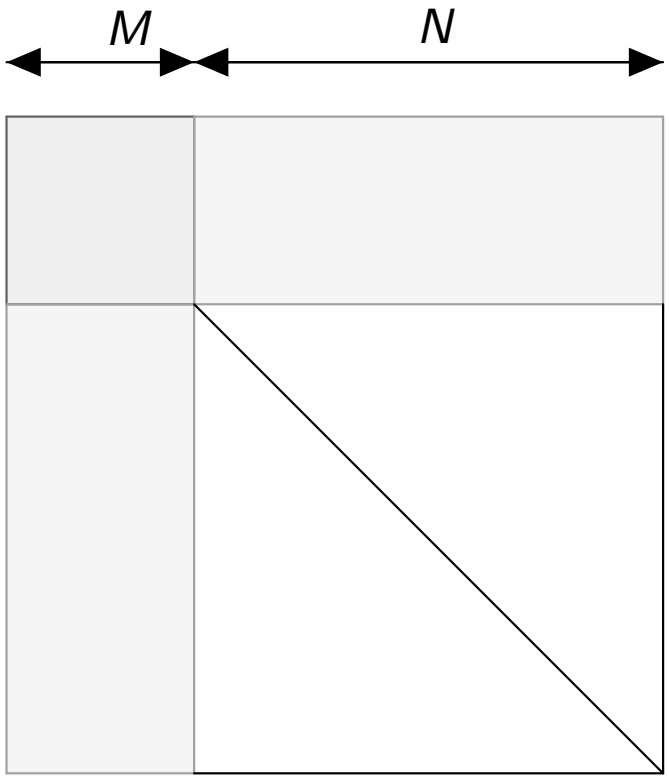
A sad fact of life:
Accurate (reliable) CI calculations require huge amount of CSFs based on large orbital sets.

CI calculations - bottlenecks

- Large number of CSFs, time consuming to construct the Hamiltonian matrix
- Large number of CSFs, time consuming to compute the expectation values
- Large files with CSFs, disk will soon get full

Where to save CPU time?

Zero- and first-order techniques ("Zero-First CI").
Divide the CSFs space into the zero-order space of size M, which accounts for the most important effects, and the first-order space of size N, that can be viewed as corrections to the zero-order space. Neglect the off-diagonal matrix elements between the CSFs in the first-order space.



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Where to save CPU time?

- Spin-angular integration gives spin-angular coefficient.
- Spin-angular coefficients combined with radial integrals give the matrix element.
- Computation of radial integrals is fast. Saved in memory.
- Spin-angular integration needs to be done for each matrix element. 10^7 CSFs means that we need to perform spin-angular integration for 10^{14} matrix elements ("**Ugah**").
- Due to the large number of matrix elements, spin-angular integration is computationally expensive.

Where to save CPU time?

- Spin-angular integration is **independent of the principal quantum numbers.**
- Using so called Configuration State Function **Generators** (CSF**G**s), spin-angular coefficients from one matrix element can be saved and used for the computation of matrix elements for a full group of CSFs.
- Potential reduction in CPU time is large

The notion of CSFGs

- Divide CSF space in a *labeling* space and a *correlation* space.

- CSFs in **labeling space** obtained allowing SDTQ... excitations from a MR according to some general rule to a set of highly occupied orbitals in **shell-closing order**, e.g.

$$\{1s, 2s, 2p\text{-}, 2p, 3s, 3p\text{-}, 3p, 3d\text{-}, 3d\}.$$

These CSFs account for major correlation effects due to close degeneracies and long-range interactions.

The notion of CSFGs – cont.

- CSFs in **correlation space** obtained by SD excitations from the above MR to a set of **symmetry-ordered** correlation orbitals

$$\underbrace{4s, 5s, 6s, 7s}_{\kappa=-1}, \underbrace{4p\text{-}, 5p\text{-}, 6p\text{-}, 7p\text{-}}_{\kappa=+1}, \underbrace{4p, 5p, 6p, 7p}_{\kappa=-2}, \underbrace{4d\text{-}, 5d\text{-}, 6d\text{-}, 7d\text{-}}_{\kappa=+2}, \underbrace{4d, 5d, 6d, 7d}_{\kappa=-3}.$$

CSFs in correlation space account for short range interactions and dynamical correlation. Correlation space is normally much larger than the labeling space.

CSFGs

- The correlation space can be divided into groups of CSFs obtained by orbital de-excitations within the symmetry-ordered orbital set from CSF**G**s, that preserve the spin-angular coupling.

- The CSF**G**s are simply CSFs at which the principal quantum numbers of orbitals in the symmetry-ordered set are taken at their highest values.

Four different types of CSFGs

Type 1: CSFs with **one** orbital in symmetry-ordered orbital set

```
1s ( 2)  2s ( 1)  4p-( 1)
             1/2      1/2
                         0-
1s ( 2)  2s ( 1)  5p-( 1)
             1/2      1/2
                         0-
....

1s ( 2)  2s ( 1)  7p-( 1)
             1/2      1/2
                         0-
```

CSFs generated by orbital de-excitations from the following CSF**G**

```
1s ( 2)  2s ( 1)  7p-( 1)
             1/2      1/2
                         0-
```

Four different types of CSFGs

Type 2: CSFs with **two** orbitals in symmetry-ordered orbital set, **different symmetry**

```
1s ( 2)  4s ( 1)  4p-( 1)
             1/2      1/2
                         0-
1s ( 2)  4s ( 1)  5p-( 1)
             1/2      1/2
                         0-
  ....

1s ( 2)  7s ( 1)  7p-( 1)
             1/2      1/2
                         0-
```

CSFs generated by orbital de-excitations from the following CSF**G**

```
1s ( 2)  7s ( 1)  7p-( 1)
             1/2      1/2
                         0-
```

Four different types of CSFGs

Type 3: CSFs with **two** orbitals in symmetry-ordered orbital set, **same symmetry**, different *n*

```
2s ( 1)  2p-( 1)  4s ( 1)  5s ( 1)
    1/2      1/2      1/2      1/2
                  1      1/2      0-
2s ( 1)  2p-( 1)  4s ( 1)  6s ( 1)
    1/2      1/2      1/2      1/2
                  1      1/2      0-
.............

2s ( 1)  2p-( 1)  6s ( 1)  7s ( 1)
    1/2      1/2      1/2      1/2
                  1      1/2      0-
```

CSFs generated by orbital de-excitations from the following CSF**G**

```
2s ( 1)  2p-( 1)  6s ( 1)  7s ( 1)
    1/2      1/2      1/2      1/2
                  1      1/2      0-
```

Four different types of CSFGs

Type 4: CSFs with a **doubly occupied** orbital in symmetry-ordered orbital set

```
  2s ( 1)  2p-( 1)  4s ( 2)
      1/2      1/2
                        0      0-
  2s ( 1)  2p-( 1)  5s ( 2)
      1/2      1/2
                        0      0-
................

  2s ( 1)  2p-( 1)  7s ( 2)
      1/2      1/2
                        0      0-
```

CSFs generated by orbital double de-excitations from the following CSF**G**

```
  2s ( 1)  2p-( 1)  7s ( 2)
      1/2      1/2
                        0      0-
```

List of CSFs vs lists of CSFGs

- In the **ordinary GRASP** program we work with lists of CSFs (three lines of configuration and coupling information for each CSF). Huge number of CSFs mean / very big files of CSFs.

- In **new GRASP** programs we work with lists of CSF**G**s. Same format as for the CSFs but we need a lot less as each CSFG spans a set of CSFs.

Program for generating list of CSFGs

`rcsfgenerate_sym`

Works as the ordinary program `rcsfgenerate` and produces `rcsf.out`

Constructing the Hamiltonian matrix

- **Old** `rci` program: matrix elements constructed one by one. Spin-angular integration done for each matrix element
- **New** `rci` program: all matrix elements between CSFs generated by one or two CSF**G**s are computed at the same time.
- Spin-angular integration done only once. Spin-angular coefficients saved and used in the computation of all matrix elements where the radial integrals are found from the fast process of orbital de-excitation.

CSF in labeling space and CSFG type 1

Spin-angular integration resolves matrix element between

```
 1s ( 2)  2s ( 1)  2p-( 1)
              1/2      1/2
                          0-
```

and

```
1s ( 2)  2s ( 1)  7p-( 1)
              1/2      1/2
                          0-
```

in

```
   1.000000000 I(2p-,7p-)
   1.000000000 R0(2s 2p-,2s 7p-)
  -0.333333333 R1(2s 2s ,7p-2p-)
   2.000000000 R0(1s 2p-,1s 7p-)
  -0.333333333 R1(1s 1s ,7p-2p-)
```

CSF in labeling space and CSFG type 1

Coupling matrix elements with the three remaining CSFs

```
1s ( 2)  2s ( 1)  6p-( 1)
1s ( 2)  2s ( 1)  5p-( 1)
1s ( 2)  2s ( 1)  4p-( 1)
```

generated by the CSFG follow by keeping the spin-angular coefficients and multiplying with appropriate radial integrals found by de-excitations of $7p-$.

CSF in labeling space and CSFG type 2

Spin-angular integration resolves matrix element between

```
 1s ( 2)  2s ( 1)  2p-( 1)
              1/2      1/2
                          0-
```

and

```
1s ( 2)  7s ( 1)  7p-( 1)
              1/2      1/2
                          0-
```

into

```
   1.000000000 R0(2s 2p-,7s 7p-)
  -0.333333333 R1(2s 2p-,7p-7s )
```

CSF in labeling space and CSFG type 2

Matrix elements with the 15 remaining CSFs generated by the CSFG follow by keeping the spin-angular coefficients and multiplying with appropriate radial integrals found by appropriate de-excitations of $7s$ and $7p-$.

Time comparisons

CI calculations for states of $1s^2 2s^2 2p^6 3s3p$ in Mg I with the Dirac-Coulomb (DC) and the Dirac-Coulomb-Breit Hamiltonian (DCB).

CSF space, SD excitations from $1s^2 2s^2 2p^6[3s3p + 3p3d]$ to increasing sets of symmetry-ordered orbitals.

	CI based on CSFs			CI based on CSF**G**s		
orbital set	CSF	CPU(DC)	CPU(DCB)	CSF**G**	CPU(DC)	CPU(DCB)
$\{5s, 5p, 5d, 5f, 5g\}$	271 588	3m59s	7m10s	115 340	1m19s	3m22s
$\{6s, 6p, 6d, 6f, 6g, 6h\}$	682 291	23m3s	42m1s	153 583	3m24s	8m52s
$\{7s, 7p, 7d, 7f, 7g, 7h\}$	1 287 898	86m13s	150m33s	158 527	6m52s	17m50s
$\{8s, 8p, 8d, 8f, 8g, 8h\}$	2 088 409	233m6s	445m52s	158 527	14m24s	35m28s
$\{9s, 9p, 9d, 9f, 9g, 9h\}$	3 083 824	376m6s	950m36s	158 527	19m25s	66m45s
$\{10s, 10p, 10d, 10f, 10g, 10h\}$	4 274 143	1074m38	2008m57s	158 527	44m13s	110m48s

Time comparisons

- Breit-interaction time consuming
- Time reduction factor of 24 for DC.
- Time reduction factor of 18 for DCB.
- The larger the orbital set, the larger the time reduction (great!)

Where to save CPU time?

- The Breit-interaction per orbital decreases rapidly with increasing n and l of the orbitals
- We can put limitations on l for the Breit integrals with small changes in the computed transition energies.
- Reduces the CPU time drastically

Time comparisons

States of $\{4s^2 4p^6 4d^2,\ 4s^2 4p^6 4d5s,\ 4s^2 4p^6 5s^2,\ 4s^2 4p^6 4d5p\}$ in Zr III. CSF space is formed by SD excitations from the above configurations to increasing sets of symmetry-ordered orbitals.

	CI based on CSFs		CI based on CSF**G**			
orbital set	CSF	CPU(full)	CSF**G**	CPU(spd)	CPU(full)	CPU ratio
$\{7s, 7p, 6d, 5f, 5g\}$	597 155	18m12s	265 939	9m6s	10m.39s	2
$\{8s, 8p, 7d, 6f, 6g, 6h\}$	1 560 620	109m31	375 373	21m25s	28m20s	5.1
$\{9s, 9p, 8d, 7f, 7g, 7h\}$	2 991 680	399m30s	389 305	32m51s	52m33s	12.2
$\{10s, 10p, 9d, 8f, 8g, 8h\}$	4 890 335	1032m39s	389 305	50m4s	94m42s	20.6
$\{11s, 11p, 10d, 9f, 9g, 9h\}$	7 256 585	1590m49s	389 305	81m10s	173m35s	19.6

Time comparisons

Corresponding energies

state	ΔE(DC)	ΔE(sp)	ΔE(spd)	ΔE(spdf)	ΔE(spdfg)	ΔE(full)
$4d^2\ {}^3F_2$	0	0	0	0	0	0
$4d^2\ {}^3F_3$	697.49	700.59	662.34	662.59	662.67	662.72
$4d^2\ {}^3F_4$	1526.61	1533.24	1451.62	1452.07	1452.30	1452.43
$4d^2\ {}^1D_2$	6064.01	6093.25	6034.29	6034.81	6034.88	6034.95
$4d^2\ {}^3P_0$	8434.63	8439.31	8417.93	8418.38	8418.46	8418.55
$4d^2\ {}^3P_1$	8699.76	8705.61	8669.28	8669.91	8670.03	8670.13
$4d^2\ {}^3P_2$	9227.18	9236.72	9164.87	9165.50	9165.77	9165.94
$4d^2\ {}^1G_4$	11635.51	11647.15	11588.07	11588.26	11588.38	11588.46
$4d5s\ {}^3D_1$	18427.19	18644.38	18494.60	18496.36	18496.78	18497.01
$4d5s\ {}^3D_2$	18848.69	19067.13	18898.51	18900.39	18900.86	18901.12
$4d5s\ {}^3D_3$	19601.54	19823.64	19615.82	19617.90	19618.47	19618.80
$4d^2\ {}^1S_0$	25292.46	25354.96	25269.45	25270.67	25270.74	25270.84
$4d5s\ {}^1D_2$	25610.69	25799.49	25629.29	25631.21	25631.68	25631.94
...	...	...	...	...	...	...
$4d5p\ {}^3P_2$	60663.40	60877.03	60679.64	60681.72	60682.27	60682.57
$4d5p\ {}^1F_3$	63288.69	63486.24	63309.35	63311.48	63311.96	63312.23
$4d5p\ {}^1P_1$	63436.43	63647.94	63451.48	63453.63	63454.19	63454.52

Time comparisons

- Reducing the orbitals to *spd* in the Breit integrals cuts the CPU time with a factor of 2.
- The change in transition energies is negligible, i.e. very good approximation.

Where to save CPU time?

- We can further reduce the CPU time by removing CSFs that are unimportant. This is known as "**condensation**".

Where to save CPU time?

A priori condensations

- We can condense by including only CSFs that interact (have non-zero matrix elements) with the CSFs in the MR. Argument based on Z-dependent perturbation theory. May not work well for neutral or near-neutral systems!

  (In GRASP this is done by running `rcsfinteract`)

- Reduces number of CSFs by a factor of 2 -3

Where to save CPU time?

A posteriori condensations

- Perform a CI for the full CSF space but using zero- and first interaction to reduce the CPU time ("Zero-First CI"),
- Sort the mixing coefficients of the CSFs and accumulate until a predefined fraction is reached
  (this is done by `rmixaccumulate` in GRASP)
- From this accumulation process, we get the condensed CSFs space for which we include all interactions.
- Works fine but we need to first perform the Zero-First CI in the full CSF space.

Where to save CPU time?

A priori condensations based on CSF**G**s

- Perform a CI with a limited set of symmetry-ordered orbitals
- Assign each CSF**G** a squared weight equal to the sum of the squared weights of the generated CSFs
- Sort the mixing coefficients of the CSF**G**s and accumulate until a predefined fraction is reached.
- To have a condensed expansion for a larger orbital set we just take the surviving CSF**G**s and set the principal quantum numbers to the highest values of the new orbital set.
- This is basically an a priori method. Can be done by the new version `rmixaccumulate_sym`.

Time comparisons

States of $\{4s^2 4p^6 4d^2,\ 4s^2 4p^6 4d5s,\ 4s^2 4p^6 5s^2,\ 4s^2 4p^6 4d5p\}$ in Zr III. CSF space is formed from increasing sets of CSF**G**s.

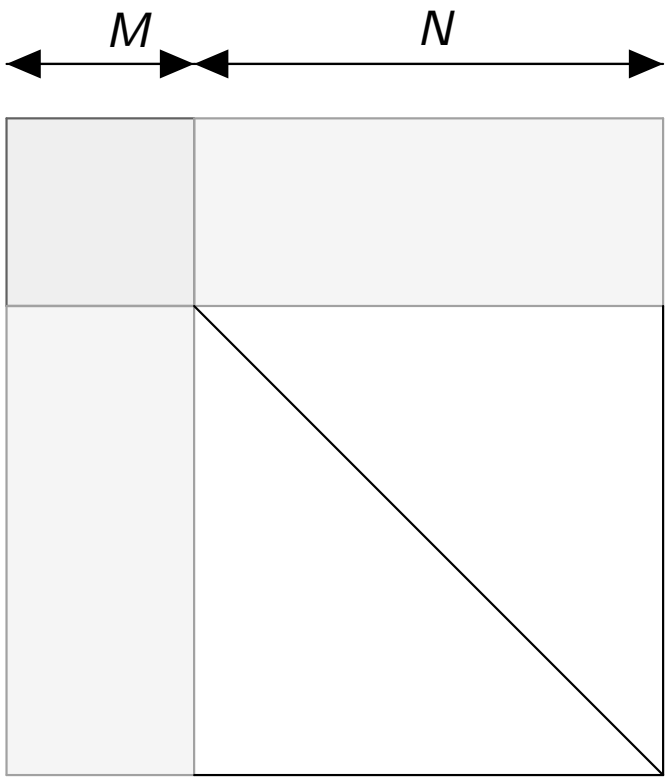
condensation	interact	0.999925	0.99995	0.99999	0.999995	full CSF space
CSF	2 674 196	2 396 072	2 694 053	4 031 414	4 593 618	7 256 585
CSF ratio	2.7	3.0	2.7	1.8	1.6	1
CPU	45m44s	37m29s	39m12s	60m46s	70m36s	173m35s
CPU ratio	3.8	4.6	4.4	2.9	2.5	1
$4d^2\ ^3F_2$	0	0	0	0	0	0.00
$4d^2\ ^3F_3$	836.07	687.98	678.19	666.47	664.62	662.72
$4d^2\ ^3F_4$	1565.51	1447.43	1448.21	1451.66	1451.89	1452.43
$4d^2\ ^1D_2$	6120.68	6064.93	6053.86	6037.56	6035.98	6034.95
$4d^2\ ^3P_0$	8841.72	8432.57	8427.83	8422.48	8420.54	8418.55
$4d^2\ ^3P_1$	8916.92	8686.67	8680.06	8672.69	8671.38	8670.13
			...			
$4d5p\ ^3D_3$	57443.66	57560.35	57546.73	57533.59	57532.56	57531.93
$4d5p\ ^3F_4$	57764.47	57783.66	57777.48	57774.15	57773.92	57774.07
$4d5p\ ^3P_1$	60218.01	60192.97	60187.48	60182.16	60181.59	60181.01
$4d5p\ ^3P_0$	60488.82	60307.24	60308.09	60314.18	60314.49	60315.03
$4d5p\ ^3P_2$	60634.12	60726.18	60710.12	60687.35	60684.89	60682.57
$4d5p\ ^1F_3$	63302.40	63337.66	63326.81	63314.24	63313.01	63312.23
$4d5p\ ^1P_1$	63890.18	63479.51	63468.35	63456.53	63455.26	63454.52
fract. error	2.2 %	0.25 %	0.15 %	0.035 %	0.017 %	0 .00 %

Where to save CPU time?

- Condensation based on interaction with CSFs in the MR does not work well.
- Condensation based on CSF**G**s and accumulation to a predefined fraction is a very powerful a priori condensation method!
- Putting everything together: CSF**G**s, restrictions for the orbitals in the Breit integrals and condensations based on accumulation to a predefined fraction, we may reduce the CPU time **with a factor 60-70** for large calculations without affecting the transition energies.

Connection to zero- and first order methods

In the zero- and first order method we include only the diagonal elements between CSFs in the first order space.



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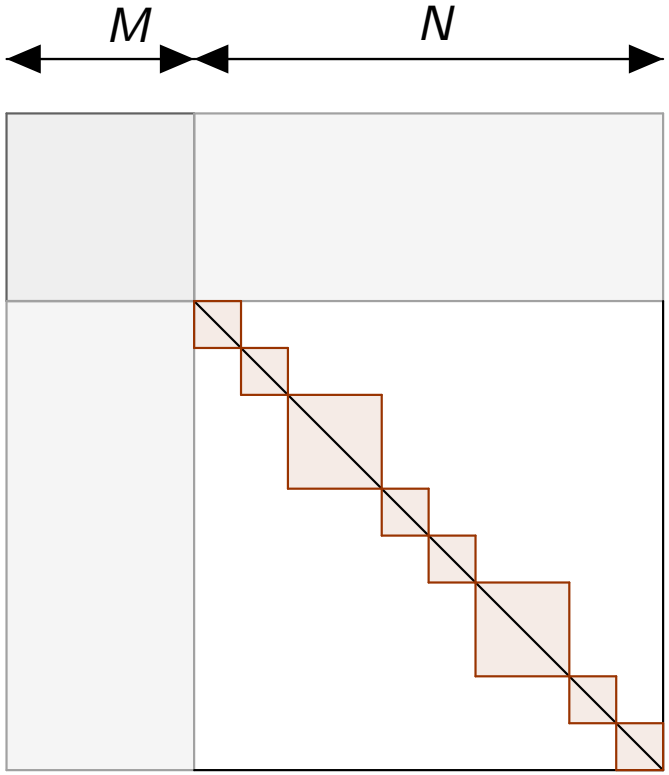
Connection to zero- and first order methods

A better approximation, but still fast, is obtained by including off-diagonal matrix elements between CSFs within CSF**G** block of the first order space. This is a block-diagonal approach.



Geddes *et al.*, PRA **98** (2018) 042508

Partitioned correlation function interaction (PCFI)

IOP PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR

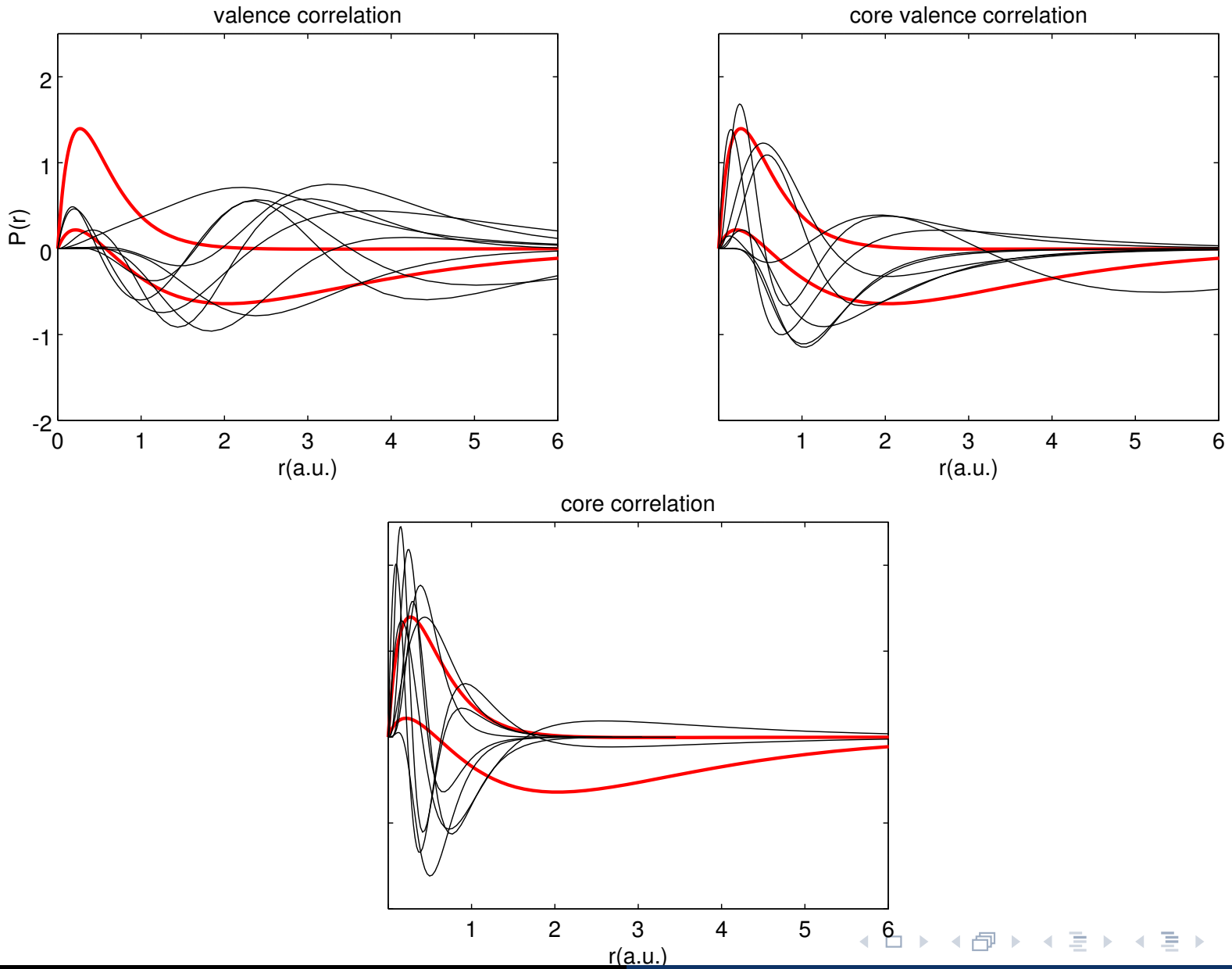
J. Phys. B: At. Mol. Opt. Phys. **46** (2013) 085003 (18pp) doi:10.1088/095

A partitioned correlation function interaction approach for describing electron correlation in atoms

S Verdebout[1], P Rynkun[2], P Jönsson[3], G Gaigalas[4], C Froese Fischer[5] and M Godefroid[1]

Verdebout *et al.*, JPB **46**(2013) 085003

Optimally localized orbital sets in $1s^2 2s^2\ {}^1S$ in Be



PCFI for $1s^2 2s^2\ {}^1S$ in Be

Tabell: $|1s^2 2s^2\ {}^1S\rangle, |1s^2 2p^2\ {}^1S\rangle, \underbrace{|\bar{\Lambda}_{VV}\rangle}_{200\text{ CSFs}}, \underbrace{|\bar{\Lambda}_{CV}\rangle}_{900\text{ CSFs}}, \underbrace{|\bar{\Lambda}_{CC}\rangle}_{1000\text{ CSFs}}$.

Energies are compared with CAS-MCHF results based on a single orthonormal orbital set.

$n \leq$	$E_{5\times5}$	$E_{CAS-MCHF}$
4	−14.660 679 48	−14.661 403 17
5	−14.665 553 46	−14.664 839 93
6	−14.666 582 83	−14.666 067 32
7	−14.666 905 87	−14.666 541 14
8	−14.667 047 86	−14.666 857 41
9	−14.667 122 76	−14.667 012 75
10	−14.667 168 08	−14.667 114 20

- CAS-MCHF 650 000 CSFs, days on a super computer cluster
- Optimally localized orbital sets, a few hours on a PC.

Connecting PCFs with Super-CSFs and CSF**G**s

In the **PCFI method** (Verdebout *et al.*, JPB **46**(2013) 085003)), we introduced the concept of Partitioned Correlation Functions. These PCFs can be generalized as **Super-CSF**s.

A Super-CSF can be taken as a linear combination of a subspace of CSFs spanned by a CSF**G**.

Example:

$$|\textbf{Super-CSF}\rangle = c_1|1s^2 2s8p\rangle + c_2|1s^2 2s9p\rangle + c_3|1s^2 2s10p\rangle + c_4|1s^2 2s11p\rangle$$

$\{c_1, \ldots, c_4\}$ can be determined perturbatively or in a smaller `rci` calculation based on a divide and conquer algorithm.

Connecting PCFs with Super-CSFs and CSF**G**s

- The use of **Super-CSFs** reduces the size of the Hamiltonian matrix: we add one basis function instead of 4
- The matrix element between an ordinary CSFs and a Super-CSF can be evaluated very efficiently using our new methods.
- The use of Super-CSFs constructed from spatially adapted radial orbitals have shown very efficient in describing the energy structure of a system.

CSFGs allow physical interpretation

The effect on expectation values can be tracked for a group of CSFs belonging to a CSF**G**

We can check the effect of the CSFs spanned by the symbolic CSF on e.g. hfs or isotope shift parameters

```
1s ( 2)  2s ( 1)  7p-( 1)
             1/2      1/2
                          0-
```

We can learn and understand what correlation effects are important **for different properties**. Program for this would be very similar to the new `rmixaccumulate_sym` code but now we rank the CSFGs according to their contribution *to the computed property*.

Thank you for your attention!