• Motivation
• Symbolic computing
• Numeric computing
• Computational challenges & future projects
Research field: development of high-precision methodologies for the calculation of the atomic properties and applications of such calculations.

This research involves:

• the study of the fundamental physics problems

• applications of atomic physics to future technological developments

http://CPEPweb.org
### MOTIVATION: FUNDAMENTAL PHYSICS

**PROPERTIES OF THE INTERACTIONS**

<table>
<thead>
<tr>
<th>Property</th>
<th>Gravitational</th>
<th>Weak (Electroweak)</th>
<th>Electromagnetic</th>
<th>Strong</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acts on:</td>
<td>Mass – Energy</td>
<td>Flavor</td>
<td>Electric Charge</td>
<td>Color Charge</td>
</tr>
<tr>
<td>Particles</td>
<td></td>
<td>Quarks, Leptons</td>
<td>Electrically charged</td>
<td>See Residual Strong Interaction Note</td>
</tr>
<tr>
<td>experiencing:</td>
<td></td>
<td></td>
<td></td>
<td>Quarks, Gluons</td>
</tr>
<tr>
<td>Particles</td>
<td>Graviton</td>
<td>W⁺ W⁻ Z⁰</td>
<td>γ</td>
<td>Hadrons</td>
</tr>
<tr>
<td>mediating:</td>
<td>(not yet observed)</td>
<td></td>
<td></td>
<td>Gluons</td>
</tr>
<tr>
<td>Strength</td>
<td></td>
<td></td>
<td></td>
<td>Mesons</td>
</tr>
<tr>
<td>relative to electromag</td>
<td>10⁻¹⁸ m</td>
<td></td>
<td>25</td>
<td>Not applicable to quarks</td>
</tr>
<tr>
<td>for two u quarks at:</td>
<td>3×10⁻¹⁷ m</td>
<td>0.8 1</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>for two protons in nucleus</td>
<td>10⁻¹⁴ m</td>
<td>10⁻⁴ 1</td>
<td>Not applicable to hadrons</td>
<td></td>
</tr>
<tr>
<td></td>
<td>10⁻¹⁴ m</td>
<td>10⁻⁷ 1</td>
<td>20</td>
<td></td>
</tr>
</tbody>
</table>

MOTIVATION: APPLICATIONS TO VARIOUS FIELDS OF PHYSICS

• Search for variation of the **fundamental fine-structure constant** with time

• Development of the **high-precision methodologies**, benchmark problems for understanding of atomic properties, tests of *ab initio* theory and experimental methods, and cross-checks of experiment

• Determination of **nuclear properties** such as nuclear magnetic and anapole moments

• Providing data for **astrophysics** studies
MOTIVATION:
NEW TECHNOLOGIES

QUANTUM COMMUNICATION, CRYPTOGRAPHY AND QUANTUM INFORMATION PROCESSING

Every 18 months microprocessors double in speed
FASTER = SMALLER

Babbage’s Engine

Silicon Wafers

Atoms

1 meter

0.000001 m

0.0000000001 m
Quantum Computer (Innsbruck)
The ability to develop more precise optical frequency standards will open ways to improve global positioning system (GPS) measurements and tracking of deep-space probes, perform more accurate measurements of the physical constants and tests of fundamental physics such as searches for gravitational waves, etc.
MOTIVATION

Atomic Clocks

NEED ATOMIC PROPERTIES

Parity Violation

Quantum information
Step 1 Derivation of the formulas

Step 2 Conducting possible analytical calculations to simplify expressions for numeric evaluation

Step 3 Writing and debugging the programs for numeric calculations

Step 4 Numeric calculations
Steps 1 – 3: Symbolic computing

Step 1 Derivation of the formulas

Step 2 Conducting possible analytical calculations to simplify expression for numerical evaluation

Step 3 Writing and debugging the programs for numerical calculations

Step 4 Numeric computation
The **coupled-cluster method** sums **infinite sets** of many-body perturbation theory terms. The wave function of the valence electron $\nu$ is represented as an expansion that includes all possible single, double, and partial triple excitations.

**Cs**: atom with single (valence) electron outside of a closed core.

$1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^66s$
\[ \left| \Psi_v \right\rangle = \text{Lowest order} \quad \left| \Psi_v^{(0)} \right\rangle \]

- Core: Green dot
- Valence electron: Orange dot
- Any excited orbital: Black dot

\[ \left| \Psi_v \right\rangle = \text{Core} \quad \left| \Psi_v^{(0)} \right\rangle \]

\[ + \sum_{ma} \rho_{ma} a_m^\dagger a_a \left| \Psi_v^{(0)} \right\rangle + \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v \left| \Psi_v^{(0)} \right\rangle \]

Single-particle excitations

\[ + \frac{1}{2} \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a \left| \Psi_v^{(0)} \right\rangle + \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_a a_v \left| \Psi_v^{(0)} \right\rangle \]

Double-particle excitations

+ ...
Need for symbolic computing

\[
H \frac{1}{2} S_2^2 \mid \Psi^{(0)}_v \rangle \rightarrow \langle a_i^+ a_j^+ a_l a_k : a_m^+ a_n^+ a_r^+ a_s^+ a_d a_c a_b a_a a_v^+ \mid 0_c \rangle
\]

800 terms!

The code was developed to implement Wick's theorem and simplify the expression.
Input: expression of the type

\[ g_{ijkl} \rho_{mnwa} : a_i^+ a_j^+ a_l a_k : : a_m^+ a_n^+ a_a a_w^+ : \]

in ASCII format.

Output: simplified resulting formula in the LaTex format, ASCII output is also generated.

\[
\begin{align*}
g_{ijkl} \rho_{mnwa} : a_i^+ a_j^+ a_l a_k : : a_m^+ a_n^+ a_a a_w^+ : & = g_{mnba} \rho_{rswc} a_m^+ a_n^+ a_r^+ a_s^+ a_a a_b a_c a_w |0\rangle - \tilde{g}_{cmba} \rho_{nrwc} a_m^+ a_n^+ a_r^+ a_a a_b a_w |0\rangle \\
& + \tilde{g}_{mnas} \tilde{\rho}_{srwb} a_m^+ a_n^+ a_r^+ a_a a_b a_w |0\rangle + \tilde{g}_{wmba} \rho_{nrwc} a_m^+ a_n^+ a_r^+ a_a a_b a_c |0\rangle \\
& - \tilde{g}_{cwba} \rho_{mnwc} a_m^+ a_n^+ a_a a_b |0\rangle + 2\tilde{g}_{wmar} \tilde{\rho}_{rwnb} a_m^+ a_n^+ a_a a_b |0\rangle - 2\tilde{g}_{bmar} \tilde{\rho}_{rnwb} a_m^+ a_n^+ a_a a_w |0\rangle \\
& - g_{mnrs} \tilde{\rho}_{srwa} a_m^+ a_n^+ a_a a_w |0\rangle - 2\tilde{g}_{bwan} \tilde{\rho}_{nmwb} a_m^+ a_a a_b |0\rangle - \tilde{g}_{wmnr} \tilde{\rho}_{rnwa} a_m^+ a_a |0\rangle \\
& + \tilde{g}_{amnr} \tilde{\rho}_{rnwa} a_m^+ a_w |0\rangle + \tilde{g}_{awmn} \tilde{\rho}_{nmwa} |0\rangle
\end{align*}
\] (1)
1) The code is set to work with two or three normal products (all possible cases) with large number of operators.

2) The code differentiates between different types of indices, i.e. core \((a,b,c,...)\), valence \((v,w,x,y,...)\), excited orbitals \((m,n,r,s,...)\), and general case \((i,j,k,l,...)\).

3) The operators are ordered as required in the same order for all terms.
\[
g_{\text{mnba}} \rho_{\text{rswe}} a_{m} a_{n} a_{r} a_{s} a_{a} a_{b} a_{c} a_{w}^{+}
\]

4) The expression is simplified to account for the identical terms and symmetry rules, \(g_{ijkl} = g_{jilk}\).

5) The direct and exchange terms are joined together,
\[
\tilde{g}_{ijkl} = g_{ijkl} - g_{ijlk}.
\]
Certain summations can be carried out analytically

Two symbolic programs are currently available:

1) KENTARO – currently interfaced with the previous program.

2) RACAH Maple code – very convenient to use, but has compatibility problems.
The resulting expressions that need to be evaluated numerically contain very large number of terms, resulting in tedious coding and debugging.

The symbolic program generator was developed for this purpose to automatically generate efficient numerical codes for coupled-cluster or perturbation theory terms.

\[
- \sum_{abcd} \sum_{k_1k_2k_3} (-1)^{J+k_1+k_2+k_3+j_c+j_d+j_w+j_{w'}} \begin{pmatrix} J & j_c & j_d \\ k_2 & j_{w'} & j_{v'} \end{pmatrix} \begin{pmatrix} J & j_a & j_b \\ k_3 & j_w & j_v \end{pmatrix} \begin{pmatrix} J & j_c & j_d \\ k_1 & j_b & j_a \end{pmatrix} \\
\times \frac{X_{k_1}(cdab) X_{k_2}(v'w'cd) Z_{k_3}(vwab)}{(\epsilon_c + \epsilon_d - \epsilon_{v'} - \epsilon_{w'})(\epsilon_a + \epsilon_b - \epsilon_{v'} - \epsilon_{w'})}
\]
Step 3: Symbolic computing for program generation

Input: list of formulas to be programmed

Output: corresponding FORTRAN code for numerical evaluation

Sample input:

```
1 subroutine term1d(nvp,kvp,nwp,kwp,nv,kv,nw,kw,jtot,res)
2   X[k1](c,d,a,b) X[k2](vp,wp,c,d) Z[k3](v,w,a,b)
3   none
4   4
xx z1=(-1)**(1+jtot+k1+k2+k3+kapc+kapd+kapw+kapwp)
xx z2=d6j(2*jtot,jc,jd,2*k2,jwp,jvp)
xx z3=d6j(ja,jb,2*jtot,jw,jv,2*k3)
xx z4=d6j(jc,jd,2*jtot,jb,ja,2*k1)
5 (e[c,d]-e[vp,wp]) (e[a,b]-e[vp,wp])
6 No
```
Features: Simple input, essentially just type in a formula.
Efficient codes are produced
Other constructs can be easily added
Safety features are build in
Works for most formulas
Future plans: interface with formula-writing codes
STEP 4: NUMERICAL COMPUTATION

1. Coupled-cluster method: iterative solution of very large number of equations

2. Relativistic many-body perturbation theory: evaluation of terms such as example considered before

3. Configuration-interaction (CI) method: finding a few eigenvalues of large matrices

4. Combination of coupled-cluster and CI: general super CI code* (in progress)
\[(\epsilon_{ab} - \epsilon_{mn})\rho_{mnab} = g_{mnab} + \sum_{cd} g_{cdab}\rho_{mncd} + \sum_{rs} g_{mnrs}\rho_{rsab} \]

\[+ \left[ \sum_{r} g_{mnr\rho_{ra}} - \sum_{c} g_{cnab}\rho_{mc} + \sum_{rc} \tilde{g}_{cnrb}\tilde{\rho}_{mrac} \right] + \begin{bmatrix} a \leftrightarrow b \\ m \leftrightarrow n \end{bmatrix} \]
The excitation coefficients $\rho$ are obtained by the iterative solution of the corresponding equations. Owing to the very large number of the equations the code needs to be very efficient. The inclusion of the triple excitations require new approaches owing to substantially larger memory and computer time requirements.

$\rho_{mnab}$  

Cs: $a,b = 1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^6$  

$m,n : \text{finite basis set} = (35 \times 13) \times (35 \times 13)$  

19 000 000 equations

$\rho_{mnrvab}$  

Extra index $r$ gives at least a factor of $(35 \times 13)$. 
These are really complicated equations!!!

- “Quadruple” term:

\[ \sum_{rs} g_{mnrs} \rho_{rsab} \]

Indices \( mnrs \) can be ANY orbitals

Basis set: \( n_{\text{max}} = 35, l_{\text{max}} = 6 \)

\( 17 \times 17 \times (35 \times 13)^4 = 5 \times 10^{12} \)

- Program has to be exceptionally efficient!
I. Efficiency of the most complicated terms

II. Efficient parallelization

III. Numerical methods

IV. Keeping up with new hardware/software and corresponding compatibility problems
1) Efficiency of the most complicated terms:
   \[ \sum_{rs} g_{mnrs} \rho_{rsab} \]
   - Can it be improved further?
   - Is any time being wasted owing to imperfect loop ordering?
   - Automated code optimization?

2) Efficient parallelization, especially for triple excitations

How to do efficient parallelization of iterative procedures with large local files?
3) Efficient parallel codes for configuration interaction method (finding few eigenvalues of large matrices)

4) New approaches for the numerical basis sets (currently using B splines)

5) Resolving convergence issues for the iterative procedure in the cases of large excitations from nearby core shells.

6) Computing on multicore machines
CONCLUSION

Fundamental Physics

Atomic Clocks

Symbolic and Numeric Computing for Atomic Calculations

Quantum information
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NSF WORKSHOP
ON CYBER-ENABLED DISCOVERY
AND INNOVATION (CDI)

NSF solicitation

Workshop page
http://www4.ncsu.edu/~kaltofen/CDI_SYMNUM_Itinerary.html