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# Software implementation and performance study of the rank-reduced relativistic coupled-cluster method

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A relativistic version of the rank-reduced coupled-cluster method accounting for double excitations (RR-RCCD) has been developed and implemented as a software package. The method is designed for accurate electronic structure calculations of systems containing heavy elements in their ground states possessing single-reference character. High computational efficiency is achieved through the simultaneous application of the Tucker approximation for the cluster amplitude tensor and the partial Cholesky decomposition for the tensor of two-electron integrals. The scalability of the developed method has been studied numerically for a series of linear molecules $(AuCN)_n$, $n = 1-5$. It has been shown that for a fixed threshold for discarding singular values identical for all studied systems, the effective rank of the cluster amplitude tensor grows approximately linearly with the number of atoms in the system. This makes possible a reduction of the computational complexity of the relativistic coupled-cluster RCCD algorithm from $O(N^6)$ to $O(N^5)$ ($N$ stands for the number of one-electron spinors).

**Keywords:** Relativistic coupled-cluster method, tensor decompositions, Tucker decomposition, partial Cholesky decomposition, effective core potentials, gold(I) cyanide.

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## Introduction

The coupled cluster (CC) method [1] is one of the most accurate and reliable approaches for describing electron correlation, particularly for systems with a pronounced dominance of a single Slater determinant in the wavefunction. This method can be formulated within a relativistic framework, which is especially important for modeling systems containing heavy elements. However, the practical application of the CC method faces a fundamental challenge of its extremely high computational complexity. Traditional software implementations of the CC versions that include double (CCD, CCSD), triple (CCSDT), and quadruple (CCSDTQ) excitations are characterized by a computational cost that scales as $O(N^6)$, $O(N^8)$, and $O(N^{10})$, respectively, with the number of molecular spinors $N$ such a scaling severely limits practical application of these approximations for electronic structure modeling of large molecular systems.

One of the most promising directions in the development of coupled-cluster methods is associated with rank-reduced (RR) approach, which is based on the Tucker decomposition [2] of an cluster amplitude tensor. For instance, the non-relativistic RR-CCSD method demonstrates $O(N^5)$ scaling [3]. In recent few years, RR versions of various non-relativistic coupled-cluster methods have been developed, including those for excited state calculations [4–6]. An efficient representation of the two-electron integral tensor is critical to accelerate rank-reduced coupled-cluster calculations. The direct use of the whole multidimensional array of these integrals, whose overall number scales as $O(M^4)$ with the number $M$ of atomic basis functions, results in high computational demands when modeling systems with a large number of electrons. To overcome this problem, approximate representations of an integral tensor are most commonly used, e. g. the resolution of the identity (RI) approximation and the partial Cholesky decomposition (PCD). These approaches significantly reduce memory requirements and accelerate computations by representing a two-electron integral tensor as products of tensor with lower dimensions.

In all the aforementioned studies considering the non-relativistic coupled-cluster method for closed-shell systems, the spin-adapted formalism was used in the derivation of the equations. The development of a relativistic version of the rank-reduced coupled-cluster method is of particular practical importance, as the advancement of RR-RCC could become a key factor enabling the study of complex systems, including materials based on $d$- and $f$-elements and high-spin electronic configurations with open shells [7]. In particular, the use of a Kramers-unrestricted CC formulation [8] within the RR-RCC approach allows for effective studies of correlated systems whose wave functions can be approximated in the first order by a single Slater determinant. The combination of RR-RCC with the Compound Tunable Embedding Potential (CTEP) technique [9–14] paves the way towards the high precision modeling of materials with unique magnetic and optical

properties. Such methods can fundamentally new possibilities for fundamental research, including the searches for effects of the physics beyond the Standard Model in experiments with solid-state systems [15–17].

In our previous study [18], the theoretical foundations for the rank-reduced relativistic coupled-cluster method were developed. It is important to note that for efficient compression of tensor representations, the Goldstone formalism have to be used (i. e., without antisymmetrization of the two-electron integral tensor). Pilot calculations for small gold clusters $Au_n$, $(AuCl)_n$ chains, and a cluster model representing a fragment of a $YbCl_2$ crystal employing the CTEP environment demonstrated the effectiveness of applying such a tensor decomposition of amplitudes to the relativistic version of the coupled-cluster method. Nevertheless, although the theoretical aspects of the method, including the derivation of all working RR-RCCD equations, were elaborated in detail in Ref. [18], the development of an optimized software implementation and a study of its computational efficiency had not been previously conducted. The present study fills this gap; in this paper we present the first program implementation of the RR-RCCD method.

This article considers the basic approximation of the coupled-cluster method, i. e. the CCD model, which assumes that the cluster operator includes only double excitations. The asymptotic computational complexity of this CC model scales as $O(N^6)$ with the number of molecular spinors $N$. The first implementation of the relativistic rank-reduced coupled-cluster method with doubles (RR-RCCD) has been developed. It should be noted that, despite its conceptual simplicity, this model allows for the thorough benchmarking of all key aspects and the identification of potential challenges in rank-reduced coupled-cluster methods. For this purpose, pilot calculations of electronic structure of linear chains $(AuCN)_n$ $(n = 1 - 5)$ were performed.

## 1. Rank-reduced relativistic coupled-cluster method

### 1.1. Representation of cluster amplitudes

Within the coupled-cluster (CC) theory, the ground state wave function $\langle\Psi\rangle$ is represented as

$$\langle\Psi\rangle = e^{\hat{T}}\langle\Phi_0\rangle, \tag{1}$$

where $\langle\Phi_0\rangle$ is a single-determinant wave function (typically a Hartree-Fock determinant), and $\hat{T}$ is a cluster operator. In the CCD approximation, it includes only a double excitation operator:

$$\hat{T}_2 = \frac{1}{2}\sum_{ijab} t_{ij}^{ab}\hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_j\hat{a}_i. \tag{2}$$

Here the $i, j, \ldots$ indices label spinors which are occupied in the vacuum determinant, and $a, b, \ldots$ label virtual spinors; $t_{ij}^{ab}$ stand for double excitation amplitudes. The amplitude equations of the CCD method have the following form:

$$t_{ij}^{ab}\varepsilon_{ij}^{ab} = R_{ij}^{ab}, \tag{3}$$

where $\varepsilon_{ij}^{ab} = \varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b$ is an energy denominator constructed from Hartree-Fock spinor energies, and the right-hand side $R_{ij}^{ab}$ depends on both cluster amplitudes and molecular integrals in a rather complicated manner.

The CCD method can be reformulated using the rank-reduced technique (resulting in the RR-RCCD approach) by representing an amplitude tensor in a factorized form *via* the Tucker decomposition [2]:

$$t_{ij}^{ab} = \sum_{XY}^{N_{\mathrm{SVD}}} T^{XY}U_{ai}^{X}U_{bj}^{Y}, \tag{4}$$

where $\mathbf{T}$ is a tensor of „compresse“ amplitudes (the „core“ tensor), and the three-index tensor $\mathbf{U}$ acts as a projector onto the subspace of compressed amplitudes. The projectors can be constructed with the use of many-body perturbation theory, e. g. the second-order (MP2) or third-order (MP3) M.ller-Plesset approximations. Although our previous study [18] indicate a structural similarity between the decomposition of MP3 amplitudes and the one of the exact tensor of coupled-cluster amplitudes, within the present paper the MP2 approximation due to the simplicity of its software implementation. A forthcoming transition to projectors from MP3 does not present any conceptual difficulties [3].

Despite the apparent similarity to the non-relativistic case, the complex arithmetic generally used within the relativistic framework to store both amplitude tensors $t_{ij}^{ab}$ and the projector $\mathbf{U}$ and operate with them necessitates significant modifications to the RR-CC computational scheme. This affects the adaptation of tensor decomposition algorithms employed and also requires to ensure that the coupled cluster equations are correctly projected onto the subspace of compressed amplitudes.

A key aspect for reducing the computational complexity of the RR-CCD method to $O(N^5)$ is the linear growth of the effective decomposition rank $N_{\mathrm{SVD}}$ with the system size [3]. In our previous study [18], we have directly confirmed that this condition is fulfilled for the relativistic formulation of the CC theory.

The properties of the projectors $\mathbf{U}$ are of great importance to construct the proper amplitude tensor factorization scheme. Columns of these projectors form an orthonormal basis in the subspace of „virtual-occupied“ spinor pairs:

$$\sum_{ai} U_{ai}^{X*}U_{ai}^{X'} = \delta_{XX'}. \tag{5}$$

Similarly to the original amplitude equations of the CCD method, the matrix of one-particle energies $E^{XX'} = \sum_{ai} U_{ai}^{X*}\varepsilon_{ia}U_{ai}^{X'}$ is defined in the „compressed“ representation, where $\varepsilon_{ia} = \varepsilon_a - \varepsilon_i$ is stands for the difference

of one-particle energies. This matrix needs to be represented using its spectral decomposition:

$$E^{XX'} = \sum_w V_w^X \varepsilon_w V_w^{X'*}. \quad (6)$$

The relations (5) and (6) allow for the projection of the right-hand side $R_{ij}^{ab}$ of the amplitude equations (3) onto the subspace of „compressed“ amplitudes. We arrive at the following form of the working amplitude equations:

$$T^{XY} = -\frac{R^{XY}}{\varepsilon_X + \varepsilon_Y}. \quad (7)$$

Here $T^{XY}$ represents the a tensor of compressed amplitudes (the Tucker decomposition core), $R^{XY} = \sum_{ijab} U_{ai}^{X*} U_{bj}^{Y*} R_{ij}^{ab}$ is the right-hand side of the amplitude equations in the compressed amplitude representation, and the energy denominator is constructed from the singular values of the matrix $E^{XX'}$. The explicit form of these working equations was previously derived and published in Ref. [18].

### 1.2. Decomposition and transformation of two-electron integrals

A reduction in the computational complexity of the coupled-cluster method can only be achieved through the simultaneous use of tensor decompositions for both the cluster amplitude and two-electron integral tensors. The most well-known approaches widely used for an efficient representation of two-electron integrals are the resolution of the identity (RI) approximation [19,20] and the partial Cholesky decomposition (PCD) [21,22]. Their combination allows one to avoid high computational cost associated with storing and directly transforming the full four-index tensor of two-electron integrals; this feature is especially critical for precision relativistic calculations employing extensive basis sets.

Within the present work a scheme for transforming two-electron integrals from the atomic basis to the molecular basis operates directly with three-index tensors is implemented. At the first stage, the two-electron integral tensor precomputed in the atomic orbital basis basis of atomic orbitals (AO) $\{\chi_\mu\}_{\mu=1}^{M}$ ($M$ is the number of basis functions) is factorized using the partial Cholesky decomposition:

$$(\mu\nu|\lambda\sigma) \approx \sum_{Q}^{M_{\text{aux}}} L_{\mu\nu}^{Q} L_{\lambda\sigma}^{Q}, \quad (8)$$

where $M_{\text{aux}}$ is the an effective rank of the decomposition in the AO basis. To achieve an acceptable accuracy, $M_{\text{aux}} \approx 4M$ is typically required. This results in a dramatic reduction in the amount of data to be stored and transformed from $O(M^4)$ to $O(M^2 M_{\text{aux}})$.

The subsequent three-index transformation to the basis of two-component molecularspinors

$$\psi_p = \sum_{\mu}^{M} C_{\mu p}^{\alpha} \chi_\mu \alpha + \sum_{\mu}^{M} C_{\mu p}^{\beta} \chi_\mu \beta \quad (9)$$

is performed for the tensors $L_{\mu\nu}^{Q}$ using the matrices $C_{p\mu}^{\alpha}$ and $C_{p\mu}^{\beta}$ containing expansion coefficients of molecular spinors:

$$V_{pr}^{Q} = \sum_{\mu} C_{\mu p}^{\alpha *} \sum_{\nu} C_{\nu r}^{\alpha} L_{\mu\nu}^{Q} + \sum_{\mu} C_{\mu p}^{\beta *} \sum_{\nu} C_{\nu r}^{\beta} L_{\mu\nu}^{Q}, \quad (10)$$

where $(pr|qs) = \sum_Q V_{pr}^{Q} V_{qs}^{Q}$. As a result, the computational complexity of the two-electron integral transformation is reduced from $O(M^5)$ to $O(M^3 M_{\text{aux}})$.

A similar procedure can be proposed for the resolution of the identity (RI) approximation. Despite the formal similarity of an algorithm with that presented for the PCD method, there are technical differences between them. Unlike PCD, the RI method uses an auxiliary basis set $\{\phi_P^{aux}\}$ to approximate products of basis function pairs ($\chi_\mu \chi_\nu \approx \sum_P D_{\mu\nu}^{P} \phi_P^{aux}$), which leads to a slightly different form of the working expressions. In this work, we use the PCD method due to its simplicity and the no need to use any external auxiliary basis set.

The presented algorithm for two-electron integrals transformation was formulated and implemented for the two-component approximation. It allows one to avoid the technical difficulties of the four-component formalism and to focus on the main idea of the method. At the same time, the algorithm can be readily extended to four-component calculations. The technical details of such a version of an integral transformation algorithm, including the use of the RI method, are described in detail in the literature (see, for example, Ref. [23]).

## 2. Program implementation

The developed software packages were fully written in the Rust programming language to ensure their high performance, code safety, and reliability. The core of the software suite developed is the *tensor-decompositions* package, which provides implementations of tensor decompositions, including the Tucker decomposition, as well as the functionality for performing tensor contractions. This package is built upon the *ndarray* library, which enables efficient work with multidimensional arrays, and the high-performance BLAS library [24] is utilized for optimizing linear algebra operations. All matrix decomposition algorithms also employ subroutines from the LAPACK library [25].

Using the *tensor-decompositions* library, a specialized package named *ccrs* for performing precise quantum-chemical calculations using the relativistic coupled-cluster method was developed. A key feature of this package is the active use of the PCD method for an efficient decomposition and transformation of molecular integrals. The *ccrs* package implements the relativistic rank-reduced coupled-cluster method with doubles (RR-RCCD), which allows one to demonstrate the key features of the RR-RCC approach.

Two-component Hartree-Fock calculations were performed using the PySCF software package [26,27], extended

with the LIBGRPP library [28,29] to compute AO integrals involving generalized relativistic pseudopotential (GRPP) operators [30].

## 3. Objects for benchmark calculations

Benchmark calculations employing the newly developed RR-RCCD method were performed for the series of linear gold(I) cyanide molecules $(AuCN)_n$, $n = 1-5$. These molecules were chosen due to the following reasons:

(a) one-dimensional systems seem to be nearly optimal for the numerical verification of the asymptotic complexity of methods exploiting the locality of electron correlation effects,

(b) the availability of X-ray structural data for the crystalline AuCN,

(c) a precise description of these systems is impossible without a balanced accounting for relativistic effects.

All calculations used the bond lengths $r$(Au-C) = 1.9717 Å, $r$(C-N) = 1.1547 Å, and $r$(N-Au) = 1.9717 Å taken from experimental data for the AuCN crystal [31]. Relativistic effects including spin-orbit coupling, the Breit electron-electron interaction [32], and finite-nucleus size corrections for Au [33], were accounted for using the generalized relativistic effective pseudopotential replacing 60 core electrons of gold. A basis set comprising $(13s11p10d10f5g)/[5s6p5d2f1g]$ compact Gaussian functions from work [18] was used to describe the valence shells of Au; $spd$-functions from the cc-pVTZ basis set [34] were used for C and N atoms, while $f$-functions were not used. The $5d$ and $6s$ orbitals of the Au atom, and the $2s$ and $2p$ orbitals of the C and N atoms were correlated at the CCD level, while sub-valence shells were kept frozen.

## 4. Results and discussion

Fig. 1 depicts the dependence of the amplitude tensor $t_{ij}^{ab}$ effective rank $N_{\mathrm{SVD}}$ on the number of monomers $n$ in the molecular chain $(AuCN)_n$. The threshold for discarding small singular values for the tensor of cluster amplitudes for the cluster amplitudes was set to $5 \cdot 10^{-5}$, and for the two-electron integrals; these thresholds approximately correspond to $N_{\mathrm{SVD}} \sim 4-5\,N$.

As the number of monomers $n$ increases, the effective rank $N_{\mathrm{SVD}}$ grows as $O(N^{1.03})$. This could be explained by the fact that as the length of the $(AuCN)_n$ chain increases, the effect of the local nature of electron correlations becomes more pronounced, allowing the correlations in such systems to be described by a relatively small number of cluster amplitudes. However, the obtained power (which is close to 1) roots in the use of the MP2 approximation to generate the projectors $U_{ai}^{X}$. It was demonstrated in Ref. [18] that this power should somewhat increase for projectors obtained at the MP3 level of theory. Fig. 1 also shows the dependence of the computation time per single iteration on the number of monomers in the $(AuCN)_n$

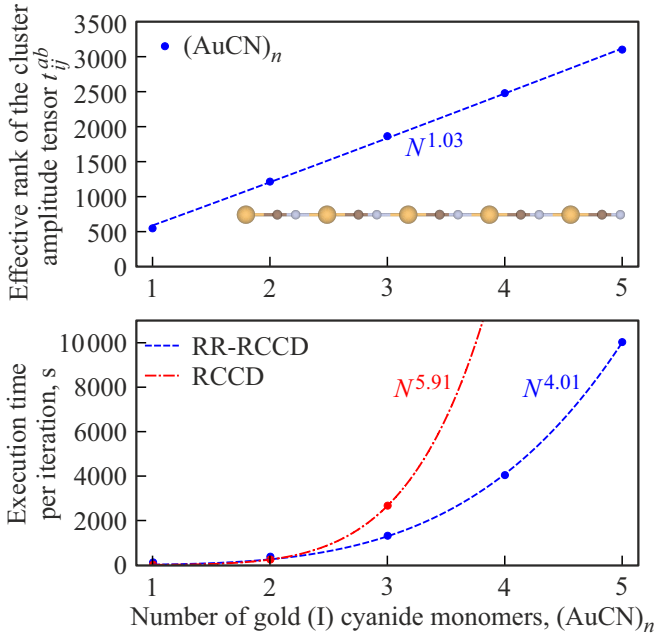



**Figure 1.** Dependence of the amplitude tensor $t_{ij}^{ab}$ effective rank $N_{\mathrm{SVD}}$ on the number of monomers $n$ in the molecular chain $(AuCN)_n$ (upper panel) and an estimate of the computational complexity of solving the RR-RCCD amplitude equations (lower panel).

chain. The computational complexity can be estimated as $O(N^{4.01})$, which agrees with the theoretical estimate of $O(N^5)$ obtained earlier for the RR-RCCD method in Ref. [18]. The overall complexity lower than $O(N^5)$ can be partly explained by the presence of terms with the $O(N^4)$ asymptotic scaling law in the amplitude equations.

The execution time of individual stages of the RR-RCCD calculation for $(AuCN)_5$ is shown in Fig. 2. It can be seen that the main portion of the computational cost (about 40% of the total time) can be attributed to the preparatory step, during which the terms remaining constant throughout the entire calculation are precomputed. At the same time, the tensor decompositions themselves require a negligible small amount of time. It is worth noting that achieving the overall $O(N^5)$ computational complexity requires the introduction of auxiliary intermediate tensors $O_{kilj}$ and $Z_{kjbc}$ (see their definitions in Refs. [3,18]). These tensors, in turn, also need to be represented *via* additional decompositions into lower-dimensional arrays.

A comparative analysis of the required computational resources (Table) demonstrates that the RR-RCCD method requires significantly less RAM than the standard full-tensor implementation of RCCD not employing any tensor decompositions. This advantage becomes of particular importance when the standard method becomes prohibitively expensive, e. g. for our supercomputer facilities. Furthermore, the RR-RCCD method provides a speedup in computations starting from the number of monomers $n = 3$.

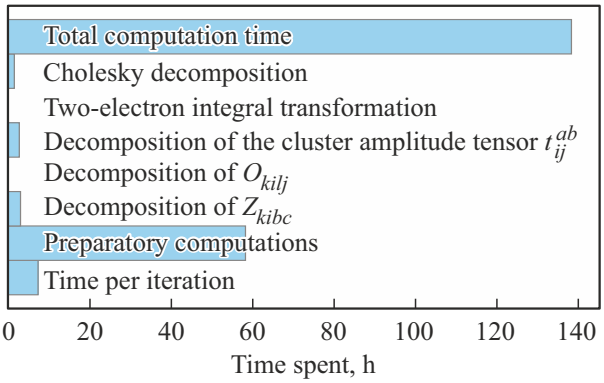



**Figure 2.** The breakdown of the time elapsed for the RR-RCCD calculation of the $(AuCN)_5$ molecule. Calculations were performed on a single compute node with an Intel Xeon E5-2680 processor.

Comparison of the maximum RAM usage and the execution time per single CC iteration for the RCCD and RR-RCCD methods

| Number of monomers AuCN ($n$) | Memory used, GB | | Execution time, s | |
|---|---|---|---|---|
| | RCCD | RR-RCCD | RCCD | RR-RCCD |
| 1 | 9 | 5 | 11 | 116 |
| 2 | 138 | 36 | 243 | 373 |
| 3 | 701 | 179 | 2669 | 1315 |
| 4 | – | 523 | – | 4043 |
| 5 | – | 1319 | – | 10030 |

## 5. Conclusions

The relativistic rank-reduced coupled-cluster method with with double excitations (RR-RCCD) has been developed and implemented as a software package in the Rust programming language. The method demonstrates a reduction in computational cost compared to the standard CCD method from $O(N^6)$ to $O(N^5)$, thus opening new prospects for high-precision modeling of complex systems containing heavy elements, including quite extended cluster models of solids.

Further developments of the RR-RCC method require addressing a number of technical challenges. A key task is the implementation of the RR version of the CCSD method, as the inclusion of single excitations is necessary for the correct calculation of properties other than the energy; chemical shifts in X-ray emission spectra are of particular interest for primary applications [13]. Furthermore, to improve the accuracy of the method, the development of an computationally efficient algorithm for evaluating the projectors $U_{ai}^X$ within the MP3 approximation is planned.

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### Conflict of interest

The authors declare no conflict of interest.

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