

# Tensor decomposition methods for high-precision relativistic modeling of electronic structure




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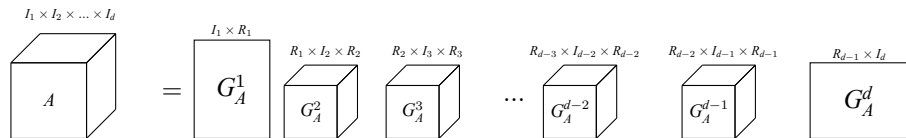
# Introduction. CC equations

CCSD		$\sum t_{ij}^{cd} \langle ab    cd \rangle \Rightarrow O(N^6)$
CCSDT		$\sum t_{ijk}^{dec} \langle ab    de \rangle \Rightarrow O(N^8)$
CCSDTQ		$\sum t_{ijkl}^{efcd} \langle ab    ef \rangle \Rightarrow O(N^{10})$

# Tensor Train

Tensor  $A$  is presented in TT format if

$$A_{i_1 i_2 \dots i_d} = \sum_{\alpha_1 \dots \alpha_d}^{R_1 \dots R_d} G_1[1, i_1, \alpha_1] G_2[\alpha_1, i_2, \alpha_2] \dots G_d[\alpha_d, i_d, 1], \text{ где } G_j \in \mathbb{C}^{R_j \times I_j \times R_{j+1}}$$



Terminology:

- $G_i$  - TT-core;
- $R_i$  - TT-dimensions;
- $R = \max_i(R_i)$  - maximum TT-dimension.

Oseledets I. V. Tensor-Train Decomposition // SIAM Journal on Scientific Computing. 2011. V.33, no. 5. PP. 2295–2317. doi: 10.1137/090752286.

# Contraction. TT-TT

$$\begin{array}{c} I_1 \times I_2 \times \dots \times K \\ \text{Cube } A \end{array} = \begin{array}{c} I_1 \times R_1 \\ \text{Cube } G_A^1 \end{array} \begin{array}{c} R_1 \times I_2 \times R_2 \\ \text{Cube } G_A^2 \end{array} \begin{array}{c} R_2 \times I_3 \times R_3 \\ \text{Cube } G_A^3 \end{array} \dots \begin{array}{c} R_{d-3} \times I_{d-2} \times R_{d-2} \\ \text{Cube } G_A^{d-2} \end{array} \begin{array}{c} R_{d-2} \times I_{d-1} \times R_{d-1} \\ \text{Cube } G_A^{d-1} \end{array} \begin{array}{c} R_{d-1} \times K \\ \text{Cube } G_A^d \end{array}$$

## TT-TT

$$\begin{array}{c} K \times J_2 \times \dots \times J_d \\ \text{Cube } B \end{array} = \begin{array}{c} K \times L_1 \\ \text{Cube } G_B^1 \end{array} \begin{array}{c} L_1 \times J_2 \times L_2 \\ \text{Cube } G_B^2 \end{array} \begin{array}{c} L_2 \times J_3 \times L_3 \\ \text{Cube } G_B^3 \end{array} \dots \begin{array}{c} L_{d-3} \times J_{d-2} \times L_{d-2} \\ \text{Cube } G_B^{d-2} \end{array} \begin{array}{c} L_{d-2} \times J_{d-1} \times L_{d-1} \\ \text{Cube } G_B^{d-1} \end{array} \begin{array}{c} L_{d-1} \times J_d \\ \text{Cube } G_B^d \end{array}$$

$$\begin{array}{c} I_1 \times I_2 \times \dots \times I_d \\ \text{Cube } A \end{array} \times_d \begin{array}{c} J_1 \times J_2 \times \dots \times J_d \\ \text{Cube } B \end{array} = \dots \begin{array}{c} R_{d-2} \times I_{d-1} \times R_{d-1} \\ \text{Cube } G_A^{d-1} \end{array} \begin{array}{c} R_{d-1} \times K \\ \text{Cube } G_A^d \end{array} \cdot \begin{array}{c} K \times R_1 \\ \text{Cube } G_B^1 \end{array} \begin{array}{c} L_1 \times J_2 \times L_2 \\ \text{Cube } G_B^2 \end{array} \dots$$

# Contraction. TT-Matrix

$$\begin{array}{c} I_1 \times I_2 \times \dots \times I_d \\ \text{---} \\ \text{Cube } A \end{array} = \begin{array}{c} I_1 \times R_1 \\ \text{---} \\ \text{Matrix } G_A^1 \end{array} \begin{array}{c} R_1 \times I_2 \times R_2 \\ \text{---} \\ \text{Cube } G_A^2 \end{array} \begin{array}{c} R_2 \times I_3 \times R_3 \\ \text{---} \\ \text{Cube } G_A^3 \end{array} \dots \begin{array}{c} R_{d-3} \times I_{d-2} \times R_{d-2} \\ \text{---} \\ \text{Cube } G_A^{d-2} \end{array} \begin{array}{c} R_{d-2} \times I_{d-1} \times R_{d-1} \\ \text{---} \\ \text{Cube } G_A^{d-1} \end{array} \begin{array}{c} R_{d-1} \times I_d \\ \text{---} \\ \text{Matrix } G_A^d \end{array}$$

## TT-Матрица

$$\begin{array}{c} I_1 \times I_2 \times \dots \times I_d \\ \text{---} \\ \text{Cube } A \end{array} \times_k \begin{array}{c} I_k \times J \\ \text{---} \\ \text{Matrix } M \end{array} = \dots \begin{array}{c} R_{k-2} \times I_{k-1} \times R_{k-1} \\ \text{---} \\ \text{Cube } G_A^{k-1} \end{array} \begin{array}{c} R_{k-1} \times I_k \times R_k \\ \text{---} \\ \text{Cube } G_A^k \end{array} \times_{\frac{1}{2}} \begin{array}{c} I_k \times J \\ \text{---} \\ \text{Matrix } M \end{array} \begin{array}{c} R_k \times I_{k+1} \times R_{k+1} \\ \text{---} \\ \text{Cube } G_A^{k-1} \end{array} \dots$$

# Some conclusions

## Advantages

- The complexity of contractions is greatly reduced and, most importantly, depends on the dimension of the tensor **linearly**;
- Data is being **compressed**.

## Disadvantages

- "The tensor **must be singular**";
- The addition operation **increases** the size of the cores.

# Applications

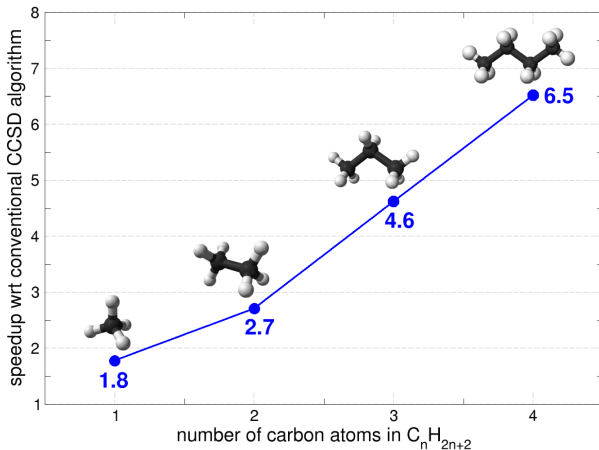


Figure 1: Speeding up the calculation of alkanes

# Conclusion

- The library is written in the Rust language and includes functions and decompositions.
- The CCSD approximation is implemented in terms of tensor trains and is almost embedded in the EXP-T software package.
- Implementation of the solution of the CCSDT and CCSDTQ equations in terms of tensor trains.



# Bibliography

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## Summation. Additionally

$A$  and  $B$  are given in TT format:

$$A = G_1^A \times_3 G_2^A \times_3 \dots \times_3 G_d^A$$

$$B = G_1^B \times_3 G_2^B \times_3 \dots \times_3 G_d^B$$

It is necessary to find

$$C = A + B.$$

Then the cores for  $C$  are defined as follows:

$$G_i^C = \begin{bmatrix} G_i^A & 0 \\ 0 & G_i^B \end{bmatrix}, \text{ для } i = 1, \dots, d.$$

Thus,  $C$  in TT format will look like this:

$$C = G_1^C \times_3 G_2^C \times_3 \dots \times_3 G_d^C$$