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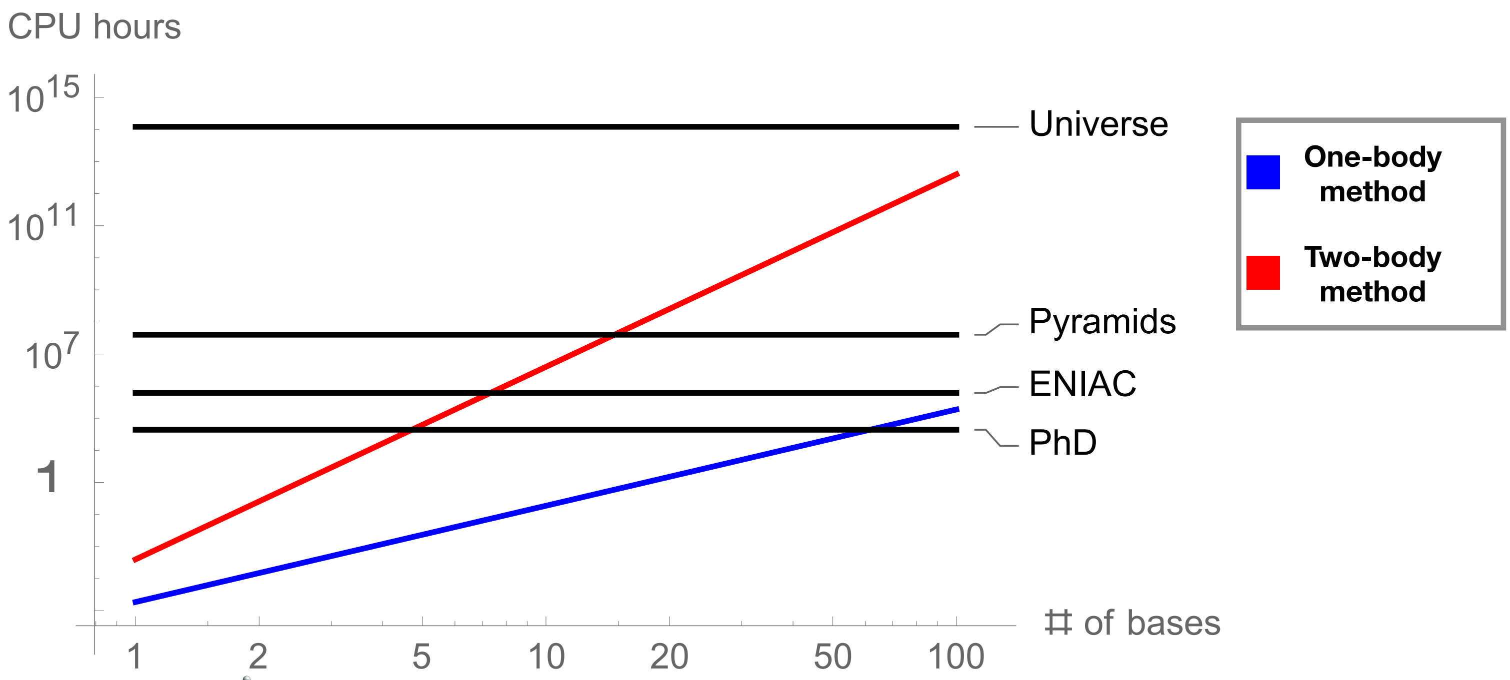
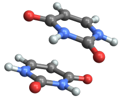
APPROXIMATING TENSOR CONTRACTIONS VIA A MATRIX-FREE TENSOR DECOMPOSITION

KARL PIERCE

The cost of molecular electronic structure methods





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The correlation between storage and computational cost

	Computational Scaling	Storage	Element of highest order tensor
CCSD	$\mathcal{O}(N^6)$	$\mathcal{O}(N^4)$	t_{ab}^{ij}
CCSDT	$\mathcal{O}(N^8)$	$\mathcal{O}(N^6)$	t_{abc}^{ijk}
CCSD(T)	$\mathcal{O}(N^7)$	$\mathcal{O}(N^4)$	t_{ab}^{ij}

Purvis, G. D.; Bartlett, R. J. *The Journal of Chemical Physics* 1982, *76*, 1910–1918.

Raghavachari, K.; Trucks, G. W.; Pople, J. A.; Head-Gordon, M . *Chemical Physics Letters* 1989, *157*, 479–483.

Noga, J.; Bartlett, R. J. *J. Chem. Phys.* 1987, *86*, 7041.

Tensor compression techniques

Matrix Decomposition

Singular Value Decomposition

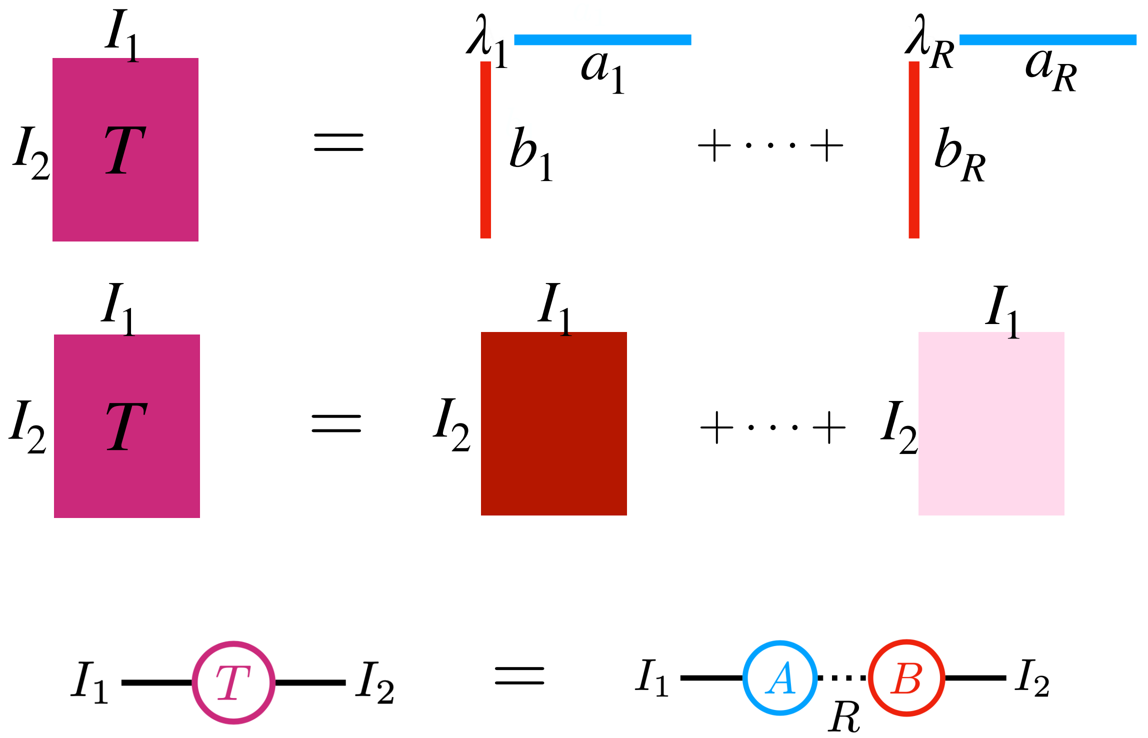
Cholesky Decomposition

Tensor Decomposition

Canonical Polyadic Decomposition

Tucker Decomposition

Singular value decomposition (SVD)



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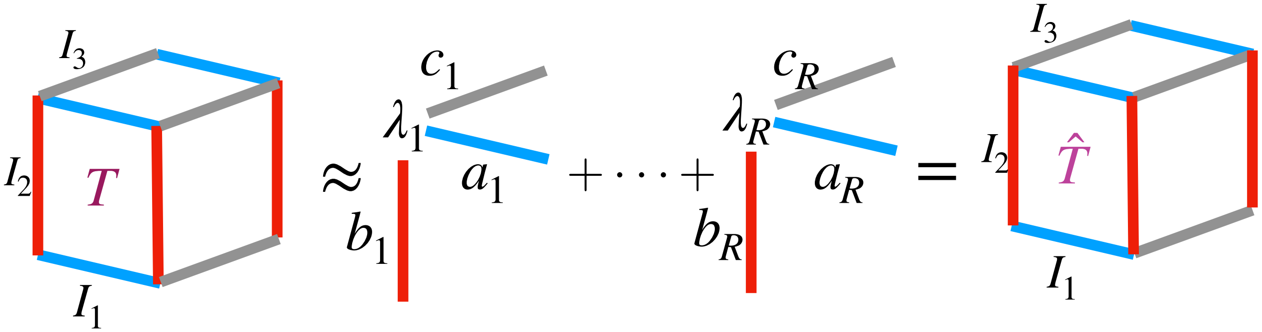
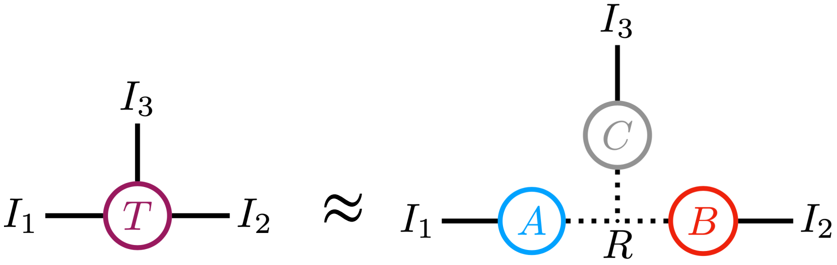
Canonical Polyadic Decomposition (CPD)



$$A = \{a_r\} \in \mathscr{R}^{I_1 \times R}$$



$$\mathcal{O}(I^3) \rightarrow \mathcal{O}(3IR)$$

Harshman, R. UCLA Work. Pap. Phonetics 1970, 16 (10), 1–84.
Carroll, J. D.; Chang, J. J. Psychometrika 1970, 35 (3), 283–319.

Coupled Cluster Optimization

Compute the coupled cluster wavefunction

$$|\Psi_{cc}\rangle = e^{\hat{T}}|\Psi_0\rangle$$

$$\hat{T} = \sum_{ia} t_i^a a_a^i + \sum_{ijab} t_{ij}^{ab} a_{ab}^{ij} + \dots$$

Truncate the cluster operator at nth-excitation

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Coupled Cluster Optimization

Compute the coupled cluster wavefunction

$$|\Psi_{cc}\rangle = e^{\hat{T}}|\Psi_0\rangle$$

$$\hat{T}_{ccsd} = \sum_{ia} t_i^a a_a^i + \sum_{ijab} \boxed{t_{ij}^{ab}} a_{ab}^{ij}$$

Goal: Optimize the n excitation tensors

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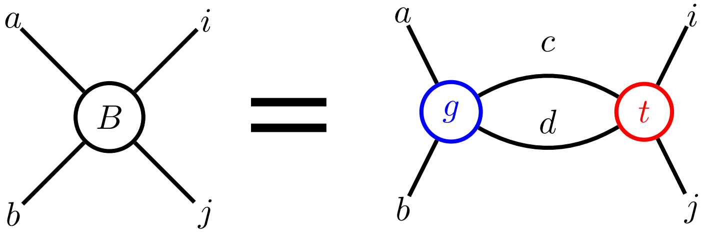
CCSD Optimization

t_{ij}^{ab} tensor optimization involves

$$^{n}R_{ij}^{ab} = A_{ij}^{ab} + B_{ij}^{ab} + C_{ij}^{ab} + D_{ij}^{ab} \qquad\qquad {}^{n}t = {}^{n-1}t + \alpha({}^{n}R)$$

Particle-Particle Ladder Diagram

$$B_{ij}^{ab} = \sum_{cd} g_{cd}^{ab} t_{ij}^{cd}$$



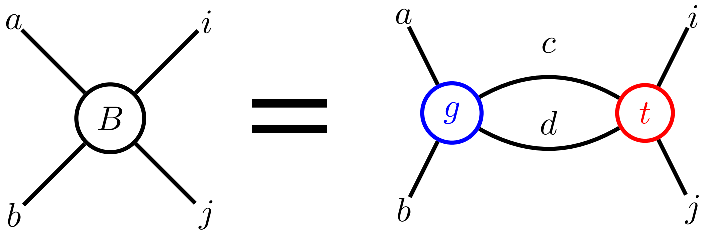
G. D. Purvis and R. J. Bartlett,
J. Chem. Phys. 76, 1910–1918 (1982).

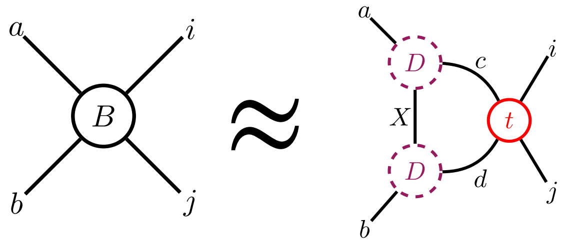
It is standard to approximate tensors in a network

$$B_{ij}^{ab} = \sum_{cd} g_{cd}^{ab} t_{ij}^{cd}$$

Density Fitting Approximation

$$B_{ij}^{ab} \approx \sum_{cdX} D_c^{aX} D_d^{bX} t_{ij}^{cd}$$





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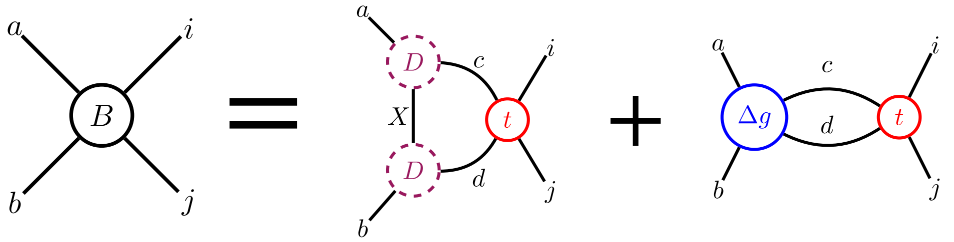
Error associated with approximated tensors in a network is amplified.

DF approximation error

$$B_{ij}^{ab} = \sum_{cdX} D_c^{aX} D_d^{bX} t_{ij}^{cd} + \sum_{cdX} \Delta g_{cd}^{ab} t_{ij}^{cd}$$



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Error associated with approximated tensors in a network is amplified.

CPD approximation

$$\sum_{cd} g_{cd}^{ab} t_{ij}^{cd} \approx \sum_{cd} \sum_{X} \hat{D}_c^{aX} D_d^{bX} t_{ij}^{cd}$$

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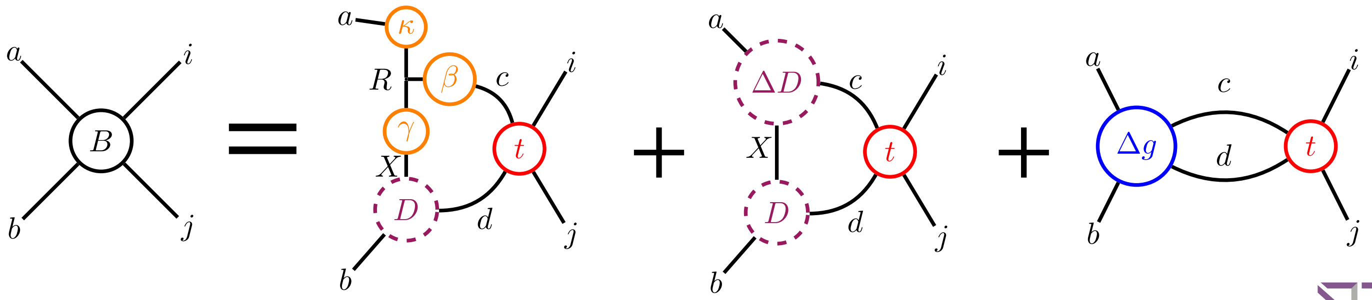
Error associated with approximated tensors in a network is amplified.

CPD approximation error

$$\sum_{cd} g_{cd}^{ab} t_{ij}^{cd} = \sum_{cd} \Big(\sum_{X} \hat{D}_c^{aX} D_d^{bX} + \sum_{X} \Delta D_c^{aX} D_d^{bX} + \Delta g_{cd}^{ab} \Big) t_{ij}^{cd}$$



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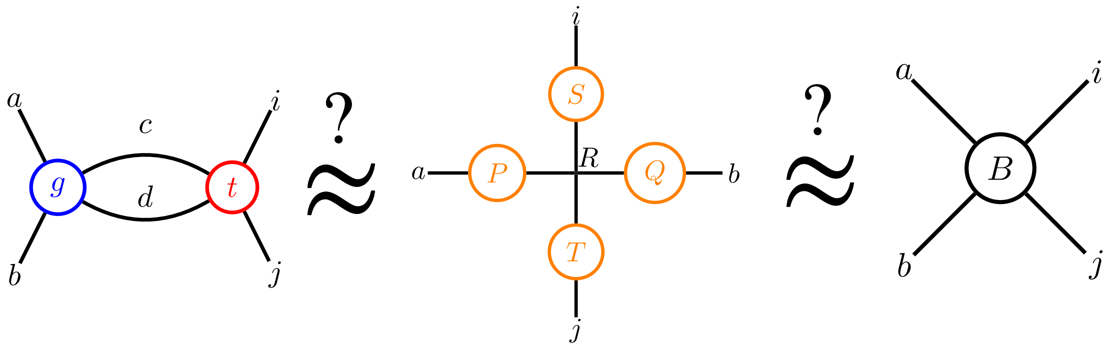
Is it possible to approximate the tensor contraction as a network?



$$f(x) = \frac{1}{2} \| \sum_{cd} g_{cd}^{ab} t_{ij}^{cd} - \hat{B}_{ij}^{ab}(x) \|_2^2 \qquad \hat{B}_{ij}^{ab}(x) = \sum_{r}^{R_{cp}} P_r^a Q_r^b S_i^r T_j^r$$

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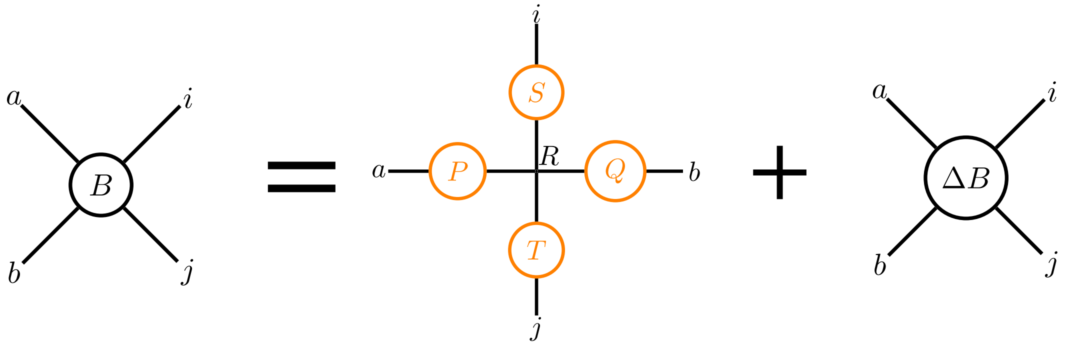
Is it possible to approximate the tensor contraction as a network?



$$B_{ij}^{ab} = \hat{B}_{ij}^{ab} + \Delta_{CPD} B_{ij}^{ab}$$

$\Delta_{CPD}B$ is directly controllable via the CPD

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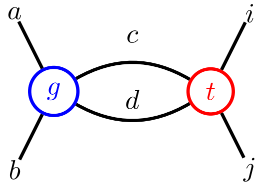
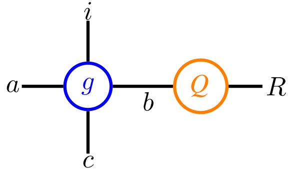
Side note: the CPD optimization of B is cheaper than the canonical contraction



$$\mathcal{O}(N^6)$$

$$\frac{\partial f(x)}{\partial P} = \sum_{cd} \boxed{\Big(\sum_{b} g^{ab}_{cd} Q^{b}_{r}\Big)} \Big(\sum_{ij} t^{cd}_{ij} S^{r}_{i} T^{r}_{j}\Big) - P^{a}_{r}(Q^{b}_{r} Q^{b}_{r'}) * (S^{r}_{i} S^{r'}_{i}) * (T^{r}_{j} T^{r'}_{j})$$



$$\mathcal{O}(N^4 R)$$

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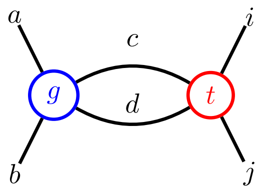
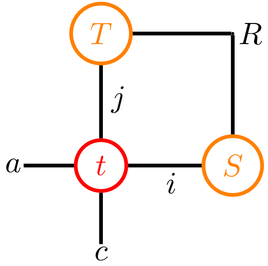
Side note: the CPD optimization of B is cheaper than the canonical contraction



$$\mathcal{O}(N^6)$$

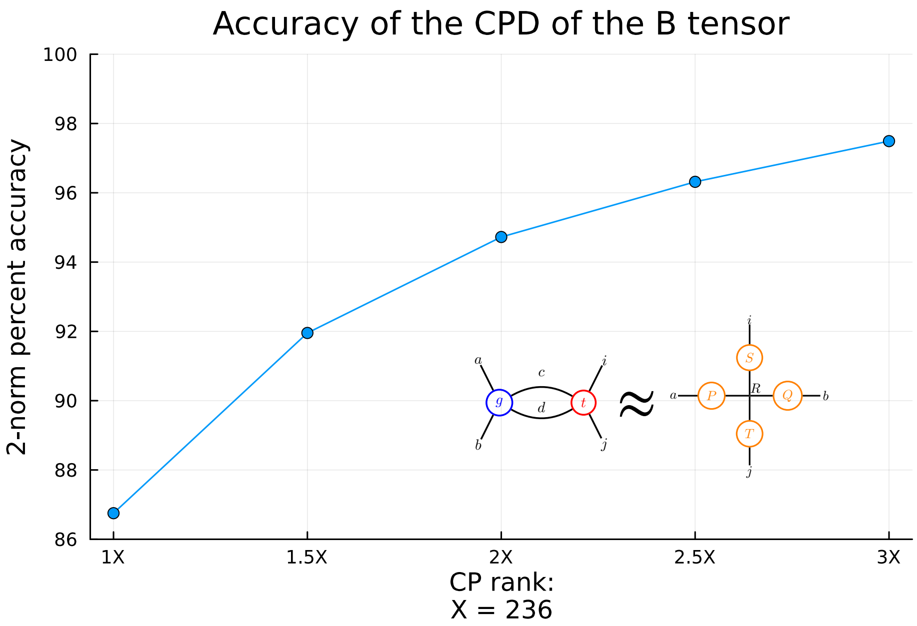
$$\frac{\partial f(x)}{\partial P} = \sum_{cd} g_{cd}^{ar}\left(\boxed{\sum_{ij} t_{ij}^{cd} S_i^r T_j^r}\right) - P_r^a (Q_r^b Q_{r'}^b) * (S_i^r S_i^{r'}) * (T_j^r T_j^{r'})$$

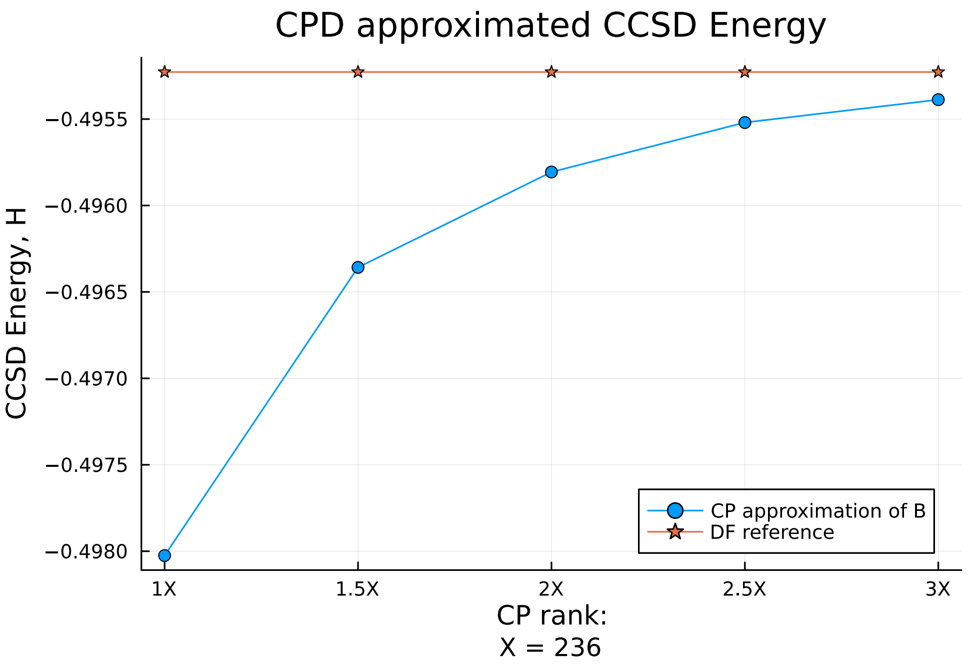


$$\mathcal{O}(N^4 R)$$

CP approximation of PPL tensor network

$(H_2O)_2$ TIP4P geometry
DZ-F12/aug-DZ-RI





$$\text{percent accuracy} = (1.0 - \|B - \hat{B}\|_2 / \|B\|_2) * 100$$

How does one choose a stopping condition?

Canonical stopping condition:
2-norm error

$$\Delta_n = \|B_{ij}^{ab} - \hat{B}_{ij}^{ab}(x_n)\|$$

$$\Delta_n - \Delta_{n-1} < \epsilon_{ALS}$$

Computational complexity: $\mathcal{O}(N^6)$

Proposed stopping condition:
2-norm error

$$\Upsilon_n = \|\hat{B}_{ij}^{ab}(x_n) - \hat{B}_{ij}^{ab}(x_{n-1})\|$$

$$\Upsilon_n < \epsilon_{ALS}$$

Computational complexity: $\mathcal{O}(N^3)$

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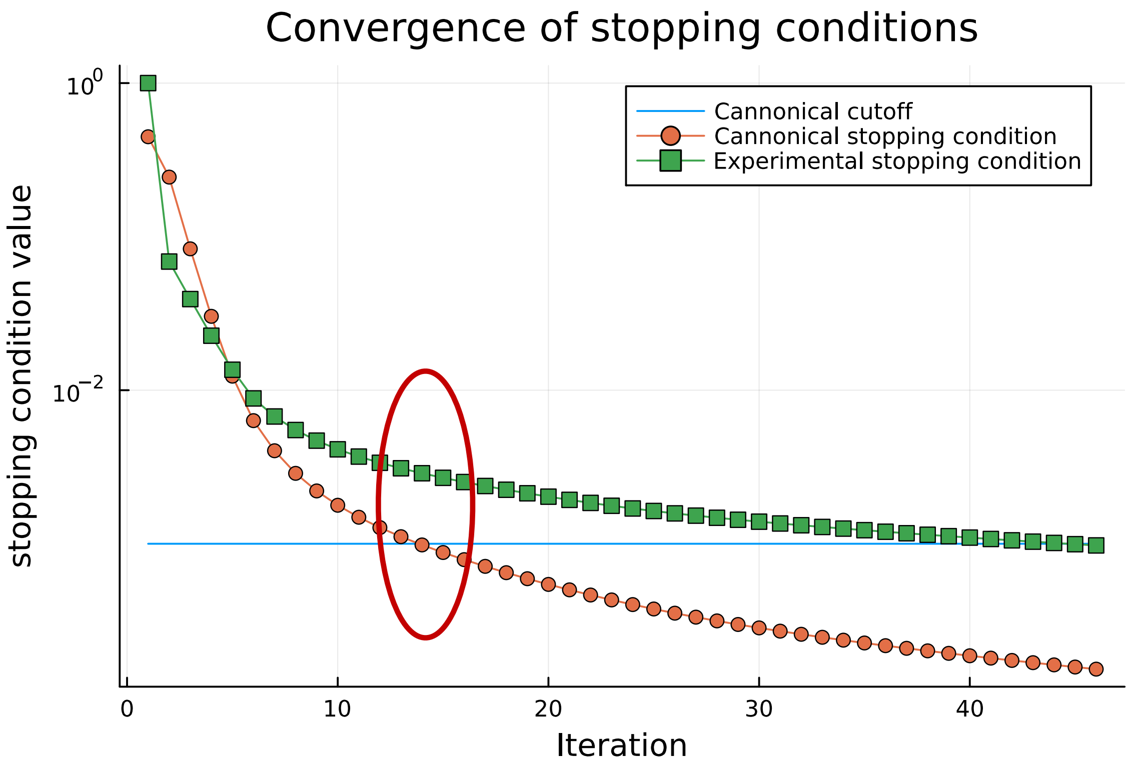
Comparing stopping conditions

$(H_2O)_2$ TIP4P geometry
DZ-F12/aug-DZ-RI



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Result

It is feasible to approximate a tensor network contraction as a matrix free tensor decomposition

Question: Can we make this CPD "contraction" more efficient?

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Is there a way to reduce the cost of the CPD?

$$ {}^{n}R_{ij}^{ab} = A_{ij}^{ab} + B_{ij}^{ab} + C_{ij}^{ab} + D_{ij}^{ab} \qquad {}^{n}t = {}^{n-1}t + \alpha({}^{n}R) $$

Iteration 1: $${}^{1}B_{ij}^{ab} = g_{cd}^{ab}({}^{1}t_{ij}^{cd})$$

Iteration 2: $${}^{2}B_{ij}^{ab} = g_{cd}^{ab}({}^{2}t_{ij}^{cd}) \qquad {}^{2}B_{ij}^{ab} \approx g_{cd}^{ab}({}^{1}t_{ij}^{cd} + \delta {}^{1}t_{ij}^{cd})$$

Idea:

The optimized ${}^{n-1}\hat{B}$ factors might be a good initial guess for the nth CC iteration's CPD

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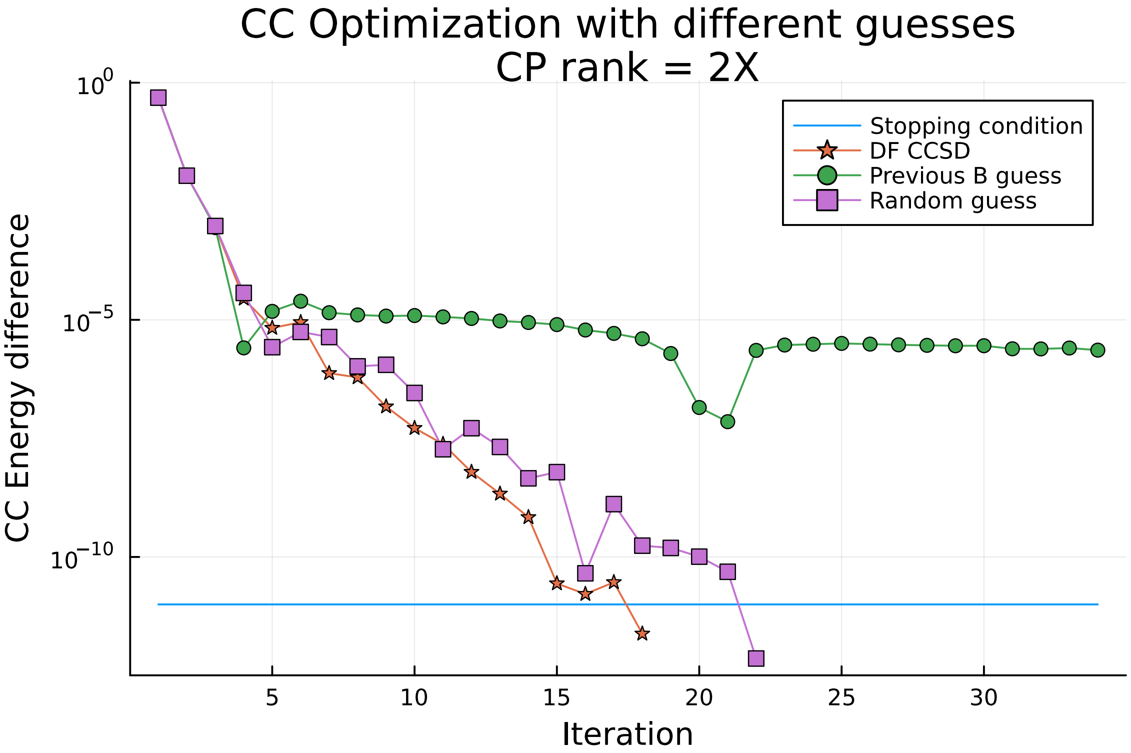
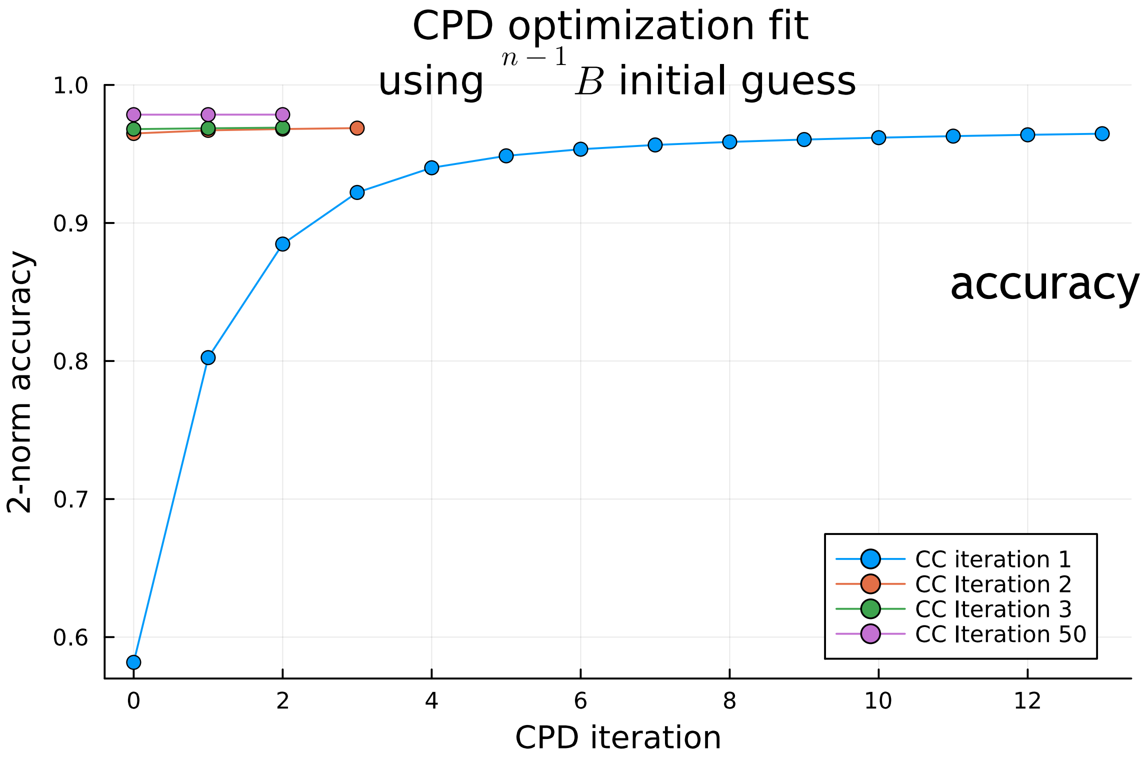
Is there a way to reduce the cost of the CPD?

$(H_2O)_2$ TIP4P geometry
DZ-F12/aug-DZ-RI



Perhaps this is border-rank optimization issue.

$(H_2O)_2$ TIP4P geometry
DZ-F12/aug-DZ-RI



$$\text{accuracy} = 1.0 - \frac{\|B - \hat{B}\|_2}{\|B\|_2}$$

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Perhaps this is border-rank optimization issue.

TAMARA G. KOLDA AND BRETT W. BADER

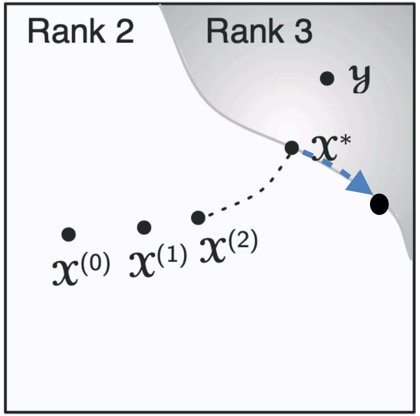

Fig. 3.2 *Illustration of a sequence of tensors converging to one of higher rank* [144].

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Perhaps this is border-rank optimization issue.

Strategy:
If CPD does 8+ iterations,
Save the factors of iteration 7
else,
Construct $\hat{B}$ and throw factors away

TAMARA G. KOLDA AND BRETT W. BADER

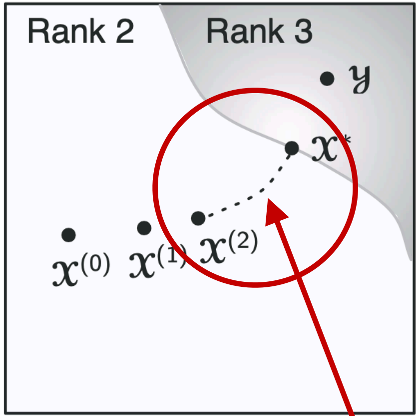

Fig. 3.2 *Illustration of a sequence of tensors converging to one of higher rank* [144].

Better idea:
Take advantage of the optimizations velocity to put us at a "good" answer

Use a set of factors from one of these iterations

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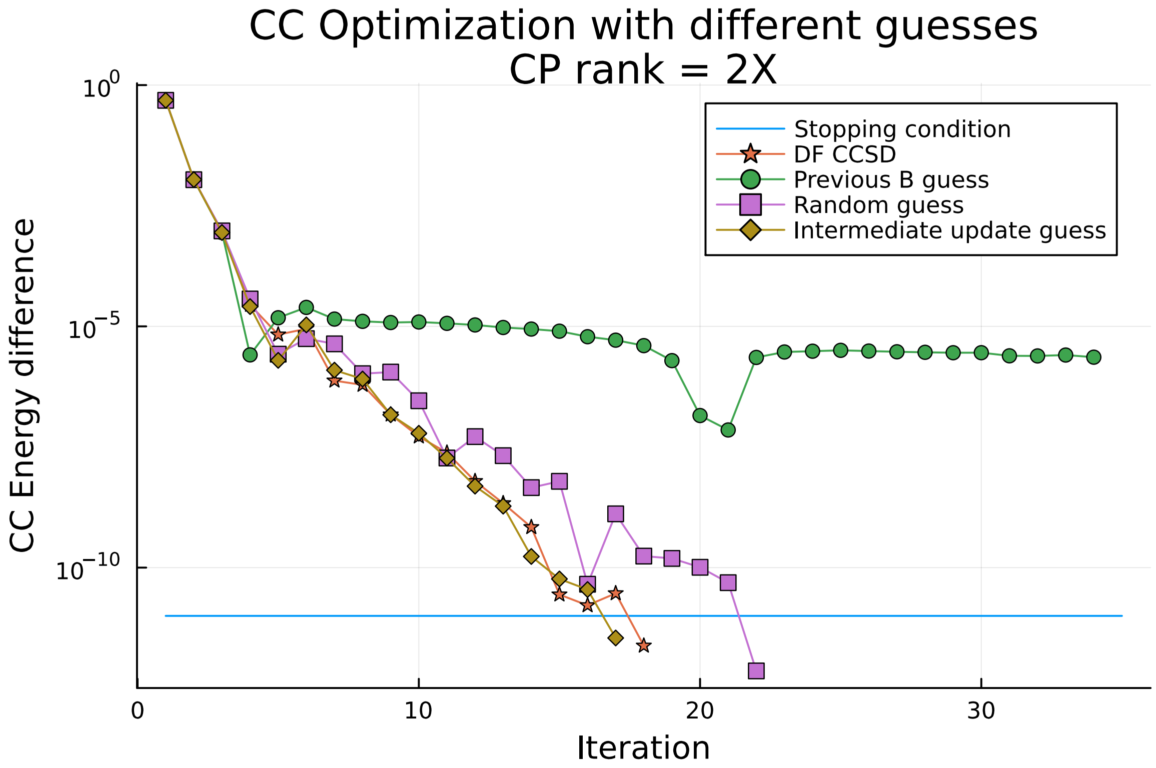
Is there a way to reduce the cost of the CPD?

$(H_2O)_2$ TIP4P geometry
DZ-F12/aug-DZ-RI



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Is there a way to reduce the cost of the CPD?

$(H_2O)_2$ TIP4P geometry
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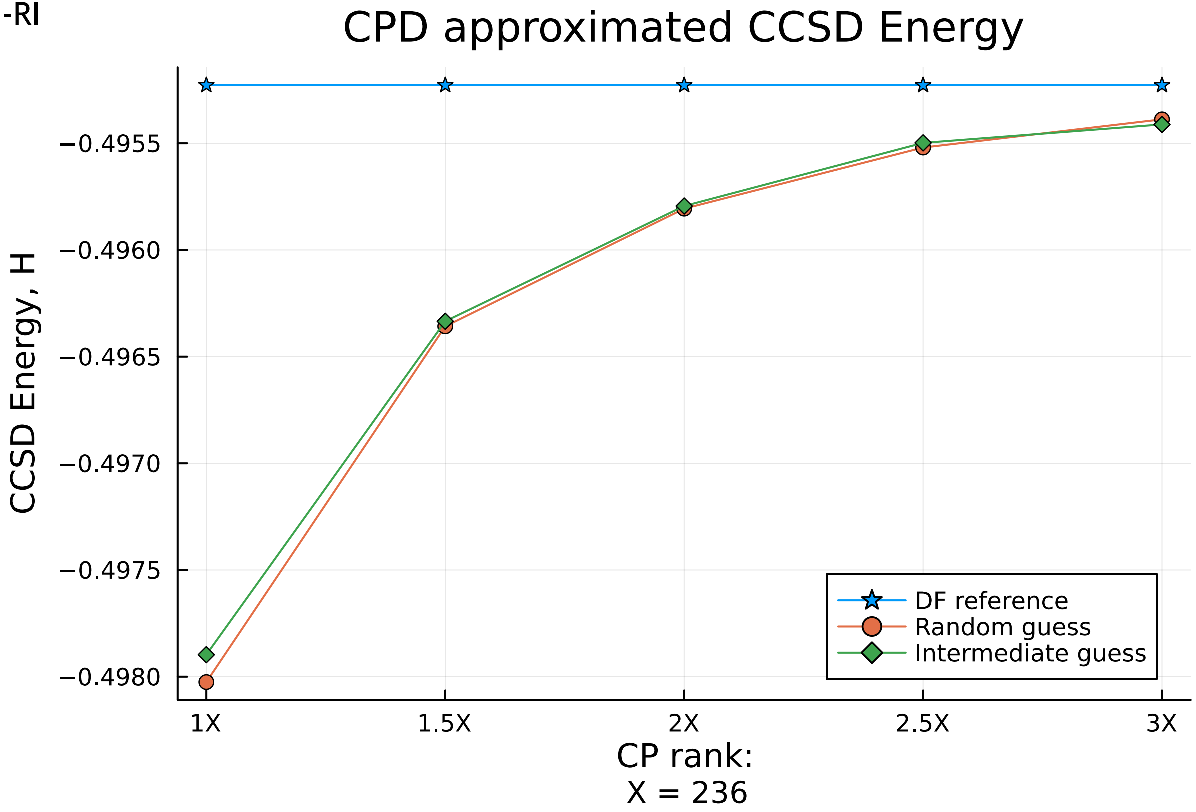
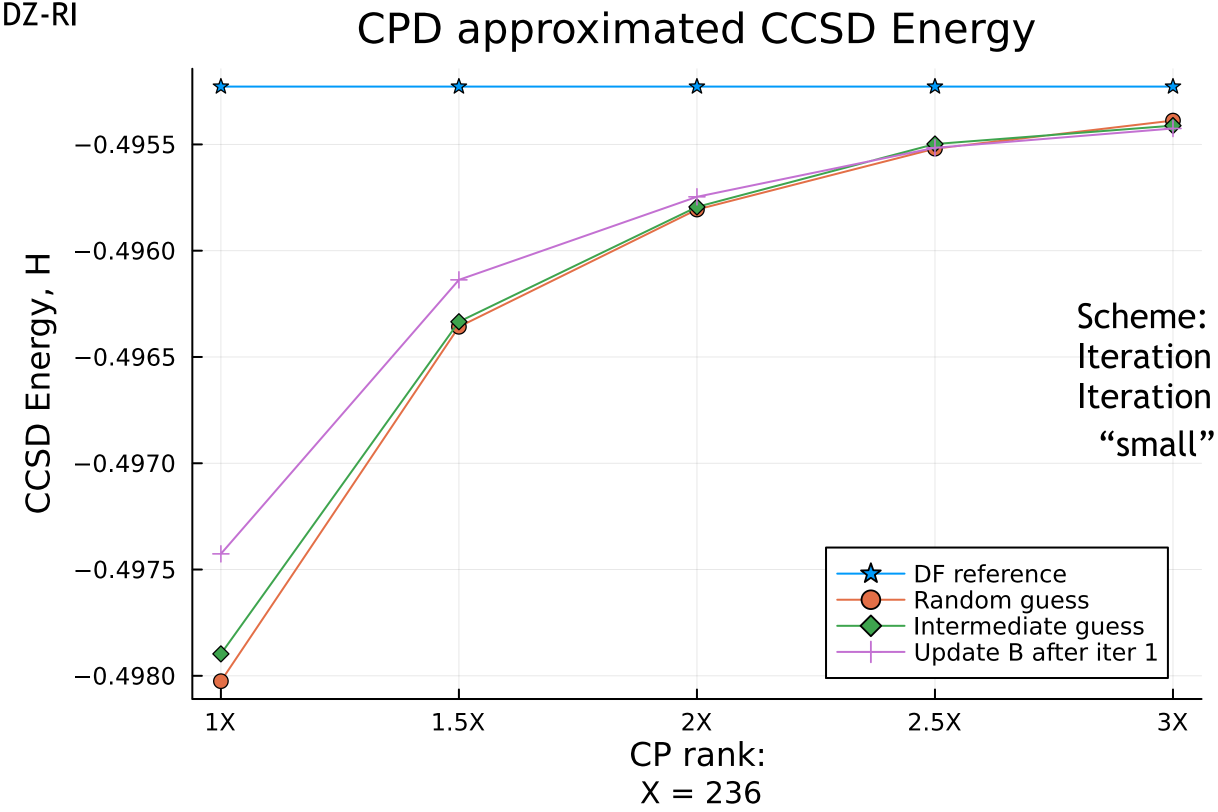


Is it necessary to recompute $\hat{B}$ every CC iteration?

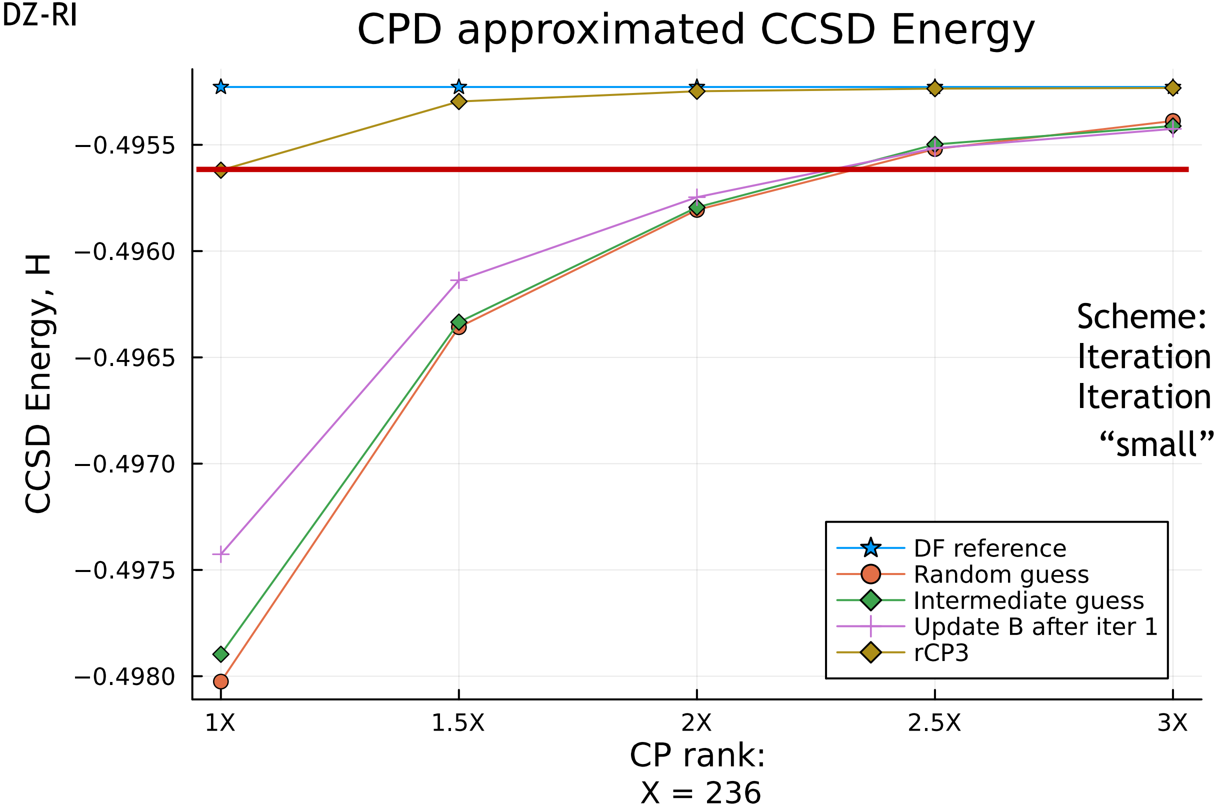
$(H_2O)_2$ TIP4P geometry
DZ-F12/aug-DZ-RI



Scheme:
Iteration 1: use full CPD rank
Iteration 2+: use fixed, "small" CPD rank (here I use X)

Is it necessary to recompute $\hat{B}$ every CC iteration?

$(H_2O)_2$ TIP4P geometry
DZ-F12/aug-DZ-RI



Accuracy threshold from previous work

Scheme:
Iteration 1: use full CPD rank
Iteration 2+: use fixed, "small" CPD rank (here I use X)

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Summary

Mina Mandic
CCQ summer student

- It is possible to replace contractions with matrix-free tensor approximations.
- We can contrive some reliable and inexpensive way to stop matrix-free optimizations.
- Finding a way to improve the CPD accuracy for sparse tensors will directly improve accuracy of this tensor contraction.
- It could be possible to use randomize algorithms to further reduce the cost of the tensor optimization.

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