EuroHPC Summit Week 2022
#PRACEdays

Massive parallel coupled cluster theory algorithms for material science

Alejandro Gallo, Andreas Irmler, and Andreas Grüneis

TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

Coupled Cluster Theory For solids: CC4S

$$\psi_p(\mathbf{r}) = \sum_{\mathbf{G}} \psi^p_G e^{i\mathbf{r}\cdot\mathbf{G}}$$

$$\Gamma^p_{q\mathbf{G}} = \sqrt{\frac{4\pi}{|\mathbf{G}|^2}} \int \mathrm{d}\mathbf{r} \psi^*_p(\mathbf{r}) \psi_q(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}}$$

$$V^{pq}_{rs} = \sum_{\mathbf{G}} \Gamma^{p\mathbf{G}}_q \Gamma^r_{s\mathbf{G}}$$


```
E[""] = T ["abij"] * V ["ijab"]

V ["ijab"] = Γ["iaG"] * Γ["jbG"]
```

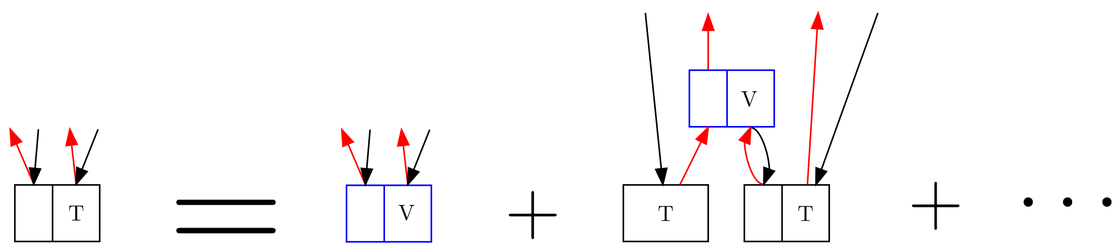
Tensor Engine Cyclops Tensor Framework

Coupled Cluster Theory in a Nutshell

→ Number of electrons
→ Number of virtual states

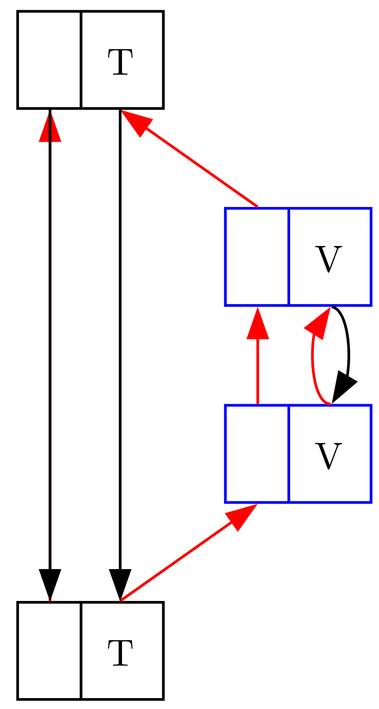
$$\hat{T} = \quad + \quad + \quad + \quad + \quad + \cdots$$

- Find tensor $\hat{T}$
- Input are one-electron integrals 
- Common approximations:
  - Restrict to the first two tensors in $\hat{T}$
  - Restrict the size in → dimension
- Equations based on tensor contractions
- Every contraction has a different optimal distributed memory layout **CTF**



Perturbative Triples [CCSD(T)] in Atrip

- CCSDT is too expensive for any non-trivial application. *Triples contributions* are introduced perturbatively to compute a correction to the correlation energy
- CCSD(T) is one of the most successful many-body theories for quantum chemistry
- Given  is one , calculated from coupled cluster theory up to doubles, the diagram on the right the main ones in a one-shot procedure to calculate the correction to the energy.
- We developed a library called **Atrip** to compute this correction
- **Atrip** is designed to calculate upt to 200 electrons (→ 100 and → 2000)
- The **Atrip** code computes the diagrams by:
  - Asynchronously communicating tensor slices using MPI
  - Overlaping computation and communication
  - Minimizing inter-node communication by optimal distribution of the tensors
  - Building a dynamic database of tensor slices
- We advocate for literate programming to ensure the clarity of the main algorithm



References

- https://alejandrogallo.github.io/atrip
- https://cc4s.org
- https://github.com/cc4s/cc4s/
- https://github.com/cyclops-community/ctf
- https://www.vasp.at

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