INNO4SCALE

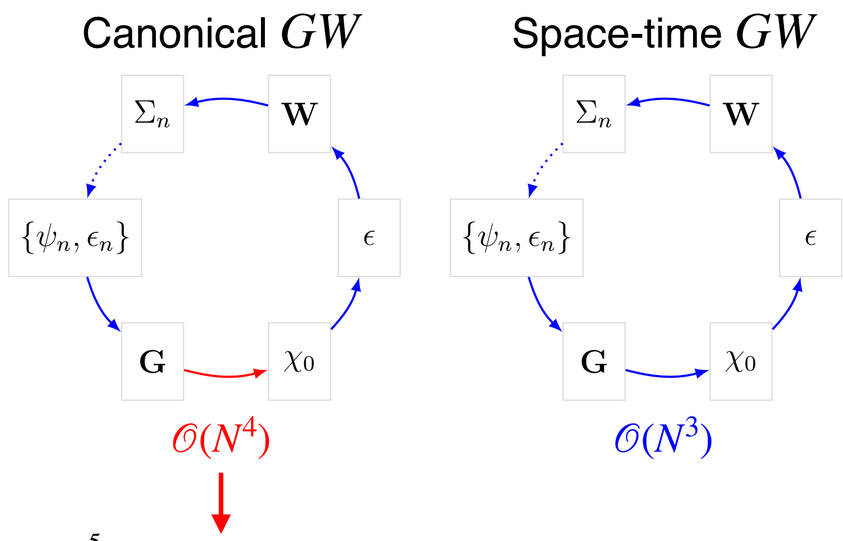
Innovative Algorithms **for** Applications on European Exa**scale** Supercomputers

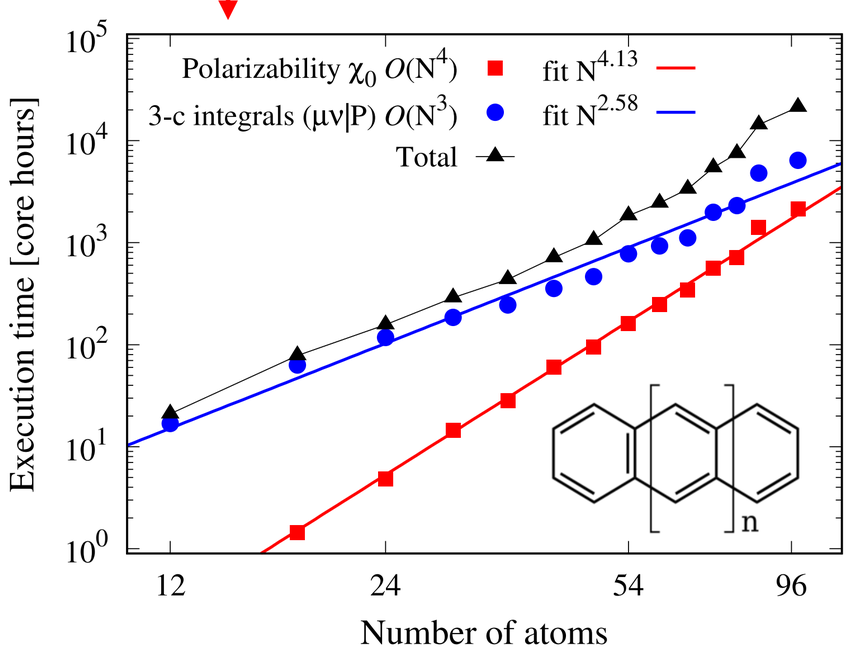
Visit our website:

Exascale-ready GW algorithms for materials interfaces

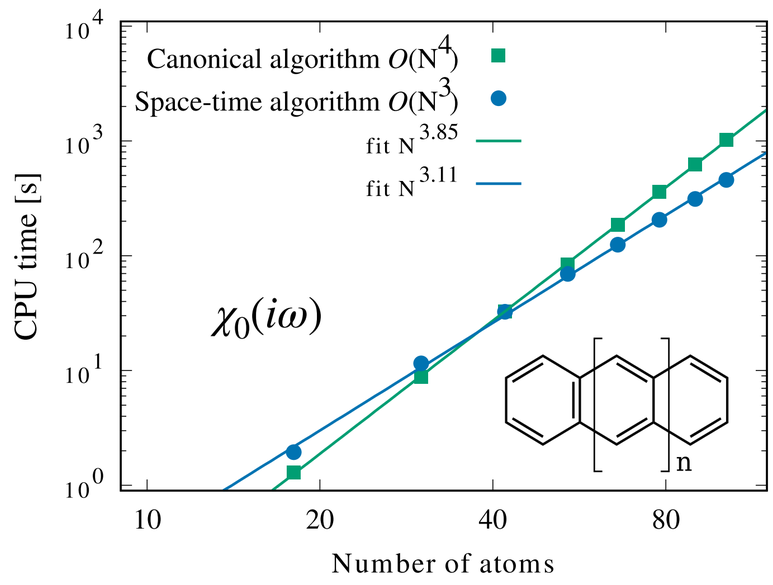
Francisco A. Delesma, Moritz Leucke, Jan Wilhelm, Dorothea Golze

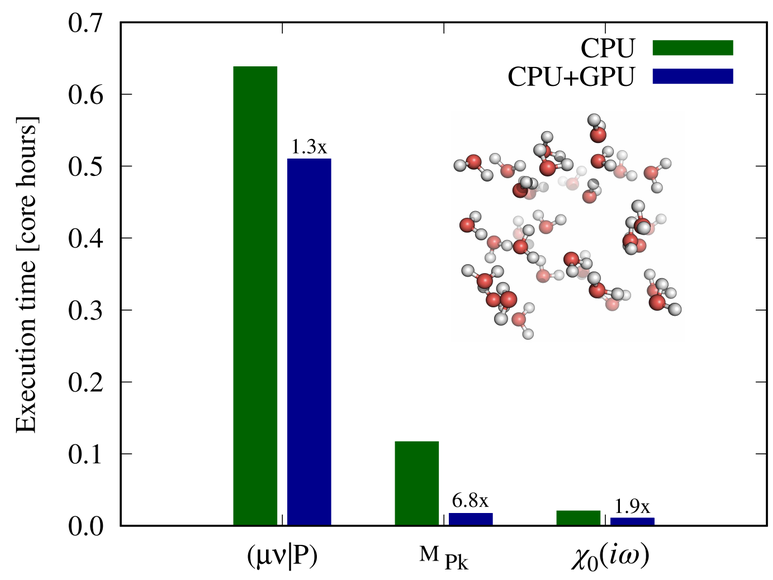
Introduction



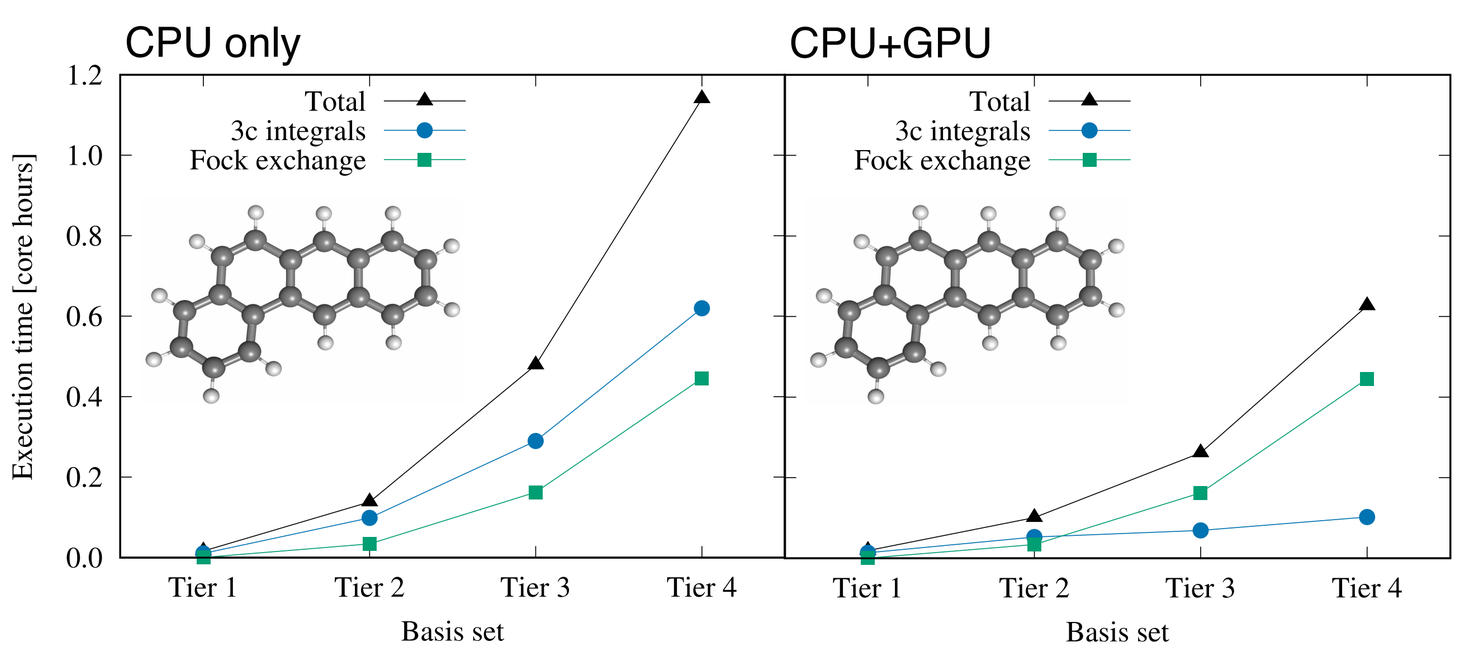


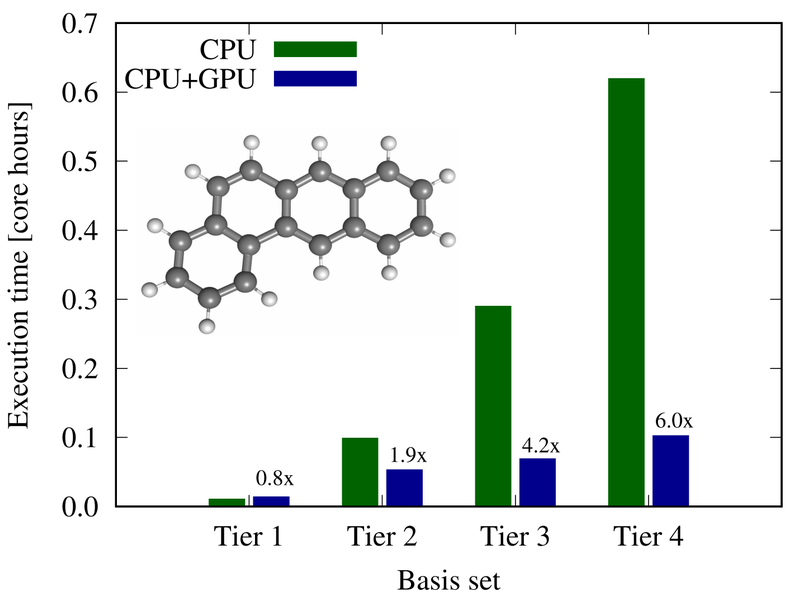
Low-scaling Implementation





GPU Acceleration of 3-center Integrals





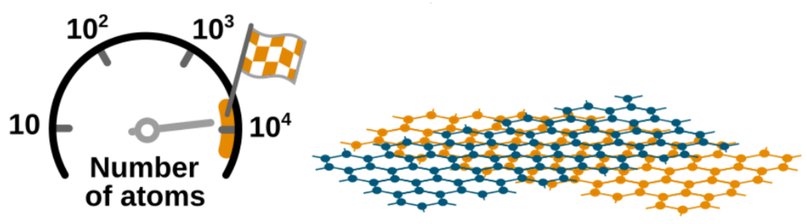
Summary

- Scaling reduction to cubic scaling GW based on space-time method [1]
- GPU accelerated 3-center integrals [2] and polarizability [3]
- Tested for up to 426 atoms on 6144 cores
- Prefactor optimization ongoing
- GPU acceleration for screened coulomb interaction W ongoing

FHI-aims The ab initio materials simulation package

CP2K

GREENX



References

(1) M.M. Rieger et al., *Comp. Phys. Comm.* **1999**, 117(3), 211-228.
(2) F.A. Delesma, M. Leucke, R.L. Panadés-Barrueta, D. Golze, *NIC Symposium Proceedings* **2025**.
(3) F.A. Delesma, M. Leucke, P. Rinke, D. Golze, *in preparation*.

Funded by the European Union

EuroHPC Joint Undertaking

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101118139. The JU receives support from the European Union's Horizon Europe Programme.