Massively parallel and GPU-accelerated evaluation of three-center integrals for numerical atomic orbitals (NAOs)

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Introduction

Four-center electron repulsion integrals appear in many electronic structure methods, such as many-body perturbation methods like the Random-Phase Approximation or GW and others. To reduce their computational cost, the resolution-of-the-identity (RI) approximation is commonly employed. RI refactors the four-center integrals into three- and two-center integrals, among which the three-center integrals remain a computational bottleneck, particularly when using NAOs. We present a global RI scheme combined with a local metric (attenuated Coulomb) within an all-electron NAO framework, treating molecules and solids on equal footing. Central to the approach is a novel GPU-accelerated algorithm for computing 3-center integrals that relies on domain decomposition to improve load balancing and strong scaling.

Resolution-of-the-Identity (RI)

RI factorization [1]: $(\mu\nu\,|\,\lambda\sigma) = \sum_{PQST} (\mu\nu\,|_m P)\; M^{-1}_{PQ}\; V_{QS}\; M^{-1}_{ST}\; (\lambda\sigma\,|_m T)$

Auxiliary basis: $\phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r}) = \sum_P \varphi_P(\mathbf{r})$

3-center integrals: $(\mu\nu\,|_m P) = \iint \phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\; m(\mathbf{r}'-\mathbf{r})\; \varphi_P(\mathbf{r}')\; d\mathbf{r}'d\mathbf{r}$

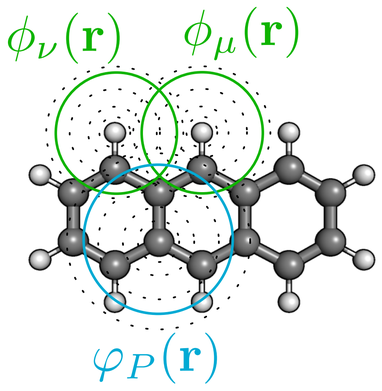
Coulomb metric (**RI-V**): $m(\mathbf{r}) = \dfrac{1}{r}$

Sigmoid attenuated coulomb metric (**RI-AtC**): $m(\mathbf{r}) = \dfrac{1/2 \cdot \mathrm{erfc}(\omega(r - r_c))}{r}$

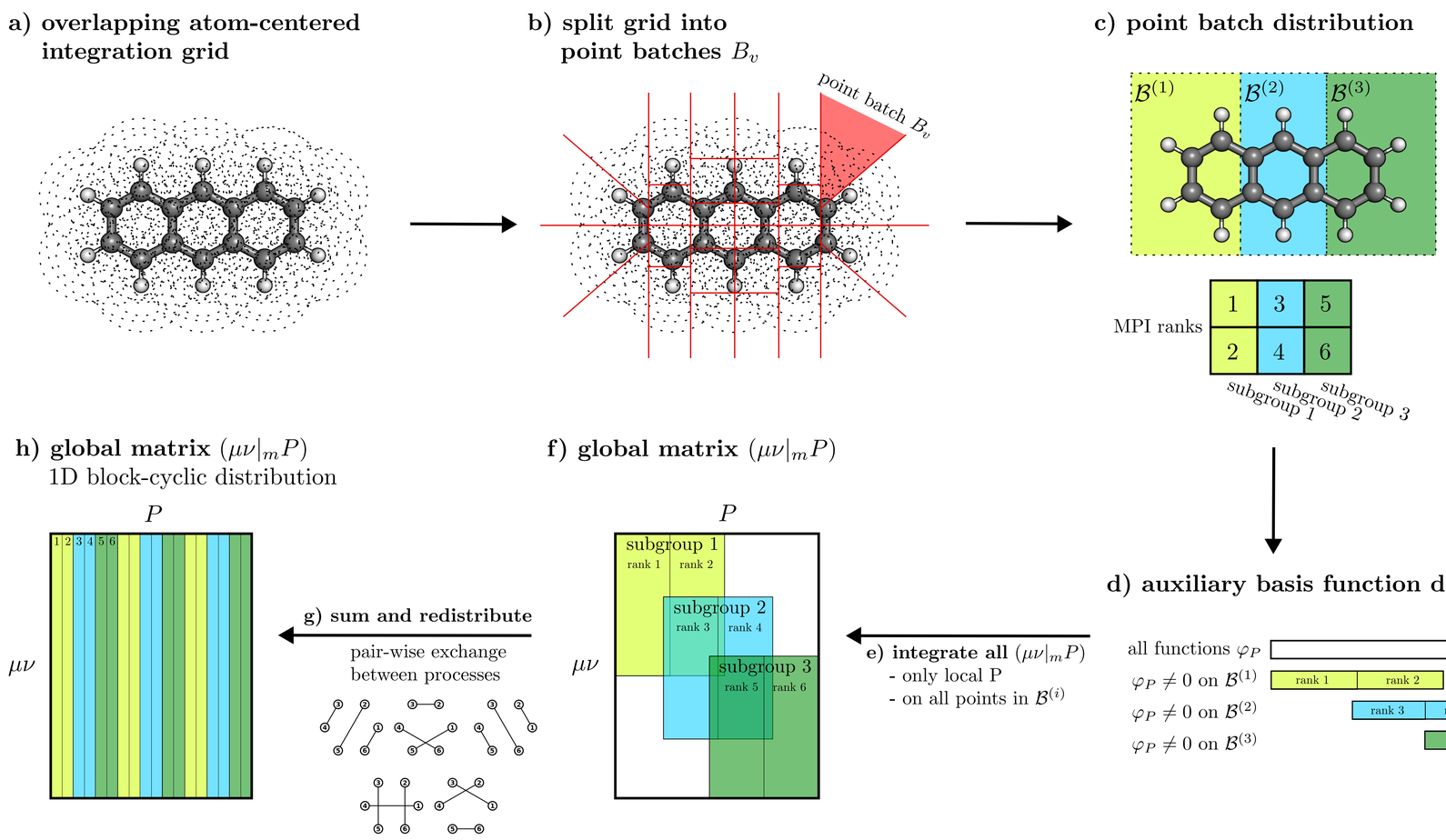
Integration algorithm $(\mu\nu\,|_m P)$

Old Algorithm [2]:

- distribute over P
- evaluate all $(\mu\nu\,|\,P)$ of local P
- integrations generated from 3 contributing atoms

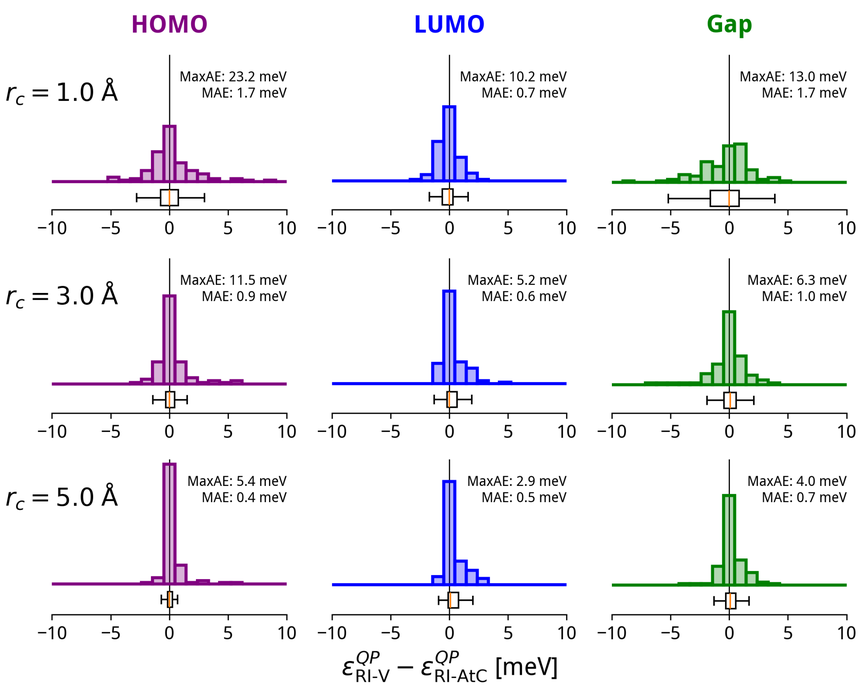


New Algorithm:

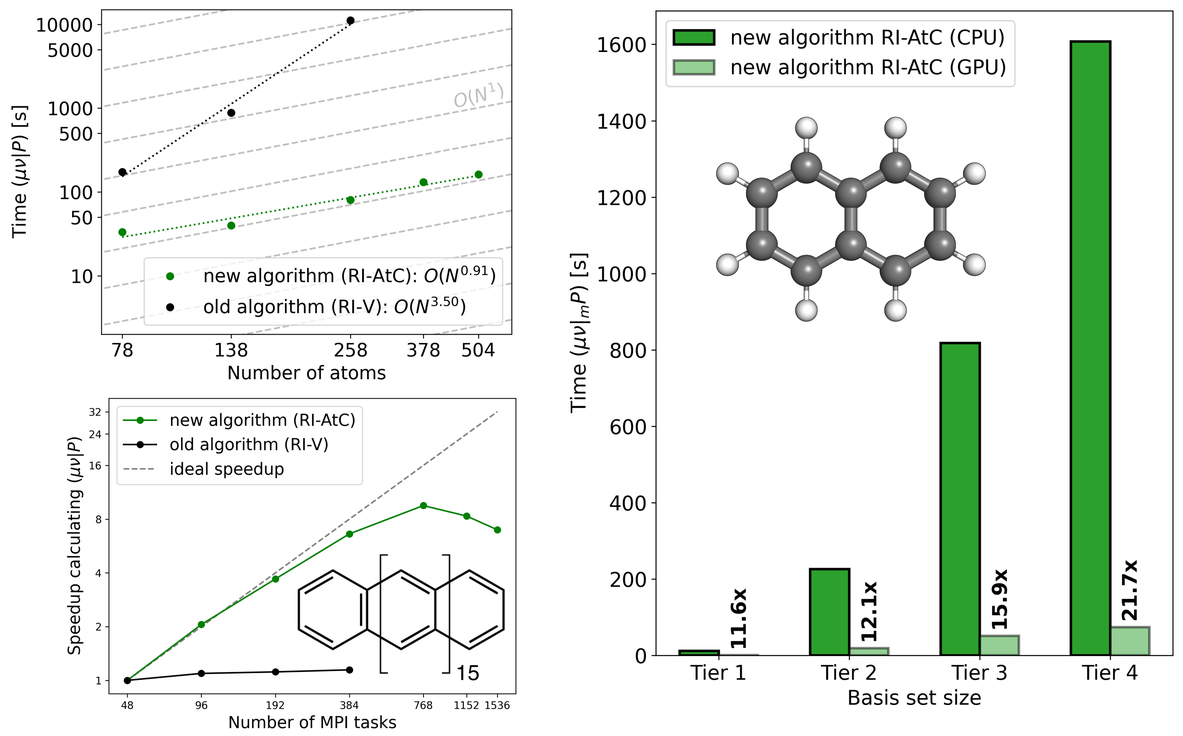


Accuracy

GW100 Benchmark:



Performance



References

[1] O. Vahtras, et al., Chem. Physics. Lett. **1993**, 213 (5), 514.

[2] X. Ren, et al., *New J. Phys.* **2012**, 14 (5), 053020.

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Computing time: GCS Gauss Centre for Supercomputing

Implemented inside: FHI-aims The ab initio materials simulation package

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