UNI WÜ

Golze Group

Computational chemistry and physics

Resolution-of-the-Identity with Domain Decomposition

Moritz Leucke, Dorothea Golze

JMU Würzburg

FHI-aims D&U Meeting Hamburg 2026

Motivation: Correlated el. Structure Methods

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Fock exchange

MP2

CC

rPT2

SOSEX

rSE

Others

GW

RPA

Antonios Talk

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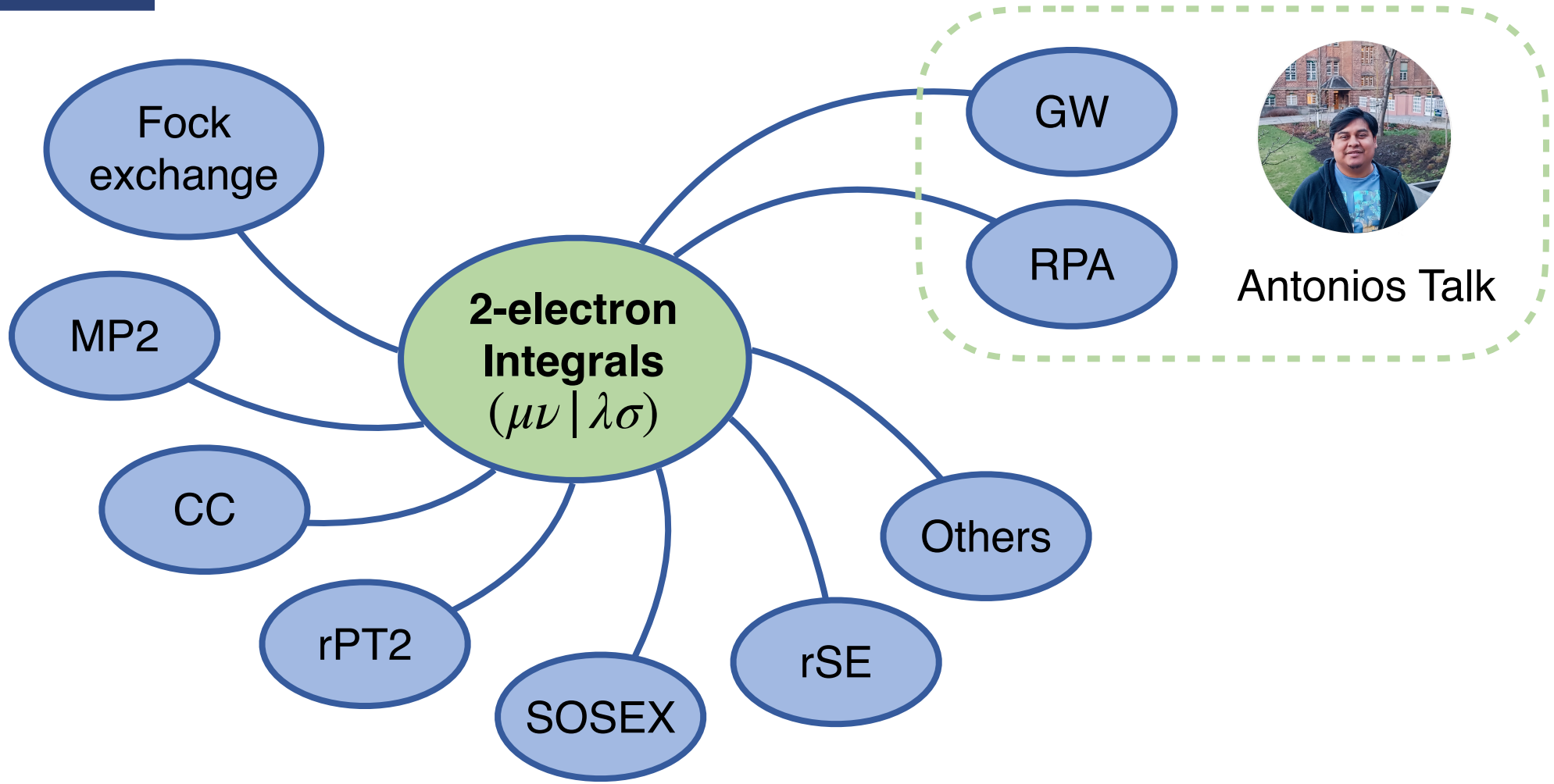

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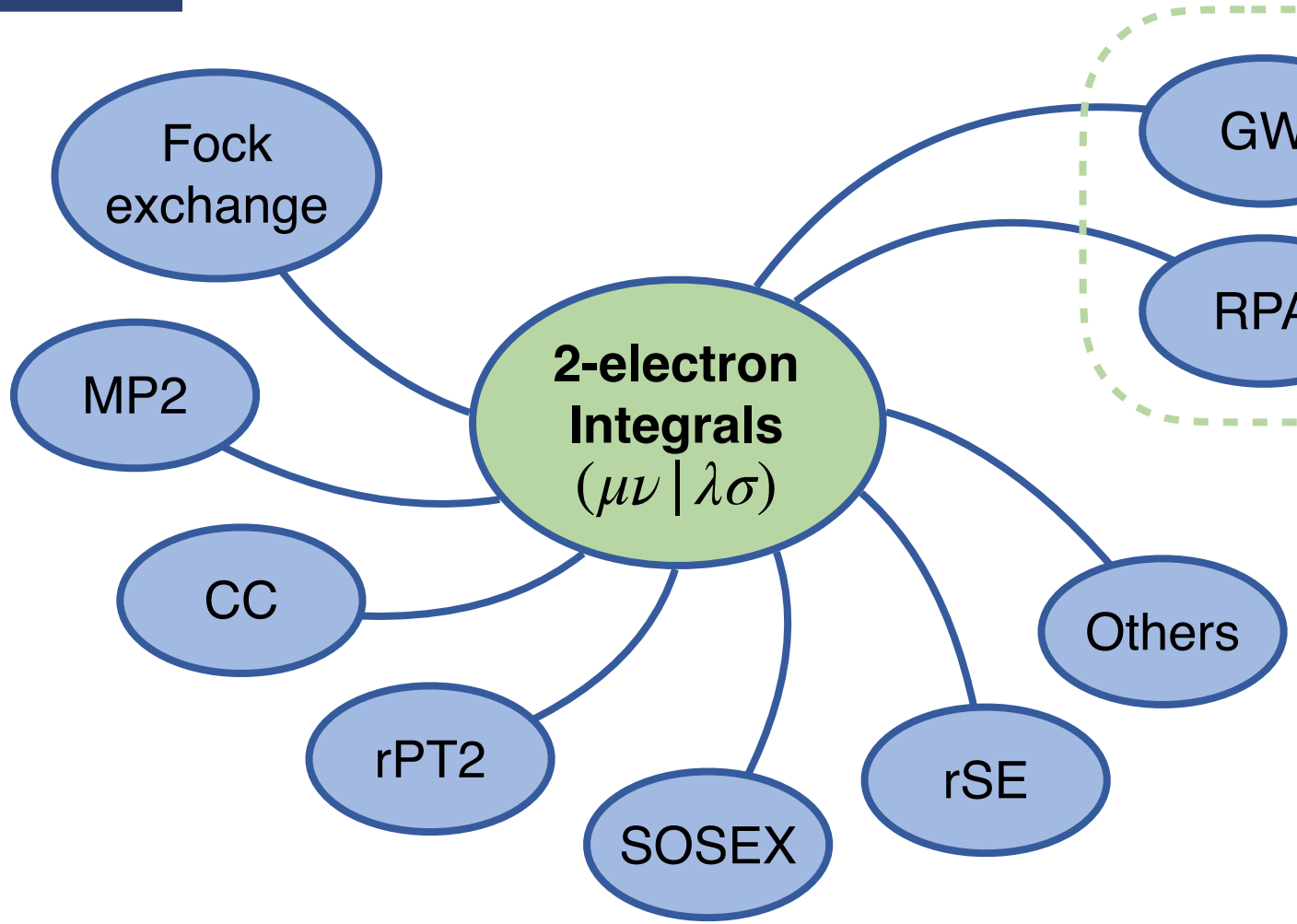

Antonios Talk

Numerical atom-centered orbitals (NAOs)

$$\phi(\mathbf{r}) = \frac{u(r)}{r} Y_{lm}(\mathbf{r})$$

FHI-aims
The ab initio materials simulation package

Blum et al., *Computer Physics Communications* **2009**, 180 (11).

Motivation

Resolution-of-the-identity (RI)

$$(\mu\nu\,|\,\lambda\sigma) = \iint \phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\frac{1}{\mathbf{r}-\mathbf{r}'}\phi_\lambda(\mathbf{r}')\phi_\sigma(\mathbf{r}')d\mathbf{r}d\mathbf{r}'$$

Vahtras et al., *Chemical Physics Letters* **1993**, 213 (5-6).

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Metric $m(\mathbf{r})$

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Motivation

Resolution-of-the-identity (RI)

- 2-electron integrals $(\mu\nu\,|\,\lambda\sigma)$ in post HF/DFT methods
- Scaling reduction
- Costly for NAOs (numerical integration)

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Goal: Accurate low-scaling core-level GW for extended Systems

- RI must be accurate for a wide energy range
- Scaling to 1000+ atomic systems
- Massively parallel

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RI methods in FHIaims

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

Restricting P
“local” RI

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Restricting P
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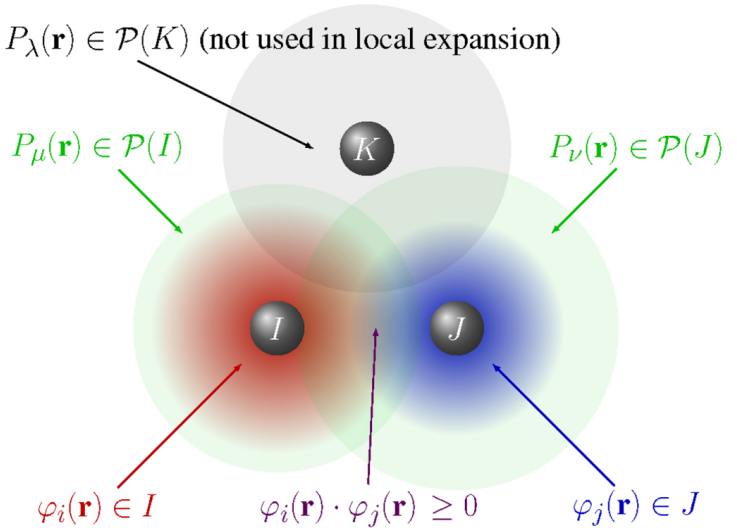
RI-LVL

$\mathcal{O}(N^1)$

Very fast, but
large aux basis



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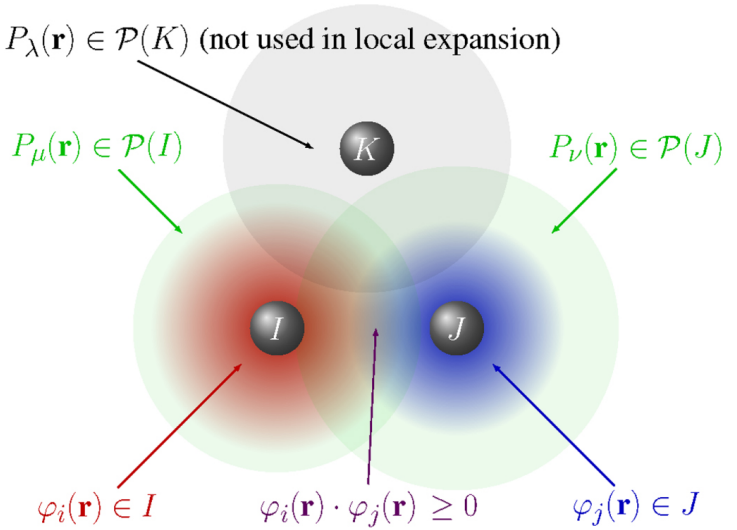

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Restricting P
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RI-V

$$m(\mathbf{r}) = \frac{1}{r}$$

$$\mathcal{O}(N^2)$$

Costly and most Accurate

Ren et al., *New Journal of Physics* **2012**, 14 (5).

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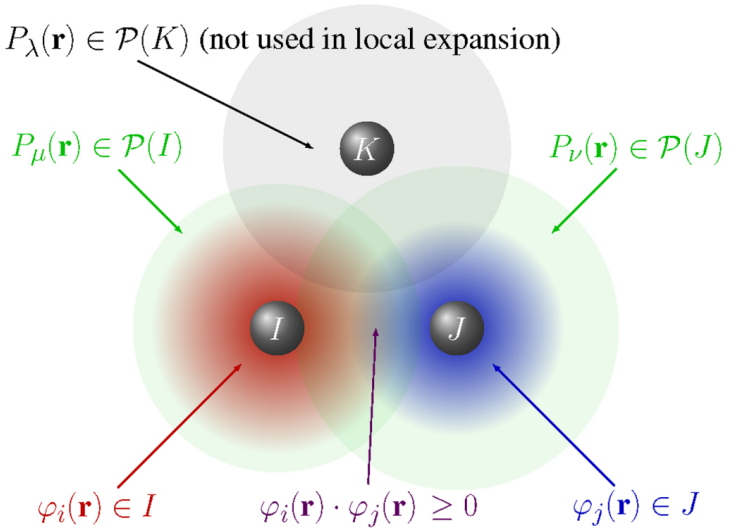

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RI-ATC
(Attenuated coulomb RI)

$$m(\mathbf{r}) = \frac{1/2 \cdot \mathrm{erfc}(\omega(r - r_c))}{r}$$

$$\mathcal{O}(N^1) - \mathcal{O}(N^2)$$

Tunable accuracy/cost

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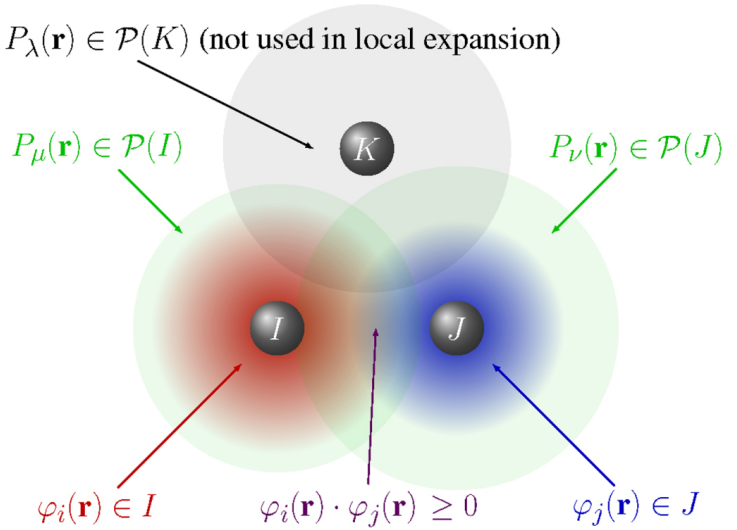

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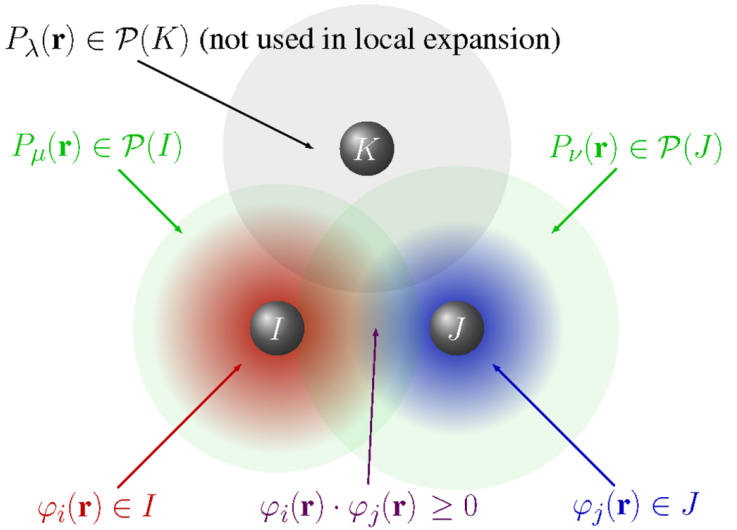

RI methods in FHIaims: RI metric

Bottleneck 3-center integrals:

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

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field of the auxiliary function:

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Attenuated metric: **small extend** $\mathcal{O}(N^1)$

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- Coulomb metric: **large extend** $\mathcal{O}(N^2)$
- Attenuated metric: **small extend** $\mathcal{O}(N^1)$
  - Sparsity leads to lower scaling

Implementation choices

Existing RI-V implementation:

- Parallelization over aux. functions P for $(\mu\nu\,|_m\,P)$
- Good for small systems
- Inefficient for big systems

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Idea for new RI-V and RI-AtC implementation:

- Better parallelization by domain decomposition
- Borrowing Idea from DFT
- RI-V ($\mathcal{O}(N^2)$) and RI-AtC ($\mathcal{O}(N^1)$)

V. Havu *et al.*, *Journal of Computational Physics* **2009**, *228*(22), 8367.

Implementation choices: Grid

Existing RI-V implementation:

$$(\mu\nu|_m P) = \int \phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\ \Omega_P[m](\mathbf{r})\ d\mathbf{r}$$

$$= \sum_{a=a_1,a_2,a_3} \sum_{st} p_3(a,\mathbf{r})w(s,t)\phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\ \Omega_P[m](\mathbf{r})$$

Ren et al., *New Journal of Physics* **2012**, 14 (5).

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Idea for new RI-V and RI-AtC implementation:

$$= \sum_{B_v} \sum_{\mathbf{r}\in B_v} p(\mathbf{r})w(\mathbf{r})\phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\ \Omega_P[m](\mathbf{r})$$

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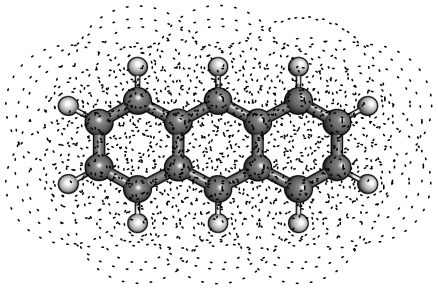
Better for GPUs

Integration using domain decomposition

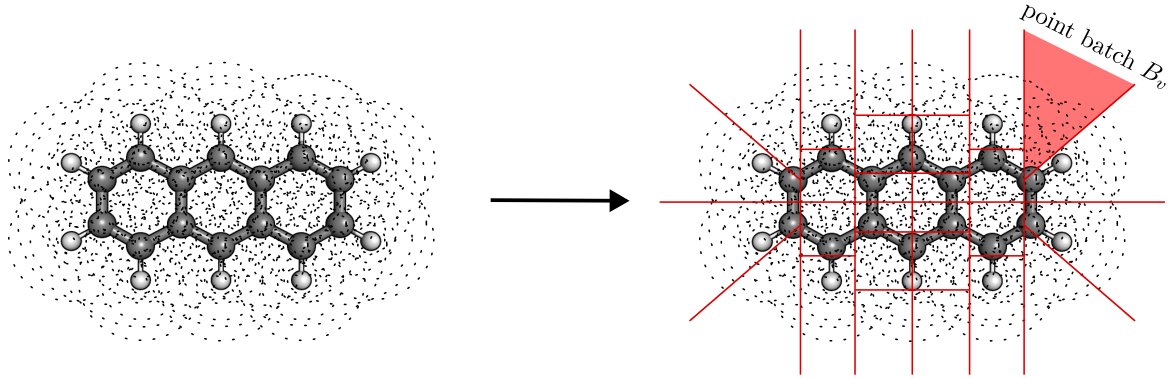
a) overlapping atom-centered integration grid



Integration using domain decomposition

a) overlapping atom-centered integration grid

b) split grid into point batches B_v



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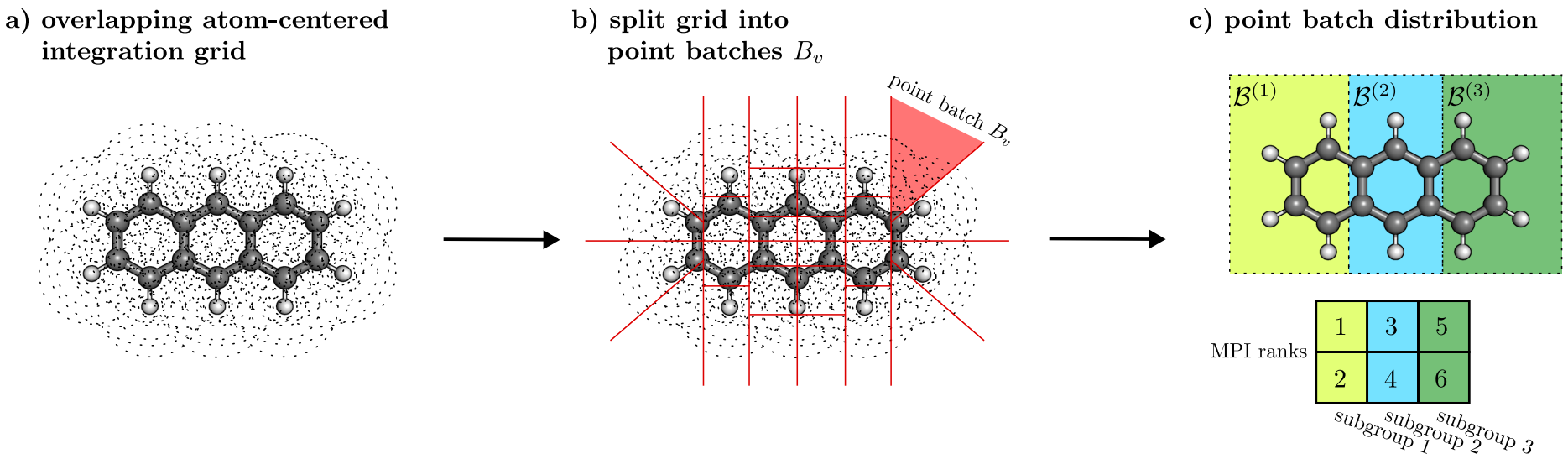

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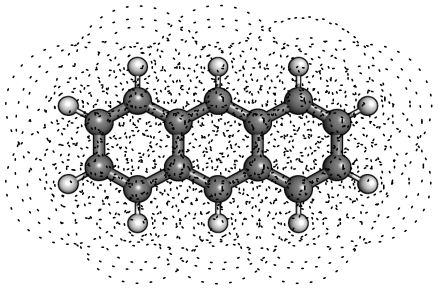

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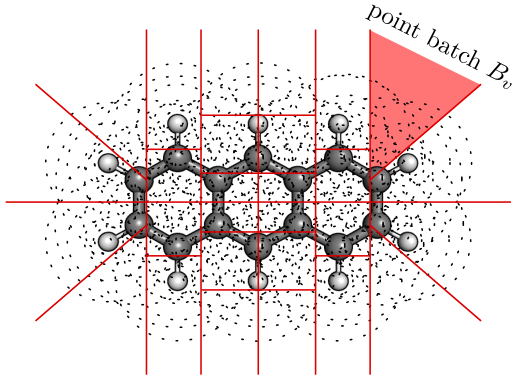
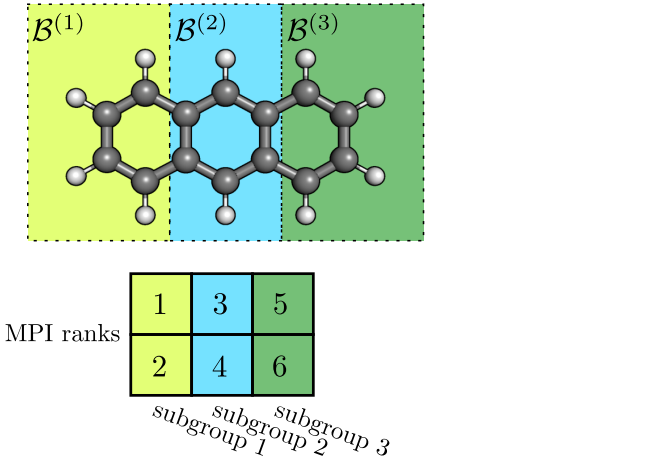
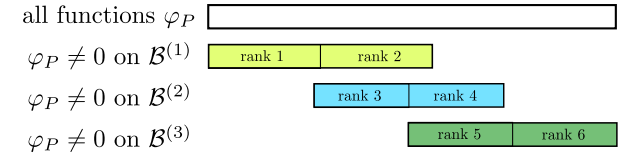


c) point batch distribution



d) auxiliary basis function distribution



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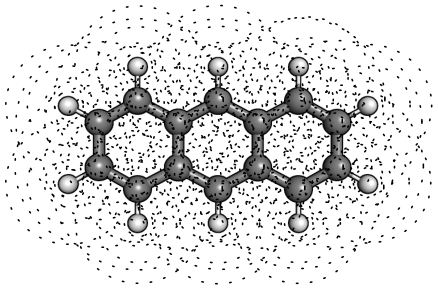

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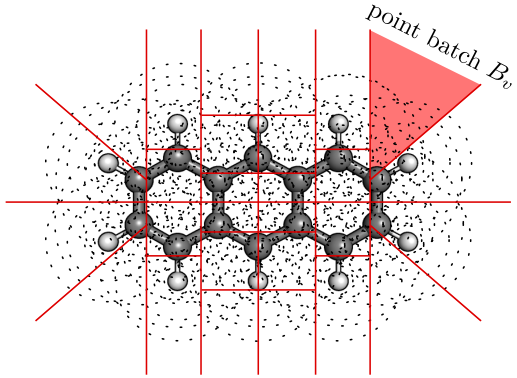

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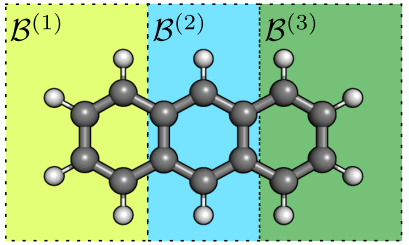

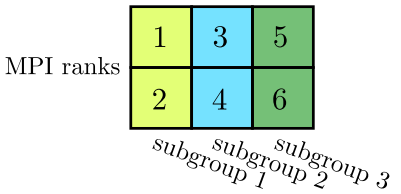

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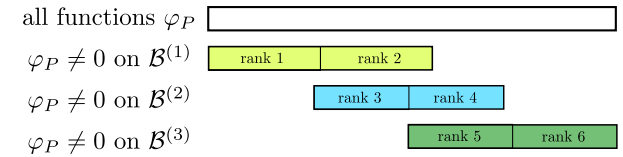
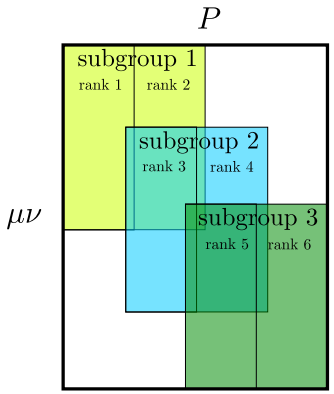


e) integrate all $(\mu\nu|_m P)$
- only local P
- on all points in $\mathcal{B}^{(i)}$

f) global matrix $(\mu\nu|_m P)$



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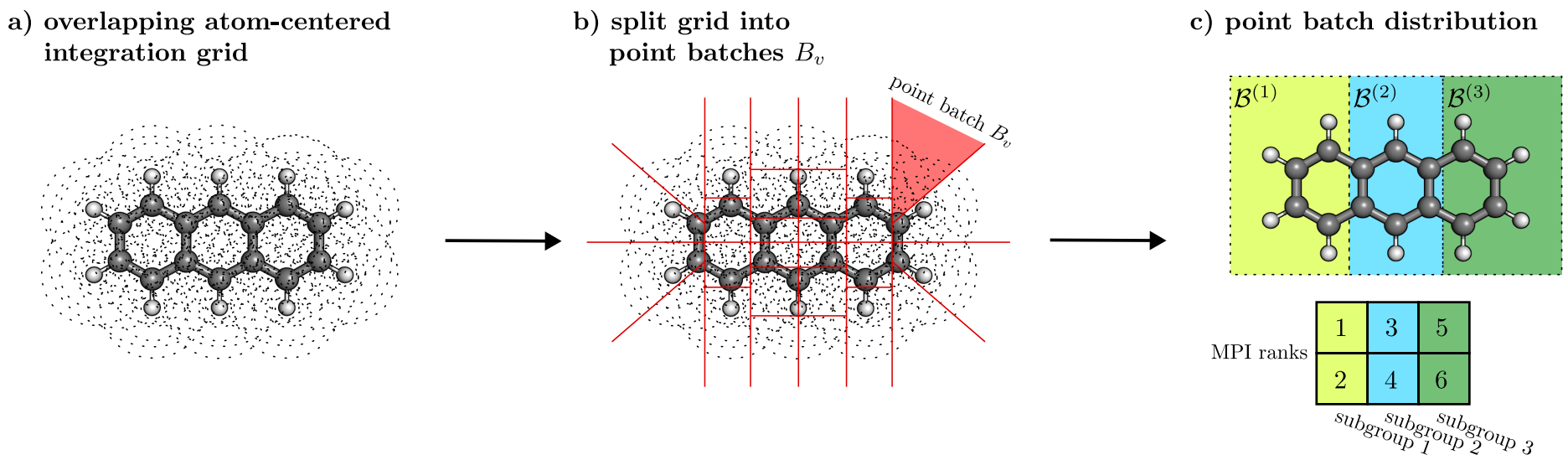
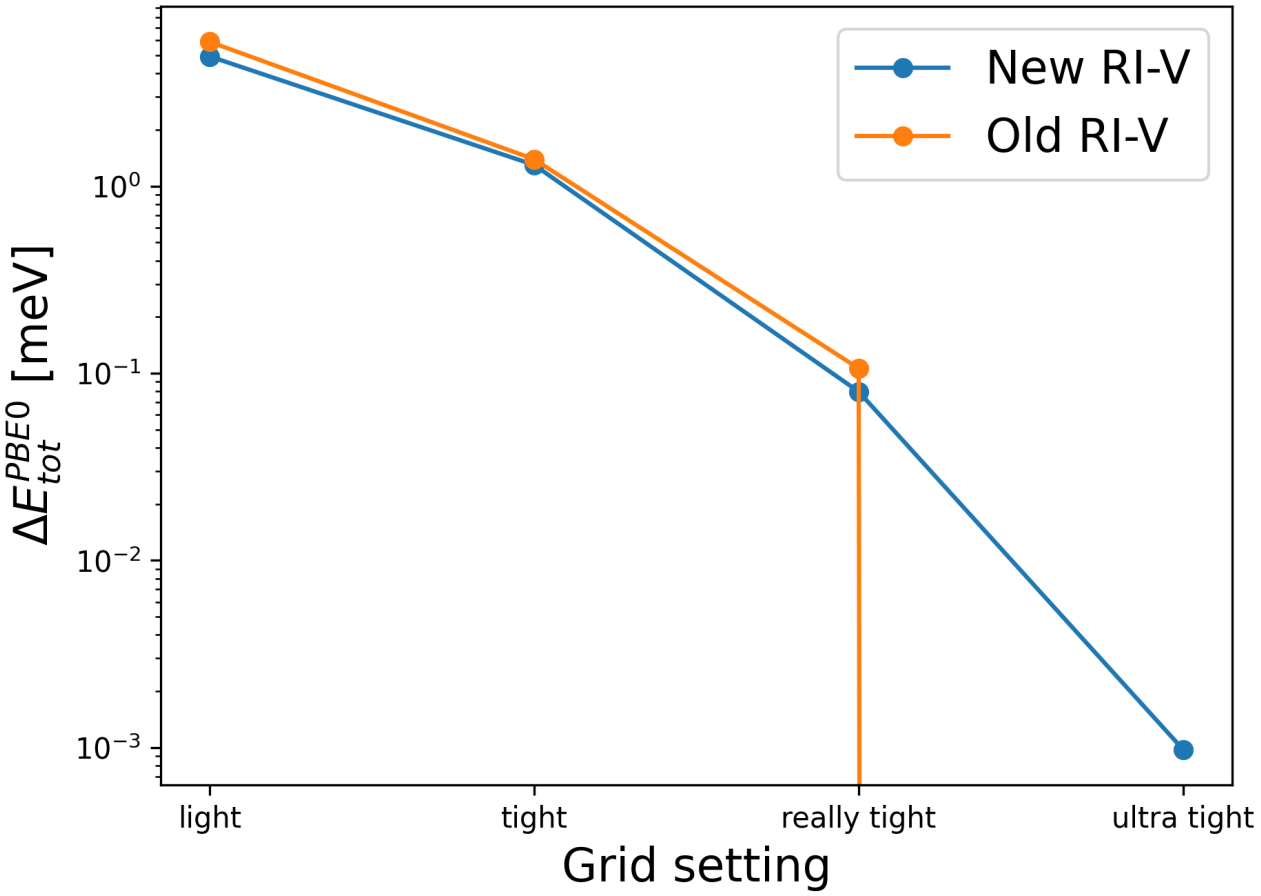


Implementation Correct?



Benzene
PBE0 // Tier 2
Reference: ultra tight old RI-V

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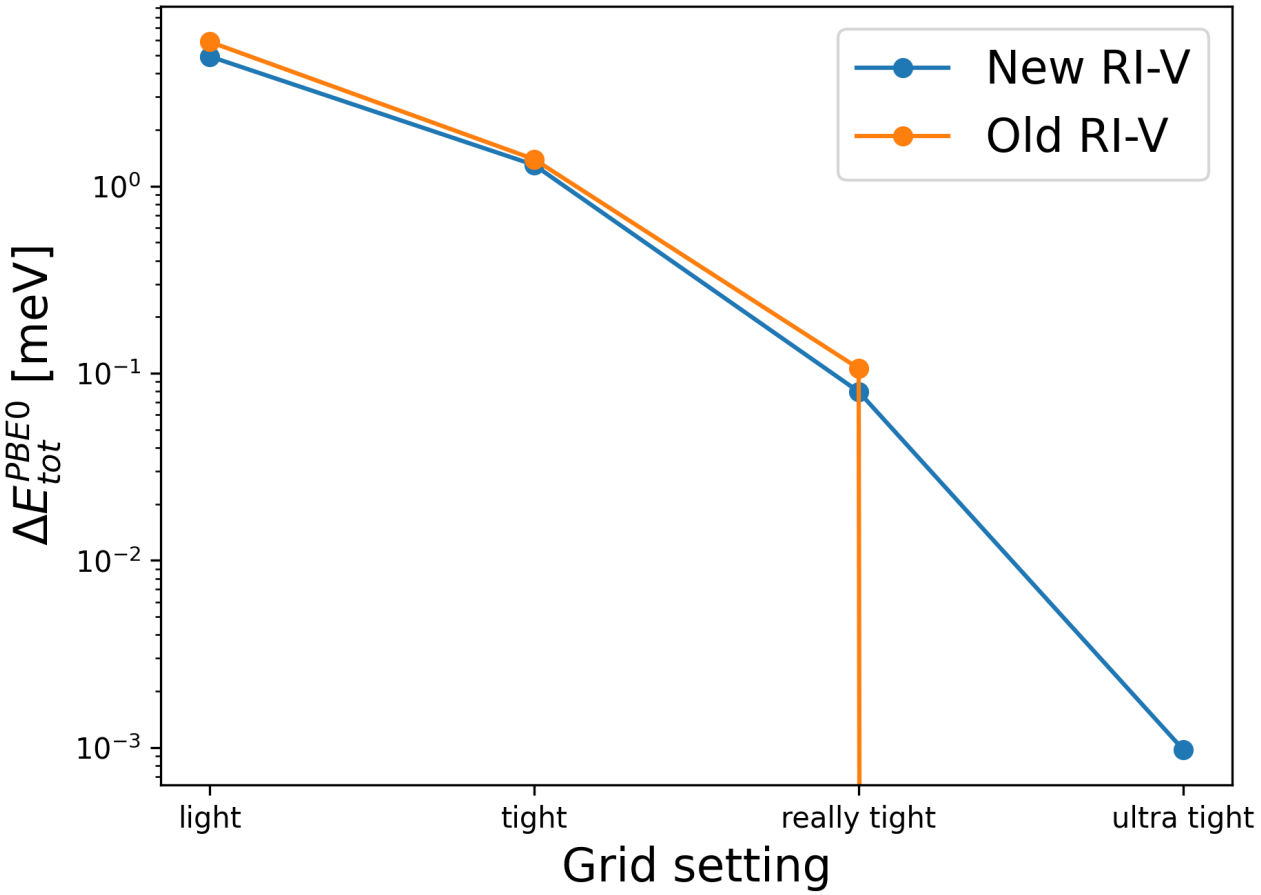

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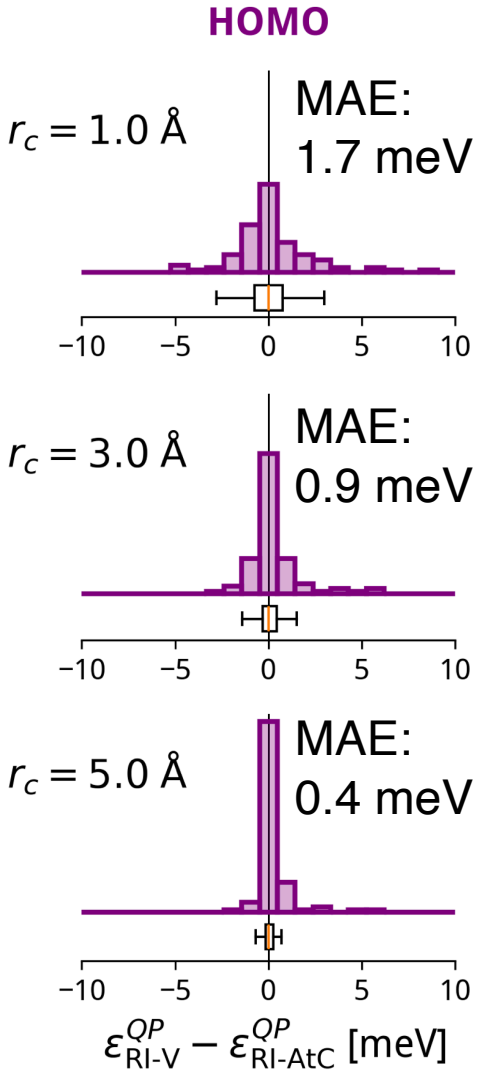
Different Grids!

But they converge to the same result

Accuracy of RI-AtC: GW 100



GW@PBE
Attenuated Coulomb metric
Tier 2 Basis

$$m(\mathbf{r}) = \frac{1/2 \cdot \operatorname{erfc}(\omega(r - r_c))}{r}$$

$$\omega = 0.75 \, \frac{1}{\text{Å}}$$

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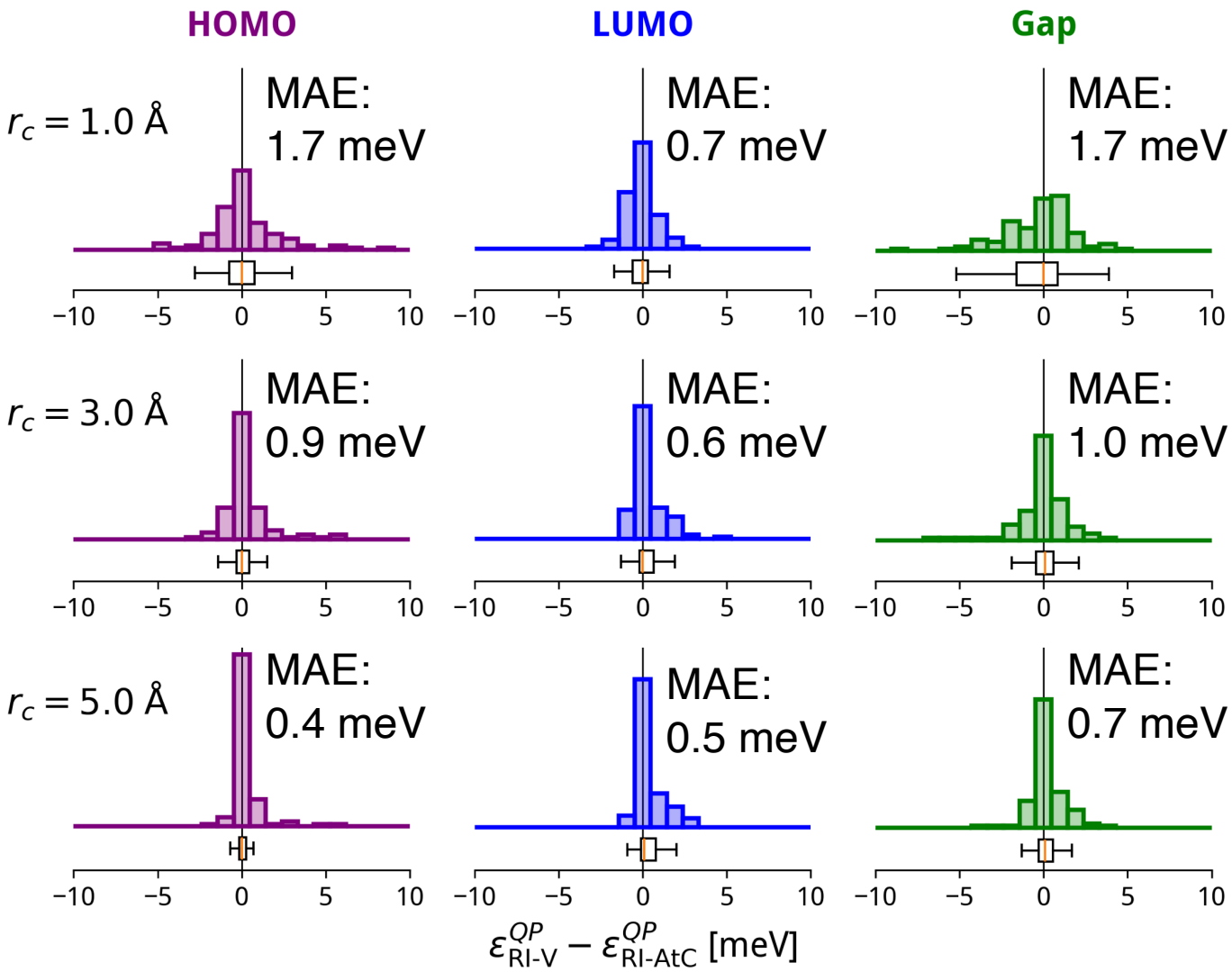

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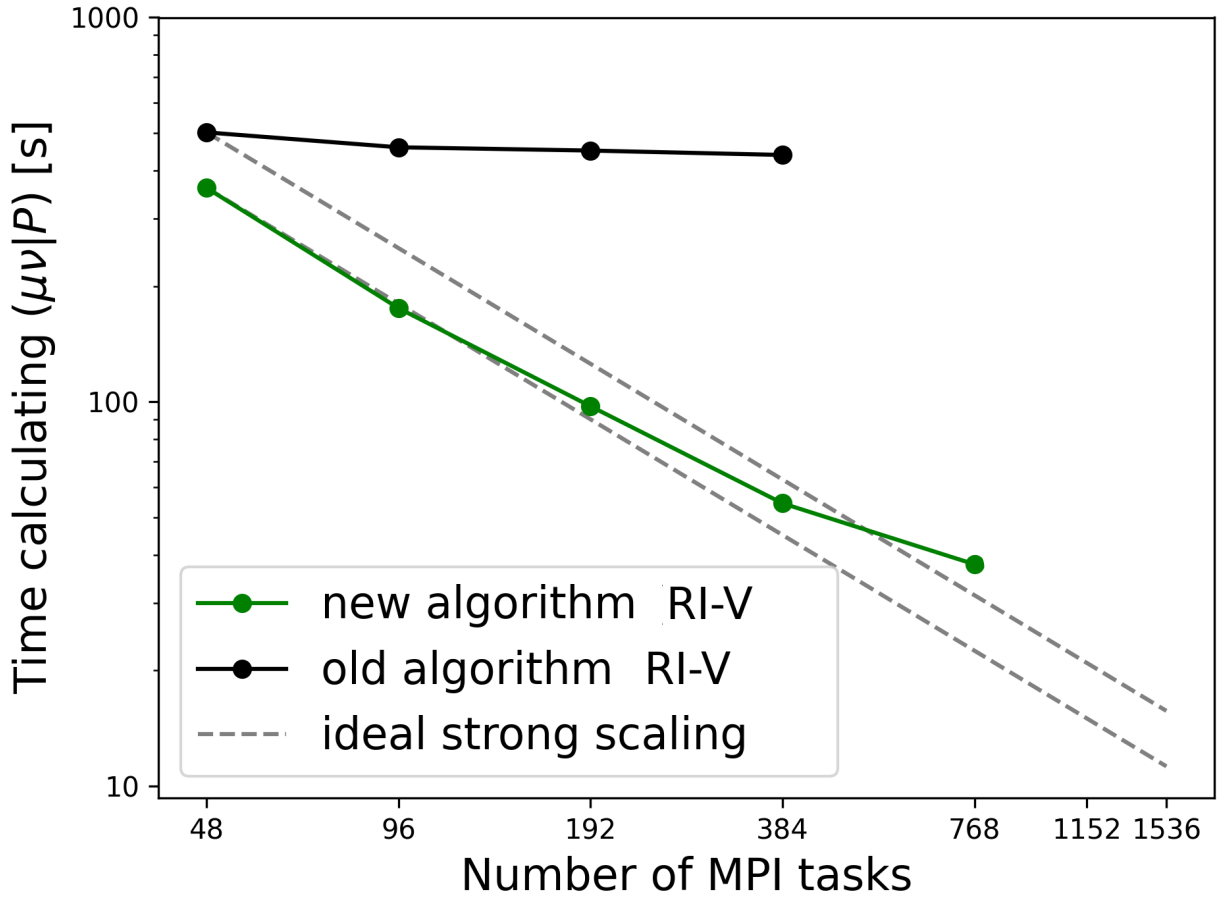
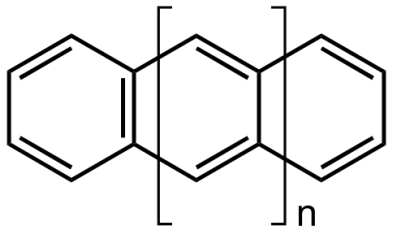
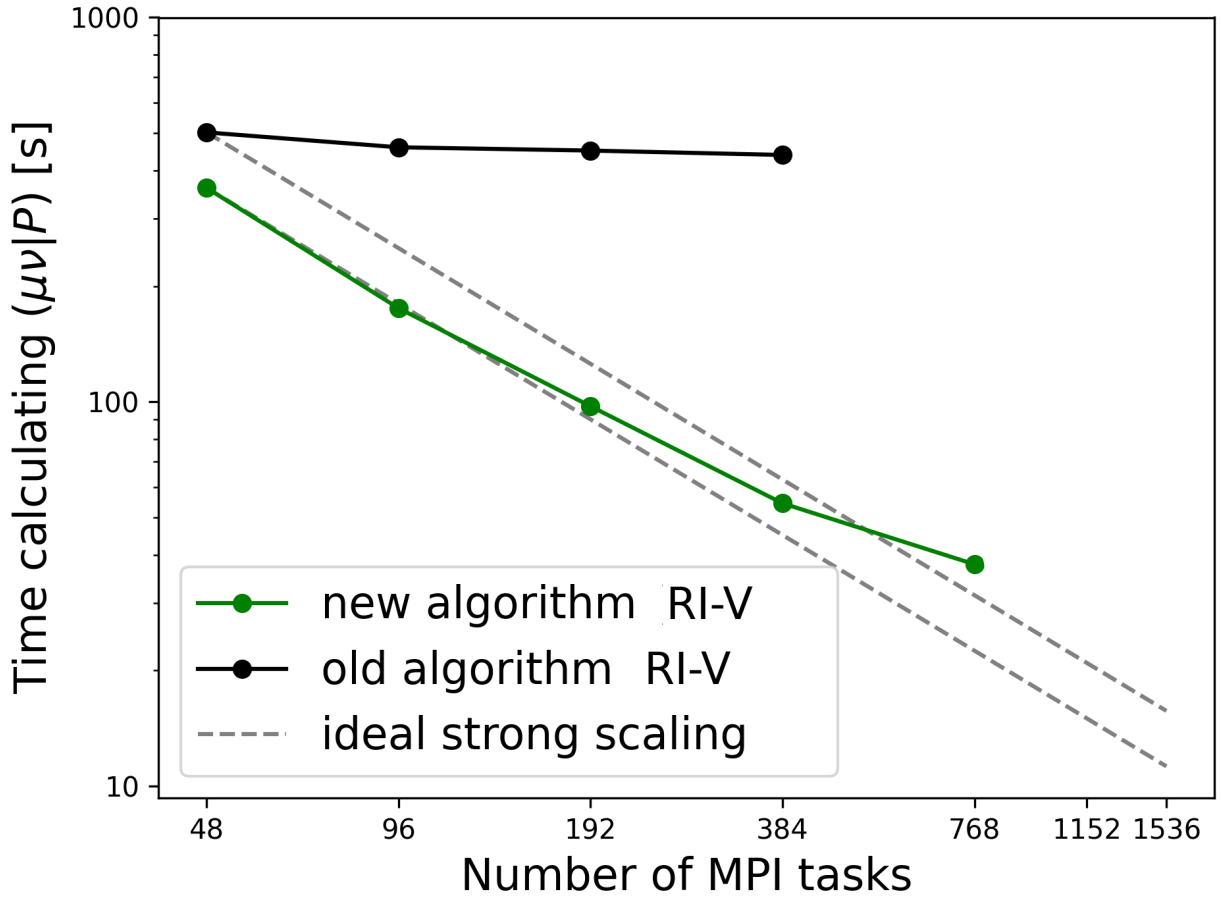
Strong Scaling: Small Systems

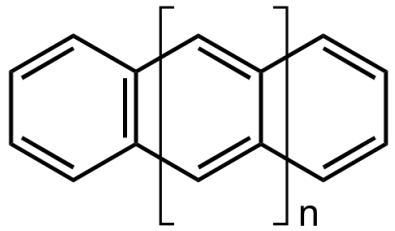




108 Atoms
Coulomb metric
Tier 1 basis
JUWELS cluster

Strong Scaling: Small Systems

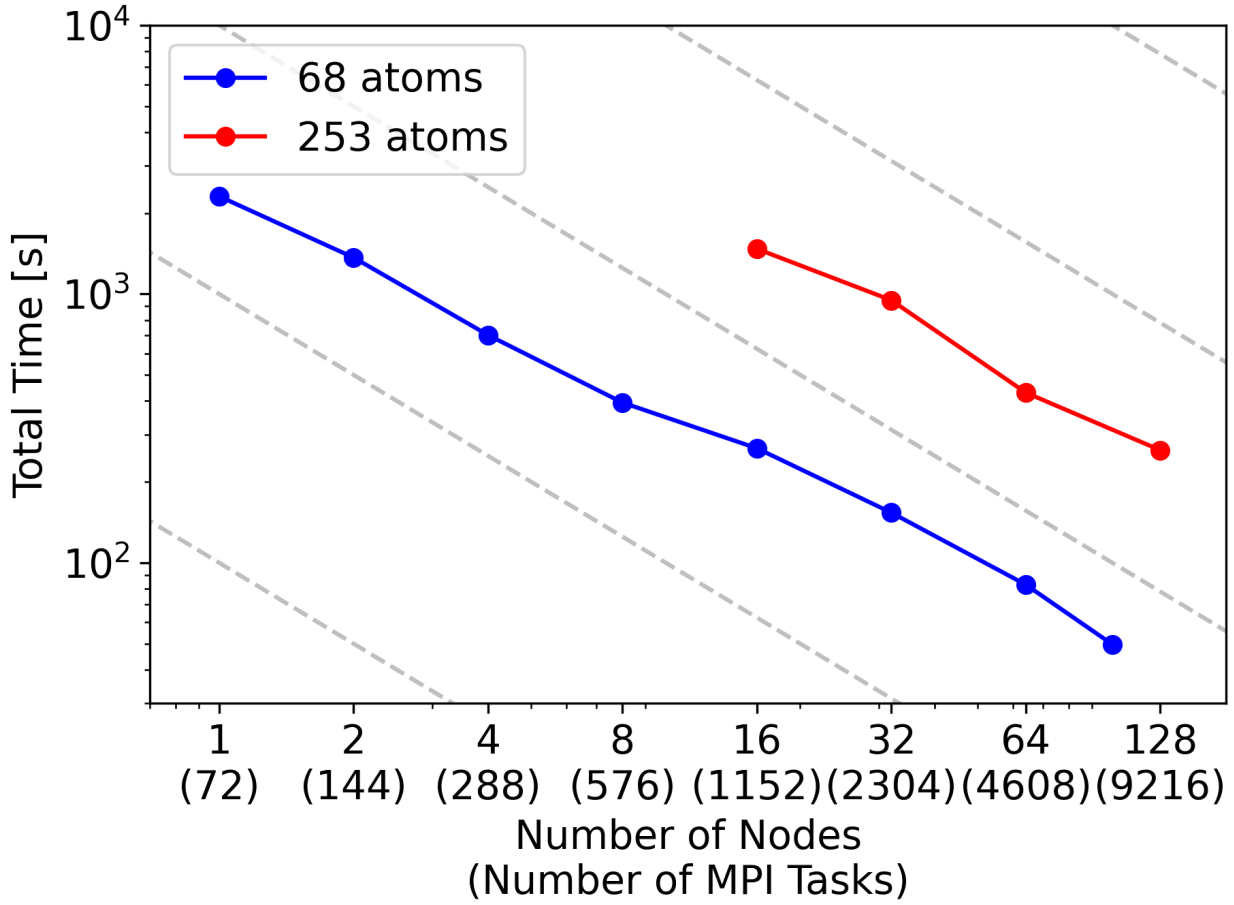


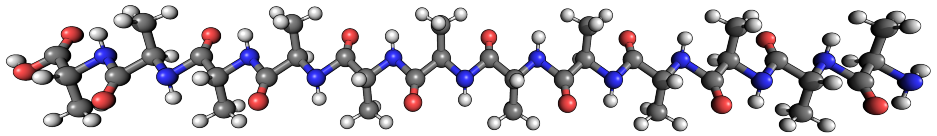


108 Atoms
Coulomb metric
Tier 1 basis
JUWELS cluster

Large, sparse systems not the scope of old implementation

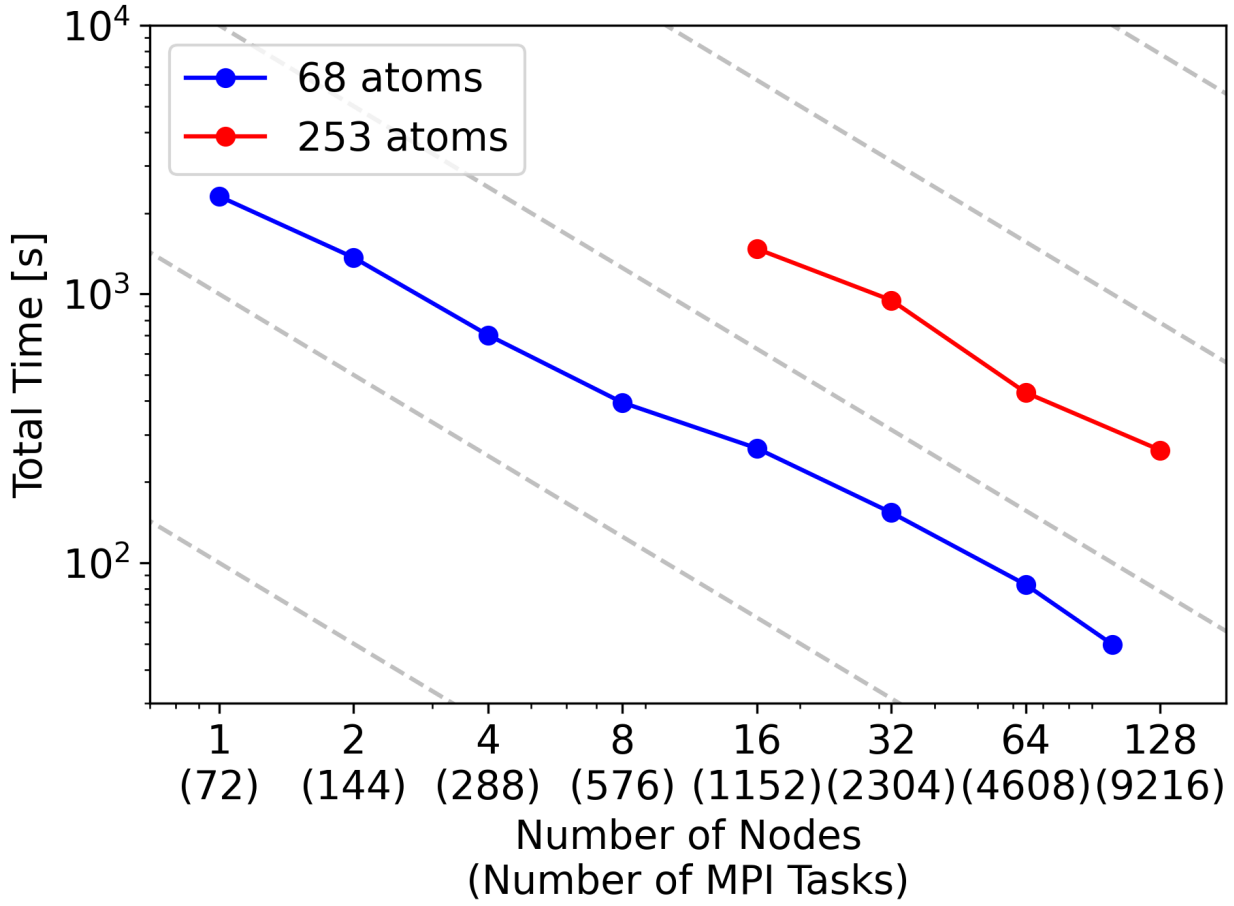
Strong Scaling: Big Systems





Alanine chains
Tier 2 basis
Coulomb metric (RI-V)
JUPITER booster

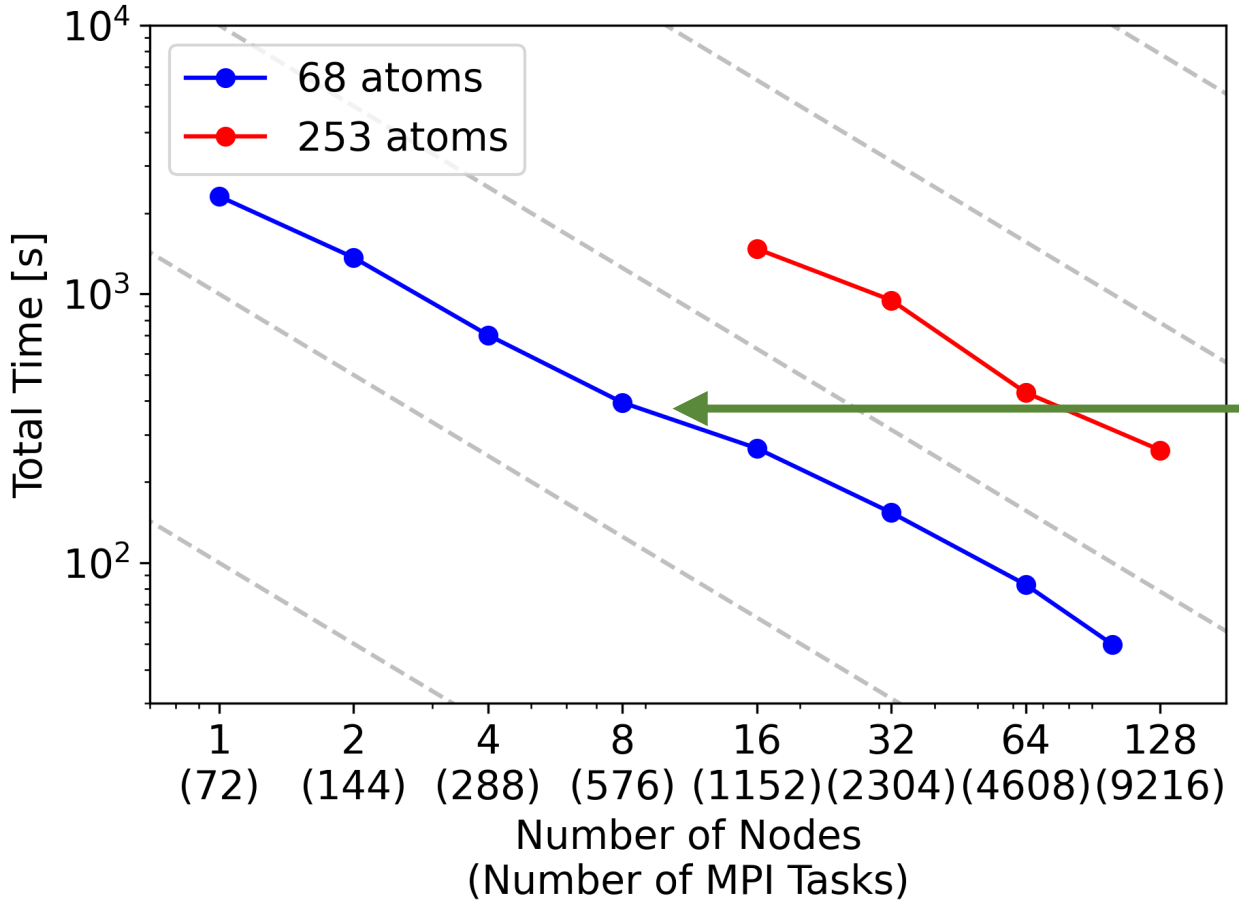
Strong Scaling: Very Important for RI



RI has high memory demand!

On how many nodes can I run my calculation?

Strong Scaling: Very Important for RI



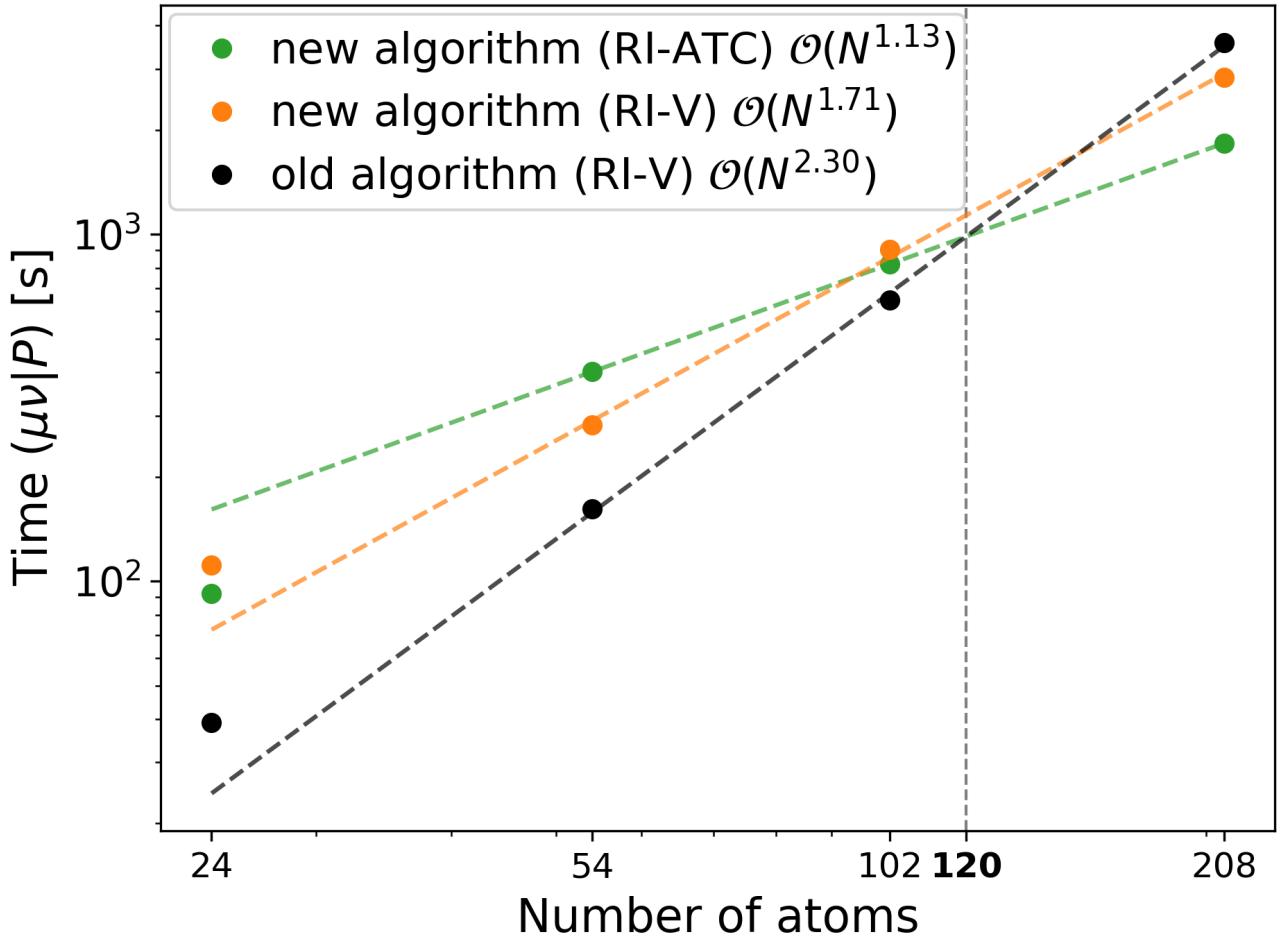
RI has high memory demand!

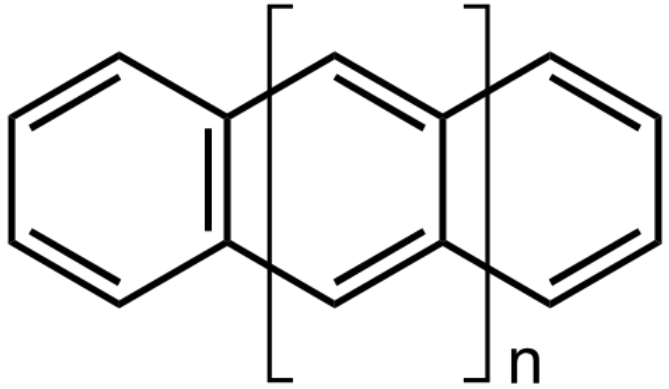
On how many nodes can I run my calculation?

Overshooting resources is ok when strong scaling is good

- No CPUh wasted
- Faster results
- HPC favors large jobs

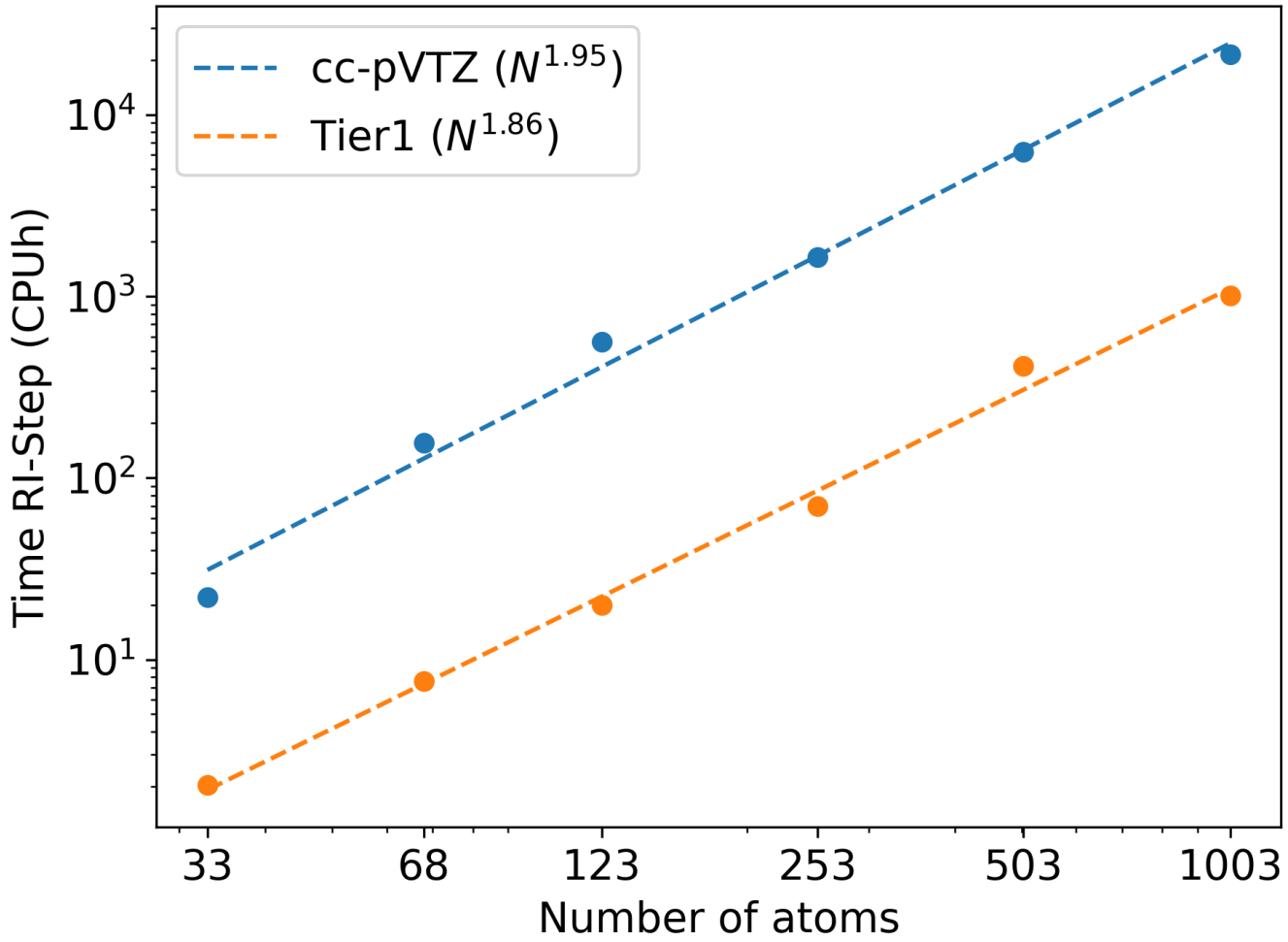
Scaling with system size

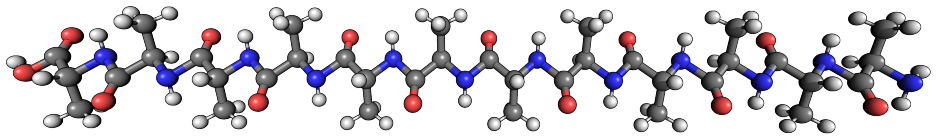




Tier 2 Basis
Juwels Cluster
10 Nodes (480 Tasks)

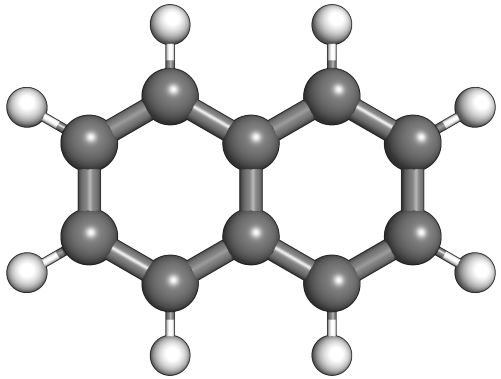
Scaling with system size: Big systems



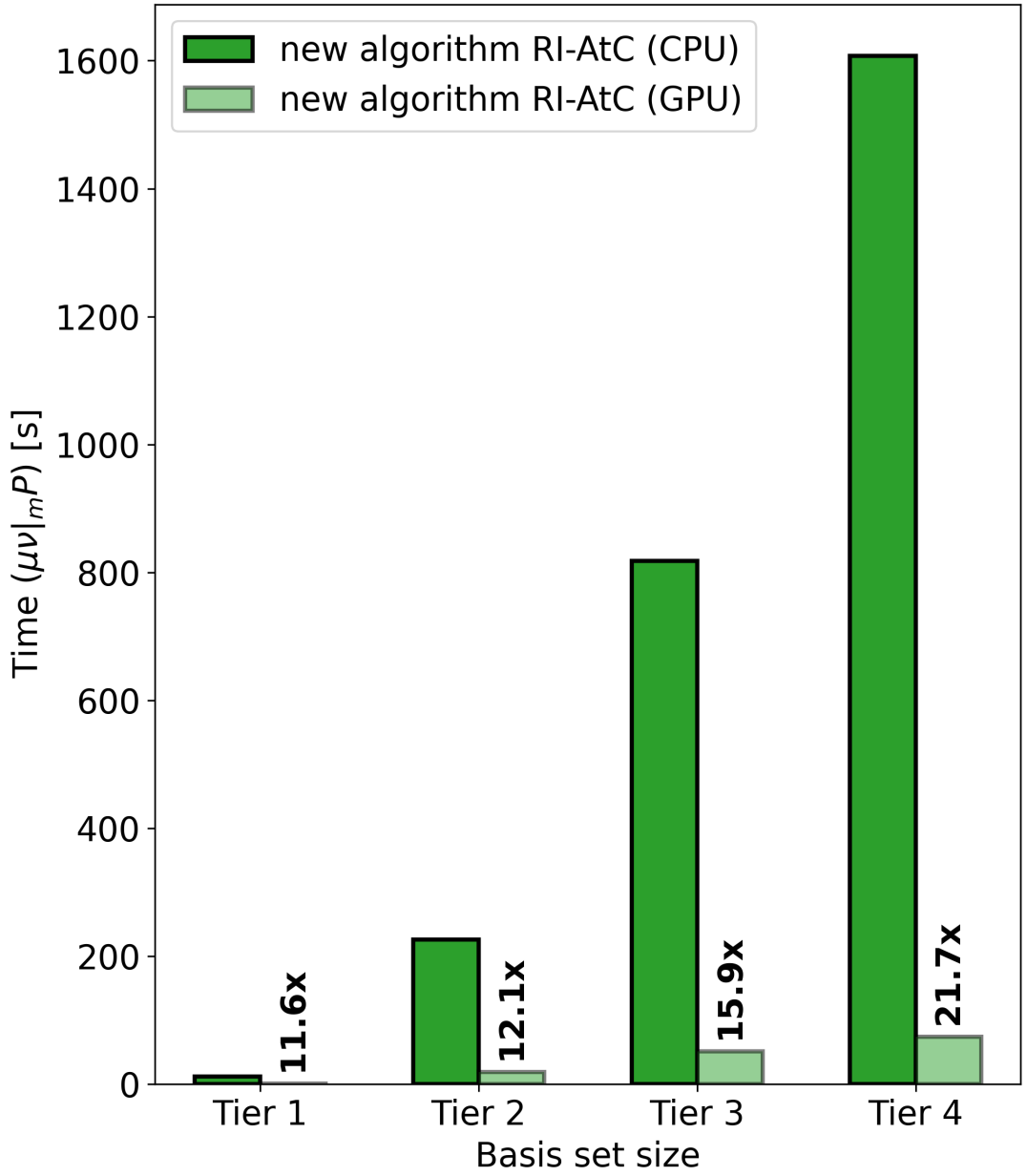


Alanine chains
Coulomb metric (RI-V)
PC2 Noctua
128 - 16 384 CPUs

GPU acceleration



Attenuated metric (RI-AtC)
Juwels Booster
1 Node (48 MPI Tasks)
+ 4 NVIDIA A100



Summary

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- Massively parallel RI-implementation

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- Very accurate

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- Linear scaling metrics or quadratic scaling RI-V

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- Scales to 1000+ atoms and 15000+ CPUs

Summary

- Massively parallel RI-implementation
- Very accurate
- Linear scaling metrics or quadratic scaling RI-V
- Scales to 1000+ atoms and 15000+ CPUs
- GPU accelerated (CUDA, HIP planned)

Acknowledgments

Golze Group
Computational chemistry and physics

- Dorothea Golze
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- Antonio Delesma
- Antonio Garcia-Blázquez

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Paderborn Center for Parallel Computing
GCS Gauss Centre for Supercomputing
JUPITER
LUMI

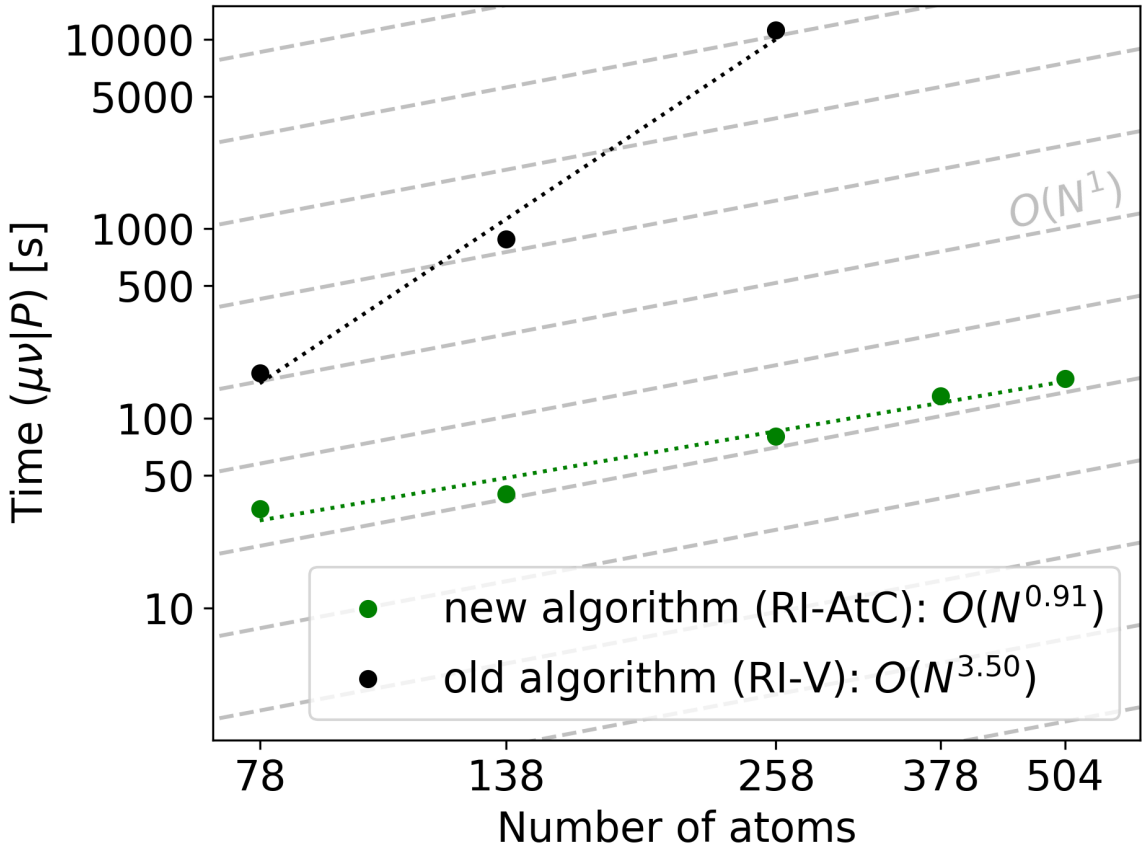
UNI WÜ

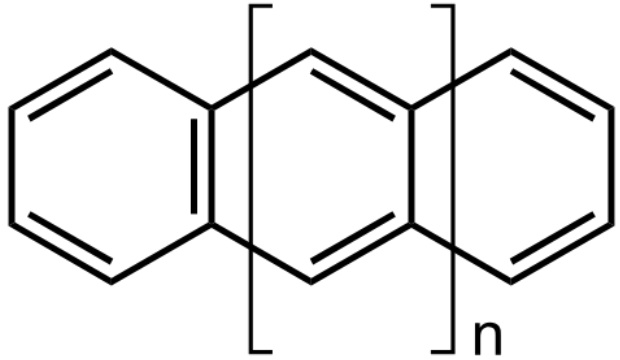
Golze Group

Computational chemistry and physics

Thanks for listening :)

Scaling





16 Nodes (768 MPI tasks)
JUWELS Cluster
Tier 1 // tight grid
Sigmoid attenuation

Integration

$$(\mu\nu|_m P) = \int \phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\ \Omega_P[m](\mathbf{r})\ d\mathbf{r}$$

$$= \sum_{a=a_1,a_2,a_3} \sum_{st} p_3(a,\mathbf{r})w(s,t)\phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\ \Omega_P[m](\mathbf{r})$$

$$= \sum_{B_v} \sum_{\mathbf{r}\in B_v} p(\mathbf{r})w(\mathbf{r})\phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\ \Omega_P[m](\mathbf{r})$$

New approach

Attenuated coulomb RI

3-center integrals:

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

$$= \int \phi_\mu(\mathbf{r})\phi_\nu(\mathbf{r})\; \Omega_P[m](\mathbf{r})\; d\mathbf{r}$$

field of the auxiliary function:

$$\Omega_P[m](\mathbf{r}) = \int m(\mathbf{r} - \mathbf{r}')\varphi_P(\mathbf{r}')\; d\mathbf{r}'$$

→ Coulomb metric: **large extend**
Attenuated metric: **small extend**

→ Sparsity leads to lower scaling

RI flavour

coulomb metric (RI-V): $$m(\mathbf{r}) = \frac{1}{r}$$

“Truncated” coulomb metric: $$m(\mathbf{r}) = \frac{\mathrm{rect}(\frac{r}{2r_c})}{r}$$

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

Analytic 3-center NAO integration

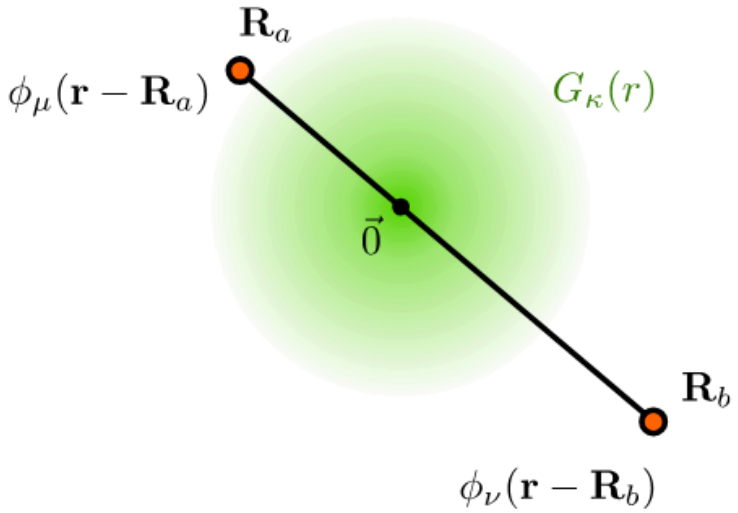


Figure 1: Codensity radial function.

$$\phi_a(|\mathbf{r}-\mathbf{R}_a|)\phi_b(|\mathbf{r}-\mathbf{R}_b|) = 4\pi \sum_{\kappa\nu} G_\kappa(r) Y_{\kappa\nu}(\hat{\mathbf{r}}) Y_{\kappa\nu}(\hat{\mathbf{R}})$$

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Multipole expansions of orbital products about an intermediate center

James D. Talman

First published: 21 April 2011 | https://doi.org/10.1002/qua.22511 | Citations: 1

Motivation

DFT

↓

2-electron Integrals

$(\mu\nu\,|\,\lambda\sigma)$

↓

Low-scaling RPA/GW
(Many body perturbation theory)

→ Antonios Talk

Numerical atom-centered orbitals (NAOs)

$$\phi(\mathbf{r}) = \frac{u(r)}{r} Y_{lm}(\mathbf{r})$$

FHI-aims
The ab initio materials simulation package

Blum et al., *Computer Physics Communications* **2009**, 180 (11).