TECHNISCHE UNIVERSITÄT DRESDEN

GreenX library

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Github Repository

GREENX

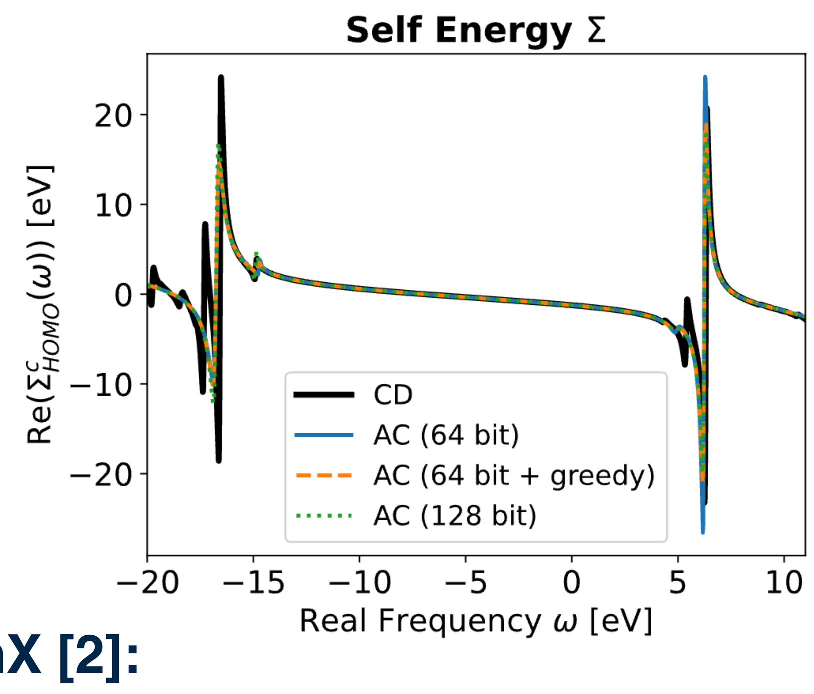
The GreenX library is a modular toolbox designed to support **Green's function-based** electronic structure methods, including RPA, GW, and Laplace-transformed direct MP2. It is organized into independent components, each dedicated to specific sub-tasks such as analytic continuation, enabling flexible integration into a variety of workflows. GreenX is built using a modern **CMake-based build system** and offers a **Fortran 2008 API** for seamless adoption in high-performance codes. The library is released under the **Apache 2.0 license** and is openly developed on GitHub. It is also available through the **Spack package manager** for easy deployment. Extensive documentation is provided through a dedicated website (accessible via QR code), and the library is already in active use by electronic structure codes such as **FHI-aims** and **CP2K**.

GreenX documentation

Analytic continuation component

Methods using analytic continuation:

- GW
- Real-time time-dependent DFT
- Many more



Analytic continuation in GreenX [2]:

- Padé functions are fitted to the reference function
- Thiele's reciprocal difference method
- Apply symmetry constraints to the Padé model

$$T_M(z) = \cfrac{a_1}{1 + \cfrac{a_2(z-z_1)}{\ddots\; 1 + \cfrac{a_p(z-z_{p-1})}{1 + \cfrac{a_{p+1}(z-z_p)}{\ddots\; 1 + a_M(z - z_{M-1})}}}}$$

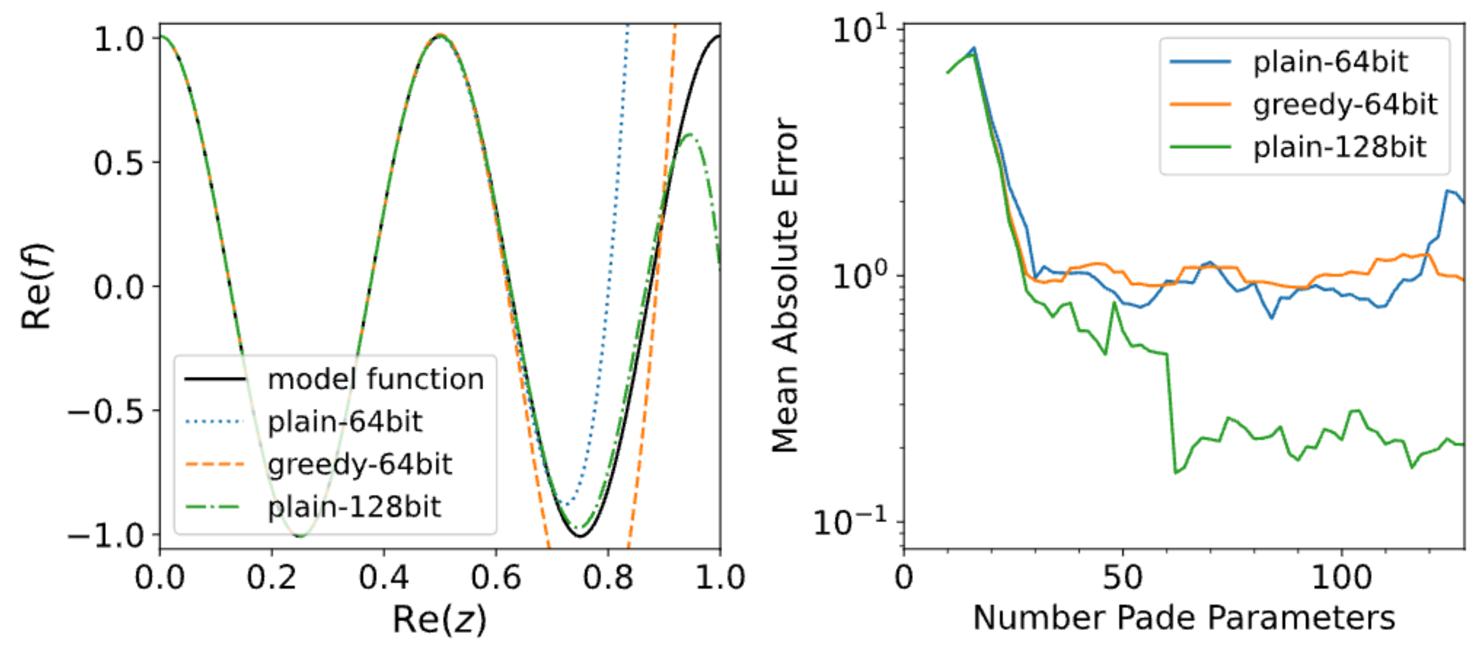
Padé rational function

Usability and advanced options [2]:

- Apply symmetry constraints (e.g. $f(z) = f(-z); f(z) = \overline{f(-z)}; \ldots$)
- Thiele's method numerically unstable [5], our approach:
  - **Multiple precision floats** > 64 bit (GNU MP library)
  - **Greedy algorithm** [4] for rearranging function arguments

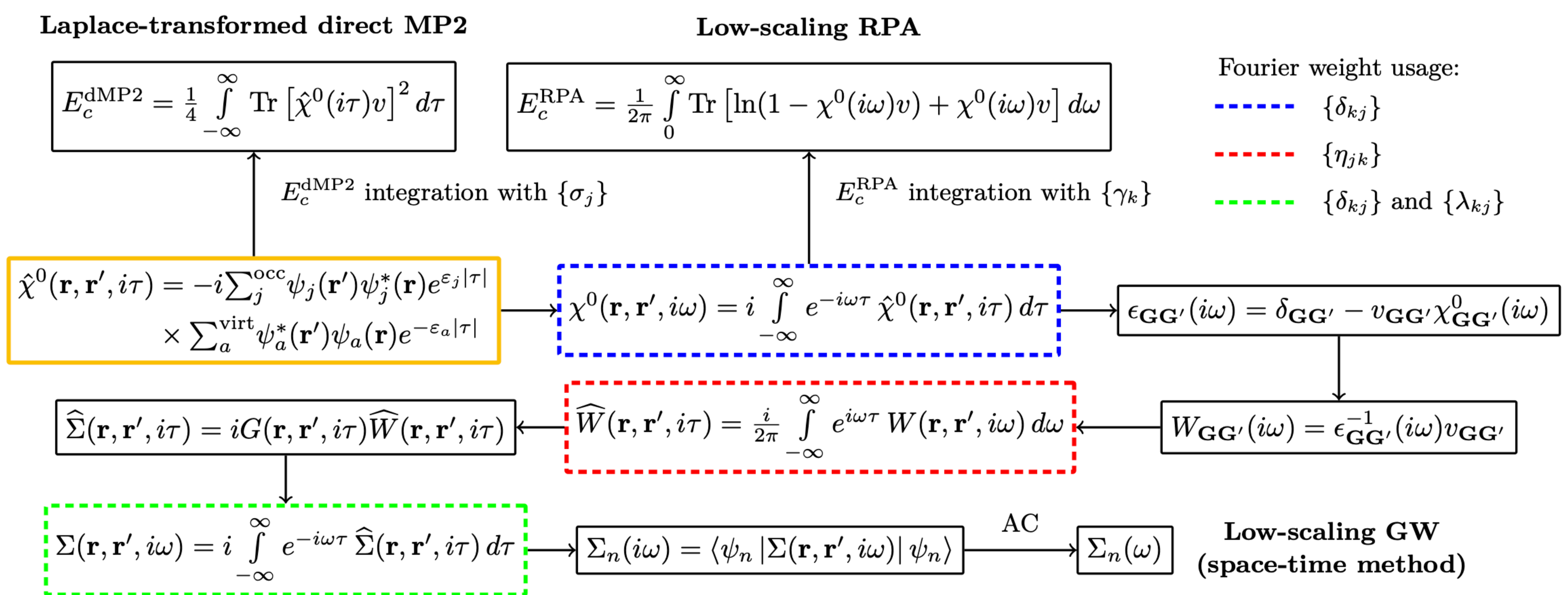
```
params_thiele = create_thiele_pade(n_par, x_ref, y_ref,      &
                                   do_greedy = .true.,       &
                                   precision = 64,           &
                                   enforce_symmetry = "none")
y_return =  evaluate_thiele_pade_at(params_thiele, x_query)
```

Performance of the analytic continuation component:



Time-frequency component

Low-scaling many-body perturbation methods using time-frequency grids:

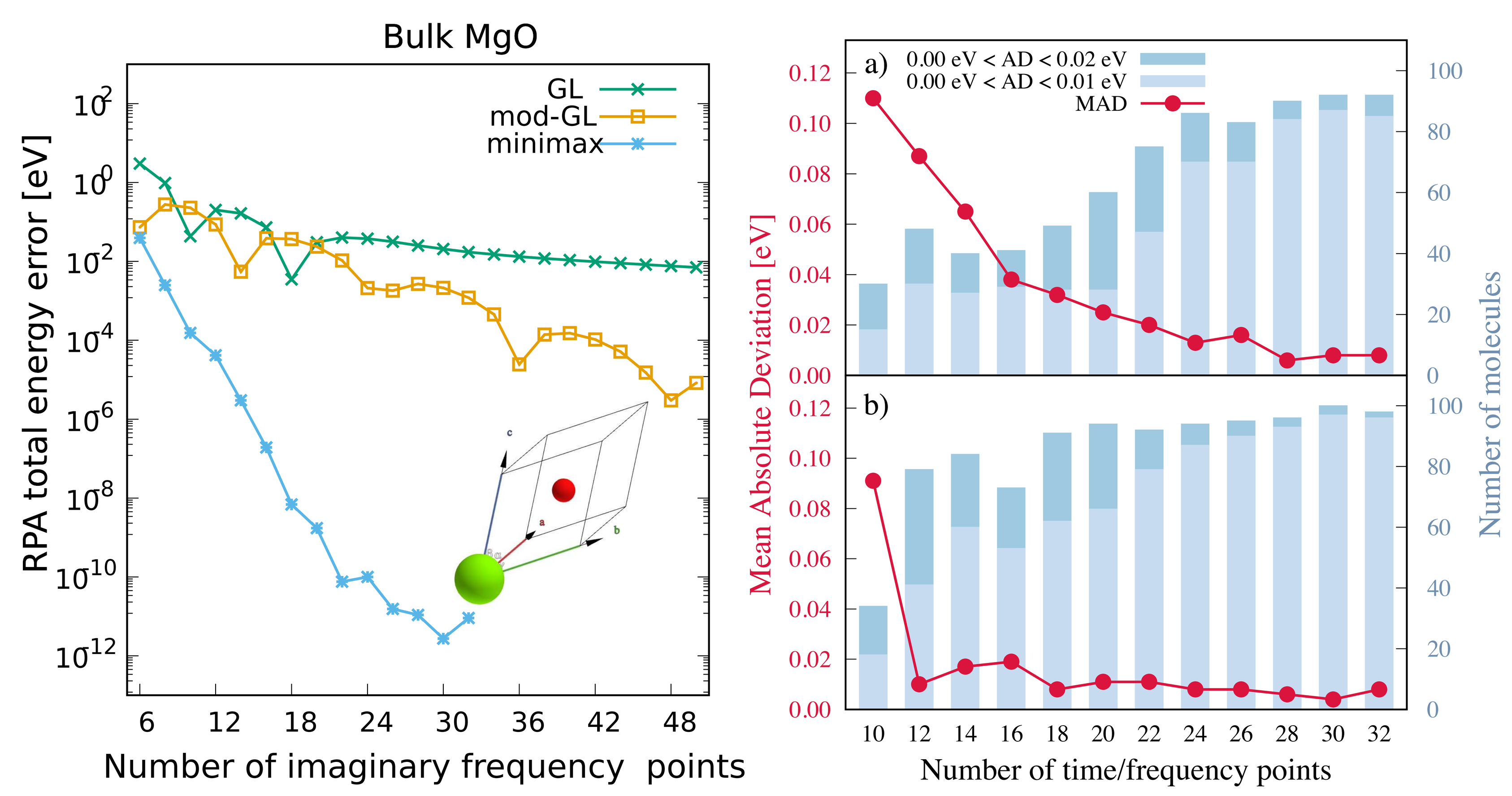


Usability of the component and provided quantities [1]:

- Minimax $\{i\tau\}$ and $\{i\omega\}$ grids + $\{\delta\}$, $\{\eta\}$ and $\{\lambda\}$ Fourier weights
- for canonical + low-scaling RPA, low-scaling GW, low-scaling LT-dMP2
- Computational pre-factor reduction for low-scaling RPA
- for molecules / solids and basis independent

```
call gx_minimax_grid(n_mesh_points, e_transition_min, e_transition_max, &
                     tau_mesh, tau_weights, &
                     freq_mesh, freq_weights, &
                     cos_tau_to_freq_weights, cos_freq_to_tau_weights, &
                     sinft_tau_to_freq_weights, &
                     max_errors, cosft_duality_error, ierr)
```

Performance of the minimax grids [3]:



References

[1] Azizi et al., *J. Open Source Softw.* **2023**, 8(90), 5570.
[2] Leucke et al., *J. Open Source Softw.* **2025**, 10(109), 7859.
[3] Azizi et al., *Phys. Rev. B* **2024**, 109, 245101.
[4] Panadés-Barrueta et al., *J. Chem. Theory Comput.* **2023**, 14(5), 053020.
[5] Beach et al., *Phys. Rev. B* **2000**, 61, 5147.

Founded by: NOMAD, INNO4SCALE
Computing time: GCS Gauss Centre for Supercomputing
GreenX is included in: FHI-aims The ab initio materials simulation package, CP2K, Spack