TECHNISCHE UNIVERSITÄT DRESDEN

GreenX library:

Time-frequency and analytic continuation component

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Flash talk reusable libraries in quantum chemistry 2025, Finland // June 30, 2025

Going beyond DFT: Green's function methods

RPA (Random Phase Approximation)
Accurate description of total energies

GW
Gold standard in photoemission spectroscopy for solids and molecules

BSE@GW (Bethe-Salpeter Equation)
Absorption spectroscopy, describing excitons

Other Methods in GreenX
- Laplace-transformed direct MP2 (LT-dMP2)
- Real-time time-dependent DFT

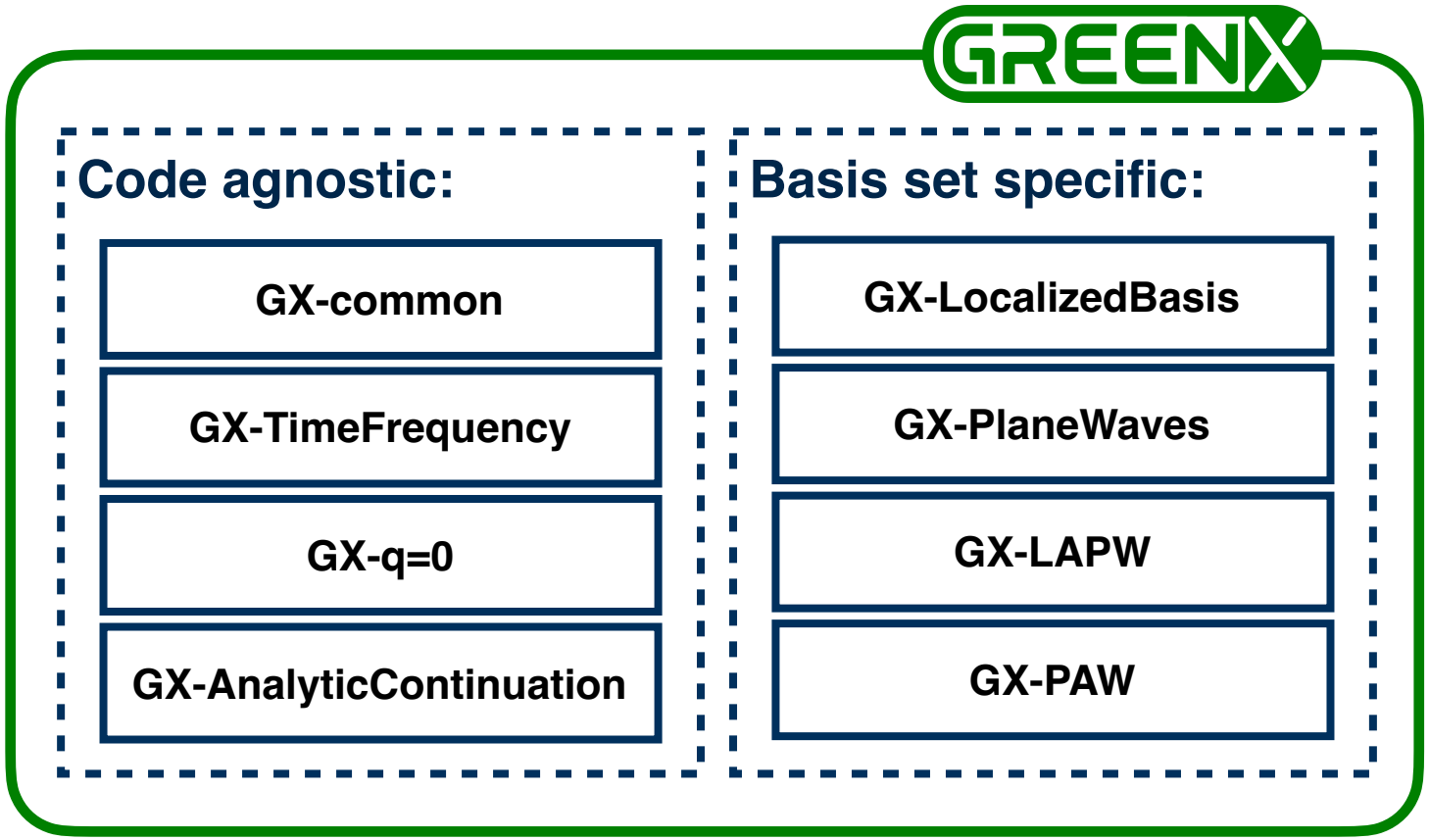
GreenX library

Motivation:

- low-scaling RPA & GW implemented or under development in many codes
- Toolbox for Green's function based methods (RPA, GW, …)

Technical details:

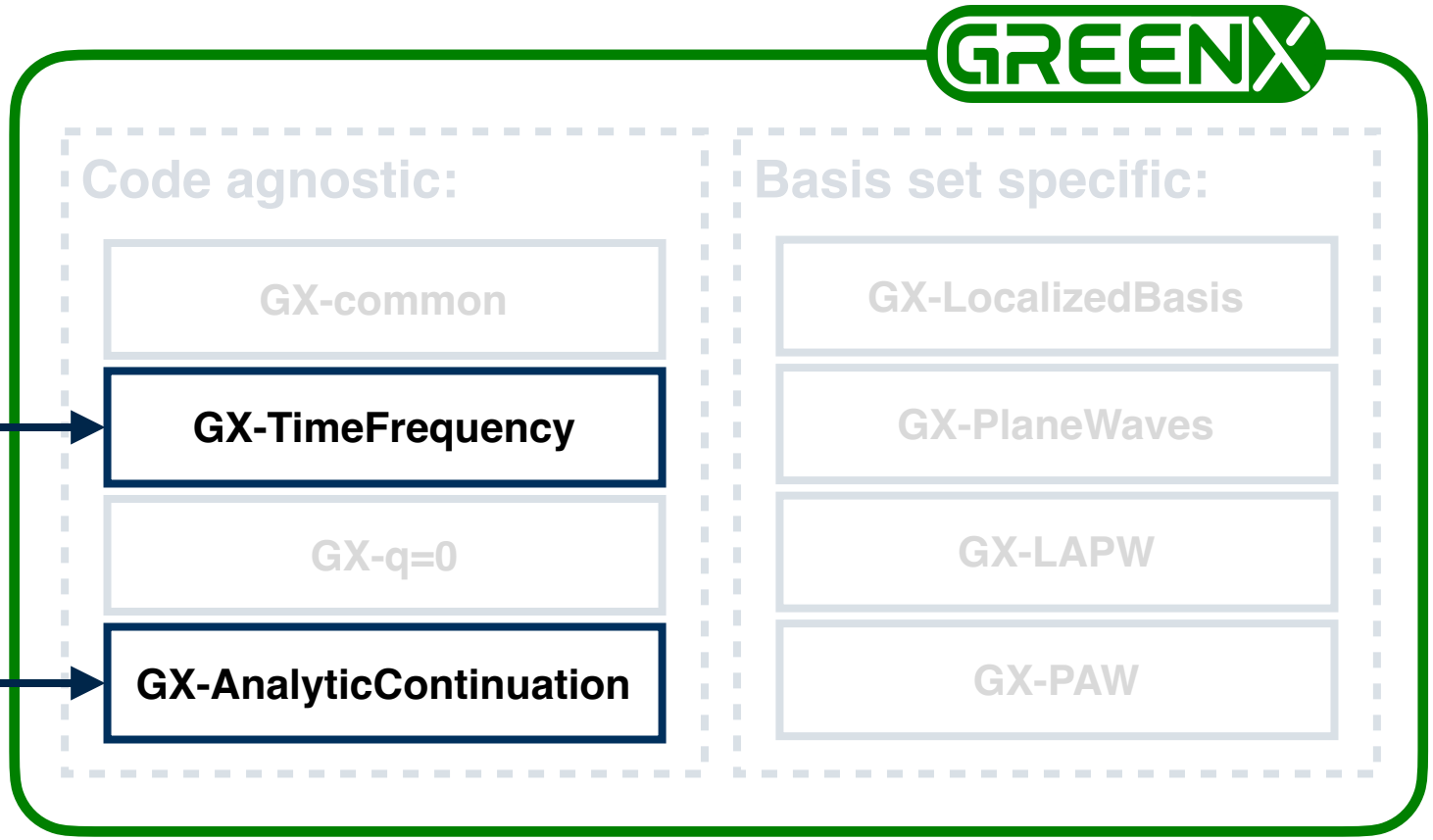
- **Fortran 2008** API
- Apache 2.0 license
- CMake build system
- Integrated into spack (package manager)



GreenX library: Components

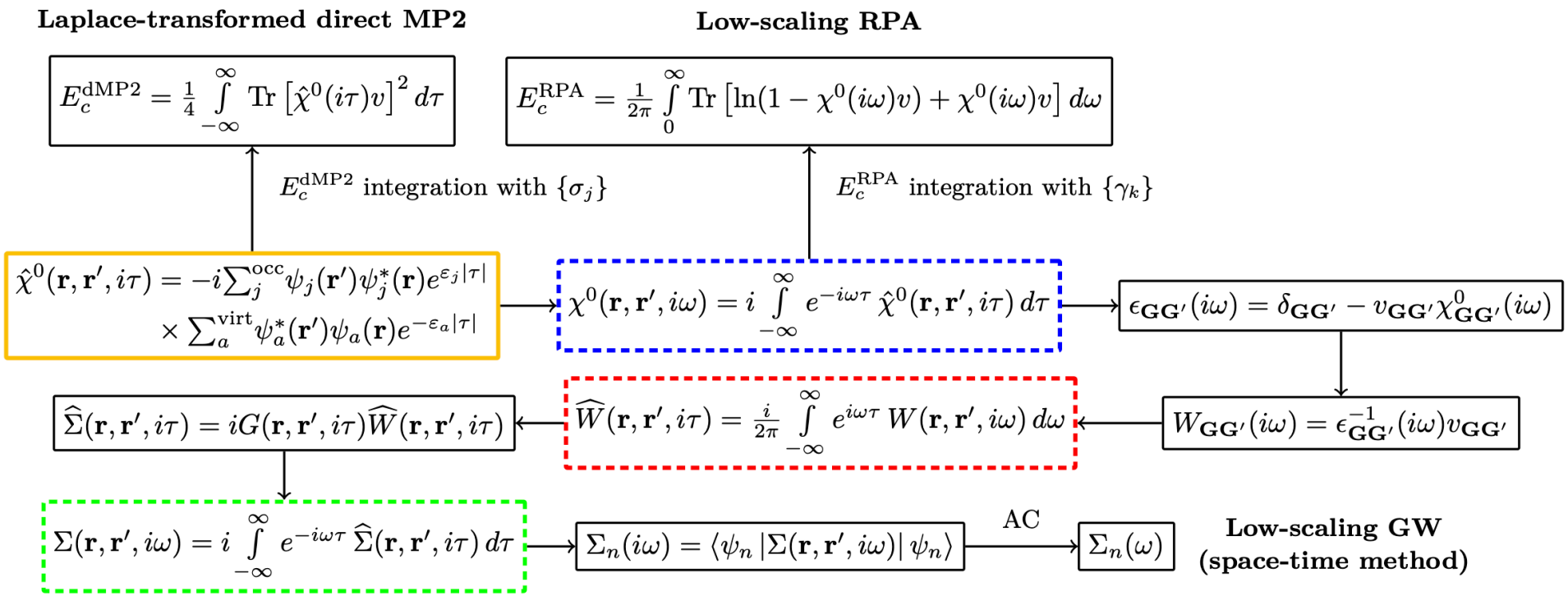
Azizi et al., *J. Open Source Softw.* **2023**, 8(90), 5570.

Leucke et al., *J. Open Source Softw.* **2025**, 10(109), 7859.



Time-Frequency component

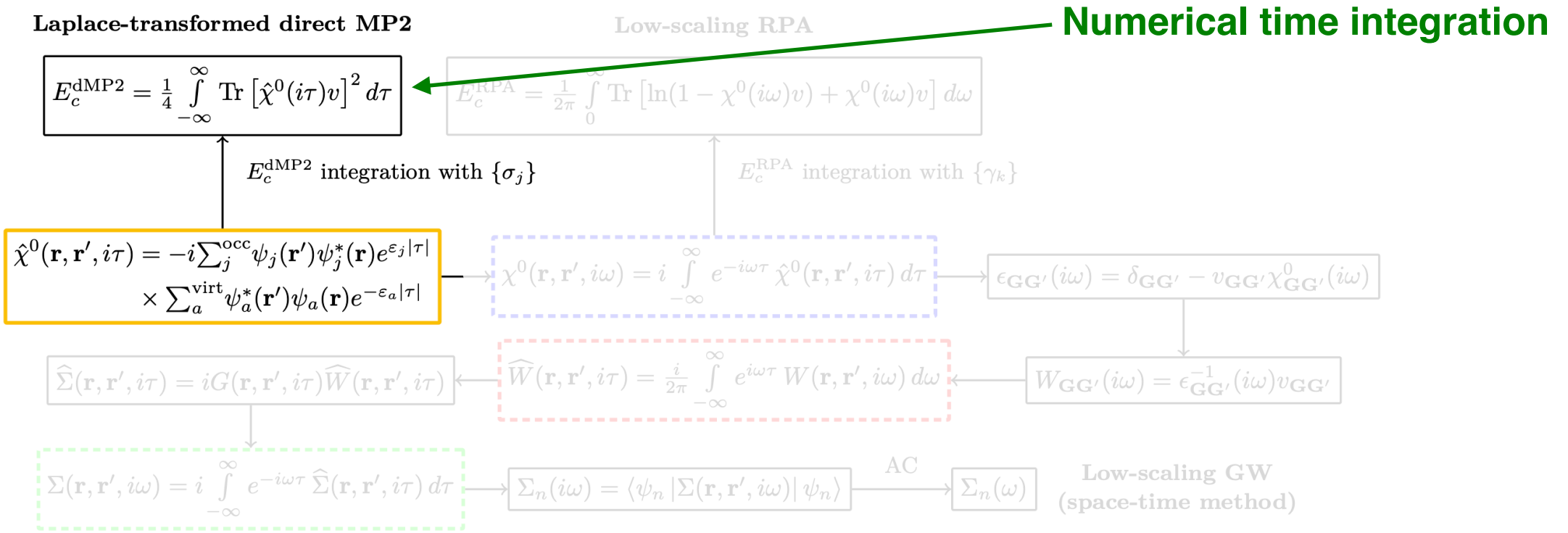
Low-scaling many-body perturbation methods:



Azizi et al., *J. Open Source Softw.* **2023**, 8(90), 5570.
Azizi et al., *Phys. Rev. B* **2024**, 109, 245101.

Time-Frequency component

Workflow low-scaling many-body perturbation methods:



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Time-Frequency component

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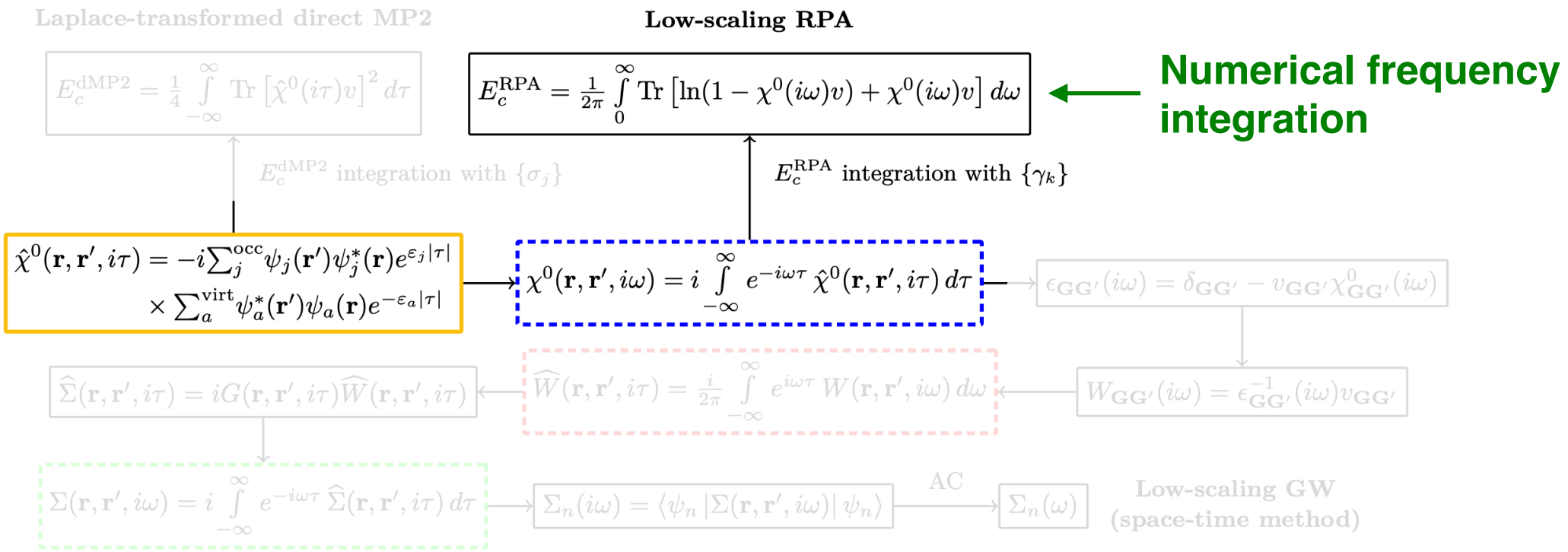

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Time-Frequency component

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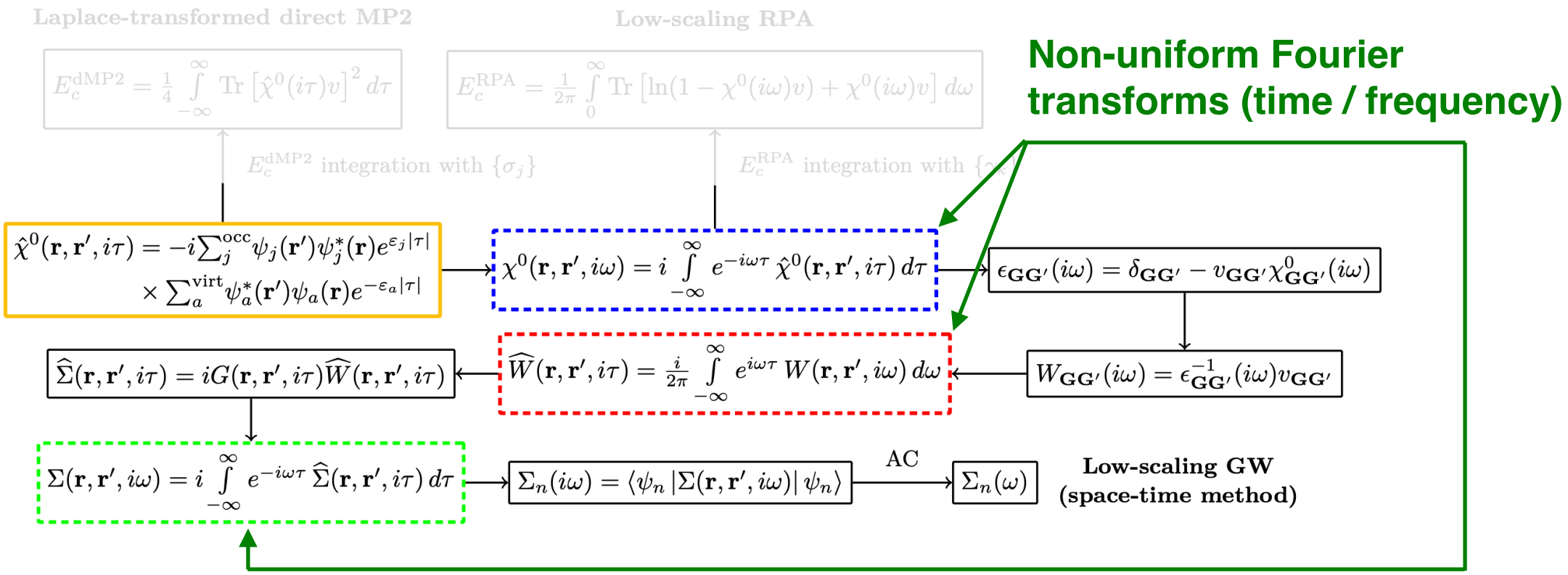

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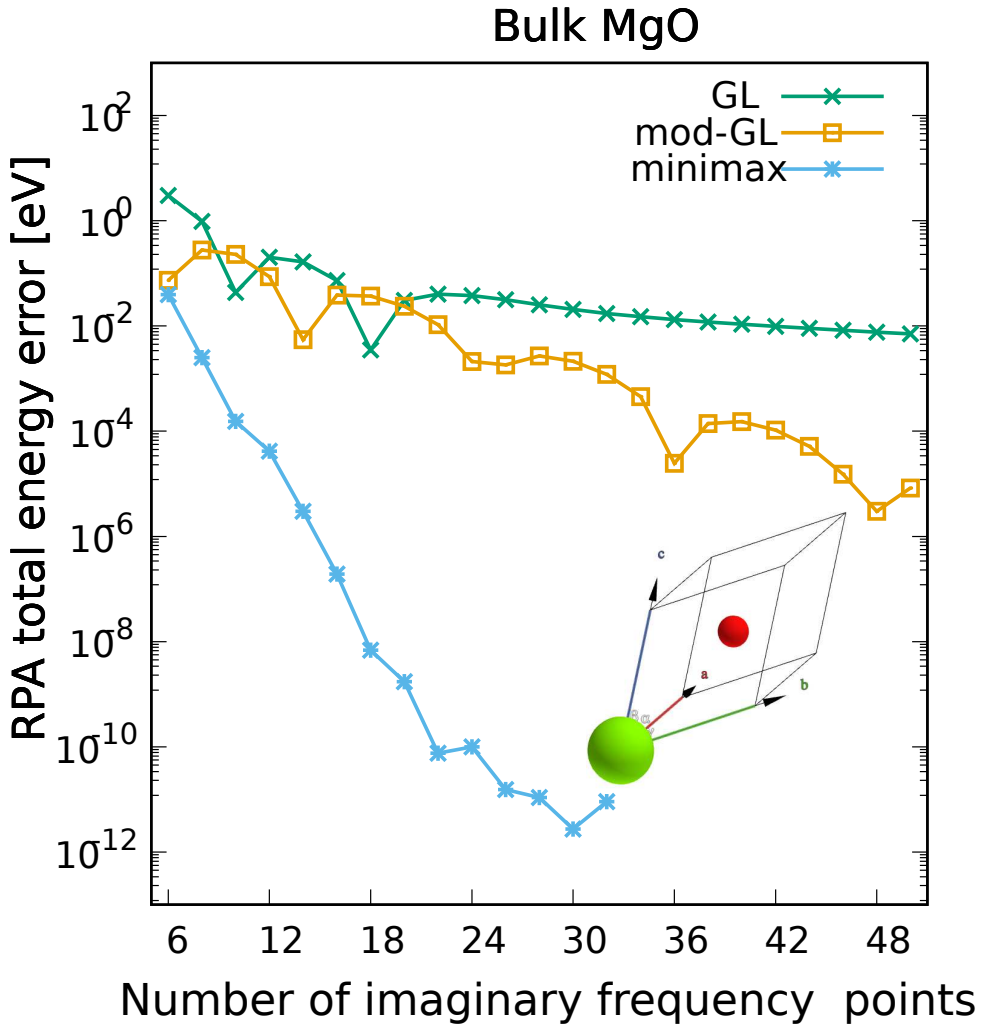
Time-Frequency component

- Tabulated Pre-optimized time/frequency grids (minimax approximation)
- Weights for non-uniform Fourier transformation
- Basis independent (plane waves, localized basis, …)
- For molecules and solids



Used by: FHI-aims The ab initio materials simulation package

CP2K

Azizi et al., *J. Open Source Softw.* **2023**, 8(90), 5570.
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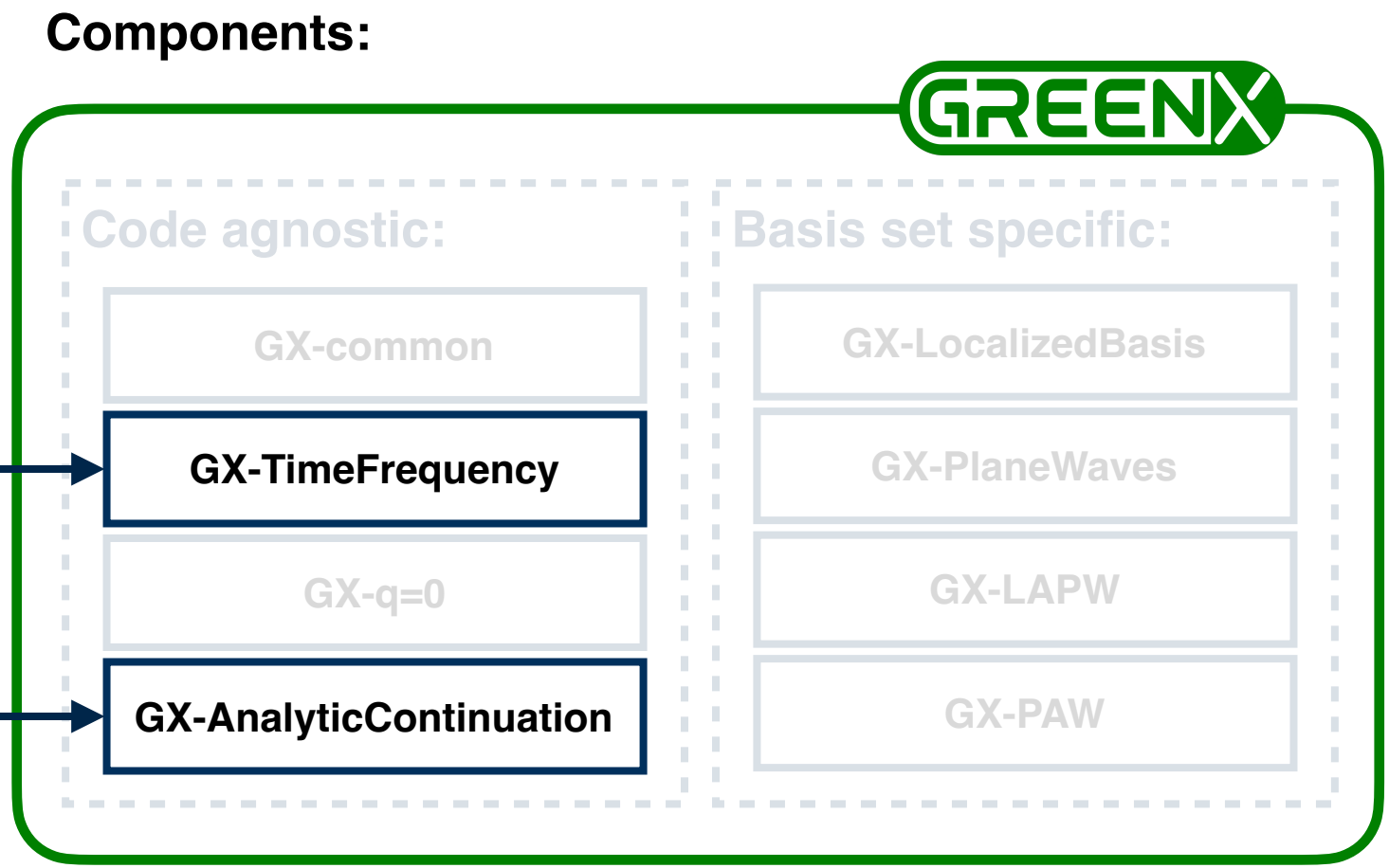
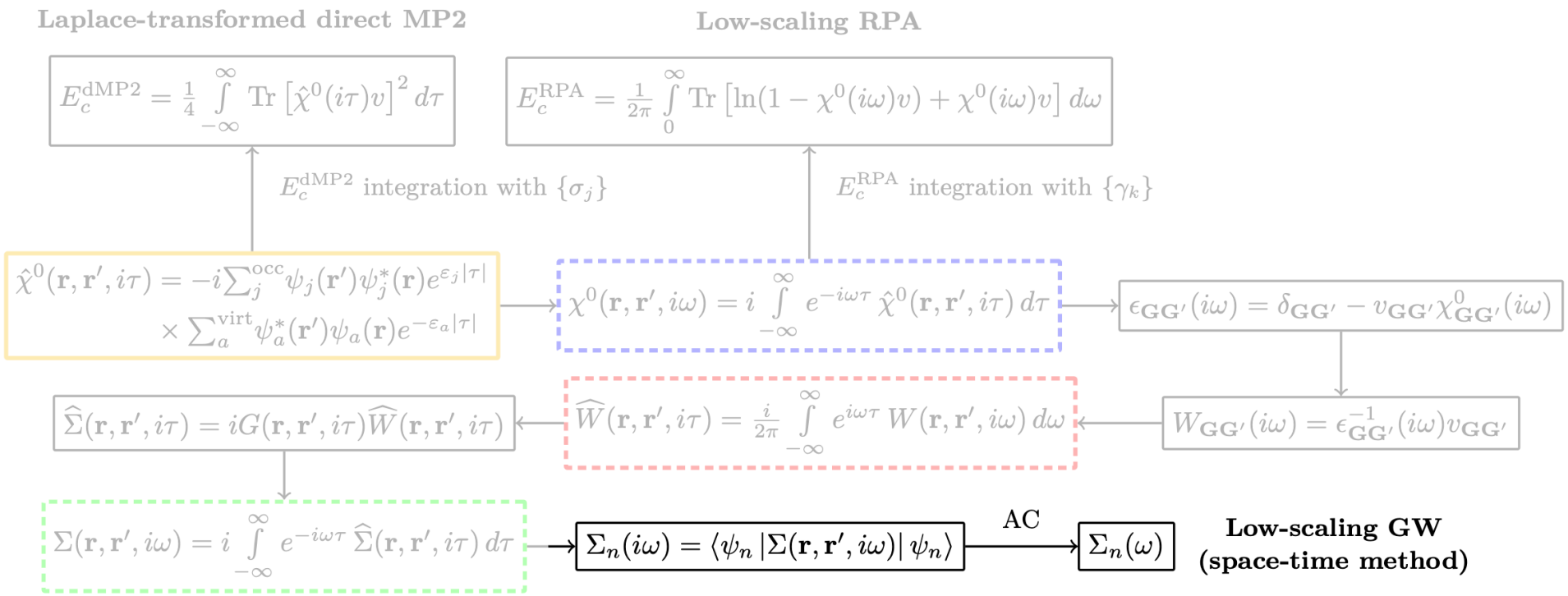


Analytic continuation component

Workflow low-scaling many-body perturbation methods:



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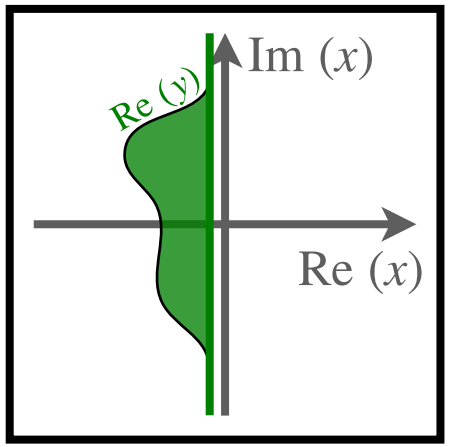
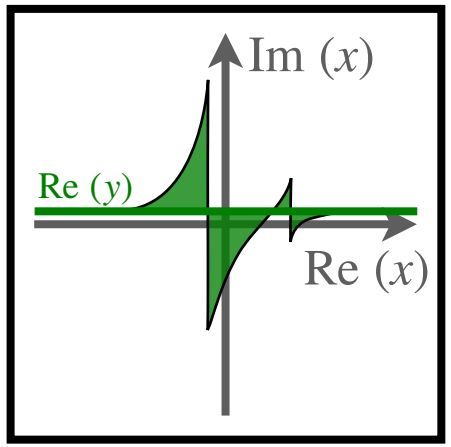
Analytic continuation component



Analytic continuation

GreenX: fit Padé function

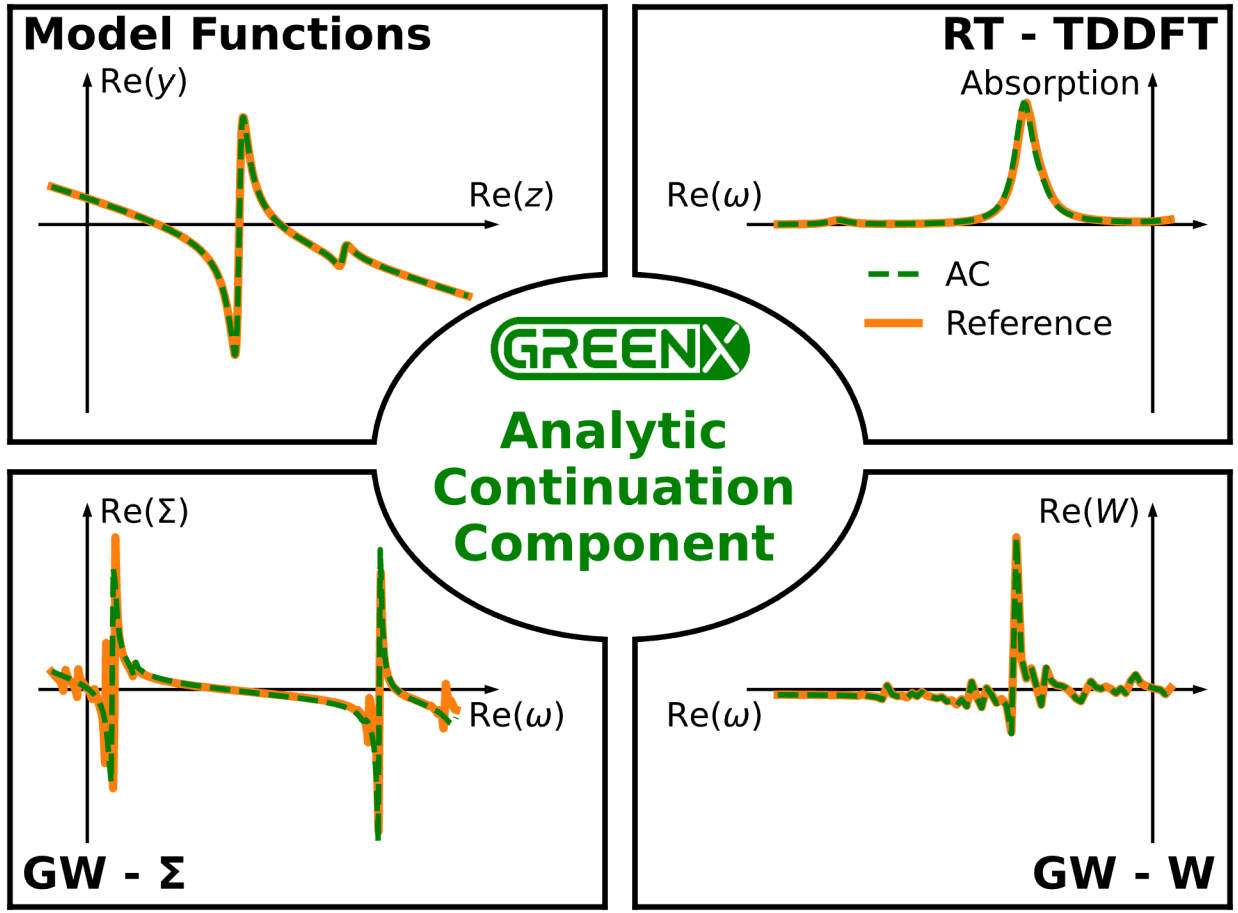


Complex function easily computed in one domain of complex plain

Evaluate in a broader domain of complex plain

Example in GW: $\Sigma(i\omega)$ $\Sigma(\omega)$

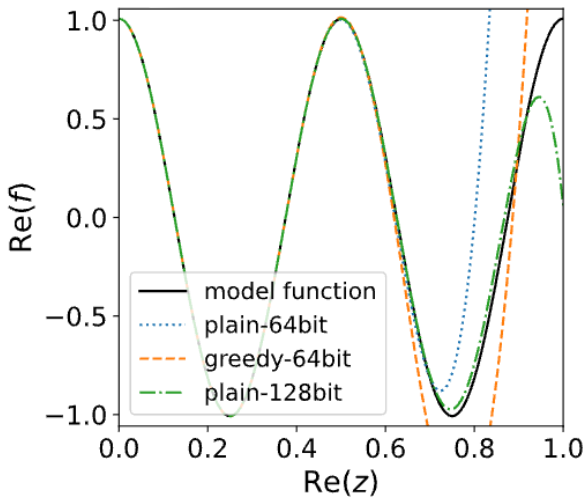
Analytic continuation component

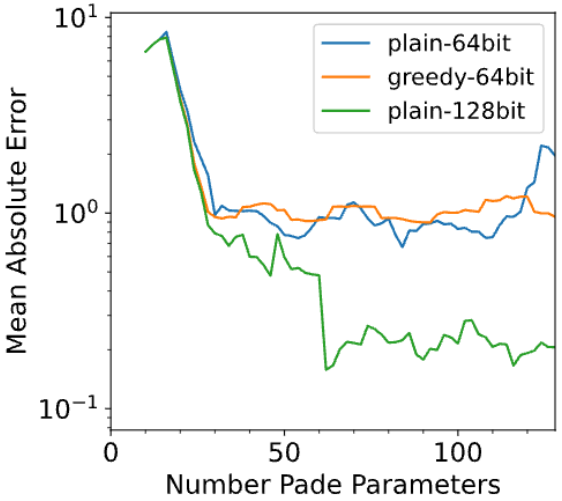


Analytic continuation component

Obtaining the Padé model:

- Thiele's reciprocal difference method
- Symmetry constraints can be applied





Numerical stability Thiele's method

➡ Multiple precision floats (> 64 bit) with GNU MP library

➡ Greedy algorithm to reorder function arguments

GMP
«Arithmetic without limitations»

Leucke et al., *J. Open Source Softw.* **2025**, 10(109), 7859.

Summary GreenX

- **Fortran 2008** library
- **Open Source** (Apache 2.0 license)
- components for Green's function based methods
- Time frequency component (ready to use)
- Analytic continuation component (ready to use)
- Interface to FHIaims and CP2K
- Basis set specific components under development

Developers:

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Dorothea Golze
Xavier Gonze
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Ramón L. Panadés-Barrueta
Patrick Rinke
Jan Wilhelm

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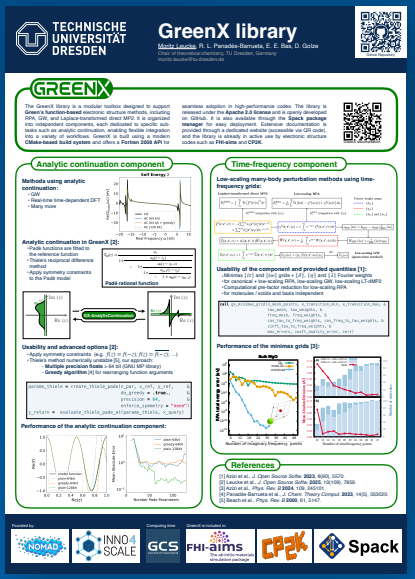
GREENX

Thank you for your attention!

Check out my Poster :)



Founding:

NOMAD

INNO4SCALE

Computing time:

GCS Gauss Centre for Supercomputing

GreenX included in:

FHI-aims The ab initio materials simulation package

CP2K

Spack

Analytic continuation component

Padé rational functions

Fraction of polynomials representation:

$$T_M(z) = \frac{A_0 + A_1 z + \cdots + A_p z^p + \cdots + A_{\frac{M-1}{2}} z^{\frac{M-1}{2}}}{1 + B_1 z + \cdots + B_p z^p + \cdots + B_{\frac{M}{2}} z^{\frac{M}{2}}}$$

Continued fraction representation:

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