








Analytic continuation component of the GreenX library: robust Padé approximants with symmetry constraints

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Summary

Analytic continuation extends the domain of a given complex-valued function to a broader region in the complex plane. This technique is widely applied across various fields, including quantum mechanical methods like the *GW* method and real-time propagation algorithms, to analytically continue a function from the imaginary axis to the real axis.

In this work, we present the analytic continuation component of the GreenX library (GX-AC), which provides a Fortran API for the use of Padé approximants with and without symmetry constraints. The component uses the Thiele Padé algorithm to create Padé approximants and uses multiple-precision floats in combination with a greedy algorithm to mitigate the numerical instabilities commonly associated with fitting Padé approximants. The GX-AC component is distributed under the Apache 2 license and freely available on GitHub.

Statement of need

Analytic continuation (AC) is used in different scientific fields where complex analysis is relevant including mathematical function theory and engineering for solving differential equations ([Lope & Tahara, 2002](#)). Another major application area is theoretical physics and chemistry, particularly in fields such as quantum mechanics ([Golze et al., 2019](#); [Li et al., 2020](#)) or quantum field theory ([Nekrasov, 2024](#)). In the following, we discuss the four examples depicted in Figure 1. The first example, shown in the top left of Figure 1, involves the application of AC to model functions, which may include Gamma functions ([Luke, 1975](#)), Zeta functions ([Iriguchi & Watanabe, 2007](#)), and others.

In quantum field theory, AC can be applied to the frequently arising, complex-valued Green's functions, like the Green's function of the Hubbard model ([Schött et al., 2016](#)). However, Green's functions also appear in *ab-initio* many-body perturbation theory methods like the *GW* approximation. The *GW* method ([Hedin, 1965](#)) is considered the method of choice for predicting band structures of solids as well as electron removal and addition energies of molecules, as measured in direct and indirect photoemission experiments ([Golze et al., 2019](#)). The complex-valued self energy is a central quantity in the *GW* method, computed as the convolution of the Green's function *G* and the screened Coulomb interaction *W*. AC is a frequently used tool for continuing the self energy from the imaginary to the real frequency axis in conventional scaling *GW* implementations ([Gonze et al., 2009](#); [Ren et al., 2012](#); [Van Setten et al., 2015](#); [Wilhelm & Hutter, 2017](#)) and low-scaling implementations ([Förster et al., 2023](#); [Förster & Visscher, 2020](#); [Förster & Visscher, 2021b, 2021a](#); [Graml et al., 2024](#); [Liu et al., 2016](#); [Wilhelm et al., 2018, 2021](#)). More recently, AC has also been applied to the screened Coulomb interaction ([Duchemin & Blase, 2020, 2021](#); [Friedrich, 2019](#); [Kehry et al.,](#)

2023; Kockläuner & Golze, 2025; Panadés-Barrueta & Golze, 2023; Samal & Voora, 2022; Springer et al., 1998; Voora, 2020) to e.g. reduce the computational scaling associated with core-level excitations (Panadés-Barrueta & Golze, 2023). The AC of a self energy Σ and a screened Coulomb interaction W are depicted as the second and third example in the bottom panel of Figure 1.

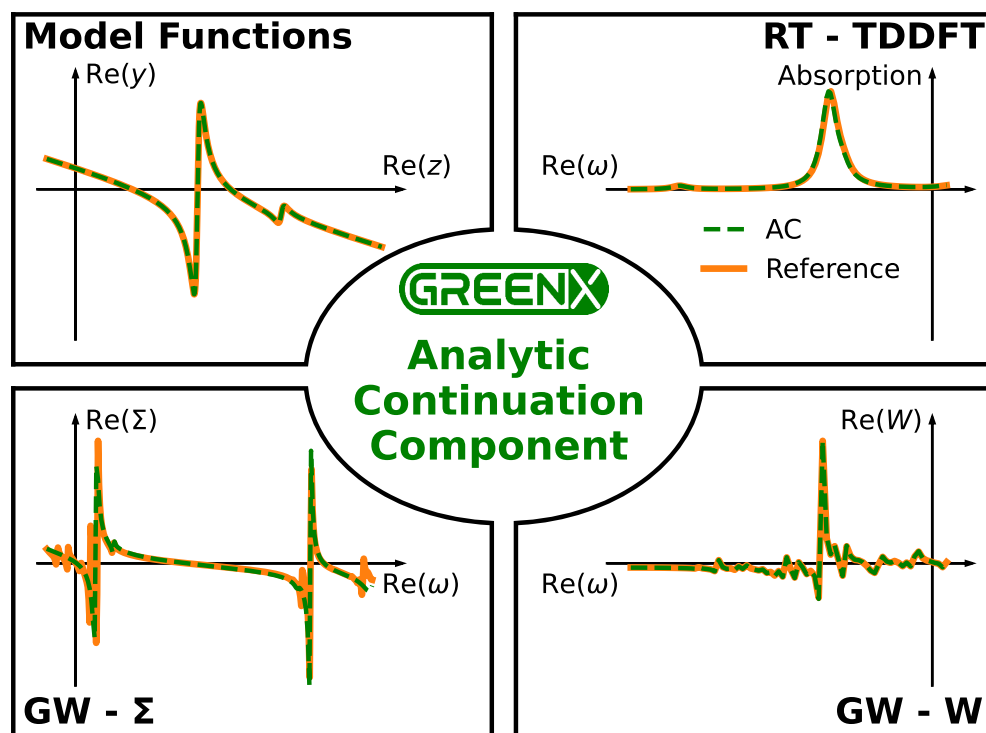


Figure 1: Application of the GX-AnalyticContinuation component to a model function with two poles (top left), an RT-TDDFT UV-vis absorption spectrum (top right), the GW self energy (bottom left) and the GW screened Coulomb interaction (bottom right). More information about the functions that are presented here can be found on the [website of the GX-AC component](#).

Our fourth and final example is the usage of AC in real-time propagation algorithms, such as real-time time-dependent density functional theory (RT-TDDFT) (Li et al., 2020). RT-TDDFT yields, for example, access to the absorption spectra of molecules and solids via the complex-valued dynamic polarizability tensor. The resolution of the RT-TDDFT absorption spectrum depends on the simulation length. It has been shown that applying Padé approximants to the dynamic polarizability tensor is an effective strategy for achieving higher spectral resolution with much shorter simulation times (Bruner et al., 2016; Mattiat & Luber, 2018). An illustrative UV-vis absorption spectrum, with and without the use of AC, is shown in the top right of Figure 1.

AC of analytic (holomorphic) functions is typically performed by approximating the function with a rational function in one domain of the complex plane, typically along the imaginary axis. According to the identity theorem, the resulting rational function can then be evaluated over a broader domain of the complex plane, for example, along the real axis. Padé approximants are an established choice for rational functions. Their flexibility enables the approximation of functions with complicated pole structures (Golze et al., 2019). Padé approximants can be expressed by the ratio of two polynomials with arbitrary order, or alternatively by a continued fraction (Baker, 1975).

The GreenX library aims to provide a suite of common tools, such as AC, for electronic

structure codes based on the GW method. The previously published first component of the GreenX library is the TimeFrequency component (Azizi et al., 2023). It provides minimax time and frequency grids for the random phase approximation (RPA) and GW methods that were validated in a comprehensive benchmark study (Azizi et al., 2024). In this work we present the second component of the GreenX library, the GX-AnalyticContinuation (GX-AC) component, which has the Apache-2.0 license. It provides a Fortran API for analytic continuation using Padé rational functions that can be easily integrated into other Fortran projects. The component uses the Thiele reciprocal difference method (Baker, 1975; Milne-Thomson, 1933; Thiele, 1909) to obtain the Padé coefficients. Although the primary focus of the GreenX library are GW -based methods, the GX-AC component is suitable for any application where AC with Padé approximants can be used. Extensive benchmarks and the full documentation of GX-AC component can be found on the [component's website](#).

Generating Padé approximants is prone to numerical instabilities caused by rounding errors that are amplified in the numerous differences in the Thiele-Padé algorithm (Beach et al., 2000; Cuyt et al., 1988; Graves-Morris, 1980; Jones & Thron, 1974). We employ two strategies to address these numerical instabilities. The first approach is to use multiple precision floating point arithmetic for the implementation of the Thiele algorithm, minimizing the numerical noise caused by rounding errors. We use the GNU Multiple Precision (GMP) library (Granlund, 2015) to handle the multiple-precision floats. The advantage of this library is that it provides highly optimized assembly code for most of the processors available. This approach allows us to exceed the 128-bit precision limit typically supported by standard Fortran compilers. The second strategy involves using a greedy algorithm for Thiele Padé approximants, that has been validated in previous work (Celis, 2023, 2024; Panadés-Barrueta & Golze, 2023). The greedy algorithm is used to rearrange the function arguments of the reference function in order to make the model numerically more stable.

Another feature of the GX-AC component is to force the Padé model to exhibit a certain symmetry. This ensures that the approximant has the same symmetry as the reference function in the case that the symmetry of the reference function is known in advance, e.g. the screened Coulomb interaction in the GW is an even function (Duchemin & Blase, 2020). Additionally, the enforced symmetry helps to increase the quality of the Padé approximant because every point of a given reference function also accounts for symmetrical equivalent points. Even, odd, conjugate and anti-conjugate function symmetry is supported by the component at this point.

State of the field

To the best of the authors' knowledge, there are no Padé AC implementations that provide symmetry constraints and floating point precision beyond 128 bit, as the GX-AC component does. An open-source project that provides a Fortran implementation is the Padé Approximants repository by Johan Schött (JohanSchott, 2016). However, it uses the Beach algorithm (Beach et al., 2000) in a quadruple precision implementation to generate Padé approximants and it provides an executable binary, rather than a Fortran API. Additionally, several Python, Julia and R implementations exist that offer an API in the specified language (Adler, 2015; bennoski, 2019; jjgoings, 2017; mjp98, 2022; Montmorency, 2014; Virtanen et al., 2020), but they do not offer a Fortran or C API.

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References

- Adler, A. (2015). *Pade: Padé Approximant Coefficients*. <https://doi.org/10.32614/CRAN.package.Pade>
- Azizi, M., Wilhelm, J., Golze, D., Delesma, F. A., Panadés-Barrueta, R. L., Rinke, P., Giantomassi, M., & Gonze, X. (2024). Validation of the GreenX library time-frequency component for efficient GW and RPA calculations. *Physical Review B*, 109(24), 245101. <https://doi.org/10.1103/PhysRevB.109.245101>
- Azizi, M., Wilhelm, J., Golze, D., Giantomassi, M., Panadés-Barrueta, R. L., Delesma, F. A., Buccheri, A., Gulans, A., Rinke, P., Draxl, C., & others. (2023). Time-frequency component of the GreenX library: Minimax grids for efficient RPA and GW calculations. *Journal of Open Source Software*, 8(90), 5570. <https://doi.org/10.21105/joss.05570>
- Baker, G. A. (1975). *Essentials of padé approximants*. Elsevier. <https://shop.elsevier.com/books/essentials-of-pade-approximants/baker/978-0-12-074855-6>
- Beach, K. S. D., Gooding, R. J., & Marsiglio, F. (2000). Reliable padé analytical continuation method based on a high-accuracy symbolic computation algorithm. *Physical Review B*, 61, 5147–5157. <https://doi.org/10.1103/PhysRevB.61.5147>
- bennoski. (2019). Pade. In *GitHub repository*. GitHub. <https://github.com/bennoski/pade>
- Bruner, A., LaMaster, D., & Lopata, K. (2016). Accelerated broadband spectra using transition dipole decomposition and padé approximants. *Journal of Chemical Theory and Computation*, 12(8), 3741–3750. <https://doi.org/10.1021/acs.jctc.6b00511.s001>
- Celis, O. S. (2023). Adaptive thiele interpolation. *ACM Commun. Comput. Algebra*, 56(3), 125–132. <https://doi.org/10.1145/3594252.3594254>
- Celis, O. S. (2024). Numerical continued fraction interpolation. *Ukrainskyi Matematychnyi Zhurnal*, 76(4), 568–580. <https://doi.org/10.3842/umzh.v74i4.7349>
- Cuyt, A. A. M., Jacobsen, L., & Verdonk, B. M. (1988). Instability and modification of thiele interpolating continued fractions. *Applied Numerical Mathematics*, 4(2-4), 253–262. [https://doi.org/10.1016/0168-9274\(83\)90005-3](https://doi.org/10.1016/0168-9274(83)90005-3)
- Duchemin, I., & Blase, X. (2020). Robust analytic-continuation approach to many-body GW calculations. *Journal of Chemical Theory and Computation*, 16(3), 1742–1756. <https://doi.org/10.1021/acs.jctc.9b01235.s001>
- Duchemin, I., & Blase, X. (2021). Cubic-scaling all-electron GW calculations with a separable density-fitting space–time approach. *Journal of Chemical Theory and Computation*, 17(4), 2383–2393. <https://doi.org/10.1021/acs.jctc.1c00101.s001>
- Förster, A., Lenthe, E. van, Spadetto, E., & Visscher, L. (2023). Two-component GW calculations: Cubic scaling implementation and comparison of vertex-corrected and partially self-consistent GW variants. *Journal of Chemical Theory and Computation*, 19(17), 5958–5976. <https://doi.org/10.1021/acs.jctc.3c00512.s002>
- Förster, A., & Visscher, L. (2020). Low-order scaling G0W0 by pair atomic density fitting. *Journal of Chemical Theory and Computation*, 16(12), 7381–7399. <https://doi.org/10.1021/acs.jctc.0c00693>
- Förster, A., & Visscher, L. (2021a). GW100: A slater-type orbital perspective. *Journal of Chemical Theory and Computation*, 17(8), 5080–5097. <https://doi.org/10.1021/acs.jctc.>

1c00308.s001

- Förster, A., & Visscher, L. (2021b). Low-order scaling quasiparticle self-consistent GW for molecules. *Frontiers in Chemistry*, 9, 736591. <https://doi.org/10.3389/fchem.2021.736591>
- Friedrich, C. (2019). Tetrahedron integration method for strongly varying functions: Application to the GT self-energy. *Physical Review B*, 100(7), 075142. <https://doi.org/10.1103/PhysRevB.100.075142>
- Golze, D., Dvorak, M., & Rinke, P. (2019). The GW compendium: A practical guide to theoretical photoemission spectroscopy. *Frontiers in Chemistry*, 7, 377. <https://doi.org/10.3389/fchem.2019.00377>
- Gonze, X., Amadon, B., Anglade, P. M., Beuken, J. M., Bottin, F., Boulanger, P., Bruneval, F., Caliste, D., Caracas, R., Côté, M., & others. (2009). ABINIT: First-principles approach to material and nanosystem properties. *Computer Physics Communications*, 180(12), 2582–2615. <https://doi.org/10.1016/j.cpc.2009.07.007>
- Graml, M., Zollner, K., Hernangómez-Pérez, D., Faria Junior, P. E., & Wilhelm, J. (2024). Low-scaling GW algorithm applied to twisted transition-metal dichalcogenide heterobilayers. *Journal of Chemical Theory and Computation*, 20(5), 2202–2208. <https://doi.org/10.1021/acs.jctc.3c01230.s001>
- Granlund, T. (2015). *GNU MP 6.3 multiple precision arithmetic library*. Samurai Media Limited. <https://gmplib.org/gmp-man-6.3.0.pdf>
- Graves-Morris, P. R. (1980). Practical, Reliable, Rational Interpolation. *IMA Journal of Applied Mathematics*, 25(3), 267–286. <https://doi.org/10.1093/imamat/25.3.267>
- Hedin, L. (1965). New method for calculating the one-particle green's function with application to the electron-gas problem. *Physical Review*, 139(3A), A796. <https://doi.org/10.1103/physrev.139.a796>
- Iriguchi, R., & Watanabe, S. (2007). Estimation of poles of zeta function in learning theory using padé approximation. *Artificial Neural Networks–ICANN 2007: 17th International Conference, Porto, Portugal, September 9–13, 2007, Proceedings, Part i* 17, 88–97. https://doi.org/10.1007/978-3-540-74690-4_10
- jjgoings. (2017). Pade: Fourier transform via pade approximants. In *GitHub repository*. GitHub. <https://github.com/jjgoings/pade>
- JohanSchott. (2016). Pade_approximants. In *GitHub repository*. GitHub. https://github.com/JohanSchott/Pade_approximants
- Jones, W. B., & Thron, W. J. (1974). Numerical stability in evaluating continued fractions. *Mathematics of Computation*, 28(127), 795–810. <https://doi.org/10.1017/cbo9780511759550.015>
- Kehry, M., Klopper, W., & Holzer, C. (2023). Robust relativistic many-body green's function based approaches for assessing core ionized and excited states. *The Journal of Chemical Physics*, 159(4). <https://doi.org/10.1063/5.0160265>
- Kockläuner, J., & Golze, D. (2025). GW plus cumulant approach for predicting core-level shakeup satellites in large molecules. *Journal of Chemical Theory and Computation*, 21(6), 3101–3119. <https://doi.org/10.1021/acs.jctc.4c01754>
- Li, X., Govind, N., Isborn, C., DePrince III, A. E., & Lopata, K. (2020). Real-time time-dependent electronic structure theory. *Chemical Reviews*, 120(18), 9951–9993. <https://doi.org/10.1021/acs.chemrev.0c00223>
- Liu, P., Kaltak, M., Klimeš, J., & Kresse, G. (2016). Cubic scaling GW: Towards fast quasiparticle calculations. *Physical Review B*, 94(16), 165109. <https://doi.org/10.1103/PhysRevB.94.165109>

- Lope, J. E. C., & Tahara, H. (2002). On the analytic continuation of solutions to nonlinear partial differential equations. *Journal de Mathématiques Pures Et Appliquées*, 81(9), 811–826. [https://doi.org/10.1016/S0021-7824\(02\)01257-6](https://doi.org/10.1016/S0021-7824(02)01257-6)
- Luke, Y. L. (1975). On the error in the padé approximants for a form of the incomplete gamma function including the exponential function. *SIAM Journal on Mathematical Analysis*, 6(5), 829–839. <https://doi.org/10.1137/0506072>
- Mattiat, J., & Luber, S. (2018). Efficient calculation of (resonance) raman spectra and excitation profiles with real-time propagation. *The Journal of Chemical Physics*, 149(17). <https://doi.org/10.1063/1.5051250>
- Milne-Thomson, L. M. (1933). *The calculus of finite differences*. Macmillan And Company. <https://archive.org/details/calculusoffinite032017mbp/page/n5/mode/2up>
- mjp98. (2022). RobustPade.jl. In *GitHub repository*. GitHub. <https://github.com/mjp98/RobustPade.jl>
- Montmorency. (2014). Pade-py. In *GitHub repository*. GitHub. <https://github.com/Montmorency/pade-py>
- Nekrasov, N. (2024). Analytic continuation and supersymmetry. *Proc. Symp. Pure Math*, 107, 167. <https://doi.org/10.48550/arXiv.2310.01654>
- Panadés-Barrueta, R. L., & Golze, D. (2023). Accelerating core-level GW calculations by combining the contour deformation approach with the analytic continuation of w. *Journal of Chemical Theory and Computation*, 19(16), 5450–5464. <https://doi.org/10.1021/acs.jctc.3c00555>
- Ren, X., Rinke, P., Blum, V., Wieferink, J., Tkatchenko, A., Sanfilippo, A., Reuter, K., & Scheffler, M. (2012). Resolution-of-identity approach to hartree–fock, hybrid density functionals, RPA, MP2 and GW with numeric atom-centered orbital basis functions. *New Journal of Physics*, 14(5), 053020. <https://doi.org/10.1088/1367-2630/14/5/053020>
- Samal, B., & Voora, V. K. (2022). Modeling nonresonant x-ray emission of second-and third-period elements without core-hole reference states and empirical parameters. *Journal of Chemical Theory and Computation*, 18(12), 7272–7285. <https://doi.org/10.1021/acs.jctc.2c00647.s002>
- Schött, J., Loch, I. L. M., Lundin, E., Grånäs, O., Eriksson, O., & Di Marco, I. (2016). Analytic continuation by averaging padé approximants. *Physical Review B*, 93(7), 075104. <https://doi.org/10.1103/physrevb.93.075104>
- Springer, M., Aryasetiawan, F., & Karlsson, K. (1998). First-principles t-matrix theory with application to the 6 eV satellite in ni. *Physical Review Letters*, 80(11), 2389. <https://doi.org/10.1103/PhysRevLett.80.2389>
- Thiele, T. N. (1909). *Interpolationsrechnung*. Leipzig B.G. Teubner. <https://archive.org/search.php?query=external-identifier%3A%22urn%3Aoclc%3Arecord%3A1047515853%22>
- Van Setten, M. J., Caruso, F., Sharifzadeh, S., Ren, X., Scheffler, M., Liu, F., Lischner, J., Lin, L., Deslippe, J. R., Louie, S. G., & others. (2015). GW 100: Benchmarking G0W0 for molecular systems. *Journal of Chemical Theory and Computation*, 11(12), 5665–5687. <https://doi.org/10.1021/acs.jctc.5b00453>
- Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., van der Walt, S. J., Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., ... SciPy 1.0 Contributors. (2020). SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods*, 17, 261–272. <https://doi.org/10.1038/s41592-019-0686-2>
- Voora, V. K. (2020). Molecular electron affinities using the generalized kohn–sham semicanon-

- ical projected random phase approximation. *The Journal of Physical Chemistry Letters*, 12(1), 433–439. <https://doi.org/10.1021/acs.jpcllett.0c03362.s001>
- Wilhelm, J., Golze, D., Talirz, L., Hutter, J., & Pignedoli, C. A. (2018). Toward GW calculations on thousands of atoms. *The Journal of Physical Chemistry Letters*, 9(2), 306–312. <https://doi.org/10.1021/acs.jpcllett.7b02740.s001>
- Wilhelm, J., & Hutter, J. (2017). Periodic GW calculations in the gaussian and plane-waves scheme. *Physical Review B*, 95(23), 235123. <https://doi.org/10.1103/PhysRevB.95.235123>
- Wilhelm, J., Seewald, P., & Golze, D. (2021). Low-scaling GW with benchmark accuracy and application to phosphorene nanosheets. *Journal of Chemical Theory and Computation*, 17(3), 1662–1677. <https://doi.org/10.1021/acs.jctc.0c01282.s001>