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Simple DFT-D3: Library first implementation of the D3 dispersion correction

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Summary

The simulation of chemical reactions or processes provides a fundamental approach to understanding chemistry. The application of Kohn-Sham density functional theory (KSDFT) (Kohn & Sham, 1965) has become an indispensable tool for computational modeling. However, semilocal KS-DFT often fails to accurately describe long-range correlation effects, such as dispersion interactions, in many exchange-correlation functionals (Stefan Grimme et al., 2016). Additive dispersion corrections, like the D3 (S. Grimme et al., 2010) or D4 (Caldeweyher et al., 2019) methods, effectively account for these effects.

Statement of Need

The D3 method is one of the most widely used dispersion corrections, however the original implementation (S. Grimme et al., 2010) has been forked and modified many times to include specific adaptations needed for integration as a library in different electronic structure software packages. Here, we present a reimplementation of the D3 method, focusing on providing a simple, library-first version with APIs defined in Fortran, C, and Python, including the latest parameters for many D3 method variants.

The `simple-dftd3` library implements several variants of the D3 method, including the original zero damping D3(0) (S. Grimme et al., 2010), rational damping D3(BJ) (S. Grimme et al., 2011), modified zero damping D3M(0) (D. G. Smith et al., 2016), and optimized power damping D3(op) (Witte et al., 2017). The main library is written in modern Fortran (Kedward et al., 2022), with additional APIs for C via Fortran-C interoperable functions and for Python via the CFFI library. A command line interface is also available for standalone usage.

Usage

The `simple-dftd3` library has been successfully adopted by several electronic structure software packages, such as DFTB+ (since version 21.2) (Hourahine et al., 2020), Psi4 (since version 1.9.0) (D. G. A. Smith et al., 2020), and Siesta (since version 5.0.0) (García et al., 2020), including recently published packages like Accelerated DFT (Ju et al., 2024) and gpu4pyscf (Wu et al., 2024). Additionally, the Python API provides interfaces for usage in ASE (Larsen et al., 2017), PySCF (Sun et al., 2020), and QCEngine (D. G. A. Smith et al., 2021). Given the accessibility of the code base, new method improvements, like the recent extension of the D3 method to actinide elements (Wittmann et al., 2024), are easily integrated. The package is already cited as tool for example in benchmark studies (Gorges et al., 2022) or for supporting experimental studies (Yu et al., 2024). With its simplicity and availability, the library is a valuable tool for the community to include dispersion corrections in their electronic structure calculations.

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References

Caldeweyher, E., Ehlert, S., Hansen, A., Neugebauer, H., Spicher, S., Bannwarth, C., & Grimme, S. (2019). A generally applicable atomic-charge dependent london dispersion correction. *J. Chem. Phys.*, *150*(15). https://doi.org/10.1063/1.5090222

García, A., Papior, N., Akhtar, A., Artacho, E., Blum, V., Bosoni, E., Brandimarte, P., Brandbyge, M., Cerdá, J. I., Corsetti, F., Cuadrado, R., Dikan, V., Ferrer, J., Gale, J., García-Fernández, P., García-Suárez, V. M., García, S., Huhs, G., Illera, S., … Junquera, J. (2020). Siesta: Recent developments and applications. *J. Chem. Phys.*, *152*(20), 204108. https://doi.org/10.1063/5.0005077

Gorges, J., Grimme, S., & Hansen, A. (2022). Reliable prediction of association (free) energies of supramolecular complexes with heavy main group elements–the HS13L benchmark set. *Phys. Chem. Chem. Phys.*, *24*(47), 28831–28843. https://doi.org/10.1039/D2CP04049B

Grimme, S., Antony, J., Ehrlich, S., & Krieg, H. (2010). A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.*, *132*, 154104. https://doi.org/10.1063/1.3382344

Grimme, S., Ehrlich, S., & Goerigk, L. (2011). Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.*, *32*, 1456–1465. https://doi.org/10.1002/jcc.21759

Grimme, Stefan, Hansen, A., Brandenburg, J. G., & Bannwarth, C. (2016). Dispersion-corrected mean-field electronic structure methods. *Chem. Rev.*, *116*(9), 5105–5154. https://doi.org/10.1021/acs.chemrev.5b00533

Hourahine, B., Aradi, B., Blum, V., Bonafé, F., Buccheri, A., Camacho, C., Cevallos, C., Deshaye, M. Y., Dumitrică, T., Dominguez, A., Ehlert, S., Elstner, M., Heide, T. van der, Hermann, J., Irle, S., Kranz, J. J., Köhler, C., Kowalczyk, T., Kubař, T., … Frauenheim, T. (2020). DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. *J. Chem. Phys.*, *152*(12), 124101. https://doi.org/10.1063/1.5143190

Ju, F., Wei, X., Huang, L., Jenkins, A. J., Xia, L., Zhang, J., Zhu, J., Yang, H., Shao, B., Dai, P., Mayya, A., Hooshmand, Z., Efimovskaya, A., Baker, N. A., Troyer, M., & Liu, H. (2024). *Acceleration without disruption: DFT software as a service*. https://doi.org/10.48550/arXiv.2406.11185

Kedward, L. J., Aradi, B., Čertík, O., Curcic, M., Ehlert, S., Engel, P., Goswami, R., Hirsch, M., Lozada-Blanco, A., Magnin, V., Markus, A., Pagone, E., Pribec, I., Richardson, B., Snyder, H., Urban, J., & Vandenplas, J. (2022). The state of Fortran. *Comput. Sci. Eng.*, *24*(2), 63–72. https://doi.org/10.1109/MCSE.2022.3159862

Kohn, W., & Sham, L. J. (1965). Self-consistent equations including exchange and correlation effects. *Phys. Rev.*, *140*(4A), A1133. https://doi.org/10.1103/PhysRev.140.A1133

Larsen, A. H., Mortensen, J. J., Blomqvist, J., Castelli, I. E., Christensen, R., Dułak, M., Friis, J., Groves, M. N., Hammer, B., Hargus, C., Hermes, E. D., Jennings, P. C., Jensen, P. B., Kermode, J., Kitchin, J. R., Kolsbjerg, E. L., Kubal, J., Kaasbjerg, K., Lysgaard, S., … Jacobsen, K. W. (2017). The atomic simulation environment—a Python library for working with atoms. *J. Phys.: Condens. Matter*, *29*(27), 273002. https:

//doi.org/10.1088/1361-648X/aa680e

Smith, D. G. A., Burns, L. A., Simmonett, A. C., Parrish, R. M., Schieber, M. C., Galvelis, R., Kraus, P., Kruse, H., Di Remigio, R., Alenaizan, A., James, A. M., Lehtola, S., Misiewicz, J. P., Scheurer, M., Shaw, R. A., Schriber, J. B., Xie, Y., Glick, Z. L., Sirianni, D. A., … Sherrill, C. D. (2020). PSI4 1.4: Open-source software for high-throughput quantum chemistry. *J. Chem. Phys.*, *152*(18), 184108. https://doi.org/10.1063/5.0006002

Smith, D. G. A., Lolinco, A. T., Glick, Z. L., Lee, J., Alenaizan, A., Barnes, T. A., Borca, C. H., Di Remigio, R., Dotson, D. L., Ehlert, S., Heide, A. G., Herbst, M. F., Hermann, J., Hicks, C. B., Horton, J. T., Hurtado, A. G., Kraus, P., Kruse, H., Lee, S. J. R., … Burns, L. A. (2021). Quantum chemistry common driver and databases (QCDB) and quantum chemistry engine (QCEngine): Automation and interoperability among computational chemistry programs. *J. Chem. Phys.*, *155*(20), 204801. https://doi.org/10.1063/5.0059356

Smith, D. G., Burns, L. A., Patkowski, K., & Sherrill, C. D. (2016). Revised damping parameters for the D3 dispersion correction to density functional theory. *J. Phys. Chem. Lett.*, *7*(12), 2197–2203. https://doi.org/10.1021/acs.jpclett.6b00780

Sun, Q., Zhang, X., Banerjee, S., Bao, P., Barbry, M., Blunt, N. S., Bogdanov, N. A., Booth, G. H., Chen, J., Cui, Z.-H., Eriksen, J. J., Gao, Y., Guo, S., Hermann, J., Hermes, M. R., Koh, K., Koval, P., Lehtola, S., Li, Z., … Chan, G. K.-L. (2020). Recent developments in the PySCF program package. *J. Chem. Phys.*, *153*(2), 024109. https://doi.org/10.1063/5.0006074

Witte, J., Mardirossian, N., Neaton, J. B., & Head-Gordon, M. (2017). Assessing DFT-D3 damping functions across widely used density functionals: Can we do better? *J. Chem. Theory Comput.*, *13*(5), 2043–2052. https://doi.org/10.1021/acs.jctc.7b00176

Wittmann, L., Gordiy, I., Friede, M., Helmich-Paris, B., Grimme, S., Hansen, A., & Bursch, M. (2024). Extension of the D3 and D4 london dispersion corrections to the full actinides series. *Phys. Chem. Chem. Phys.* https://doi.org/10.1039/D4CP01514B

Wu, X., Sun, Q., Pu, Z., Zheng, T., Ma, W., Yan, W., Yu, X., Wu, Z., Huo, M., Li, X., Ren, W., Gong, S., Zhang, Y., & Gao, W. (2024). *Enhancing GPU-acceleration in the Python-based simulations of chemistry framework*. https://doi.org/10.48550/arXiv.2404.09452

Yu, S., Gautam, A. K., Gao, D., Kuhn, A. N., He, H., Mironenko, A. V., & Yang, H. (2024). Implication of surface oxidation of nanoscale molybdenum carbide on electrocatalytic activity. *J. Mater. Chem. A*. https://doi.org/10.1039/D4TA01746C