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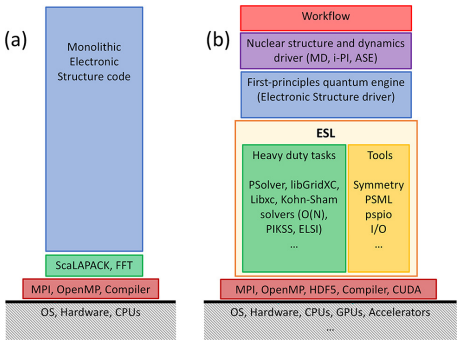
The Electronic Structure Library (ESL) has created an effective collaboration platform for a better way to develop software that utilizes electronic structure theory.



Electronic structure theory, which describes the motion of electrons in atoms and molecules, has wide-ranging applications for condensed matter physics, chemistry, materials science, biological sciences, and engineering. While research efforts have developed codes that implement certain aspects of the theory, the resulting software packages tend to be built independently from one another, which can be inefficient for increasingly complex simulations.

Oliveira et al. report on a coding paradigm trying to move away from the status quo. The Electronic Structure Library (ESL), initiated by the European Centre for Atomic and Molecular Calculations (CECAM), aims to create an effective collaboration platform for shared software development.

The effort to build ESL began in 2014 by extracting tasks common to electronic structure programs and redesigning them as open-source libraries for anyone in the community to use. Such a modular paradigm, as opposed to the monolithic approach of the past, avoids the re-coding of well-known algorithms and allows scientists to focus on higher-level coding.

The authors describe the different libraries ESL currently contains, plans to include future libraries, and various challenges faced by the project and how to address them, such as the difficulty to build a code that depends on various libraries.

The contents of the ESL are already being actively used by leading programs in the field. Any improvements made to the ESL will benefit many programs at once, without the need to re-engineer all of them separately.

Source: "The CECAM electronic structure library and the modular software development paradigm," by Micael J. T. Oliveira, Nick Papior, Yann Pouillon, Volker Blum, Emilio Artacho, Damien Caliste, Fabiano Corsetti, Stefano de Gironcoli, Alin M. Elena, Alberto Garcia, Victor M. Garcia-Suarez, Luigi Genovese, William P. Huhn, Georg Huhs, Sebastian Kokott, Emine Küçükbenli, Ask H. Larsen, Alfio Lazzaro, Irina V. Lebedeva, Yingzhou Li, David López-Durán, Pablo López-Tarifa, Martin Lüders, Miguel A. L. Marques, Jan Minar, Stephan Mohr, Arash A. Mostofi, Alan O'Cais, Mike C. Payne, Thomas Ruh, Daniel G. A. Smith, José M. Soler, David A. Strubbe, Nicolas Tancogne-Dejean, Dominic J. Tildesley, Marc Torrent, and Victor Wen-zhe Yu, *Journal of Chemical Physics* (2020). The article can be accessed at http://doi.org/10.1063/5.0012901.