Sanna, N.; **Baccarelli, I.**; **Morelli, G.**

SCELib3.0: the new revision of SCELib, the parallel computational library of molecular properties in the single center approach. (English) Zbl 1197.82017

Comput. Phys. Commun. 180, No. 12, 2544-2549 (2009).

Summary: SCELib is a computer program which implements the Single Center Expansion (SCE) method to describe molecular electronic densities and the interaction potentials between a charged projectile (electron or positron) and a target molecular system. The first version (CPC Catalog identifier ADMG_v1_0) was submitted to the CPC Program Library in 2000, and version 2.0 (ADMG_v2_0) was submitted in 2004.We here announce the new release 3.0 which presents additional features with respect to the previous versions aiming at a significative enhance of its capabilities to deal with larger molecular systems. SCELib 3.0 allows for ab initio effective core potential (ECP) calculations of the molecular wavefunctions to be used in the SCE method in addition to the standard all-electron description of the molecule. The list of supported architectures has been updated and the code has been ported to platforms based on accelerating coprocessors, such as the NVIDIA GPGPU and the new parallel model adopted is able to efficiently run on a mixed many-core computing system.

MSC:

82-04 Software, source code, etc. for problems pertaining to statistical mechanics

81-04 Software, source code, etc. for problems pertaining to quantum theory

Keywords:

single center expansion library; SCE molecular properties; electron-molecule scattering; SCELib

Software:

SCELib; GAUSSIAN; SCELib3.0

Full Text: DOI

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[21] Please, refer to the code documentation for the detailed timings of the GX2 two-core runs of our test cases given in Table 1, Table 2, and Fig. 2. Despite the outstanding performance, the multi-(GPU)core version of SCELib3 has to be intended as experimental until the numerical stability of the code will be tested over the Tesla S1070 or future multi-(GPU)core nVIDIA devices