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May 23, 2017

VISITORS

Software development experience

Dear Visitors,

PSI4: scalar relativistic module using C++ & Python

- Implemented relevant integral ($W_{\mu\nu} = \langle\chi_\mu|\vec{p}.(V\vec{p})|\chi_\nu\rangle$, $\vec{p}$ is the momentum operator) needed for constructing X2C (exact-two-component) one-electron relativistic Hamiltonian, by taking derivatives w.r.t nuclear coordinates of the nuclear-electron attraction integrals (V) (see github.com/psi4/psi4/blob/master/psi4/src/psi4/libmints/rel_potential.cc).
- Implemented various matrix manipulations steps to obtain relativistic kinetic energy and electron-nucleus interaction potential using PSI4 linear algebra libraries (see github.com/psi4/psi4/blob/master/psi4/src/psi4/libmints/x2cint.cc).
- Implementation details and sample application can be found in J. Chem. Theory Comput. **12**, 144 (2016))

ACES 3: CCSD density linear response module using Fortran 77 & SIP/SIAL

- Implemented one-electron and two-electron spin-orbital integrals using already existing integral packages.
- Developed massively parallel linear-response coupled-cluster (CCSD) module in ACES3 using domain specific language SIP/SIAL.
- Unfortunately source code is part of private repository, but the implementation details and sample applications can be found in Mol. Phys. **114** , 547 (2016) & J. Chem. Phys. **139** , 174103 (2013).

NWChem: 2c-ZORA-DFT ESR parameters using Global arrays & Fortran 77

- Developed computation tools in NWChem program system to calculate ESR parameters (A-and g-tensor) using two-component quasi-relativistic ZORA- (Zero Order Regular Approximation) DFT (Density Functional Theory) approaches.
- Unfortunately source code is part of private repository, but the implementation details and sample applications can be found in J. Chem. Theory Comput. **9**, 1052 (2013) & J. Chem. Theory Comput. **9**, 1932 (2013).

ACES II : various aspects of DFT using Fortran 77

- Implemented DFT analytical gradient in ACESII, both variational and non-variational DFT gradient procedures are implemented. In non-variational DFT, Hartree-Fock density is used to evaluate DFT energy functional, while in variational DFT Kohn-Sham density is used. (see Chem. Phys. Lett. **524**, 10 (2012))
- Implemented self-consistent solution of *ab initio* DFT approach where functionals are taken from wave function method such as random phase approximation, linear CCD and CCD. (see J. Chem. Phys. **136**, 044105 (2012))

Sincerely,

Prakash Verma