

# Prakash Verma

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VISITORS

## Software development experience

Dear Visitors,

### **PSI4: scalar relativistic module using C++ & Python**

- Implemented relevant integral ( $W_{\mu\nu} = \langle \chi_\mu | \vec{p} \cdot (V \vec{p}) | \chi_\nu \rangle$ ,  $\vec{p}$  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](https://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](https://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**

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