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| Initial timings and MPI setup initialize_mpi, initialize_timings, initial_mpi_report | |
| Read input data: Parse control.in, geometry.in for initial dimensions, allocate input data structures, read full content of control.in, geometry.in and verify consistency read_input_data | |
| Prepare data for all s.c.f. cycles: per-species integration grids, spherical free-atom DFT potentials and densities, radial basis functions $u(r)$ for each species prepare_scf | |
| Initial s.c.f. iteration: Partition and prepare 3-d integration grid, obtain overlap matrix, initial superposition-of-free-atoms Hamiltonian, Kohn-Sham eigenvalues and eigenvectors initialize_scf | |
| Full s.c.f. cycle - starting from initial Kohn-Sham eigenvectors, obtain self-consistent potential electron density, wave function, total energy and forces; track wall-time, s.c.f. convergence scf_solver | |
| No | Geometry optimization or molecular dynamics requested? |
| | Yes |
| | Predict next geometry step; check validity of forces; check geometry convergence predict_new_geometry |
| | While (enough walltime left) and (geometry not converged) and (valid forces) |
| | <div> Repartition 3-d integration grids, recompute overlap matrix and fixed sums of free atoms for updated geometry: reinitialize_scf </div> <div> Full s.c.f. cycle - starting from previous Kohn-Sham eigenvectors, obtain self-consistent potential, electron density, wave function, total energy and forces; track wall-time, s.c.f. convergence scf_solver </div> <div> Predict next geometry step; check validity of forces; check geometry convergence predict_new_geometry </div> |
| If requested, post-processing of wave function and density: Electrostatic moments, Mulliken & Hirshfeld charge analyses, volumetric (cube) output, MP2 perturbative correlation energy, GW or MP2 self-energy corrections output_dipole_moment, output_quadrupole_moment, mulliken_analysis, hirshfeld_analysis, output_cube_files, prepare_corr_energy_calc, qpe_calculation, mp2_calculation | |
| Final tasks: Deallocations, final timing output, finalize MPI infrastucture final_deallocations, finalize_scalapack, final_timings, finalize_mpi | |