In this paper we present the Uppsala Quantum Chemistry package (UQUANTCHEM), a new and versatile computational platform with capabilities ranging from simple Hartree-Fock calculations to state of the art First principles Extended Lagrangian Born Oppenheimer Molecular Dynamics (XL-BOMD) and diffusion quantum Monte Carlo (DMC). The UQUANTCHEM package is distributed under the general public license and can be directly downloaded from the code web-site.[1] Together with a presentation of the different capabilities of the uquantchem code and a more technical discussion on how these capabilities have been implemented, a presentation of the user-friendly aspect of the package on the basis of the large number of default settings will also be presented. Furthermore, since the code has been parallelized within the framework of the message passing interface (MPI), the timing of some benchmark calculations are reported to illustrate how the code scales with the number of computational nodes for different levels of chemical theory.

I. INTRODUCTION

One of the main motives behind the recent development of the Uppsala Quantum Chemistry package, UQUANTCHEM[1], has been to complement the broad selection of quantum chemistry codes available with an “easy to use”, open source, development friendly and yet versatile computational framework. The other motive, which has perhaps been the most important driving force, is to provide a pedagogical platform for students and scientists active in the computational chemistry community that are harboring intermediate to basic programming skills, but nevertheless are interested in learning how to implement new computational tools in quantum chemistry. The didactical design of the code has been achieved by limiting the level of optimization, not to obscure the connection between the different quantum chemical methods implemented in the package, and the actual text-book algorithms [2, 3], upon which the construction of the code rests.

The user-friendliness of the UQUANTCHEM package has been ascertained by a large set of default values for the computational parameters, in order for the inexperienced user not to get overwhelmed by technical details. Furthermore, thanks to the limited number of pre-installed computational libraries required prior to the installation of the UQUANTCHEM code (only the linear algebra package (LAPACK)[4] and the basic linear algebra subprograms (BLAS)[5] are required) the package is also very simple to install. The UQUANTCHEM code has been written completely in Fortran90 and comes in three versions; A serial version, an openmp version and a MPI version. In the case of the serial and the openmp version, more or less generic make files are provided for the ifortran and gfortran[6] compilers. The MPI version of the UQUANTCHEM code comes with pre-constructed make files for five of the largest computer clusters in Sweden, the Lindgren cluster[7], the Matter Cluster[8], the Triolith cluster[9], the Abisko cluster[10] and the Kalkyl cluster[11]. These makefiles can be used as templates to create makefiles for a broad selection of clusters.

The wide range of capabilities of the UQUANTCHEM package is perhaps best illustrated by the different levels of chemical theory in which the electron correlation can be treated by UQUANTCHEM, ranging from Hartree-Fock and Møller plesset second order perturbation theory (MP2) [12] to configuration interaction[2], density functional theory (DFT)[13, 14] and diffusion quantum Monte Carlo (DQMC)[15].

The UQUANTCHEM package provides a platform on which further development can easily be made, since the implementation of the different electronic structure techniques in UQUANTCHEM has, to a large extent, been made almost in one to one correspondence with the text books of Szabo and Ostlund[2] and Cook[3], i.e the code has been transparently written and well commented in reference to these texts. The developer friendliness is further enhanced by the explicit calculation of all relevant data structures such as kinetic energy integrals, potential energy integrals and their gradients with respect to electron and nuclear coordinates. Furthermore, since the UQUANTCHEM is constructed from a very limited number of subroutines and modules, an overview of the data structure and design of the code is easily achieved, simplifying any future modification of the program.

II. CAPABILITIES

The UQUANTCHEM code is a versatile computational package with a number of features useful to any computational chemist. The main ingredient in any quantum chemical calculation is the level of theory in which the correlation of the electrons are treated, here
FIG. 1: Total energy of a Born-Oppenheimer molecular dynamics (BOMD) calculation of a H$_2$O molecule, where the density matrix from the previous time step, is used as the initial guess to the SCF optimization with the energy converged to $< 0.01 \mu$Hartree, blue dotted line. The total energy of a Extended Lagrangian Born-Oppenheimer molecular dynamics (XL-BOMD) calculation of a H$_2$O molecule with 5 scf iterations per time step, full black line.

the UQUANTCHEM package is no exception. The least computational demanding level of theory explored by the UQUANTCHEM code is the Hartree-Fock level of theory, where the electron correlation is completely ignored.

In the context of Hartree-Fock total energy calculations it is also possible to calculate analytical interatomic forces, enabling the user to either relax the molecular structure with respect to the Hartree-Fock total energy, or perform molecular dynamics (MD) calculations. Here the user can either choose to run a Born-Oppenheimer Molecular Dynamics calculation (BOMD), or an extended Lagrangian Molecular Dynamics calculation (XL-BOMD), where the density matrix of the next time-step is propagated from the previous time step by means of an auxiliary recursion relation. The advantage of the XL-BOMD methodology over the BOMD approach is that in the case of XL-BOMD, there is no need of a thermostat and an accompanying rescaling of the nuclear velocities in order to suppress any energy drift. In Figure 1 the results obtained with the UQUANTCHEM code for a H$_2$O molecule using the XL-BOMD and BOMD schemes without thermostat are shown. Here the superiority of the XL-BOMD approach over the BOMD scheme is manifested by the lack of energy drift in the former’s total energy.

On the intermediate level of electron correlation theory implemented in the package one finds MP2, CISD and DFT. When using the DFT level of electron correlation it is also possible to calculate analytical interatomic forces, and therefore also perform structural relaxation and molecular dynamics calculations. Here the DFT forces are analytical to the extent that the gradients with respect to nuclear coordinates of the exchange correlation energy are calculated as analytical gradients of the quadrature expression used to calculate the exchange correlation energy.

The highest level of electron correlation theory possible to utilize within the UQUANTCHEM package is DQMC. Here it is possible, within the fixed node approximation, to calculate total ground state energies of medium sized molecules taking into account $> 90\%$ of the correlation energy. In Figure 2 the estimated charge density of a H$_2$O molecule is shown, here calculated with DQMC as implemented in UQUANTCHEM.

Apart from the different methods involved in dealing with electron correlation implemented in the UQUANTCHEM package, a number of other capabilities can also be found within the package. Amongst these capabilities is the ability to provide graphical information about the highest occupied and the lowest unoccupied orbitals (HOMO and LUMO), deal with charged systems as well as calculating Mulliken charges, plot the Hartree-Fock and Kohn-Sham orbitals as well as the corresponding charge density, calculate the velocity auto-correlation

FIG. 2: The estimated charge density in water using a diffusion quantum Monte Carlo algorithm as implemented in the UQUANTCHEM code. Here red colors correspond to high values of the charge density and blue or bluish colors correspond to low values. The charge density was estimated from 2000 walkers and $4.0 \cdot 10^6$ time steps with a time step of $\Delta t = 1.0 \cdot 10^{-4}$ au, and a cusp corrected cc-pVTZ basis. The resulting ground state energy was $E_0 = -76.4409 \pm 0.0002$ a.u. The rendering of the charge density map was obtained by using the UQUANTCHEM output file CHARGEDENS.dat as input to the Matlab script chargdens2DIM.m, which is a script provided with the UQUANTCHEM package.
function and relax the molecular structure with respect to interatomic forces by utilizing a conjugate gradient scheme. However, it should be stressed that the code can only deal with finite systems, thus excluding any calculation of periodic systems.

III. IMPLEMENTATION DETAILS

The code utilizes a localized atomic basis set, where each basis function, \( \phi_i \), is constructed from a contraction of primitive cubic Gaussian orbitals [3]

\[
\phi_i(x, y, z) = \sum_n d_n(x - X_i) L_i^L_j(y - Y_i) M_j^M_j(z - Z_i)^N_i e^{-\alpha_i(r - R_i)}. \tag{1}
\]

Here, \( d_n \) are the contraction coefficients, \( R_i = (X_i, Y_i, Z_i) \) are the atomic coordinates at which the basis function is centered, \( \alpha_i \) are the primitive Gaussian exponents and \( L_i, M_j \) and \( N_i \) integer numbers determining the angular momentum, \( l = L_i + M_j + N_i \), of the corresponding basis function. In what follows we will suppress the spin part of the basis functions and assume that the spin degrees of freedom are treated implicitly, i.e., have been integrated out.

Thanks to the use of primitive Gaussians almost all the matrices involved in the different implementations, such as the overlap matrix, \( S \), the kinetic energy matrix, \( T \) and the nuclear attraction matrix, \( V \) defined by

\[
S_{ij} = \int d^3r \phi_i(r) \phi_j(r), \tag{2}
\]

\[
T_{ij} = -\frac{1}{2} \int d^3r \phi_i(r) \nabla^2 \phi_j(r), \tag{3}
\]

\[
V_{ij} = -\sum_n Z_n \int d^3r \frac{\phi_i(r) \phi_j(r)}{|r - R_n|}, \tag{4}
\]

have been calculated analytically. Here, \( Z_n \) denotes the atomic numbers of the nuclei. The implementation of the analytic evaluation of the above integrals follows almost exactly the outline given in D. B. Cook’s book *Handbook of Computational Chemistry*. [3]

In order to enhance the performance of the code, the electron-electron integrals,

\[
(ij|kl) = \int d^3r \int d^3r' \frac{\phi_i(r) \phi_j(r') \phi_k(r') \phi_l(r')}{|r - r'|}, \tag{5}
\]

have been calculated by Rys quadrature [21], even though they can be calculated analytically as is described in Cook’s book [3].

The exchange correlation energy, \( E_{xc} \) and the corresponding exchange correlation matrix elements, \( V_{ij}^{xc} \)

\[
E_{xc} = \int d^3r \epsilon_{xc}(\rho, \nabla \rho) \rho(r), \tag{6}
\]

\[
V_{ij}^{xc} = \int d^3r \frac{\delta E_{xc}}{\delta \rho} \phi_i(r) \phi_j(r) = \int d^3r \phi_i(r) \frac{d(\epsilon_{xc}(\rho))}{d\rho} \phi_j(r) + \tilde{V}_{ij}^{xc}, \tag{7}
\]

\[
\tilde{V}_{ij}^{xc} = \int \frac{d^3r}{|\nabla \rho|} \left( \nabla \phi_i \cdot \nabla \rho \phi_j + \phi_i \nabla \rho \cdot \nabla \phi_j \right) \frac{d(\epsilon_{xc}(\rho))}{d|\nabla \rho|} \tag{8}
\]

defined through the exchange correlation energy density, \( \epsilon_{xc}(\rho) \), and the functional derivative of the exchange correlation energy [20],

\[
V_{xc}(r) = \frac{\delta E_{xc}}{\delta \rho} \equiv \frac{d(\epsilon_{xc}(\rho))}{d\rho} - \frac{d}{dx} \left( \frac{d(\epsilon_{xc}(\rho))}{d(\nabla \rho)_x} \right) - \frac{d}{dy} \left( \frac{d(\epsilon_{xc}(\rho))}{d(\nabla \rho)_y} \right) - \frac{d}{dz} \left( \frac{d(\epsilon_{xc}(\rho))}{d(\nabla \rho)_z} \right),
\]

have been calculated by decomposing the above spatial integrals into sums of integrals over atom-centered “fuzzy” polyhedra, as described by Becke [22]. Each one of these polyhedral integrals is computed by the use of Gauss-Chebyshev quadrature of second order [23], and Lebedev quadrature [24]. Here, \( \rho \) denotes the charge density.

The only difference between the implementation of the above integrals in UQUANTCHEM and the outline given by Becke [22], is that in the UQUANTCHEM implementation, the mapping of the interval \( x \in [-1, 1] \) into the radial integration interval \( r \in [0, \infty] \) enables the use of Gauss-Chebyshev quadrature, and the use of Slater atomic covalent radius [25] of the atom at which the corresponding “fuzzy” tetrahedron is centered. It has been shown by Mura et al. [26] that the above mapping results in a much more accurate numerical integration as compared to what is achieved with the mapping proposed by Becke [22].

The density functionals provided with the UQUANTCHEM package are the local density approximation (LDA) functional of Vosko et al. [27], the revised gradient corrected functional of Perdew et al. [28] (revPBE) [29] and the B3LYP hybrid functional [27, 30–32].

The MP2 implementation and the CISD implementation very closely follow the outline given in the text-book of Szabo and Ostlund [2].

The implementation of the DQMC algorithm in UQUANTCHEM follows closely the algorithm outlined in the work of Umrigar et al. [15]. However, in UQUANTCHEM the trial function is constructed with a much simplier Jastrow factor, \( J \), and the slater determinants are constructed from cusp corrected Gaussian
orbitals, instead of Slater type orbitals (STO), as in the work of Umrigar et al. The implementation of the cusp correction in UQUANTCHEM follows the prescription given by S. Manten and A. Liechow [19]. The explicit form of the trial function used for the importance sampling in the DQMC of UQUANTCHEM is given by:

\[ \Psi_T = D_\uparrow D_\downarrow \mathcal{J}. \]  

(10)

Where

\[ \mathcal{J} = \exp\left( \sum_{i<j} \frac{\delta \cdot b \cdot r_{ij}}{(1 + c \cdot r_{ij})} \right), \]  

(11)

\[ r_{ij} = |r_i - r_j| \]  
is the distance between electron \( i \) and \( j \), \( D_\uparrow \) and \( D_\downarrow \) are the slater determinants created from spin up respectively spin down orbitals. The orbitals are constructed from the unrestricted Hartree-Fock (URHF) self consistent solution. Here \( \delta = 0.25 \) if the spin of the electrons \( i \) and \( j \) are identical otherwise if the spins are opposite, \( \delta = 0.5 \). Here, \( b \) and \( c \) are Jastrow parameters that can be chosen and optimized by the user.

IV. TECHNICAL DETAILS

As was mentioned in the introduction, the UQUANTCHEM package has been written with the aim of keeping a high level of transparency in order to facilitate further development, with the result of a somewhat limited computational speed for the serial implementation of the code. A quantitative illustration of the performance limitation of the UQUANTCHEM code is obtained by comparing the total execution times of the UQUANTCHEM code with corresponding times of the GAMESS code [37]. When comparing the execution times for a HF total energy calculation employing a cc-pVTZ basis set, the GAMESS code is about 15 times faster on a dual intel core processor. And if one instead would compare the performance of the execution times for a HF total energy calculation of the UQUANTCHEM MPI version is displayed. Here the most effective parallelization, when using around 500 processors, is found in the Hartree-Fock (HF) and diffusion quantum Monte Carlo (DQMC) implementations, where the speed-ups of \( \sim 380 \), in the case of the HF implementation, and \( \sim 280 \), in the case of the DQMC implementation, correspond to efficiencies of the respective parallelizations of 76% respectively 56%.

The speed-up of the MP2 and CISD implementations, at the same number of processors, only reaches \( \sim 30\% \) efficiency, with the DFT parallelization performing slightly better. When using more than 1000 processors the HF level of theory prevails as the most effectively parallelized method, at which point the speed-up of DQMC method has already saturated and been overtaken by the CISD method. Before we continue, we note in passing that the number of processors at which the speed-up (at any level of theory) is saturated strongly depends on the serial execution time, \( t_1 \), i.e on the system size and the number of basis functions used in the calculation. Therefore it should be stressed that it is more informative to compare the efficiency of the different parallelizations rather than the number of processors at which the speed-up saturates.

The difference in efficiency between parallel HF calculations and the parallel MP2 and CISD calculations, comes from the fact that in the case of the HF calculation, only the computation of two-electron integrals, \( \langle ij|kl \rangle \), and the contraction of these integrals with the density matrices \( P_{ij} \) into Fock, \( J_{ij} \), and exchange, \( K_{ij} \), matrices, i.e

\[ J_{ij} = \sum_{kl} \langle ij|kl \rangle P_{kl}, \quad K_{il} = \sum_{jk} \langle ij|kl \rangle P_{jk}, \]  

(12)

are parallelized. Whereas in the case of the MP2 calculation, also the sum of two-particle excitations [2] are made in parallel, and in the case of the CISD calculations, both the construction of the Hamiltonian and the diagonalization are made in parallel, thanks to the utilization of the Scalable Linear Algebra Package (scaLAPACK) [33].
FIG. 3: Computational time as a function of number of basis functions in (a-d), and number of electrons in (e), for the different levels of theory implemented in the UQUANTCHEM code. In all panels (a-e) the logarithm of the computational times are represented by black circles in the upper sub-panels and the finite difference, $\frac{\Delta \ln(t)}{\Delta \ln(N)}$ (in (e) $\frac{\Delta \ln(t)}{\Delta \ln(Z)}$), as red squares in the lower sub-panels. In (a) the computational times and finite differences of the Hartree-Fock implementation, in (b) the computational times and finite differences of the DFT (revPBE functional) implementation, in (c) the computational times and finite differences of the MP2 implementation, in (d) the computational times and finite differences of the CISD implementation and in (e) the computational times and finite differences of the DQMC implementation. The calculations presented in panels (a-d) were performed for the atoms with atomic number $Z = 2, 10, 18, 36, 54$. In all calculations a 3-21G basis set was used except for the DQMC calculations where the cc-pVTZ basis-set was employed.
FIG. 4: Speed-up as a function of the number of processors used for calculations performed at different levels of theory. Here the black circles is the speed-up of a Hartree-Fock calculation of H₂O using a cc-pVQZ basis set, the red squares is the speed-up of a density functional theory (DFT) [13, 14] calculation of H₂O using the Perdew, Burke and Ernzerhof (PBE) functional [25] and a cc-pVTZ basis set, the green triangles is the speed-up of a second order Möller Plesset (MP2) [12] calculation of H₂O using a cc-pVTZ basis set, the empty blue diamonds is the speed up of a singles and doubles configuration interaction (CISD) calculation of H₂ using a cc-pVTZ basis set and the violet crosses is the speed-up of a quantum diffusion Monte Carlo (QDMC) [15] calculation of a single Be atom utilizing a cc-pV5Z basis set. In all the calculations. Here the computational time on one single processor, \( t_1 \), was the following: \( t_1 = 13547 \) s for the Hartree-Fock calculation, \( t_1 = 1764 \) s, for the DFT calculation, \( t_1 = 5995 \) s for the MP2 calculation, \( t_1 = 3381 \) s for the CISD calculation and \( t_1 = 44300 \) s for the QDMC calculation. The inset shows an enlarged portion of the figure in order to more clearly expose the region in which the different parallelizations are close to maximum efficiency.

Furthermore, in order to accelerate the convergence of the HF and DFT self consistent calculations, the direct inversion of the iterative subspace algorithm (DIIS) of P. Pulay [35, 36] has also been implemented in both the serial and parallel versions of UQUANTCHEM.

V. USING THE CODE

The UQUANTCHEM package has been developed to be easily installed and run on UNIX-type platforms. The code has been compiled without any problems on machines running under Mac OSX 10.7, Red-Hat Linux and Ubuntu, using either the gfortran or ifort compilers.

The interface of the code with the user goes mainly through one single file, the INPUTFILE-file, through which the user specifies what type of calculation is going to be performed on what type of molecule. Below, the INPUTFILE-file specifying a DFT calculation of the total energy and HOMO-LUMO orbitals of a water molecule is given.

```
CORRLEVEL B3LYP
TOL 1.0E-8
WHOMOLUMO .T.
Ne 10
NATOMS 3
ATOM 1 0.4535 1.7512 0.0000
ATOM 8 0.0000 0.0000 0.0000
ATOM 1 -1.8090 0.0000 0.0000
```

Apart from the INPUTFILE-file the user is only required to provide the code with the so called BASISFILE-file, specifying which type of Gaussian basis set to use in the calculation. The most common basis-sets used in modern quantum chemistry are provided within the UQUANTCHEM package. There is also the possibility to use the information at the Basis Exchange Portal, located at https://bse.pnl.gov/bse/portal, to extend the default library of basis-sets that comes with the UQUANTCHEM package.

Once the user has made sure that the files INPUTFILE and BASISFILE are located in the same directory as the code is being executed, then, in order to run for instance the serial version of the code, it is just a matter of giving the command:

```
"command-prompt"/uquantchem.s"
```

on the command line.

Thus from the above given exposé, it becomes apparent that the user can, after the code has been compiled, quickly start performing quantum chemical calculations without getting overwhelmed by a plethora of input-parameters and input-files. However, when necessary, the user can always bypass the default settings and more carefully specify the calculation with the computational input-parameters that were initially "hidden".

divide and conquer diagonalization routine PDSYEV[34]. Furthermore, since the storage of the CISD Hamiltonian is shared amongst all the computational nodes taking part in the calculation, memory bottlenecks can be avoided, permitting the computation and diagonalization of Hamiltonians of substantial size.

The difference in the performance between parallel implementations of HF and DFT comes from the fact that in the DFT implementation, not only the computation of two-electron integrals and their contraction are parallelized, as in the HF implementation, but also the calculation of the exchange-correlation potential and exchange correlation energy by means of numerical quadrature is parallelized.
VI. BENCHMARKING OF DFT

In Table I and Table II we show the results of a series of geometry optimization calculations obtained with Uquantchem and the well established Gamess code \[^{[37]}\]. Here the results obtained with Uquantchem are virtually indistinguishable from the results obtained with the Gamess code, especially when comparing the results obtained with the B3LYP hybrid functional. In order to calculate the exchange correlation potential matrix elements in these Uquantchem calculations, Gauss-Chebyshev quadrature of the second kind with 100 grid points was used for the radial integration, and Lebedev quadrature \[^{[24]}\] using 194 angular grid points was used for the angular part of the integration. The structures of the molecules were considered optimized when the absolute values of the interatomic forces had been relaxed down to $< 10^{-6}$ a.u.

In Table III, the corresponding experimental structural parameters are also displayed.

VII. TEST-CALCULATIONS

In order to test that the compilation of the UQUANTCHEM package have been successful, seven different test-calculations have been provided within the package. The input files of these calculations are located in the subdirectories RUN1, RUN2, ..., RUN7 of the TESTS -directory. Here follows a brief description of these tests:

- **RUN1**: An unrestricted Hartree-Fock total energy calculation of a single water molecule.
- **RUN2**: A DFT total energy calculation using the revPBE functional of a single water molecule.
- **RUN3**: A DFT total energy calculation and interatomic force calculation using the B3LYP functional of a single water molecule.
- **RUN4**: A MP2 total energy calculation of a single water molecule.
- **RUN5**: A CISD total energy calculation of a single Be atom.
- **RUN6**: A DQMC total energy calculation of a single He atom, using a cc-PVTZ basis set.
- **RUN7**: An unrestricted Hartree-Fock structural relaxation of a single water molecule, using a STO-3G basis set.

In all tests listed above the 6-31G** basis is used except in test calculations RUN6 and RUN7. To run the test calculations the user just have to execute the command: .\runtests.pl, in the root directory of the UQUANTCHEM code.

FIG. 5: The highest occupied molecular orbital (HOMO) iso-surface, (a), and the lowest unoccupied molecular orbital (LUMO) iso-surface, (b), of the Alanine amino acid calculated with UQUANTCHEM using a 6-31G** basis set together with the B3LYP functional. Here the rendering of the iso-surfaces was obtained by using the UQUANTCHEM output files HOMO.xsf and LUMO.xsf as input to the XCrySDen graphical software package \[^{[38]}\].

VIII. INTERFACING WITH OTHER COMPUTATIONAL SOFTWARE

The UQUANTCHEM software comes with a set of supporting utility scripts for generating two-dimensional charge-density plots and three-dimensional iso-density plots with Matlab. See for example Figure 2 showing a two-dimensional charge-density plot of a water molecule generated with the chargdens2DIM.m Matlab script included in the software package.

The UQUANTCHEM has been adapted to work with the graphical software package XCrySDen \[^{[38]}\], by generating a number of files in the xsf-format. In Figure 3 the highest occupied molecular orbital (HOMO) iso-surface and the lowest unoccupied molecular orbital (LUMO) iso-surface of Alanine are shown. The rendering of the iso-surfaces was obtained by using the UQUANTCHEM output files HOMO.xsf and LUMO.xsf as input to the xcrysden graphical software package. 

TABLE I: Results from geometry optimization using the revPBE [29] functional, with 6-31G**. Here, $\alpha$, is the equilibrium angle, d, in units of [Å], the equilibrium distance between nearest neighbor atoms and, E, the total energy for the optimized structure.

| Code     | $\alpha$(HOH) d(OH) E [a.u.] | $\alpha$(HNH) d(NH) E [a.u.] | $\alpha$(HCH) d(CH) E [a.u.] |
|----------|-------------------------------|-------------------------------|-------------------------------|
| Gamess   | 102.571 0.9736 -76.3940       | 104.495 1.0271 -56.5378       | 109.471 1.0696 -40.5050       |
| Uquantchem | 102.598 0.9734 -76.3956       | 104.508 1.0269 -56.5391       | 109.469 1.0994 -40.5059       |

TABLE II: Results from geometry optimization using the B3LYP functional [27, 30–32], with 6-31G**. Here $\alpha$ is the equilibrium angle, d, in units of [Å], the equilibrium distance between nearest neighbor atoms and, E, the total energy for the optimized structure.

| Code     | $\alpha$(HOH) d(OH) E [a.u.] | $\alpha$(HNH) d(NH) E [a.u.] | $\alpha$(HCH) d(CH) E [a.u.] |
|----------|-------------------------------|-------------------------------|-------------------------------|
| Gamess   | 103.720 0.9656 -76.3826       | 105.719 1.0183 -56.5212       | 109.470 1.0922 -40.4881       |
| Uquantchem | 103.741 0.9656 -76.3825       | 105.717 1.0183 -56.5211       | 109.470 1.0922 -40.4878       |

TABLE III: Experimental data for the equilibrium geometries for H$_2$O, NH$_3$ and CH$_4$ [29].

|       | $\alpha$ | d [Å] |
|-------|----------|-------|
| H$_2$O | 103.9    | 0.959 |
| NH$_3$ | 106.0    | 1.012 |
| CH$_4$ | 109.5    | 1.086 |

IX. CONCLUSION

In this work the recently developed quantum chemistry package UQUANTCHEM has been presented together with the results of some performance benchmark calculations. Here, even though the scaling of the computational time with respect to system size, especially the MP2 and CISD implementations, leave room for much improvement, the MPI-implementation of the package compensates rather well for the limited performance in the serial version, enabling the UQUANTCHEM package to be utilized as a "proof of principle" platform for new computational ideas in quantum chemistry, or to be utilized in standard quantum chemistry calculations of molecules with $\leq$ 100 atoms.

Acknowledgements

Thanks to Professor Olle Eriksson for his patience and to Carl Caleman and Anders Niklasson for their inspiration.

The manual for the UQUANTCHEM software package can be obtained at: [http://www.anst.uu.se/pesou087/UU-SITE/Webbplats_2/UQUANTCHEM_files/manual.pdf](http://www.anst.uu.se/pesou087/UU-SITE/Webbplats_2/UQUANTCHEM_files/manual.pdf)
[10] Abisko is comprised of 322 nodes with a total of 15456 CPU cores. Each node is equipped with 4 AMD Opteron 6238 (Interlagos) 12 core 2.6 GHz processors. The Abisko cluster is located at HPC2N, Umeå University, Sweden., URL http://www.hpc2n.umu.se/resources/abisko.

[11] The Kalkyl cluster has a total of 2784 64-bit processor cores. The Kalkyl cluster is located at Uppmax, Uppsala University, Sweden., URL http://www.uppmax.uu.se/the-kalkyl-cluster.

[12] C. Møller and M. S. Plesset, Phys. Rev. 46, 618 (1934).
[13] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
[14] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
[15] C. J. Umrigar, M. P. Nightingale, and R. K. J., J. Phys. Chem. 99, 2865 (1993).
[16] A. M. N. Niklasson, P. Steneteg, A. Odell, N. Bock, M. Challacombe, C. J. Tymczak, E. Holmström, G. Zheng, and V. Weber, J. Chem. Phys. 130, 214109 (2009).
[17] B. G. Johnson, P. M. W. Gill, and J. A. Pople, J. Chem. Phys. 98, 5612 (1993).
[18] A. Lüchow and R. F. Fink, J. Chem. Phys. 113, 8457 (2000).
[19] S. Manten and A. Lüchow, J. Chem. Phys. 115, 5362 (2001).

[20] Here the conventional definition of the functional derivative is used as opposed to the more unconventional definitions:

\[ \frac{\delta E_{xc}}{\delta \rho(x)} = \frac{1}{\rho(x)} \int d^3 r \epsilon_{xc}(\rho, \nabla \rho) \rho \equiv \frac{d(\epsilon_{xc}(\rho))}{d\rho}, \]

\[ \frac{\delta E_{xc}}{\delta (\nabla \rho)_x} = \frac{1}{\rho(x)} \int d^3 r \epsilon_{xc}(\rho, \nabla \rho) \rho \equiv \frac{d(\epsilon_{xc}(\rho))}{d(\nabla \rho)_x}, \]

\[ \frac{\delta E_{xc}}{\delta (\nabla \rho)_y} = \frac{1}{\rho(x)} \int d^3 r \epsilon_{xc}(\rho, \nabla \rho) \rho \equiv \frac{d(\epsilon_{xc}(\rho))}{d(\nabla \rho)_y}, \]

\[ \frac{\delta E_{xc}}{\delta (\nabla \rho)_z} = \frac{1}{\rho(x)} \int d^3 r \epsilon_{xc}(\rho, \nabla \rho) \rho \equiv \frac{d(\epsilon_{xc}(\rho))}{d(\nabla \rho)_z}, \]

which were used in the Comp. Phys. Comm. -version of this article.

[21] J. D. Augspurger, D. E. Bernholdt, and C. E. Dykstra, J. Comp. Chem. 11, 972 (1990).
[22] A. D. Becke, J. Chem. Phys. 88, 2547 (1988).
[23] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, 1972), 10th ed.
[24] V. I. Lebedev, Zh. Vychisl. Mat. Mat. Fiz. 16, 293 (1976).
[25] J. C. Slater, J. Chem. Phys. 41, 3199 (1964).
[26] M. E. Mura and P. J. Knowles, J. Chem. Phys. 104, 9848 (1996).
[27] S. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. 58, 1200 (1980).
[28] J. P. Perdew., K. Burke., and M. Ernzerhof, Phys. Rev. Lett 77, 3865 (1996).
[29] Y. Zhang and W. Yang, Phys. Rev. Lett 80, 890 (1998).
[30] A. D. Becke, Phys. Rev. A 38, 3098 (1988).
[31] C. Lee, W. Yang, and R. G. Parr, Phys. Rev. B. 37, 785 (1988).
[32] P. J. Stephens, F. J. Devlin, C. F. Chabalowski, and M. J. Frisch, J. Phys. Chem. 98, 11623 (1994).
[33] The Scalable Linear Algebra Package (LAPACK) can be obtained free of charge from the address listed here: URL http://www.netlib.org/scalapack.
[34] Information about the PDSEVD SCALAPACK routine can be found at the address listed here: URL http://www.netlib.org/scalapack.
[35] P. Pulay, Chem. Phys. Lett. 73, 323 (1980).
[36] P. Pulay, J. Comp. Chem. 3, 556 (1982).
[37] M.F. Guest, I. J. Bush, H.J.J. van Dam, P. Sherwood, J.M.H. Thomas, J.H. van Lenthe, R.W.A Havenith, J. Kendrick, "The GAMESS-UK electronic structure package: algorithms, developments and applications", Molecular Physics, 103, 719-747 (2005).
[38] A. Kokalj, J. Mol. Graphics Modelling 17, 176-179 (1999).