The deMon Suite of Programs

www.demonsoft.com

The deMon Developers

demon is a system of programs for density functional theory (DFT) calculations of primarily molecules, but they may also be used for atoms and a version exists for solids. The deMon Suite of Programs is maintained and distributed by an international group known as the deMon Developers, located in a number of countries, including France, Germany, Sweden, Switzerland, Canada, Mexico, and Brazil. The programs are available directly from the deMon Developer groups. Obtaining the program requires signing and returning a “non-disclosure agreement” to Dennis R. Salahub at the University of Calgary in Alberta, Canada, and to the Developers who provided the particular version of deMon. This agreement simply says that the code will not be distributed to anyone without the knowledge of the deMon Developers and is basically intended to prevent the situation where the code is used without proper recognition of the work of the deMon Developers. The deMon codes are free for academic groups, with the exception of computer centers which are charged. Companies are also charged for the codes. This money is used to help defray the cost of the deMon Developers meetings which have been held once a year for the last 6 years (e.g. by financing student lodging.)

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<tr>
<th>Year</th>
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<td>Germany</td>
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<td>2006</td>
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The Game of the Name

The first widely available version of deMon [1] appeared in 1992. deMon stands for “densité de Montréal.” The unusual capitalisation emphasizes the roots of the code at the Université de Montréal (UdM) simultaneously by its implicit separation into two words [de-Mon(réal)] and by its resemblance to the main edifice of UdM with its tall central tower.

History and Capabilities

One way to understand deMon is to look at it in its historical context [2]. During the 1970’s Slater’s Xα method had been tried and abandoned by quantum chemists. Part of the difficulty was in the scattered wave, muffin-tin implementation of the time. Major numerical
Improvements came about through the introduction of Gaussian-type orbitals (GTO) and the use of auxiliary fitting functions in the LCAO-Xα program [3,4]. This allowed GTO technology to be borrowed from existant *ab initio* codes. Other major advances were Axel Becke’s introduction of efficient, accurate, atom-centered numerical integration, Vosko, Wilk and Nusair’s parameterization of the local density approximation [5] based upon Ceperly and Alder’s accurate quantum Monte Carlo calculations of the correlation energy of the homogeneous electron gas, as well as the emergence of good quality generalized gradient approximations such as those of Becke [6] and Perdew [7].

By the 1980’s, it had become clear that it was time to update the old LCAO-Xα strategy and write a modern DFT program with analytic derivatives capable of automatic geometry optimizations. This goal was realized simultaneously in deMon and in another program (namely DGauss developed at Cray for use on their computers).

Shortly after its appearance the original deMon code was substantially modified for commercialization by BIOSYM Technologies. The beta-release of this version appeared in 1993. It was the basis of the deMon-KS1 [8] series of programs developed in Montreal until 1997. Meanwhile the original deMon version was further developed in Montpellier and Stockholm. These developments were initially independent from each other. In 1997 they merged to become the deMon-KS3 [9] series of programs.

Over the years, many important method developments in DFT can be attributed to work originating with deMon and related programs. This includes, but is not limited to, NMR chemical shifts [10] and time-dependent density functional theory [11]. Several different versions of deMon developed

The ALLCHEM [12] project started in Hannover in 1995 independently of the deMon project. The aim of this project was to write a well structured DFT code from scratch. The first ALLCHEM version appeared in 1997. The structured programming of ALLCHEM proved very useful for the development and testing of new DFT approaches and algorithms.

The deMon and ALLCHEM developers agreed at the first deMon Developers meeting in Ottawa to merge their codes in order to keep a Tower of Babel from arising. As a result the new code couples the deMon functionality with the stable and efficient integral part from ALLCHEM, including for example $f$, $g$, and higher angular momentum type Hermite gaussian auxiliary functions. The merged code was presented for the first time at the third deMon Developers meeting in Geneva. The present version of the code is now known as deMon2k [13] to distinguish it from the earlier (premerge) codes.

It is difficult to know whether we should be more proud of our contributions extending DFT to new types of molecular properties or whether to focus on program efficiency. Since some of the contributions of the deMon Developers to property calculations have already been mentioned, let us just mention one example of the type of geometry optimization which can now be performed with deMon2k. The optimization of a mordenite model consisting of 404 atoms without symmetry took 720 hours on a single 2.4 GHz Xeon CPU with 2 GB of memory. Parallelization over 6 processors reduces the optimization time by about 5 times.
**Optimization calculation**

Basis DZVP (5820)

Auxis A2 (10128)

Functional VWN

404 Atoms

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The mordenite model: H, white; Si, yellow; O, red; Al, blue; Na, pink. Note that dangling bonds have been capped with hydrogens whose positions were fixed during the geometry optimization. All other atoms were allowed to move.

The ability to optimize a molecule of this size means that we now have access to the study of a particularly large range of chemical and physical chemical phenomenal.

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<tr>
<th>Number of Processors</th>
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<td>Dual Xeon Node</td>
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</tr>
<tr>
<td>Dual Xeon Nodes with Myrinet</td>
<td>6.5 days</td>
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More or less, all that remains of the original UdM connection is history and the name deMon since the original contributors have all left UdM and no further work with the program is being carried out there. The present version of deMon2k has several attractive features, including but not limited to parallelization, effective and model core potentials, property calculations (NMR, TDDFT, polarizability, and first hyperpolarizability), sophisticated visualisation through interface with the VU (http://www.invisu.ca/e/vu.php), Molden (http://www.cmbi.ru.nl/molden/molden.html), Molekel (http://www.cscs.ch/molekel/), and OpenDX (www.opendx.org) programs, Bader topological analysis of the density, the electron localisation function (ELF), improved geometry optimizers, and molecular dynamics methods.

**deMon2k Platforms and Code Requests**

deMon2k is a FORTRAN90 code. Standard platforms on which deMon2k runs (and so has optimized compile flags included in the distribution package) are:

1. IBM AIX
   - AIX 4.3
   - AIX 4.3 (64 bit)
   - AIX 5.1 (64 bit)

2. IRIX
   - IRIX 6.5 (IP27)
   - IRIX 6.5 (IP35)

3. Alpha
   - OSF1 4.0
   - OSF1 5.1

4. Linux
   - AMD i686
   - Intel i686
   - Intel ia64 (Itanium2)
   - x86_64 (Athlon 64 bit/Xeon 64 bit)

Other platforms on which deMon2k runs but are not yet considered part of the standard package are:

1. PowerPc G5 (Mac, Darwin Kernel version 7.9.0)

2. SunOS 5.8

Requests for deMon2k should be addressed directly to the individual deMon developers [such as MEC (Mark.Casida@UJF-Grenoble.FR) or PC (pcalamin@cinvestav.mx)].
References


