



ADF Newsletter March 2003

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1. New Releases

a. ADF2002.03

The ADF2002.03 release is available on the SCM website since the beginning of this year. It includes many improvements compared to previous versions.

New functionality:

- Time-Dependent DFT in BAND for frequency-dependent dielectric functions
- Distance cut-offs and confinement options for improved performance of BAND
- AddRemove link model for QM/MM calculations (Int. J. Quant. Chem. **91**, 177 (2003))
- Improved regular basis sets TZ2P+ for transition metals Sc to Zn and
- Improved even-tempered basis set ET-pVQZ for elements H to Kr.

Bug fixes:

- Important bug fix for geometry optimizations in Z-matrix coordinates
- Various other bug fixes for both geometry optimizations and various types of single-point calculations.

Technical improvements:

- An easier way to work with files for parallel ADF runs.

Further information is available in the Updates document on the SCM website at <http://www.scm.com/Doc/Doc2002/Updates.pdf>

b. The ADFinput module (menu-based input builder for ADF)

ADFinput is a menu-based input builder for ADF. It greatly facilitates the task of preparing an ADF input file. With ADFinput, you can:

- build your molecule from scratch
- import a structure from file (e.g. PDB or XYZ formats)
- use pre-defined or user-defined templates
- use the tutorial to get started quickly
- use help balloons while you work
- pre-optimize your structure with a simple force field
- set up your calculation such that results can be visualized with ADFview

The first picture on <http://www.scm.com/Products/GUIInfo.html> shows an early version of ADFinput. The first release will be made available through the SCM website soon. Check the News items on the website for updates.

c. New platforms

With assistance from HP, ADF is now available for the HP Itanium2 with Linux platform. Ports to other Itanium2 systems are in progress. The HP Itanium2 executables will soon be made available on the SCM website. A port to the HP AlphaServerSC will be tackled next.

d. Speed-ups for PC-Linux binaries

Preliminary timings for ADF binaries built with the Intel 7.0 Fortran compiler indicate that significant speed-ups can be achieved with respect to the ADF2002.03 executables. Performance improvements are seen from 25% (Athlon and PentiumIII) to even about a factor of 2 (PentiumIV). This makes it likely that faster PC-Linux executables can be made available with the next release, or even before.

2. SCM and ADF at conferences

a. Sanibel Symposium

At the moment of writing, the Sanibel Symposium has just ended. Erik van Lenthe (SCM) and Myrta Grüning demonstrated ADF, ADFinput, and ADFview to the participants. Lasse Jensen presented his results on the Direct Reaction Field (DRF) model (J. Chem. Phys. **118**, 514 (2003)) to describe solvent effects, as implemented in his private ADF version. Myrta Grüning presented very encouraging results obtained with new exchange-correlation meta-GGA energy functionals. Meta van Faassen showed new results on time-dependent current-density-functional theory applications to polymers (Phys. Rev. Lett. **88**, 186401 (2002); J. Chem. Phys. in press).

b. ACS National meeting, New Orleans, 24-26 March 2003

Marcel Swart and Stan van Gisbergen (SCM) will show recent developments in ADF, BAND, and the ADF-GUI in booth 1913 of the expo at the ACS Spring Meeting in New Orleans, 24-26 March 2003.

QM/MM options available in ADF are discussed in Marcel's oral presentation in the Division of Inorganic Chemistry, (session Bioinorganic Chemistry) on Sunday. Prof. Evert-Jan Baerends, Prof. Tom Ziegler, and Dr. Jochen Autschbach will all present their work with ADF in the section on Time-dependent DFT (COMP Division).

c. Quantum Inorganic Chemistry conference, York, UK, April 14-16, 2003

A conference will be held in York, UK, from 14-16 April 2003. The topic is computational chemistry applied to complex inorganic systems. ADF is particularly popular for this research area. About half the presentations in the provisional programme feature ADF users (or developers) as presenters or co-authors.

For more information: <http://www.scm.com/News/York.html>

d. ADF lecture series in Japan, May 26-30, 2003

Ryoka Systems Inc. and SCM plan to co-organize a lecture series on ADF in Japan, in the week of 26-30 May this year. Prof. Baerends, Dr. van Gisbergen, and Dr. Swart will give scientific presentations on various recent developments in the ADF package. All details of this trip (such as the places to visit) still need to be determined. If you are interested in attending one of the lecture series in your region, contact SCM (info@scm.com) or Ryoka (adf@cubs.bio.rsi.co.jp).

e. DFT 2003 conference, Brussels, September 7-12, 2003

From the conference website, we quote:

"The 10th edition of the International Congress on the Applications of Density Functional Theory in Chemistry and Physics will be held from September 7 to September 12 2003 in

Brussels (Belgium) at the Vrije Universiteit Brussel (VUB). This edition succeeds previous successful editions in Madrid (2001), Rome (1999), Vienna (1997), Paris (1995), ... It will be devoted to both fundamental and applied aspects of Density Functional Theory within Chemistry and Physics.”
For more information: <http://www.vub.ac.be/dft2003>

3. Other news / recent developments

a. Parallelization project NMR and analytic second derivatives

An optimization project has started to significantly speed up the NMR and SD programs. These serve to calculate NMR properties (shieldings and spin-spin coupling constants) and for the analytic calculation of the Hessian, normal modes and IR spectra. Preliminary timings indicate that at least an order of magnitude speed-up can be achieved in parallel calculations. This work will continue in the following months and will enable NMR and SD calculations on much larger molecules than currently accessible. The scientists involved in this project are Steve Wolff and Jochen Autschbach.

b. Environment modeling

Several ADF developers are currently developing better ways to model the environment of a QM system, for a more realistic description of the real system. The models range from very simple but efficient point charge models, to QM/MM models (with or without inclusion of polarization effects), to QM models of the environment. SCM is preparing an interface between ADF and various property programs that will facilitate inclusion of environment effects on molecular properties in future ADF releases.

c. Molecular properties

Circular Dichroism spectra (J. Chem. Phys. **116**, 6930 (2002)) will be available in the next ADF release. The Optical Rotatory Dispersion (J. Chem. Phys. **117**, 517 (2002)) functionality will become available one version later. This has been agreed between SCM and Jochen Autschbach, primary author of these new parts of the ADF code.

Self-Interaction-Corrected LDA (SIC-LDA) and GGA (SIC-GGA) functionals will be included in the next ADF version. These functionals cure difficult cases, both for energy barriers (J. Chem. Phys. **116**, 7806 (2002)) and for NMR chemical shieldings (J. Chem. Phys. **115**, 26 (2002)). The SIC functionals are contributed by Serguei Patchkovskii.

d. Older news

- If you observe a non-negligible difference between CPU and elapsed time for your ADF or BAND jobs, this can be solved by setting the environment variable `SCM_IOBUFFERSIZE` to a larger value. More info: <http://www.scm.com/News/iobuf.html>
- DGrid is a separate program that computes the density, density gradient, density Laplacian, one-electron potential, and electron localization function (ELF) on an equidistant grid, starting from TAPE21. Basin is a program for the analysis of the bonding situation based on the data grid file from DGrid. Dr. Kohout is making these utilities available. More info: <http://www.scm.com/News/DGrid.html>

- Marcel Swart received his Ph.D. degree for the thesis entitled "Density Functional Theory Applied to Copper Proteins". If you are interested in receiving a copy of this thesis, contact SCM.
- PDB2ADF is a utility developed by Marcel Swart to create an ADF input file from a PDB file, for a subsequent QM/MM calculation using ADF.
More info: <http://theochem.chem.rug.nl/~swart/manuals/pdb2adf>

4. Science Papers with ADF: Actinide-Noble Gas Complexes and Au₂₀ Molecule

Recently two remarkable scientific research works using the Amsterdam Density Functional (ADF) program have been published in *Science* magazine (<http://www.sciencemag.org>) by Pacific Northwest National Laboratory scientist Dr. Jun Li and his collaborators. This research involves the relativistic density functional theoretical investigations of the first-ever actinide-noble gas (Ng) complexes CUO(Ng)_x (*Science*, **2002**, 295, 2242-2245) and a surprisingly stable Au₂₀ pyramid molecule (*Science*, **2003**, 299, 864-867).

Dr. Li et al. used the ADF program to perform calculations of geometry optimizations, vibrational frequencies, energetics, excited states properties, solvent effects, and some other physico-chemical properties of the systems mentioned above.

"The unique relativistic quantum chemistry features of the ADF program greatly facilitate our research," said Li. "The problems that we are investigating are highly challenging because of the complexity of the heavy-element systems and the size of the molecules. We benefited a great deal from ADF because of its superb efficiency, robust parallel scalability, and high accuracy. Without ADF and the high performance computing resources we have in our laboratory, it would be difficult for us to fulfill what we have accomplished. We have been very pleased with many of the state-of-the-art features available in ADF for tackling transition-metal and heavy-element systems".

Dr. Li (http://emslbios.pnl.gov/id/li_j) is currently a senior research scientist working at the Molecular Science Computing Facility in the William R. Wiley Environmental Molecular Sciences Laboratory, a US Department of Energy national user facility at PNNL. Li's collaborators include his former mentor Professor Bruce Bursten at Ohio State University, Professor Lai-Sheng Wang at Washington State University, and Professor Lester Andrews at University of Virginia.

Questions, comments, contributions

Any questions or comments regarding the above, or other questions related to ADF, are very welcome and can be sent to info@scm.com. Feel free to contact us also in case you have some information that may be of interest to other current or future ADF users (such as extraordinary applications with ADF), and that may be suitable material for a future Newsletter.