10th Seminar on Computational Methods in Quantum Chemistry

COMPUTATIONAL CHEMISTRY FROM A PERSONAL PERSPECTIVE

(Closing Remarks)

Geerd HF Diercksen

I would like to start by expressing my thanks to Dr Alain Veillard for joining me in starting this series of *Seminars on Computational Methods in Quantum Chemistry*. I do regret very much that he has decided not to participate in this seminar. I would have loved to share memories with him about the pioneering time of research in computational chemistry which, for a short period, I had the privilege to share with him. At the same time I feel deep sympathy for his decision. He has retired just at the right time. I wish I had the possibility do to the same, now.

I would like to continue by thanking the organizers of this series of seminars. First of all, of course, Alain Veillard and his colleagues for organizing the seminar four times in Strasbourg. I would like to thank in particular Chantal Daniel and Marie Madeleine Rohmer, the organizers of this 10th Seminar on Computational Methods in Quantum Chemistry. Finally, I would like to express my thanks to the organizers of the other seminars in this series, in chronological order: Bjorn Roos (Örenäs ,1978), Wim Nieuwpoort (Groningen, 1981), Wolfgang Kraemer (Tegernsee, 1984), Brian T Sutcliffe (York, 1987), Jens N Oddershede (Gl Avernäs, 1990) and Ramon Carbo (Girona, 1993).

In 1969, when the 1st Seminar on Computational Methods in Quantum Chemistry was held, quantum-mechanical calculations were still in its infancy. The first computers that were powerful enough to permit self-consistent field all-electron calculations for small polyatomic molecules employing an orbital basis seemingly large enough to expect some reliability of the calculated properties, mostly orbital and total energies, just became commercially available. At that time the IBM 360/91 computer, the top model of the IBM 360 series, was probably the most powerful computer. The first two computer codes for molecular structure calculations of polyatomic molecules employing Gaussian functions as basis sets had just been developed: IBMOL by Enrico Clementi and Alain Veillard in the Large Scale Computation Department at the IBM Research Laboratories in San Jose, California, headed by Enrico Clementi, and POLYTOM by Imre G Czismadia, Macolm C Harrison, Jules W Moskowitz, Shirly Seung, Brian T Sutcliffe and Michael P Barnett in the laboratory of John C Slater at MIT, Cambridge, Massachusetts. Actually, when I first met Alain Veillard in autumn 1967 in the Large Scale Computation Department at the IBM Research Laboratories in San Jose he was developing IBMOL II for the new series of IBM 360 computers. Both codes were limited to the self-consistent field approximation. Typical studies at that time, like a self-consistent field calculation of the water molecule, employing a basis set of 35 contracted Gaussian functions, according to my laboratory notebooks, took about 30 minutes CPU time on an IBM

360/91 using IBMOL II while the water-dimer, employing 70 functions, took about 2 hours.

From there we have gone a long way, quite successfully, as it seems to me, at least what concerns the tools. The further development of computational physics in general and of computational chemistry in particular has been strongly dependent on the progress in computer technology, in particular concerning processor speed and storage size. A big step in processor speed was achieved by the development of vector processors. Later, the overall computer speed was further increased by the development of massively parallel computer architectures tying together several hundreds of processors. But the development in computer architecture that has changed research in computational physics most dramatically has been the development of (single user) workstations.

Parallel to and inspired by the availability of more and more powerful computers progress has been made both in the development of computational methods and algorithms and in the development of the corresponding software. The advances in the development of computational methods concern solving the time-independent non-relativistic Schrödinger equation in different approximations and, in particular in recent years, solving the four-component relativistic Schrödinger equation and its two-component approximations. Often well known methods established a long time ago have become computationally feasible by the development of new algorithms fully exploiting the specifics of the computer architecture. This is in particular true for the development of new algorithms and software for vector processors and for massively parallel computer architectures. A similarly successful development has taken place in heavy particle dynamics, an area of computational chemistry traditionally ignored by conventional quantum chemists in the past. The progress concerns solving the heavy-particle Schrödinger equation for studying vibrational-rotational spectroscopy and scattering processes. It concerns equally solving the classical equations of motion for investigating bulk properties of condensed phases.

Before reflecting further on the development of Quantum Chemistry I would like to raise the question: What is science? Let me quote from the book *Heraclitean Fire* by Erwin Chargaff. (Erwin Chargaff, Heraclitean Fire, The Rockefeller University Press, New York, 1978.) *Truly a big question about which large books have been written that I have great difficulty in reading. I shall give a simple answer. Science is the attempt to learn the truth about those parts of nature that are explorable. Science, therefore, is not a mechanism to explore the unexplorable; and it is not its task to decide on the existence or nonexistence of God or to measure the weight of a soul.*

There can be no reasonable doubts that computational chemistry has contributed to explore nature. But how much it has actually contributed to our knowledge about nature has still to be evaluated and definitely not on a scale set by ourselves! It is true as well that many questions are still awaiting exploration. Among them are the properties of electronically excited states and, even more so, reactions of molecules in condensed phases and on surfaces.

I am afraid, applying the most fashionable, usually identical with the most heavily advertised, computer program to badly formulated or fake questions, often with the only purpose to outrun other colleagues with whom we are in competition, provide little hope to learn the truth about those parts of nature that are explorable. This is, at best, technology. I respect technology. It forms not only the basis of the prosperity of

our society and thus the financial basis of the sciences but it forms in particular the basis of the computational sciences. But even technology addressing fake questions is simply a waste of resources, both human and financial. Similar arguments hold for variants of methods, algorithms and software developed without an attempt to open routes to the exploration of still unexplored parts of nature.

In the book *Heraclitean Fire*, published first in 1978, about twenty years ago, Erwin Chargaff has expressed it much more drastically: *Modern science lives only in the day and for the day; it resembles much more a stock-market speculation than a research for truth about nature: a search in which I thought, perhaps mistakenly, of engaging when I entered science nearly fifty years ago*.

Conferences devoted mainly to the presentation of routine results or incremental improvements of methods, in my mind, resemble the floor of stock markets. Discussions, on the other hand, focusing on a well formulated question that has not been addressed so far or has resisted exploration form an important attempt to research for truth about nature. I would like to see such focused discussions organized. I would enjoy participating in it if only for the purpose of satisfying my curiosity about nature.

I would like to close by reminding us: Research can be carried out by others, often even more successfully than by us, and, if it is a research for truth about nature, it has always been and it will be in future. But our life is limited and much too precious to be wasted in front of a terminal pushing the button and waiting for the *truth*. Therefore: let's enjoy both work and life, and life and work at the right time and in proper proportion.

Strasbourg, 06 September 1996 Geerd HF Diercksen