

**THE HISTORY OF THE
1st SEMINAR
ON COMPUTATIONAL METHODS IN QUANTUM CHEMISTRY**

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(from memory in July 1996)

On the occasion of the 10th *Seminar on Computational Methods in Quantum Chemistry* to be held, once again, in Strasbourg, 4-6 September 1996, I am trying to recall how this series of seminars got started. The following account is based entirely on my memory and therefore will be biased and may even be wrong in some places.

In early May 1968 (probably on the 9th of May) I traveled with my wife and our two children to San Jose, California, to take up a post-doc position in the Large Scale Computation Department at the IBM Research Laboratories in San Jose, California, headed by Dr Enrico Clementi. An apartment had been arranged for us in the Round Table Drive housing area by Dr Alain Veillard who had arrived earlier in the department and was living with his wife and son in the same apartment area. It was there in San Jose that I first met Alain Veillard, actually already in autumn 1967 on the occasion of a short visit to the department. We were the first in a program which became established shortly afterwards as a formal post-doc program sponsored by IBM from which many young European colleagues have profited for more than a decade. At that time we were the only two visitors from Europe in the department. I seem to remember that Alain Veillard and myself never shared an office. But in case we did it must have been for a rather short time because a couple of weeks after I had arrived the department moved into trailers and everyone of us got his private office (without windows!). At that time Alain Veillard was actively looking for a position back in France and that year in early autumn he was offered a CNRS position at the Louis Pasteur University of Strasbourg. I do not recall precisely the occasion at which the idea of what is now being called the *Seminars on Computational Methods in Quantum Chemistry* was born. But I remember that at that time no *platform existed for discussing the development of methods and software in quantum chemistry*, the most pressing challenge in establishing computational chemistry. Moreover, most of the traditional chemists were rather reserved towards computational chemistry, in order not to say hostile. Thus we decided to organize a seminar, today probably called a workshop, bringing together young colleagues active in developing methods and software in computational chemistry. *In order to achieve close scientific contact among participants and to discuss methodology and software in sufficient depth we limited the number of colleagues to be invited to about 20.* We discussed this proposal with Enrico Clementi and he enthusiastically supported the idea. At the beginning of November 1968 Alain Veillard left for Strasbourg to take up his position. At about the same time an IBM 360/91 computer was delivered to the Max-Planck-Institut für Plasmaphysik, Garching, and I had to return to München for reporting about my experiences with using this computer model. Actually, Alain Veillard and myself took

the same flight to Paris which, as I remember, was delayed for many hours until after midnight. Before leaving for Europe Enrico Clementi had arranged for me to meet in Germany with the IBM representative responsible for the companies contacts to the Academia. While in Germany we met and I was offered full financial support for the seminar (travel and subsistence for about 20 persons) without any conditions on the choice of the participants. After the funds had been raised Alain Veillard and myself finalized the list of colleagues to be invited. Shortly afterwards Alain Veillard and colleagues in his laboratory started with the local organization of the seminar. Just before Christmas 1968 I went back to San Jose, and to my family, in order to continue my post-doc work. Eventually, we returned back home to München at the end of July 1969. The 1st Seminar *on Computational Methods in Quantum Chemistry* finally was held at the Louis Pasteur University of Strasbourg in September 1969. It was attended by 25 participants from 9 countries and 16 contributions were presented.

In spring 1970, about half a year after the seminar, Alain Veillard and myself decided to organize another seminar on the same subject in the same format. But this time I completely failed to raise funds from IBM, getting the subtle indication that some established colleagues had severely complained with IBM about not having been invited. Last not least it were them who were most important to IBM because after all it were them who decided what computer to buy! After the failure to raise funds we did not follow up the idea any further. But by the end of 1971 we had been asked repeatedly by participants of the 1st seminar to organize a follow up seminar. Therefore we decided to contact about 20 colleagues, including a large number of participants in the 1st seminar, and to suggest to organize a seminar without support by IBM. To our great surprise all invited colleagues accepted to participate and to cover their expenses from local funds. As a result the 2nd *Seminar on Computational Methods in Quantum Chemistry* was held in September 1972, again in Strasbourg, attended by 24 participants from 8 countries and 19 contributions were presented. This was the beginning of a series now established as the *Seminars on Computational Methods in Quantum Chemistry*.

Strasbourg, 06 September 1996

Geerd HF Diercksen

10th Seminar on Computational Methods in Quantum Chemistry

**SEMINARS
ON COMPUTATIONAL METHODS IN QUANTUM CHEMISTRY**

Year	Place (Country)	Organizer(s)	# Participants
1969	Strasbourg (France)	GHF Diercksen, A Veillard	25
1972	Strasbourg (France)	GHF Diercksen, A Veillard, BT Sutcliffe	24
1975	Strasbourg (France)	GHF Diercksen, A Veillard, BT Sutcliffe	30
1978	Örenäs (Sweden)	BO Roos	40
1981	Groningen (The Netherlands)	PT van Duijnen, WC Niewpoort	41
1984	Tegernsee (Germany)	WP Kraemer, R Beardsworth	33
1987	York (Great Britain)	BT Sutcliffe	39
1990	Gl. Aversaes (Denmark)	J Oddershede	46
1993	Girona (Spain)	R Carbo	43
1996	Strasbourg (France)	C Daniel, MM Rohmer	66