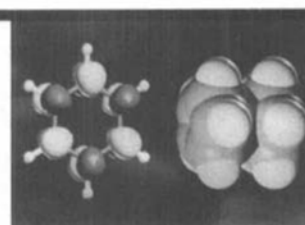


COMPUTATIONAL CHEMISTRY COLUMN

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The Group of Swiss Computational Chemists (GSCC)

Hans P. Lüthi*

The Group of Swiss Computational Chemists (GSCC) was initiated in the mid-eighties by a collegium of Swiss chemists headed by Profs. E. Schumacher (Bern) and J. Weber (Geneva). The main goal of this special interest group was to establish contacts and to exchange know-how and software. Once a small 'Club', this group has grown into an organization which is now an integral part of the Swiss chemistry scene. This development reflects the tremendous change the computer and its application has had on chemical research. The need to communicate these new developments has led to a rapid growth of the GSCC, and activities such as workshops and regular meetings evolved naturally. Most recently, the GSCC became an official affiliate of the New Swiss Chemical Society, a fact which shows that it is now a mature and well-respected organization.

Structure and Organization

The GSCC is a non-profit organization directed by a Board currently composed of a representative from each Swiss university (see *Box 1* below). The Board deter-

mines the policies of the GSCC and also prepares the different activities. The chairman of the Board, or, alternatively, a delegate or a group of delegates, execute the resolutions taken by the Board. There is no formal membership to the GSCC. However, the organization keeps a mailing list to communicate news or other informations to the 'members'. The mailing list currently contains nearly 100 addresses. The main source of income of the GSCC is from its workshops (*i.e.* tuition fees and advertising contracts).

Box 1. The Board of the Group of Swiss Computational Chemists

Dr. Hans Peter Lüthi, ETH-Zürich (Chairman)
Prof. Claude Daul, Fribourg (Vice Chairman)
Dr. Pierre-Alain Carrupt, University of Lausanne (Treasurer)
Dr. Pierre-Yves Morgantini, University of Geneva
Dr. Daniel Stahl, EPF Lausanne
Prof. Helen Stoeckli-Evans, University of Neuchâtel
Prof. Samuel Leutwyler, University of Bern
Prof. Hanspeter Huber, University of Basel
Prof. Walter Thiel, University of Zürich

Current Activities

The GSCC Business Meetings

The Board of the GSCC usually meets twice a year, with one meeting held open to the public. This has usually been the 'Spring Meeting', and it has been framed by a small scientific program. At this meeting the Board informs its 'members' about the activities of the GSCC, and, at the same time, takes the input from the public.

Political Activities

Since the computer is a vital tool for the computational chemist, the national supercomputer policy is of special interest to the GSCC. The GSCC has observed the activities around the evaluation of the NEC SX-3 supercomputer and the Centro Svizzero di Calcolo Scientifico rather carefully. A 'Supercomputing Task Force' consisting of Board members has been formed. Its main responsibility is to ensure that the interests of the computational chemists are well taken care of at all levels (supercomputing policies, evaluations, grants, *etc.*)

The 'Computer Based Chemistry' Minisymposium

As an affiliate of the New Swiss Chemical Society, the GSCC has been partly responsible for the organization of the 'Computer Based Chemistry' section of the annual Autumn Meeting. It assists the organizers in setting up and executing the program.

The GSCC Workshops

One of the most important activities of the GSCC were its workshops.

Starting in 1989, a series of workshops, each focusing on a particular item of computational chemistry, was held in fall. The events, hosted by the Ecole de Pharmacie of the University of Lausanne, were well visited. The target audience was academic and industrial researchers from all levels, *i.e.* from graduate students to senior researchers. *Box 2* shows the workshops held so far. Since fall is the main conference season, the Board of the GSCC

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Box 2. *The Workshops Organized by the GSCC*

1994	Density Functional Theory an Its Application
1992	Molecular Structure Optimization
1991	Molecular Modelling
1990	Molecular Mechanics and Molecular Dynamics Simulations
1989	Quantum Chemistry Software on Supercomputers

at its last business meeting in April, has decided to hold its workshops in spring. The next workshop, which will be on Density Functional Theory, will be held in April 1994, and will be hosted by the Swiss National Supercomputer Center (Centro Svizzero di Calcolo Scientifico) in Manno (Lugano).

Future Activities

The 'Spring Meetings' gradually changed their character from pure business meetings to predominantly scientific meetings. Given the large interest these extend-

ed business meetings have drawn, the Board of the GSCC decided to make it a full-day event. The idea is to invite senior researchers of the Swiss and of the neighboring computational chemistry scene to present their research. The goal is to provide a better overview of the activities in this area of research in and around our country.

The GSCC now also became the host organization of the 'Symposium für Theoretische Chemie', the biggest theoretical and computational chemistry conference of the German-speaking countries. The 30th 'Symposium für Theoretische Che-

mie' will be organized by Prof. H. Huber (Basel), and will be held in Fiesch (VS) in September 1994. The plan for the GSCC is to also become a host organization for the 'Conférence de Chimistes Théoriciens d'Expression Latine'.

Numerical quantum chemistry and molecular simulation are now becoming part of the undergraduate curriculum at all Swiss universities. Unfortunately, there are no well established text books available yet, a fact which often turns the task of preparing lectures into a heavy burden. The GSCC plans to arrange a small symposium for the computational chemistry lecturers in order to facilitate the exchange of experience.

Joining the GSCC

For more information about the GSCC, or for requests to be put on the mailing list, please contact *H.P.L.*

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'[Es] könnte langfristig viel Geld gespart werden, wenn ein Konzept hier Schule machte, das die Universität Zürich mit verblüffendem Erfolg und zur Begeisterung der Studenten eingeführt hat.'

Die Zeit

'[Das neuartige Konzept] dürfte wegweisend für die zukünftige Gestaltung von Praktika an Hochschulen sein.'

Chemie in unserer Zeit

