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Bringing Theory to the Classroom: Summer School in Computational Quantum Chemistry (CQCS-98)

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The use of modern quantum-chemical methods in research was the topic of the 1st 'Summer School in Computational Quantum Chemistry CQCS-98' held at the Centro Svizzero di Calcolo Scientifico (CSCS) from July 27–31 in Manno (Lugano). The focus of the summer school, organized by *Hans Peter Lüthi*, was to provide 'hands-on' experience using a modern computational infrastructure.

Computational chemistry has become a 'must-have-tool' [1] in chemical research. Such a development, most naturally, puts a demand on education and training. Even though most university chemistry curricula cover instruction in computational chemistry, the demand for training is still growing. This became very evident also for CQCS-98 where the classrooms filled much faster than ever anticipated.

History

In December 1997, a small group of Swiss and Italian computational chemists met in Milan to discuss collaboration in education in computational quantum chemistry. The idea was to gather instructors with expertise in different areas of application of electronic structure methods in order to generate a body of practical exercises in a unified format. These materials, similar to the exercises collected by *J.V. Foresman* and *Æ. Frisch* [2], were to be archived on a Web server and made accessible to the members of this consortium. The plan was to introduce the newly developed course materials at a summer school to be held at CSCS Manno under the direction of the Swiss Association of Computational Chemistry (SACC/ACSS). The target audience were masters and freshman PhD students in chemistry and physics from Italy and Switzerland. The idea of mixing content (computational chemistry) with modern electronic education technology was received enthusiastically by the various sponsors, including the COST Action D9 of the European Community. Given this broad support, the summer school was advertised at the European level. Within a few weeks only, 60 registrations were obtained and the classrooms were more than full.

Table. *Lectures and Keynote-Lectures*

Keynote-Lectures: Speakers	Titles
G. Scuseria (Rice University, Houston, Texas)	Recent Developments in Linear Scaling Electronic Structure Methods for Applications to Large Molecules
H.-J. Böhm (*Roche*, Basel)	The Role of Computational Chemistry in Pharmaceutical Research
W. Kutzelnigg (Ruhr Universität, Bochum)	*Ab Initio* Calculation of NMR Chemical Shifts with Application to Structural Chemistry
H.F. Schaefer III (University of Georgia, Athens, Georgia)	Planar and Twisted Ethylene: An Important Model System for Electronic Spectroscopy and Photochemistry
Lecturers	**Lectures**
V. Barone (Napoli)	Solute-Solvent Interactions
A. Bencini (Firenze)	EPR/Molecular Magnetism
C. Daul (Fribourg)	Exited States and Photochemical Properties
P. Fantucci (Milano)	Molecular-Orbital Analysis and Properties
A. Goursot (Montpellier)	Density-Functional Theory
W. Klopper (Oslo)	Electron Correlation
H.F. Schaefer III (Athens, Georgia, USA)	*Hartree-Fock* Theory
J. Weber (Geneva)	Exploration of Potential-Energy Surfaces
C. Adamo (Napoli) *R. Bruyndonckx* (Fribourg), *S. I. Ciofini* (Fribourg) *L. de Gioia* (Milano), *P. Morgantini* (Geneva) *F. Totti* (Firenze), *S. Portmann* (CSCS, program supervisor)	Practical Assignments

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The Event

On Monday, July 27, 1998, 45 students plus 15 lecturers and assistants representing seven European countries and the United States, arrived at CSCS for the start of the summer school. The program was split into two parts: a block of lectures and keynote-lectures, and a series of practical exercises. The keynote-lectures were also teleconferenced to the ETH Zürich and EPF Lausanne. The lectures covered the basics necessary for the practical assignments. The keynote-lectures, on the other hand, presented topics of current interest in method development and research (see *Table* for details). During the practical assignments the participants were lead through basic problem-solving all the way to addressing specific problems in the areas of magnetic properties, solute/solvent interactions, photochemical properties, and others (see [3] for the complete list/content of assignments) (*Fig. 1*).

Twenty workstations were available to generate input and to postprocess the results. The actual computations were performed with Gaussian94 and ADF2.3 (Amsterdam Density Functional) on the NEC SX-4 supercomputer of CSCS. For the practical work, the students formed teams of two or three participants sharing one keyboard (*Fig. 2*).

All exercises were provided as Web documents. This has several advantages, one of them being the efficiency in generating (errorless) input. The pages are available also after the summer school, offering the students to work on a topic which they couldn't address during the event [3].

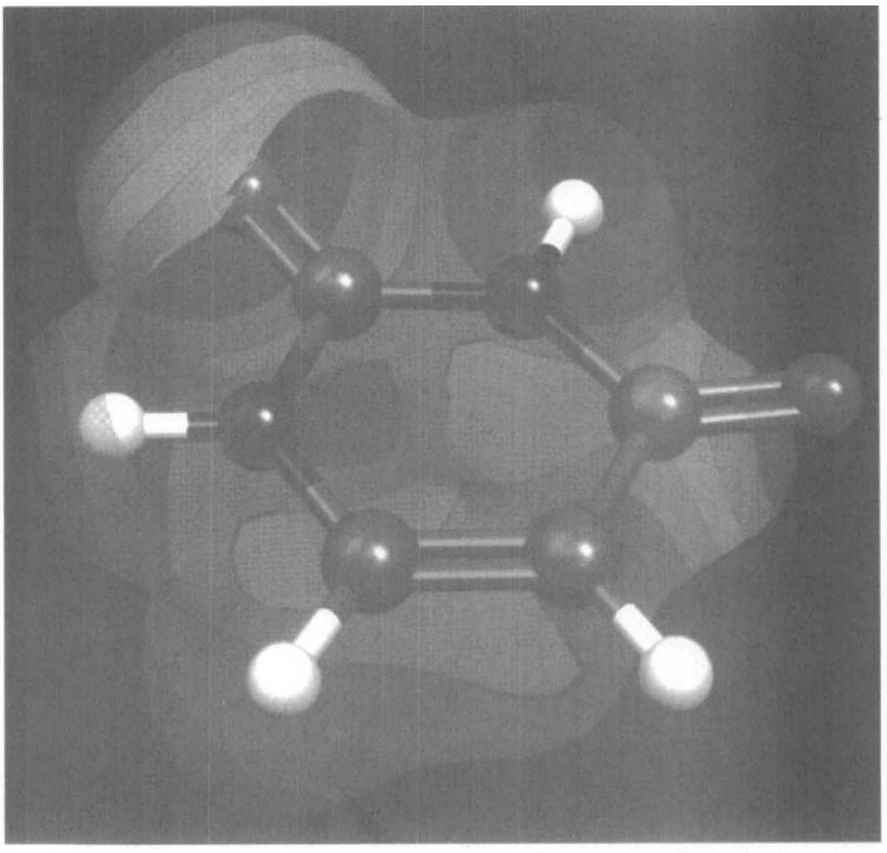

Fig. 1. *The computation of the ^{1}H, ^{13}C-NMR chemical shift of uracil was the topic of one of the advanced assignments*

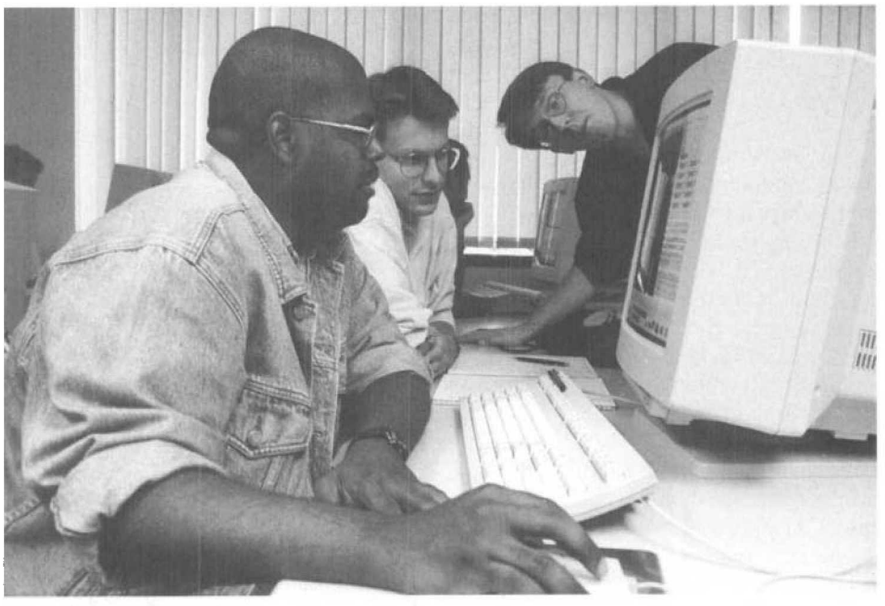

Fig. 2. *Students at work*

An Initiative with a Future

The summer school showed that the progress in quantum-chemical method development is so fast, that training programs with a goal to transfer these modern technologies to the user in a very compact and time-efficient form are highly appreciated. For some of the senior participants the summer school also had 'continuous-education' character. The combination of application-oriented (*i.e.*, 'practical') computational chemistry with modern education technology was a very successful approach and shows significant potential for the future. The ratings of the event by the students gave a very encouraging feedback to the organizers. The program and, most of all, the practical assignments obtained very good ratings, indicating that the event reached the educational target set. The technical infrastructure and especially the high quality of assistantship during the practical assignments (7 assistants and 45 students) were highly appreciated.

The summer school will be continued, and its next edition will be hosted by the Consorzio Interuniversitario Lombardo per l'Elaborazione Automatica (CILEA) in Milano, one of the sponsors of CQCS-98.

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[1] J.H. Krieger, *Chem. Eng. News* **1997**, *May 12*, 30–40: 'Computational Chemistry Impact'.

[2] J.V. Foresman, Æ. Frisch, 'Exploring Chemistry with Electronic Structure Methods', Gaussian, Inc. Pittsburgh.

[3] CQCS-98 on-line: http://www.cscs.ch/Official/SummerSchool.