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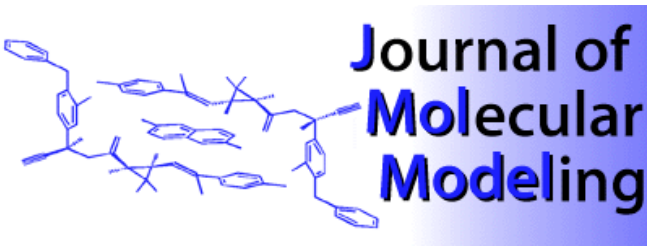

CONFERENCE REPORT

High Performance Computing in Chemistry

Research Centre Jülich, 16.-18.2.1998

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The current use of high performance computers in chemical research encompasses a wide spectrum of subjects and corresponding techniques. Structures and properties of individual molecules are accessible with accurate quantum mechanical methods while macroscopic properties of solids and liquids and interactions between large molecules are derived from sophisticated modelling approaches. Mathematical modelling and optimizations of industrial processes have an increasing impact on productivity. The retrieval and analysis of the vast amounts of genetic information resulting from genome analysis projects pose new computational challenges. Modern computational chemistry clearly has close ties into the neighbouring fields of solid state physics, genetics, computer science, and engineering. Computers have become an established research tool also in the hands of non-experts due to the increasing availability of high performance hardware and sophisticated software packages.

The Research Centre Jülich is a major contributor to the field of computer-aided chemistry through its own research programs in solid state physics, materials research and soft matter physics. The Central Institute for Applied Mathematics (ZAM) of the Research Centre Jülich operates the largest German supercomputer complex with an aggregate peak power of 0.5 TeraFlops. The Cray/SGI hardware is a combination of two massively parallel (T3E-600/512 and T3E-900/256) and three parallel vector machines (T90/16 and two J90) with a combined memory of over 100 GByte. Major chemistry software packages installed on these machines are UniChem (DGauss, CADPAC, Gaussian, MNDO), Molpro, GAMESS, CPMD, Amber and GROMOS. HLRZ (Höchstleistungsrechenzentrum, High Performance Computing Centre) is a cooperation of the Research Centre Jülich, DESY (Hamburg) and GMD-Forschungszentrum Informationstechnik (Bonn) which makes a major fraction of these computer resources available to academic and industrial users through peer-reviewed projects. Currently about a third of the HLRZ projects and a significant fraction of the Research Centre's own computational science activities fall into the broader area of chemistry. The rapidly increasing use of the Jülich supercomputers by the chemistry community is the background of the initiative of ZAM to organize a scientific conference on the subject of "High Performance Computing in Chemistry".

A particular focus of the meeting was the impact of computational chemistry on industrial research and productivity. The meeting was held 16.-18.2.1998 and brought together about 180 participants from academic and industrial research institutions. With the intention of creating a forum for the exchange of ideas between method developers concentrated in academia and scientists in industrial R&D the program committee had invited 30 renowned speakers from both communities. The invited lecturers impressively demonstrated the multifaceted and interdisciplinary character

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of modern computer-aided research. Their subjects included drug design, polymer simulations, the computation of material's properties, bioinformatics, plant and process optimization, and catalysis. The lecture program was complemented with numerous posters presenting ongoing research and an exhibition of hardware vendors and chemistry software providers.

A recurring theme was the use of density functional theory (DFT) as a computational tool in diverse areas including high performance ceramics, polymerisation reactions and catalysis. DFT has recently evolved into a versatile and universally accepted quantum chemical technique which also allows the direct monitoring of dynamical processes. Two major contributors to the popularisation of this method, M. Parrinello and R. O. Jones, were present as speakers. M. Parrinello reported detailed dynamic investigations of polymerisation reactions in the presence of a Ziegler-Natta catalyst. The dynamic information from the CPMD-code developed in Parrinello's group allowed R. O. Jones to arrive at a molecular understanding of the exceptional thermal properties of the lithio-alumo-silicate β-eucryptite. Further applications of the DFT-method to catalytic problems, sometimes in combination with conventional ab initio methods, were presented by R. Meier, J. Sauer, J. Lohrenz, and A. Schäfer. Semiempirical quantum chemical approaches are of great importance for the treatment of large molecules and biological complexes. The systematic improvement of these techniques and their embedding into molecular mechanics schemes was demonstrated by W. Thiel.

Simulations of macroscopic systems are generally based on empirical potential models. The power of these methods was illustrated with applications to polymers, complex liquids, and biological membranes. U. Suter adressed the question of the prediction of slow events from finite length simulations of the elastic properties of polymers. The complex behaviour of supercooled water and of surfactant solutions was discussed by A. Geiger. The long range character of Coulomb interactions requires special simulation techniques for polyelectrolytes, which were presented by Ch. Holm. The self assembly and the rearrangement dynamics of biological membranes were the subjects of the contributions from H. J. C. Berendsen and A. Baumgärtner. O. Evers discussed simulation techniques for mesoscopic systems.

The design of new pharmacologically active compounds is a field of major industrial importance and makes heavy use of advanced modelling techniques. The presentations of H. J. Böhm and G. Barnickel highlighted significant successes in this field but also addressed the difficulties in the systematic identification of fundamentally new lead structures. The complexity and context dependence of biological interactions were among the themes of the lecture delivered by G. Folkers, which examined the functional ambivalence of protein segments and the resulting ambiguities for drug design. P. Erk presented the successful prediction of crystal structures of industrial pigments on the basis of empirical models. Reliable thermodynamic data are essential for the calculation of phase distribution equilibria in chemical processes but are not always easily measurable. A successful combination of quantum chemical calculations and electrostatic embedding for the computation of these quantities was presented by A. Klamt.

Large systems of coupled differential equations are the mathematical basis of the description of chemical production plants and the modelling of reactive flows. Combustion modelling combines the challenges of turbulent flow simulations with the molecular aspects of elementary chemical reactions taking place on a vast range of time scales. J. Warnatz described smart reduction techniques which allow the identification and parametrization of the dominant chemical processes in combustion engines and thereby permit the numerical treatment of the turbulent reactive flow in simple geometries. The optimization of production plants with respect to throughput, chemical yield and purity, and controllability figures among the commercially most important computer applications in the chemical industry. Key ingredients are thermodynamic and kinetic data and mixing and flow properties. The simulation of entire production processes as demonstrated by R. Bachmann helps to identify bottlenecks and to study the scaling and startup behaviour. These simulations routinely require the simultaneous treatment of many thousands of coupled differential equations.

The storage, classification, and intelligent reduction of genetic and biochemical information emphasizes an important non-numerical aspect of high performance computing. Modern approaches aiming at the prediction of protein structure and functionality from genome data with the goal of discovering qualitatively new therapeutic pathways were the subject of the lectures of R. Schneider, R. Zimmer and D. Schomburg. The use of the internet for the automatic retrieval of data from heterogeneous data bases distributed around the world plays an important role in this process. The daily quantity of new sequence data amounts to about 50 MByte. The fast analysis and classification of the immense quantities of data require the fast I/O-capabilities of supercomputers and the availability of parallel processing.

E. Wimmer reviewed the parallel evolution of computing hardware and of theoretical methods and their software implementations and emphasized the role of software companies in the process of turning collections of research codes into user friendly integrated software tools with graphical interfaces, detailed documentation, and competent user support for the non-expert. The rapid incorporation of new algorithmic developments and the adaptation to the rapidly changing computer architectures are key software design problems. Easy company wide access to supercomputing expertise was the subject of the presentation of M. Schlenkrich who introduced the web based CrunchServer developed by Silicon Graphics Inc.. Ch. Henriet stressed the importance of a multidisciplinary team of high performance computing experts in his case studies of the tuning of chemistry codes for the NEC SX-4 parallel vector computer at the Swiss supercomputer center CSCS in Manno, TI. The close interaction with program authors and end users led to highly successful adaptations of important codes like MNDO94, CPV, GROMDO, and DALTON. The scientific program was closed with a lecture by J. Grotendorst from ZAM, who presented

the hardware and chemistry software available on the Jülich Cray complex and the procedures for academic and industrial users to get access to these facilities.

While quantitatively accurate numerical predictions still remain limited to small molecules, important qualitative questions can be reliably answered also for large systems. This meeting repeatedly demonstrated unexpected insights into chemical processes gained from modern simulation techniques. Algorithmic progress has been impressive in the past and is expected to continue. However, the continuously growing demand for advanced computing resources was underlined by many speakers. Competent advice on the proper exploitation of computing resources is as important as their ready availability. High performance computing consulting requires experts with multiple qualifications from computer science, mathematics, and one of the relevant scientific disciplines. This expert know-how can be supplied by research centres like the one in Jülich, which can act as a hub to bring together basic research and industrial applications and to promote technology transfer in chemistry.

The extended abstracts of the lectures and posters with bibliographies are available at: http://www.kfa-juelich.de/compchem/proceedings/.