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Centro Svizzero di Calcolo Scientifico (CSCS)

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The Swiss Scientific Computing Centre CSCS (Centro Svizzero di Calcolo Scientifico) is managed by the Swiss Federal Institute of Technology (ETH-Zürich) on behalf of the Swiss scientific community. The center was established by the government to further advance the usage of high-performance computing in education, research and industry.

As a national resource, the centre's overall objective is to provide high-performance computing to universities and research institutes. Towards these objectives, it provides besides computing power the user support needed to solve complex scientific problems.

CSCS users represent diverse disciplines; physics, chemistry, materials science, biology, engineering, forecasting and environmental sciences. They benefit from well focused and intensive support in the areas of algorithmic consulting and development, the evaluation, installation and optimisation of applications and the development of graphical visualisation techniques.

Computer simulation and numerical modelling are widely accepted as a new branch of science, complementing and linking theoretical and experimental methods. In order to solve complex problems, CSCS develops integrated program environments containing state-of-the-art computational methods. In particular, program environments for computational chemistry and materials science (*i.e.* PECCAM) offer advanced tools for calculations of structure, dynamics and electronic properties of macromolecules, drugs, and new materials.

Modules for semi-empirical, density-functional and *ab-initio* electronic structure calculations as well as for molecular dynamics simulations are ported and optimised on the most suited computer architectures (vector, vector parallel with shared memory or workstation cluster).

Graphical user interface and visualisation tools guarantee user friendly input preparation (3D molecular builder), output visualisation and analysis.

Modern techniques for database searches represent a further subject of applied research at CSCS. The developed methods will provide a further tool for biochemical engineering at the Centre.

Fig. 1. *The Swiss Scientific Computing Centre CSCS*

Some Technical Notes on the CSCS Computing Environment

The central computational element is a *NEC SX-3/24R* vector computer. Its peak performance is 12.8 GFlops (12.8 milliards of floating point operations per second). In early 1993 a *Convex C3820* was added as a front-end system to the *SX-3*, helping to optimise the use of the super computer.

In 1994 a *HP* workstation cluster (consisting of eight *Hewlett-Packard* workstations grouped together) was opened to the users for production.

While the *SX-3* is optimised towards large and well-vectorised jobs, the *Convex*

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as an interactive platform is the users' workplace. Interactive work such as file editing, code writing and submitting of NQS batch jobs can be done on the front end.

The front end system is also manager for a large archive system and handles massive amounts of data. Its capacity amounts to more then 4 TBytes.

The CSCS local network is linked to the worldwide Internet community through *PTT-Telecom* leased SWITCH lines. These lines, linking CSCS to ETHZ, EPFL, CERN, and all Swiss universities, are currently rated at 2MBits/s.

If you are interested in more information or documentation, please feel free to contact us.

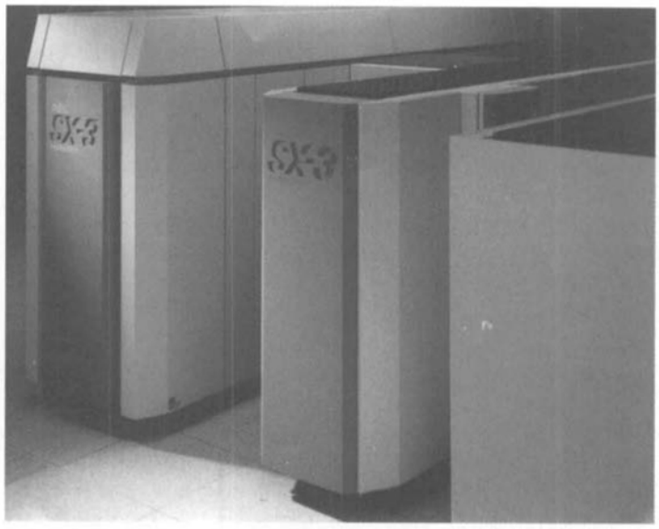

Fig. 2. NEC SX-3124R
vector computer

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Quantum Chemistry and Drug Design

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Abstract. The state-of-the-art computational chemistry software, visualization tools and high performance computing infrastructure are employed to assist the design of new and more effective drugs. At present a project focuses on the quantitative structure activity relationships of antimalarial drugs.

1. Introduction

Computational methods today play an important role in modeling applications in molecular sciences such as chemistry and biology. In particular, drug design techniques based on computational tools recently have proved to be very efficient in predicting the potency of possibly active compounds among a large series of molecular systems [1]. In this article we concentrate on this specific field of drug design and mainly on its relationship with high performance computing. We also briefly describe the results of such an investigation we are currently carrying out on antimalarial compounds derived from the lead system artemisinin, known in China as the traditional medicament *Qinghaosu*.

The key steps in rationalizing and predicting the biological activity of a given molecule start invariably with the determination of the structure of this compound. Traditionally, this has been done using experimental techniques such as X-ray crystallography. Nowadays, however, progress in both computer hardware and computational chemistry methods is such that this determination can be performed theoretically with considerable reliability. Quantum chemistry is indeed in principle able to reproduce the structural parameters of molecules to a high accuracy (*i.e.* ± 0.01 Å on bond lengths and ± 2° on bond and torsion angles) provided that ample computational resources, such as those provided by a supercomputer, are available. The second step is more heuristic: how to correlate the structure, and possibly some molecular properties, with the biological activity of the compound? This is generally achieved using the approach of structure activity relationship (SAR) correlation, or quantitative SAR (QSAR) correlation if the relationship is of a quantitative nature. In other words, mathematical equations are developed to correlate biological effects of a set of compounds with their structural and molecular properties.

Of course, a better, but very difficult, procedure would consist of a comprehensive description of 'what is happening' in the biological system under the effect of the drug. This includes the whole path followed *in vivo* by the drug from the intake up to its binding to the active site, and the chemical reactions which are induced by the drug or in which the drug takes part. Needless to say, the comprehensive knowledge of this complex process would enable one accurately to ration-

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