How Computer Science is Taught to Our Students in Chemistry. Part II

Heiner G. Bühhrr

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Finally, we would like to give an example from the real world of quantum chemistry, where people are not 'cheating' their processors, but nevertheless similar effects can be found. Lüthi et al. [3] reported results from a calculation on a Cray Y-MP/8-128 supercomputer with the DISCO-program for bis(2,6-dimethylphenyl) carbonate (C_13H_{18}O), a molecule with 38 atoms (314 contracted / 610 primitive basis functions), in which one iteration took about 400 s (this number is different from the one in [3], which was wrong, due to an input error [4]) and a performance of 1531 Mflops was achieved. The speedup for 8 processors was 7.65. Brode [5] has carried out a very similar calculation on the same molecule (356 contracted/592 primitive basis functions) with the TURBOMOLE-program on a workstation cluster of 14 machines performing to a maximum rate of 660 Mflops. The speedup was only 11.6. Although the loss in parallelization was higher and the Mflop-rate was much smaller (the formal rate for the 8 Cray processors would even be 2660 Mflops) the time for the first iteration (taking usually most time) was only 524 s, i.e. slightly more than with DISCO. Similar experiences have been made by Vogel et al. [6] with a version of DISCO on a network of workstations.

Summarizing, we can state that the Mflop- and the speedup-measure are often not very useful criteria for the real world of vector- and parallel-computers, but that a comparison between programs solving problems as similar as possible is the best way to estimate the performance of computers for a specific task. Policies such as that of CSCS in Manno, enforcing that only programs yielding 275 Mflops should run on the NEC, are questionable in view of the difficulty to accurately estimate the efficiency of application programs running on vector processors. An alternative policy would be to supply a supplementary national cluster of workstations or a super parallel computer for codes performing badly on a vector processor making the scientists choose the most efficient facility for their purpose.

We thank Dr. Stefan Brode, BASF Aktiengesellschaft, Ludwigshafen/Rhein and Dr. Hans Peter Lüthi, Interdisziplinäres Projektzentrum für Supercomputing, ETH, Zürich for the example.


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CH-8401 Winterthur
Table

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<td>new curriculum</td>
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</table>

*) Not comparable; the general computer training is part of a two year course preceding chemical engineering studies.

Contents:

Burgdorf: Introduction to computer architecture and WINDOWS user interface, general application software, chemical data bases, molecular modelling

Fribourg: Introduction to programming, general application software (WINDOWS programs), data comprehension, processing and modelling, molecular design

Genève: Introduction to computer science and laboratory applications

Muttenz: Introduction to computer architecture and to an operating system, introduction to programming, general application software, overview of computer applications in chemistry

Sion: Introduction to computer science, introduction to programming, Excel

Winterthur: Introduction to computer architecture, networks and operating systems, general application software (chemical word-processing, spreadsheets), introduction to molecular modelling, chemical data bases


ANNOUNCEMENTS

29. Symposium für Theoretische Chemie

Oberwiesenthal (Sachsen), BRD, 28. Sept.–1. Okt. 1993

Organisiert durch Joachim Reinhold, Fachbereich Chemie, Universität Leipzig, Talstr. 35, 0–7010 Leipzig, Deutschland EM: reinhold@theorie.chemie.uni-leipzig.dbp.de

European Summer School in Quantum Chemistry (ESQC)

Tjörnarps Kursgård, Sweden, 15.–28. August 1993

Organized by Björn Roos, Dept. of Theoretical Chemistry, Chemical Centre, P.O.B. 124, S–221 00 Lund, Sweden EM: teobor@garm.teokem.lu.se