Computational chemistry on the FPS-X64 scientific computers

Experience on single- and multi-processor systems

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1. Introduction

The purpose of this paper is to review the impact and use of the FPS-X64 scientific computers in computational chemistry, focusing attention on experience gained on both an FPS-164/MAX, installed at the Science and Engineering Research Council’s Daresbury Laboratory, UK, and on the distributed system, composed of an IBM 4381-3 front end processor and 10 FPS-164 attached array processors, at the ECSEC facility in Rome, Italy.

The review is necessarily selective, and is divided into several sections. In Sect. 2 we outline some general characteristics of the FPS-X64 machines. We consider their performance in various computational chemistry kernels in Sect. 3, where the general strategy adopted in code implementation is outlined. In Sect. 4 we consider the implementation and performance on FPS X64 scientific computers of a typical \textit{ab initio} program, GAMESS, and provide in Sect. 5 estimates of the cost-effectiveness of these machines in the context of supercomputers exemplified by the Cray-1S and CDC Cyber-205.

In Sect. 6 we consider the feasibility of migrating computational chemistry codes to the different architectures characteristic of the next generation of multiprocessors. Finally, in Sect. 7 we describe our initial attempts at adapting codes to run on the distributed system of multiple FPS processors at the ECSEC facility in Rome.

1.1. Cost-effective computing in chemistry

The introduction in 1976 of the VAX 11/780 by Digital provided arguably the greatest impetus to the use of minicomputers in large scale chemical computations, and led to the migration of many theoretical chemists from the less cost-effective alternative offered by the large scalar mainframes that typified the central computing facility of the 1960s and 1970s. Since 1976 use of the VAX-11/780 “superminicomputer” or its equivalents in chemical computations has proliferated to the extent of becoming a \textit{de facto} standard. Yet even the new generation of superminis, from Data General, Digital, Gould/SEL, Prime, Harris, IBM and Perkin-Elmer [1], that provide speeds several times that of the VAX-11/780,