

Identifying 3D maximal common substructures using Transputer networks

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This paper describes the use of a multiprocessor system for identifying the maximal common substructure (MCS) between pairs of three-dimensional (3D) chemical structures. The system is constructed from Transputers, 32-bit RISC microprocessors produced by Inmos Ltd., linked together in a tree network. The MCS algorithm used, developed by Crandell and Smith, identifies the MCS by a breadth-first search in which individual atoms common to the structures are extended one atom at a time until no further extension of the common substructure can be obtained. Experiments using a Pascal-based simulation package demonstrate the feasibility of using a multiprocessor system to increase the speed of MCS identification. Experiments with networks of Transputers demonstrate that substantial increases in speed can be achieved in practice if, and only if, the MCS is large.

Keywords: atom-by-atom searching, transputer networks, maximal common substructure, parallel processing

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The increasing computational demands of applications such as protein crystallography, molecular modeling, and chemical graphics has led to interest in the use of parallel computer hardware for processing a variety of types of chemical information. Many parallel computers have been designed or built, although the way in which parallelism is manifested differs drastically from one machine type to another. Thus, pipelining and multiple functional units have been used to increase the efficiency of uniprocessors, while a few sophisticated uniprocessors can be coupled together via the sharing of global memory, as in commercial multiprocessor systems. Array processors, conversely, contain many simple processing elements, all of which execute the same instructions on their local stores. Other architectures under active investigation include associative processors and data-flow machines. Overviews of research and development in this area are presented by Zakharov¹ and by Hwang and Briggs.²

Most scientific applications of parallel processing have been used to increase the efficiency of numeric computations of various sorts. However, parallel-processing techniques can also be used for processing nonnumeric

data. In this paper, we are interested in the use of microprocessor-based, multiprocessor networks for processing three-dimensional (3D) chemical structure information. In a multiprocessor system, each processor in the network is fully programmable and can execute its own program while communicating with others over the network; a multiprocessor system is thus an example of a multiple-instruction stream, multiple-data stream (MIMD) architecture.³

Recently, several types of 32-bit microprocessors have become available that can be used as building blocks for constructing multiprocessors that offer the prospect of extremely high processing rates at cost levels substantially less than those associated with conventional mainframes or supercomputers. An example of a microprocessor building block is the Transputer produced by Inmos Ltd., which has been designed specifically for concurrent processing.^{4,5} A Transputer contains a high-performance RISC (reduced instruction set computer) processor, local memory, and multiple communication links, called channels, that provide direct connections to other Transputers and to external memory and backing storage. A programming language called Occam has been developed not only for the design of concurrent systems based on linked microprocessors but also for programming the individual microprocessors in the network. Thus, a program can be developed on one Transputer and implemented on a network of Transputers, linked together in the configuration that seems most appropriate for the particular application.⁶ See the Appendix for details of the Transputer and of Occam.

Our interest in multiprocessor systems stems from a paper by Wipke and Rogers that considers the simulation of a star network of multiprocessors to increase the efficiency of atom-by-atom searching in chemical substructure search systems.⁷ In such systems, a query substructure (i.e., a set of atoms and the bonds connecting them together) must be mapped onto each of the structures in a database to determine whether the substructure is present. A simulation approach has also been used in our department to investigate an alternative method of substructure searching called relaxation searching.⁸ This involves comparing a query substructure with a structure in a database by iteratively examining correspondences between the two sets of atoms; the aim is to reduce the number of possible correspondences that must be considered in the final, atom-by-atom

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