MEETING REPORTS

Molecular dynamics on parallel computers

The Molecular Modelling Transputer Applications Community Club (MMTACC) recently organized a one day seminar at the Rutherford Appleton Laboratory where five invited speakers described their work on molecular dynamics. The audience participated in a discussion on the aims of the club and future activities.

G.S. Pawley presented an exciting paper describing his work at Edinburgh University on combining hetero architectures, using each where they were most appropriate on applications to simulation of a molecular lattice gas and the modelling of hydrodynamics of liquids using cellular automata. The Department of Trade and Industry (DTI) and the UK Science and Engineering Research Council (SERC) support a project at the Edinburgh Parallel Computer Centre to make a fast interface between two types of parallel computer, the AMT Distributed Array processor and the Meiko Computing Surface. The use of the High Performance Parallel Interface (HiPPI) means that the results will be applicable to a range of parallel hardware, not just to the two particular machines.

Monte Carlo methods are used in work on the Ising model. In the molecular lattice gas two atoms touch to form a molecule, a process favored by the term in the Hamiltonian describing the system. When more than two atoms are joined, they form an aggregate, and this is discriminated against. There is a chemical potential that acts like pressure. Increasing it forces the molecules together, forming crystallites first, then aggregates. Generation of the configurations is an ideal operation for the DAP, but their subsequent analysis is better done on the Meiko Computing Surface.

Another project combines a lattice gas simulation of a polymer diffusing into a liquid modelled with cellular automata. The liquid is modelled on a hexagonal grid with automata that move between the grid nodes. This work is ideal for the DAP, to model the basic cellular automata operations for the liquid. However, the collisions of the polymer molecules with those of the liquid must obey the conservation laws of energy and momentum. This calculation is better done on the transputers, since the energy and momentum have to be redistributed over the large molecule, which is not a local operation. There are problems of synchronization of the two machines; these may be overcome by running two separate simulations concurrently, thereby interleaving their usage of the two different machines.

P. Adams, from the Department of Biochemistry at Edinburgh University, described work on molecular dynamics on the Meiko Computing Surface. He is studying proteins to try to find an effective inhibitor to the process that enables some bacteria to become resistant to penicillin. The substrate has been modelled into the active site using computer graphics, but energy minimization is needed to determine the global substrate minimum. The FORTRAN source of the GROMOS87 program has been mounted on a transputer farm and energy minimization run on 32 processors simultaneously, but so far only local minima have been found. In another approach, a parallel implementation of GROMOS has been made, using two rings of transputers, one for bonded and the other for non-bonded force calculations. He reported that programs that previously took 900 seconds for one time step on a VAX 11/750 took only 22 seconds on the transputer system. He also mentioned EGO, the system built by Schulten et al. at the University of Illinois that has special hardware containing a systolic ring of transputers for use on molecular dynamics problems.

A. Raine, from the NMR Group at Cambridge University, is working on methods of determining protein structures, where simulation is an important tool used with X-ray and NMR methods of finding structures of biological macromolecules. SLS-PRO has been written in Occam II to run on a Meiko computing surface. A spherical distance cut off is imposed to reduce the amount of computing needed for each time step; adjacent residues are calculated on adjacent processors, which can introduce load balancing problems.

S.L. Fornili, from the University of Palermo, described his work on the hydrogen bond pathways that develop in liquids, for example, in water containing ions such as ammonium or hydroxyl ions. These calculations were initially done on computers such as a VAX 11/750 or a CRAY in Bologna, but the VAX was too slow and it was too difficult to get the data into the CRAY via the network. They now use a more cost-effective array of transputers hosted by an IBM PC-AT microcomputer with an Inmos B007 graphics board. The program has been written in Occam II to simulate the two-dimensional (2D) spinodal phase separation of a large Lennard-Jones system with over 7000 particles. It uses geometric decomposition and includes a distributed dynamic load balancer. Plots of the state of the systems were shown at several time periods up to 450 ps from the starting position. The execution time for a single time step (0.01 ps) on a VAX 11/750 was 26 sec. On a single T800 transputer using sequential FORTRAN it was 14 sec, but using parallel programming in Occam on 26 T800 transputers it was only 0.43 sec.

The last speaker, U.C. Klump from Shell Thornton Research Labs, spoke on the simulation of organic liquids. He is interested in the elasto-hydrodynamic properties of lu-

bricating oils between fast moving metal parts. These oils form thin films. Experimental measurements are extremely difficult, so computer simulations are the best way to understand and improve the lubricating action. He models the shear viscosity of the liquid, with sliding boundary conditions, on an array of 36 T800 transputers, with color displays on an associated SUN workstation. A box of liquid containing 10,000 atoms is divided into columns and each is assigned to a transputer that holds lists of all the atoms in the column and of their neighbors in the liquid. The forces between pairs of atoms in each column are calculated, the columns sheared, the lists updated, and the forces recalculated. The bending and torsional stress on each atom are calculated and hence find the parts of the molecule that most contribute to the stress. These are the parts that would need to be changed when new lubricants are designed with the ability to withstand higher shear stress.

The MMTACC is supported by the Transputer Initiative, which has joint funding from the SERC and the DTI. It aims to provide better information for the community by organizing seminars and providing a software library, a bibliography, a directory of members' interests, an electronic bulletin board, demonstrators of molecular modelling for the Transputer Initiative, and better liaison with suppliers and other computing research activities in molecular modelling. The Transputer Initiative publishes a monthly mailshot with details of new hardware, software, meetings, and so forth. We welcome further contributions to our bibliography. Please send them to the address below where a copy of the current bibliography may be obtained.

The next Transputer Initiative meeting is scheduled for 21 November 1990 at the University of Edinburgh. The topic, "Graphics and Transputers," was suggested by members of MMTACC who have found it much more difficult to move the graphics than the molecular modelling. Speakers include Roger Hubbold from the University of Manchester, who will talk about "Graphics Standards and parallel computers"; David White from the University of Glasgow, who will describe his general graphics library; Terry Barnaby from Beam Ltd, who will describe "An implementation of X-Windows for transputers"; and we are hoping a speaker from the Edinburgh Parallel Computing Centre will describe "Molecular graphics and the Illinois molecular modelling code on the Meiko computing Surface." There will be an opportunity to visit the Edinburgh Parallel Computing Centre after the meeting. If interested, please let the Chairman know (GSP@uk.ac.edinburgh), and indicate any particular interests you may have. Further details may be obtained from the address below.

Membership of MTACC is free and open to anyone interested in molecular modelling. To join, please contact: Mr. T. Mawby, Building R1, SERC/DTI Transputer Initiative, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK, tel (0235) 445787 or e-mail MMTACC@uk.ac.rl.inf.

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MOLECULAR MODELLING ON TRANSPUTERS REFERENCES

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