

METHODS IN MOLECULAR SIMULATION

CCP5 Spring School 11–15 April

Mike Allen

The Spring School was held at Southampton University, with lectures in the Chemistry Department each morning, hands-on computer workshops in the afternoon at the University's Data Visualization Suite, and a 'guest seminar' before dinner each evening. The principal lecturers were Mike Allen (Bristol), Julian Clarke (UMIST) and Dominic Tildesley (Southampton), with supplementary lectures from Tim Forester (Daresbury) and Stephen Warde (Molecular Simulations). Evening guest seminars were given by Julia Goodfellow (Birkbeck), Geoffrey Luckhurst (Southampton), Paul Madden (Oxford) and Mark Rodger (Reading).

The course began with lectures and workshops on basic and advanced techniques in Monte Carlo and molecular dynamics, and then moved on to topics in molecular modelling and scientific data visualization. Towards the end of the week, more specialized subjects were introduced: nonequilibrium methods, phase transitions, and Fortran 90. For each afternoon, a selection of exercises was provided: enough to give a reasonable choice of new material, while still permitting the student to look back at work from earlier in the week. For almost every exercise, a 'solution' was provided about two-thirds of the way through the afternoon. This allowed students to look at problems that they did not wish, or have time, to attempt, as well as being able to check their own work. The early part of the week concentrated on programming and simulation algorithms, but from Wednesday onwards other software was introduced. Cerius² (Molecular Simulations) was used to model zeolite adsorption, Collage (NCSA) was used to visualize large data sets, Iris Explorer (SGI/NAG) was used to illustrate module assembly for visualization, and PV-Wave (Precision Visuals) was also made available. The DL_POLY package was used to run example simulations of water and valinomycin. Finally, on the Friday, there was an exercise involving the progressive introduction of Fortran-90 constructs into a Fortran-77 molecular dynamics program, and an exercise involving programs run on several workstations at once, with message-passing by PVM.

This was an ambitious and intensive programme for both students and lecturers. The 16 Silicon Graphics R3000 Indigos worked almost faultlessly (just one machine was out of action for about an hour). The software was also extremely reliable: Cerius² crashed once or twice due to running out of swap space, but otherwise performed very well, and there was a minor glitch with the DL_POLY programs which needed to be recompiled on the R3000-chip Indigos (binaries from an R4000 turned out not to be compatible). None of these minor hiccups caused any real problems. After the course the students were allowed to copy their work, the original exercise programs, and the solutions to all the exercises, back home by ftp.

At the end of the course, the students filled in, anonymously, a set of questionnaires. These will provide some useful feedback and information essential to the planning of future courses, and they will be studied in detail. The overall tone was very positive indeed: all the students seem to have enjoyed their week, and gained something from it. The 'guest seminars' especially were appreciated: they were all delivered in an enthusiastic and inspiring manner. The food and accommodation at Glen Eyre hall of residence also received general approval.

One or two points emerged that need further consideration. There was a larger split than anticipated in background and expectations between 'programmers' and 'package users': if this had been fully appreciated we could have targetted and tailored the course a little better. This split is itself something that needs some attention: our contacts with the commercial sector of molecular modelling suggest that there is a need for more Ph.D.'s who know something of what is inside these packages, rather than just knowing how to use them. Secondly, the students would have appreciated an afternoon off (to see Southampton), and a few more informal opportunities (round tables, poster sessions) to discuss simulations with the lecturers. It would be very desirable to include these in a future programme, but the Spring School would have to extend beyond one week, or we would have to trim down the material to be covered. Additional comments on the questionnaires concerning the level and pace of lectures will also be very useful to us.

I would like to thank my co-lecturers, all the 'guest seminar' speakers, and our two supplementary lecturers, for the effort they put in to present all this material in an interesting and informative way. Dominic Tildesley also deserves thanks for handling registration and all the domestic arrangements. Southampton University provided the lecture theatre and visualization suite free of charge. We could not have mounted this course without the assistance of Southampton Computer Centre staff, notably Ian Hardy, who helped set things up on the DV Suite machines, and worked behind the scenes during the week to keep things running smoothly. Thanks are also due to Mike Stapleton, Stephen Warde and Jeremy Turvey of Molecular Simulations for allowing us to use Cerius² during the workshops, and (to Stephen and Jeremy) for setting up the zeolite exercise, and attending the afternoon session to provide advice; to Robert Morell of NAG for allowing us to use their Fortran-90 compiler; to Jeremy Walton of NAG for files and advice on the Iris Explorer exercise; and to Tim Forester of Daresbury Laboratory, for providing the DL_POLY exercise and attending in the afternoon to help with it. Finally, thanks to the students, who, to their credit, attended every lecture and every workshop session, in a packed programme, and demonstrated plenty of enthusiasm and team spirit.