

METHODS IN MOLECULAR SIMULATION

CCP5 Spring School 27–31 March

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The general format of this year's Spring School was similar to that adopted last year, with minor changes following the feedback we obtained at that time. As before, the event was held at Southampton University, with lectures in the Chemistry Department each morning, and a 'guest seminar' after lunch (plus a couple of extra seminars in the morning). The principal lecturers were Mike Allen (Bristol), Julian Clarke (UMIST) and Dominic Tildesley (Southampton), and guest speakers were Steve Parker (Bath), Tim Forester (Daresbury), Clive Freeman (Biosym), David Edwards (York), Jeremy Walton (NAG), Mike Gillan (Keele) and Dave Kofke (Buffalo). Hands-on computer workshops took place in the afternoon at the University's Data Visualization Suite; these were linked as much as possible to the material covered in lectures and seminars that day. Two poster sessions were held, to allow the students to explain in detail their research interests and the simulation techniques of most interest to them, and there was a round-table question and answer session on the last day which generated much discussion.

The majority of the students came from U.K. institutions, with one or two from continental Europe, and one from Canada. 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 parallel simulation methods, molecular modelling and scientific data visualization. Towards the end of the week, more specialized subjects were introduced: nonequilibrium methods, phase transitions, *ab initio* MD. 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 using small programs and simple models, but the DL_POLY package was introduced on Tuesday, and molecular modelling using the Biosym suite on Wednesday. Collage (NCSA) was used to visualize large data sets, and Iris Explorer (SGI/NAG) was used to illustrate the modular approach to visualization. Finally, on the Friday, there was an exercise involving the progressive introduction of Fortran-90 constructs into a Fortran-77 molecular dynamics program.

This was an ambitious and intensive programme for both students and lecturers. The computer system worked almost faultlessly (a server failure caused one short-term glitch), and the software was also extremely reliable. After the course the students were allowed to copy their work, the original exercise programs, and the solutions to all the exercises, back home from a Web site set up at Bristol.

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 introduction of poster sessions and the round table were especially well received, while the food and accommodation at Glen Eyre hall of residence also met with general approval.

I would like to thank my co-lecturers, and all the ‘guest seminar’ speakers, 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; Sean Jordan and Martin Bates also helped during the workshops. Thanks are also due to Allan Price, Clive Freeman and Glenn Mills of Biosym for allowing us to use their software, and (to Clive and Glenn) for coming to Southampton to supervise its use. We are grateful to Robert Morell of NAG for allowing us to use their Fortran-90 compiler. Finally, thanks to the students, who attended every lecture and workshop session, put on an impressive display of posters, and showed plenty of enthusiasm and good humour.