

CCP5 visit of Dennis Rapaport

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During the course of an extended visit to the Physics Department at Edinburgh University, which was sponsored by the TRACS program of the Edinburgh Parallel Computing Center (EPCC), a short lecture tour was arranged for me under the auspices of CCP5. So, during a hot week in August 1997, I found myself visiting the Daresbury Laboratory, UMIST (Manchester), and Reading University, with lots of train mileage in between (despite using a sophisticated algorithm to minimize the distance).

The visit began in Daresbury where my hosts were Bill Smith and Phil Lindan. I had visited the lab on two previous occasions to work on parallel processing, so this provided a welcome opportunity to renew old acquaintances. I gave a talk on interactive simulation and visualization (some of this material is described in [1,2]) with live demonstrations using a Silicon Graphics workstation and large-screen projector kindly arranged by Phil. The visit gave me a chance to talk at length with Bill about subjects of mutual interest, parallel computing in particular.

It was only a short hop to Manchester, where my my host at UMIST was Julian Clarke. I gave a seminar describing some of my recent work on granular material simulation (see [3-5]). There was time for plenty of discussion with Julian, with Les Woodcock who came over from Bradford and who also finds granular matter fascinating, and with the members of Julian's group.

Then south to Reading, home also to a famous place of incarceration. My hosts were Mark Rodger and Mike Drew. The colloquium was on the methodology of molecular dynamics, based on my recent book [6]. A number of members of the audience who had come from universities nearby were people I had encountered in various places in the past but had not met for many years, so it was nice to see some familiar faces. I had discussions with Mark and Mike and the members of their groups; it was also an opportunity to catch up on the latest Australian news from Mark, a fellow antipodean expatriate.

I would like to thank my hosts at each of the ports of call for their warm hospitality and for making this little trip a most rewarding experience. It provided a welcome opportunity to talk to people working on challenging computational problems in a number of different fields, and it was encouraging to see that computer simulation has such a dedicated following in the physics and chemistry communities. Thanks also to CCP5 for sponsoring the trip, and to Stuart Pawley, who was my host in Edinburgh, for putting the program together.

References:

- [1] *An Introduction to Interactive Molecular Dynamics Simulations*, D. C. Rapaport, *Computers in Physics* **11** (4), 337 (1997).
- [2] *Interactive Molecular Dynamics*, D. C. Rapaport, *Physica A*, **240**, 246 (1997).

[3] *Molecular Dynamics Studies of Grain Segregation in Sheared Flow*, D. Hirshfeld and D. C. Rapaport, Phys. Rev. E **56**, 2012 (1997).

[4] *Molecular Dynamics Studies of Granular Flow Through an Aperture*, D. Hirshfeld, Y. Radzyner and D. C. Rapaport, Phys. Rev. E **56**, 4404 (1997).

[5] *Subharmonic Surface Waves in Vibrated Granular Media*, D. C. Rapaport, Physica A (in press, 1997).

[6] *The Art of Molecular Dynamics Simulation*, D. C. Rapaport (Cambridge University Press, 1995); paperback edn. (1997).